Full wwPDB EM Validation Report ⓘ

Mar 20, 2024 – 05:23 AM JST

PDB ID	:	6M5S
EMDB ID	:	EMD-30091
Title	:	The coordinates of the apo hexameric terminase complex
Authors	:	Yang, Y.X.; Yang, P.; Wang, N.; Chen, Z.H.; Zhou, Z.H.; Rao, Z.H.; Wang, X.X.
Deposited on	:	2020-03-11
Resolution	:	3.90 Å(reported)

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

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

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

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

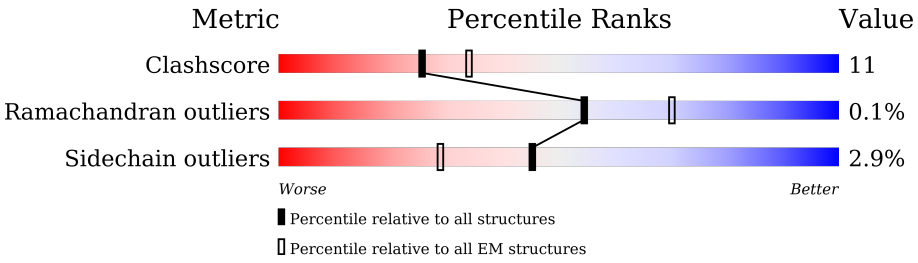
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.90 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A	693	60% 71% 21% • 7%
2	B	774	25% 66% 22% • 11%
3	C	118	33% 66% 22% • 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11055 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 Tripartite terminase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	646	Total	C	N	O	S	0	0
			4924	3153	871	879	21		

- Molecule 2 is a protein called Tripartite terminase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	689	Total	C	N	O	S	0	0
			5296	3332	976	962	26		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	216	SER	ARG	engineered mutation	UNP P10212
B	312	GLN	ARG	engineered mutation	UNP P10212

- Molecule 3 is a protein called Tripartite terminase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	105	Total	C	N	O	S	0	0
			833	523	149	158	3		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

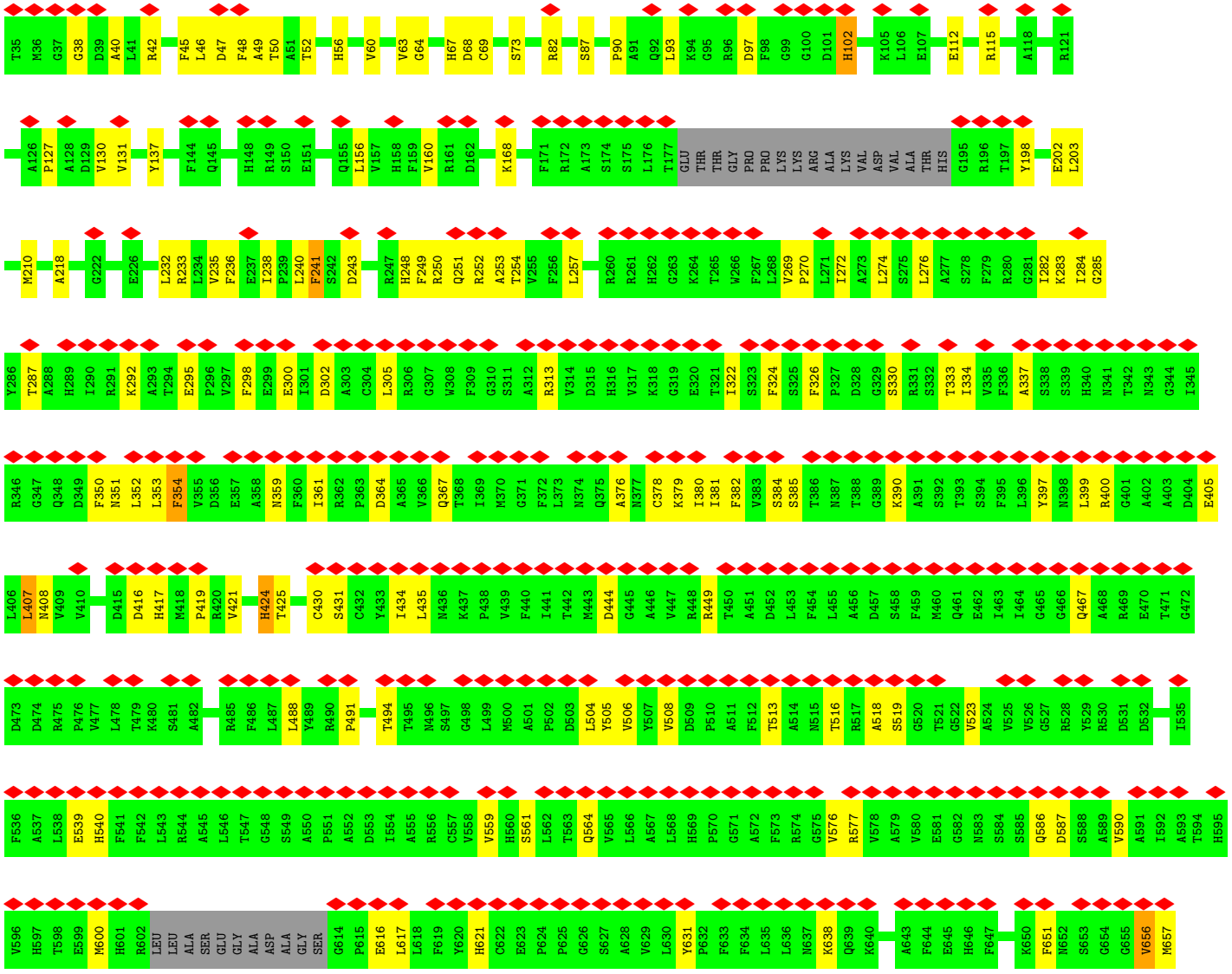
Mol	Chain	Residues	Atoms		AltConf
4	B	2	Total	Zn	0
			2	2	

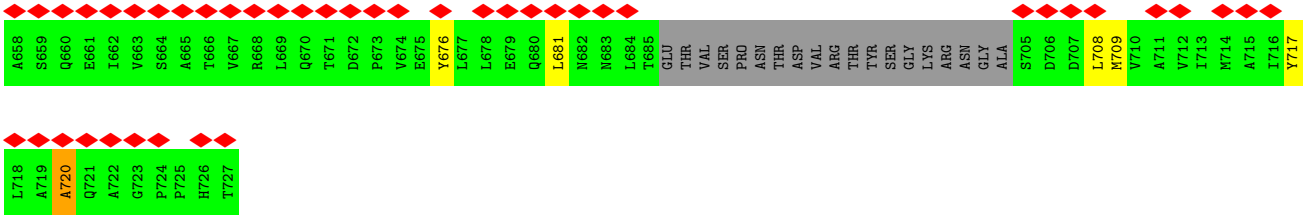
3 Residue-property plots (i)

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: Tripartite terminase subunit 3

