



Full wwPDB EM Validation Report ⓘ

Sep 7, 2026 – 06:16 PM JST

PDB ID : 25FQ / pdb_000025fq
EMDB ID : EMD-80076
Title : BAM-SurA complex (Core only)
Authors : Kohga, H.; Miyazaki, R.; Tsukazaki, T.
Deposited on : 2026-04-01
Resolution : 3.60 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.dev133
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) : 2.50

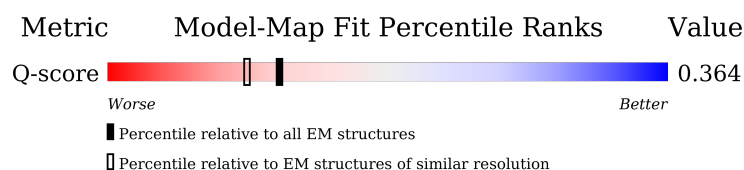
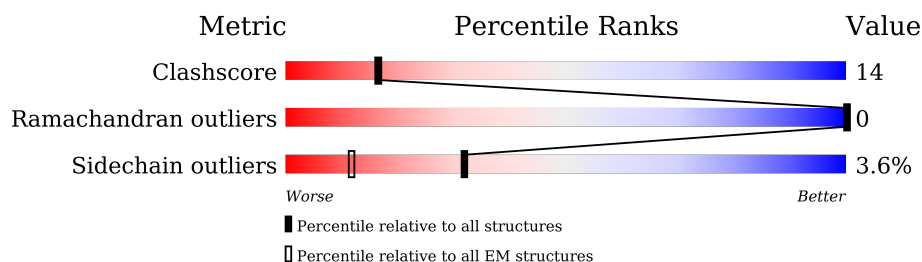
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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	1222	
1	F	1222	
2	B	392	
3	C	344	

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Mol	Chain	Length	Quality of chain
4	D	245	 66% 23% 11%
5	E	123	 53% 19% 28%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 14923 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 Chaperone SurA, Outer membrane protein assembly factor BamA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	783	Total	C	N	O	S	0	0
			6194	3907	1043	1228	16		
1	F	177	Total	C	N	O	S	0	0
			1417	870	265	271	11		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLY	-	linker	UNP P0ABZ8
A	18	GLY	-	linker	UNP P0ABZ8
A	19	SER	-	linker	UNP P0ABZ8
F	429	GLY	-	linker	UNP P0ABZ8
F	430	GLY	-	linker	UNP P0ABZ8
F	431	SER	-	linker	UNP P0ABZ8

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	369	Total	C	N	O	S	0	0
			2776	1739	476	555	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	272	Total	C	N	O	S	0	0
			2081	1293	366	414	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	218	Total	C	N	O	S	0	0
			1761	1109	309	336	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	89	Total	C	N	O	S	0	0
			694	436	122	134	2		

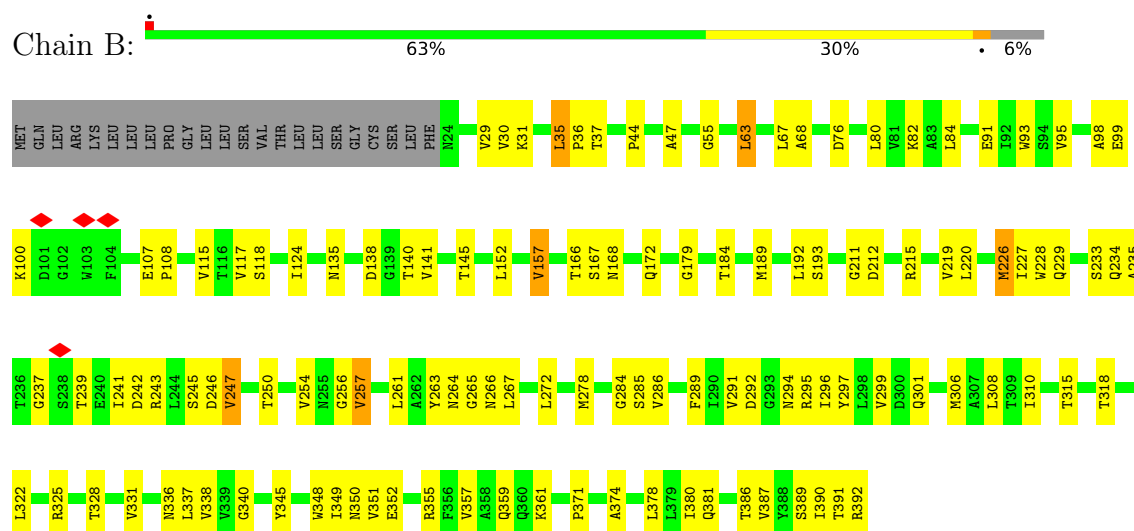
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	114	GLY	-	expression tag	UNP P0A938
E	115	GLY	-	expression tag	UNP P0A938
E	116	HIS	-	expression tag	UNP P0A938
E	117	HIS	-	expression tag	UNP P0A938
E	118	HIS	-	expression tag	UNP P0A938
E	119	HIS	-	expression tag	UNP P0A938
E	120	HIS	-	expression tag	UNP P0A938
E	121	HIS	-	expression tag	UNP P0A938
E	122	HIS	-	expression tag	UNP P0A938
E	123	HIS	-	expression tag	UNP P0A938

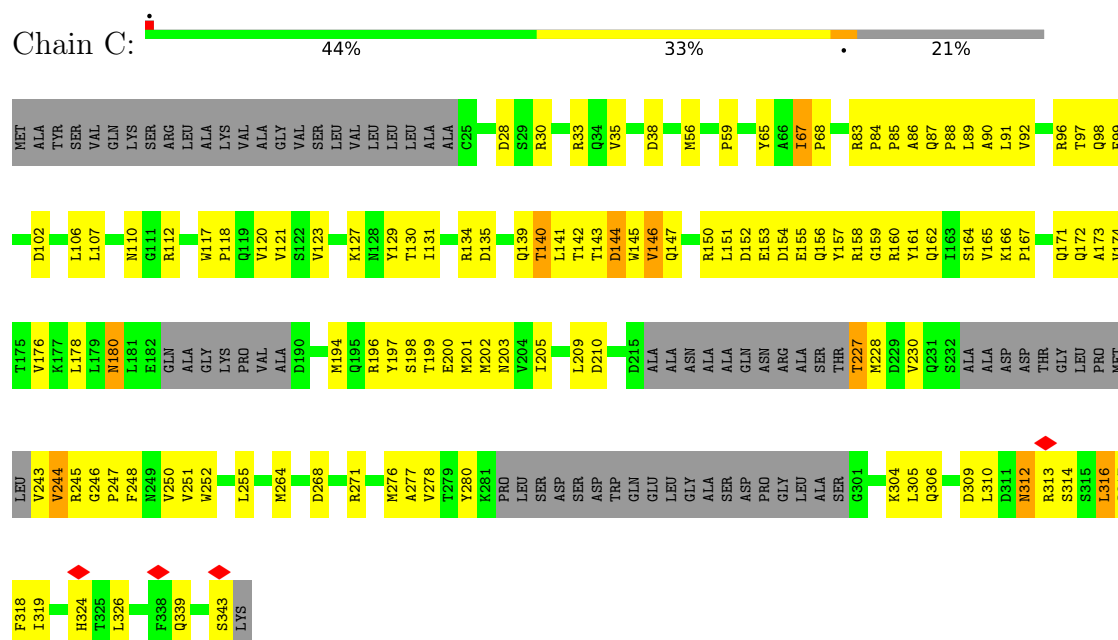


[illegible]

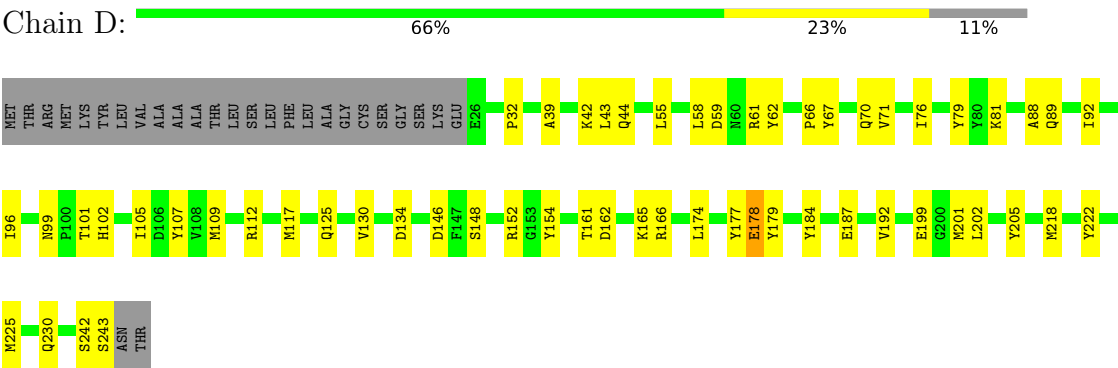
- Molecule 2: Outer membrane protein assembly factor BamB



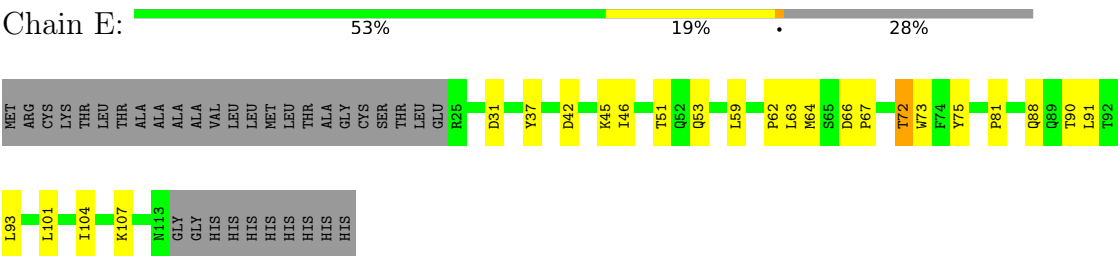
- Molecule 3: Outer membrane protein assembly factor BamC



● Molecule 4: Outer membrane protein assembly factor BamD



● Molecule 5: Outer membrane protein assembly factor BamE



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	107150	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.692	Depositor
Minimum map value	-0.249	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.08	Depositor
Map size ($\text{\AA}$)	240.63998, 240.63998, 240.63998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.752, 0.752, 0.752	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	0.24	0/6337	0.35	0/8598
1	F	0.69	0/1426	0.93	0/1913
2	B	0.21	0/2826	0.41	1/3854 (0.0%)
3	C	0.46	0/2113	0.69	1/2867 (0.0%)
4	D	0.28	0/1801	0.42	0/2447
5	E	0.39	0/709	0.53	0/967
All	All	0.35	0/15212	0.51	2/20646 (0.0%)

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	F	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	312	ASN	N-CA-C	-8.03	103.32	113.43
2	B	257	VAL	N-CA-C	6.32	117.68	108.58

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	129	ARG	Sidechain
1	F	399	ARG	Sidechain
1	F	404	ARG	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	6194	0	5907	128	0
1	F	1417	0	1445	55	0
2	B	2776	0	2718	74	0
3	C	2081	0	2043	121	0
4	D	1761	0	1699	48	0
5	E	694	0	674	17	0
All	All	14923	0	14486	415	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 14.

