



## Full wwPDB EM Validation Report ⓘ

May 18, 2025 – 03:30 AM EDT

PDB ID : 9AYR / pdb\_00009ayr  
EMDB ID : EMD-43997  
Title : Structure of a Ric1-Rgp1-Rab6 activation intermediate  
Authors : Feathers, J.R.; Fromme, J.C.  
Deposited on : 2024-03-08  
Resolution : 3.30 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev118  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

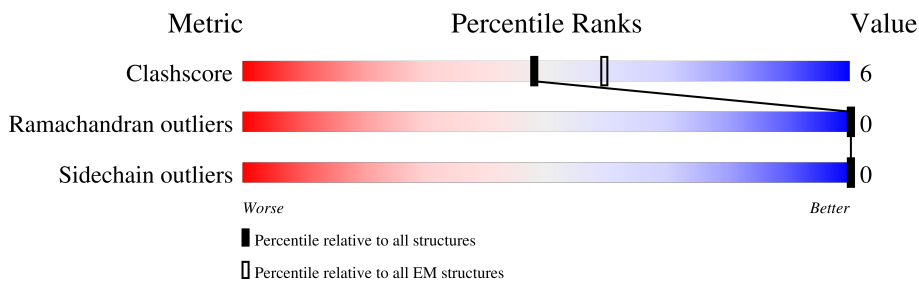
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1056	
2	B	663	
3	C	215	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23897 atoms, of which 11935 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 Guanine nucleotide exchange factor subunit RIC1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	910	Total	C	H	N	O	S	0	0
			14474	4683	7226	1178	1355	32		

There are 49 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	998	UNK	ASP	conflict	UNP P40395
A	999	UNK	GLU	conflict	UNP P40395
A	1000	UNK	GLU	conflict	UNP P40395
A	1001	UNK	LEU	conflict	UNP P40395
A	1002	UNK	MET	conflict	UNP P40395
A	1003	UNK	LEU	conflict	UNP P40395
A	1004	UNK	LYS	conflict	UNP P40395
A	1005	UNK	VAL	conflict	UNP P40395
A	1006	UNK	LEU	conflict	UNP P40395
A	1007	UNK	GLU	conflict	UNP P40395
A	1008	UNK	LEU	conflict	UNP P40395
A	1009	UNK	LEU	conflict	UNP P40395
A	1010	UNK	VAL	conflict	UNP P40395
A	1011	UNK	THR	conflict	UNP P40395
A	1012	UNK	SER	conflict	UNP P40395
A	1013	UNK	ALA	conflict	UNP P40395
A	1014	UNK	ALA	conflict	UNP P40395
A	1015	UNK	ASN	conflict	UNP P40395
A	1019	UNK	PRO	conflict	UNP P40395
A	1020	UNK	ILE	conflict	UNP P40395
A	1021	UNK	LYS	conflict	UNP P40395
A	1022	UNK	ALA	conflict	UNP P40395
A	1023	UNK	THR	conflict	UNP P40395
A	1024	UNK	ASP	conflict	UNP P40395
A	1025	UNK	SER	conflict	UNP P40395
A	1026	UNK	TRP	conflict	UNP P40395
A	1027	UNK	ASP	conflict	UNP P40395
A	1028	UNK	MET	conflict	UNP P40395

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1029	UNK	CYS	conflict	UNP P40395
A	1030	UNK	PHE	conflict	UNP P40395
A	1031	UNK	GLN	conflict	UNP P40395
A	1032	UNK	LEU	conflict	UNP P40395
A	1033	UNK	ILE	conflict	UNP P40395
A	1034	UNK	ARG	conflict	UNP P40395
A	1035	UNK	LEU	conflict	UNP P40395
A	1036	UNK	LEU	conflict	UNP P40395
A	1037	UNK	LYS	conflict	UNP P40395
A	1038	UNK	GLU	conflict	UNP P40395
A	1039	UNK	LEU	conflict	UNP P40395
A	1047	UNK	LEU	conflict	UNP P40395
A	1048	UNK	VAL	conflict	UNP P40395
A	1049	UNK	GLN	conflict	UNP P40395
A	1050	UNK	LYS	conflict	UNP P40395
A	1051	UNK	ALA	conflict	UNP P40395
A	1052	UNK	LEU	conflict	UNP P40395
A	1053	UNK	GLU	conflict	UNP P40395
A	1054	UNK	ARG	conflict	UNP P40395
A	1055	UNK	PHE	conflict	UNP P40395
A	1056	UNK	LYS	conflict	UNP P40395

- Molecule 2 is a protein called Guanine nucleotide exchange factor subunit RGP1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	424	Total	C	H	N	O	S	0	0
			6645	2150	3300	548	636	11		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	379	UNK	LYS	conflict	UNP P16664
B	380	UNK	ARG	conflict	UNP P16664
B	381	UNK	VAL	conflict	UNP P16664
B	382	UNK	LYS	conflict	UNP P16664
B	383	UNK	LYS	conflict	UNP P16664
B	384	UNK	ASN	conflict	UNP P16664
B	385	UNK	PHE	conflict	UNP P16664
B	386	UNK	ILE	conflict	UNP P16664
B	387	UNK	GLU	conflict	UNP P16664
B	388	UNK	LEU	conflict	UNP P16664
B	389	UNK	VAL	conflict	UNP P16664

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Chain	Residue	Modelled	Actual	Comment	Reference
B	390	UNK	GLU	conflict	UNP P16664
B	398	UNK	ASP	conflict	UNP P16664
B	399	UNK	ILE	conflict	UNP P16664
B	400	UNK	ASP	conflict	UNP P16664
B	401	UNK	GLU	conflict	UNP P16664
B	402	UNK	LEU	conflict	UNP P16664
B	403	UNK	ILE	conflict	UNP P16664
B	404	UNK	ASP	conflict	UNP P16664
B	405	UNK	LEU	conflict	UNP P16664
B	406	UNK	GLN	conflict	UNP P16664
B	407	UNK	MET	conflict	UNP P16664
B	408	UNK	GLY	conflict	UNP P16664
B	409	UNK	VAL	conflict	UNP P16664

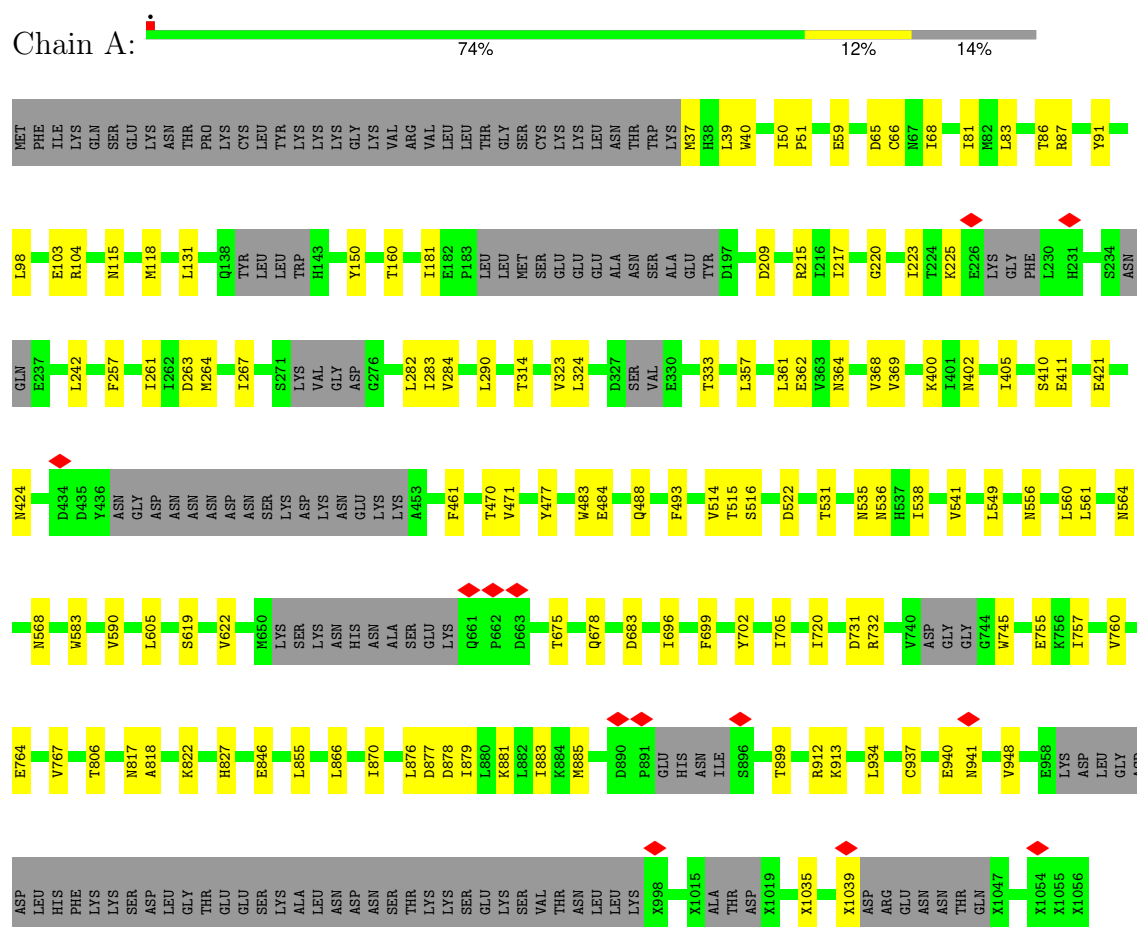
- Molecule 3 is a protein called GTP-binding protein YPT6.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	167	Total	C	H	N	O	S	0	0
			2778	883	1409	223	259	4		