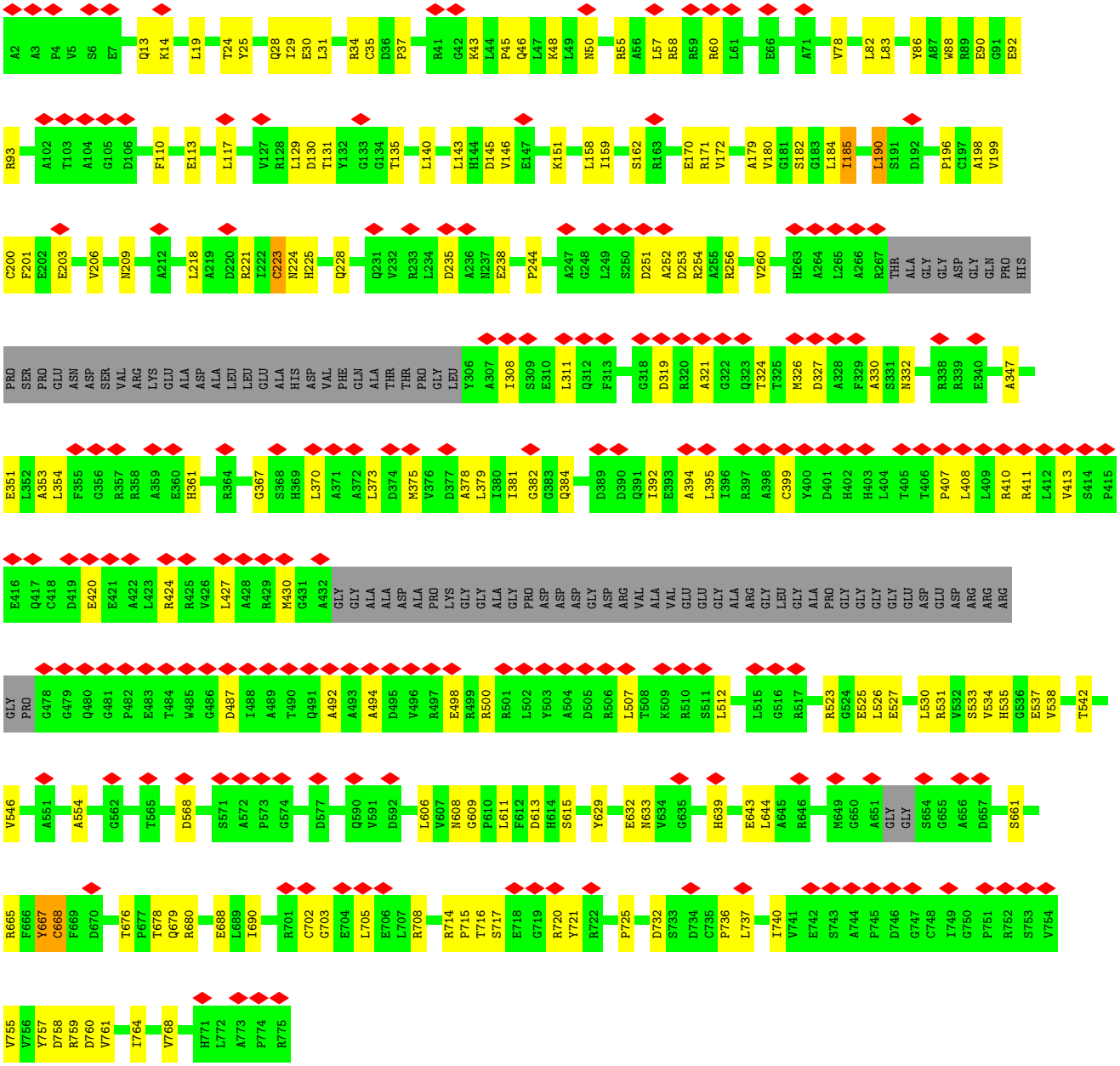
Chain A:





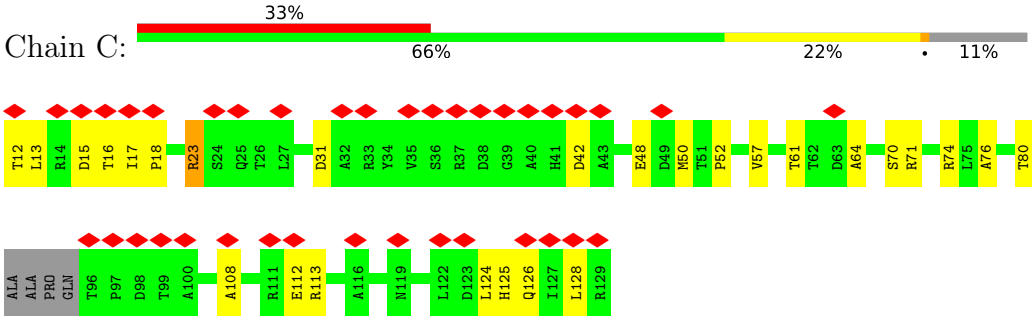
• Molecule 2: Tripartite terminase subunit 1

Chain B:



• Molecule 3: Tripartite terminase subunit 2

Chain C:


33%
66%
22%
11%
T12 L13 R14 D15 T16 I17 P18 R23 S24 Q25 T26 L27 D31 A32 R33 Y34 V35 S36 R37 D38 G39 A40 H41 D42 A43 E48 D49 M50 T51 P52 V57 T61 T62 D63 A64 S70 R71 R74 L75 A76 T80 Y81 A82 GLY PRO ILE LYS ALA PRO ASP ASP ALA
ALA ALA PRO GLN T96 P97 D98 T99 A100 A108 R111 E112 R113 A116 N119 L122 D123 L124 H125 Q126 I127 L128 R129

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25249	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 ($e^-/Å^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.146	Depositor
Minimum map value	-0.070	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0407	Depositor
Map size (Å)	374.4, 374.4, 374.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.35	0/5038	0.51	0/6849
2	B	0.27	0/5403	0.43	0/7336
3	C	0.26	0/847	0.42	0/1151
All	All	0.31	0/11288	0.46	0/15336

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

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	4924	0	4831	126	0
2	B	5296	0	5224	131	0
3	C	833	0	822	32	0
4	B	2	0	0	0	0
All	All	11055	0	10877	250	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 11.

