



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 08:24 PM UTC

PDB ID : 9D0T / pdb_00009d0t
EMDB ID : EMD-46461
Title : Proteasome core particle assembly intermediate Blm10:13S purified from *Saccharomyces cerevisiae*
Authors : Chen, X.; Kaur, M.; Roelofs, J.; Walters, K.J.
Deposited on : 2024-08-07
Resolution : 2.84 Å (reported)
Based on initial models : 7LSX, 4V7O

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

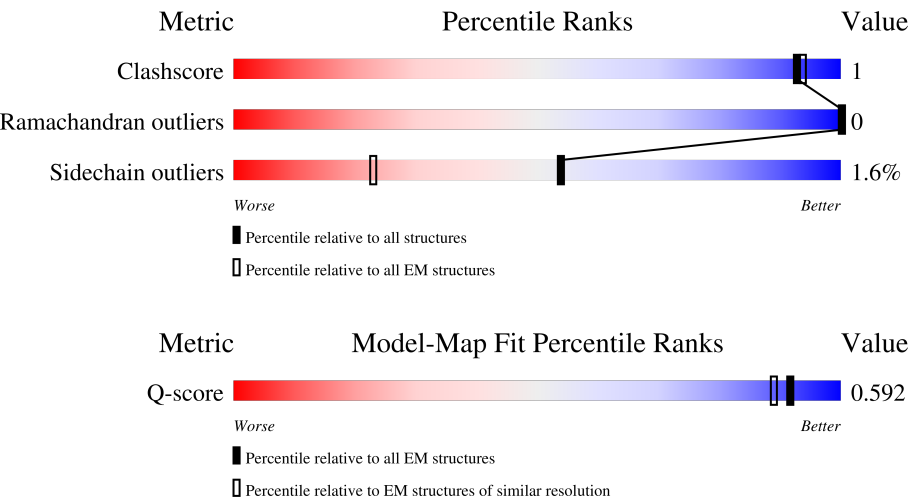
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.84 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	11884 (2.34 - 3.34)

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	252	
2	B	250	
3	C	258	
4	D	254	

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Mol	Chain	Length	Quality of chain
5	E	260	92% 5%
6	F	234	95%
7	G	288	81% 14%
8	I	261	78% 19%
9	J	205	82% 8% 9%
10	K	198	87% 6% 7%
11	O	2143	86% 10%
12	P	200	44% 55%

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 68083 atoms, of which 34010 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 Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	244	Total	C	H	N	O	S	0	0
			3834	1222	1912	323	369	8		

- Molecule 2 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	246	Total	C	H	N	O	S	0	0
			3775	1200	1894	308	370	3		

- Molecule 3 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	239	Total	C	H	N	O	S	0	0
			3713	1175	1858	306	371	3		

- Molecule 4 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	249	Total	C	H	N	O	S	0	0
			3924	1220	1967	343	389	5		

- Molecule 5 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	246	Total	C	H	N	O	S	0	0
			3760	1190	1864	312	386	8		

- Molecule 6 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	234	Total	C	H	N	O	S	0	0
			3614	1134	1811	313	351	5		

- Molecule 7 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	247	Total	C	H	N	O	S	0	0
			3820	1217	1904	333	362	4		

- Molecule 8 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	I	212	Total	C	H	N	O	S	0	0
			3191	1012	1588	277	309	5		

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	J	186	Total	C	H	N	O	S	0	0
			2897	935	1447	233	274	8		

- Molecule 10 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	K	184	Total	C	H	N	O	S	0	0
			2959	942	1479	249	283	6		

- Molecule 11 is a protein called Proteasome activator BLM10.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	O	1919	Total	C	H	N	O	S	0	0
			31119	10023	15558	2574	2893	71		

- Molecule 12 is a protein called Proteasome maturation factor UMP1,Myosin light chain kinase 2, skeletal/cardiac muscle.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	P	90	Total	C	H	N	O	S	0	0
			1477	463	728	136	145	5		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	149	GLY	-	linker	UNP P38293
P	150	ARG	-	linker	UNP P38293
P	151	ARG	-	linker	UNP P38293

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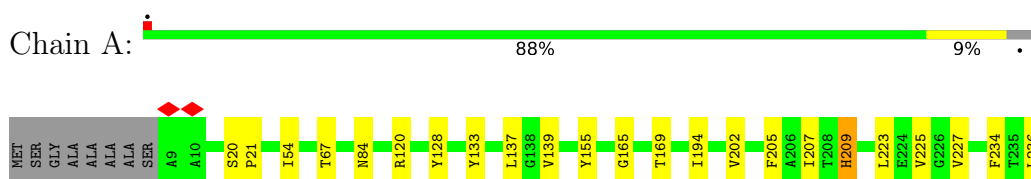
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Chain	Residue	Modelled	Actual	Comment	Reference
P	152	ILE	-	linker	UNP P38293
P	153	PRO	-	linker	UNP P38293
P	154	GLY	-	linker	UNP P38293
P	155	LEU	-	linker	UNP P38293
P	156	ILE	-	linker	UNP P38293
P	157	ASN	-	linker	UNP P38293
P	158	PRO	-	linker	UNP P38293
P	159	TRP	-	linker	UNP P38293
P	186	ASP	-	expression tag	UNP A4IFM7
P	187	TYR	-	expression tag	UNP A4IFM7
P	188	ASP	-	expression tag	UNP A4IFM7
P	189	ILE	-	expression tag	UNP A4IFM7
P	190	PRO	-	expression tag	UNP A4IFM7
P	191	THR	-	expression tag	UNP A4IFM7
P	192	THR	-	expression tag	UNP A4IFM7
P	193	ALA	-	expression tag	UNP A4IFM7
P	194	SER	-	expression tag	UNP A4IFM7
P	195	GLU	-	expression tag	UNP A4IFM7
P	196	ASN	-	expression tag	UNP A4IFM7
P	197	LEU	-	expression tag	UNP A4IFM7
P	198	TYR	-	expression tag	UNP A4IFM7
P	199	PHE	-	expression tag	UNP A4IFM7
P	200	GLN	-	expression tag	UNP A4IFM7

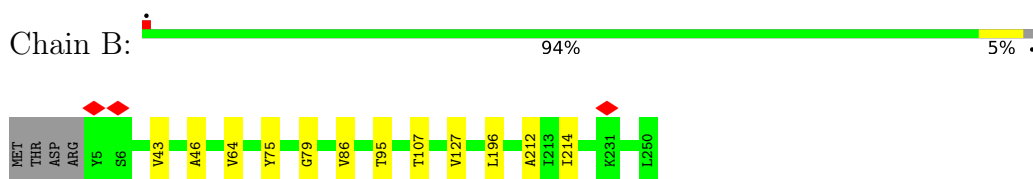
3 Residue-property plots [i](#)

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

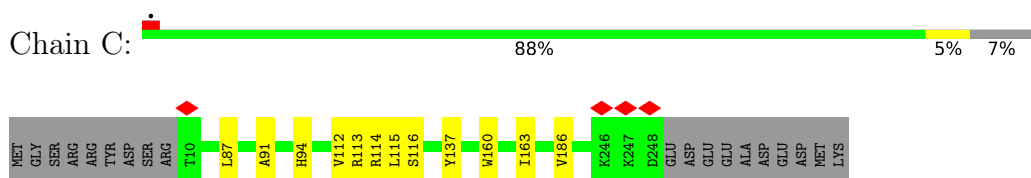
- Molecule 1: Proteasome subunit alpha type-1



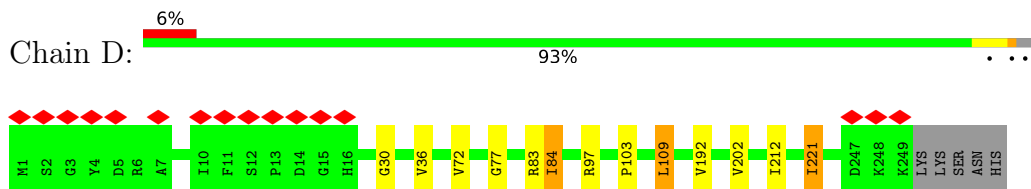
- Molecule 2: Proteasome subunit alpha type-2



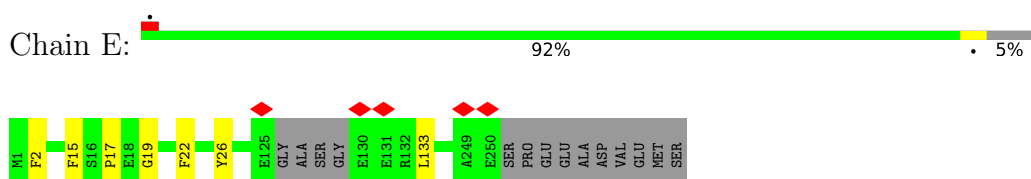
- Molecule 3: Proteasome subunit alpha type-3



