



## Full wwPDB EM Validation Report ⓘ

May 13, 2025 – 05:26 AM EDT

PDB ID : 7KIN / pdb\_00007kin  
EMDB ID : EMD-22888  
Title : Mycobacterium tuberculosis WT RNAP transcription open promoter complex  
with WhiB7 promoter  
Authors : Lilic, M.; Darst, S.A.; Campbell, E.A.  
Deposited on : 2020-10-23  
Resolution : 2.74 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

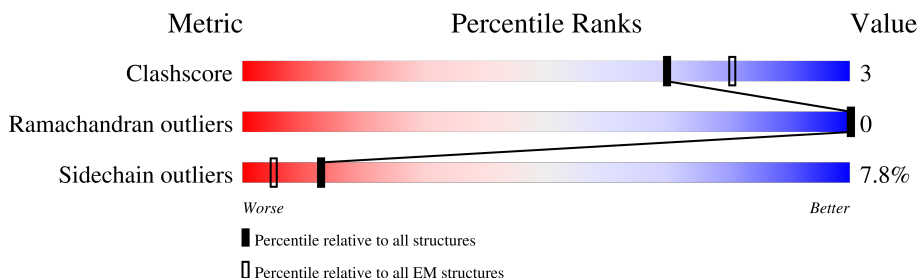
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.74 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	347	
1	B	347	
2	C	1172	
3	D	1318	
4	E	110	
5	F	528	
6	J	111	
7	M	162	

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Mol	Chain	Length	Quality of chain
8	O	100	<div><div><div></div><div></div><div></div></div><div>46%8%46%</div></div>
9	P	100	<div><div><div></div><div></div><div></div></div><div>40%9%51%</div></div>

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 29379 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	225	Total	C	N	O	S	0	0
			1716	1080	296	338	2		
1	B	237	Total	C	N	O	S	0	0
			1765	1115	301	346	3		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0
			8606	5392	1511	1664	39		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1270	Total	C	N	O	S	0	0
			9914	6208	1802	1862	42		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP A0A045J9E2
D	0	ALA	-	expression tag	UNP A0A045J9E2

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	83	Total	C	N	O	0	0
			649	414	108	127		

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	317	Total	C	N	O	S	0	0
			2510	1566	455	480	9		

- Molecule 6 is a protein called RNA polymerase-binding protein RbpA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	107	Total	C	N	O	S	0	0
			870	537	164	166	3		

- Molecule 7 is a protein called RNA polymerase-binding transcription factor CarD.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	159	Total	C	N	O	S	0	0
			1241	777	224	239	1		

- Molecule 8 is a DNA chain called DNA (54-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	54	Total	C	N	O	P	0	0
			1096	522	189	331	54		

- Molecule 9 is a DNA chain called DNA (49-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	49	Total	C	N	O	P	0	0
			1009	477	195	288	49		

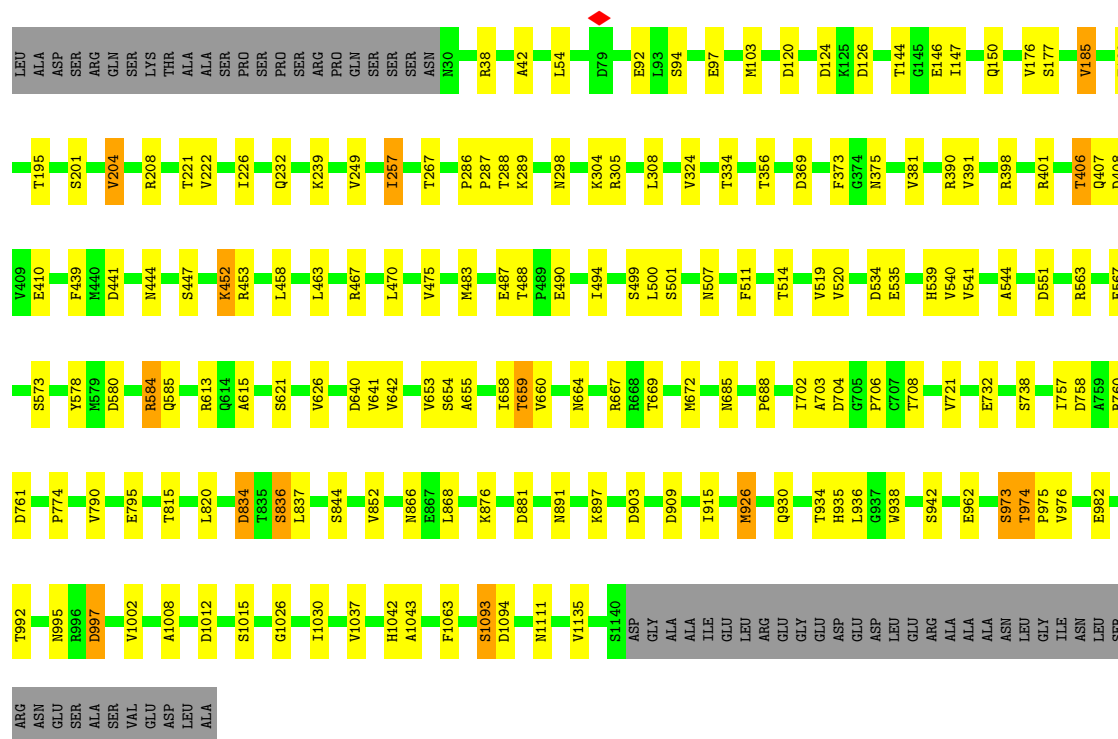
- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
10	D	2	Total	Zn	0
			2	2	

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

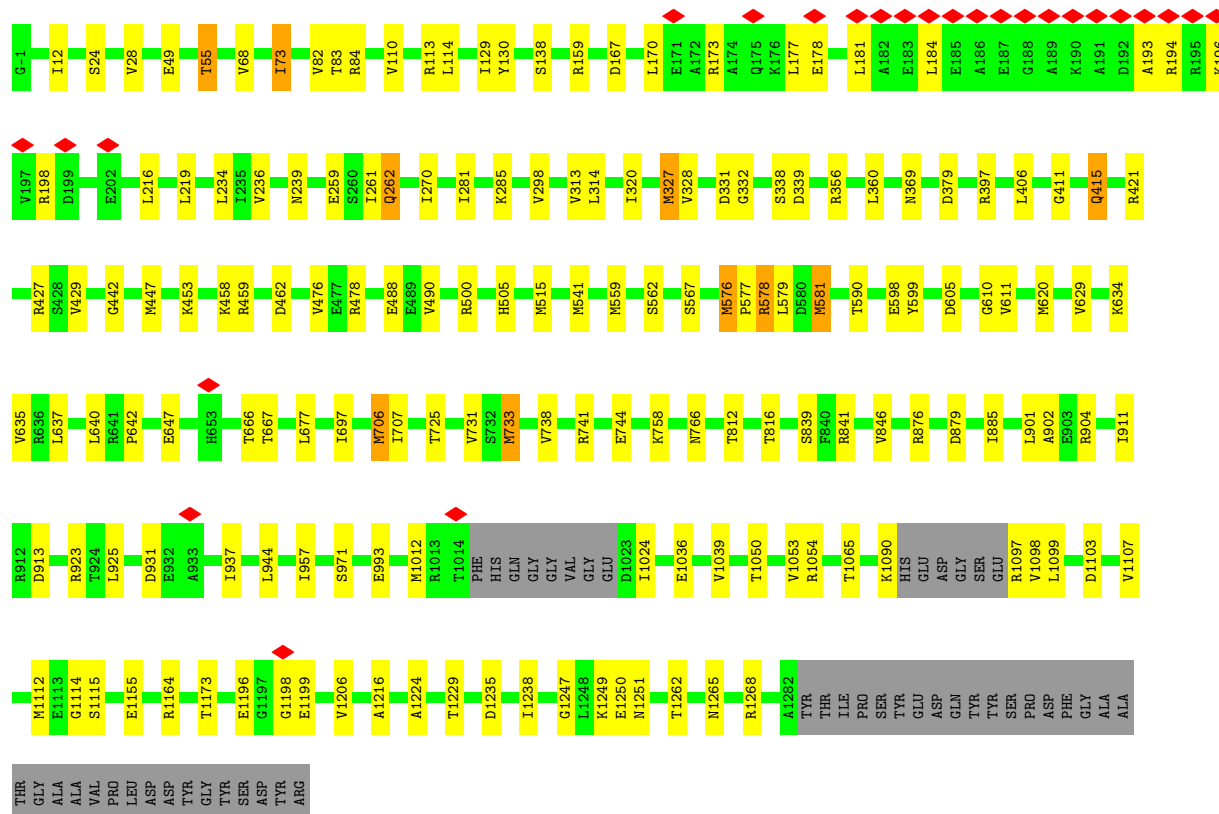
Mol	Chain	Residues	Atoms		AltConf
11	D	1	Total	Mg	0
			1	1	