All (250) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:17:ILE:HD12	3:C:48:GLU:OE2	1.41	1.21
1:A:491:PRO:HG2	1:A:657:MET:SD	1.84	1.15
1:A:269:VAL:HG11	1:A:300:GLU:HG3	1.35	1.05
1:A:491:PRO:CG	1:A:657:MET:SD	2.43	1.05
1:A:269:VAL:CG2	1:A:270:PRO:HD3	1.94	0.96
1:A:272:ILE:CG2	1:A:334:ILE:HD12	1.99	0.92
1:A:269:VAL:HG23	1:A:270:PRO:HD3	1.51	0.91
1:A:272:ILE:HG21	1:A:334:ILE:CD1	2.01	0.90
1:A:681:LEU:HD23	1:A:709:MET:HG3	1.53	0.88
3:C:17:ILE:HG23	3:C:18:PRO:HD3	1.57	0.84
1:A:272:ILE:HG21	1:A:334:ILE:HD12	1.60	0.83
3:C:17:ILE:CD1	3:C:48:GLU:OE2	2.26	0.81
1:A:488:LEU:CD1	2:B:507:LEU:HG	2.12	0.80
2:B:606:LEU:HD12	2:B:690:ILE:HD11	1.63	0.79
1:A:269:VAL:HG11	1:A:300:GLU:CG	2.13	0.79
1:A:488:LEU:HD11	2:B:507:LEU:HG	1.65	0.78
1:A:269:VAL:CG1	1:A:300:GLU:HG3	2.16	0.73
1:A:272:ILE:HG23	1:A:334:ILE:HD12	1.69	0.72
1:A:359:ASN:HD21	1:A:390:LYS:HE3	1.53	0.72
1:A:284:ILE:HG12	1:A:352:LEU:HD12	1.72	0.72
1:A:269:VAL:HG22	1:A:270:PRO:HD3	1.70	0.71
2:B:373:LEU:HD21	2:B:381:ILE:HD11	1.73	0.70
1:A:508:VAL:HG23	1:A:523:VAL:HG22	1.72	0.70
2:B:203:GLU:OE1	2:B:221:ARG:NH2	2.25	0.69
2:B:527:GLU:HB3	2:B:531:ARG:HE	1.58	0.69
2:B:30:GLU:O	2:B:34:ARG:NH2	2.25	0.69
2:B:546:VAL:HG23	2:B:611:LEU:HD12	1.76	0.68
2:B:223:CYS:O	2:B:225:HIS:ND1	2.26	0.68
2:B:50:ASN:ND2	3:C:50:MET:SD	2.64	0.68
3:C:17:ILE:HG23	3:C:18:PRO:CD	2.24	0.67
2:B:408:LEU:HD13	3:C:128:LEU:HD13	1.77	0.66
1:A:67:HIS:HD2	1:A:69:CYS:H	1.43	0.66
1:A:269:VAL:HG23	1:A:270:PRO:CD	2.24	0.65
2:B:758:ASP:HB3	2:B:764:ILE:HG12	1.80	0.64
2:B:381:ILE:HG22	3:C:74:ARG:HB3	1.80	0.64
3:C:17:ILE:CG2	3:C:18:PRO:HD3	2.28	0.64
1:A:276:LEU:HD11	1:A:334:ILE:HB	1.81	0.63
2:B:244:PRO:O	2:B:254:ARG:NH2	2.32	0.63
1:A:516:THR:HG22	1:A:518:ALA:H	1.62	0.63
2:B:708:ARG:NH1	2:B:725:PRO:O	2.31	0.63
1:A:539:GLU:O	1:A:708:LEU:CD2	2.47	0.62
1:A:676:TYR:HE2	1:A:708:LEU:CD1	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:PRO:HA	1:A:130:VAL:HG12	1.80	0.62
1:A:540:HIS:HB2	1:A:708:LEU:HD11	1.81	0.61
2:B:308:ILE:HD11	2:B:330:ALA:HA	1.82	0.61
1:A:434:ILE:HG22	1:A:435:LEU:H	1.65	0.61
1:A:421:VAL:HA	1:A:424:HIS:HB2	1.82	0.61
2:B:382:GLY:HA2	3:C:71:ARG:HE	1.64	0.61
1:A:651:PHE:HA	1:A:656:VAL:HG13	1.81	0.61
1:A:676:TYR:CE2	1:A:708:LEU:CD1	2.83	0.61
2:B:716:THR:OG1	2:B:717:SER:N	2.33	0.61
2:B:256:ARG:NH2	2:B:353:ALA:O	2.33	0.61
1:A:494:THR:HG21	2:B:500:ARG:HH22	1.66	0.60
2:B:223:CYS:O	2:B:225:HIS:N	2.35	0.60
2:B:373:LEU:HB3	2:B:378:ALA:HB2	1.85	0.59
3:C:17:ILE:CG2	3:C:18:PRO:CD	2.80	0.59
1:A:305:LEU:HD21	1:A:324:PHE:HD1	1.67	0.59
1:A:491:PRO:CD	1:A:657:MET:SD	2.91	0.59
1:A:444:ASP:HB2	1:A:449:ARG:HE	1.67	0.59
2:B:48:LYS:HD2	3:C:23:ARG:HD2	1.85	0.59
1:A:252:ARG:HA	1:A:379:LYS:HG3	1.84	0.58
1:A:38:GLY:O	1:A:42:ARG:NH1	2.37	0.58
1:A:240:LEU:HD22	2:B:537:GLU:HG3	1.85	0.58
1:A:488:LEU:HD12	2:B:507:LEU:HD11	1.86	0.58
1:A:539:GLU:O	1:A:708:LEU:HD21	2.03	0.58
1:A:241:PHE:CE2	2:B:203:GLU:HG2	2.39	0.58
1:A:559:VAL:HG13	1:A:600:MET:CE	2.34	0.58
2:B:55:ARG:NE	2:B:92:GLU:OE2	2.29	0.57
2:B:367:GLY:HA2	2:B:370:LEU:HD23	1.85	0.57
1:A:676:TYR:HE2	1:A:708:LEU:HD11	1.70	0.57
1:A:112:GLU:OE2	1:A:115:ARG:NH2	2.38	0.57
1:A:218:ALA:HB2	1:A:250:ARG:HH21	1.69	0.56
1:A:252:ARG:NH1	1:A:376:ALA:O	2.39	0.56
2:B:384:GLN:OE1	3:C:71:ARG:NH1	2.39	0.56
1:A:251:GLN:HE21	1:A:254:THR:HG22	1.70	0.56
2:B:140:LEU:HD23	2:B:146:VAL:HG22	1.87	0.56
1:A:45:PHE:CE1	1:A:47:ASP:HB3	2.41	0.55
2:B:151:LYS:HD3	2:B:198:ALA:HB2	1.86	0.55
2:B:534:VAL:HG23	2:B:535:HIS:H	1.72	0.55
2:B:30:GLU:OE2	2:B:182:SER:OG	2.21	0.55
1:A:351:ASN:HA	1:A:378:CYS:HA	1.87	0.55
1:A:202:GLU:HG2	1:A:203:LEU:H	1.71	0.55
1:A:397:TYR:OH	1:A:400:ARG:NH2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:HIS:CD2	1:A:69:CYS:H	2.23	0.55
2:B:159:ILE:HD11	2:B:678:THR:HB	1.88	0.55
2:B:24:THR:O	2:B:28:GLN:HG2	2.06	0.54
2:B:117:LEU:HA	3:C:80:THR:HG22	1.90	0.54
2:B:311:LEU:HB3	2:B:326:MET:CE	2.37	0.54
1:A:240:LEU:HB2	2:B:199:VAL:HG21	1.89	0.54
1:A:253:ALA:HA	1:A:380:ILE:O	2.07	0.54
1:A:82:ARG:NH2	2:B:537:GLU:OE2	2.40	0.54
2:B:494:ALA:O	2:B:498:GLU:HG3	2.07	0.54
2:B:702:CYS:SG	2:B:703:GLY:N	2.80	0.54
1:A:491:PRO:HG3	1:A:657:MET:SD	2.45	0.54
1:A:97:ASP:O	2:B:714:ARG:NH1	2.40	0.54
2:B:45:PRO:HB3	3:C:23:ARG:HG2	1.90	0.54
1:A:488:LEU:HD12	2:B:507:LEU:CD1	2.38	0.54
2:B:43:LYS:HD2	2:B:46:GLN:HG3	1.90	0.53
2:B:384:GLN:HB3	3:C:71:ARG:HD3	1.90	0.53
2:B:324:THR:HG22	3:C:126:GLN:HE22	1.73	0.53
2:B:523:ARG:O	2:B:527:GLU:HG3	2.09	0.53
2:B:705:LEU:HD21	2:B:768:VAL:HG11	1.90	0.52
2:B:151:LYS:HD2	2:B:633:ASN:HB3	1.91	0.52
1:A:127:PRO:O	1:A:131:VAL:HG23	2.10	0.52
2:B:525:GLU:OE2	3:C:113:ARG:NE	2.42	0.52
1:A:156:LEU:HD21	1:A:232:LEU:HD21	1.92	0.52
2:B:256:ARG:O	2:B:260:VAL:HG23	2.10	0.52
1:A:676:TYR:CE2	1:A:708:LEU:HD12	2.45	0.52
2:B:185:ILE:HD11	3:C:70:SER:HB2	1.92	0.51
2:B:758:ASP:OD1	2:B:759:ARG:N	2.42	0.51
2:B:668:CYS:SG	2:B:759:ARG:NH2	2.82	0.51
1:A:576:VAL:HG22	1:A:617:LEU:HD12	1.93	0.51
1:A:63:VAL:HG12	1:A:64:GLY:H	1.74	0.51
1:A:251:GLN:NE2	1:A:405:GLU:O	2.27	0.51
1:A:399:LEU:HD22	1:A:407:LEU:HD23	1.91	0.51
1:A:425:THR:HG22	1:A:425:THR:O	2.10	0.51
2:B:399:CYS:HB3	3:C:125:HIS:CD2	2.45	0.51
2:B:93:ARG:NH1	2:B:113:GLU:O	2.43	0.50
2:B:253:ASP:HA	2:B:256:ARG:HG2	1.92	0.50
2:B:129:LEU:HG	2:B:131:THR:HG22	1.94	0.50
2:B:179:ALA:HB1	2:B:190:LEU:HD13	1.93	0.50
1:A:494:THR:HG21	2:B:500:ARG:NH2	2.27	0.50
2:B:715:PRO:HB3	2:B:721:TYR:CE1	2.46	0.50
1:A:272:ILE:HD11	1:A:354:PHE:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:76:ALA:O	3:C:80:THR:HG23	2.11	0.50
1:A:285:GLY:O	1:A:354:PHE:N	2.44	0.49
1:A:40:ALA:HB3	1:A:87:SER:HB2	1.94	0.49
1:A:559:VAL:HG13	1:A:600:MET:HE2	1.95	0.49
2:B:140:LEU:HD21	2:B:172:VAL:HG22	1.94	0.49
1:A:233:ARG:NH2	1:A:243:ASP:OD2	2.45	0.49
