Full wwPDB EM Validation Report (i)

Aug 26, 2026 – 07:23 pm BST

PDB ID	:	6TEH / pdb_00006teh
EMDB ID	:	EMD-10490
Title	:	Baseplate of native GTA particle computed with C3 symmetry
Authors	:	Bardy, P.; Fuzik, T.; Hrebik, D.; Pantucek, R.; Beatty, J.T.; Plevka, P.
Deposited on	:	2019-11-12
Resolution	:	3.99 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

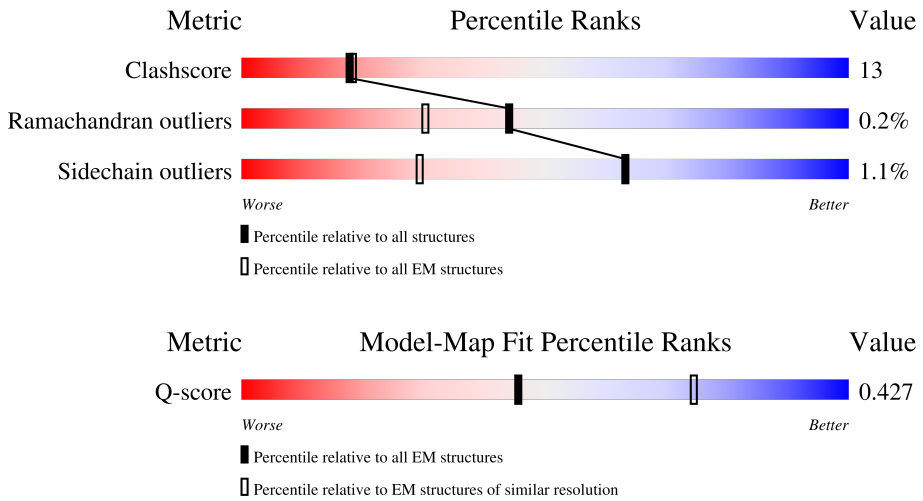
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.99 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	7463 (3.49 - 4.49)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	296	75% 23%
2	D	1304	26% 8% 66%
3	A	210	7% 42% 21% 36%
3	B	210	5% 43% 20% 36%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7545 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 Putative gene transfer agent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C	292	2179	1369	395	408	7	0	0

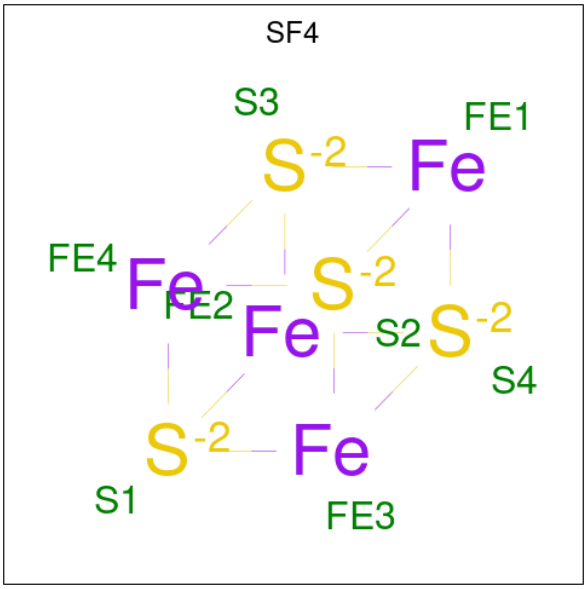
- Molecule 2 is a protein called Putative gene transfer agent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	439	3246	2028	590	621	7	0	0

- Molecule 3 is a protein called Putative gene transfer agent protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	B	134	1056	665	198	193	0	0
3	A	134	1056	665	198	193	0	0

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



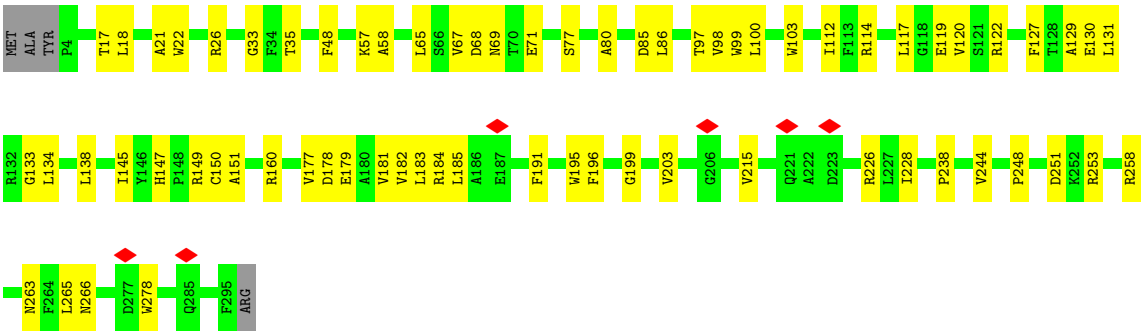
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
4	C	1	8	4	4	0

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.

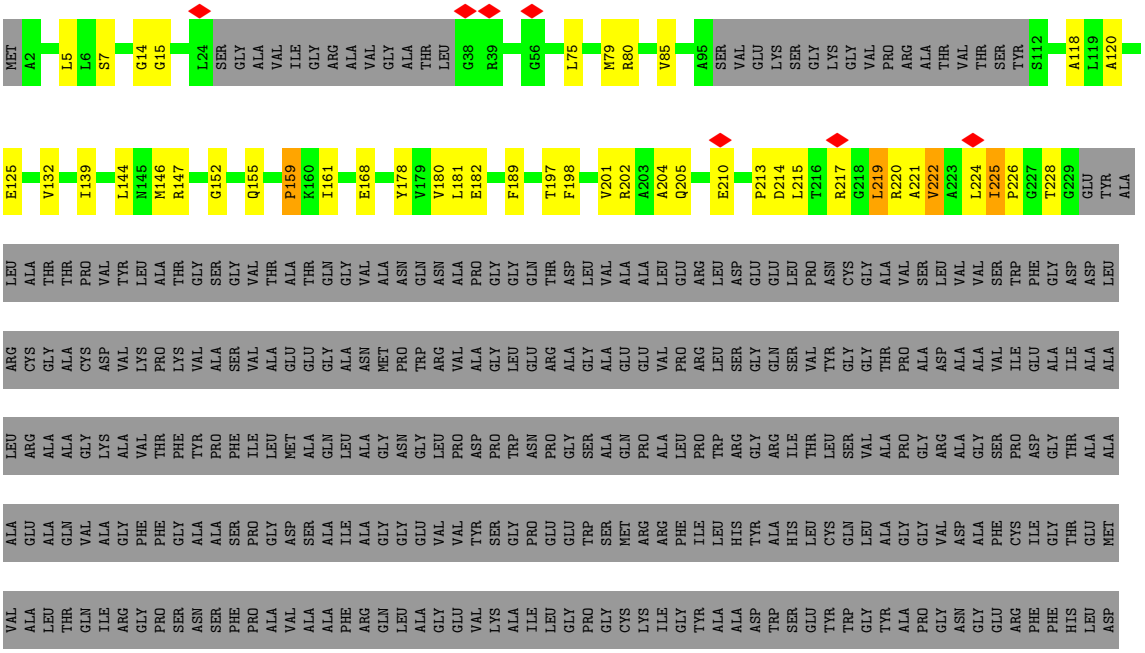
- Molecule 1: Putative gene transfer agent protein