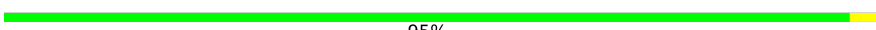
- Molecule 4: Proteasome subunit alpha type-4



- Molecule 5: Proteasome subunit alpha type-5



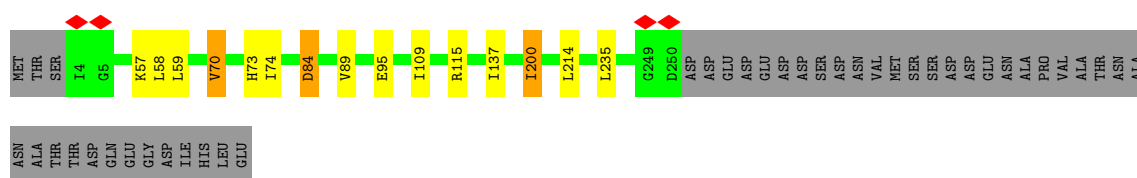
- Molecule 6: Proteasome subunit alpha type-6

Chain F:  95%



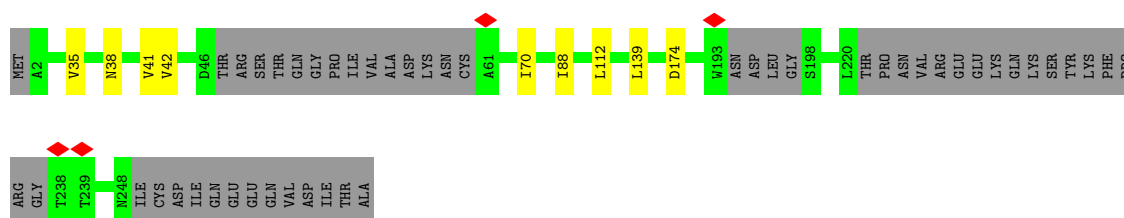
- Molecule 7: Probable proteasome subunit alpha type-7

Chain G:  81% 14%



- Molecule 8: Proteasome subunit beta type-2

Chain I:  78% 19%



- Molecule 9: Proteasome subunit beta type-3

Chain J:  82% 8% 9%



- Molecule 10: Proteasome subunit beta type-4

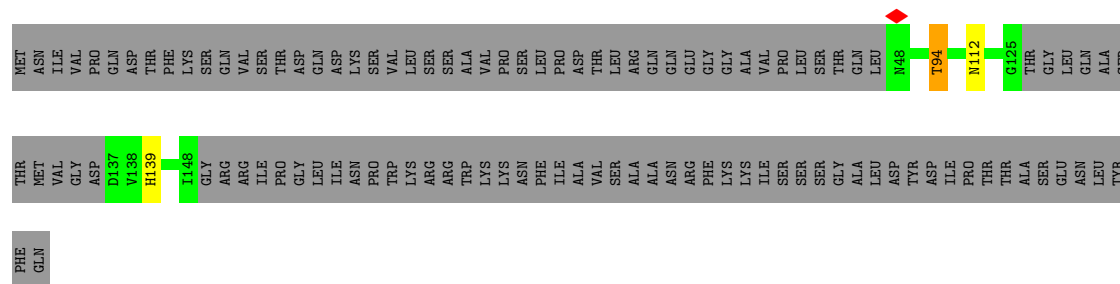
Chain K:  87% 6% 7%



- Molecule 11: Proteasome activator BLM10

Chain O:  86% 10%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	573652	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	23.596	Depositor
Minimum map value	-0.483	Depositor
Average map value	0.028	Depositor
Map value standard deviation	0.604	Depositor
Recommended contour level	3	Depositor
Map size (Å)	363.12, 363.12, 363.12	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.068, 1.068, 1.068	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	0.81	0/1960	1.31	0/2654
2	B	0.73	0/1918	1.30	0/2597
3	C	0.72	0/1884	1.30	0/2552
4	D	0.77	0/1986	1.35	0/2685
5	E	0.72	0/1922	1.25	0/2591
6	F	0.79	0/1831	1.32	0/2473
7	G	0.77	0/1956	1.35	0/2641
8	I	0.76	0/1631	1.33	0/2210
9	J	0.76	0/1478	1.28	0/1995
10	K	0.74	0/1507	1.26	0/2030
11	O	0.74	0/15910	1.31	0/21559
12	P	0.71	0/762	1.38	0/1025
All	All	0.75	0/34745	1.31	0/47012

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	1922	1912	1911	11	0
2	B	1881	1894	1893	4	0
3	C	1855	1858	1855	5	0
4	D	1957	1967	1969	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1896	1864	1858	4	0
6	F	1803	1811	1809	5	0
7	G	1916	1904	1904	7	0
8	I	1603	1588	1584	4	0
9	J	1450	1447	1445	10	0
10	K	1480	1479	1478	5	0
11	O	15561	15558	15545	36	0
12	P	749	728	727	3	0
All	All	34073	34010	33978	96	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 1.