1:A:257:LEU:HD12	1:A:407:LEU:HD13	1.95	0.49
2:B:162:SER:OG	2:B:554:ALA:HB2	2.13	0.49
1:A:90:PRO:HD2	1:A:93:LEU:HD12	1.95	0.48
2:B:311:LEU:HB3	2:B:326:MET:HE3	1.94	0.48
2:B:117:LEU:HG	3:C:80:THR:HG22	1.94	0.48
1:A:50:THR:HG22	1:A:52:THR:H	1.78	0.48
1:A:364:ASP:HA	1:A:367:GLN:HE22	1.79	0.48
3:C:15:ASP:OD2	3:C:16:THR:N	2.40	0.48
1:A:431:SER:O	1:A:431:SER:OG	2.30	0.47
1:A:283:LYS:HA	1:A:333:THR:O	2.15	0.47
1:A:505:TYR:CE2	1:A:577:ARG:HD2	2.50	0.47
1:A:49:ALA:O	1:A:50:THR:OG1	2.30	0.47
2:B:568:ASP:HA	2:B:757:TYR:HB2	1.96	0.47
2:B:420:GLU:O	2:B:424:ARG:HG3	2.14	0.47
1:A:717:TYR:O	1:A:720:ALA:HB3	2.14	0.47
2:B:407:PRO:O	2:B:408:LEU:HG	2.15	0.47
2:B:526:LEU:HD23	2:B:526:LEU:HA	1.77	0.47
2:B:135:THR:O	2:B:135:THR:OG1	2.28	0.46
1:A:283:LYS:O	1:A:350:PHE:HA	2.16	0.46
1:A:292:LYS:HA	1:A:292:LYS:HD3	1.71	0.46
3:C:15:ASP:HB3	3:C:18:PRO:HD2	1.97	0.46
1:A:384:SER:OG	1:A:385:SER:N	2.49	0.46
1:A:210:MET:HG2	1:A:236:PHE:CE2	2.51	0.46
2:B:180:VAL:HG23	2:B:535:HIS:CE1	2.51	0.46
2:B:629:TYR:O	2:B:633:ASN:ND2	2.36	0.46
1:A:272:ILE:HD11	1:A:354:PHE:HD2	1.80	0.46
1:A:283:LYS:HG3	1:A:350:PHE:HA	1.98	0.45
2:B:86:TYR:CZ	2:B:90:GLU:HG3	2.51	0.45
1:A:73:SER:HB3	2:B:184:LEU:HD13	1.98	0.45
1:A:248:HIS:CD2	1:A:405:GLU:HB3	2.50	0.45
1:A:516:THR:HB	1:A:519:SER:HB3	1.99	0.45
1:A:540:HIS:HB2	1:A:708:LEU:HD21	1.99	0.45
2:B:25:TYR:CZ	2:B:29:ILE:HD11	2.52	0.45
2:B:57:LEU:HD12	2:B:57:LEU:HA	1.81	0.45
1:A:46:LEU:HD22	2:B:13:GLN:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:643:GLU:OE1	2:B:680:ARG:NE	2.43	0.45
2:B:170:GLU:OE1	2:B:171:ARG:NH2	2.49	0.44
1:A:513:THR:O	1:A:519:SER:HB2	2.17	0.44
3:C:12:THR:HG23	3:C:13:LEU:HG	1.99	0.44
1:A:417:HIS:HB2	1:A:467:GLN:HB2	2.00	0.44
2:B:200:CYS:HA	2:B:203:GLU:HG3	1.99	0.44
2:B:347:ALA:O	2:B:351:GLU:HG3	2.17	0.44
2:B:130:ASP:HA	2:B:135:THR:HB	1.99	0.44
2:B:354:LEU:HD23	2:B:354:LEU:HA	1.86	0.44
1:A:102:HIS:CE1	2:B:717:SER:HA	2.52	0.43
1:A:326:PHE:HB2	1:A:330:SER:HB2	1.99	0.43
2:B:58:ARG:C	2:B:60:ARG:H	2.22	0.43
1:A:361:ILE:HD12	1:A:361:ILE:HA	1.92	0.43
3:C:124:LEU:O	3:C:128:LEU:HG	2.18	0.43
2:B:31:LEU:HD23	2:B:31:LEU:HA	1.85	0.43
2:B:55:ARG:HD3	3:C:31:ASP:OD1	2.18	0.43
2:B:159:ILE:HD12	2:B:679:GLN:HG3	2.01	0.43
2:B:375:MET:O	2:B:379:LEU:HB2	2.19	0.43
2:B:392:ILE:HD11	2:B:530:LEU:HB2	2.00	0.43
1:A:274:LEU:HD13	1:A:274:LEU:HA	1.85	0.43
2:B:740:ILE:HG12	2:B:755:VAL:HG12	2.00	0.43
3:C:23:ARG:HD3	3:C:23:ARG:HA	1.71	0.43
3:C:108:ALA:O	3:C:112:GLU:HG2	2.18	0.43
1:A:302:ASP:OD2	1:A:322:ILE:HD13	2.19	0.43
1:A:564:GLN:CB	2:B:492:ALA:HB2	2.49	0.43
2:B:88:TRP:O	2:B:92:GLU:HG3	2.19	0.43
2:B:410:ARG:HA	2:B:413:VAL:HG22	2.01	0.43
1:A:269:VAL:CG2	1:A:270:PRO:CD	2.81	0.43
1:A:621:HIS:HA	1:A:631:TYR:O	2.19	0.42
2:B:14:LYS:HE3	2:B:14:LYS:HB2	1.70	0.42
2:B:608:ASN:OD1	2:B:609:GLY:N	2.51	0.42
2:B:667:TYR:HB2	2:B:736:PRO:HG3	2.00	0.42
1:A:333:THR:OG1	1:A:334:ILE:N	2.52	0.42
1:A:334:ILE:HG12	1:A:334:ILE:O	2.18	0.42
1:A:60:VAL:HG23	1:A:63:VAL:HB	2.00	0.42
2:B:308:ILE:HD12	2:B:308:ILE:HA	1.84	0.42
1:A:408:ASN:HA	2:B:209:ASN:O	2.19	0.42
2:B:201:PHE:CZ	2:B:632:GLU:HG2	2.54	0.42
1:A:488:LEU:CD1	2:B:507:LEU:CG	2.90	0.42
2:B:37:PRO:HG3	2:B:110:PHE:CD2	2.54	0.42
1:A:168:LYS:O	1:A:198:TYR:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ILE:HG22	1:A:351:ASN:HD22	1.85	0.42
2:B:78:VAL:O	2:B:82:LEU:HG	2.19	0.42
2:B:143:LEU:HD23	2:B:143:LEU:HA	1.87	0.42
2:B:427:LEU:HA	2:B:430:MET:HG2	2.01	0.42
2:B:758:ASP:OD1	2:B:760:ASP:N	2.52	0.42
1:A:56:HIS:O	1:A:68:ASP:HB2	2.20	0.42
1:A:287:THR:HG22	1:A:337:ALA:HB3	2.01	0.42
1:A:353:LEU:HD23	1:A:380:ILE:HG12	2.02	0.42
2:B:661:SER:OG	2:B:688:GLU:OE2	2.28	0.42
1:A:361:ILE:HB	2:B:430:MET:HE2	2.02	0.41
1:A:488:LEU:HD12	2:B:507:LEU:CG	2.50	0.41
2:B:19:LEU:HD11	2:B:83:LEU:HD12	2.02	0.41
2:B:228:GLN:O	2:B:533:SER:HA	2.20	0.41
1:A:238:ILE:HG12	1:A:241:PHE:CD1	2.55	0.41
2:B:251:ASP:OD1	2:B:252:ALA:N	2.45	0.41
1:A:47:ASP:N	1:A:47:ASP:OD1	2.40	0.41
1:A:381:ILE:HD13	1:A:381:ILE:HA	1.92	0.41
2:B:373:LEU:HD12	2:B:373:LEU:HA	1.88	0.41
2:B:737:LEU:HD12	2:B:759:ARG:O	2.20	0.41
1:A:45:PHE:HA	1:A:137:TYR:CE2	2.55	0.41
1:A:249:PHE:HZ	2:B:206:VAL:HG12	1.85	0.41
2:B:319:ASP:OD2	2:B:321:ALA:N	2.54	0.41
2:B:737:LEU:HD13	2:B:761:VAL:HA	2.03	0.41
1:A:63:VAL:HG12	1:A:64:GLY:N	2.35	0.41
1:A:295:GLU:O	1:A:298:PHE:HB2	2.20	0.41
1:A:313:ARG:HH21	1:A:326:PHE:HA	1.85	0.41
2:B:28:GLN:HB2	3:C:50:MET:HE2	2.02	0.41
2:B:411:ARG:NH1	2:B:512:LEU:HB3	2.36	0.41
2:B:35:CYS:HA	2:B:361:HIS:CD2	2.56	0.41
1:A:586:GLN:O	1:A:590:VAL:HG23	2.20	0.41
2:B:43:LYS:NZ	3:C:52:PRO:HA	2.36	0.41
2:B:332:ASN:HB3	2:B:394:ALA:HB1	2.02	0.41
2:B:411:ARG:CZ	2:B:512:LEU:HB3	2.51	0.41
2:B:538:VAL:O	2:B:542:THR:HG23	2.20	0.41
2:B:235:ASP:HB2	2:B:238:GLU:HG2	2.03	0.41
2:B:613:ASP:O	2:B:615:SER:N	2.54	0.41
1:A:494:THR:CG2	2:B:500:ARG:NH2	2.84	0.40
2:B:716:THR:CG2	2:B:720:ARG:HB3	2.52	0.40
1:A:156:LEU:O	1:A:160:VAL:HG23	2.22	0.40
3:C:61:THR:HG22	3:C:64:ALA:H	1.87	0.40
2:B:60:ARG:HD2	3:C:42:ASP:OD1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ASP:O	1:A:419:PRO:HD2	2.21	0.40
1:A:416:ASP:HA	1:A:467:GLN:HG2	2.03	0.40
2:B:196:PRO:HG3	2:B:218:LEU:HG	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	A	638/693 (92%)	578 (91%)	59 (9%)	1 (0%)	47 79
2	B	681/774 (88%)	617 (91%)	63 (9%)	1 (0%)	51 84
3	C	101/118 (86%)	92 (91%)	9 (9%)	0	100 100
All	All	1420/1585 (90%)	1287 (91%)	131 (9%)	2 (0%)	54 84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	224	ASN
1	A	720	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	507/573 (88%)	491 (97%)	16 (3%)	39	63
2	B	538/608 (88%)	523 (97%)	15 (3%)	43	66
3	C	89/98 (91%)	87 (98%)	2 (2%)	52	71
All	All	1134/1279 (89%)	1101 (97%)	33 (3%)	45	65