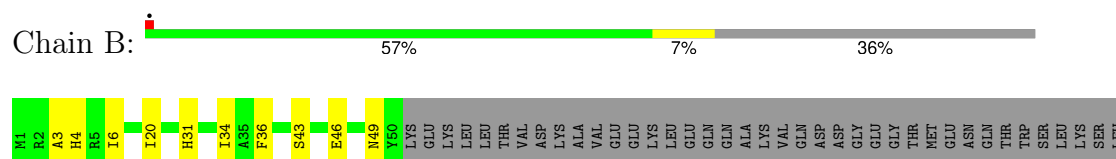
### 3 Residue-property plots

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.

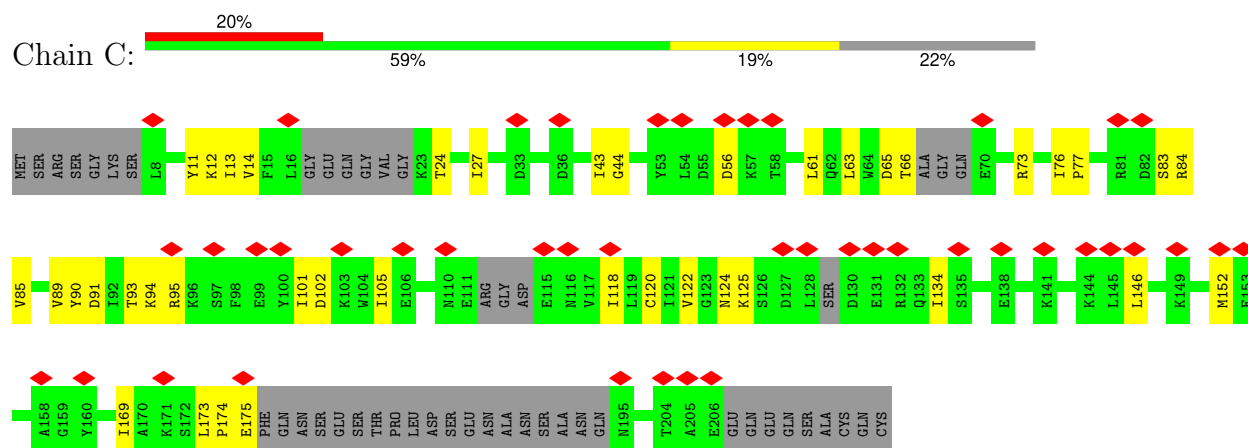
- Molecule 1: Guanine nucleotide exchange factor subunit RIC1



- Molecule 2: Guanine nucleotide exchange factor subunit RGP1



- Molecule 3: GTP-binding protein YPT6



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT, POINT, POINT	Depositor
Number of particles used	69399, 69399, 69399, 69399	Depositor
Resolution determination method	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50.00	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.118	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	245.0, 245.0, 245.0	wwPDB
Map dimensions	196, 196, 196	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.25, 1.25, 1.25	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	0.11	0/7142	0.29	0/9680
2	B	0.09	0/3293	0.24	0/4448
3	C	0.11	0/1387	0.31	0/1857
All	All	0.11	0/11822	0.28	0/15985

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7248	7226	7173	85	0
2	B	3345	3300	3276	33	0
3	C	1369	1409	1403	25	0
All	All	11962	11935	11852	135	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 6.