All (96) 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)
4:D:72:VAL:CG2	4:D:221:ILE:HD11	2.22	0.69
11:O:2136:VAL:HG23	11:O:2137:LEU:HD12	1.76	0.67
9:J:23:ILE:HD11	9:J:110:ALA:HB3	1.77	0.67
11:O:1034:PHE:HB2	11:O:1173:HIS:NE2	2.10	0.66
3:C:112:VAL:HG12	3:C:137:TYR:CG	2.32	0.63
11:O:1034:PHE:HB2	11:O:1173:HIS:CE1	2.35	0.62
10:K:5:LEU:HD13	10:K:6:GLY:N	2.15	0.61
11:O:662:ILE:HG21	11:O:695:ILE:CD1	2.34	0.57
5:E:15:PHE:HB3	5:E:19:GLY:HA2	1.86	0.56
4:D:97:ARG:CG	4:D:103:PRO:HA	2.36	0.55
1:A:120:ARG:NH1	12:P:112:ASN:HB2	2.23	0.54
6:F:176:LEU:HD12	7:G:58:LEU:HD23	1.91	0.53
9:J:21:VAL:HG11	9:J:110:ALA:HB1	1.90	0.53
11:O:1805:LEU:HD23	11:O:1886:TRP:CD1	2.43	0.53
5:E:2:PHE:HA	11:O:520:THR:HG21	1.91	0.52
10:K:5:LEU:HD12	10:K:161:LEU:HD13	1.91	0.52
4:D:72:VAL:HG22	4:D:221:ILE:HD11	1.91	0.51
11:O:1035:ASN:CG	11:O:1274:SER:OG	2.54	0.51
9:J:58:THR:HG21	10:K:122:LEU:HB3	1.92	0.50
9:J:175:ALA:HB2	9:J:183:TRP:CH2	2.47	0.50
2:B:75:TYR:CE2	2:B:79:GLY:HA2	2.47	0.50
4:D:72:VAL:HG23	4:D:221:ILE:HD11	1.93	0.50
11:O:230:ILE:HG13	11:O:1149:ILE:HG22	1.94	0.49
3:C:116:SER:HB2	4:D:83:ARG:NH2	2.28	0.49
10:K:34:LYS:HA	10:K:46:PHE:CZ	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:O:1034:PHE:CB	11:O:1173:HIS:CE1	2.95	0.49
2:B:43:VAL:HG22	2:B:214:ILE:HB	1.94	0.49
5:E:22:PHE:O	5:E:26:TYR:CD2	2.66	0.49
6:F:175:THR:HG22	6:F:178:THR:HB	1.95	0.48
11:O:1009:GLY:HA2	11:O:1200:MET:HE1	1.94	0.48
8:I:35:VAL:O	8:I:41:VAL:HA	2.13	0.48
9:J:98:ARG:HG3	9:J:103:TYR:CE2	2.48	0.48
11:O:1998:LEU:O	11:O:2007:ARG:HD2	2.13	0.48
11:O:1018:VAL:O	11:O:1022:THR:HG23	2.13	0.48
4:D:192:VAL:HG13	4:D:212:ILE:CD1	2.43	0.48
4:D:97:ARG:HG2	4:D:103:PRO:HA	1.95	0.48
7:G:200:ILE:HG21	7:G:214:LEU:HD13	1.96	0.48
9:J:15:MET:HE2	9:J:150:CYS:SG	2.54	0.47
9:J:112:ILE:O	9:J:113:ASN:C	2.57	0.47
10:K:5:LEU:HD13	10:K:6:GLY:H	1.79	0.47
11:O:273:VAL:HG22	11:O:1402:ILE:HG22	1.96	0.47
6:F:213:ILE:HD12	6:F:230:VAL:HG13	1.95	0.47
11:O:1806:THR:HG21	11:O:1889:GLU:HG3	1.97	0.47
5:E:17:PRO:CG	11:O:2115:ALA:HB1	2.45	0.47
6:F:179:PHE:HA	6:F:182:ILE:CD1	2.44	0.47
11:O:1450:LEU:HB2	11:O:1464:ILE:HG21	1.97	0.46
3:C:91:ALA:HB2	3:C:115:LEU:HD11	1.97	0.46
3:C:94:HIS:CD2	3:C:114:ARG:HG2	2.51	0.46
11:O:2003:PHE:HB2	11:O:2006:VAL:HB	1.98	0.46
11:O:920:ILE:HG21	11:O:1022:THR:HG22	1.98	0.45
11:O:1427:ALA:HA	11:O:1430:LYS:HD2	1.99	0.45
8:I:38:ASN:HB2	8:I:174:ASP:HA	1.99	0.45
11:O:904:TYR:CE1	11:O:1018:VAL:HG22	2.52	0.44
11:O:1009:GLY:CA	11:O:1200:MET:HE1	2.47	0.44
11:O:1291:LEU:H	11:O:1291:LEU:HD23	1.82	0.44
1:A:205:PHE:CZ	1:A:209:HIS:HD2	2.36	0.44
2:B:46:ALA:HB1	2:B:196:LEU:HD11	1.99	0.44
4:D:109:LEU:HD13	4:D:109:LEU:O	2.16	0.44
7:G:58:LEU:O	7:G:59:LEU:C	2.60	0.44
11:O:331:TYR:OH	11:O:1518:ASP:CG	2.61	0.44
11:O:1019:MET:HE1	11:O:1182:PHE:CE1	2.52	0.44
1:A:20:SER:O	1:A:21:PRO:C	2.60	0.44
11:O:1749:MET:HG3	11:O:1763:LYS:HB3	1.99	0.44
1:A:225:VAL:HG11	1:A:236:LEU:HD12	2.00	0.43
8:I:88:ILE:HG21	8:I:112:LEU:HG	2.00	0.43
9:J:21:VAL:HG12	9:J:22:ALA:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:O:1016:VAL:HA	11:O:1019:MET:HE3	1.99	0.43
11:O:160:ILE:HD11	11:O:1395:ILE:HG21	2.00	0.43
11:O:904:TYR:CE1	11:O:1018:VAL:CG2	3.02	0.43
7:G:73:HIS:CD2	7:G:109:ILE:HD11	2.53	0.42
1:A:54:ILE:HD12	1:A:225:VAL:HG22	2.01	0.42
7:G:84:ASP:OD1	7:G:84:ASP:N	2.51	0.42
2:B:64:VAL:HG11	2:B:212:ALA:HB3	2.02	0.42
4:D:84:ILE:HG12	12:P:139:HIS:NE2	2.35	0.42
11:O:254:ASP:OD1	11:O:254:ASP:N	2.53	0.42
1:A:137:LEU:HB3	1:A:139:VAL:HG22	2.01	0.42
4:D:30:GLY:HA3	4:D:77:GLY:H	1.84	0.42
7:G:70:VAL:HG23	7:G:74:ILE:HB	2.02	0.42
7:G:95:GLU:OE2	7:G:115:ARG:HD3	2.20	0.42
11:O:230:ILE:CG1	11:O:1149:ILE:HG22	2.49	0.42
11:O:1880:THR:HG23	11:O:1914:LEU:HD11	2.02	0.42
6:F:216:VAL:HG13	6:F:216:VAL:O	2.19	0.42
11:O:520:THR:HG23	11:O:521:PHE:CD1	2.55	0.42
1:A:227:VAL:HB	1:A:234:PHE:CZ	2.55	0.41
3:C:160:TRP:CE2	3:C:163:ILE:HD12	2.55	0.41
9:J:22:ALA:HB2	9:J:163:LEU:CD1	2.50	0.41
11:O:1982:LEU:HD22	11:O:1986:GLU:HB3	2.02	0.41
9:J:46:TYR:HB3	9:J:71:THR:HG21	2.03	0.41
11:O:697:ILE:HG22	11:O:793:ILE:HG21	2.02	0.41
11:O:1994:VAL:HG21	11:O:2017:ILE:HD12	2.03	0.41
1:A:133:TYR:CE2	12:P:94:THR:HG21	2.56	0.41
8:I:35:VAL:HB	8:I:42:VAL:HB	2.03	0.41
1:A:155:TYR:CD1	1:A:165:GLY:HA2	2.56	0.41
1:A:194:ILE:HD11	1:A:202:VAL:HG13	2.02	0.41
1:A:194:ILE:HD13	1:A:205:PHE:CD1	2.56	0.41
11:O:2004:VAL:HG13	11:O:2007:ARG:NH2	2.37	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	242/252 (96%)	234 (97%)	8 (3%)	0	100	100
2	B	244/250 (98%)	237 (97%)	7 (3%)	0	100	100
3	C	237/258 (92%)	227 (96%)	10 (4%)	0	100	100
4	D	247/254 (97%)	238 (96%)	9 (4%)	0	100	100
5	E	242/260 (93%)	233 (96%)	9 (4%)	0	100	100
6	F	232/234 (99%)	219 (94%)	13 (6%)	0	100	100
7	G	245/288 (85%)	232 (95%)	13 (5%)	0	100	100
8	I	204/261 (78%)	199 (98%)	5 (2%)	0	100	100
9	J	182/205 (89%)	173 (95%)	9 (5%)	0	100	100
10	K	180/198 (91%)	168 (93%)	12 (7%)	0	100	100
11	O	1913/2143 (89%)	1845 (96%)	68 (4%)	0	100	100
12	P	86/200 (43%)	80 (93%)	6 (7%)	0	100	100
All	All	4254/4803 (89%)	4085 (96%)	169 (4%)	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	206/210 (98%)	199 (97%)	7 (3%)	32	57
2	B	205/209 (98%)	201 (98%)	4 (2%)	48	72
3	C	198/216 (92%)	195 (98%)	3 (2%)	57	77
4	D	221/226 (98%)	216 (98%)	5 (2%)	44	68
5	E	202/215 (94%)	201 (100%)	1 (0%)	81	90
6	F	193/193 (100%)	189 (98%)	4 (2%)	47	70
7	G	203/239 (85%)	196 (97%)	7 (3%)	32	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	170/214 (79%)	168 (99%)	2 (1%)	63	80
9	J	156/173 (90%)	155 (99%)	1 (1%)	78	89
10	K	163/175 (93%)	156 (96%)	7 (4%)	26	50
11	O	1760/1963 (90%)	1740 (99%)	20 (1%)	65	81
12	P	85/180 (47%)	84 (99%)	1 (1%)	63	80
All	All	3762/4213 (89%)	3700 (98%)	62 (2%)	54	76

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	THR
1	A	84	ASN
1	A	128	TYR
1	A	169	THR
1	A	207	ILE
1	A	209	HIS
1	A	223	LEU
2	B	86	VAL
2	B	95	THR
2	B	107	THR
2	B	127	VAL
3	C	87	LEU
3	C	113	ARG
3	C	186	VAL
4	D	36	VAL
4	D	84	ILE
4	D	109	LEU
4	D	202	VAL
4	D	221	ILE
5	E	133	LEU
6	F	35	THR
6	F	74	LEU
6	F	176	LEU
6	F	220	THR
7	G	57	LYS
7	G	70	VAL
7	G	84	ASP
7	G	89	VAL
7	G	137	ILE
7	G	200	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	235	LEU
8	I	70	ILE
8	I	139	LEU
9	J	124	PHE
10	K	4	ILE
10	K	5	LEU
10	K	7	ILE
10	K	35	THR
10	K	60	ILE
10	K	92	ILE
10	K	119	ILE
11	O	85	ARG
11	O	111	TRP
11	O	238	VAL
11	O	254	ASP
11	O	425	ASP
11	O	518	ILE
11	O	605	LEU
11	O	889	LEU
11	O	926	THR
11	O	1148	ASP
11	O	1244	ASN
11	O	1266	LEU
11	O	1344	LEU
11	O	1474	ASN
11	O	1553	GLU
11	O	1693	LEU
11	O	1710	TYR
11	O	1979	LEU
11	O	1980	LEU
11	O	2116	ASP
12	P	94	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	GLN
1	A	176	GLN
1	A	193	HIS
1	A	209	HIS
2	B	20	GLN
2	B	180	ASN

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Continued from previous page...