• Molecule 3: DNA-directed RNA polymerase subunit beta'

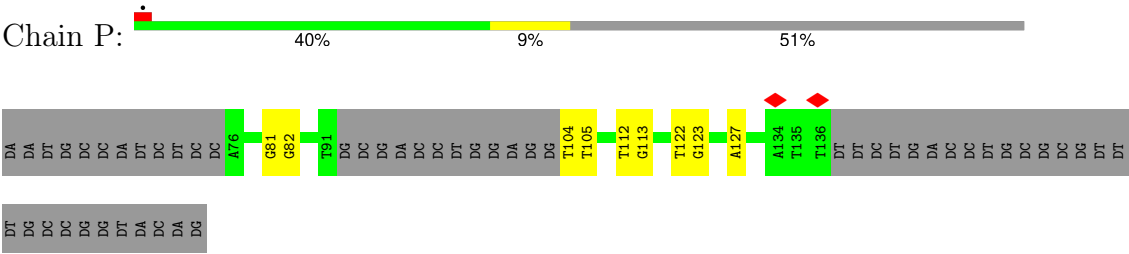
Chain D: 84% 12%







● Molecule 9: DNA (49-MER)



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	296097	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.851	Depositor
Minimum map value	-3.227	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.119	Depositor
Recommended contour level	0.3	Depositor
Map size ( $\text{\AA}$ )	330.0, 330.0, 330.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.1, 1.1, 1.1	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN

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	0.66	0/1742	0.58	0/2370
1	B	0.54	0/1792	0.56	0/2442
2	C	0.70	0/8765	0.63	0/11885
3	D	0.69	1/10078 (0.0%)	0.64	2/13624 (0.0%)
4	E	0.63	0/662	0.64	0/901
5	F	0.44	0/2541	0.55	0/3427
6	J	0.38	0/886	0.52	0/1196
7	M	0.29	0/1257	0.61	2/1700 (0.1%)
8	O	0.40	0/1223	0.53	0/1881
9	P	0.38	0/1133	0.55	0/1744
All	All	0.63	1/30079 (0.0%)	0.61	4/41170 (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
2	C	0	3
3	D	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	442	GLY	C-N	-6.36	1.24	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	578	ARG	CA-C-N	7.18	135.25	121.54
3	D	578	ARG	C-N-CA	7.18	135.25	121.54
7	M	147	ASP	CA-C-N	6.31	133.59	121.54
7	M	147	ASP	C-N-CA	6.31	133.59	121.54

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	1093	SER	Peptide
2	C	774	PRO	Peptide
2	C	962	GLU	Peptide
3	D	579	LEU	Mainchain

## 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	1716	0	1756	13	0
1	B	1765	0	1794	15	0
2	C	8606	0	8544	67	0
3	D	9914	0	9986	67	0
4	E	649	0	645	5	0
5	F	2510	0	2537	25	0
6	J	870	0	848	10	0
7	M	1241	0	1259	10	0
8	O	1096	0	611	6	0
9	P	1009	0	549	5	0
10	D	2	0	0	0	0
11	D	1	0	0	0	0
All	All	29379	0	28529	197	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 3.