All (135) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:877:ASP:OD1	1:A:881:LYS:NZ	2.11	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ILE:HG21	1:A:471:VAL:HG21	1.66	0.78
1:A:324:LEU:HD22	1:A:357:LEU:HD13	1.66	0.76
2:B:514:ASP:OD1	2:B:586:ARG:NH1	2.19	0.75
1:A:104:ARG:NH1	1:A:115:ASN:OD1	2.21	0.73
1:A:424:ASN:ND2	1:A:755:GLU:OE2	2.22	0.73
2:B:133:LEU:HD22	2:B:294:VAL:HG12	1.73	0.71
3:C:66:THR:O	3:C:73:ARG:NH2	2.24	0.70
3:C:91:ASP:OD2	3:C:94:LYS:NZ	2.26	0.68
1:A:357:LEU:HD12	1:A:369:VAL:HG13	1.75	0.68
1:A:937:CYS:O	1:A:941:ASN:N	2.26	0.68
1:A:209:ASP:OD2	1:A:215:ARG:NH1	2.26	0.68
1:A:477:TYR:OH	2:B:573:ASP:OD2	2.12	0.67
2:B:46:GLU:O	2:B:49:ASN:ND2	2.29	0.66
1:A:59:GLU:OE1	1:A:59:GLU:N	2.29	0.66
2:B:512:THR:OG1	2:B:658:GLU:OE2	2.14	0.64
2:B:494:ARG:NH1	2:B:643:GLU:OE1	2.31	0.64
1:A:912:ARG:NH1	3:C:44:GLY:O	2.32	0.63
1:A:150:TYR:CE2	1:A:282:LEU:HD21	2.33	0.63
1:A:257:PHE:CD2	1:A:261:ILE:HD11	2.34	0.63
1:A:590:VAL:HG22	1:A:605:LEU:HD12	1.81	0.62
3:C:13:ILE:HD13	3:C:61:LEU:HG	1.81	0.62
1:A:65:ASP:OD1	1:A:66:CYS:N	2.35	0.60
1:A:675:THR:OG1	1:A:678:GLN:O	2.07	0.60
1:A:870:ILE:HG23	1:A:876:LEU:HD11	1.86	0.57
1:A:131:LEU:HD12	1:A:267:ILE:HD11	1.86	0.57
2:B:619:SER:O	2:B:637:LYS:NZ	2.38	0.57
2:B:6:ILE:HG12	2:B:20:ILE:HG23	1.86	0.56
1:A:361:LEU:HD23	1:A:362:GLU:N	2.20	0.56
1:A:535:ASN:O	1:A:556:ASN:ND2	2.38	0.56
1:A:223:ILE:HG22	1:A:225:LYS:H	1.71	0.56
1:A:899:THR:HG21	1:A:940:GLU:HB2	1.86	0.56
1:A:514:VAL:O	1:A:515:THR:OG1	2.24	0.56
3:C:175:GLU:N	3:C:175:GLU:OE1	2.39	0.56
1:A:515:THR:OG1	1:A:516:SER:N	2.39	0.56
3:C:124:ASN:OD1	3:C:125:LYS:N	2.38	0.56
1:A:878:ASP:OD1	1:A:879:ILE:N	2.40	0.55
1:A:98:LEU:HD21	2:B:622:LEU:HD11	1.88	0.55
2:B:3:ALA:O	2:B:4:HIS:ND1	2.41	0.54
3:C:120:CYS:SG	3:C:169:ILE:HD11	2.48	0.54
2:B:122:GLN:OE1	2:B:124:GLN:N	2.41	0.53
1:A:531:THR:HG21	1:A:536:ASN:ND2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:43:SER:OG	2:B:46:GLU:OE1	2.27	0.53
2:B:521:LEU:H	2:B:521:LEU:HD23	1.74	0.53
1:A:257:PHE:HD2	1:A:261:ILE:HD11	1.73	0.53
1:A:522:ASP:OD1	1:A:827:HIS:NE2	2.40	0.53
1:A:37:MET:O	1:A:402:ASN:ND2	2.42	0.53
1:A:81:ILE:O	1:A:118:MET:HE1	2.08	0.52
3:C:65:ASP:OD1	3:C:66:THR:N	2.42	0.52
1:A:402:ASN:OD1	1:A:405:ILE:N	2.42	0.52
2:B:593:THR:HG23	2:B:603:HIS:CE1	2.44	0.52
2:B:583:LEU:H	2:B:583:LEU:HD23	1.74	0.52
3:C:91:ASP:OD2	3:C:93:THR:OG1	2.28	0.52
1:A:705:ILE:HD11	1:A:745:TRP:CZ2	2.45	0.52
1:A:806:THR:HA	1:A:855:LEU:HD21	1.91	0.52
3:C:24:THR:HG22	3:C:24:THR:O	2.10	0.51
1:A:103:GLU:OE1	1:A:103:GLU:N	2.44	0.51
1:A:757:ILE:HG12	1:A:767:VAL:HG12	1.92	0.51
1:A:263:ASP:OD1	1:A:264:MET:N	2.44	0.50
1:A:361:LEU:HD21	1:A:400:LYS:HD2	1.92	0.50
1:A:461:PHE:HB3	1:A:470:THR:HG22	1.92	0.50
2:B:46:GLU:OE1	2:B:46:GLU:N	2.45	0.49
3:C:85:VAL:HG13	3:C:118:ILE:O	2.13	0.49
1:A:619:SER:O	1:A:622:VAL:HG12	2.12	0.49
1:A:899:THR:HG22	1:A:899:THR:O	2.12	0.49
1:A:560:LEU:HD23	1:A:561:LEU:N	2.28	0.49
2:B:504:LEU:HD22	2:B:517:LEU:HD11	1.95	0.48
2:B:266:THR:HG21	2:B:334:LYS:HB2	1.95	0.48
2:B:34:ILE:HD13	2:B:288:LEU:HD13	1.95	0.48
3:C:11:TYR:OH	3:C:174:PRO:O	2.28	0.48
2:B:122:GLN:OE1	2:B:123:LYS:N	2.47	0.47
1:A:364:ASN:ND2	1:A:421:GLU:OE1	2.48	0.47
1:A:912:ARG:NE	1:A:948:VAL:O	2.47	0.47
1:A:181:ILE:HG13	1:A:181:ILE:O	2.15	0.47
1:A:324:LEU:HD21	1:A:333:THR:HG22	1.96	0.46
2:B:36:PHE:HZ	2:B:138:VAL:HG21	1.80	0.46
3:C:122:VAL:HA	3:C:152:MET:O	2.16	0.46
3:C:169:ILE:O	3:C:173:LEU:HD23	2.14	0.46
1:A:83:LEU:HB2	1:A:118:MET:HE2	1.98	0.46
2:B:133:LEU:CD2	2:B:294:VAL:HG12	2.45	0.46
1:A:131:LEU:HD11	1:A:283:ILE:HD11	1.97	0.46
1:A:549:LEU:HD23	1:A:583:TRP:CH2	2.51	0.45
1:A:817:ASN:OD1	1:A:818:ALA:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:12:LYS:O	3:C:84:ARG:N	2.50	0.45
1:A:39:LEU:HD23	1:A:483:TRP:O	2.17	0.45
1:A:160:THR:HG22	1:A:160:THR:O	2.17	0.45
1:A:866:LEU:HD12	1:A:883:ILE:CD1	2.47	0.45
1:A:822:LYS:NZ	3:C:56:ASP:OD2	2.44	0.44
1:A:870:ILE:CG2	1:A:876:LEU:HD11	2.47	0.44
1:A:217:ILE:HD12	2:B:612:VAL:HG13	1.99	0.44
1:A:493:PHE:HZ	1:A:720:ILE:HD12	1.81	0.44
2:B:36:PHE:CZ	2:B:138:VAL:HG21	2.52	0.44
1:A:50:ILE:HG22	1:A:91:TYR:OH	2.18	0.44
3:C:90:TYR:CD2	3:C:101:ILE:HD11	2.53	0.44
3:C:95:ARG:HG2	3:C:134:ILE:HD11	1.99	0.44
3:C:102:ASP:HA	3:C:105:ILE:HG22	2.00	0.44
1:A:220:GLY:O	2:B:570:ILE:HD11	2.18	0.43
1:A:261:ILE:HG23	1:A:284:VAL:HG23	2.00	0.43
1:A:731:ASP:OD1	1:A:732:ARG:N	2.51	0.43
1:A:51:PRO:O	1:A:87:ARG:NH2	2.42	0.43
1:A:37:MET:SD	1:A:37:MET:N	2.92	0.43
1:A:39:LEU:HD21	1:A:484:GLU:OE1	2.17	0.43
3:C:76:ILE:N	3:C:77:PRO:HD2	2.32	0.43
1:A:150:TYR:HB2	1:A:264:MET:HE1	2.00	0.43
1:A:760:VAL:HG13	1:A:764:GLU:O	2.19	0.43
1:A:913:LYS:CE	3:C:43:ILE:HD11	2.49	0.43
3:C:14:VAL:HG23	3:C:83:SER:HB3	2.00	0.43
1:A:531:THR:HG21	1:A:536:ASN:HD21	1.83	0.43
1:A:696:ILE:HD12	1:A:699:PHE:CZ	2.54	0.43
1:A:361:LEU:O	1:A:368:VAL:N	2.40	0.43
2:B:31:HIS:ND1	2:B:265:SER:O	2.48	0.43
2:B:515:ILE:HG22	2:B:517:LEU:HD13	2.01	0.42
1:A:314:THR:HG22	1:A:323:VAL:HG22	2.00	0.42
2:B:326:LEU:HD12	2:B:600:VAL:HG22	2.01	0.42
3:C:89:VAL:HG12	3:C:122:VAL:HG13	2.02	0.42
3:C:27:ILE:HD13	3:C:63:LEU:HD22	2.01	0.42
1:A:683:ASP:OD2	1:A:702:TYR:HB2	2.19	0.42
1:A:846:GLU:N	1:A:885:MET:HE1	2.34	0.42
2:B:276:TYR:CD1	2:B:593:THR:HG21	2.55	0.42
1:A:65:ASP:OD2	1:A:86:THR:OG1	2.31	0.42
1:A:934:LEU:HA	1:A:937:CYS:SG	2.60	0.42
2:B:521:LEU:O	2:B:525:THR:OG1	2.38	0.42
3:C:105:ILE:HG21	3:C:146:LEU:HD12	2.02	0.42
1:A:242:LEU:HD13	1:A:535:ASN:HB3	2.02	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:GLN:NE2	1:A:541:VAL:O	2.50	0.42
1:A:410:SER:OG	1:A:411:GLU:N	2.53	0.41
2:B:628:ASP:OD1	2:B:629:LYS:N	2.52	0.41
1:A:98:LEU:HD21	2:B:622:LEU:CD1	2.50	0.41
1:A:1035:UNK:O	1:A:1039:UNK:N	2.53	0.41
1:A:564:ASN:O	1:A:568:ASN:N	2.54	0.41
1:A:290:LEU:HD21	1:A:314:THR:HG21	2.02	0.40
1:A:40:TRP:O	1:A:483:TRP:N	2.42	0.40
2:B:493:ASN:N	2:B:493:ASN:OD1	2.53	0.40
1:A:150:TYR:CZ	1:A:282:LEU:HD21	2.57	0.40
1:A:538:ILE:CG2	1:A:541:VAL:HG23	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	839/1056 (80%)	787 (94%)	52 (6%)	0	100	100
2	B	388/663 (58%)	376 (97%)	12 (3%)	0	100	100
3	C	155/215 (72%)	147 (95%)	8 (5%)	0	100	100
All	All	1382/1934 (72%)	1310 (95%)	72 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	813/945 (86%)	813 (100%)	0	100	100
2	B	373/589 (63%)	373 (100%)	0	100	100
3	C	153/191 (80%)	153 (100%)	0	100	100
All	All	1339/1725 (78%)	1339 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	HIS
1	A	326	HIS
1	A	638	HIS
1	A	661	GLN
1	A	701	GLN
1	A	771	HIS
1	A	850	HIS
2	B	45	HIS
2	B	562	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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

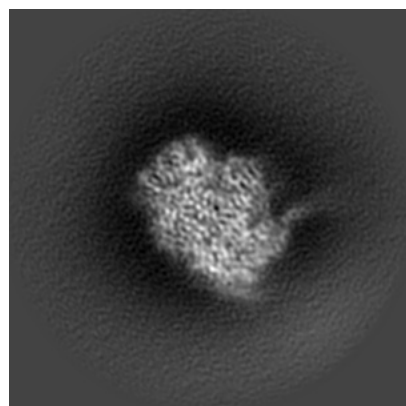
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43997. These allow visual inspection of the internal detail of the map and identification of artifacts.