All (415) 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:59:PRO:HG3	5:E:67:PRO:HB2	1.61	0.81
1:F:72:GLU:HA	1:F:75:ILE:HD12	1.64	0.79
3:C:244:VAL:HG13	3:C:316:LEU:HD23	1.66	0.77
3:C:243:VAL:HA	3:C:316:LEU:H	1.51	0.76
3:C:131:ILE:HG13	3:C:134:ARG:HH11	1.50	0.75
2:B:55:GLY:HA2	2:B:76:ASP:HB2	1.68	0.74
4:D:117:MET:HE1	4:D:166:ARG:HE	1.53	0.74
1:F:69:GLN:HE22	1:F:73:ARG:HH11	1.33	0.73
3:C:151:LEU:HB2	4:D:44:GLN:HB3	1.72	0.71
4:D:92:ILE:HG21	4:D:112:ARG:HB2	1.71	0.71
3:C:96:ARG:HH21	3:C:98:GLN:HB2	1.57	0.70
4:D:148:SER:HB2	4:D:152:ARG:HH21	1.56	0.70
3:C:33:ARG:HG3	3:C:83:ARG:HH12	1.57	0.70
3:C:244:VAL:HG22	3:C:316:LEU:HB3	1.74	0.70
3:C:304:LYS:HB3	3:C:319:ILE:HB	1.74	0.69
5:E:66:ASP:HB2	5:E:72:THR:HG22	1.72	0.69
3:C:305:LEU:HD12	3:C:317:GLN:O	1.92	0.69
1:F:65:THR:HA	1:F:68:HIS:CE1	2.27	0.68
3:C:92:VAL:HG22	3:C:210:ASP:HB2	1.75	0.68
2:B:381:GLN:HG3	2:B:386:THR:HA	1.76	0.68
1:A:76:ARG:HB2	1:A:87:GLN:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:197:TYR:HA	3:C:200:GLU:HG3	1.75	0.68
1:A:99:PHE:HB3	1:A:167:LEU:HB2	1.74	0.68
3:C:130:THR:OG1	3:C:144:ASP:HB3	1.93	0.68
1:A:79:ARG:H	1:F:25:VAL:HG21	1.57	0.67
3:C:155:GLU:HG2	3:C:157:TYR:CE1	2.29	0.67
1:A:269:SER:HB2	1:A:334:THR:HB	1.76	0.67
3:C:88:PRO:HA	3:C:199:THR:HG23	1.77	0.67
3:C:86:ALA:HB3	3:C:196:ARG:HA	1.77	0.66
3:C:310:LEU:HB2	3:C:313:ARG:C	2.20	0.66
3:C:180:ASN:N	3:C:180:ASN:OD1	2.28	0.66
1:F:67:ARG:HG3	1:F:71:MET:HE3	1.77	0.66
3:C:91:LEU:HD13	4:D:67:TYR:HE2	1.61	0.66
3:C:276:MET:HB2	3:C:305:LEU:HB3	1.77	0.65
1:F:143:ASN:HA	1:F:406:PHE:HZ	1.62	0.65
1:A:396:GLU:HG2	1:A:397:THR:HG22	1.78	0.64
1:A:549:LEU:HD12	1:A:554:GLU:HB2	1.78	0.64
1:A:701:LYS:HZ1	1:A:758:PRO:HD2	1.60	0.64
1:A:173:VAL:HB	2:B:29:VAL:HG22	1.79	0.64
1:A:54:VAL:HG12	1:A:56:ASP:H	1.61	0.63
3:C:310:LEU:HB2	3:C:313:ARG:O	1.99	0.63
1:A:54:VAL:HG11	1:A:79:ARG:HH12	1.63	0.63
3:C:155:GLU:CG	3:C:157:TYR:CE1	2.81	0.63
1:A:185:ASN:HB3	1:A:260:ILE:HD11	1.80	0.62
1:A:74:ASP:HB3	1:A:89:LYS:HB3	1.80	0.62
3:C:159:GLY:CA	3:C:180:ASN:HB3	2.29	0.62
1:F:92:SER:HB3	1:F:95:GLN:HG3	1.81	0.62
1:A:719:ILE:HD13	1:A:736:SER:HB2	1.79	0.62
2:B:256:GLY:O	2:B:272:LEU:HD22	1.99	0.62
3:C:305:LEU:HD13	3:C:318:PHE:CD2	2.34	0.62
2:B:211:GLY:H	2:B:247:VAL:HG13	1.65	0.61
1:A:615:THR:HB	1:A:633:THR:HG23	1.83	0.61
1:F:32:VAL:HG21	1:F:78:GLN:HB3	1.81	0.61
2:B:243:ARG:HE	2:B:264:ASN:HD21	1.49	0.61
1:F:67:ARG:O	1:F:71:MET:HE2	2.00	0.61
1:A:67:PHE:HD2	1:F:36:VAL:HB	1.65	0.61
3:C:147:GLN:HA	3:C:158:ARG:HA	1.82	0.61
1:A:581:LEU:HD13	1:A:587:PRO:HG3	1.83	0.61
3:C:165:VAL:HG13	3:C:174:VAL:HG22	1.83	0.61
4:D:32:PRO:HG3	4:D:62:TYR:CZ	2.36	0.61
5:E:62:PRO:HG3	5:E:73:TRP:CD2	2.35	0.61
1:A:719:ILE:HD12	1:A:734:ARG:HE	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:264:MET:HE1	3:C:318:PHE:CZ	2.36	0.60
3:C:155:GLU:CG	3:C:157:TYR:CZ	2.84	0.60
1:F:46:MET:HE1	1:F:67:ARG:HA	1.83	0.60
3:C:131:ILE:HG13	3:C:134:ARG:NH1	2.15	0.60
4:D:117:MET:HE1	4:D:166:ARG:NE	2.17	0.60
3:C:112:ARG:HH12	3:C:209:LEU:HB3	1.67	0.60
1:F:398:TYR:O	1:F:402:MET:HG2	2.01	0.59
5:E:51:THR:HG23	5:E:53:GLN:H	1.65	0.59
1:A:750:ASP:HB3	1:A:753:GLN:HB2	1.84	0.59
2:B:212:ASP:HA	2:B:246:ASP:HB2	1.85	0.59
4:D:125:GLN:HB3	4:D:130:VAL:HB	1.85	0.59
1:A:684:PRO:HG2	1:A:687:ASP:HB2	1.85	0.58
1:A:754:TYR:HA	1:A:757:TYR:HD2	1.68	0.58
3:C:139:GLN:HB2	3:C:165:VAL:HB	1.84	0.58
1:A:94:ILE:HD12	1:A:97:ILE:HD11	1.85	0.58
3:C:167:PRO:HA	3:C:172:GLN:HG3	1.85	0.58
1:A:215:GLN:HB2	1:A:218:LYS:HB2	1.85	0.58
3:C:305:LEU:HD11	3:C:316:LEU:HD13	1.85	0.58
5:E:90:THR:HB	5:E:107:LYS:HB3	1.85	0.58
2:B:345:TYR:HE1	2:B:361:LYS:HB2	1.68	0.57
3:C:145:TRP:HE1	3:C:160:ARG:NH1	2.02	0.57
1:A:466:GLN:HB2	1:A:494:PHE:HB2	1.85	0.57
2:B:336:ASN:HD22	2:B:348:TRP:HE3	1.51	0.57
3:C:59:PRO:HD2	4:D:202:LEU:HD21	1.87	0.57
1:A:630:LEU:HB3	1:A:717:GLU:HB2	1.84	0.57
1:A:377:LEU:HD22	1:A:412:VAL:HG11	1.86	0.57
3:C:247:PRO:HD2	3:C:250:VAL:HB	1.86	0.57
1:A:536:LEU:HD11	1:A:648:PHE:HZ	1.68	0.57
2:B:107:GLU:HG3	2:B:108:PRO:HD2	1.85	0.57
1:F:107:ASN:HD22	1:F:114:MET:HE1	1.70	0.57
2:B:215:ARG:HD3	2:B:229:GLN:HE21	1.69	0.57
3:C:244:VAL:HG13	3:C:316:LEU:CD2	2.35	0.57
2:B:99:GLU:HB2	2:B:107:GLU:HB3	1.87	0.56
1:A:67:PHE:CD2	1:F:36:VAL:HB	2.41	0.56
4:D:96:ILE:HD12	4:D:105:ILE:HD11	1.88	0.56
1:A:170:GLN:HA	3:C:324:HIS:HE2	1.71	0.56
3:C:268:ASP:HB3	3:C:277:ALA:HB3	1.87	0.56
2:B:322:LEU:HD23	2:B:325:ARG:HD3	1.89	0.55
3:C:145:TRP:HA	3:C:159:GLY:C	2.32	0.55
1:A:476:PRO:HA	1:A:484:SER:HB2	1.87	0.55
3:C:83:ARG:HG3	3:C:84:PRO:HD2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:155:GLU:HG2	3:C:157:TYR:CZ	2.41	0.55
1:F:96:LEU:HD21	1:F:129:ARG:HB3	1.89	0.55
1:F:73:ARG:HA	1:F:76:MET:SD	2.47	0.54
3:C:145:TRP:HB2	3:C:158:ARG:HE	1.72	0.54
1:A:675:PHE:HD1	1:A:676:PRO:HD2	1.72	0.54
4:D:178:GLU:HB3	4:D:201:MET:HE2	1.89	0.54
2:B:291:VAL:HG22	2:B:296:ILE:HG12	1.89	0.54
3:C:264:MET:HG2	3:C:280:TYR:HA	1.90	0.54
2:B:172:GLN:HG2	2:B:184:THR:HG22	1.87	0.54
4:D:162:ASP:O	4:D:166:ARG:HG3	2.08	0.54
5:E:42:ASP:HA	5:E:45:LYS:HZ2	1.73	0.54
1:A:204:PRO:HG2	1:A:207:ASN:HB2	1.89	0.54
1:A:322:VAL:HG13	1:A:341:VAL:HG22	1.89	0.54
3:C:118:PRO:O	3:C:121:VAL:HB	2.08	0.54
1:F:69:GLN:O	1:F:72:GLU:HG2	2.07	0.54
1:A:130:ILE:HG13	1:A:131:ALA:N	2.22	0.54
1:A:206:TRP:H	1:A:206:TRP:CD1	2.25	0.54
2:B:295:ARG:HH21	2:B:351:VAL:HG22	1.73	0.53
3:C:143:THR:O	3:C:160:ARG:HG3	2.09	0.53
1:A:663:PHE:HA	1:A:799:ALA:HA	1.91	0.53
1:A:138:GLU:HG3	1:A:151:VAL:HG22	1.89	0.53
2:B:118:SER:HB3	2:B:157:VAL:HG11	1.90	0.53
3:C:178:LEU:HD13	3:C:198:SER:HB3	1.91	0.53
3:C:107:LEU:HD13	3:C:173:ALA:HB2	1.91	0.53
2:B:35:LEU:HD13	2:B:36:PRO:HD2	1.91	0.53
5:E:75:TYR:HB2	5:E:91:LEU:HB3	1.91	0.52
1:A:91:ARG:HH21	1:A:126:ASP:HA	1.73	0.52
2:B:115:VAL:HG22	2:B:124:ILE:HD12	1.91	0.52
1:A:546:TRP:HH2	1:A:563:ASN:HD21	1.57	0.52
2:B:345:TYR:CE1	2:B:361:LYS:HB2	2.44	0.52
4:D:162:ASP:OD2	4:D:166:ARG:HD2	2.09	0.52
1:A:198:GLN:HG3	1:A:218:LYS:HE3	1.92	0.52
1:A:376:TRP:CZ3	5:E:37:TYR:HB3	2.45	0.52
3:C:28:ASP:HB3	3:C:30:ARG:HD2	1.92	0.52
1:F:39:GLU:O	1:F:42:VAL:HG13	2.10	0.52
3:C:155:GLU:HG3	3:C:157:TYR:CE1	2.45	0.52
5:E:46:ILE:HG13	5:E:59:LEU:HD11	1.92	0.52
2:B:308:LEU:HG	2:B:315:THR:HA	1.91	0.51
1:F:126:ASN:HA	1:F:129:ARG:HD2	1.92	0.51
2:B:234:GLN:HB3	2:B:266:ASN:ND2	2.26	0.51