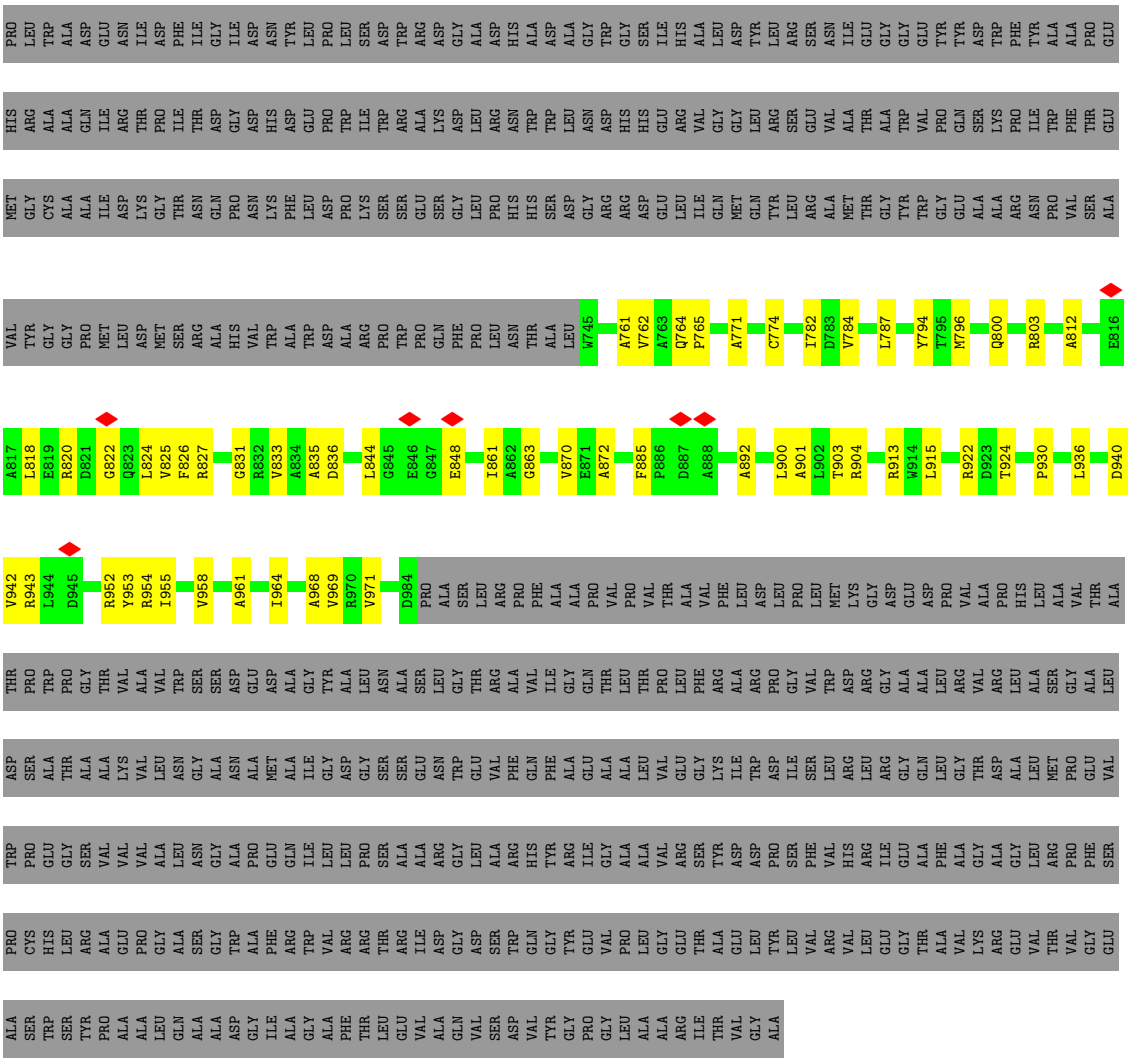
Chain C:



- Molecule 2: Putative gene transfer agent protein

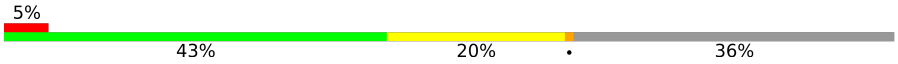
Chain D:

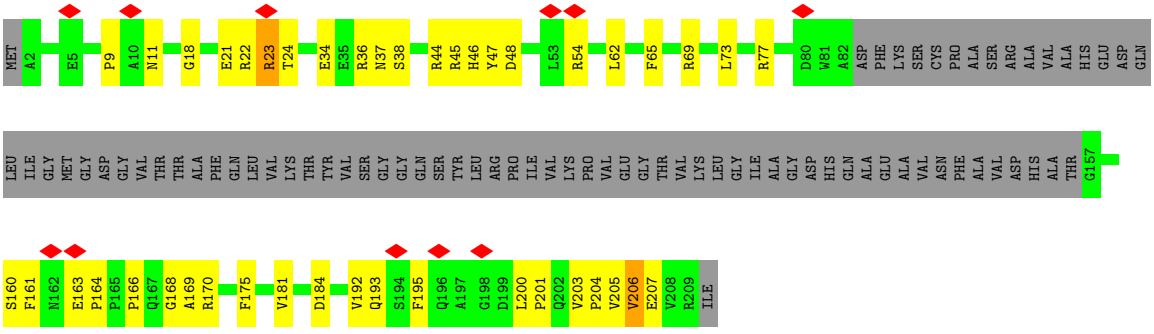




• Molecule 3: Putative gene transfer agent protein

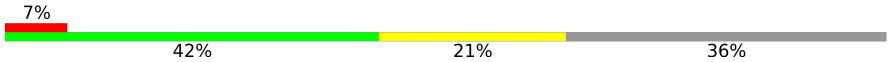
Chain B:

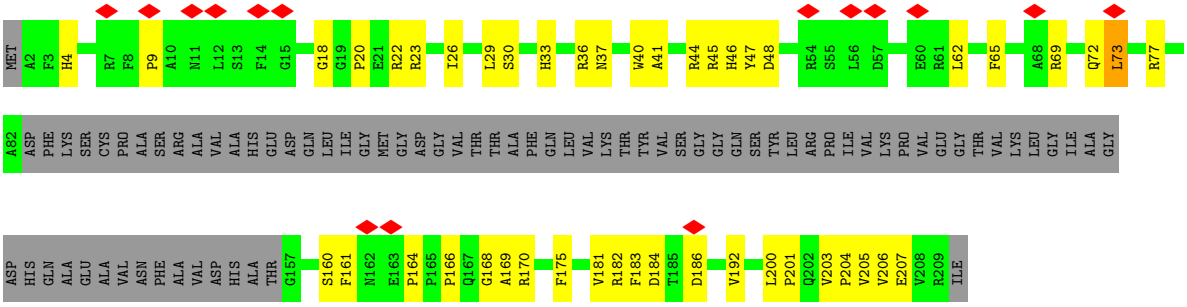




• Molecule 3: Putative gene transfer agent protein

Chain A:




MET A2 F3 H4 R7 F8 P9 A10 N11 L12 S13 F14 G15 G18 G19 P20 E21 R22 R23 I26 L29 S30 H33 R36 N37 W40 A41 R44 R45 H46 Y47 D48 R54 S55 L56 D57 E60 R61 L62 F65 A68 R69 Q72 L73 R77
A82 ASP PHE LYS SER CYS PRO ALA SER ARG ALA VAL ALA HIS GLU ASP GLN LEU ILE GLY MET GLY ASP GLY VAL THR THR ALA PHE GLN LEU VAL LYS THR TYR VAL SER GLY GLY GLN SER TYR LEU ARG PRO ILE VAL LYS PRO VAL GLU GLY THR VAL LYS LEU GLY ILE ALA GLY
ASP HIS GLN ALA GLU ALA VAL ASN PHE ALA VAL ASP HIS ALA THR G157 S160 F161 N162 E163 P164 P165 P166 Q167 G168 A169 R170 F175 V181 R182 F183 D184 T185 D186 V192 L200 P201 Q202 V203 P204 V205 V206 E207 V208 R209 ILE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	42242	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	42.75	Depositor
Minimum defocus (nm)	-1000	Depositor
Maximum defocus (nm)	-3000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.205	Depositor
Minimum map value	-0.058	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0268	Depositor
Map size (Å)	318.9, 318.9, 318.9	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.063, 1.063, 1.063	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4

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	C	0.51	0/2222	0.83	0/3010
2	D	0.51	0/3292	0.79	4/4459 (0.1%)
3	A	0.27	0/1085	0.58	0/1472
3	B	0.27	0/1085	0.58	0/1472
All	All	0.46	0/7684	0.75	4/10413 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	225	ILE	CA-C-N	5.79	125.47	119.05
2	D	225	ILE	C-N-CA	5.79	125.47	119.05
2	D	159	PRO	CA-C-N	5.16	131.40	121.54
2	D	159	PRO	C-N-CA	5.16	131.40	121.54

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	C	2179	0	2125	57	0
2	D	3246	0	3223	85	0
3	A	1056	0	1000	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1056	0	1000	39	0
4	C	8	0	0	0	0
All	All	7545	0	7348	199	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 13.