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	PHE
1	A	102	HIS
1	A	235	VAL
1	A	241	PHE
1	A	354	PHE
1	A	382	PHE
1	A	407	LEU
1	A	424	HIS
1	A	430	CYS
1	A	504	LEU
1	A	506	VAL
1	A	561	SER
1	A	587	ASP
1	A	616	GLU
1	A	638	LYS
1	A	656	VAL
2	B	145	ASP
2	B	158	LEU
2	B	185	ILE
2	B	190	LEU
2	B	223	CYS
2	B	327	ASP
2	B	395	LEU
2	B	487	ASP
2	B	639	HIS
2	B	644	LEU
2	B	665	ARG
2	B	667	TYR
2	B	668	CYS
2	B	676	THR
2	B	732	ASP
3	C	23	ARG
3	C	57	VAL

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

Mol	Chain	Res	Type
1	A	67	HIS
1	A	102	HIS
1	A	135	ASN
1	A	211	HIS
1	A	316	HIS
1	A	340	HIS
1	A	343	ASN
1	A	351	ASN
1	A	359	ASN
1	A	367	GLN
1	A	670	GLN
2	B	46	GLN
2	B	53	GLN
2	B	124	HIS
2	B	152	GLN
2	B	522	GLN
2	B	579	HIS
2	B	614	HIS
2	B	621	GLN
3	C	103	HIS
3	C	126	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

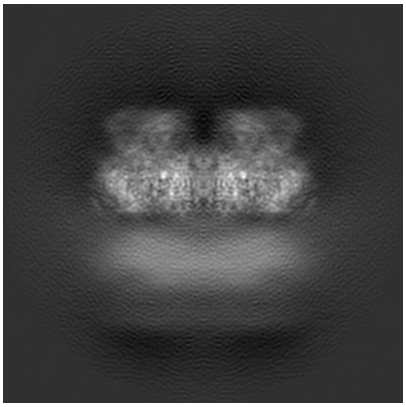
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30091. These allow visual inspection of the internal detail of the map and identification of artifacts.