All (197) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:VAL:HA	1:B:188:ASP:H	1.51	0.73
1:A:40:ARG:HH12	2:C:903:ASP:HB3	1.60	0.66
5:F:306:LEU:HD11	5:F:348:THR:HG23	1.77	0.65
3:D:1265:ASN:OD1	3:D:1268:ARG:NH2	2.31	0.64
3:D:181:LEU:HA	3:D:198:ARG:HH21	1.64	0.63
4:E:60:ARG:HH22	4:E:80:GLY:HA3	1.64	0.61
3:D:167:ASP:HA	3:D:170:LEU:HD12	1.82	0.61
5:F:336:ASP:OD1	6:J:89:ARG:NH2	2.33	0.61
3:D:1053:VAL:HG12	3:D:1103:ASP:H	1.66	0.61
7:M:36:VAL:HG12	7:M:47:ARG:HG2	1.83	0.61
1:B:72:ASP:OD1	1:B:72:ASP:N	2.35	0.59
3:D:178:GLU:HA	3:D:181:LEU:HD12	1.85	0.59
5:F:466:THR:OG1	5:F:519:ARG:NH1	2.37	0.58
3:D:741:ARG:NH1	3:D:744:GLU:OE2	2.38	0.57
2:C:369:ASP:O	2:C:375:ASN:ND2	2.33	0.57
2:C:42:ALA:HB2	2:C:975:PRO:HG2	1.87	0.57
7:M:73:VAL:O	7:M:109:ARG:NH1	2.38	0.56
2:C:659:THR:HB	2:C:669:THR:HG22	1.87	0.56
3:D:113:ARG:NH2	3:D:1235:ASP:OD2	2.38	0.56
3:D:49:GLU:OE2	3:D:55:THR:OG1	2.24	0.56
6:J:69:LEU:HB3	6:J:71:GLU:HG3	1.86	0.56
2:C:146:GLU:OE2	7:M:11:TYR:OH	2.24	0.55
2:C:97:GLU:O	2:C:401:ARG:NH1	2.40	0.55
2:C:467:ARG:NH1	8:O:64:DA:OP2	2.40	0.55
3:D:338:SER:O	3:D:338:SER:OG	2.17	0.55
3:D:1247:GLY:O	3:D:1251:ASN:ND2	2.40	0.55
1:B:167:ILE:HG23	3:D:620:MET:HE1	1.87	0.55
2:C:38:ARG:HG2	2:C:973:SER:HB3	1.88	0.55
2:C:507:ASN:HD22	2:C:511:PHE:HB2	1.73	0.54
2:C:514:THR:OG1	2:C:585:GLN:NE2	2.40	0.54
1:B:37:SER:O	1:B:41:THR:OG1	2.26	0.54
2:C:997:ASP:OD1	2:C:997:ASP:N	2.39	0.54
2:C:544:ALA:HB2	2:C:580:ASP:HB2	1.88	0.54
3:D:902:ALA:H	3:D:913:ASP:HB2	1.72	0.54
2:C:761:ASP:OD1	2:C:866:ASN:ND2	2.40	0.54
3:D:1054:ARG:HB2	3:D:1065:THR:HB	1.90	0.53
2:C:995:ASN:OD1	2:C:995:ASN:N	2.40	0.53
2:C:239:LYS:NZ	2:C:267:THR:O	2.40	0.53
3:D:130:TYR:OH	3:D:379:ASP:OD2	2.27	0.53
3:D:458:LYS:NZ	3:D:462:ASP:OD2	2.42	0.53
2:C:654:SER:OG	2:C:655:ALA:N	2.40	0.53
5:F:501:GLU:OE2	5:F:504:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:LEU:HB3	1:B:110:ILE:HB	1.92	0.52
2:C:408:ASP:N	2:C:408:ASP:OD1	2.40	0.52
2:C:760:ARG:HD2	3:D:332:GLY:HA2	1.92	0.52
3:D:500:ARG:HB2	3:D:541:MET:HE2	1.90	0.52
3:D:184:LEU:O	3:D:194:ARG:NH1	2.42	0.52
6:J:58:ASN:HB2	6:J:60:MET:HG2	1.92	0.52
2:C:758:ASP:N	2:C:758:ASP:OD1	2.42	0.51
2:C:820:LEU:HD23	5:F:460:LEU:HD21	1.92	0.51
6:J:79:ARG:HD2	6:J:84:MET:HE2	1.93	0.51
1:B:84:VAL:HG22	1:B:119:HIS:HB2	1.92	0.51
6:J:20:ARG:NH1	6:J:23:ASP:O	2.35	0.51
3:D:577:PRO:HB3	3:D:581:MET:HB2	1.93	0.51
7:M:111:LEU:HD11	7:M:127:MET:HE3	1.92	0.51
5:F:386:LEU:O	5:F:390:LEU:HB2	2.12	0.50
1:A:151:GLN:NE2	2:C:795:GLU:OE1	2.44	0.50
1:B:102:PRO:HD3	1:B:131:LYS:HG2	1.92	0.50
5:F:342:LYS:NZ	8:O:53:DC:OP2	2.45	0.50
1:B:6:ARG:NH1	1:B:235:GLY:O	2.44	0.50
2:C:757:ILE:HD12	2:C:837:LEU:HB2	1.93	0.50
3:D:83:THR:OG1	3:D:84:ARG:N	2.45	0.50
3:D:1198:GLY:N	3:D:1199:GLU:OE1	2.43	0.49
5:F:498:VAL:HG13	8:O:23:DG:H5"	1.95	0.49
5:F:269:ARG:NH1	5:F:271:GLU:OE1	2.45	0.49
3:D:194:ARG:O	3:D:198:ARG:NH1	2.46	0.49
2:C:1093:SER:OG	3:D:421:ARG:O	2.30	0.49
2:C:487:GLU:OE2	2:C:613:ARG:NH1	2.45	0.49
2:C:881:ASP:OD1	2:C:881:ASP:N	2.42	0.49
3:D:578:ARG:H	3:D:581:MET:HE3	1.78	0.49
2:C:563:ARG:HB2	2:C:567:GLU:HB2	1.94	0.49
2:C:658:ILE:HD11	2:C:688:PRO:HB3	1.95	0.49
3:D:1090:LYS:O	3:D:1097:ARG:N	2.46	0.49
1:A:175:THR:OG1	1:A:176:TYR:N	2.45	0.49
2:C:406:THR:OG1	2:C:407:GLN:N	2.46	0.49
3:D:605:ASP:OD1	3:D:605:ASP:N	2.43	0.49
2:C:891:ASN:ND2	2:C:930:GLN:OE1	2.46	0.48
3:D:159:ARG:HE	3:D:216:LEU:HD22	1.78	0.48
5:F:379:LEU:HD12	5:F:403:MET:HE1	1.96	0.48
1:B:198:THR:OG1	1:B:199:LYS:O	2.30	0.48
2:C:664:ASN:OD1	2:C:664:ASN:N	2.47	0.48
2:C:834:ASP:OD1	2:C:836:SER:OG	2.31	0.48
7:M:26:THR:OG1	7:M:31:GLN:OE1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:721:VAL:HG23	2:C:915:ILE:HG23	1.95	0.48
3:D:515:MET:HB3	3:D:515:MET:HE2	1.70	0.48
9:P:122:DT:H2'	9:P:123:DG:C4	2.49	0.47
3:D:931:ASP:OD1	3:D:931:ASP:N	2.46	0.47
5:F:488:THR:OG1	5:F:490:ASP:OD1	2.24	0.47
7:M:121:SER:OG	7:M:122:ALA:N	2.44	0.47
1:A:170:PRO:HG2	1:A:202:ILE:HD11	1.96	0.47
1:A:94:THR:HG22	1:A:139:VAL:HG22	1.97	0.47
7:M:8:THR:HB	7:M:141:LEU:HD11	1.96	0.47
7:M:125:LYS:HA	7:M:125:LYS:HD3	1.57	0.47
3:D:331:ASP:OD1	3:D:331:ASP:N	2.44	0.47
7:M:23:GLU:OE2	7:M:47:ARG:NH1	2.47	0.47
9:P:81:DG:H2'	9:P:82:DG:C8	2.49	0.47
2:C:208:ARG:NH1	2:C:304:LYS:O	2.46	0.46
3:D:1024:ILE:HD11	3:D:1114:GLY:HA2	1.97	0.46
2:C:704:ASP:OD1	2:C:708:THR:OG1	2.34	0.46
3:D:356:ARG:O	3:D:360:LEU:HB2	2.15	0.46
2:C:92:GLU:OE2	2:C:390:ARG:NE	2.40	0.46
3:D:611:VAL:HG12	3:D:634:LYS:HB2	1.98	0.46
3:D:193:ALA:HA	3:D:196:LYS:HG2	1.98	0.46
2:C:54:LEU:HD22	2:C:452:LYS:HD2	1.97	0.46
3:D:1164:ARG:NH2	3:D:1216:ALA:O	2.49	0.45
3:D:453:LYS:HG3	3:D:476:VAL:HG11	1.97	0.45
5:F:524:ARG:HH22	5:F:527:LEU:HB2	1.81	0.45
1:B:95:MET:HE2	1:B:110:ILE:HD11	1.98	0.45
3:D:879:ASP:OD2	3:D:1249:LYS:NZ	2.38	0.45
5:F:524:ARG:O	5:F:524:ARG:NH2	2.50	0.45
6:J:31:ARG:HG2	6:J:41:GLU:HG2	1.98	0.45
2:C:1012:ASP:OD2	2:C:1015:SER:OG	2.33	0.45
3:D:411:GLY:O	3:D:415:GLN:HB3	2.17	0.45
3:D:923:ARG:NH2	3:D:1155:GLU:OE1	2.49	0.45
1:B:55:ARG:HG3	1:B:161:ARG:HA	1.97	0.45
3:D:459:ARG:NH2	4:E:88:GLN:OE1	2.50	0.45
2:C:453:ARG:NH2	2:C:501:SER:O	2.50	0.45
3:D:339:ASP:OD2	3:D:397:ARG:NH2	2.50	0.45
6:J:89:ARG:HD3	6:J:89:ARG:HA	1.81	0.45
2:C:982:GLU:OE1	3:D:841:ARG:NH2	2.50	0.44
2:C:640:ASP:HB3	2:C:706:PRO:HD2	1.99	0.44
3:D:576:MET:HG2	3:D:697:ILE:HD12	1.98	0.44
2:C:1043:ALA:HB2	3:D:447:MET:HG2	1.98	0.44
3:D:73:ILE:HG23	6:J:27:ARG:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:GLU:OE2	2:C:876:LYS:NZ	2.37	0.44
1:A:82:SER:O	1:A:82:SER:OG	2.29	0.44
2:C:1111:ASN:ND2	4:E:66:ASP:OD2	2.51	0.44
3:D:599:TYR:HA	3:D:610:GLY:HA3	1.99	0.44
3:D:129:ILE:HG22	3:D:261:ILE:HG13	2.00	0.43
3:D:173:ARG:HH22	3:D:177:LEU:HD22	1.83	0.43
3:D:1112:MET:HE3	3:D:1112:MET:HB3	1.88	0.43
2:C:621:SER:O	2:C:621:SER:OG	2.31	0.43
1:A:72:ASP:OD1	1:A:72:ASP:N	2.44	0.43
2:C:185:VAL:HG12	2:C:204:VAL:HB	2.00	0.43
2:C:298:ASN:O	2:C:305:ARG:NH2	2.51	0.43
2:C:758:ASP:OD2	2:C:760:ARG:NH2	2.52	0.43
8:O:24:DG:H2'	8:O:25:DT:H71	2.00	0.43
5:F:524:ARG:HA	5:F:524:ARG:HD2	1.92	0.43
2:C:1002:VAL:HG22	2:C:1008:ALA:HB2	2.00	0.43
3:D:285:LYS:HA	3:D:285:LYS:HD2	1.77	0.43
3:D:24:SER:O	6:J:57:ARG:NH2	2.52	0.43
3:D:766:ASN:OD1	3:D:766:ASN:N	2.39	0.42
3:D:937:ILE:HD13	3:D:957:ILE:HD11	2.00	0.42
5:F:345:THR:OG1	8:O:52:DC:O2	2.32	0.42
1:A:187:THR:O	1:A:187:THR:OG1	2.36	0.42
2:C:891:ASN:OD1	2:C:891:ASN:N	2.41	0.42
3:D:239:ASN:OD1	3:D:239:ASN:N	2.50	0.42
1:B:123:MET:HE2	1:B:123:MET:HB3	1.93	0.42
2:C:286:PRO:HA	2:C:287:PRO:HD3	1.88	0.42
3:D:707:ILE:HD11	4:E:32:PRO:HB3	2.01	0.42
1:B:176:TYR:HB3	1:B:194:LEU:HD23	2.02	0.42
2:C:580:ASP:OD2	2:C:580:ASP:N	2.52	0.42
2:C:1135:VAL:HG22	3:D:12:ILE:HG13	2.01	0.42
3:D:327:MET:HB2	3:D:327:MET:HE2	1.76	0.42
5:F:315:MET:HE2	5:F:319:ASP:HB3	2.01	0.42
2:C:541:VAL:HG22	2:C:578:TYR:HB2	2.02	0.42
2:C:974:THR:O	2:C:974:THR:OG1	2.36	0.42
1:A:225:LEU:HD11	1:B:208:LEU:HD23	2.02	0.42
2:C:935:HIS:CD2	3:D:733:MET:HG2	2.55	0.42
2:C:938:TRP:HB2	2:C:1026:GLY:HA2	2.00	0.42
3:D:876:ARG:NH2	3:D:1036:GLU:OE2	2.51	0.42
5:F:448:VAL:HA	5:F:451:VAL:HG12	2.02	0.42
9:P:104:DT:H4'	9:P:105:DT:H5'	2.01	0.42
3:D:1224:ALA:O	3:D:1229:THR:OG1	2.29	0.41
5:F:372:MET:HE3	5:F:372:MET:HB3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:257:ILE:H	2:C:257:ILE:HG13	1.59	0.41
1:B:185:GLN:H	1:B:185:GLN:HG3	1.67	0.41
2:C:304:LYS:HE3	2:C:304:LYS:HB3	1.91	0.41
3:D:637:LEU:HD13	3:D:640:LEU:HD12	2.02	0.41
3:D:262:GLN:HB2	3:D:313:VAL:HG21	2.01	0.41
3:D:666:THR:OG1	3:D:667:THR:N	2.52	0.41
4:E:47:VAL:HG21	4:E:53:LEU:HB2	2.02	0.41
5:F:401:LYS:HD3	5:F:401:LYS:HA	1.90	0.41
1:A:73:VAL:O	1:A:77:ILE:HG12	2.21	0.41
2:C:444:ASN:ND2	2:C:615:ALA:O	2.54	0.41
5:F:251:LYS:HB2	5:F:251:LYS:HE3	1.90	0.41
1:A:172:LEU:HD13	1:A:199:LYS:HB3	2.02	0.41
5:F:503:ILE:HD13	5:F:503:ILE:HA	1.94	0.41
5:F:504:ARG:HH12	9:P:127:DA:H2'	1.85	0.41
2:C:150:GLN:HG2	7:M:44:LEU:HB3	2.03	0.41
3:D:812:THR:O	3:D:816:THR:HG23	2.21	0.41
1:A:226:ASN:OD1	1:A:226:ASN:N	2.53	0.40
3:D:369:ASN:OD1	5:F:322:GLN:NE2	2.52	0.40
3:D:642:PRO:HG2	3:D:647:GLU:HB2	2.03	0.40
6:J:79:ARG:HA	6:J:79:ARG:HD3	1.91	0.40
5:F:427:ILE:HD12	5:F:427:ILE:HA	1.87	0.40
5:F:483:ASP:OD1	5:F:483:ASP:N	2.53	0.40
9:P:112:DT:H2''	9:P:113:DG:C8	2.56	0.40
2:C:642:VAL:HB	2:C:703:ALA:HB3	2.03	0.40
2:C:584:ARG:HE	2:C:584:ARG:HB3	1.70	0.40
2:C:942:SER:OG	2:C:992:THR:OG1	2.37	0.40
3:D:706:MET:H	3:D:706:MET:HG3	1.65	0.40
2:C:289:LYS:HD2	2:C:289:LYS:HA	1.80	0.40
2:C:447:SER:OG	2:C:613:ARG:O	2.39	0.40
2:C:535:GLU:O	2:C:539:HIS:ND1	2.53	0.40
2:C:926:MET:HB2	2:C:926:MET:HE2	1.69	0.40
8:O:35:DC:H2'	8:O:36:DT:H71	2.04	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	223/347 (64%)	210 (94%)	13 (6%)	0	100	100
1	B	235/347 (68%)	220 (94%)	15 (6%)	0	100	100
2	C	1109/1172 (95%)	1036 (93%)	73 (7%)	0	100	100
3	D	1264/1318 (96%)	1198 (95%)	66 (5%)	0	100	100
4	E	81/110 (74%)	76 (94%)	5 (6%)	0	100	100
5	F	315/528 (60%)	305 (97%)	10 (3%)	0	100	100
6	J	105/111 (95%)	92 (88%)	13 (12%)	0	100	100
7	M	157/162 (97%)	145 (92%)	12 (8%)	0	100	100
All	All	3489/4095 (85%)	3282 (94%)	207 (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	194/297 (65%)	171 (88%)	23 (12%)	4	7
1	B	195/297 (66%)	171 (88%)	24 (12%)	4	6
2	C	937/993 (94%)	854 (91%)	83 (9%)	8	15
3	D	1048/1095 (96%)	981 (94%)	67 (6%)	14	26
4	E	69/90 (77%)	63 (91%)	6 (9%)	8	15
5	F	264/427 (62%)	250 (95%)	14 (5%)	19	34
6	J	92/97 (95%)	86 (94%)	6 (6%)	14	25
7	M	129/131 (98%)	123 (95%)	6 (5%)	22	39
All	All	2928/3427 (85%)	2699 (92%)	229 (8%)	13	19