All (199) 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)
2:D:219:LEU:HD11	2:D:222:VAL:HB	1.62	0.81
1:C:65:LEU:HD13	2:D:803:ARG:HB2	1.63	0.78
1:C:178:ASP:HB3	1:C:182:VAL:HG23	1.63	0.78
2:D:784:VAL:HG13	2:D:787:LEU:HD12	1.67	0.76
3:B:163:GLU:HG2	3:A:69:ARG:HH12	1.50	0.76
1:C:134:LEU:CD2	2:D:824:LEU:HB2	2.16	0.76
3:A:181:VAL:HA	3:A:207:GLU:HA	1.70	0.73
2:D:5:LEU:HG	2:D:7:SER:H	1.55	0.72
3:A:9:PRO:HG2	3:A:62:LEU:HD23	1.71	0.72
2:D:774:CYS:HB2	2:D:782:ILE:HD12	1.72	0.71
1:C:134:LEU:HD23	2:D:824:LEU:HB2	1.72	0.71
1:C:150:CYS:SG	1:C:151:ALA:N	2.64	0.70
1:C:67:VAL:HB	1:C:133:GLY:H	1.56	0.69
1:C:100:LEU:O	1:C:100:LEU:HD23	1.94	0.68
3:A:184:ASP:OD2	3:A:206:VAL:HG13	1.93	0.67
2:D:214:ASP:CG	2:D:765:PRO:HG3	2.19	0.67
2:D:774:CYS:SG	2:D:782:ILE:HD12	2.35	0.67
3:B:9:PRO:HG2	3:B:62:LEU:HD23	1.76	0.67
1:C:100:LEU:HB2	1:C:112:ILE:HD11	1.78	0.66
3:B:181:VAL:HA	3:B:207:GLU:HA	1.77	0.65
3:B:21:GLU:HG2	3:B:44:ARG:HB2	1.77	0.65
1:C:195:TRP:HD1	1:C:196:PHE:HD1	1.43	0.65
2:D:774:CYS:CB	2:D:782:ILE:HD12	2.26	0.65
3:A:184:ASP:HB2	3:A:204:PRO:HG2	1.78	0.64
1:C:196:PHE:HB3	1:C:248:PRO:HA	1.81	0.62
3:B:34:GLU:OE2	3:A:182:ARG:NH2	2.31	0.62
1:C:178:ASP:HB3	1:C:182:VAL:CG2	2.29	0.62
3:B:184:ASP:HB2	3:B:204:PRO:HG2	1.82	0.62
2:D:132:VAL:HG22	2:D:198:PHE:CD1	2.35	0.61
1:C:258:ARG:NH1	2:D:168:GLU:O	2.33	0.61
1:C:251:ASP:OD2	1:C:253:ARG:NH1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:784:VAL:HG12	2:D:784:VAL:O	2.00	0.60
2:D:955:ILE:HA	2:D:968:ALA:HA	1.83	0.60
3:B:184:ASP:N	3:B:204:PRO:O	2.29	0.60
2:D:784:VAL:HG22	2:D:826:PHE:HB2	1.84	0.59
2:D:954:ARG:HE	2:D:971:VAL:HG21	1.67	0.58
2:D:848:GLU:HG3	2:D:848:GLU:O	2.03	0.58
3:A:164:PRO:HB2	3:A:166:PRO:HD2	1.85	0.58
2:D:771:ALA:HA	2:D:782:ILE:HD13	1.86	0.57
3:B:18:GLY:HA3	3:B:47:TYR:HA	1.86	0.57
2:D:820:ARG:NH2	2:D:940:ASP:OD1	2.37	0.57
1:C:18:LEU:O	3:A:37:ASN:ND2	2.24	0.57
3:B:48:ASP:HA	3:B:204:PRO:HA	1.85	0.57
1:C:114:ARG:HD3	2:D:822:GLY:HA3	1.87	0.57
3:B:181:VAL:HB	3:B:205:VAL:HB	1.86	0.57
3:B:168:GLY:O	3:B:170:ARG:NH2	2.38	0.57
3:B:164:PRO:HB2	3:B:166:PRO:HD2	1.85	0.57
2:D:120:ALA:HA	2:D:178:TYR:HA	1.87	0.56
3:B:46:HIS:HA	3:B:206:VAL:HA	1.87	0.56
2:D:796:MET:HE3	2:D:800:GLN:HB3	1.88	0.56
2:D:139:ILE:HD12	2:D:144:LEU:HD21	1.86	0.56
2:D:125:GLU:HG2	2:D:152:GLY:HA2	1.87	0.56
2:D:818:LEU:HD22	2:D:820:ARG:HG3	1.88	0.55
1:C:26:ARG:NH2	1:C:85:ASP:OD2	2.40	0.55
3:B:23:ARG:HH11	3:B:23:ARG:HA	1.70	0.55
1:C:97:THR:HG22	1:C:114:ARG:HG2	1.87	0.55
3:B:36:ARG:HE	3:A:73:LEU:HA	1.72	0.55
3:B:193:GLN:HA	3:B:193:GLN:OE1	2.07	0.55
3:A:26:ILE:HD13	3:A:36:ARG:HB3	1.88	0.54
3:A:168:GLY:O	3:A:170:ARG:NH2	2.40	0.54
3:B:184:ASP:OD2	3:B:206:VAL:HG13	2.07	0.54
2:D:215:LEU:HD22	2:D:761:ALA:O	2.08	0.54
2:D:836:ASP:HA	2:D:943:ARG:HB3	1.89	0.54
3:B:161:PHE:HD2	3:B:168:GLY:HA3	1.73	0.54
1:C:17:THR:OG1	1:C:103:TRP:NE1	2.42	0.53
2:D:835:ALA:HB2	2:D:936:LEU:HD11	1.90	0.53
1:C:97:THR:OG1	1:C:99:TRP:NE1	2.41	0.53
1:C:134:LEU:HD21	2:D:824:LEU:HB2	1.91	0.53
2:D:924:THR:HG22	2:D:969:VAL:HG23	1.91	0.53
3:A:77:ARG:HH22	3:A:175:PHE:H	1.57	0.53
3:B:77:ARG:HH22	3:B:175:PHE:H	1.58	0.52
2:D:220:ARG:O	2:D:220:ARG:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:18:GLY:HA3	3:A:47:TYR:HA	1.92	0.52
1:C:122:ARG:HA	1:C:127:PHE:HA	1.91	0.52
1:C:77:SER:H	1:C:80:ALA:HB3	1.74	0.52
1:C:138:LEU:HB3	2:D:803:ARG:HB3	1.92	0.52
1:C:147:HIS:NE2	1:C:150:CYS:O	2.40	0.52
2:D:794:TYR:HD1	2:D:900:LEU:HB3	1.75	0.52
2:D:215:LEU:HD13	2:D:761:ALA:HA	1.92	0.52
2:D:833:VAL:HG11	2:D:943:ARG:HB2	1.92	0.51
3:A:45:ARG:H	3:A:207:GLU:HG2	1.75	0.51
2:D:844:LEU:HB2	3:A:30:SER:HB3	1.92	0.51
1:C:199:GLY:H	1:C:215:VAL:HG12	1.76	0.51
3:B:206:VAL:O	3:B:207:GLU:HG3	2.09	0.51
2:D:118:ALA:HA	2:D:180:VAL:HA	1.91	0.51
2:D:861:ILE:HG22	2:D:922:ARG:HD3	1.93	0.51
1:C:65:LEU:HB2	2:D:803:ARG:NH2	2.26	0.51
1:C:183:LEU:HD22	1:C:228:ILE:HD11	1.93	0.51
2:D:146:MET:HB3	2:D:181:LEU:HD23	1.93	0.51
1:C:160:ARG:O	1:C:263:ASN:ND2	2.44	0.51
3:B:46:HIS:ND1	3:B:206:VAL:HG12	2.26	0.51
1:C:65:LEU:CD1	2:D:803:ARG:HB2	2.38	0.51
2:D:812:ALA:O	2:D:913:ARG:NH1	2.44	0.50
3:B:45:ARG:HB2	3:B:207:GLU:HG2	1.93	0.50
2:D:818:LEU:HB3	2:D:825:VAL:HG13	1.93	0.50
3:A:46:HIS:ND1	3:A:206:VAL:HG12	2.26	0.50
2:D:219:LEU:CD1	2:D:222:VAL:HB	2.40	0.50
2:D:848:GLU:O	2:D:848:GLU:CG	2.60	0.50
3:A:161:PHE:HD2	3:A:168:GLY:HA3	1.77	0.49
1:C:184:ARG:O	1:C:185:LEU:HB3	2.12	0.49
2:D:147:ARG:NH2	2:D:159:PRO:O	2.45	0.49
3:A:184:ASP:N	3:A:204:PRO:O	2.37	0.49
1:C:86:LEU:HD11	1:C:120:VAL:HG21	1.94	0.49