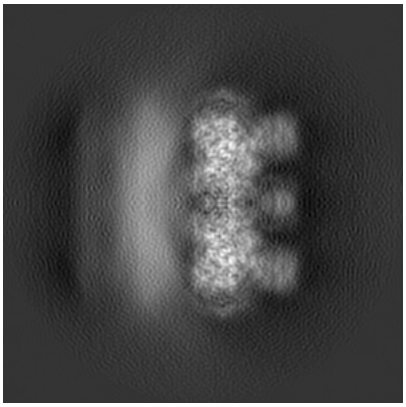
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

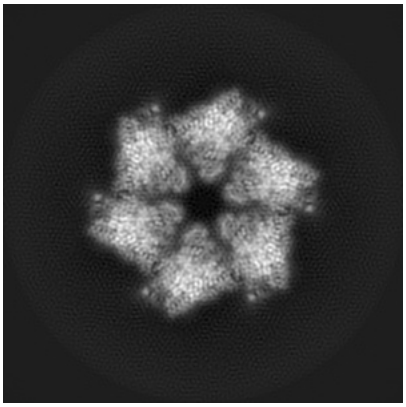
6.1.1 Primary map



X



Y

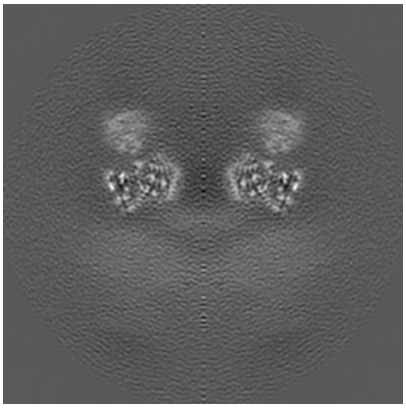


Z

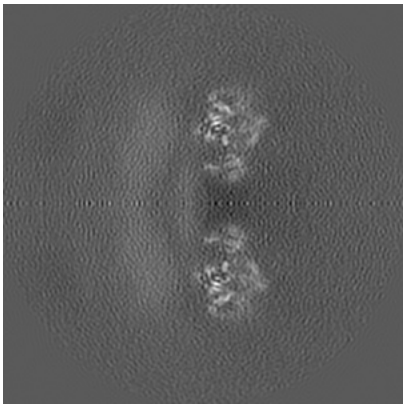
The images above show the map projected in three orthogonal directions.

6.2 Central slices

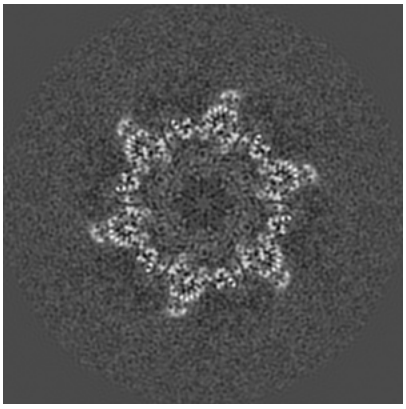
6.2.1 Primary map



X Index: 180



Y Index: 180

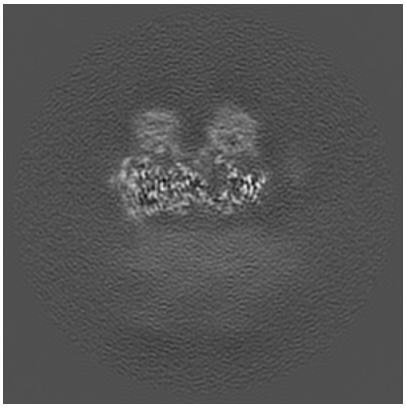


Z Index: 180

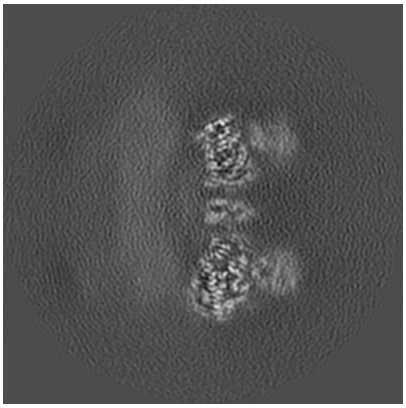
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

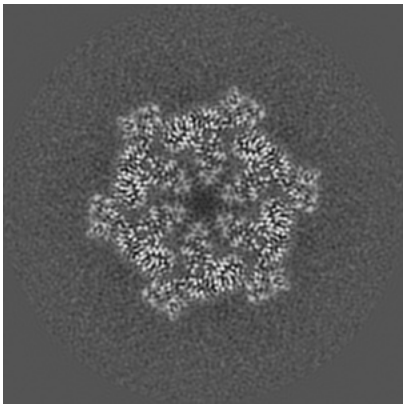
6.3.1 Primary map



X Index: 240



Y Index: 152

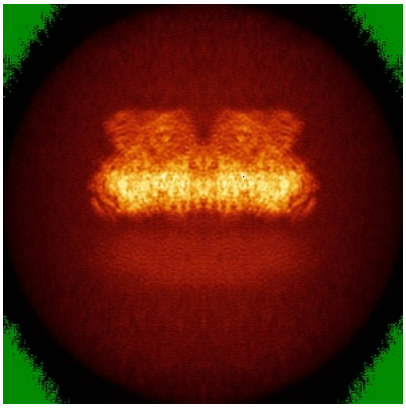


Z Index: 198

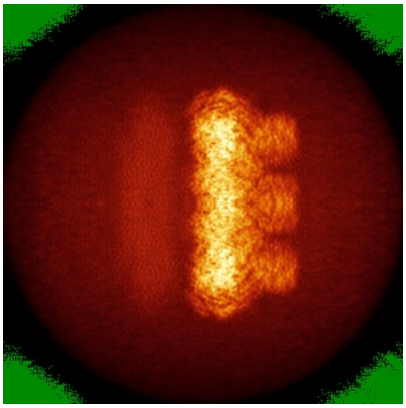
The images above show the largest variance slices of the map in three orthogonal directions.

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

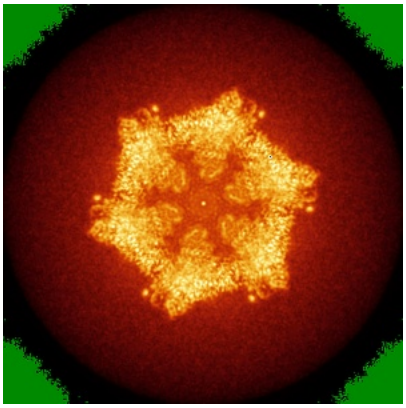
6.4.1 Primary map



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 0.0407. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