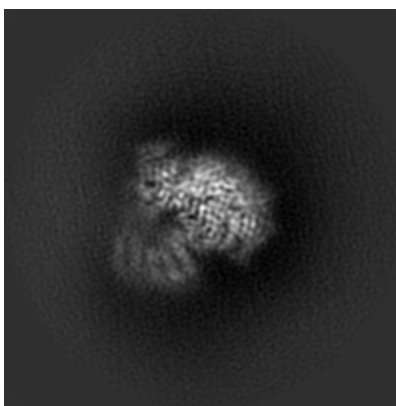
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

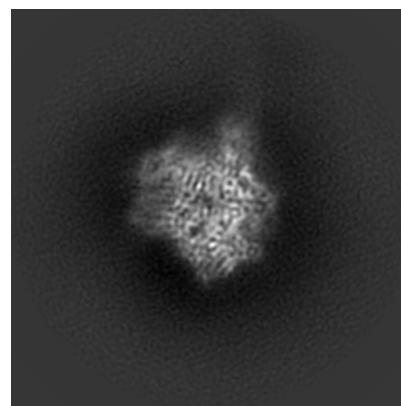
#### 6.1.1 Primary map



X

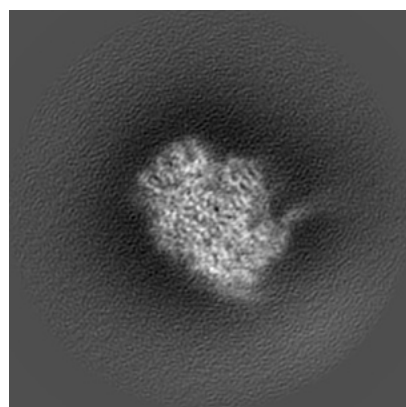


Y

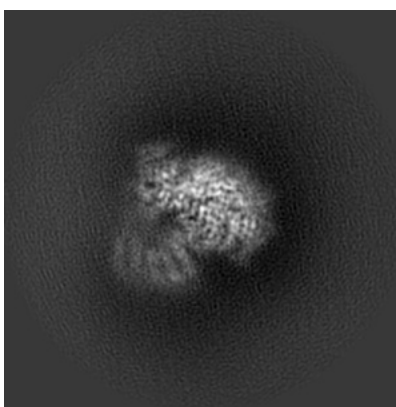


Z

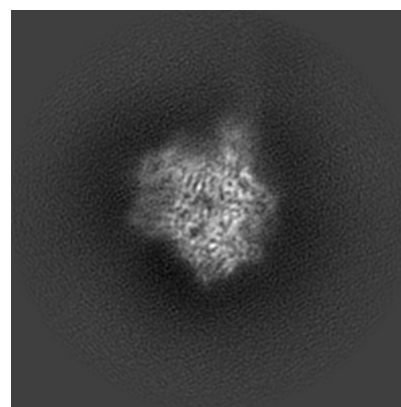
#### 6.1.2 Raw map



X



Y



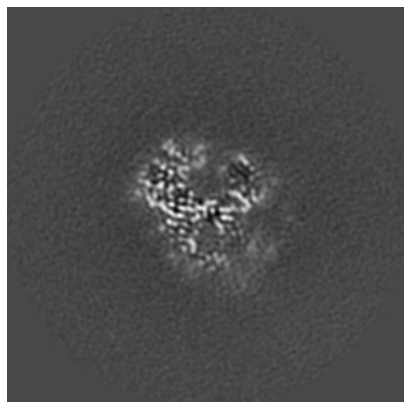
Z

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

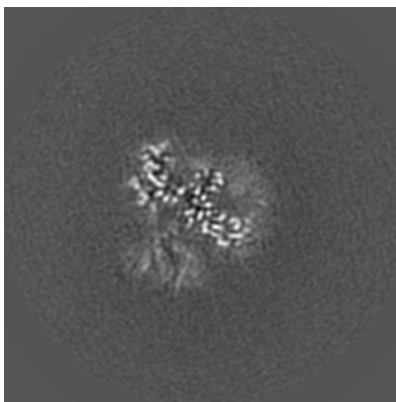


## 6.2 Central slices [i](#)

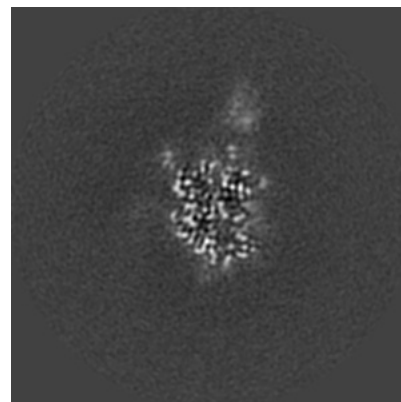
### 6.2.1 Primary map



X Index: 98

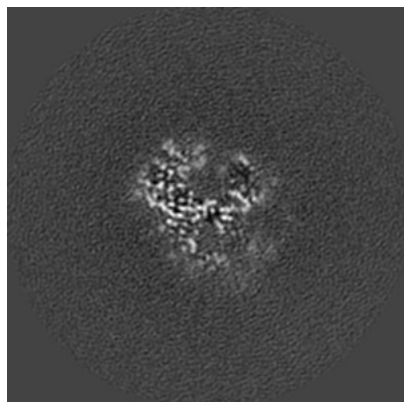


Y Index: 98

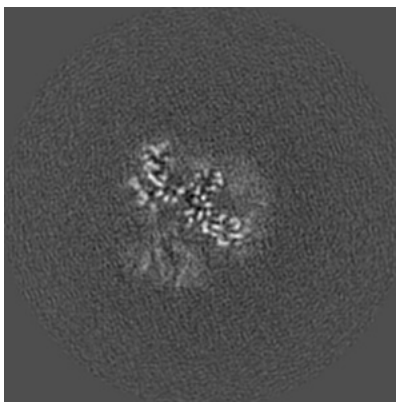


Z Index: 98

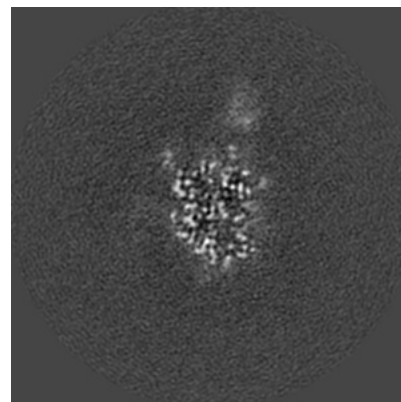
### 6.2.2 Raw map



X Index: 98



Y Index: 98

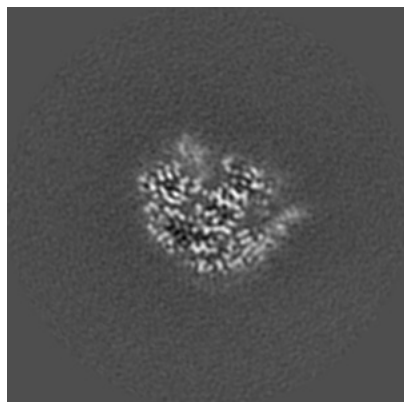


Z Index: 98

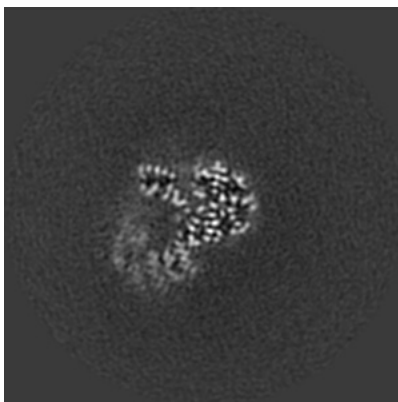
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