Mol	Chain	Res	Type
3	C	94	HIS
3	C	96	GLN
3	C	97	ASN
3	C	147	GLN
4	D	79	ASN
6	F	91	GLN
6	F	185	ASN
7	G	12	ASN
7	G	21	ASN
7	G	183	HIS
7	G	195	GLN
8	I	122	HIS
8	I	201	ASN
9	J	72	ASN
10	K	65	GLN
10	K	86	GLN
10	K	101	ASN
10	K	112	ASN
10	K	118	GLN
10	K	133	HIS
11	O	100	HIS
11	O	314	GLN
11	O	473	ASN
11	O	484	GLN
11	O	546	HIS
11	O	571	HIS
11	O	683	ASN
11	O	795	ASN
11	O	994	ASN
11	O	1181	HIS
11	O	1226	ASN
11	O	1242	HIS
11	O	1270	ASN
11	O	1338	GLN
11	O	1420	GLN
11	O	1532	ASN
11	O	1594	ASN
11	O	1870	GLN
11	O	1981	GLN
11	O	2088	ASN
12	P	92	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

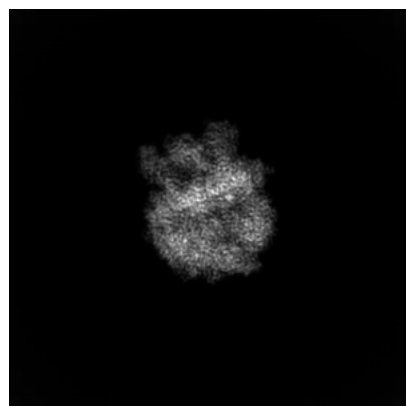
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46461. These allow visual inspection of the internal detail of the map and identification of artifacts.

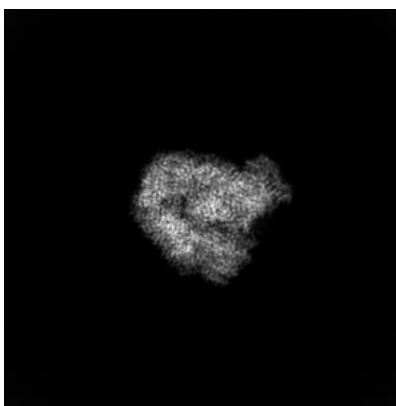
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