All (229) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	VAL
1	A	59	VAL
1	A	69	VAL
1	A	81	LYS
1	A	84	VAL
1	A	85	VAL
1	A	91	GLU
1	A	95	MET
1	A	111	VAL
1	A	116	VAL
1	A	127	THR
1	A	136	VAL
1	A	138	LEU
1	A	150	VAL
1	A	159	ILE
1	A	164	VAL
1	A	166	SER
1	A	178	VAL
1	A	188	ASP
1	A	202	ILE
1	A	213	LYS
1	A	218	LEU
1	A	221	LEU
1	B	2	LEU
1	B	34	LEU
1	B	38	LEU
1	B	52	THR
1	B	69	VAL
1	B	84	VAL
1	B	93	VAL
1	B	94	THR
1	B	95	MET
1	B	99	LYS
1	B	110	ILE
1	B	111	VAL
1	B	147	VAL
1	B	150	VAL
1	B	164	VAL
1	B	171	VAL
1	B	175	THR
1	B	177	LYS
1	B	178	VAL
1	B	192	LEU

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Mol	Chain	Res	Type
1	B	216	VAL
1	B	217	GLU
1	B	223	ARG
1	B	227	VAL
2	C	94	SER
2	C	103	MET
2	C	120	ASP
2	C	124	ASP
2	C	126	ASP
2	C	144	THR
2	C	147	ILE
2	C	176	VAL
2	C	177	SER
2	C	185	VAL
2	C	190	THR
2	C	195	THR
2	C	201	SER
2	C	204	VAL
2	C	221	THR
2	C	222	VAL
2	C	226	ILE
2	C	232	GLN
2	C	249	VAL
2	C	257	ILE
2	C	288	THR
2	C	308	LEU
2	C	324	VAL
2	C	334	THR
2	C	356	THR
2	C	373	PHE
2	C	381	VAL
2	C	391	VAL
2	C	398	ARG
2	C	406	THR
2	C	410	GLU
2	C	439	PHE
2	C	441	ASP
2	C	452	LYS
2	C	458	LEU
2	C	463	LEU
2	C	470	LEU
2	C	475	VAL

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Mol	Chain	Res	Type
2	C	483	MET
2	C	488	THR
2	C	490	GLU
2	C	494	ILE
2	C	499	SER
2	C	500	LEU
2	C	519	VAL
2	C	520	VAL
2	C	534	ASP
2	C	540	VAL
2	C	551	ASP
2	C	573	SER
2	C	584	ARG
2	C	626	VAL
2	C	641	VAL
2	C	653	VAL
2	C	659	THR
2	C	660	VAL
2	C	667	ARG
2	C	672	MET
2	C	685	ASN
2	C	702	ILE
2	C	732	GLU
2	C	738	SER
2	C	790	VAL
2	C	815	THR
2	C	834	ASP
2	C	836	SER
2	C	844	SER
2	C	852	VAL
2	C	868	LEU
2	C	897	LYS
2	C	909	ASP
2	C	926	MET
2	C	934	THR
2	C	936	LEU
2	C	973	SER
2	C	974	THR
2	C	976	VAL
2	C	997	ASP
2	C	1030	ILE
2	C	1037	VAL