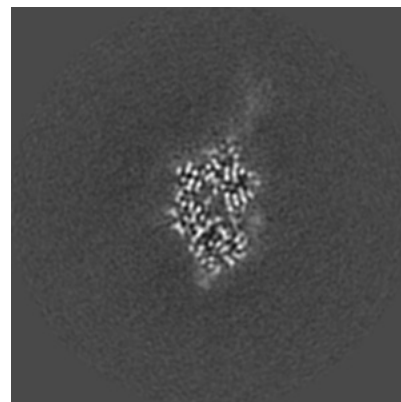
### 6.3.1 Primary map



X Index: 105

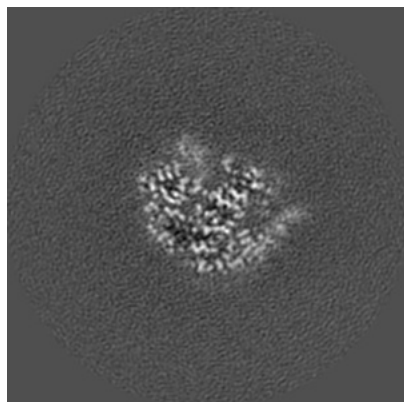


Y Index: 114

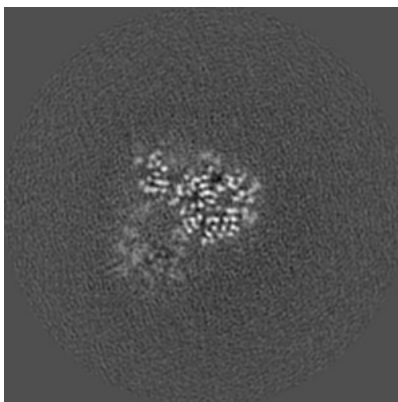


Z Index: 103

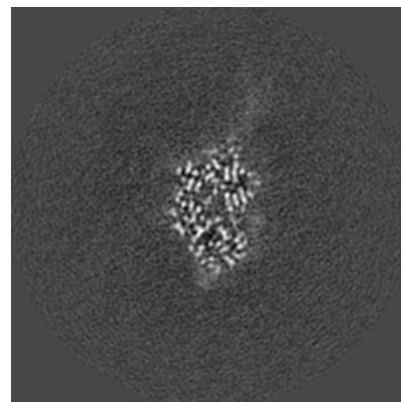
### 6.3.2 Raw map



X Index: 105



Y Index: 108

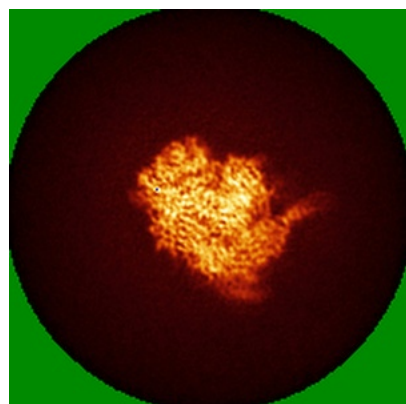


Z Index: 103

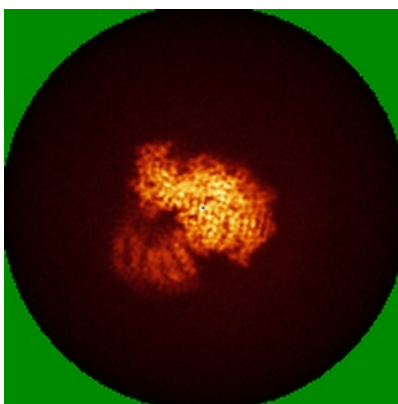
The images above show the largest variance slices of the map in three orthogonal directions.

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

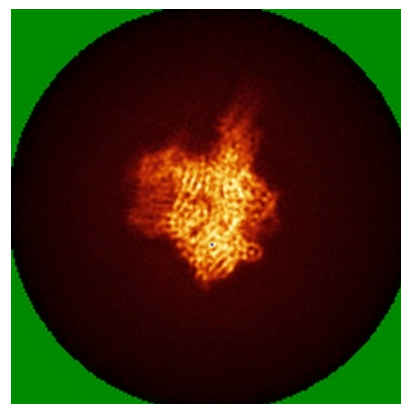
### 6.4.1 Primary map



X

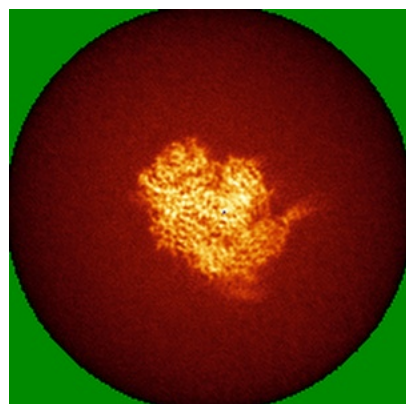


Y

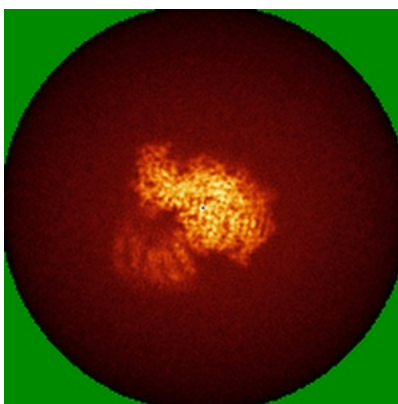


Z

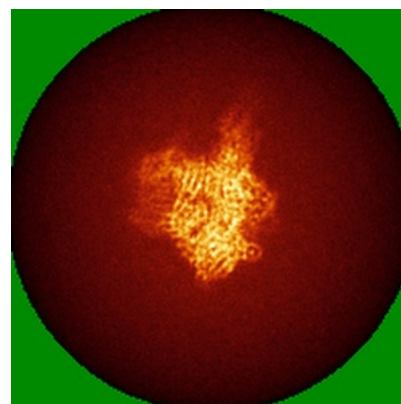
### 6.4.2 Raw map



X



Y

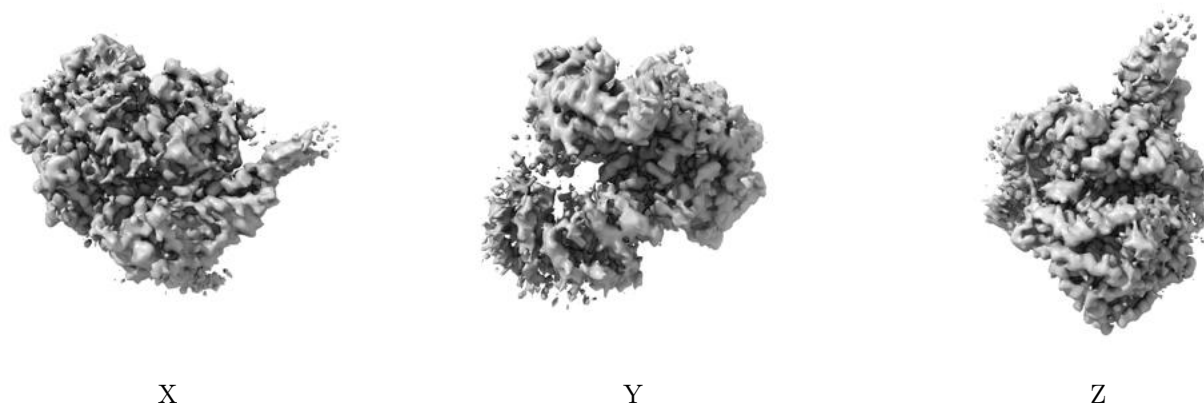


Z

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.

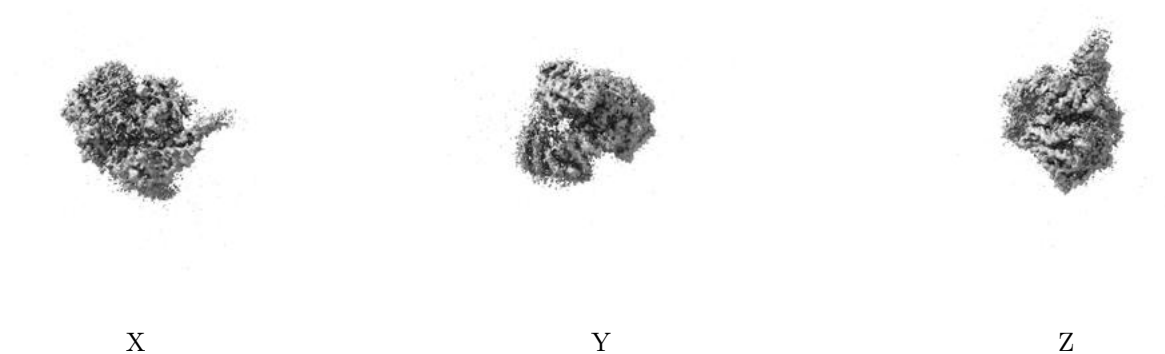
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. 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.