3:C:67:ILE:HD12	3:C:68:PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:THR:HA	1:A:304:MET:HE1	1.91	0.51
1:A:668:ILE:HD11	1:A:767:ARG:NE	2.26	0.51
3:C:87:GLN:HB3	4:D:70:GLN:OE1	2.11	0.51
3:C:110:ASN:HB2	3:C:171:GLN:HA	1.92	0.51
1:F:93:ASP:HA	1:F:96:LEU:HB3	1.91	0.51
1:A:159:PRO:HG2	1:A:160:ARG:HH21	1.74	0.51
2:B:219:VAL:HG22	2:B:226:MET:HA	1.93	0.51
3:C:89:LEU:HB2	3:C:203:ASN:CG	2.36	0.51
4:D:55:LEU:HD12	4:D:71:VAL:HG13	1.90	0.51
3:C:96:ARG:HB3	3:C:107:LEU:HB3	1.92	0.51
1:F:68:HIS:HA	1:F:71:MET:HG2	1.92	0.51
1:A:62:THR:O	1:A:66:LEU:HD22	2.10	0.51
1:F:30:ALA:HB2	1:F:425:ILE:HD12	1.92	0.51
3:C:127:LYS:HB3	3:C:129:TYR:CD2	2.46	0.50
4:D:89:GLN:HA	4:D:92:ILE:HG12	1.93	0.50
2:B:296:ILE:HG13	2:B:310:ILE:HG22	1.93	0.50
2:B:135:ASN:HB3	2:B:138:ASP:OD1	2.12	0.50
2:B:338:VAL:HG21	2:B:378:LEU:HD11	1.94	0.50
2:B:378:LEU:HD22	2:B:390:ILE:HB	1.94	0.50
1:F:161:ALA:HB1	1:F:394:LYS:HE2	1.94	0.50
1:A:393:GLY:HA2	1:A:584:GLY:HA3	1.94	0.50
3:C:83:ARG:HE	3:C:196:ARG:CZ	2.25	0.50
3:C:264:MET:HE2	3:C:280:TYR:HB2	1.94	0.50
4:D:161:THR:O	4:D:165:LYS:HG2	2.12	0.50
1:A:321:ARG:HB3	1:A:342:ASP:HB2	1.94	0.49
1:A:111:LYS:HE3	1:A:111:LYS:HA	1.95	0.49
2:B:285:SER:HB2	2:B:301:GLN:CD	2.37	0.49
3:C:135:ASP:HB3	3:C:140:THR:HG23	1.94	0.49
3:C:318:PHE:HB2	3:C:326:LEU:HD22	1.94	0.49
3:C:117:TRP:CZ3	3:C:141:LEU:HG	2.48	0.49
1:F:158:GLU:O	1:F:162:GLN:HG2	2.12	0.49
1:A:170:GLN:HG2	3:C:324:HIS:CD2	2.48	0.49
1:A:676:PRO:HD3	1:A:699:LEU:HD23	1.95	0.49
2:B:98:ALA:HB3	2:B:100:LYS:HE2	1.94	0.49
1:A:244:GLN:HG2	2:B:189:MET:HE2	1.94	0.49
2:B:145:THR:HG21	2:B:179:GLY:HA2	1.95	0.49
1:A:365:LEU:HD21	1:A:395:PHE:HZ	1.76	0.49
1:A:583:ARG:HB2	1:A:587:PRO:HA	1.95	0.49
1:A:701:LYS:HZ3	1:A:757:TYR:HB3	1.76	0.49
1:A:719:ILE:HD12	1:A:734:ARG:NE	2.27	0.49
4:D:178:GLU:HB3	4:D:201:MET:CE	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:192:VAL:HG22	5:E:64:MET:SD	2.53	0.48
1:F:110:THR:H	1:F:113:GLN:HB2	1.78	0.48
3:C:305:LEU:HD11	3:C:316:LEU:CD1	2.42	0.48
3:C:85:PRO:HD3	4:D:107:TYR:CE2	2.49	0.48
1:A:127:ARG:O	1:A:130:ILE:HG12	2.14	0.48
1:A:405:VAL:HG13	1:A:407:GLY:H	1.79	0.48
4:D:222:TYR:CE2	4:D:230:GLN:HG3	2.48	0.48
1:F:393:GLN:HB2	1:F:394:LYS:HE3	1.96	0.48
1:A:29:ILE:HD11	1:A:43:LEU:HD13	1.95	0.48
2:B:350:ASN:HB2	2:B:355:ARG:HG2	1.95	0.48
4:D:117:MET:CE	4:D:166:ARG:HE	2.24	0.48
1:A:670:PRO:HB3	1:A:760:TYR:CD2	2.49	0.48
3:C:129:TYR:CE1	3:C:146:VAL:HG21	2.49	0.48
3:C:106:LEU:HD13	3:C:202:MET:HE2	1.96	0.48
3:C:159:GLY:HA3	3:C:180:ASN:HB3	1.96	0.48
1:A:152:LYS:HD3	1:A:152:LYS:HA	1.58	0.47
4:D:134:ASP:HA	4:D:177:TYR:HD1	1.79	0.47
1:A:785:PHE:HE1	1:A:804:PHE:CD1	2.32	0.47
1:A:608:TYR:HA	1:A:640:GLY:HA2	1.96	0.47
3:C:97:THR:HG22	3:C:106:LEU:HB2	1.95	0.47
3:C:155:GLU:HG3	3:C:157:TYR:CZ	2.48	0.47
1:F:100:ILE:HD11	1:F:129:ARG:HG2	1.96	0.47
1:A:231:LEU:HD12	1:A:231:LEU:HA	1.79	0.47
1:A:99:PHE:HE2	1:A:111:LYS:NZ	2.13	0.47
2:B:241:ILE:HD12	2:B:241:ILE:H	1.79	0.47
3:C:145:TRP:HE1	3:C:160:ARG:CZ	2.28	0.47
4:D:109:MET:HE1	4:D:154:TYR:CE1	2.49	0.47
3:C:140:THR:HA	3:C:164:SER:HA	1.95	0.47
1:F:134:LYS:HA	1:F:137:ILE:HG22	1.96	0.47
1:F:394:LYS:HE3	1:F:394:LYS:N	2.28	0.47
2:B:67:LEU:HD23	2:B:374:ALA:HB3	1.95	0.47
2:B:261:LEU:HD21	2:B:267:LEU:HD12	1.96	0.47
4:D:76:ILE:HD12	4:D:92:ILE:HD13	1.97	0.47
2:B:31:LYS:HE3	2:B:31:LYS:HB3	1.74	0.47
2:B:237:GLY:HA3	2:B:243:ARG:HD2	1.97	0.47
4:D:99:ASN:HD21	4:D:102:HIS:CD2	2.33	0.47
3:C:33:ARG:HG3	3:C:83:ARG:NH1	2.29	0.47
2:B:242:ASP:HB3	2:B:243:ARG:HH12	1.80	0.47
3:C:247:PRO:O	3:C:251:VAL:HG22	2.14	0.46
1:A:227:ARG:HA	1:A:238:PHE:HE2	1.81	0.46
3:C:120:VAL:O	3:C:123:VAL:HB	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63:ASP:O	1:F:67:ARG:HB2	2.16	0.46
1:A:232:ASP:HA	1:A:297:ASN:HA	1.96	0.46
1:A:465:TYR:C	1:A:497:ASP:HB2	2.41	0.46
1:A:701:LYS:NZ	1:A:757:TYR:HB3	2.31	0.46
1:A:749:TRP:CZ3	1:A:760:TYR:HB2	2.50	0.46
3:C:245:ARG:HG3	3:C:313:ARG:HD3	1.97	0.46
1:A:323:GLN:HB3	1:A:340:ASN:OD1	2.15	0.46
1:A:365:LEU:HD21	1:A:395:PHE:CZ	2.50	0.46
1:F:91:ILE:HB	1:F:133:ARG:HD2	1.96	0.46
1:A:107:ASP:O	1:A:111:LYS:HG2	2.16	0.46
1:F:137:ILE:O	1:F:140:GLU:HG3	2.16	0.46
1:A:449:TRP:HB2	1:A:456:VAL:HG12	1.97	0.46
2:B:306:MET:HB3	2:B:306:MET:HE2	1.72	0.46
3:C:33:ARG:NH1	3:C:153:GLU:HA	2.30	0.46
1:A:627:TRP:HA	1:A:719:ILE:O	2.16	0.45
1:A:543:VAL:HG12	1:A:673:VAL:HG22	1.98	0.45
2:B:391:THR:O	2:B:392:ARG:C	2.59	0.45
4:D:58:LEU:HD22	4:D:71:VAL:HG21	1.99	0.45
1:F:91:ILE:H	1:F:133:ARG:CZ	2.29	0.45
3:C:145:TRP:CD1	3:C:160:ARG:HB2	2.50	0.45
5:E:93:LEU:HD23	5:E:101:LEU:HD11	1.97	0.45
1:F:50:LYS:HE2	1:F:60:LEU:HD13	1.98	0.45
1:F:70:ILE:O	1:F:74:LEU:HG	2.16	0.45
3:C:65:TYR:HE2	4:D:174:LEU:HD13	1.81	0.45
4:D:43:LEU:HD23	4:D:43:LEU:HA	1.81	0.45
1:A:288:THR:HA	1:A:304:MET:CE	2.46	0.45
4:D:79:TYR:HB3	4:D:88:ALA:HB2	1.98	0.45
1:F:69:GLN:HA	1:F:72:GLU:CD	2.42	0.45
1:A:72:PHE:CE2	1:A:88:VAL:HG13	2.52	0.45
2:B:220:LEU:HB2	2:B:227:ILE:HD11	1.99	0.45
4:D:225:MET:HB3	5:E:88:GLN:HE22	1.82	0.45
1:A:350:ARG:HH21	1:A:405:VAL:HG23	1.82	0.45
2:B:166:THR:HG23	2:B:168:ASN:H	1.81	0.45
3:C:141:LEU:HD23	3:C:141:LEU:HA	1.85	0.45
2:B:152:LEU:HD12	2:B:167:SER:HB3	1.99	0.44
3:C:127:LYS:HD3	3:C:127:LYS:HA	1.76	0.44
1:F:109:MET:HB2	1:F:113:GLN:HB2	1.99	0.44
1:F:132:ILE:HG23	1:F:136:MET:SD	2.56	0.44
1:A:600:THR:OG1	1:A:607:GLU:HA	2.17	0.44
2:B:227:ILE:HG22	2:B:228:TRP:CD1	2.52	0.44
3:C:30:ARG:HA	3:C:33:ARG:HE	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ARG:H	1:F:25:VAL:CG2	2.29	0.44
1:A:738:PHE:HZ	1:A:788:ALA:HB2	1.82	0.44
2:B:36:PRO:HG2	2:B:359:GLN:NE2	2.31	0.44
2:B:352:GLU:H	2:B:352:GLU:HG3	1.70	0.44
3:C:201:MET:O	3:C:205:ILE:HG12	2.18	0.44
3:C:227:THR:HG22	3:C:343:SER:HA	1.99	0.44
4:D:81:LYS:HD2	4:D:81:LYS:HA	1.69	0.44
2:B:93:TRP:HZ3	2:B:95:VAL:HG22	1.83	0.44
3:C:88:PRO:HD3	3:C:99:PHE:CD2	2.53	0.44
4:D:39:ALA:HB1	4:D:55:LEU:HD22	1.99	0.44
1:F:76:MET:HA	1:F:79:ILE:HG12	1.99	0.44
1:A:72:PHE:CD2	1:A:75:VAL:HG12	2.53	0.44
2:B:233:SER:HB2	2:B:245:SER:HB2	1.99	0.44
1:F:392:ALA:O	1:F:396:ARG:HG3	2.18	0.44
1:A:586:PHE:HB2	1:A:734:ARG:CZ	2.47	0.44
3:C:271:ARG:NH2	4:D:61:ARG:HG2	2.33	0.44
1:F:78:GLN:O	1:F:82:GLN:HG2	2.17	0.44
1:A:300:LYS:HE2	1:A:300:LYS:HB2	1.87	0.44
2:B:328:THR:HG22	2:B:340:GLY:H	1.83	0.44
3:C:252:TRP:CZ2	3:C:276:MET:HE1	2.53	0.44