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Mol	Chain	Res	Type
2	C	1042	HIS
2	C	1063	PHE
2	C	1094	ASP
3	D	28	VAL
3	D	55	THR
3	D	68	VAL
3	D	73	ILE
3	D	82	VAL
3	D	110	VAL
3	D	114	LEU
3	D	138	SER
3	D	219	LEU
3	D	234	LEU
3	D	236	VAL
3	D	259	GLU
3	D	262	GLN
3	D	270	ILE
3	D	281	ILE
3	D	298	VAL
3	D	314	LEU
3	D	320	ILE
3	D	327	MET
3	D	328	VAL
3	D	406	LEU
3	D	415	GLN
3	D	427	ARG
3	D	429	VAL
3	D	478	ARG
3	D	488	GLU
3	D	490	VAL
3	D	505	HIS
3	D	559	MET
3	D	562	SER
3	D	567	SER
3	D	576	MET
3	D	581	MET
3	D	590	THR
3	D	598	GLU
3	D	629	VAL
3	D	635	VAL
3	D	677	LEU
3	D	706	MET

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Mol	Chain	Res	Type
3	D	725	THR
3	D	731	VAL
3	D	733	MET
3	D	738	VAL
3	D	758	LYS
3	D	839	SER
3	D	846	VAL
3	D	885	ILE
3	D	901	LEU
3	D	904	ARG
3	D	911	ILE
3	D	925	LEU
3	D	944	LEU
3	D	971	SER
3	D	993	GLU
3	D	1012	MET
3	D	1039	VAL
3	D	1050	THR
3	D	1098	VAL
3	D	1099	LEU
3	D	1107	VAL
3	D	1115	SER
3	D	1173	THR
3	D	1196	GLU
3	D	1206	VAL
3	D	1238	ILE
3	D	1250	GLU
3	D	1262	THR
4	E	31	THR
4	E	33	LEU
4	E	35	ILE
4	E	49	SER
4	E	92	LEU
4	E	105	GLU
5	F	280	ASP
5	F	281	MET
5	F	284	ILE
5	F	306	LEU
5	F	370	VAL
5	F	375	VAL
5	F	387	LEU
5	F	415	GLN

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Mol	Chain	Res	Type
5	F	446	VAL
5	F	464	LEU
5	F	468	SER
5	F	489	LEU
5	F	498	VAL
5	F	511	MET
6	J	21	ASN
6	J	24	LEU
6	J	27	ARG
6	J	58	ASN
6	J	86	LEU
6	J	105	ILE
7	M	24	THR
7	M	39	VAL
7	M	125	LYS
7	M	128	LEU
7	M	133	GLN
7	M	141	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	142	ASN
2	C	603	ASN
2	C	935	HIS
2	C	941	HIS
2	C	1129	GLN
3	D	213	GLN
3	D	233	GLN
3	D	369	ASN
3	D	396	ASN
3	D	416	ASN
3	D	465	HIS
3	D	653	HIS
3	D	792	HIS
3	D	810	ASN
3	D	1084	GLN
3	D	1109	GLN
3	D	1153	HIS
5	F	242	ASN
5	F	261	GLN
5	F	322	GLN

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Mol	Chain	Res	Type
7	M	13	HIS

### 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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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.

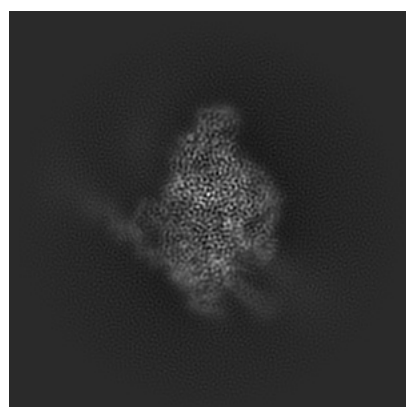
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22888. These allow visual inspection of the internal detail of the map and identification of artifacts.

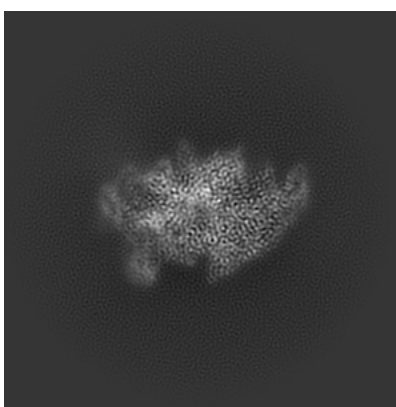
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

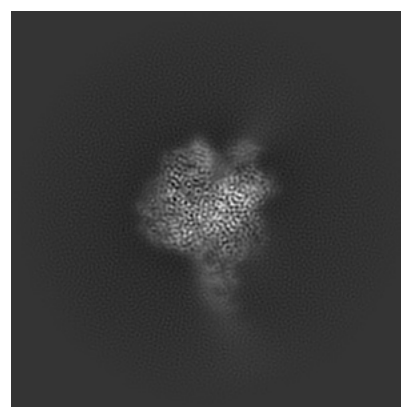
#### 6.1.1 Primary map



X



Y

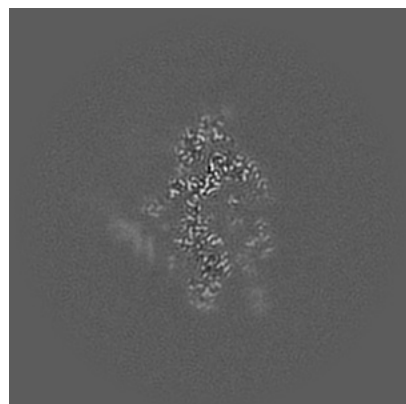


Z

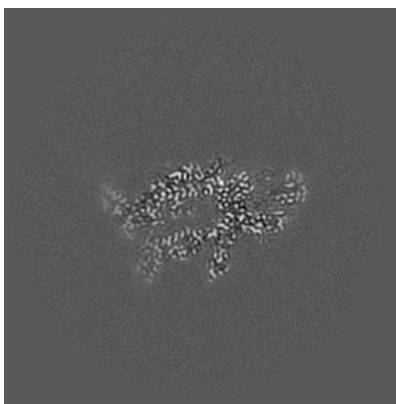
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

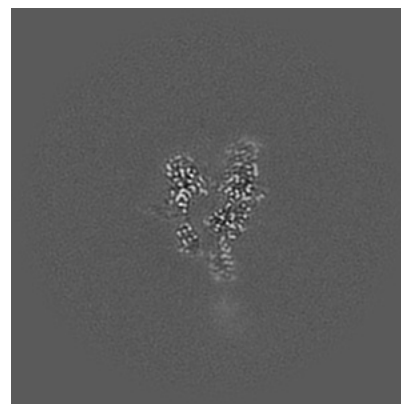
#### 6.2.1 Primary map



X Index: 150



Y Index: 150

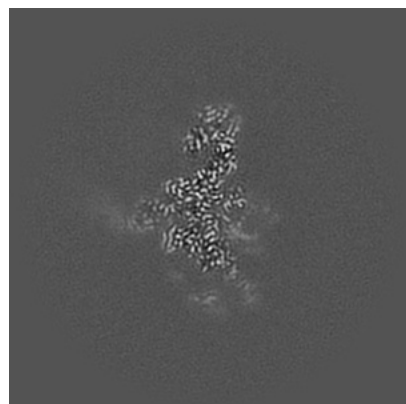


Z Index: 150

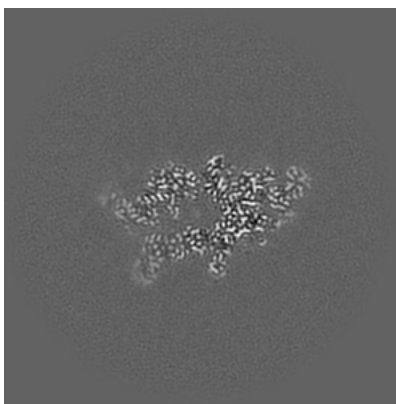
The images above show central slices of the map in three orthogonal directions.