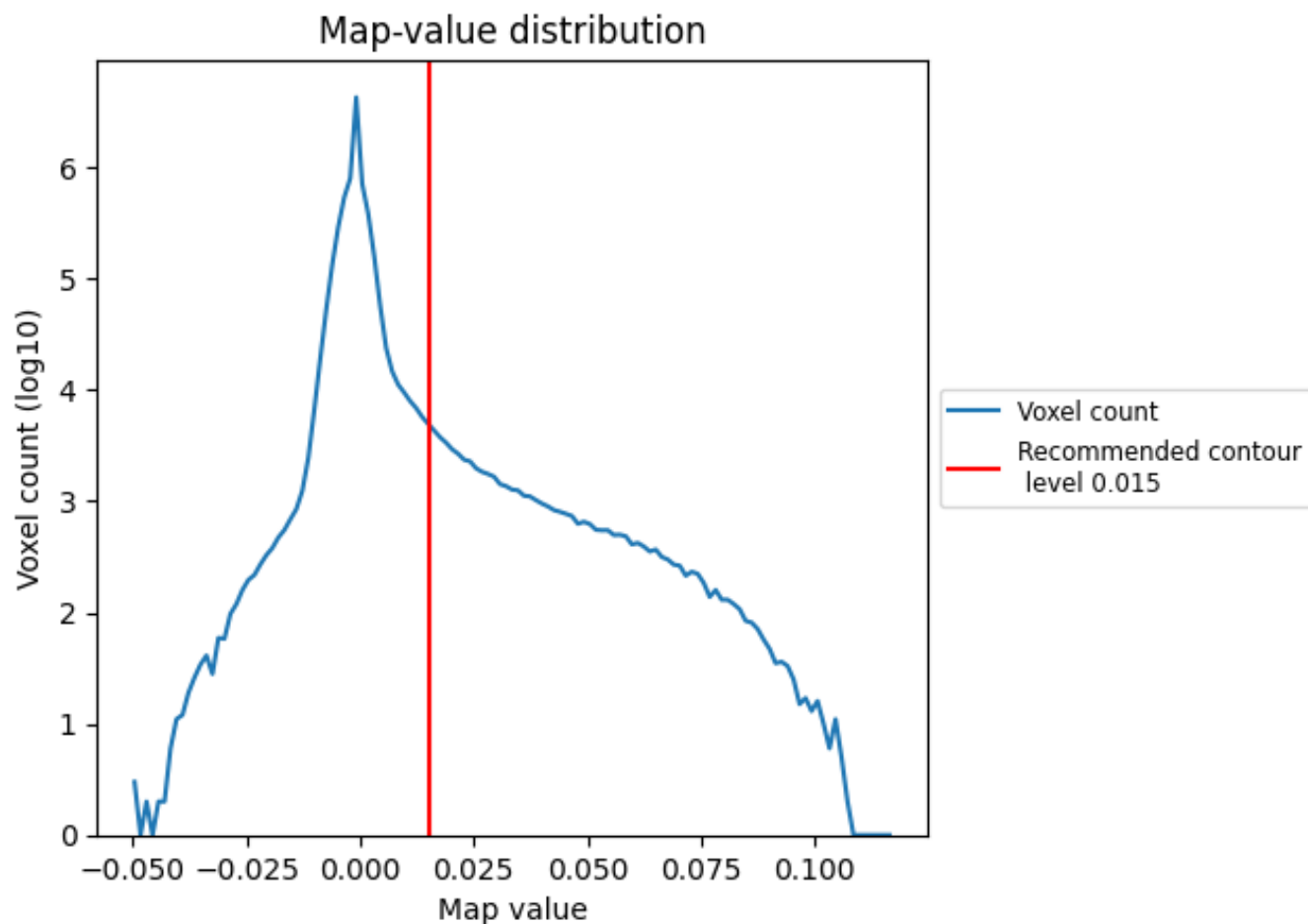
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

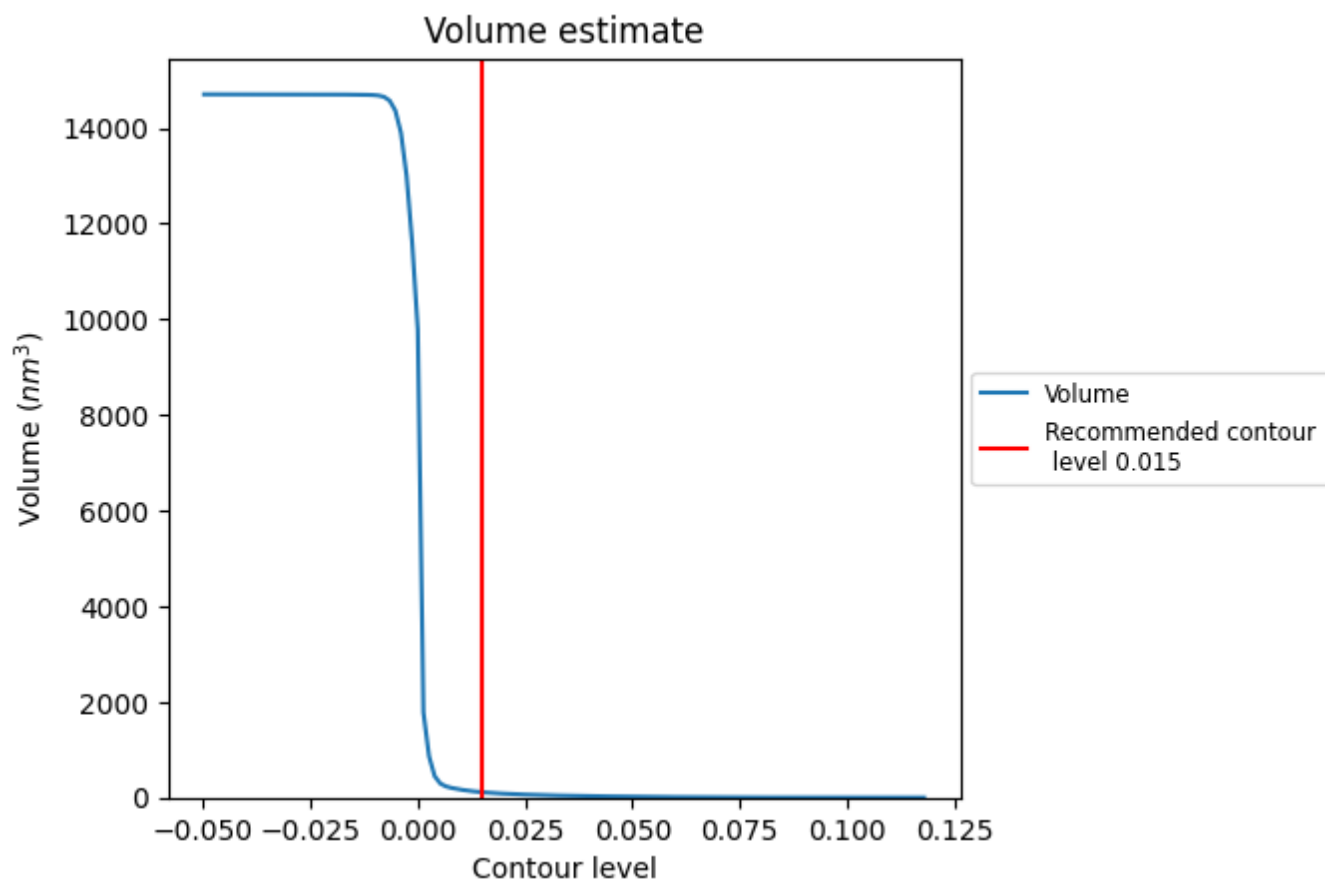
This section contains the results of statistical analysis of the map.