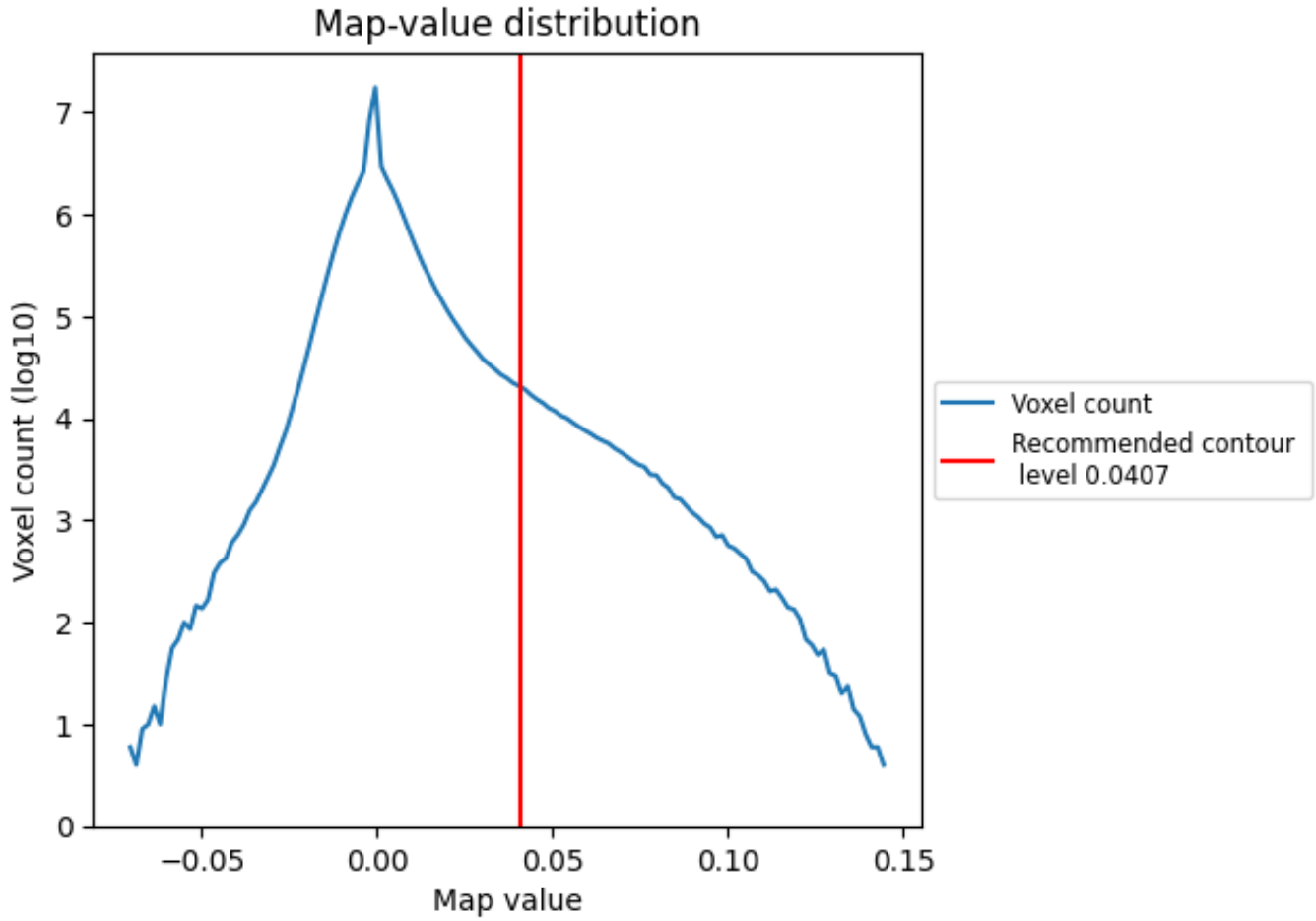
6.6 Mask visualisation (i)

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

7 Map analysis

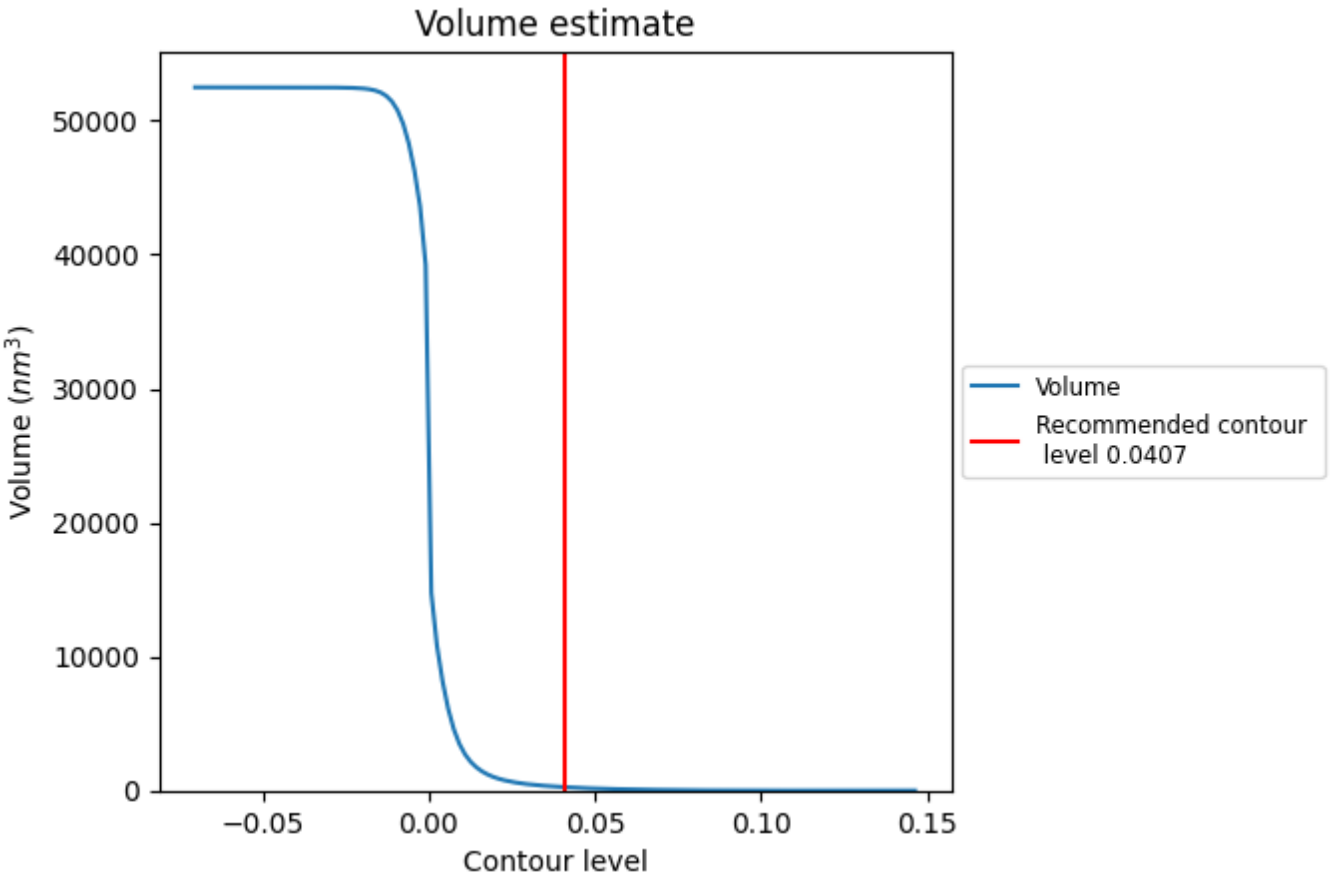
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