1:F:110:THR:O	1:F:114:MET:N	2.48	0.44
4:D:202:LEU:C	4:D:202:LEU:HD23	2.43	0.43
1:F:65:THR:HA	1:F:68:HIS:HE1	1.77	0.43
1:A:165:LEU:HD23	1:A:165:LEU:HA	1.83	0.43
3:C:246:GLY:N	3:C:312:ASN:O	2.51	0.43
3:C:248:PHE:HB2	3:C:309:ASP:OD2	2.19	0.43
1:A:266:TYR:HD1	1:A:333:LYS:HA	1.83	0.43
3:C:305:LEU:HA	3:C:317:GLN:O	2.18	0.43
4:D:59:ASP:HB2	4:D:71:VAL:HG11	1.99	0.43
2:B:80:LEU:HD21	2:B:82:LYS:HG3	2.01	0.43
3:C:145:TRP:CE3	3:C:159:GLY:HA2	2.53	0.43
5:E:93:LEU:HB3	5:E:101:LEU:HD21	2.00	0.43
1:F:75:ILE:O	1:F:79:ILE:HG23	2.19	0.43
1:F:159:SER:O	1:F:163:GLN:HG2	2.18	0.43
3:C:145:TRP:HA	3:C:159:GLY:O	2.18	0.43
3:C:165:VAL:HA	3:C:174:VAL:HG13	1.99	0.43
1:A:77:VAL:HB	1:F:26:ASP:HB3	2.01	0.43
2:B:286:VAL:HG22	2:B:299:VAL:O	2.19	0.43
2:B:289:PHE:HE1	2:B:291:VAL:HG23	1.84	0.43
3:C:90:ALA:O	4:D:66:PRO:HB3	2.19	0.43
3:C:131:ILE:HD12	3:C:142:THR:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:140:THR:HG22	3:C:164:SER:HB2	1.99	0.43
3:C:145:TRP:CD1	3:C:145:TRP:H	2.36	0.43
3:C:38:ASP:OD1	3:C:38:ASP:C	2.62	0.43
3:C:145:TRP:HB2	3:C:158:ARG:NE	2.33	0.43
2:B:337:LEU:HB2	2:B:349:ILE:HB	2.01	0.43
1:A:303:LYS:HE2	1:A:303:LYS:HB2	1.81	0.42
4:D:42:LYS:HB2	4:D:42:LYS:HE2	1.79	0.42
1:A:246:SER:HA	2:B:193:SER:O	2.19	0.42
1:A:711:MET:HB2	1:A:744:VAL:HG22	2.00	0.42
2:B:239:THR:O	2:B:243:ARG:HG2	2.19	0.42
5:E:63:LEU:HD12	5:E:63:LEU:HA	1.73	0.42
1:F:143:ASN:HA	1:F:406:PHE:CZ	2.48	0.42
1:F:400:MET:HE3	1:F:400:MET:HB3	1.92	0.42
2:B:63:LEU:HD13	2:B:63:LEU:HA	1.76	0.42
3:C:230:VAL:HG23	3:C:339:GLN:OE1	2.19	0.42
4:D:88:ALA:O	4:D:92:ILE:HG12	2.18	0.42
2:B:84:LEU:HD23	2:B:91:GLU:HA	2.01	0.42
1:A:105:VAL:HG13	1:A:109:MET:SD	2.60	0.42
1:A:364:VAL:HG12	1:A:365:LEU:HD23	2.01	0.42
1:A:619:VAL:HB	1:A:629:VAL:HG13	2.00	0.42
2:B:235:ALA:HB1	2:B:243:ARG:HB3	2.01	0.42
2:B:380:ILE:HD12	2:B:381:GLN:H	1.83	0.42
3:C:84:PRO:HA	4:D:107:TYR:CZ	2.54	0.42
3:C:159:GLY:HA2	3:C:180:ASN:HB3	1.99	0.42
4:D:179:TYR:HA	4:D:201:MET:HE1	2.02	0.42
1:A:157:PRO:O	3:C:309:ASP:N	2.43	0.42
1:A:166:LYS:HD2	1:A:166:LYS:HA	1.76	0.42
1:A:268:LEU:HD23	1:A:290:ILE:HG21	2.02	0.42
1:A:280:HIS:O	1:A:284:ILE:HD12	2.20	0.42
1:A:561:GLN:HE21	1:A:680:SER:HB2	1.85	0.42
2:B:47:ALA:HB3	2:B:389:SER:HB3	2.01	0.42
2:B:263:TYR:O	2:B:285:SER:HA	2.19	0.42
3:C:88:PRO:HD3	3:C:99:PHE:CE2	2.54	0.42
3:C:228:MET:HE3	3:C:246:GLY:HA2	2.00	0.42
1:A:91:ARG:H	1:A:91:ARG:HG3	1.59	0.42
1:A:112:GLN:H	1:A:112:GLN:CD	2.28	0.42
1:A:493:ASP:HA	1:A:507:LYS:HA	2.01	0.42
3:C:161:TYR:CD2	3:C:201:MET:HG3	2.54	0.42
3:C:166:LYS:HD2	3:C:167:PRO:HD2	2.02	0.42
3:C:252:TRP:HA	3:C:255:LEU:HG	2.02	0.42
1:F:64:ALA:HA	1:F:67:ARG:HE	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:GLN:HE21	1:A:542:GLN:HB3	1.75	0.42
1:A:677:HIS:O	1:A:692:THR:HA	2.20	0.42
1:A:682:TYR:CZ	1:A:684:PRO:HD3	2.55	0.42
2:B:138:ASP:OD1	2:B:140:THR:HG22	2.20	0.42
5:E:31:ASP:OD1	5:E:81:PRO:HA	2.19	0.42
1:A:571:THR:HG22	1:A:600:THR:HG22	2.01	0.42
1:A:735:THR:HB	1:A:774:LEU:HD12	2.02	0.42
3:C:87:GLN:HG2	3:C:88:PRO:HD2	2.01	0.42
1:A:158:LEU:HD23	1:A:158:LEU:HA	1.88	0.42
4:D:242:SER:O	4:D:243:SER:C	2.63	0.42
5:E:91:LEU:HD12	5:E:91:LEU:HA	1.87	0.42
1:F:403:ASN:O	1:F:404:ARG:C	2.63	0.42
2:B:295:ARG:HB2	2:B:297:TYR:CE1	2.55	0.41
4:D:55:LEU:HD13	4:D:55:LEU:HA	1.92	0.41
1:A:660:VAL:HG23	1:A:740:ASP:HB3	2.01	0.41
1:A:786:SER:OG	1:A:803:GLN:HB2	2.20	0.41
1:F:80:ILE:HG21	1:F:138:ILE:HG23	2.01	0.41
1:A:296:TYR:HB2	1:A:335:VAL:HG21	2.01	0.41
1:A:640:GLY:HA3	1:A:644:LYS:O	2.20	0.41
2:B:371:PRO:HB3	2:B:380:ILE:HB	2.02	0.41
1:A:32:GLU:HG3	1:A:87:GLN:HA	2.03	0.41
3:C:197:TYR:N	3:C:197:TYR:CD1	2.88	0.41
1:F:114:MET:O	1:F:118:LEU:HG	2.20	0.41
2:B:68:ALA:HB2	2:B:117:VAL:HG11	2.03	0.41
4:D:146:ASP:OD1	4:D:146:ASP:C	2.62	0.41
3:C:154:ASP:O	3:C:156:GLN:NE2	2.54	0.41
1:A:248:THR:C	1:A:250:ASP:H	2.29	0.41
2:B:331:VAL:HB	2:B:338:VAL:HG23	2.02	0.41
1:A:541:PRO:HB3	1:A:546:TRP:HE1	1.86	0.41
2:B:44:PRO:HA	2:B:392:ARG:C	2.46	0.41
2:B:265:GLY:HA2	2:B:284:GLY:HA3	2.02	0.41
3:C:150:ARG:HB3	3:C:152:ASP:OD1	2.21	0.41
1:A:135:LYS:HA	1:A:135:LYS:HD3	1.85	0.41
1:A:367:ARG:HA	4:D:184:TYR:OH	2.21	0.41
2:B:294:ASN:HA	2:B:310:ILE:HD13	2.02	0.41
3:C:162:GLN:O	3:C:176:VAL:HA	2.21	0.41
3:C:243:VAL:N	3:C:316:LEU:HG	2.36	0.41
3:C:244:VAL:O	3:C:314:SER:O	2.39	0.41
4:D:109:MET:HE3	4:D:109:MET:HB2	1.92	0.41
1:F:47:GLN:O	1:F:51:LEU:HD22	2.21	0.41
1:A:480:VAL:HB	4:D:187:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:LYS:HE3	1:A:580:LYS:HB3	1.86	0.41
2:B:355:ARG:HH12	2:B:357:VAL:HG13	1.86	0.41
1:F:32:VAL:CG1	1:F:75:ILE:HG23	2.51	0.40
1:A:223:LEU:HD12	1:A:240:ILE:HD13	2.02	0.40
1:A:268:LEU:HA	1:A:268:LEU:HD12	1.88	0.40
1:A:463:ASN:HB3	1:A:466:GLN:H	1.86	0.40
2:B:192:LEU:HD12	2:B:192:LEU:HA	1.74	0.40
1:A:389:LEU:HD23	1:A:389:LEU:HA	1.91	0.40
2:B:192:LEU:HD23	2:B:241:ILE:O	2.20	0.40
2:B:257:VAL:HG12	2:B:278:MET:HE1	2.02	0.40
2:B:306:MET:HG3	2:B:308:LEU:CD1	2.50	0.40
3:C:117:TRP:O	3:C:120:VAL:HG22	2.22	0.40
3:C:252:TRP:HZ3	3:C:271:ARG:HG3	1.87	0.40
1:A:156:THR:HG21	3:C:306:GLN:HG3	2.02	0.40
3:C:56:MET:C	3:C:56:MET:SD	3.05	0.40
3:C:102:ASP:HB2	3:C:178:LEU:HB3	2.04	0.40
3:C:305:LEU:HD13	3:C:318:PHE:CE2	2.56	0.40
3:C:306:GLN:HB3	3:C:317:GLN:HB2	2.02	0.40
4:D:199:GLU:OE2	5:E:67:PRO:HB3	2.22	0.40
1:A:29:ILE:HD12	1:A:31:PHE:HZ	1.85	0.40
1:A:92:PRO:HB2	1:A:163:VAL:HB	2.04	0.40
1:A:284:ILE:HG23	1:A:308:ILE:HD12	2.04	0.40
1:A:392:LEU:HD23	1:A:392:LEU:HA	1.79	0.40
1:A:683:ASP:OD1	1:A:688:TYR:HB3	2.22	0.40
1:A:727:ASP:HA	1:A:730:ALA:HB2	2.03	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	781/1222 (64%)	727 (93%)	54 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	173/1222 (14%)	165 (95%)	8 (5%)	0	100	100
2	B	367/392 (94%)	335 (91%)	32 (9%)	0	100	100
3	C	262/344 (76%)	256 (98%)	6 (2%)	0	100	100
4	D	216/245 (88%)	210 (97%)	6 (3%)	0	100	100
5	E	87/123 (71%)	83 (95%)	4 (5%)	0	100	100
All	All	1886/3548 (53%)	1776 (94%)	110 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	668/1027 (65%)	646 (97%)	22 (3%)	33	58
1	F	154/1027 (15%)	148 (96%)	6 (4%)	28	54
2	B	300/321 (94%)	287 (96%)	13 (4%)	26	52
3	C	225/276 (82%)	214 (95%)	11 (5%)	22	49
4	D	183/204 (90%)	179 (98%)	4 (2%)	45	65
5	E	77/103 (75%)	75 (97%)	2 (3%)	40	62
All	All	1607/2958 (54%)	1549 (96%)	58 (4%)	32	56