3:B:22:ARG:O	3:B:24:THR:HG22	2.13	0.49
3:A:206:VAL:O	3:A:207:GLU:HG3	2.13	0.49
2:D:903:THR:OG1	2:D:904:ARG:N	2.46	0.49
1:C:119:GLU:O	1:C:130:GLU:N	2.45	0.48
2:D:125:GLU:O	2:D:205:GLN:NE2	2.45	0.48
3:B:65:PHE:HA	3:B:69:ARG:HH21	1.78	0.48
1:C:120:VAL:HA	1:C:129:ALA:HA	1.95	0.48
1:C:22:TRP:HB3	1:C:98:VAL:HA	1.95	0.48
2:D:872:ALA:HB2	2:D:901:ALA:HB1	1.96	0.48
2:D:831:GLY:O	2:D:952:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:TRP:CH2	3:A:41:ALA:HB2	2.50	0.47
1:C:117:LEU:HD23	1:C:117:LEU:O	2.15	0.47
2:D:75:LEU:HD12	2:D:79:MET:HB3	1.96	0.47
2:D:787:LEU:HD23	2:D:787:LEU:HA	1.74	0.47
2:D:930:PRO:HG3	3:A:29:LEU:HD12	1.96	0.46
1:C:195:TRP:HD1	1:C:196:PHE:CD1	2.30	0.46
1:C:265:LEU:HB3	2:D:155:GLN:CD	2.40	0.46
2:D:784:VAL:CG1	2:D:787:LEU:HD12	2.42	0.46
2:D:214:ASP:O	2:D:215:LEU:C	2.58	0.46
2:D:885:PHE:HB2	2:D:915:LEU:HD11	1.97	0.46
3:A:65:PHE:HA	3:A:69:ARG:HH21	1.81	0.46
1:C:177:VAL:HG21	1:C:238:PRO:O	2.16	0.46
1:C:58:ALA:HA	2:D:961:ALA:HB2	1.98	0.46
1:C:179:GLU:C	1:C:181:VAL:H	2.24	0.46
3:A:29:LEU:HB3	3:A:33:HIS:O	2.15	0.46
3:A:46:HIS:HA	3:A:206:VAL:HA	1.97	0.45
1:C:57:LYS:HD2	1:C:71:GLU:HB2	1.98	0.45
1:C:103:TRP:CZ2	3:A:41:ALA:HB2	2.52	0.45
2:D:204:ALA:H	2:D:764:GLN:HG2	1.79	0.45
2:D:215:LEU:HG	2:D:219:LEU:HD23	1.97	0.45
2:D:14:GLY:HA2	2:D:15:GLY:HA2	1.61	0.45
2:D:213:PRO:HB3	2:D:217:ARG:NE	2.32	0.45
2:D:833:VAL:HA	2:D:941:VAL:HG13	1.98	0.45
2:D:835:ALA:HB3	2:D:942:VAL:HA	1.98	0.45
3:B:181:VAL:HG12	3:B:207:GLU:HB3	1.98	0.45
3:B:11:ASN:ND2	3:B:54:ARG:HG2	2.32	0.45
3:A:181:VAL:HG12	3:A:207:GLU:HB3	1.98	0.45
1:C:69:ASN:N	1:C:69:ASN:OD1	2.50	0.44
1:C:21:ALA:HA	1:C:35:THR:HA	1.98	0.44
2:D:228:THR:HG22	2:D:228:THR:O	2.16	0.44
2:D:80:ARG:HH21	2:D:197:THR:HG21	1.82	0.44
3:B:45:ARG:H	3:B:207:GLU:CG	2.31	0.44
3:A:181:VAL:HB	3:A:205:VAL:HB	1.98	0.44
2:D:161:ILE:HG12	2:D:182:GLU:HG2	1.99	0.44
2:D:820:ARG:HH12	2:D:827:ARG:HE	1.64	0.44
1:C:278:TRP:HZ3	2:D:85:VAL:HG21	1.83	0.43
3:B:37:ASN:OD1	3:B:38:SER:N	2.51	0.43
3:A:48:ASP:HA	3:A:204:PRO:HA	2.00	0.43
2:D:132:VAL:HG22	2:D:198:PHE:HD1	1.81	0.43
2:D:863:GLY:H	2:D:892:ALA:HB3	1.84	0.43
3:B:77:ARG:HH22	3:B:175:PHE:N	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:77:ARG:HH22	3:A:175:PHE:N	2.16	0.43
3:B:192:VAL:O	3:B:192:VAL:HG13	2.19	0.43
3:A:200:LEU:HA	3:A:201:PRO:HD3	1.84	0.43
3:A:20:PRO:HA	3:A:44:ARG:O	2.19	0.43
2:D:782:ILE:O	2:D:782:ILE:HG23	2.19	0.42
2:D:159:PRO:HB2	2:D:161:ILE:HG22	2.01	0.42
3:B:22:ARG:NH2	3:B:170:ARG:HH11	2.17	0.42
3:A:22:ARG:NH2	3:A:170:ARG:HH11	2.17	0.42
3:A:192:VAL:O	3:A:192:VAL:HG13	2.18	0.42
1:C:203:VAL:HB	1:C:244:VAL:HG12	2.02	0.42
1:C:68:ASP:H	1:C:133:GLY:HA3	1.84	0.42
2:D:225:ILE:HA	2:D:226:PRO:HD3	1.91	0.42
2:D:941:VAL:HA	2:D:954:ARG:HA	2.01	0.42
2:D:224:LEU:CD2	2:D:224:LEU:O	2.68	0.42
2:D:201:VAL:HG13	2:D:762:VAL:HG13	2.02	0.42
3:A:186:ASP:OD1	3:A:186:ASP:N	2.53	0.42
1:C:145:ILE:HD13	1:C:145:ILE:HG21	1.81	0.42
2:D:953:TYR:HB3	2:D:968:ALA:HB1	2.02	0.42
2:D:958:VAL:HG13	2:D:964:ILE:HG23	2.02	0.42
3:A:72:GLN:HA	3:A:183:PHE:CZ	2.55	0.41
3:B:47:TYR:O	3:B:205:VAL:N	2.40	0.41
3:B:160:SER:HA	3:B:169:ALA:H	1.85	0.41
1:C:147:HIS:CD2	1:C:149:ARG:HB2	2.56	0.41
2:D:125:GLU:N	2:D:205:GLN:HE22	2.19	0.41
1:C:263:ASN:HD21	1:C:266:ASN:HD22	1.68	0.41
2:D:224:LEU:O	2:D:224:LEU:HD22	2.21	0.41
3:B:21:GLU:CG	3:B:44:ARG:HB2	2.45	0.41
1:C:33:GLY:HA3	1:C:48:PHE:HA	2.02	0.41
1:C:131:LEU:HD13	1:C:131:LEU:HA	1.87	0.41
3:B:24:THR:OG1	3:A:72:GLN:HG2	2.20	0.41
3:B:45:ARG:H	3:B:207:GLU:HG2	1.86	0.41
3:B:163:GLU:HG2	3:A:69:ARG:NH1	2.28	0.41
3:B:195:PHE:H	3:B:195:PHE:HD2	1.69	0.41
3:A:23:ARG:H	3:A:40:TRP:NE1	2.19	0.41
2:D:210:GLU:HA	2:D:217:ARG:HH22	1.84	0.41
3:A:4:HIS:CD2	3:A:77:ARG:HD2	2.56	0.41
1:C:98:VAL:HG23	1:C:112:ILE:HB	2.03	0.40
1:C:191:PHE:HB2	1:C:226:ARG:HH22	1.85	0.40
3:A:160:SER:HA	3:A:169:ALA:H	1.85	0.40
2:D:774:CYS:HB2	2:D:782:ILE:CD1	2.48	0.40
3:B:200:LEU:HA	3:B:201:PRO:HD3	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:75:LEU:O	2:D:202:ARG:HD2	2.21	0.40
2:D:79:MET:HE1	2:D:870:VAL:HG11	2.02	0.40
1:C:17:THR:OG1	1:C:17:THR:O	2.33	0.40
1:C:185:LEU:HD23	1:C:226:ARG:HB3	2.03	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	C	290/296 (98%)	255 (88%)	35 (12%)	0	100	100
2	D	431/1304 (33%)	375 (87%)	55 (13%)	1 (0%)	43	75
3	A	130/210 (62%)	101 (78%)	29 (22%)	0	100	100
3	B	130/210 (62%)	102 (78%)	27 (21%)	1 (1%)	16	52
All	All	981/2020 (49%)	833 (85%)	146 (15%)	2 (0%)	44	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	221	ALA
3	B	206	VAL