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

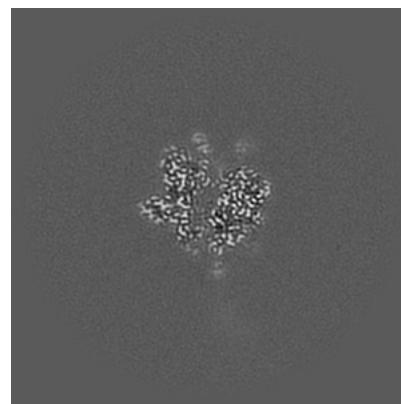
### 6.3.1 Primary map



X Index: 160



Y Index: 154

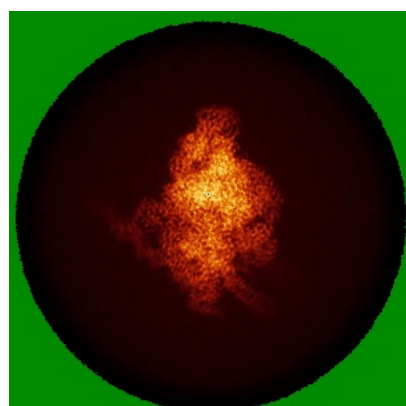


Z Index: 158

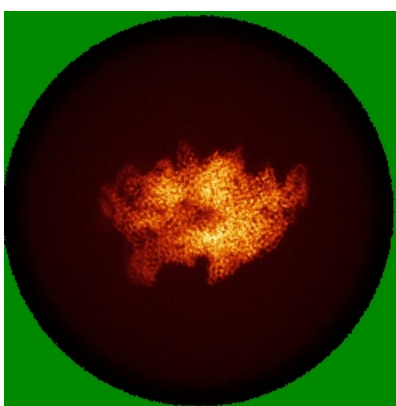
The images above show the largest variance slices of the map in three orthogonal directions.

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

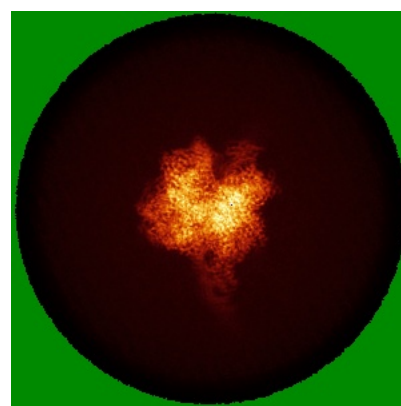
### 6.4.1 Primary map



X



Y

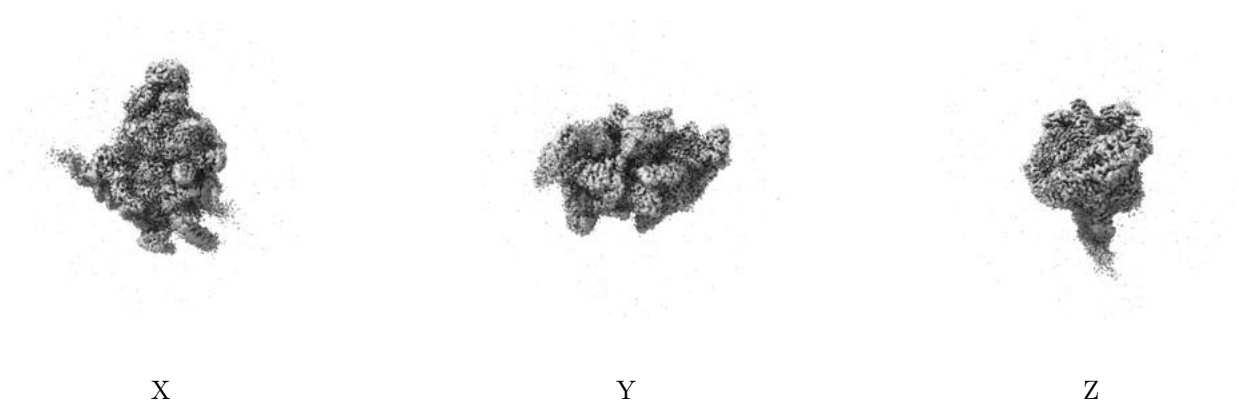


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

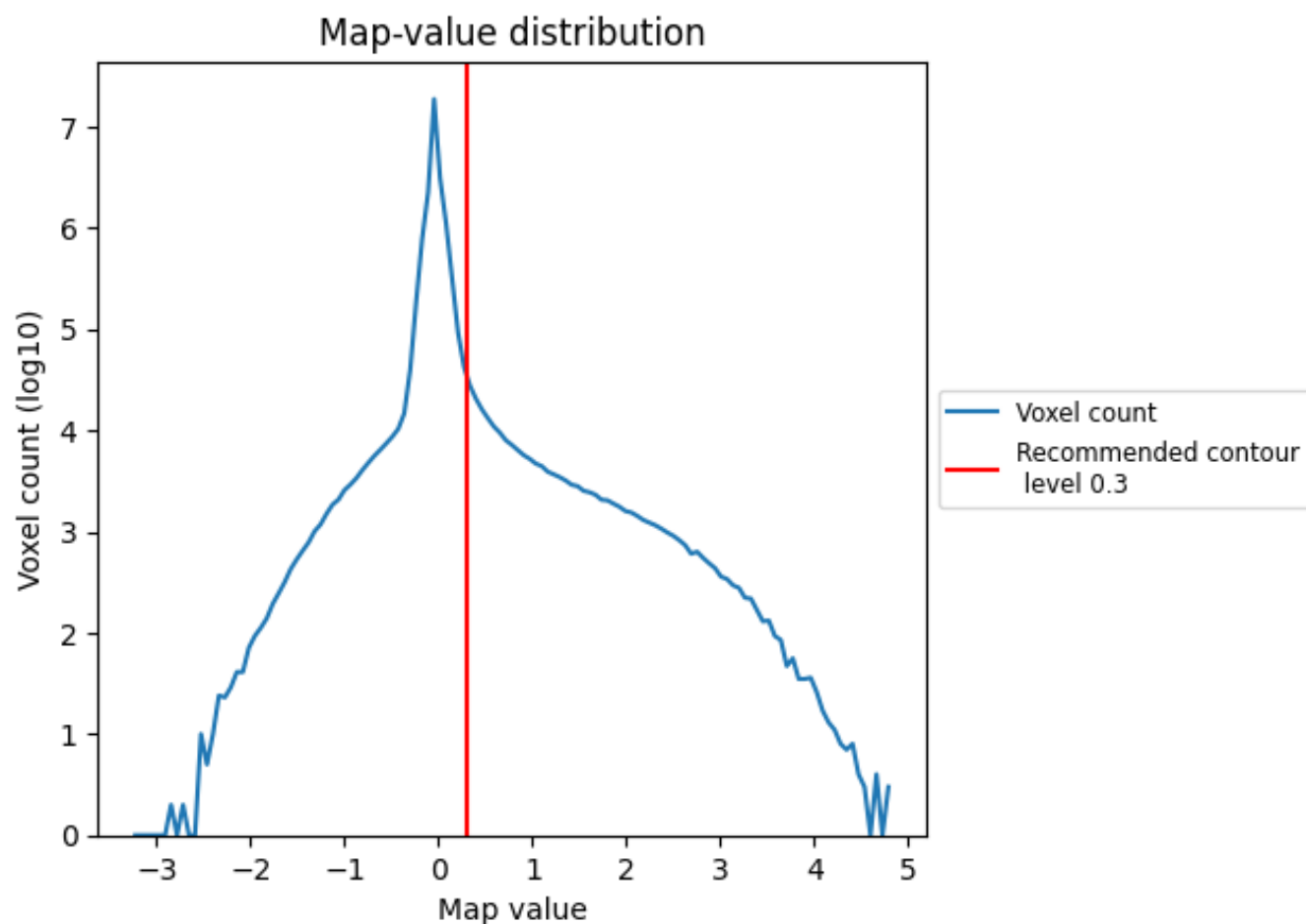
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