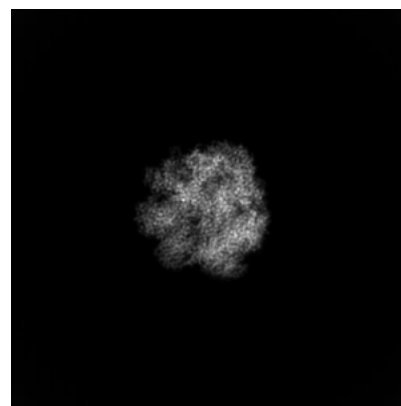
6.1.1 Primary map



X

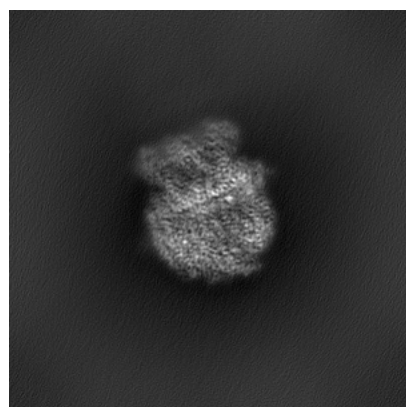


Y

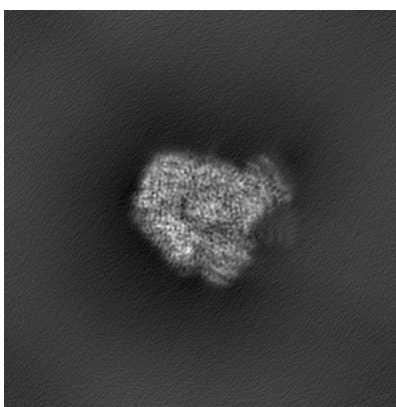


Z

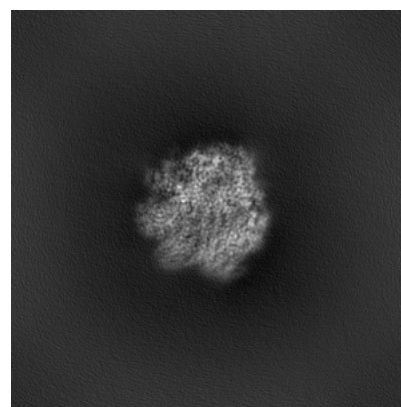
6.1.2 Raw map



X



Y

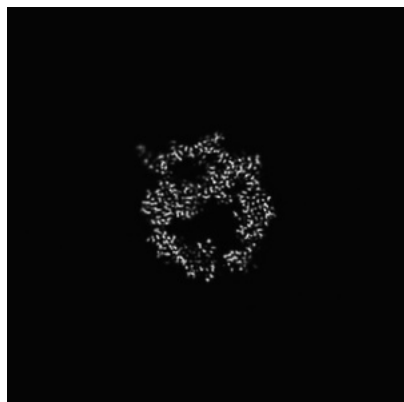


Z

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

6.2 Central slices [i](#)

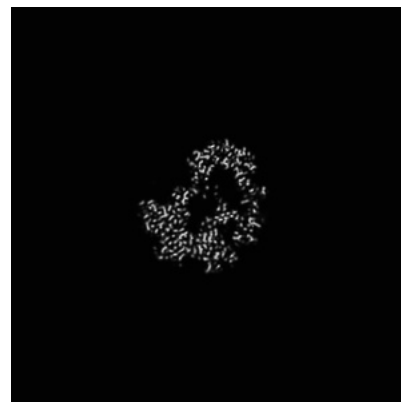
6.2.1 Primary map



X Index: 170

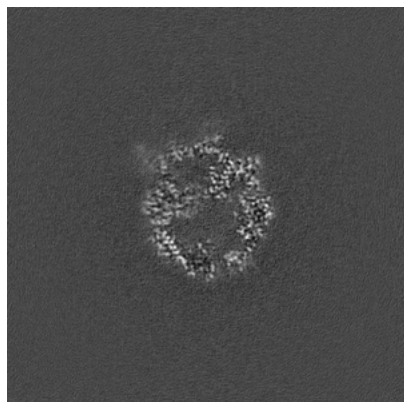


Y Index: 170

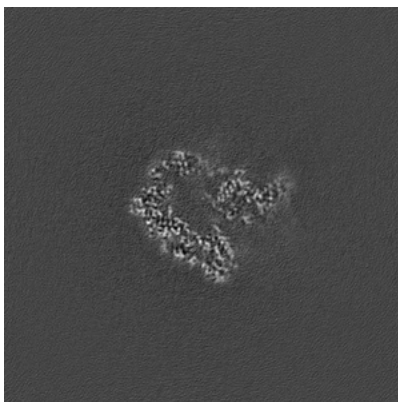


Z Index: 170

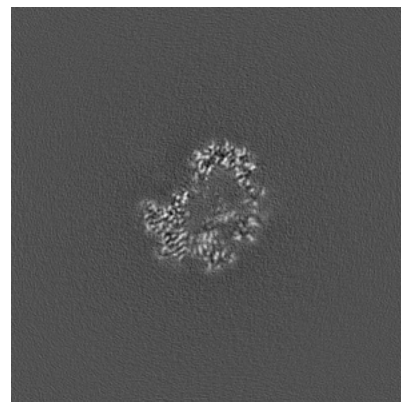
6.2.2 Raw map



X Index: 170



Y Index: 170

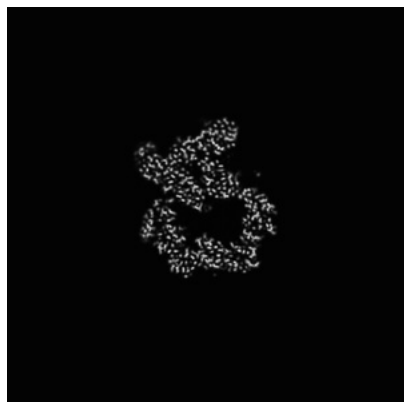


Z Index: 170

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

6.3 Largest variance slices [i](#)

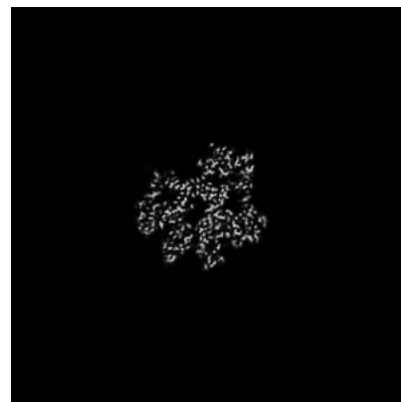
6.3.1 Primary map



X Index: 183

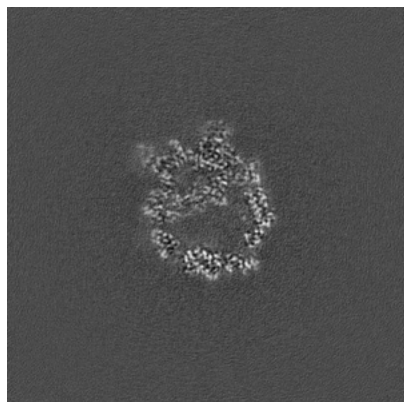


Y Index: 175

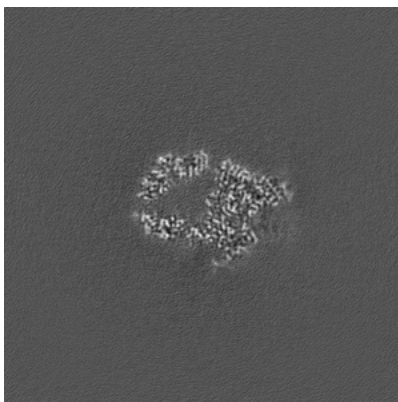


Z Index: 178

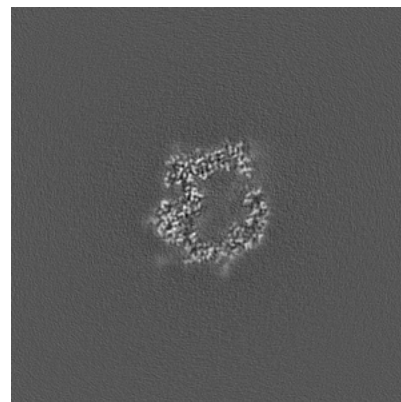
6.3.2 Raw map



X Index: 175



Y Index: 182

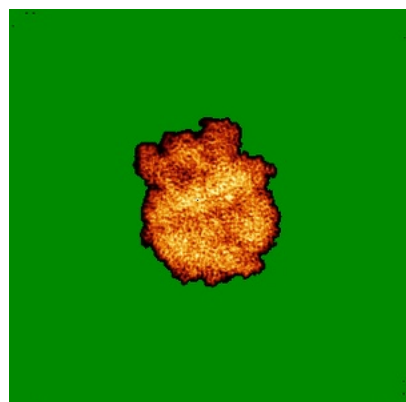


Z Index: 147

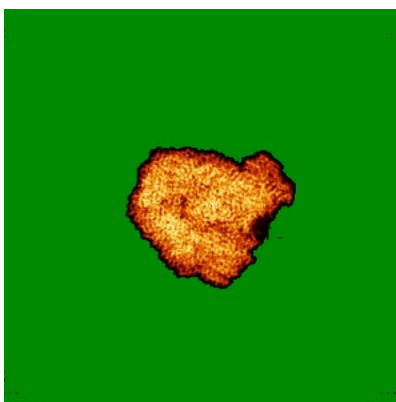
The images above show the largest variance slices of the map in three orthogonal directions.

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

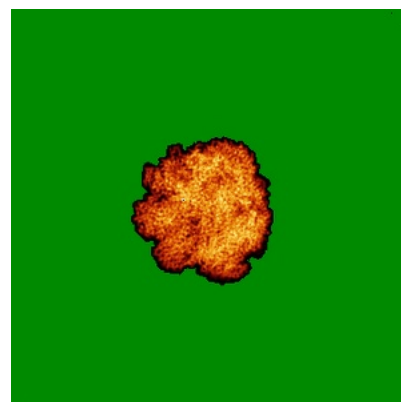
6.4.1 Primary map



X

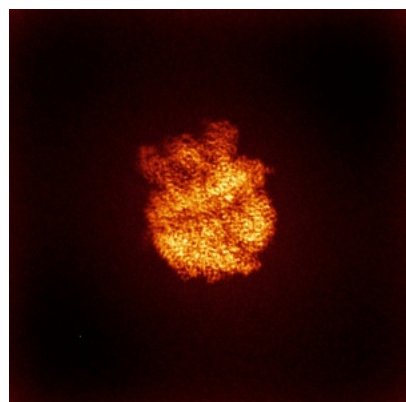


Y

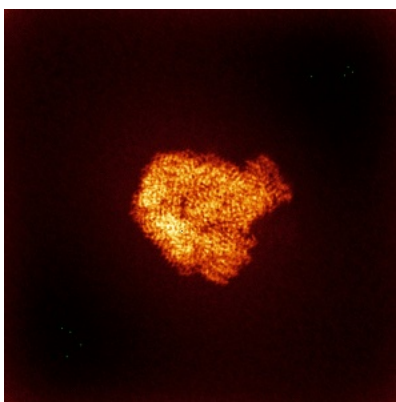


Z

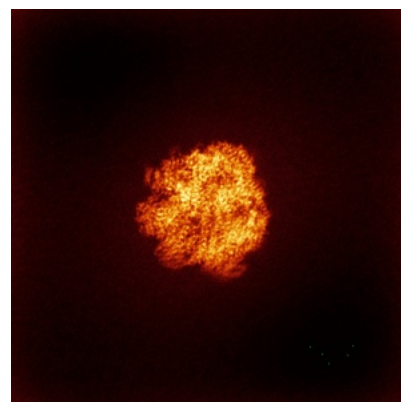
6.4.2 Raw map



X



Y

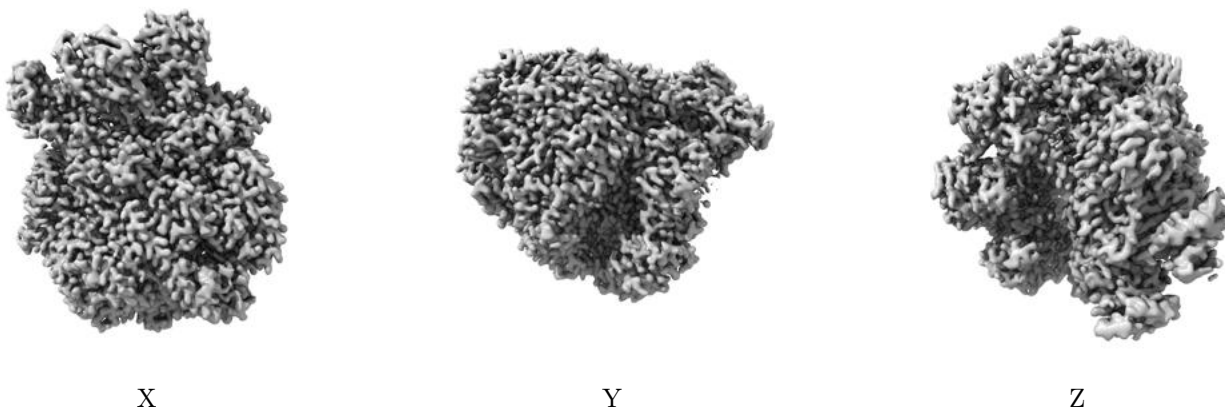


Z

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.

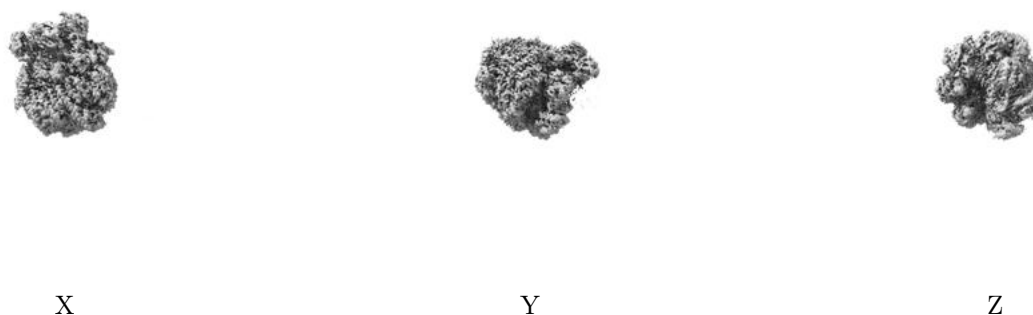
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

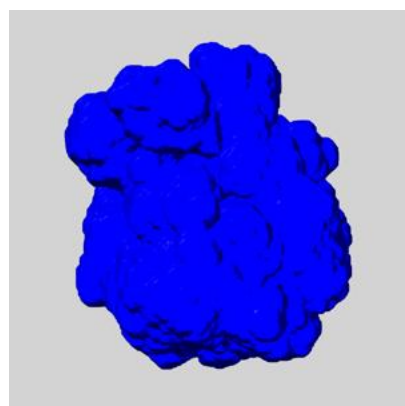
6.6 Mask visualisation [i](#)