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	C	212/218 (97%)	212 (100%)	0	100	100
2	D	310/952 (33%)	307 (99%)	3 (1%)	68	76
3	A	109/169 (64%)	107 (98%)	2 (2%)	51	68
3	B	109/169 (64%)	106 (97%)	3 (3%)	38	60
All	All	740/1508 (49%)	732 (99%)	8 (1%)	63	74

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	189	PHE
2	D	219	LEU
2	D	222	VAL
3	B	23	ARG
3	B	73	LEU
3	B	203	VAL
3	A	73	LEU
3	A	203	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	263	ASN
1	C	266	ASN
2	D	205	GLN
2	D	755	HIS
2	D	764	GLN
3	B	196	GLN
3	A	72	GLN

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)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SF4	C	301	-	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	C	301	-	-	-	0/6/5/5

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.

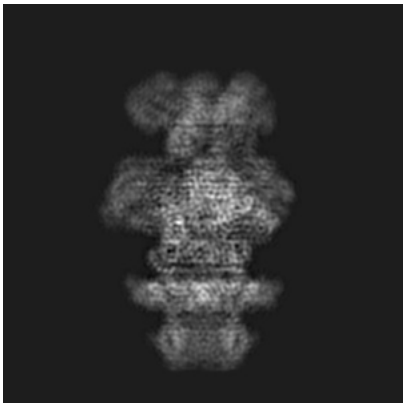
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10490. These allow visual inspection of the internal detail of the map and identification of artifacts.

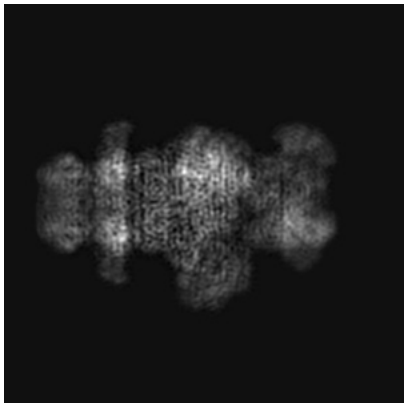
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

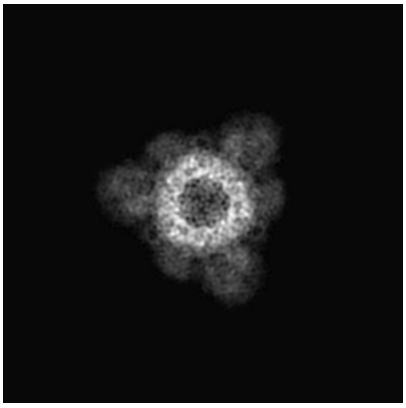
6.1.1 Primary map



X



Y



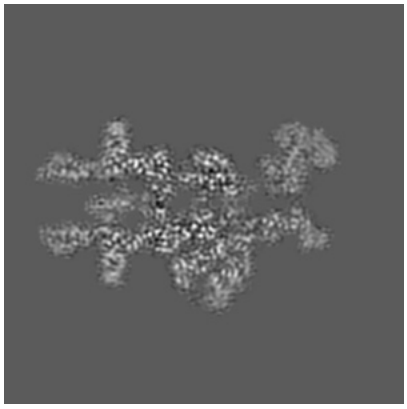
Z

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

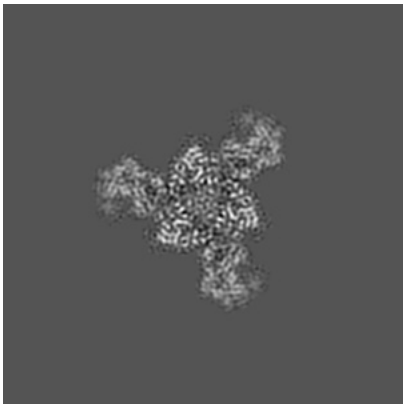
6.2 Central slices (i)

6.2.1 Primary map

X Index: 150



Y Index: 150

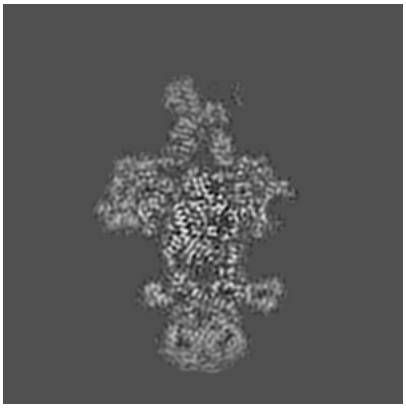


Z Index: 150

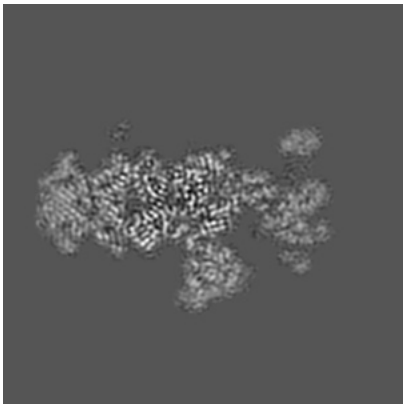
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

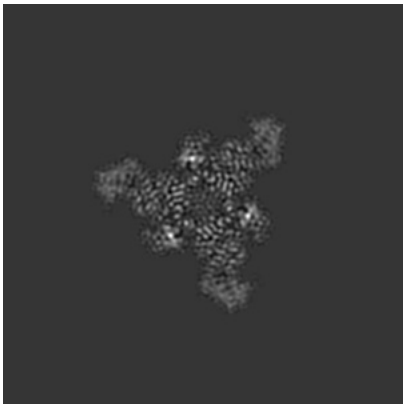
6.3.1 Primary map



X Index: 170



Y Index: 170

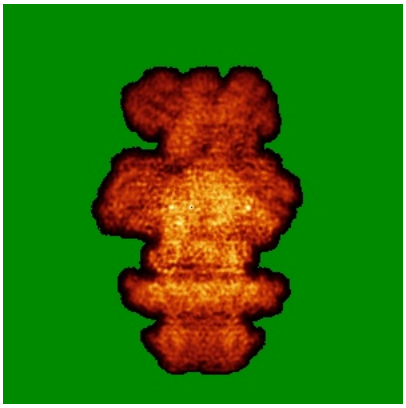


Z Index: 146

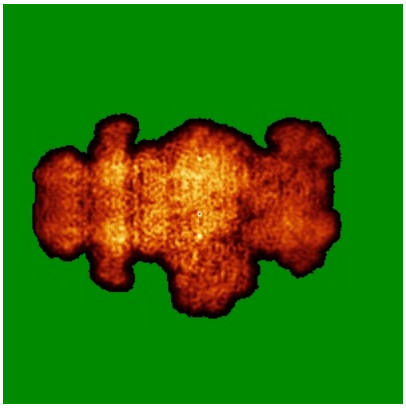
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

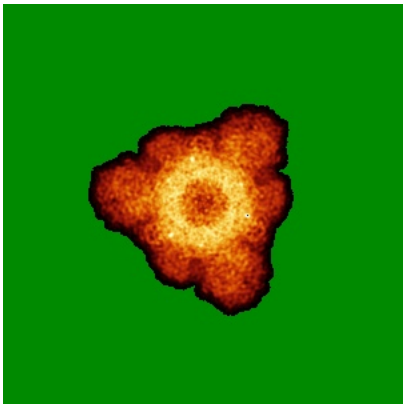
6.4.1 Primary map



X



Y

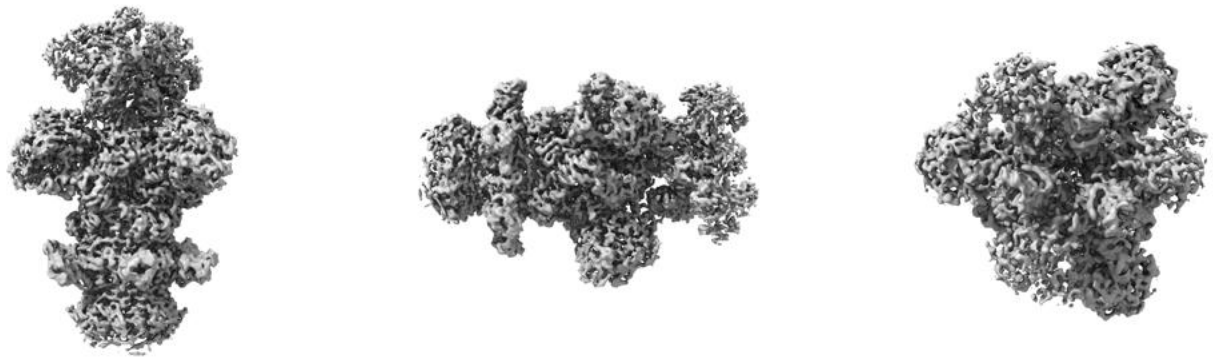


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0268. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