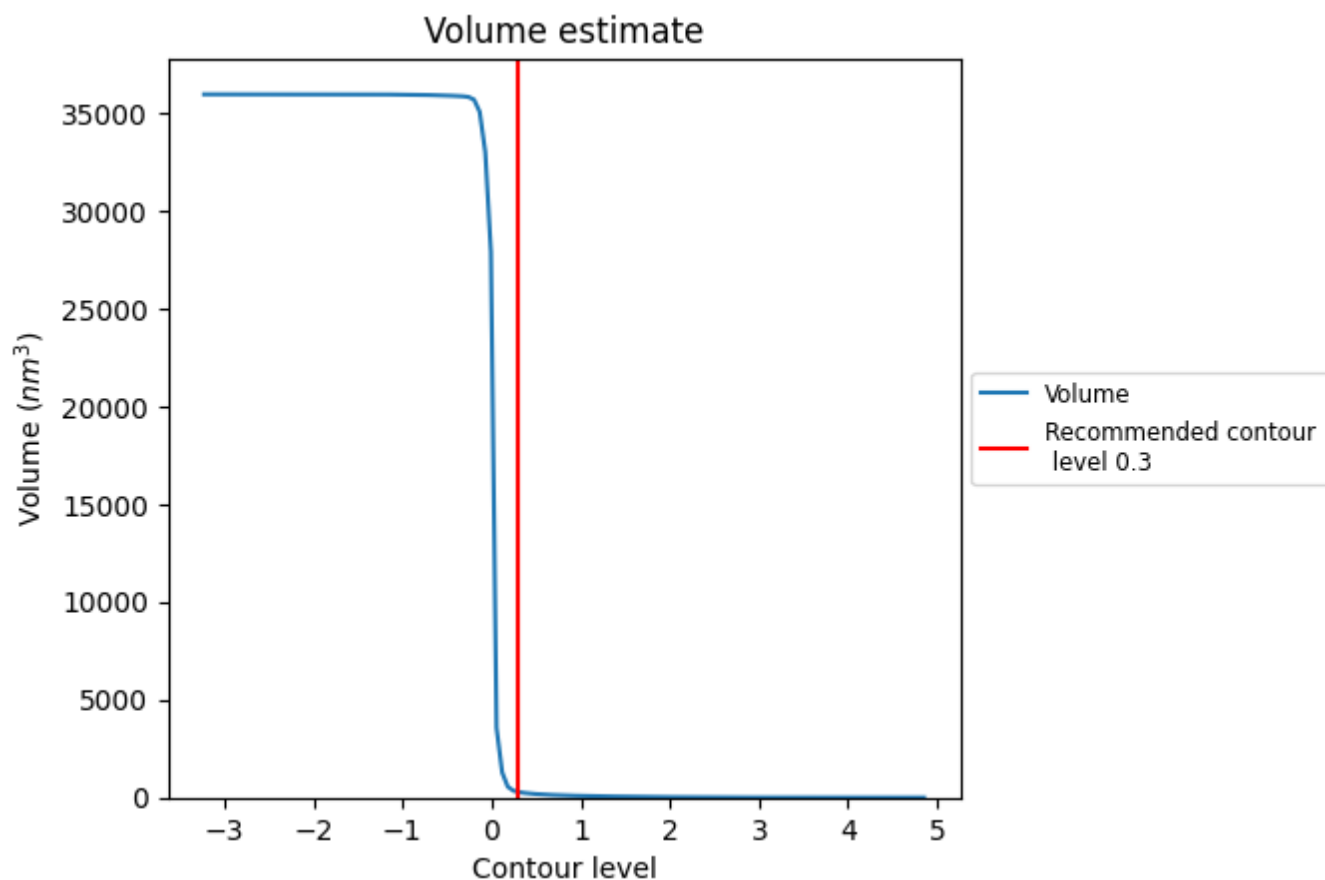
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

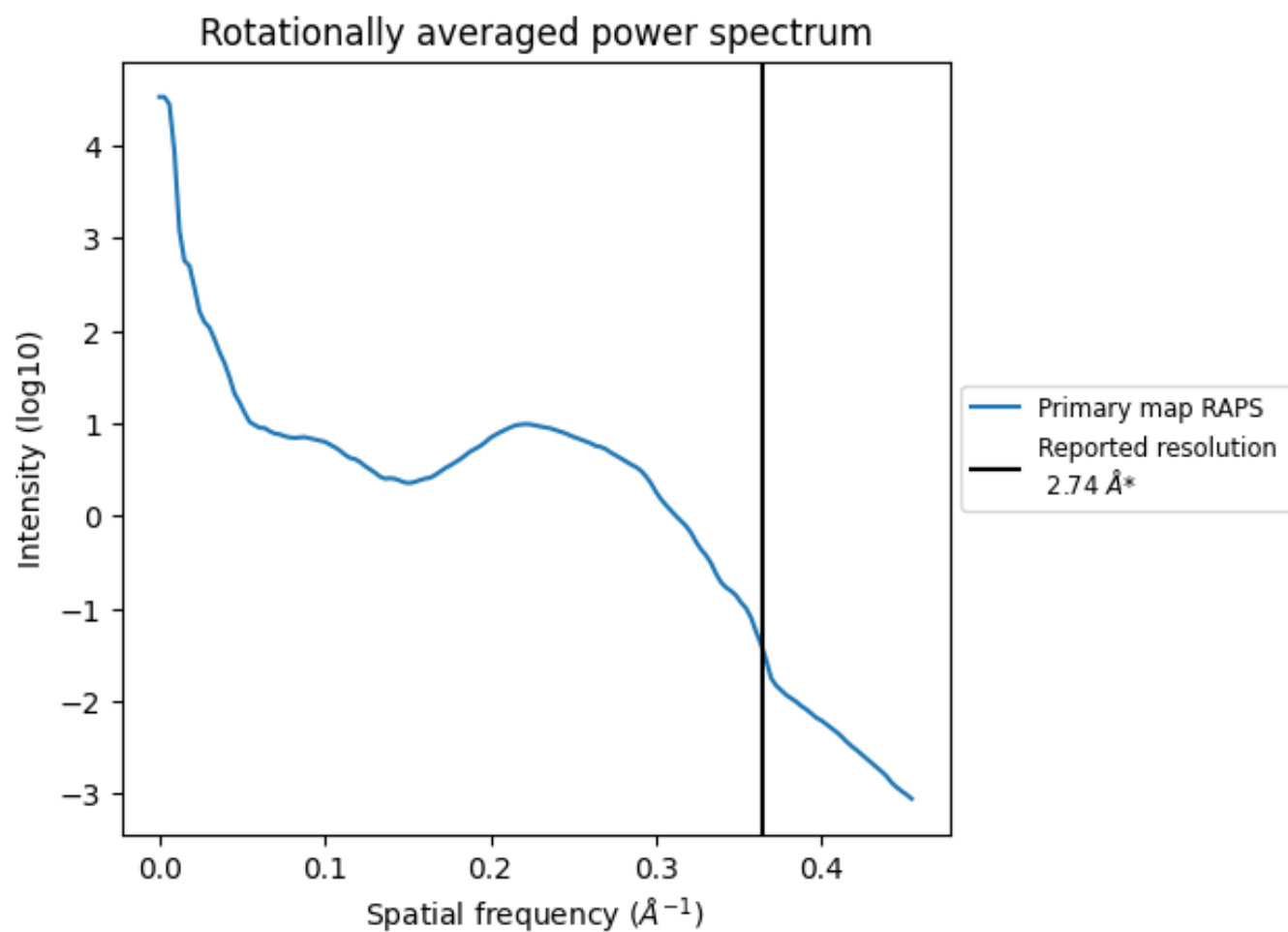
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 286 nm<sup>3</sup>; this corresponds to an approximate mass of 258 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 0.365 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

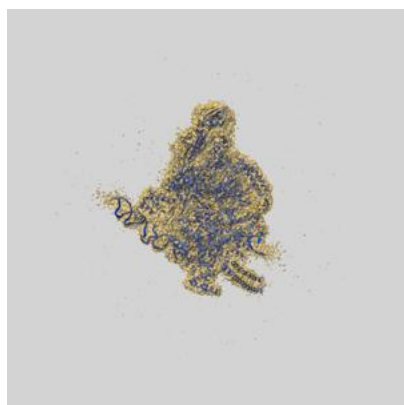
This section was not generated. No FSC curve or half-maps provided.



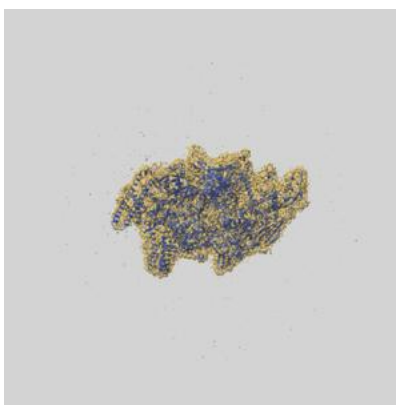
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22888 and PDB model 7KIN. Per-residue inclusion information can be found in section [3](#) on page [6](#).