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	VAL
1	A	125	LEU
1	A	177	ILE
1	A	230	TYR
1	A	243	THR
1	A	312	LEU
1	A	346	ARG
1	A	397	THR

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Mol	Chain	Res	Type
1	A	398	VAL
1	A	444	VAL
1	A	461	THR
1	A	494	PHE
1	A	531	TYR
1	A	542	GLN
1	A	633	THR
1	A	673	VAL
1	A	677	HIS
1	A	713	VAL
1	A	716	LEU
1	A	735	THR
1	A	784	VAL
1	A	804	PHE
2	B	30	VAL
2	B	35	LEU
2	B	37	THR
2	B	63	LEU
2	B	141	VAL
2	B	157	VAL
2	B	226	MET
2	B	247	VAL
2	B	250	THR
2	B	254	VAL
2	B	292	ASP
2	B	318	THR
2	B	387	VAL
3	C	35	VAL
3	C	67	ILE
3	C	140	THR
3	C	144	ASP
3	C	146	VAL
3	C	180	ASN
3	C	194	MET
3	C	227	THR
3	C	244	VAL
3	C	278	VAL
3	C	316	LEU
4	D	101	THR
4	D	178	GLU
4	D	205	TYR
4	D	218	MET

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Mol	Chain	Res	Type
5	E	72	THR
5	E	104	ILE
1	F	31	VAL
1	F	41	ASP
1	F	42	VAL
1	F	114	MET
1	F	394	LYS
1	F	423	VAL

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

Mol	Chain	Res	Type
1	A	87	GLN
1	A	207	ASN
1	A	244	GLN
1	A	445	GLN
1	A	801	GLN
2	B	144	GLN
2	B	336	ASN
2	B	359	GLN
3	C	147	GLN
3	C	317	GLN
4	D	99	ASN
5	E	33	ASN
5	E	89	GLN
1	F	68	HIS
1	F	69	GLN
1	F	82	GLN
1	F	107	ASN
1	F	126	ASN
1	F	403	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 [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.

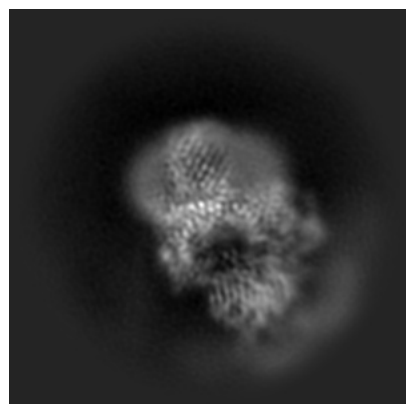
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-80076. These allow visual inspection of the internal detail of the map and identification of artifacts.

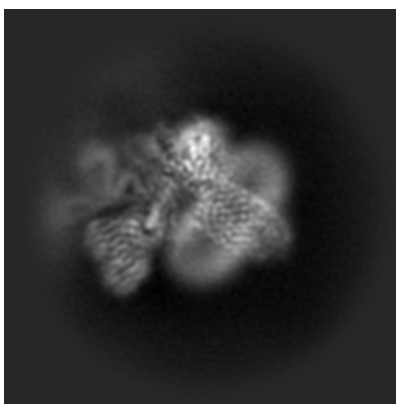
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

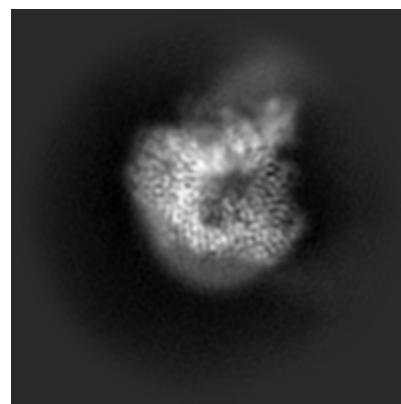
6.1.1 Primary map



X

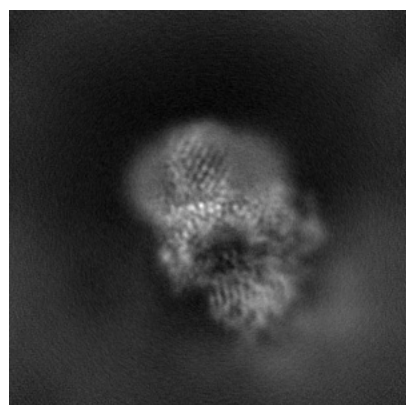


Y

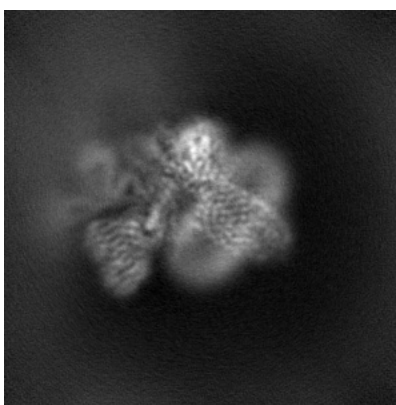


Z

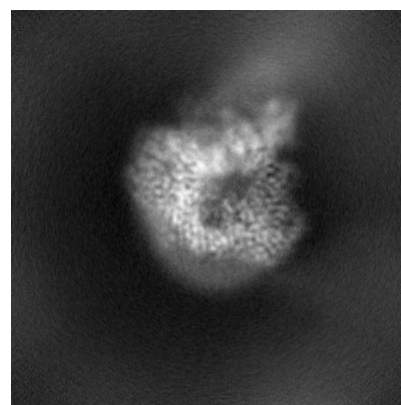
6.1.2 Raw map



X



Y

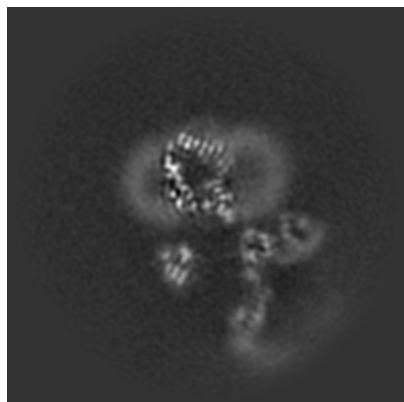


Z

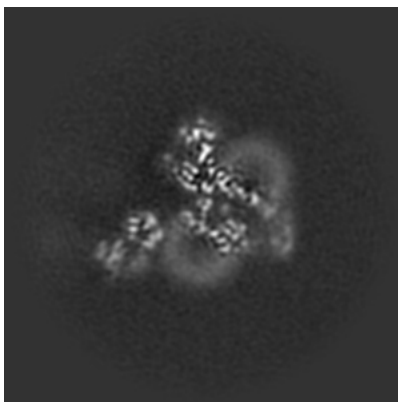
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