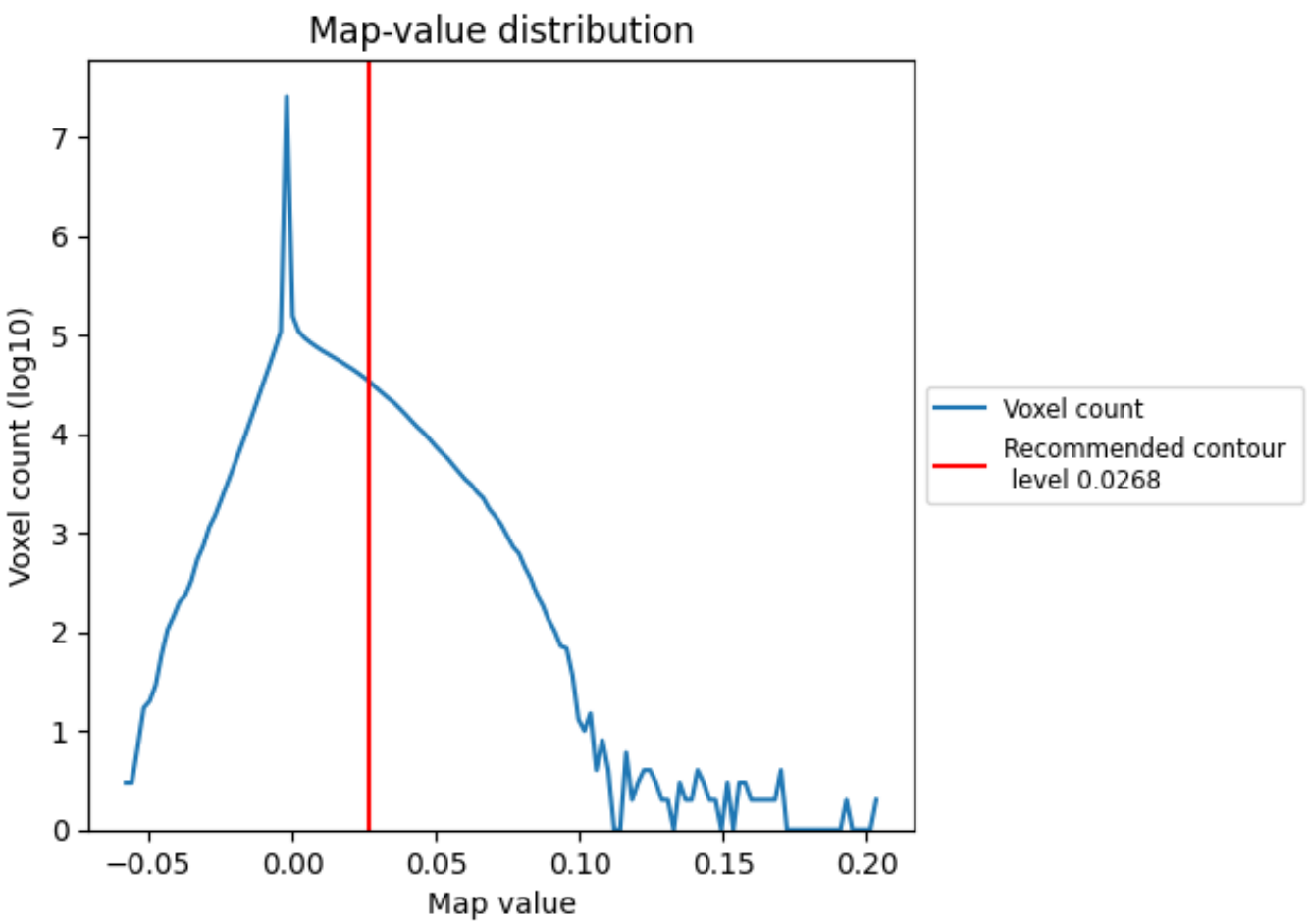
6.6 Mask visualisation (i)

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

7 Map analysis (i)

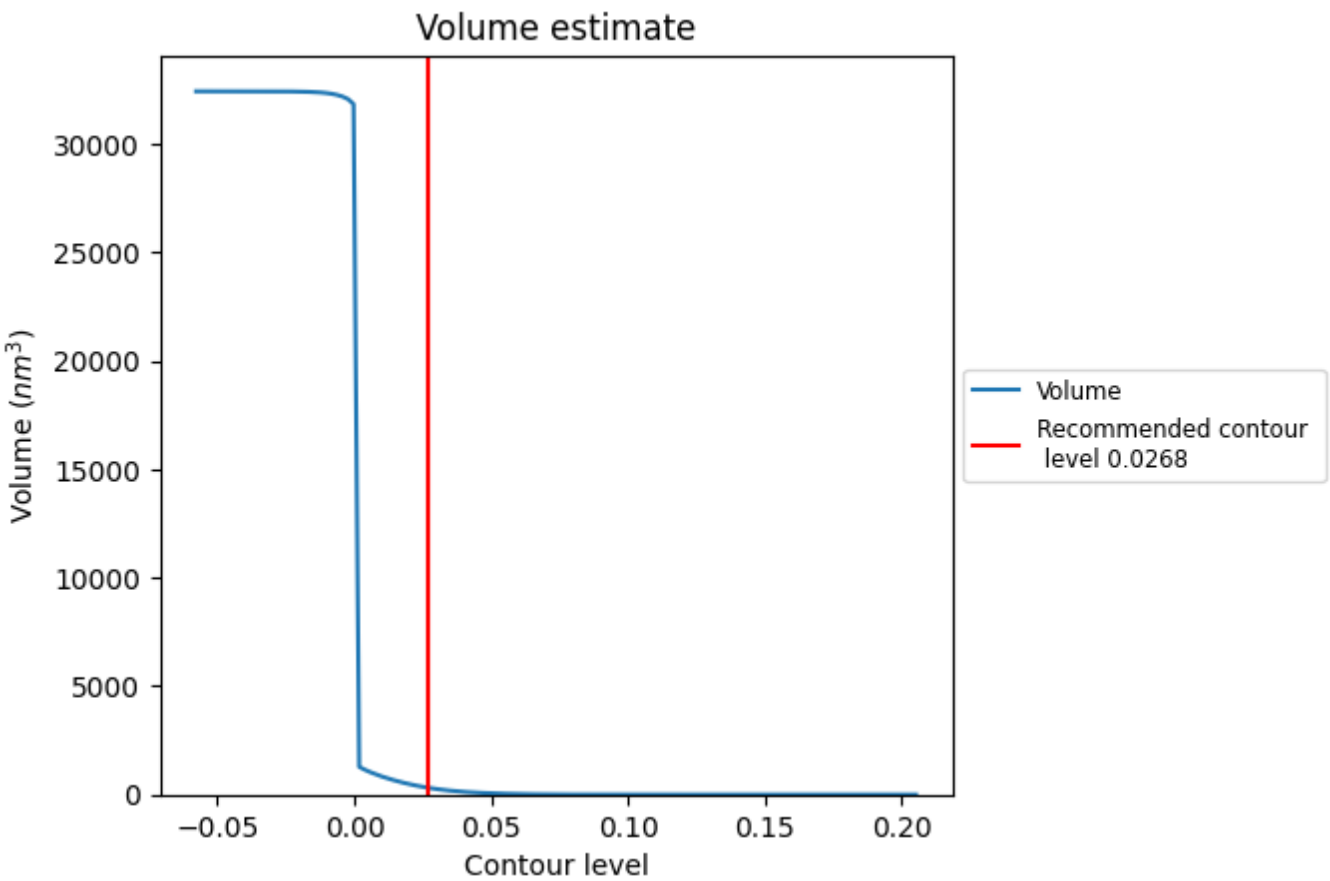
This section contains the results of statistical analysis of the map.

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.