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

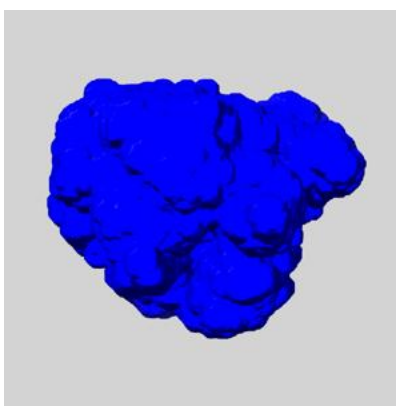
A mask typically either:

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

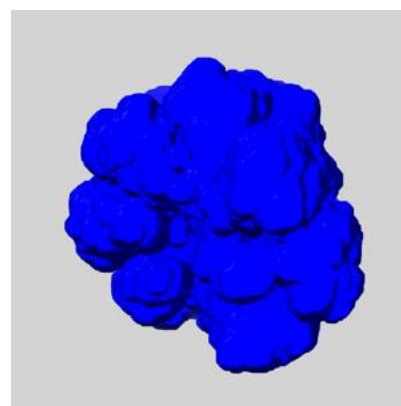
6.6.1 emd_46461_msk_1.map [i](#)



X



Y

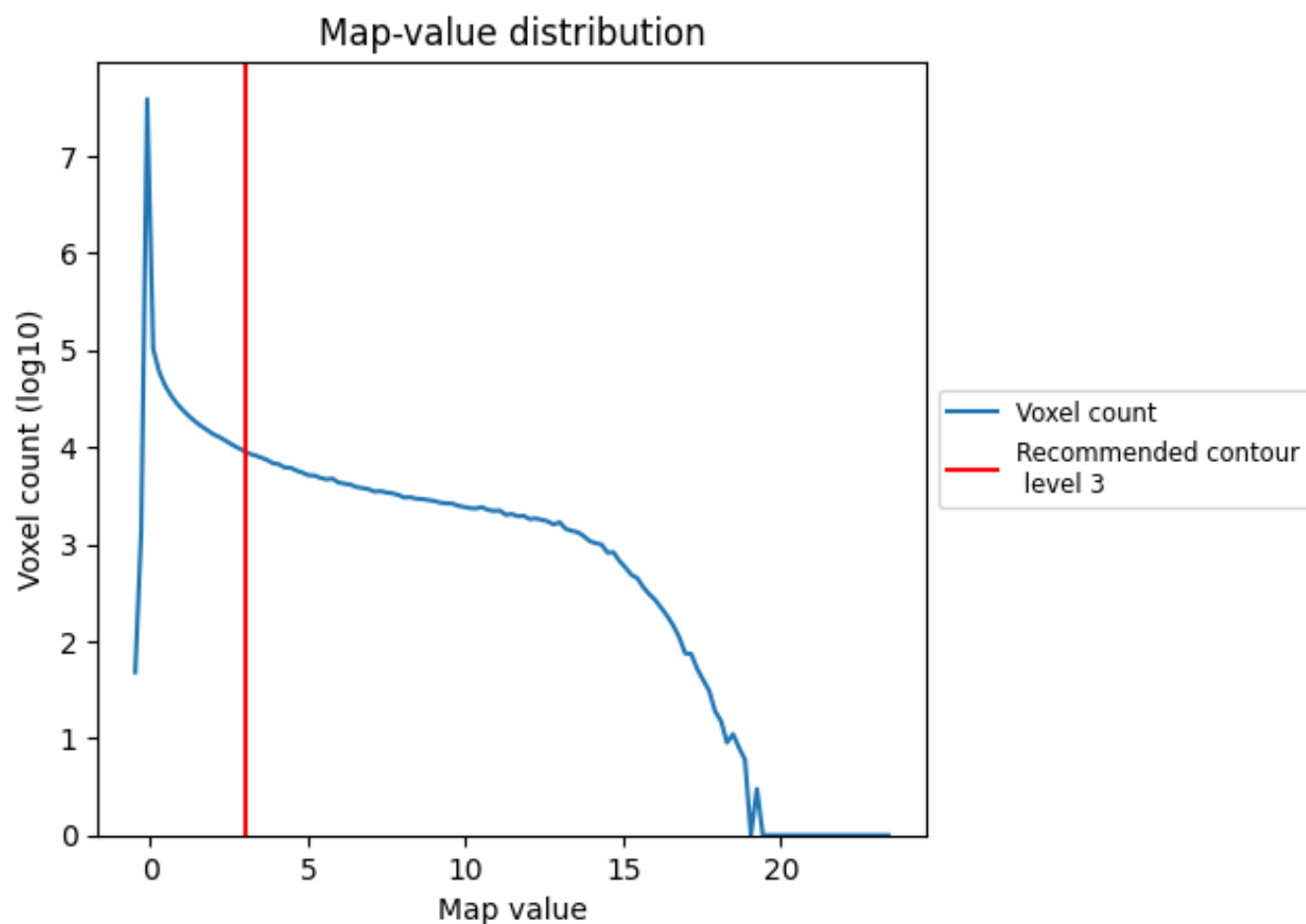


Z

7 Map analysis [i](#)

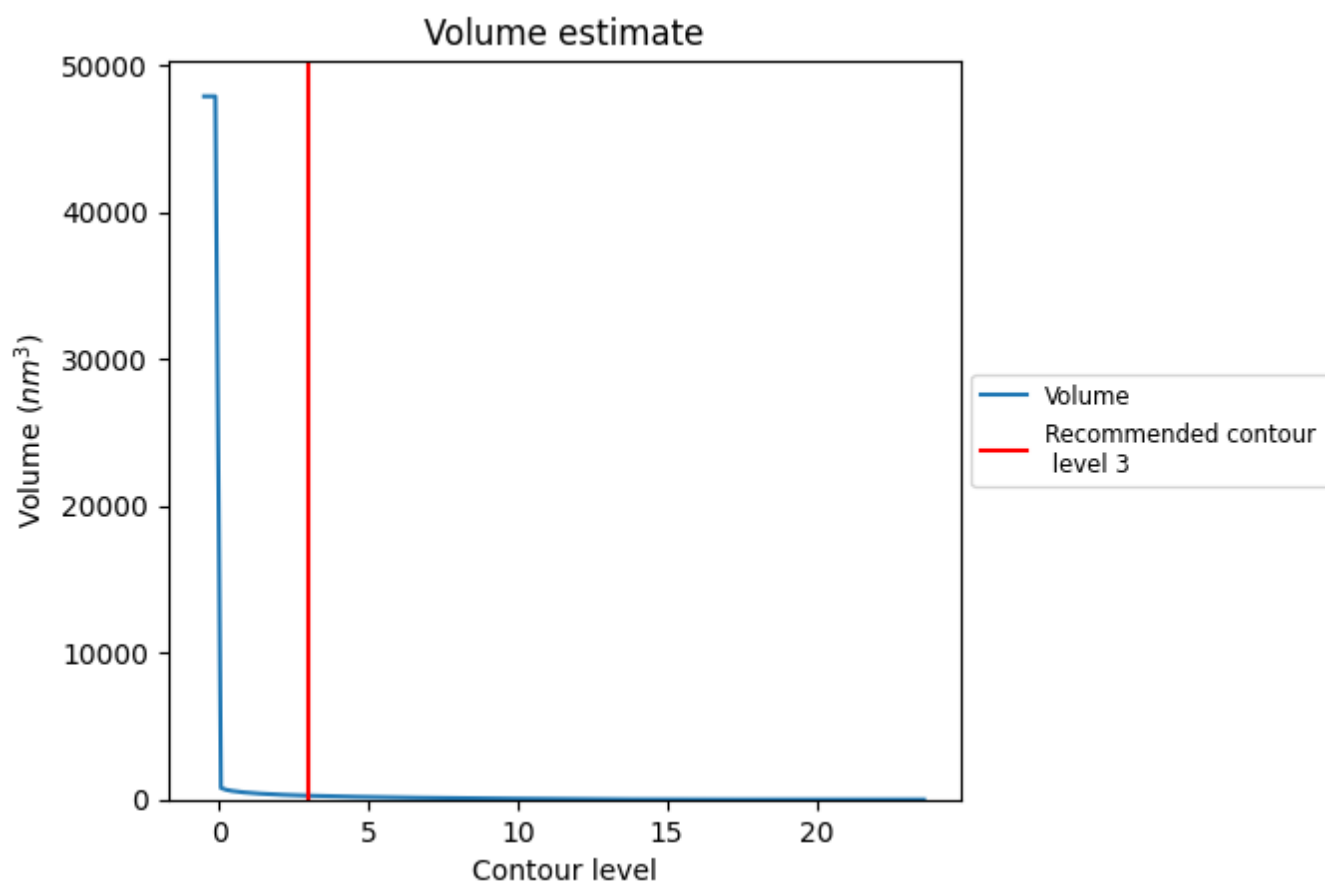
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