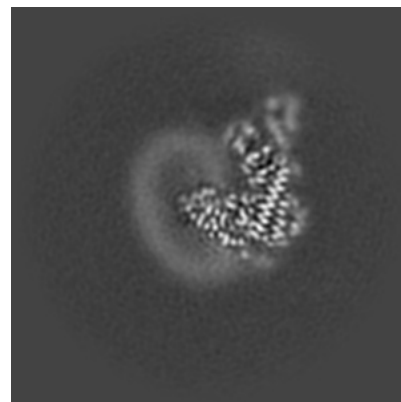
6.2.1 Primary map



X Index: 160

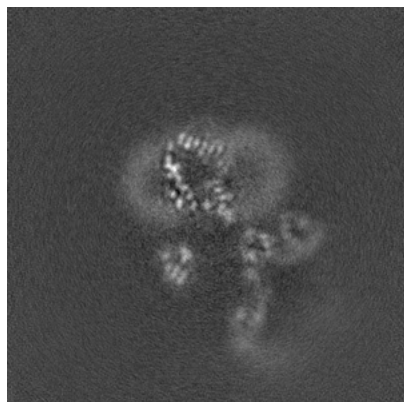


Y Index: 160

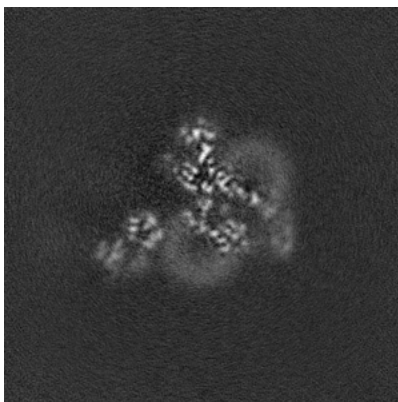


Z Index: 160

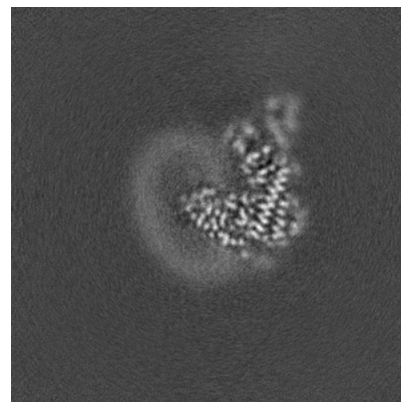
6.2.2 Raw map



X Index: 160



Y Index: 160

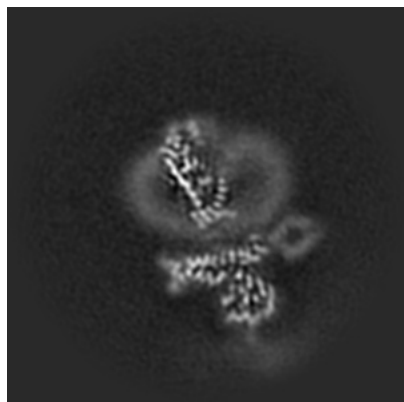


Z Index: 160

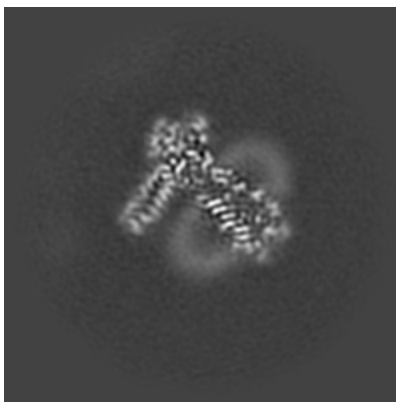
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

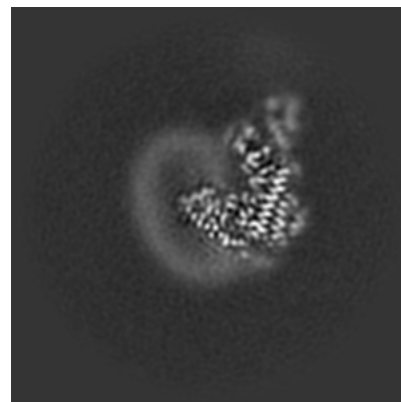
6.3.1 Primary map



X Index: 147

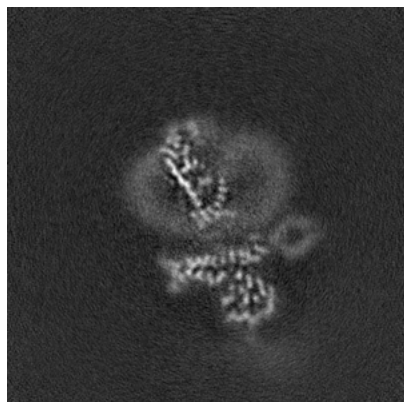


Y Index: 139

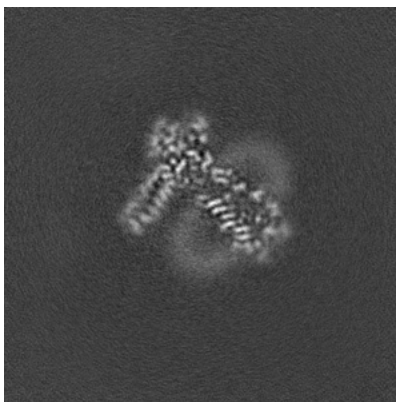


Z Index: 161

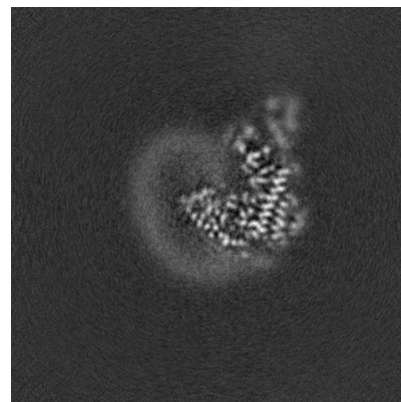
6.3.2 Raw map



X Index: 147



Y Index: 139

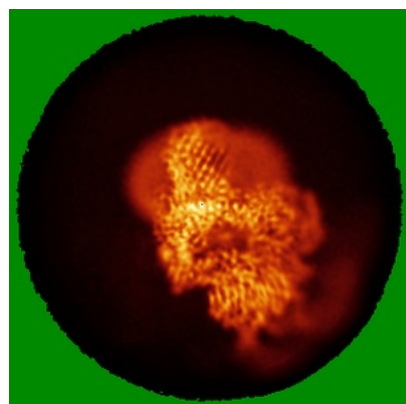


Z Index: 161

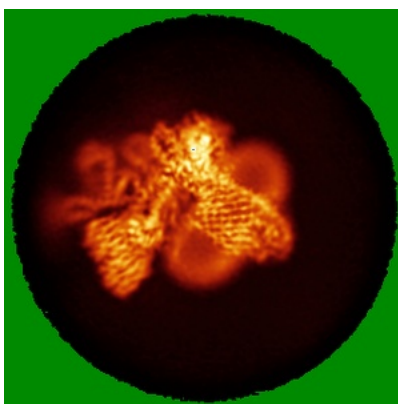
The images above show the largest variance slices of the map in three orthogonal directions.

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

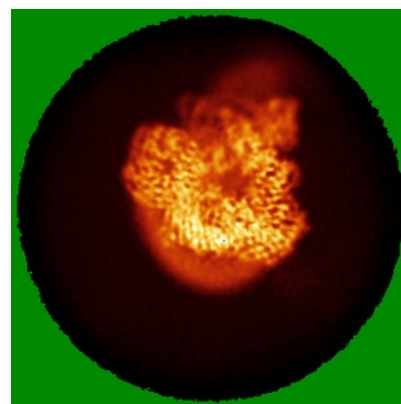
6.4.1 Primary map



X

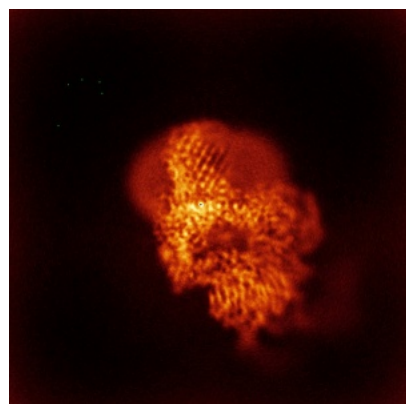


Y

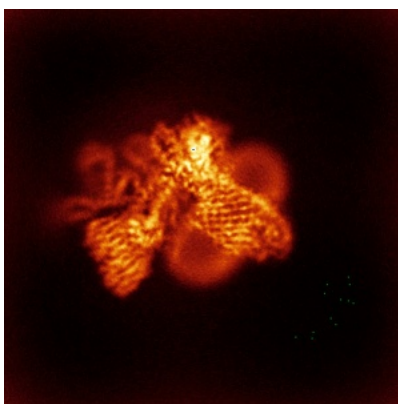


Z

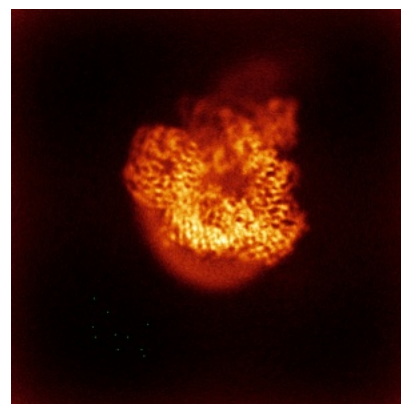
6.4.2 Raw map



X



Y

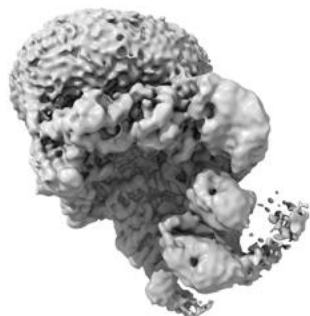


Z

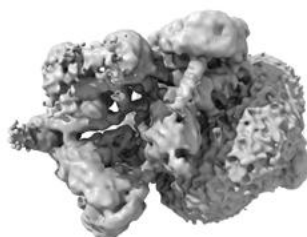
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

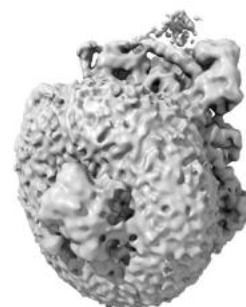
6.5.1 Primary map



X



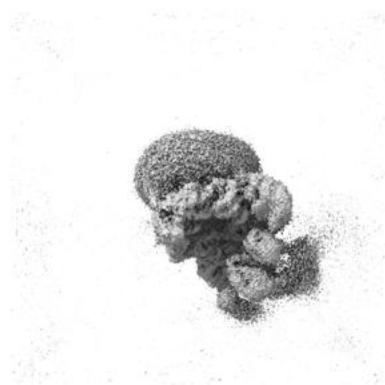
Y



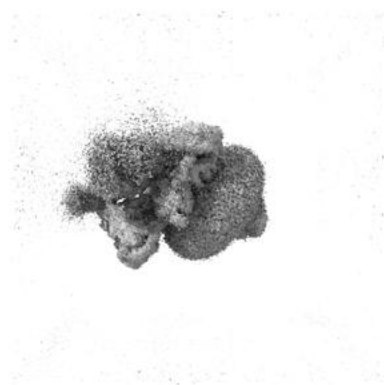
Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