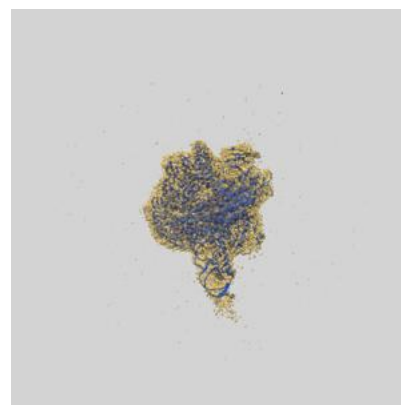
### 9.1 Map-model overlay [i](#)



X



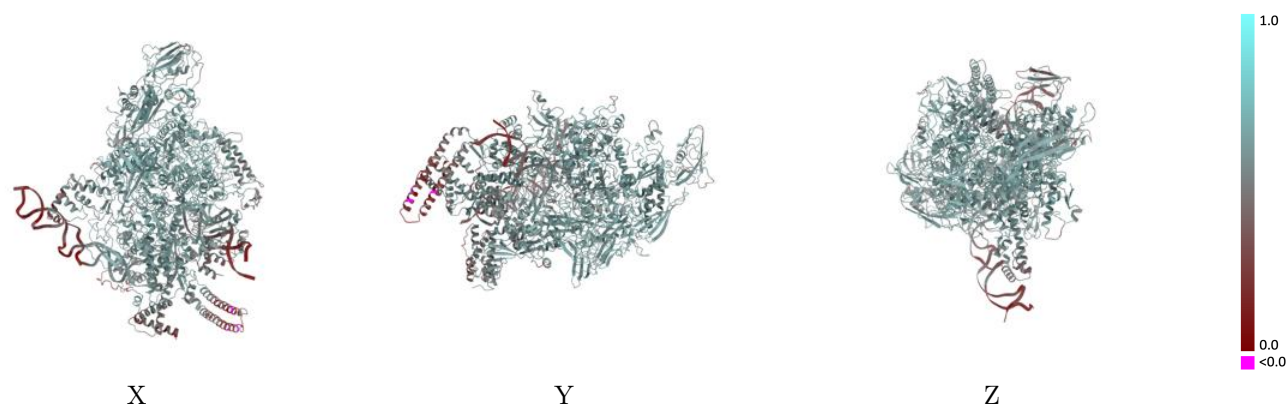
Y



Z

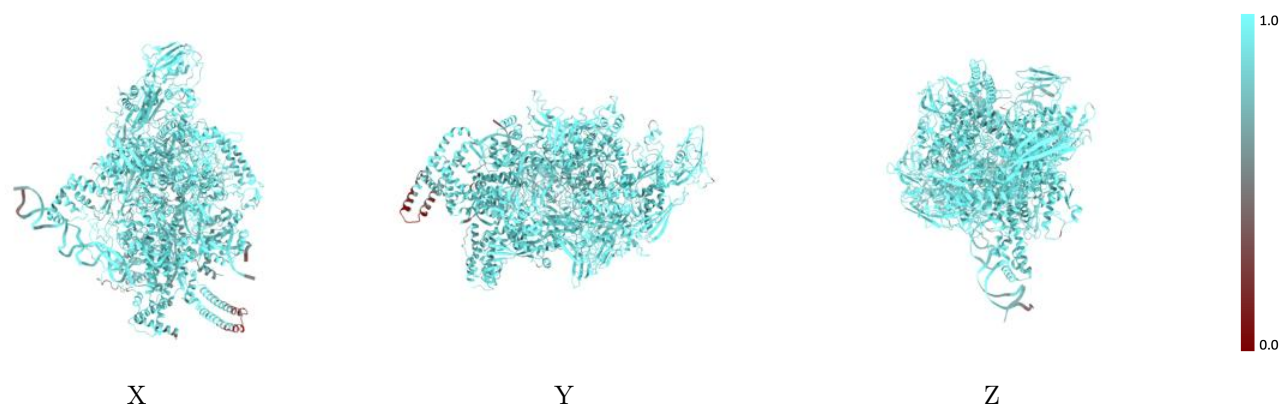
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



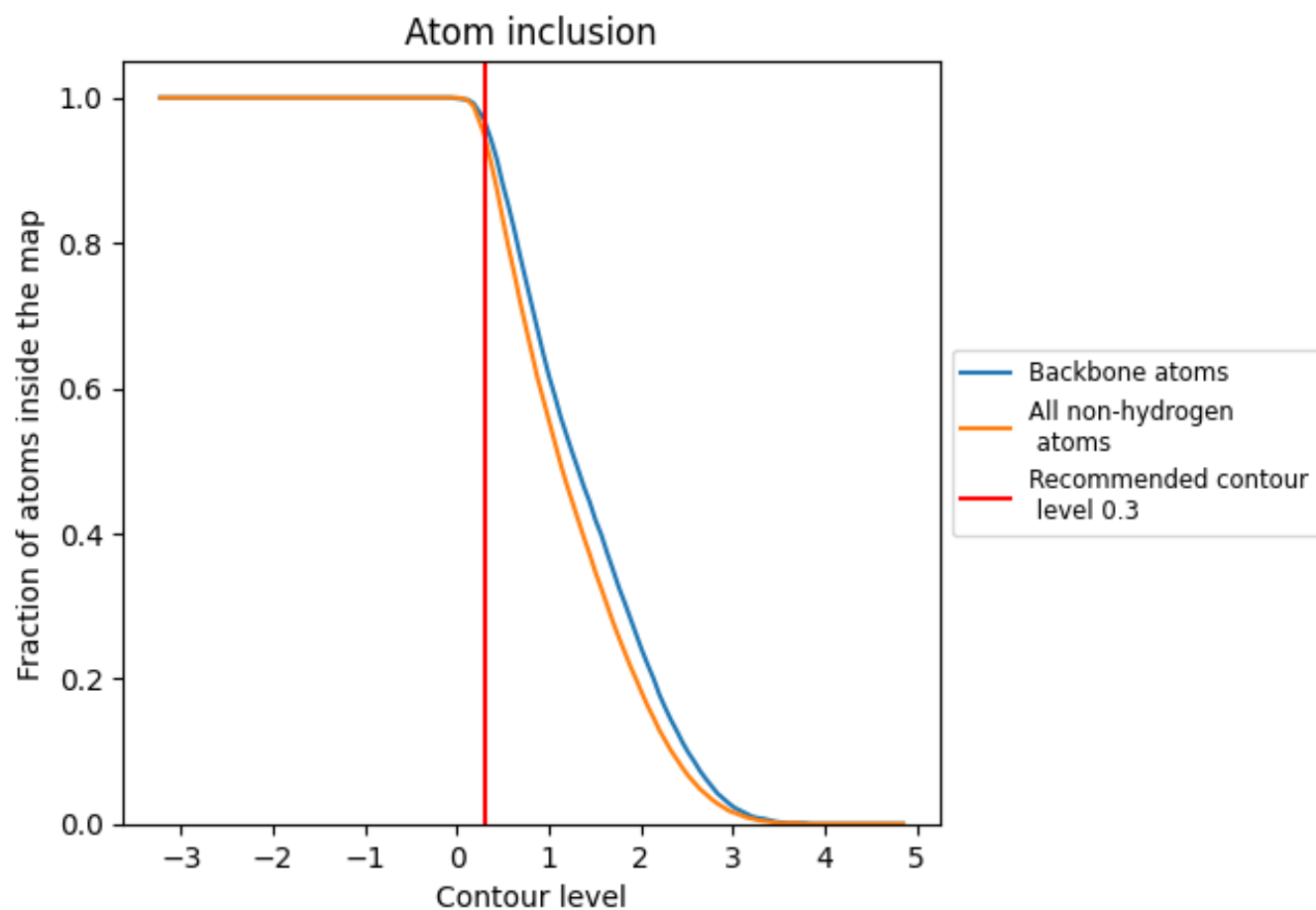
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 95% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9480	<div><div></div></div> 0.5560
A	<div><div></div></div> 0.9770	<div><div></div></div> 0.6000
B	<div><div></div></div> 0.9520	<div><div></div></div> 0.5650
C	<div><div></div></div> 0.9690	<div><div></div></div> 0.5930
D	<div><div></div></div> 0.9510	<div><div></div></div> 0.5740
E	<div><div></div></div> 0.9510	<div><div></div></div> 0.5870
F	<div><div></div></div> 0.9450	<div><div></div></div> 0.5330
J	<div><div></div></div> 0.8840	<div><div></div></div> 0.5010
M	<div><div></div></div> 0.9030	<div><div></div></div> 0.4750
O	<div><div></div></div> 0.8650	<div><div></div></div> 0.3730
P	<div><div></div></div> 0.8780	<div><div></div></div> 0.3620

1.0

0.0

<0.0