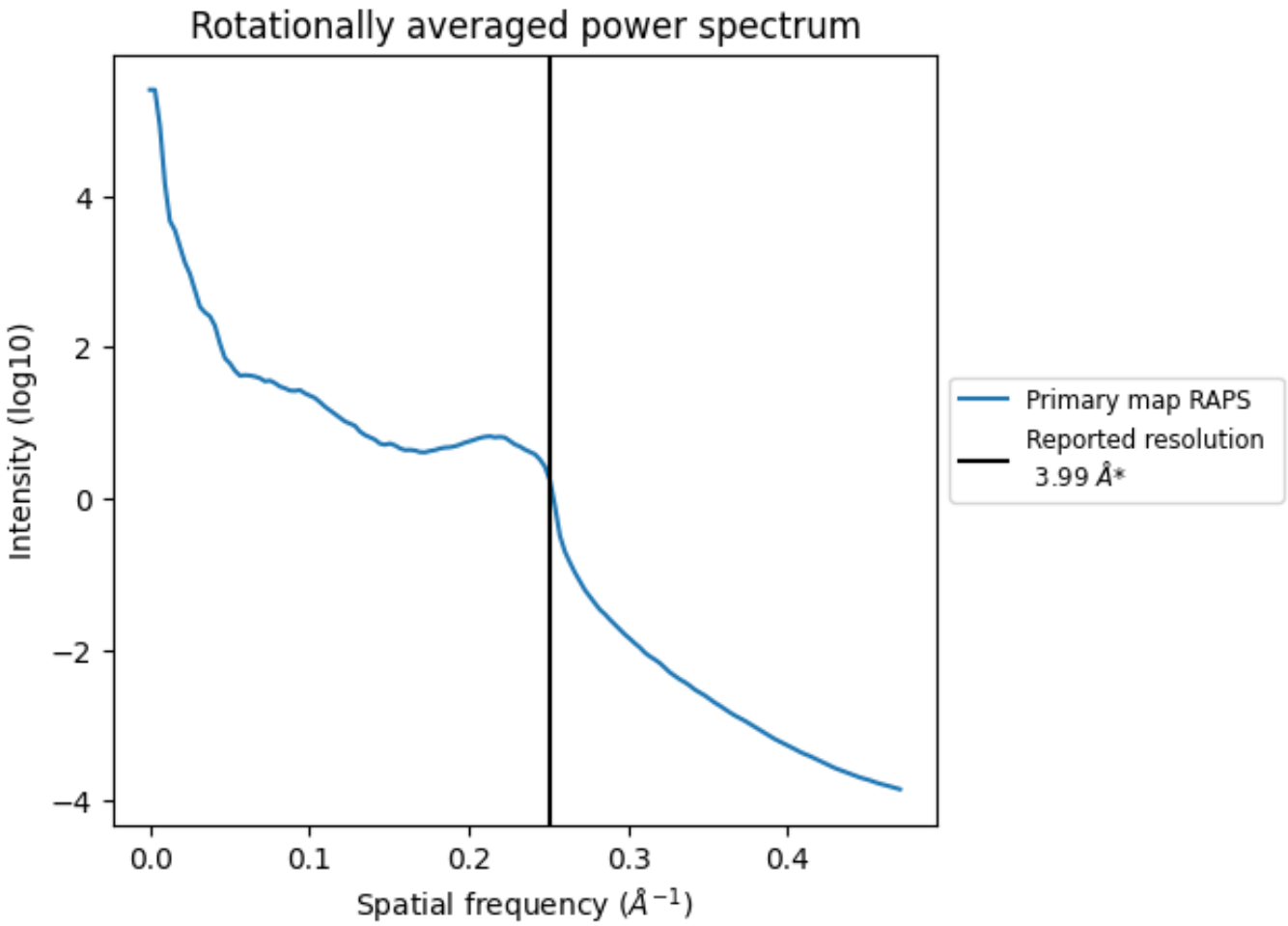
7.2 Volume estimate (i)



The volume at the recommended contour level is 318 nm^3; this corresponds to an approximate mass of 287 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 (i)

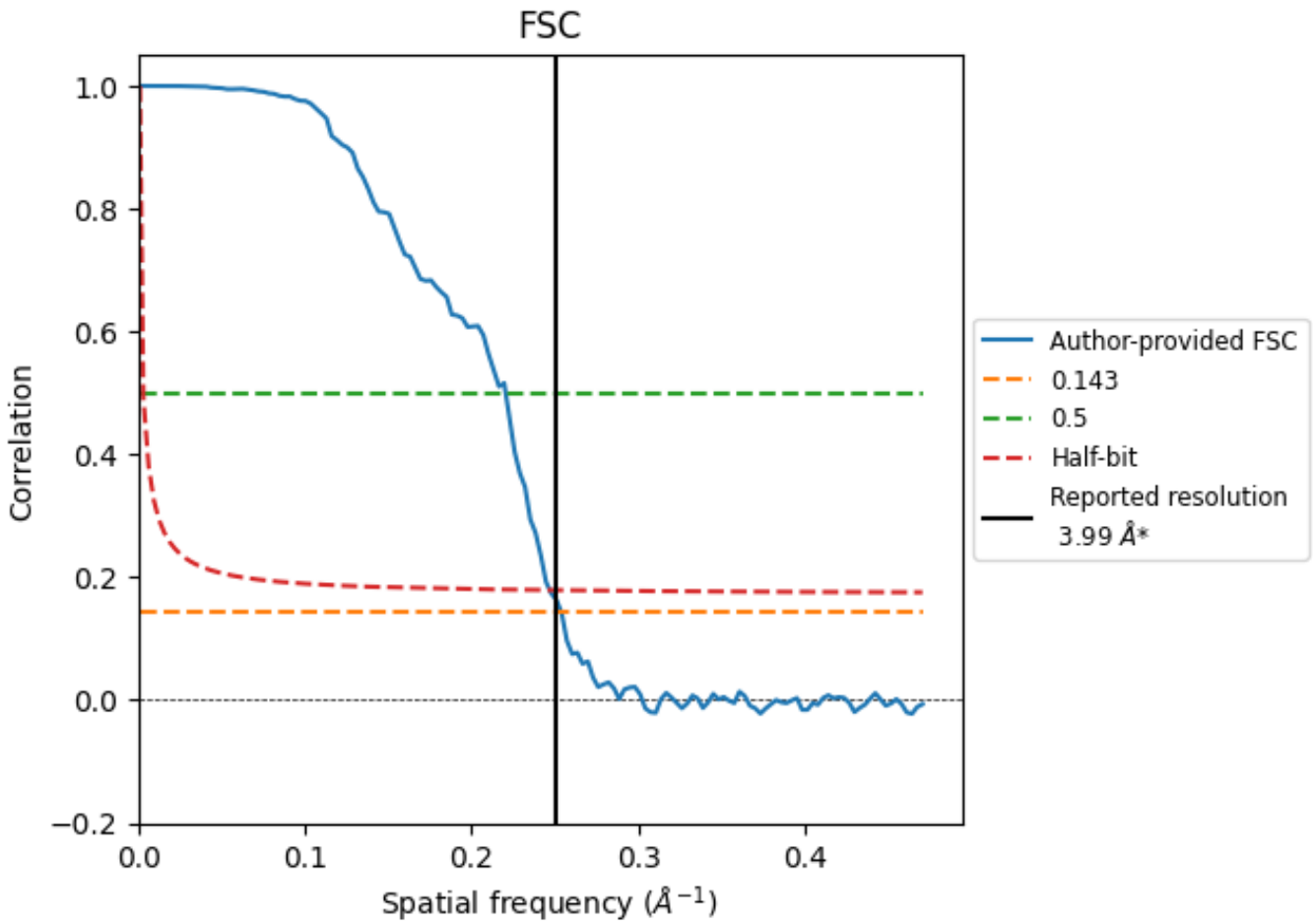


*Reported resolution corresponds to spatial frequency of 0.251 Å^{-1}

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 0.251 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.99	-	-
Author-provided FSC curve	3.94	4.54	4.05
Unmasked-calculated*	-	-	-

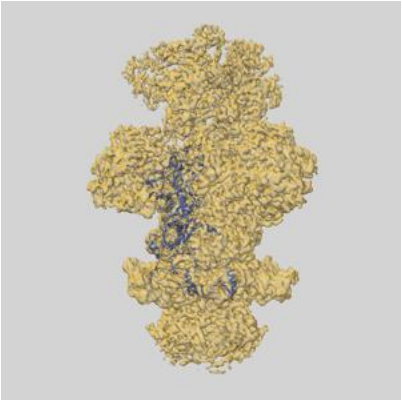
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit (i)

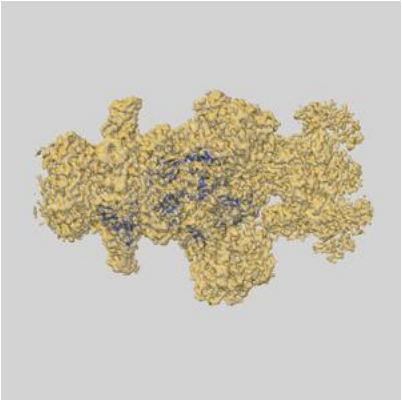
This section contains information regarding the fit between EMDB map EMD-10490 and PDB model 6TEH. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

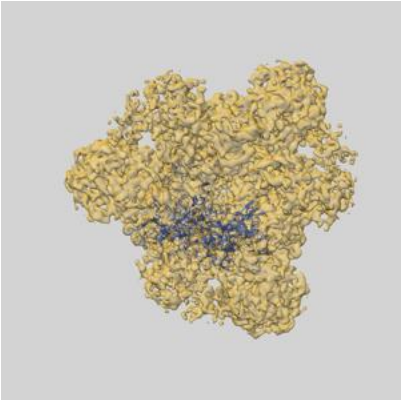
9.1.1 Map-model overlay (i)