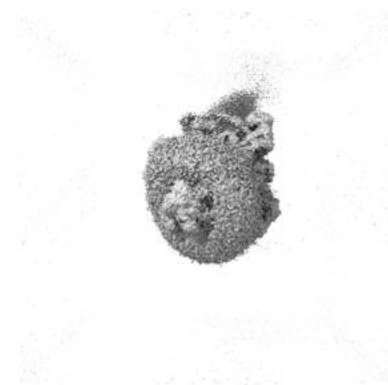
6.5.2 Raw map



X



Y



Z

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

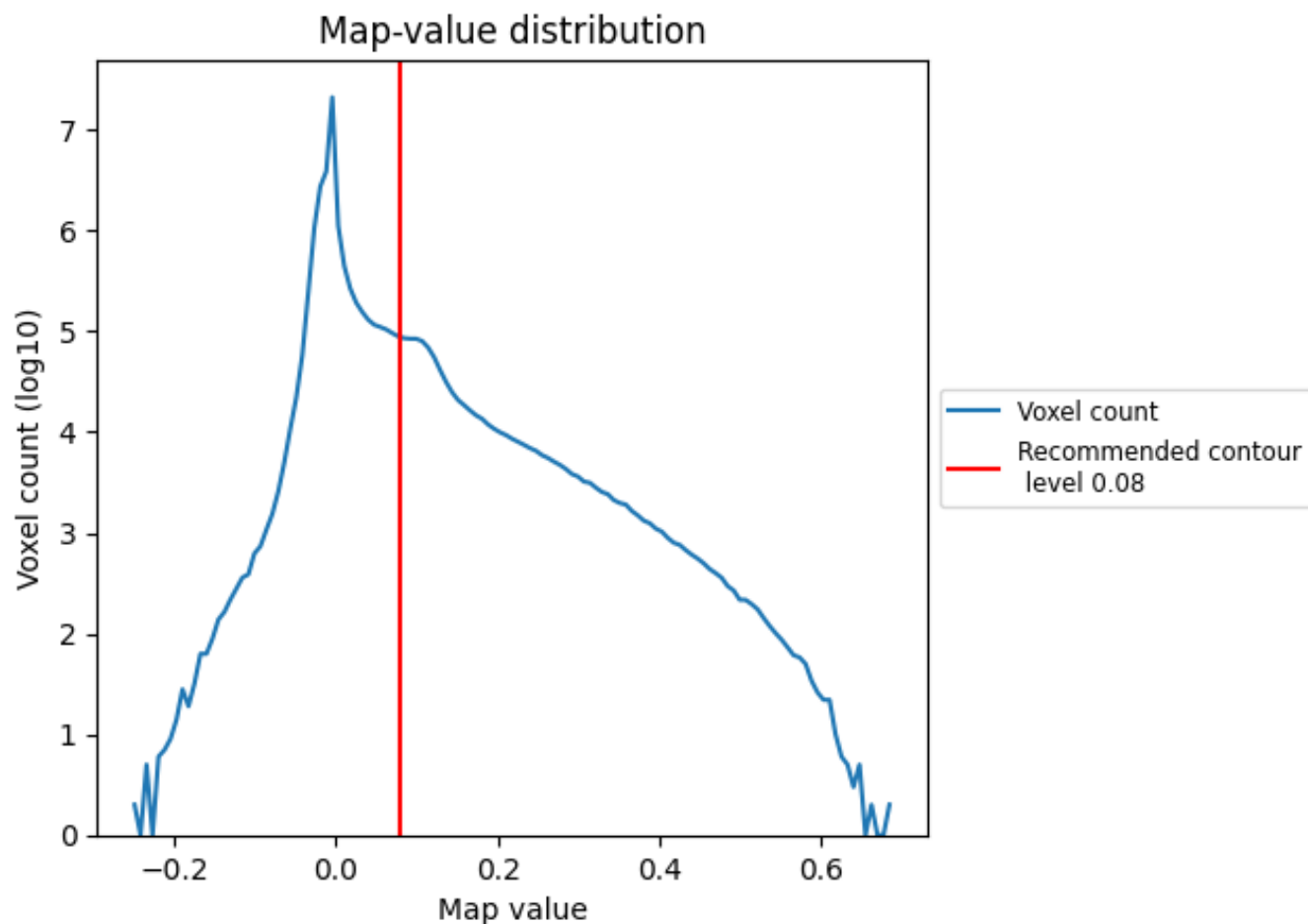
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

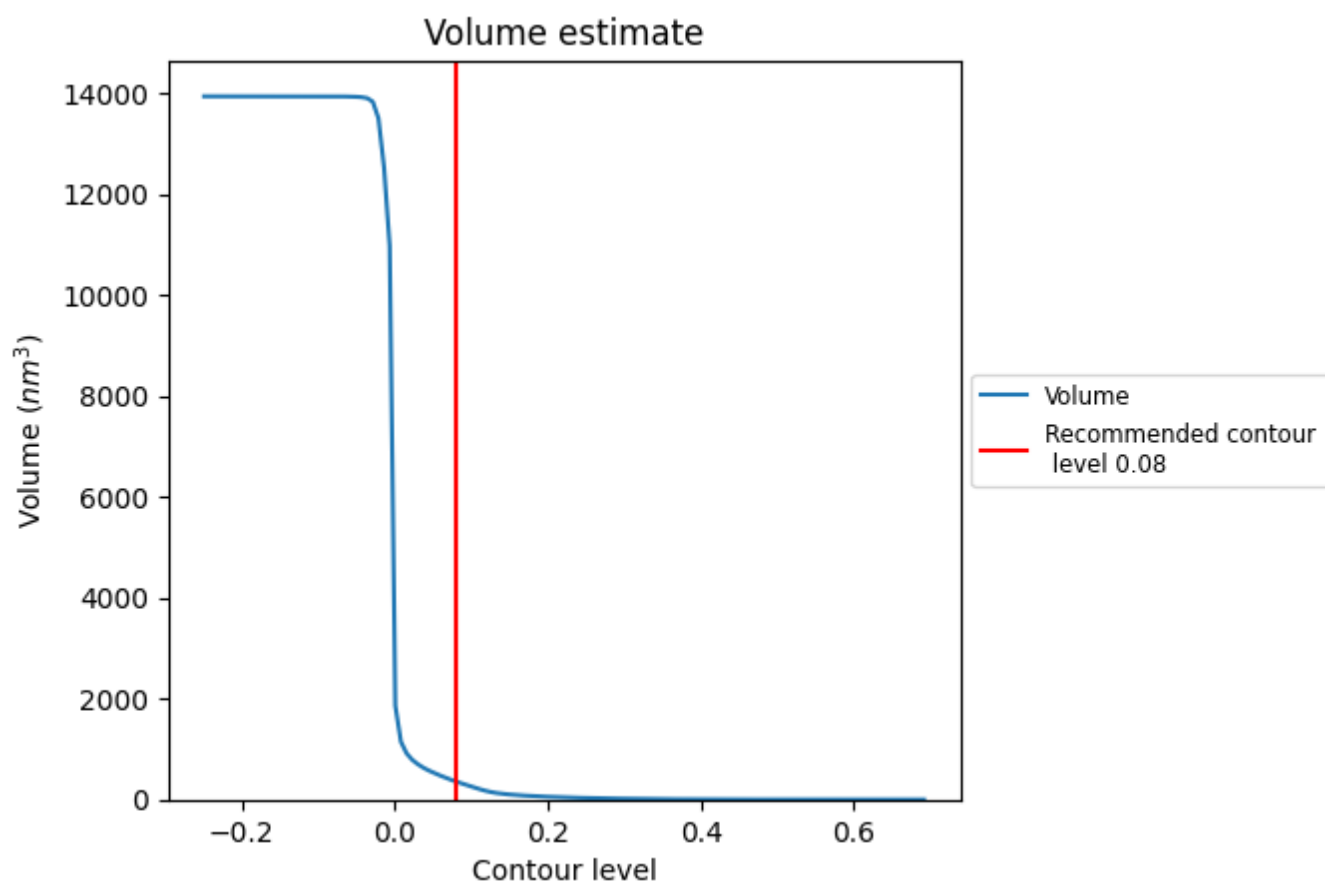
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

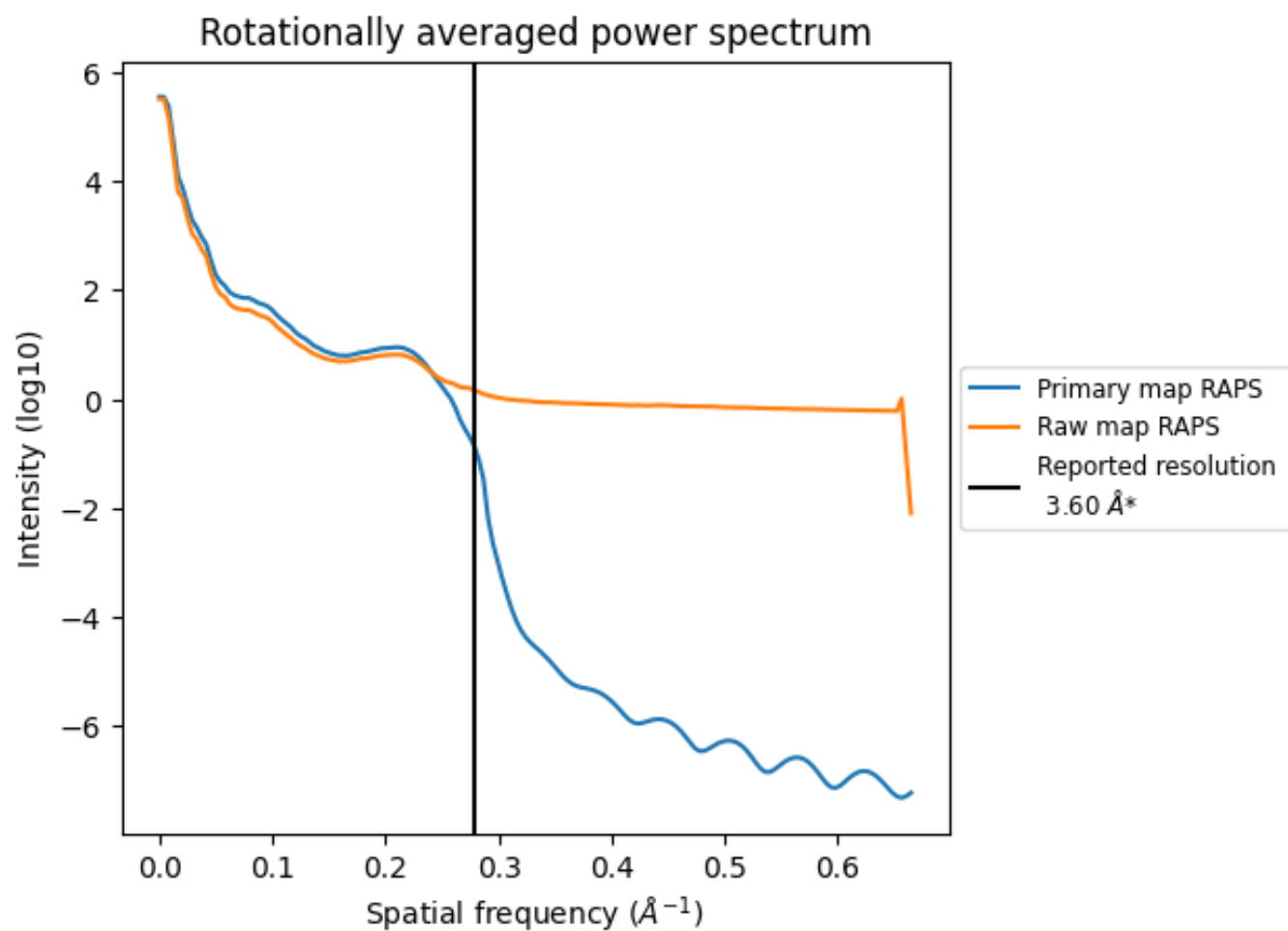
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 358 nm³; this corresponds to an approximate mass of 323 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 ⓘ