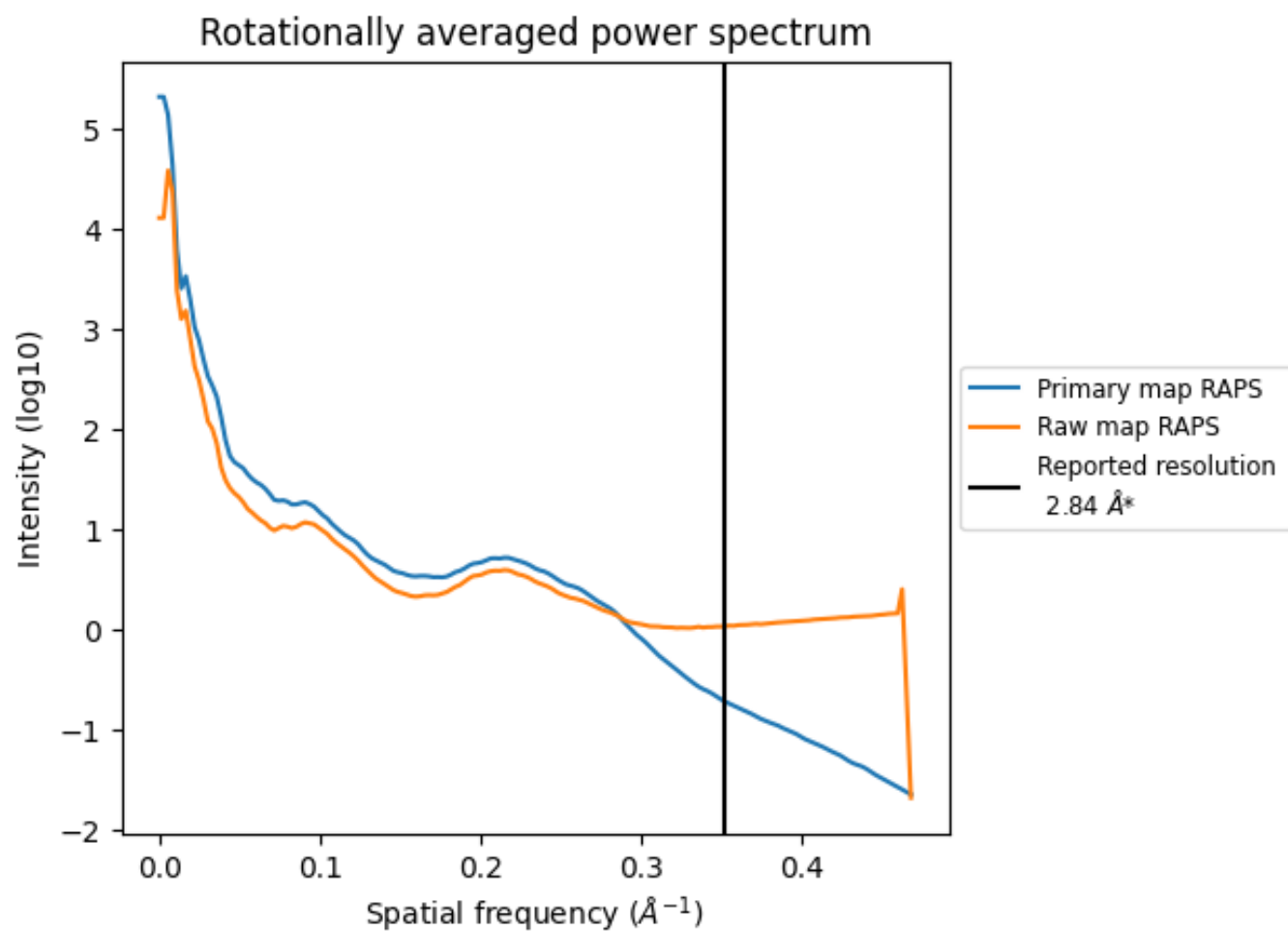
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 264 nm³; this corresponds to an approximate mass of 239 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 ⓘ

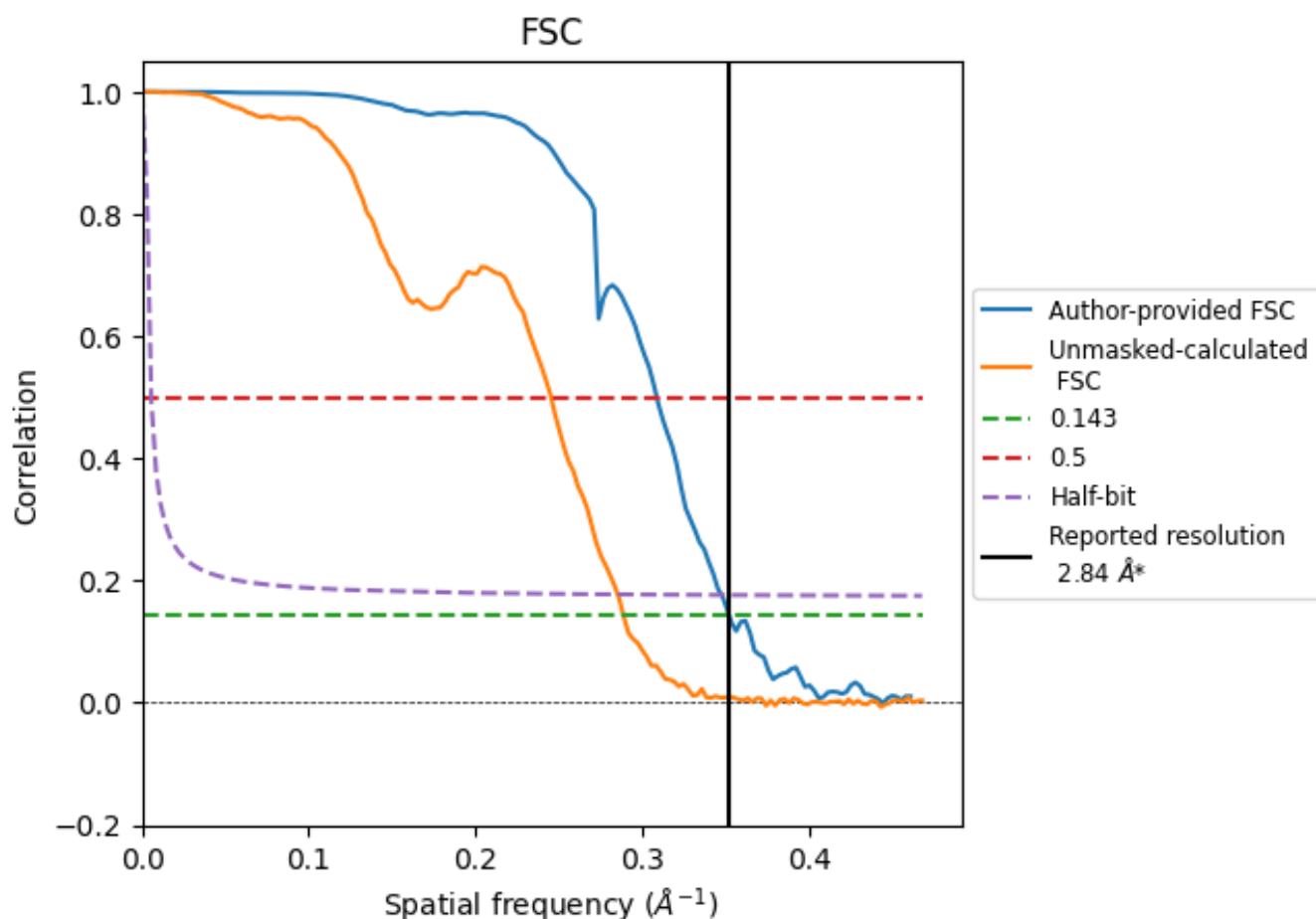


*Reported resolution corresponds to spatial frequency of $0.352 \text{ \AA}^{-1}$

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 $0.352 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

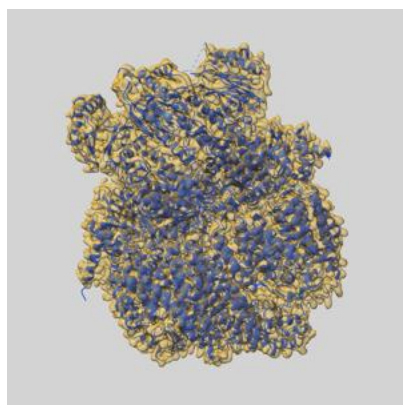
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	2.84	3.24	2.88
Unmasked-calculated*	3.46	4.07	3.50

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.46 differs from the reported value 2.84 by more than 10 %

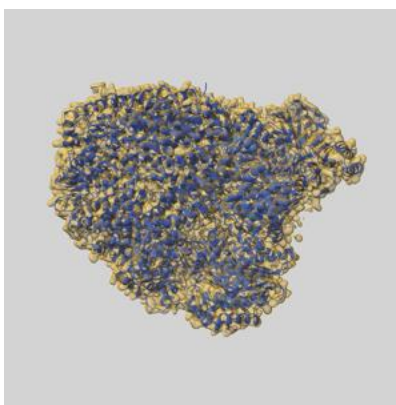
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-46461 and PDB model 9D0T. Per-residue inclusion information can be found in section [3](#) on page [7](#).