X

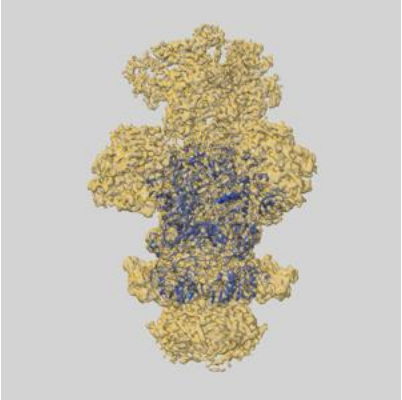


Y

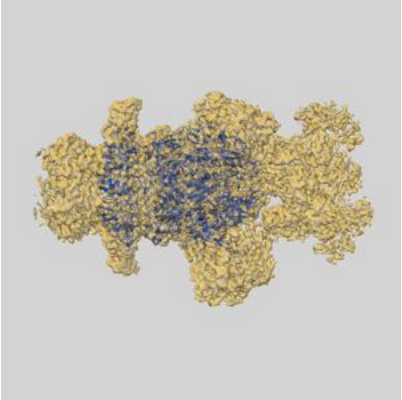


Z

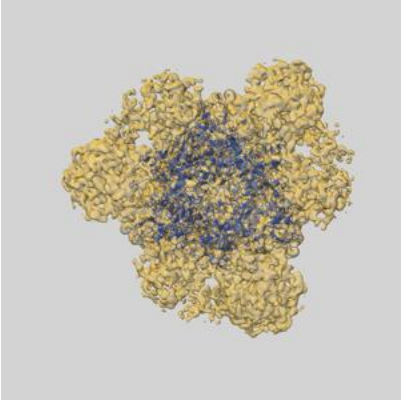
9.1.2 Map-model assembly overlay (i)



X



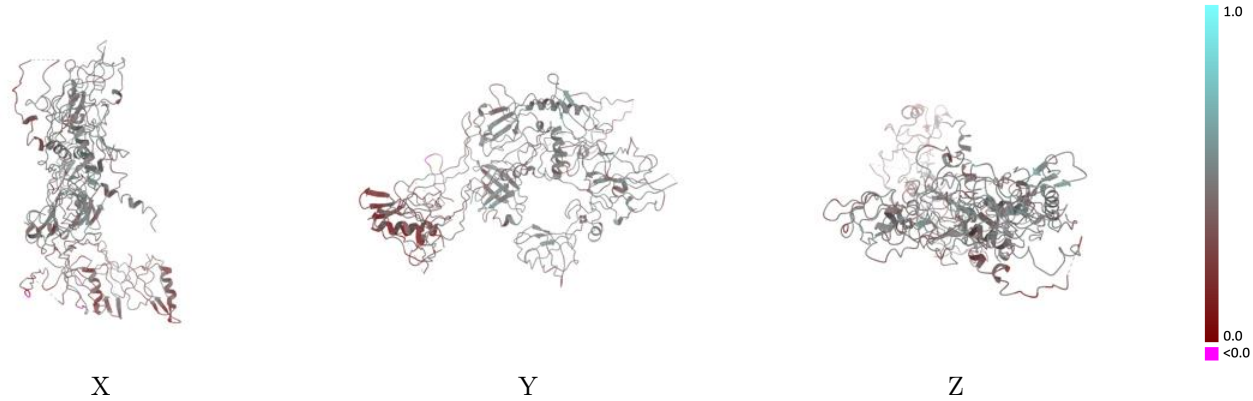
Y



Z

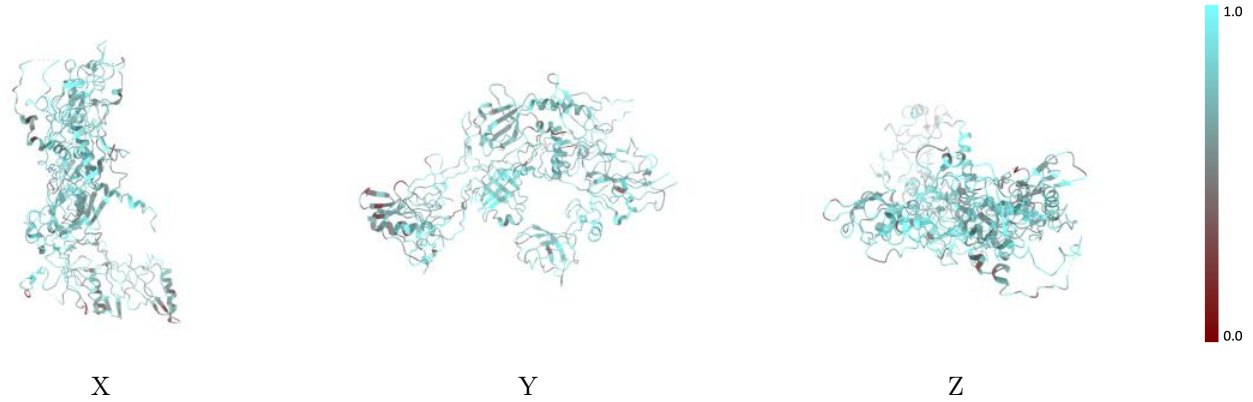
The images above show the 3D surface view of the map at the recommended contour level 0.0268 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



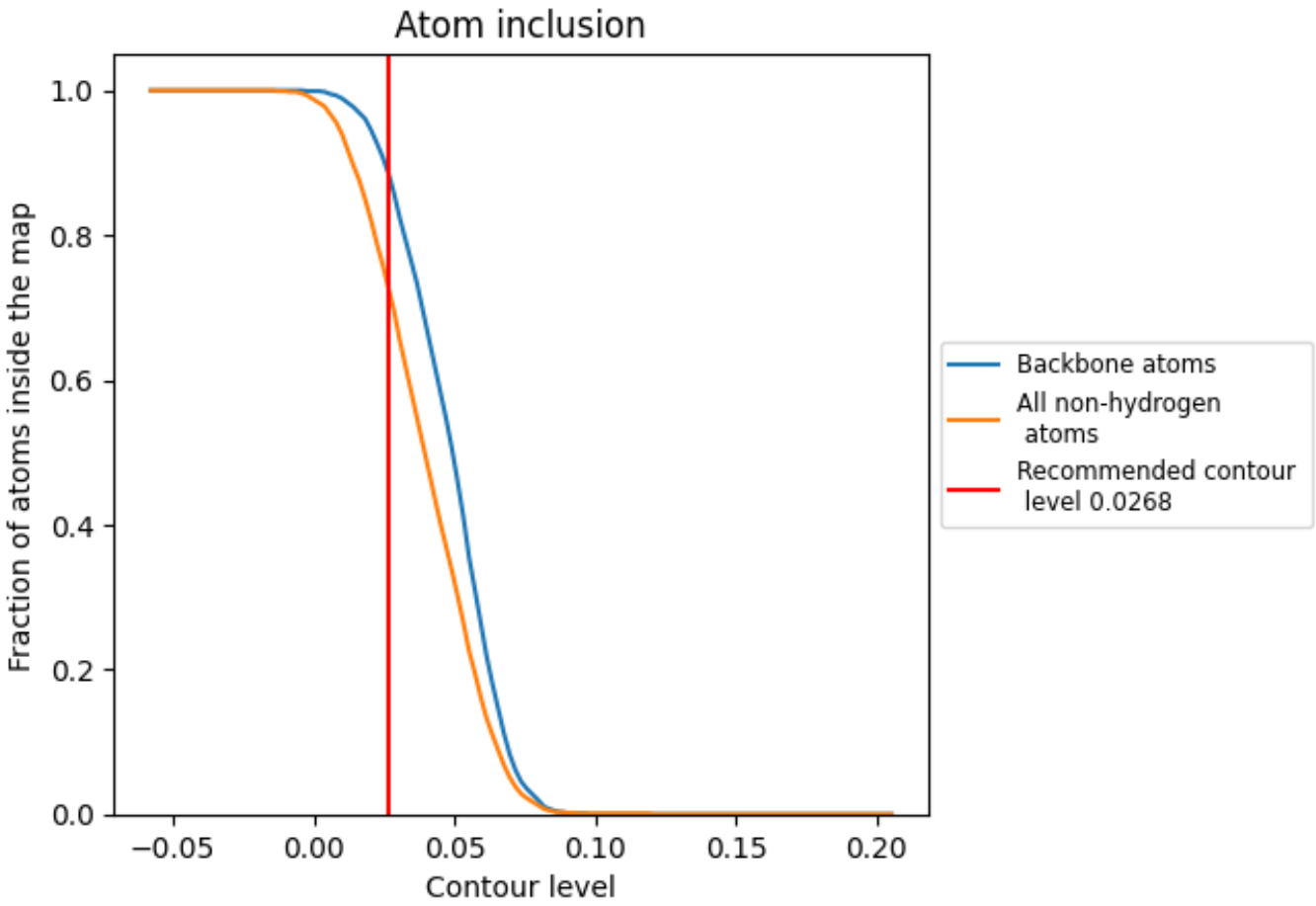
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0268).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0268) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7240	0.4270
A	0.6820	0.3490
B	0.6800	0.3570
C	0.7640	0.4540
D	0.7260	0.4580