### 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.

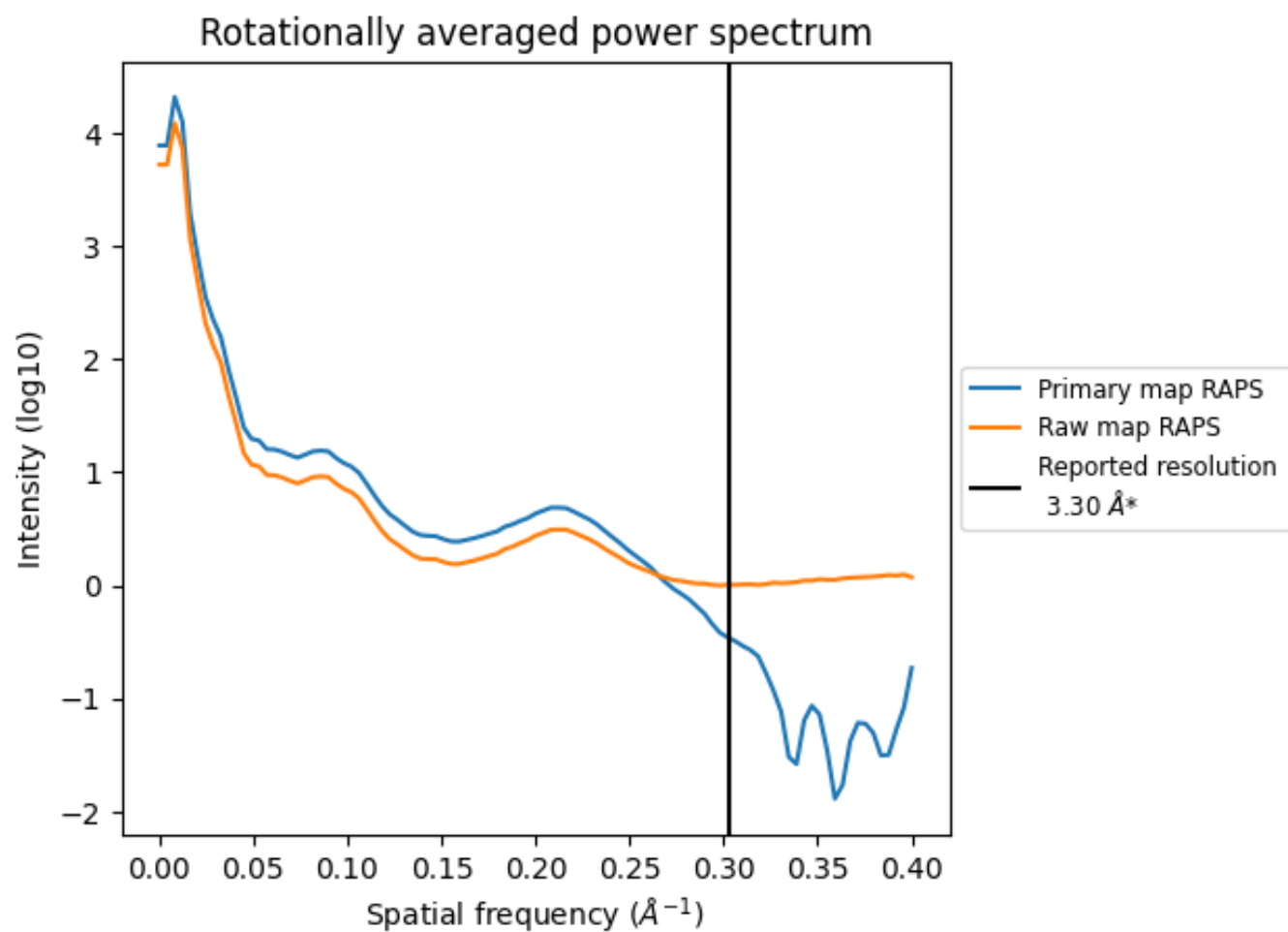
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 113  $\text{nm}^3$ ; this corresponds to an approximate mass of 102 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 ⓘ

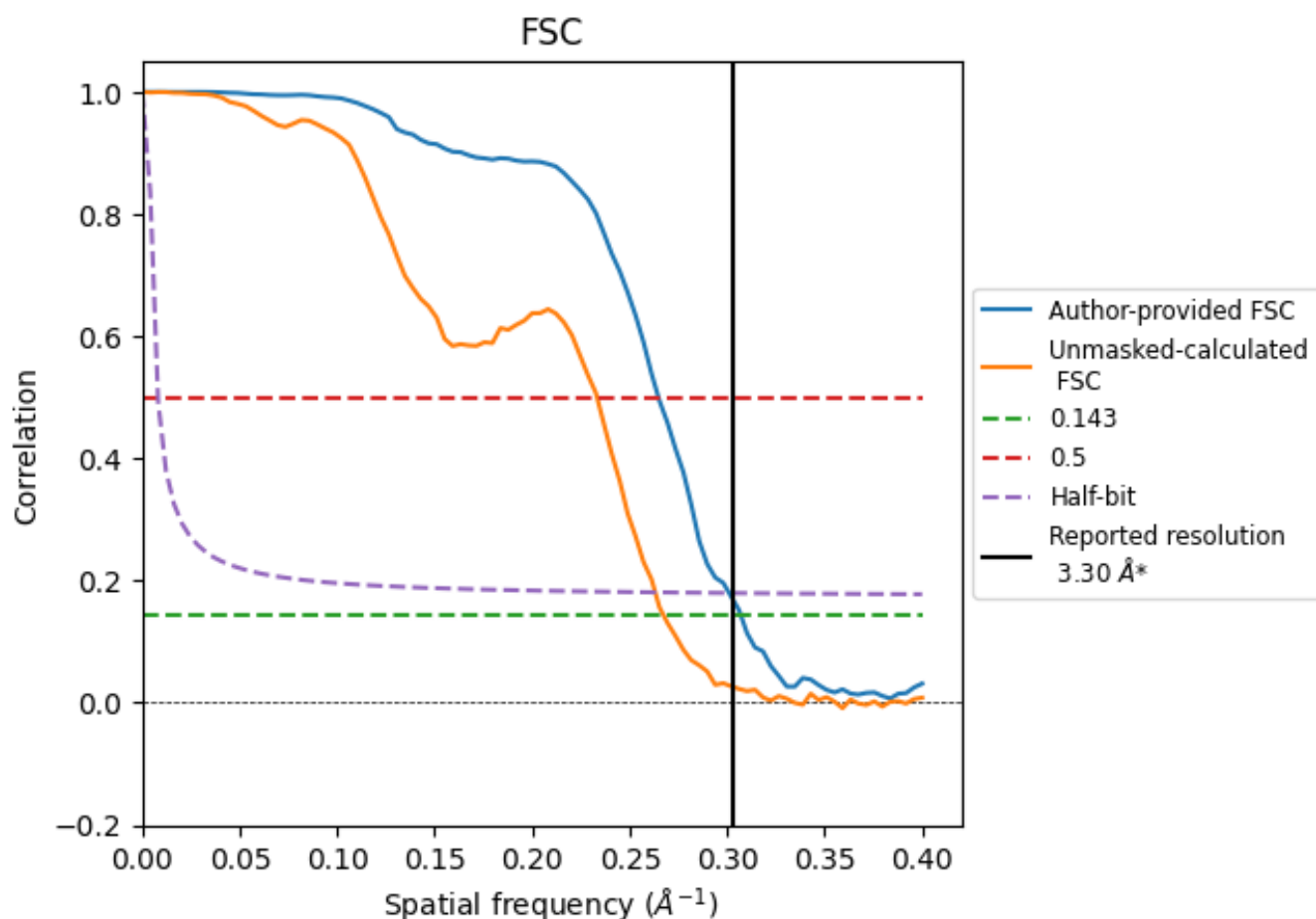


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 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 0.303  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

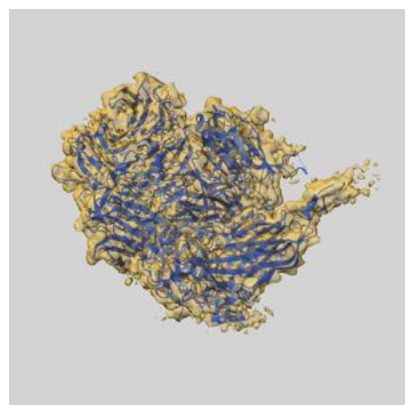
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	3.26	3.78	3.32
Unmasked-calculated*	3.74	4.29	3.80

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

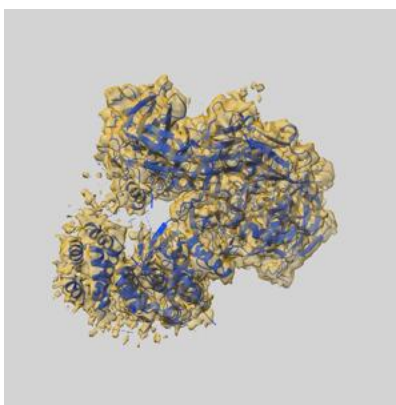
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-43997 and PDB model 9AYR. Per-residue inclusion information can be found in section 3 on page 6.