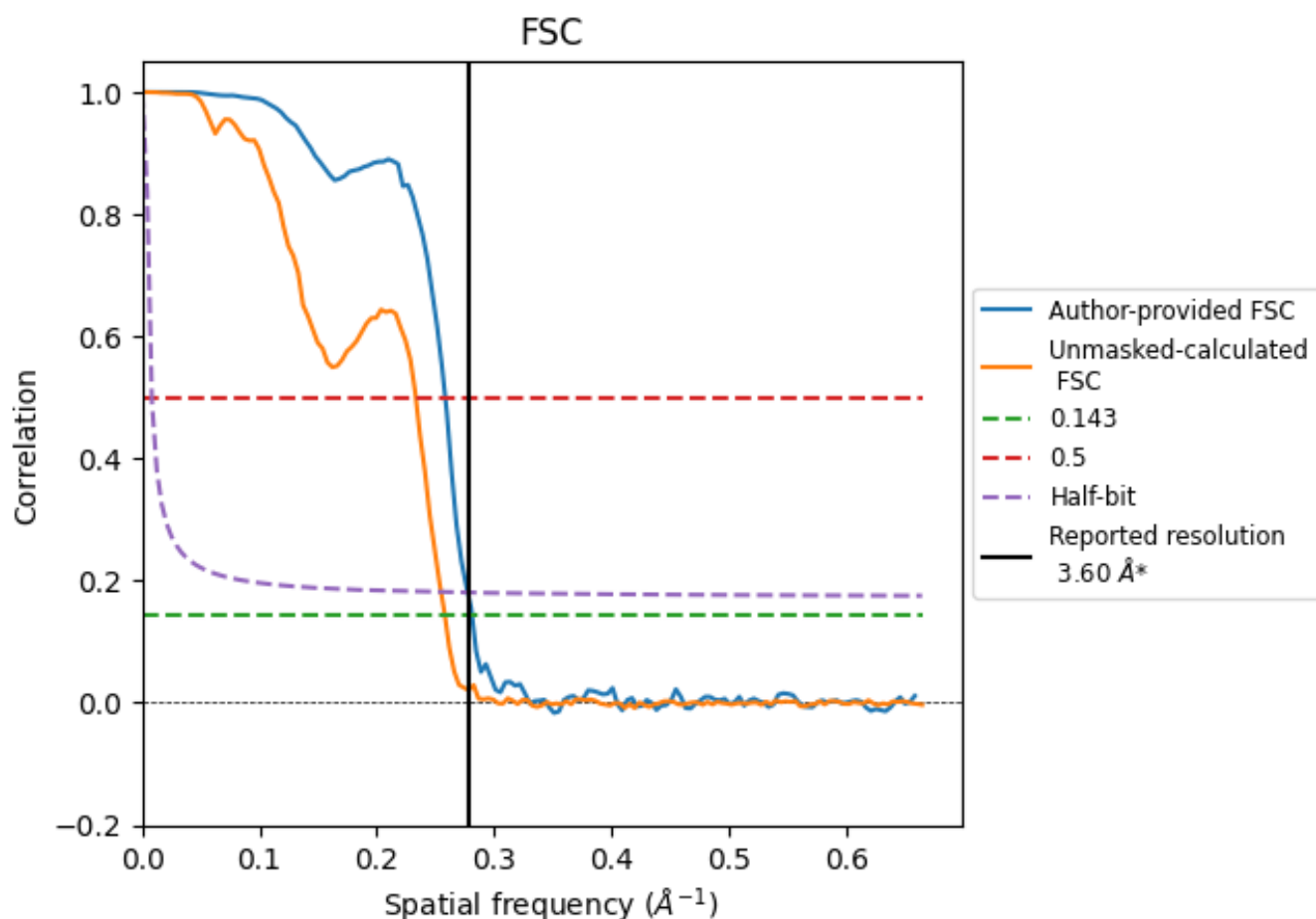


*Reported resolution corresponds to spatial frequency of 0.278 $\text{\AA}^{-1}$

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 0.278 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

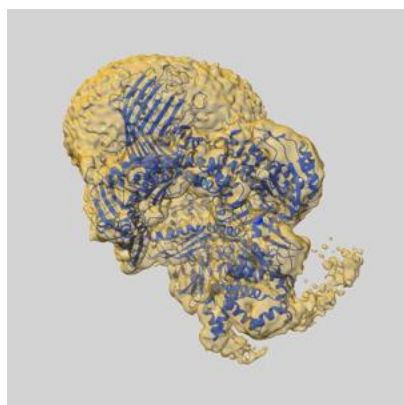
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.56	3.87	3.60
Unmasked-calculated*	3.87	4.29	3.92

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

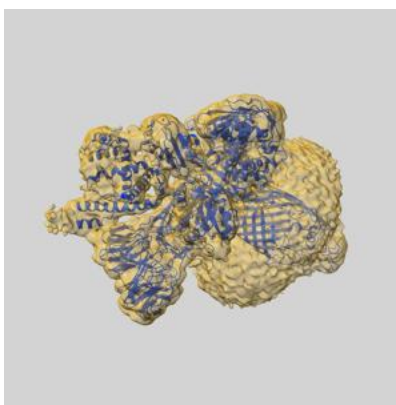
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-80076 and PDB model 25FQ. Per-residue inclusion information can be found in section [3](#) on page [6](#).

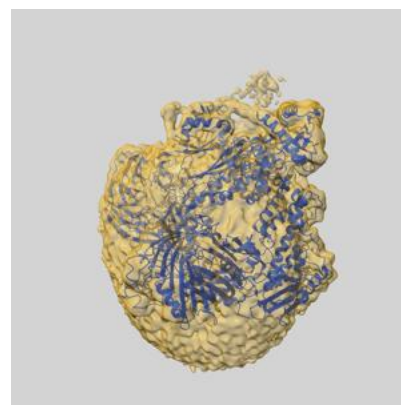
9.1 Map-model overlay [i](#)



X



Y



Z

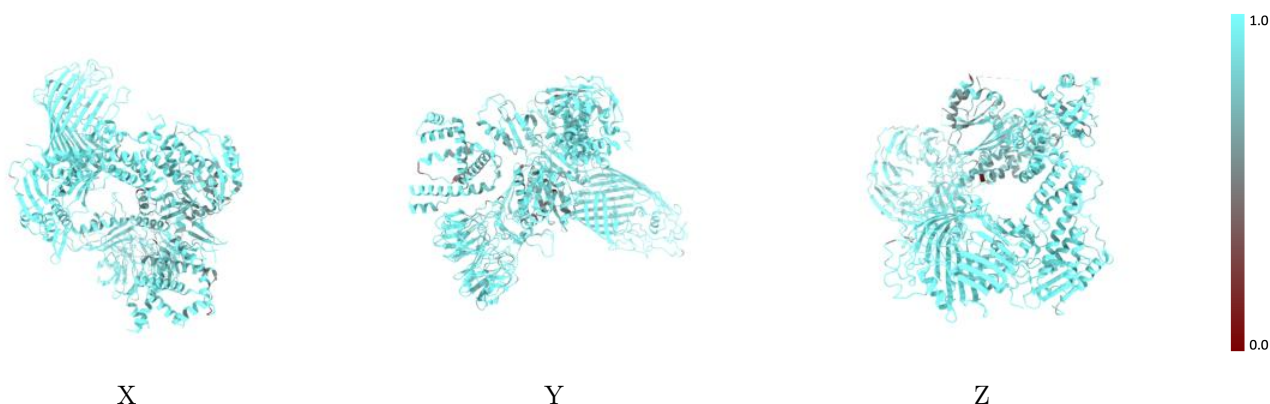
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



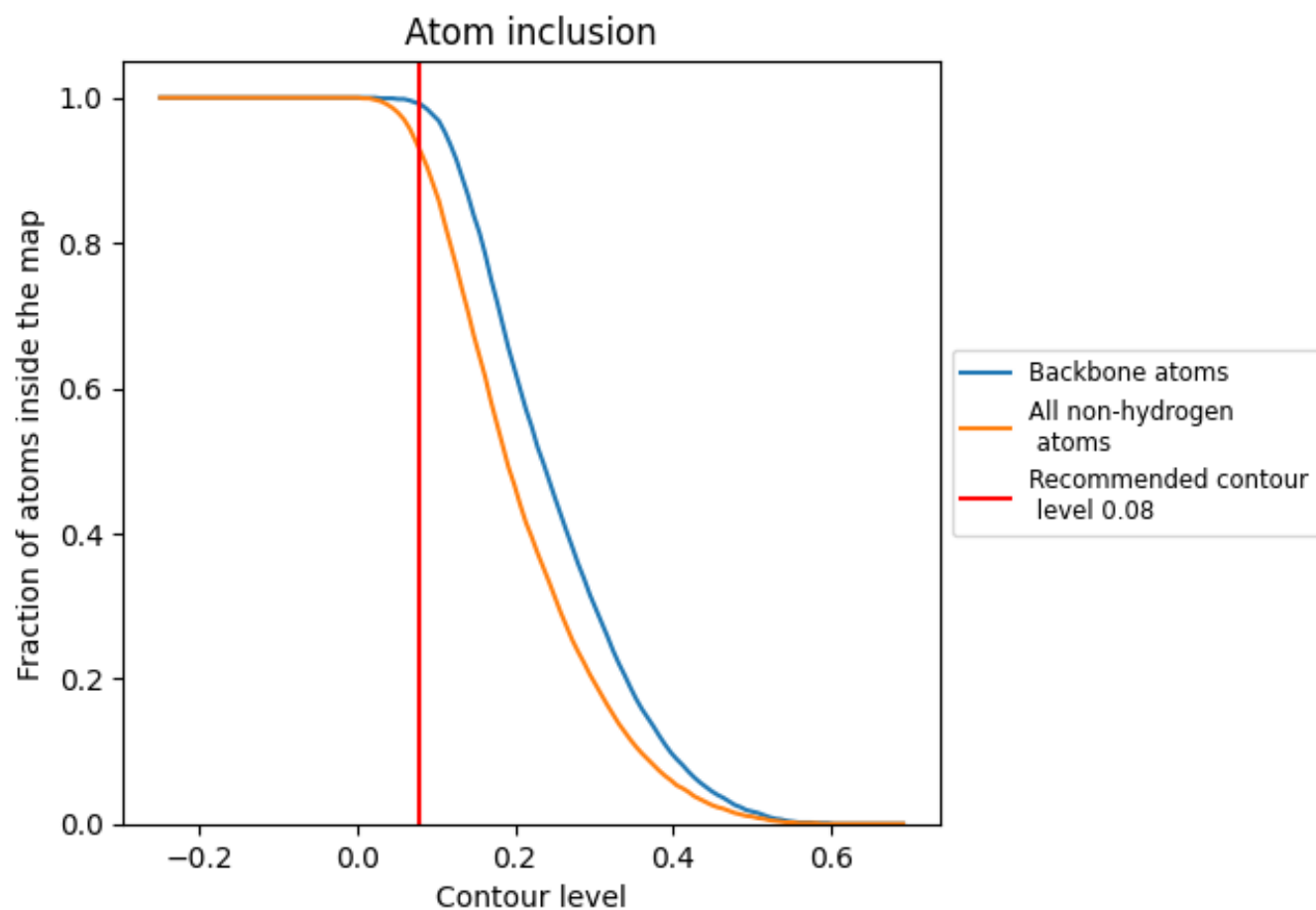
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 93% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9270	0.3640
A	0.9470	0.4000
B	0.9260	0.3770
C	0.8470	0.2580
D	0.9720	0.4260
E	0.9720	0.4280
F	0.8810	0.2360

1.0

0.0

<0.0