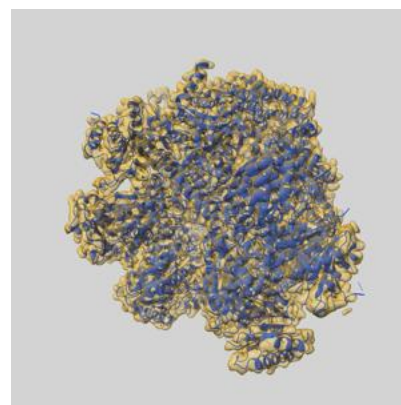
9.1 Map-model overlay [i](#)



X



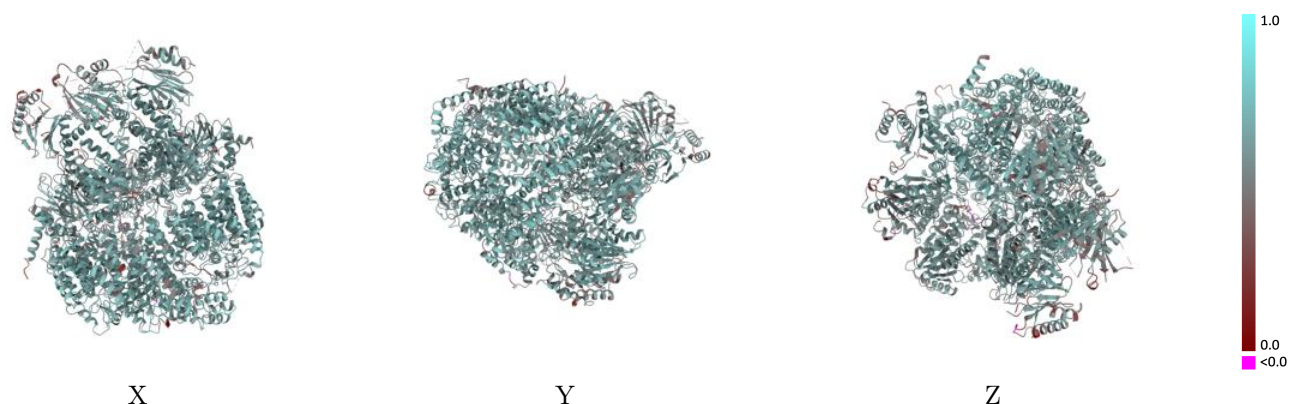
Y



Z

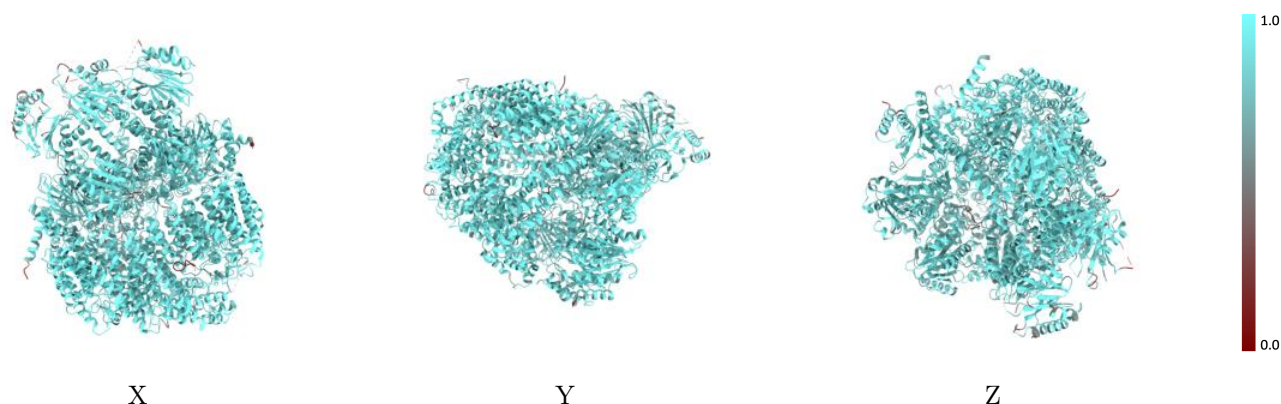
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



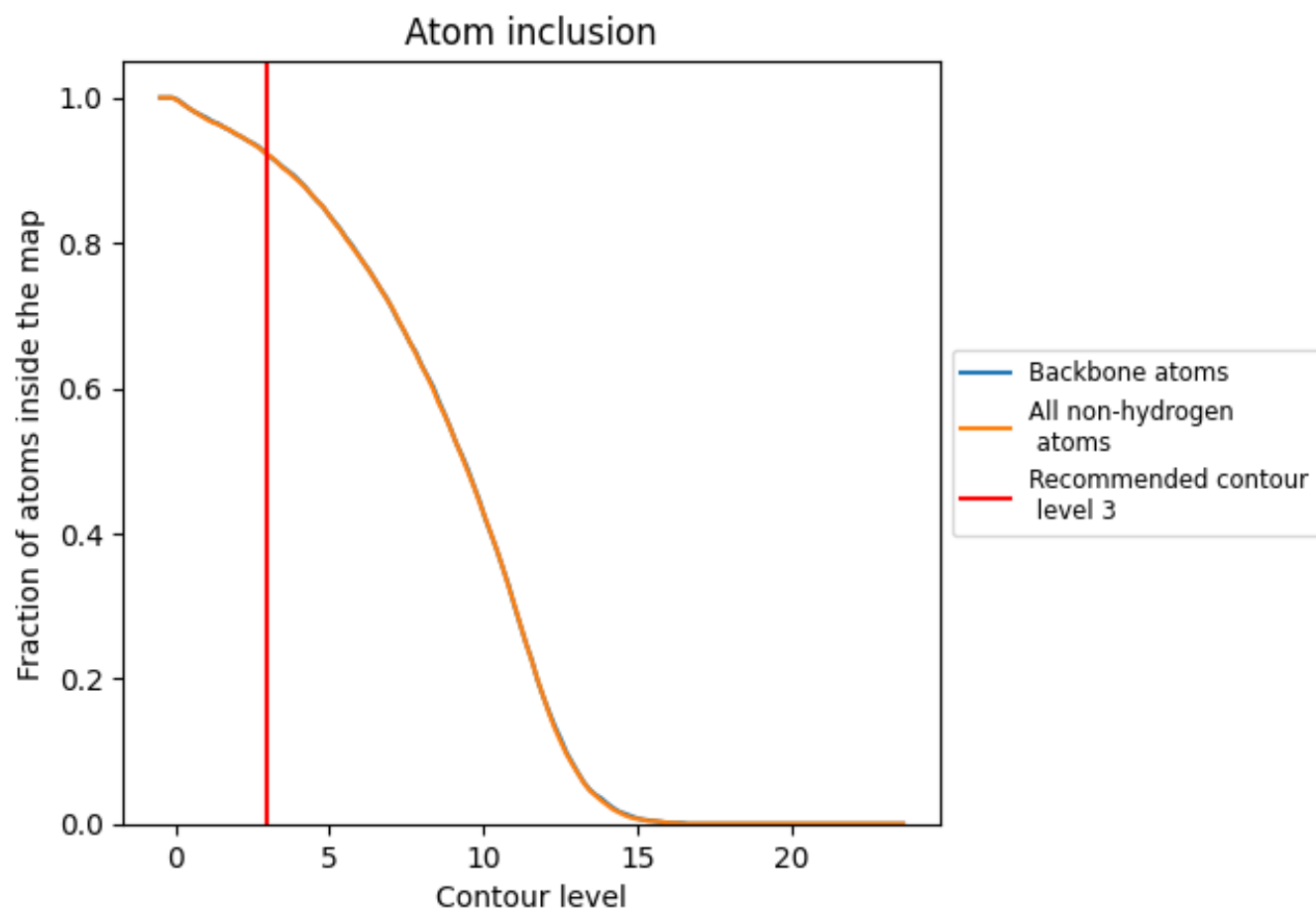
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9210	0.5920
A	0.9360	0.5950
B	0.9360	0.6010
C	0.9190	0.5830
D	0.8710	0.5560
E	0.8970	0.5530
F	0.9310	0.5650
G	0.9160	0.5820
I	0.9130	0.5650
J	0.8890	0.5490
K	0.8570	0.5270
O	0.9480	0.6190
P	0.9250	0.5970