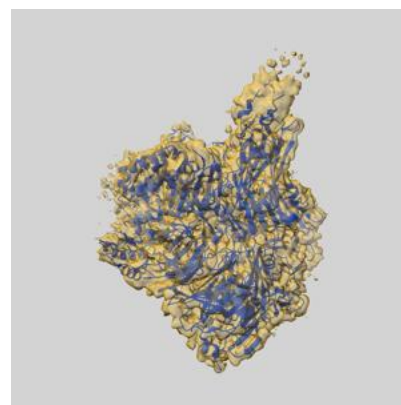
### 9.1 Map-model overlay [i](#)



X



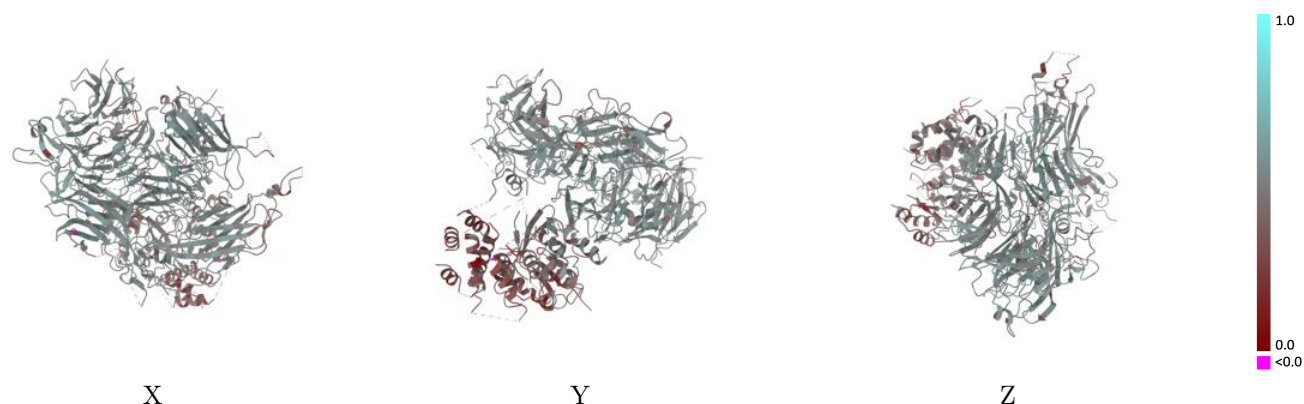
Y



Z

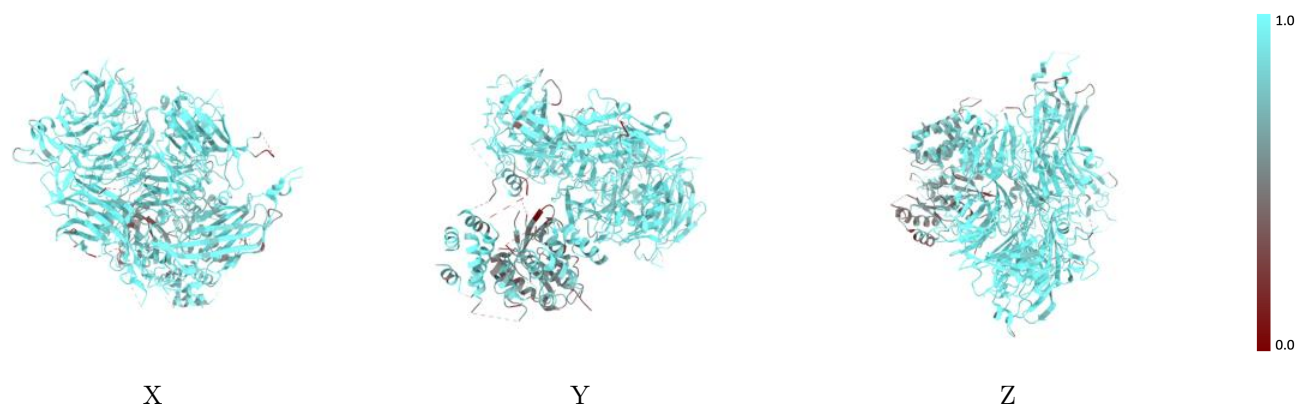
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



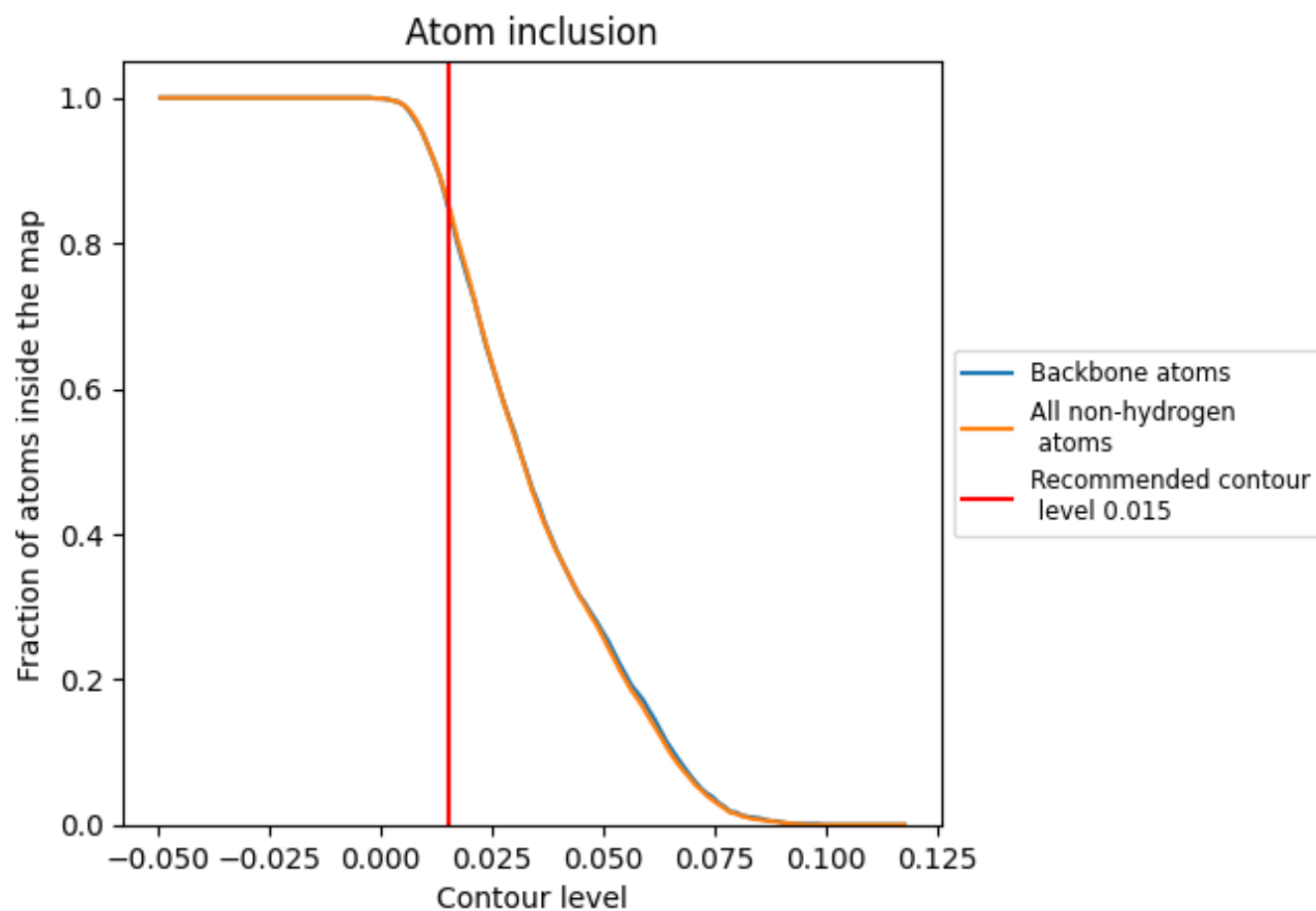
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 86% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8570	<div></div> 0.4730
A	<div></div> 0.9020	<div></div> 0.4840
B	<div></div> 0.9010	<div></div> 0.4930
C	<div></div> 0.5490	<div></div> 0.3660