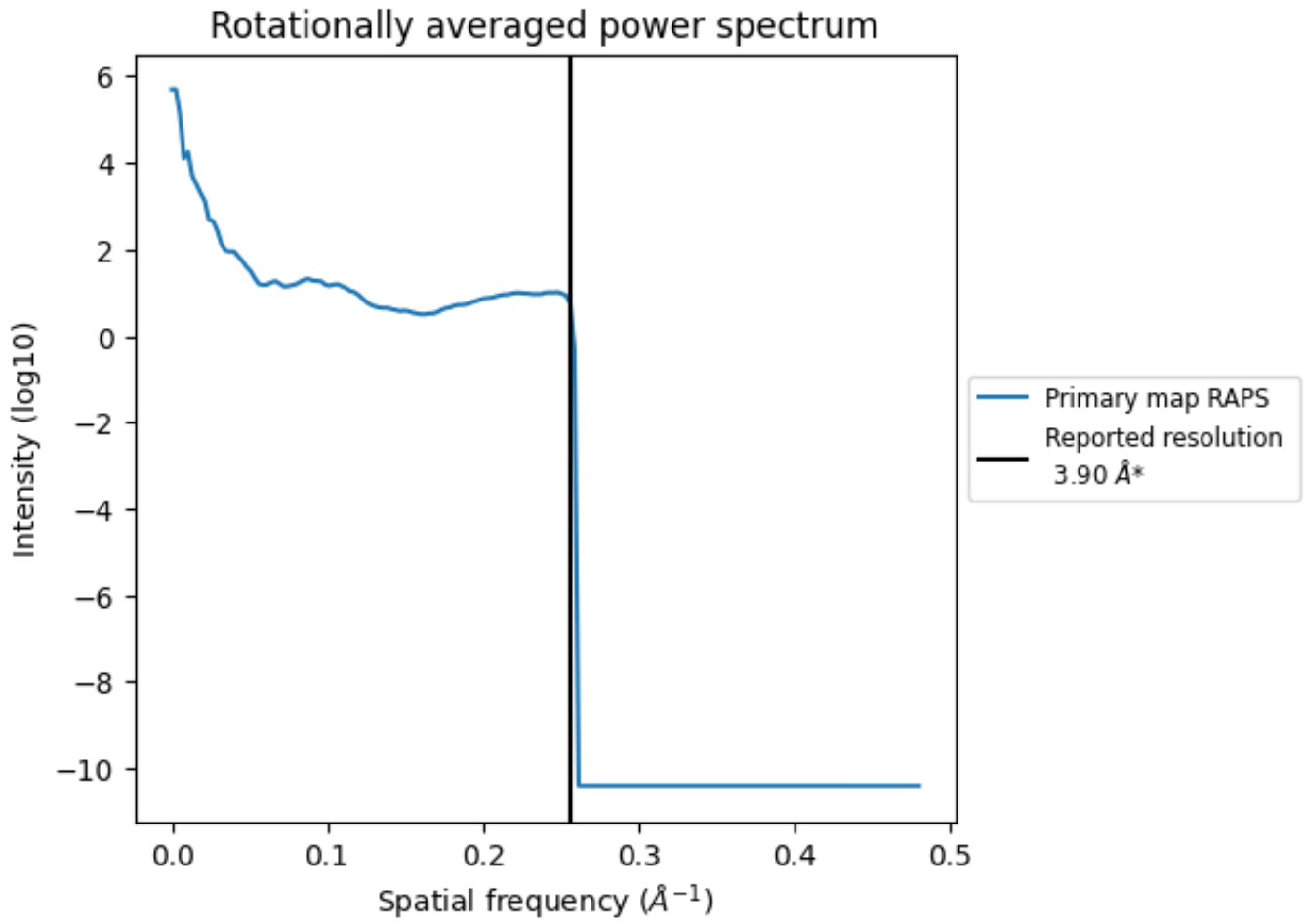
7.2 Volume estimate



The volume at the recommended contour level is 258 nm^3; this corresponds to an approximate mass of 233 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 0.256 Å^{-1}

8 Fourier-Shell correlation (i)

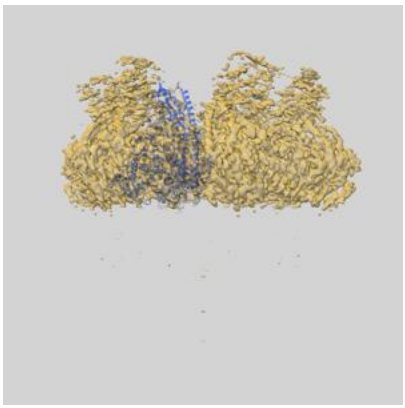
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

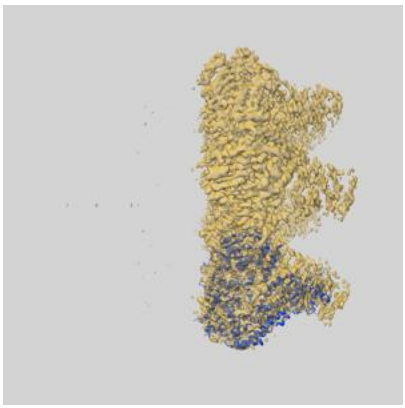
This section contains information regarding the fit between EMDB map EMD-30091 and PDB model 6M5S. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlays

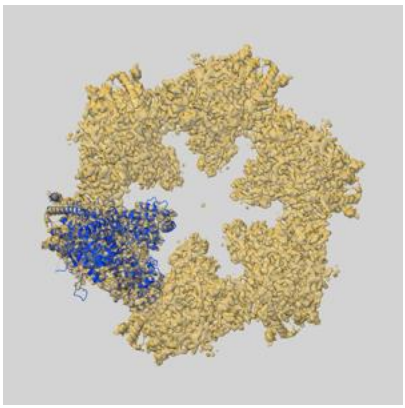
9.1.1 Map-model overlay



X

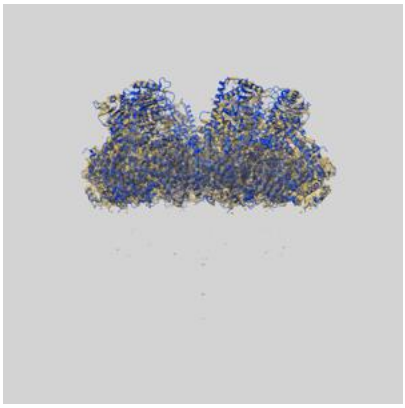


Y

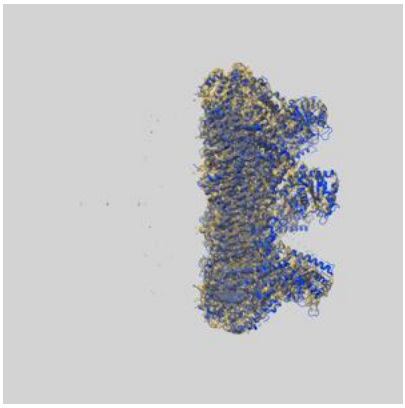


Z

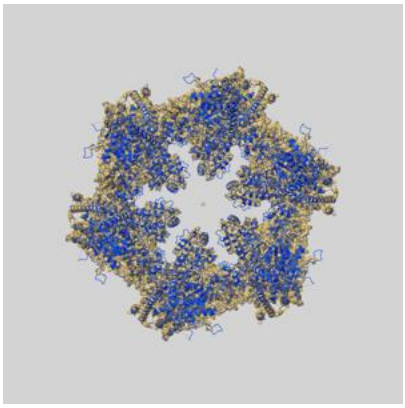
9.1.2 Map-model assembly overlay



X



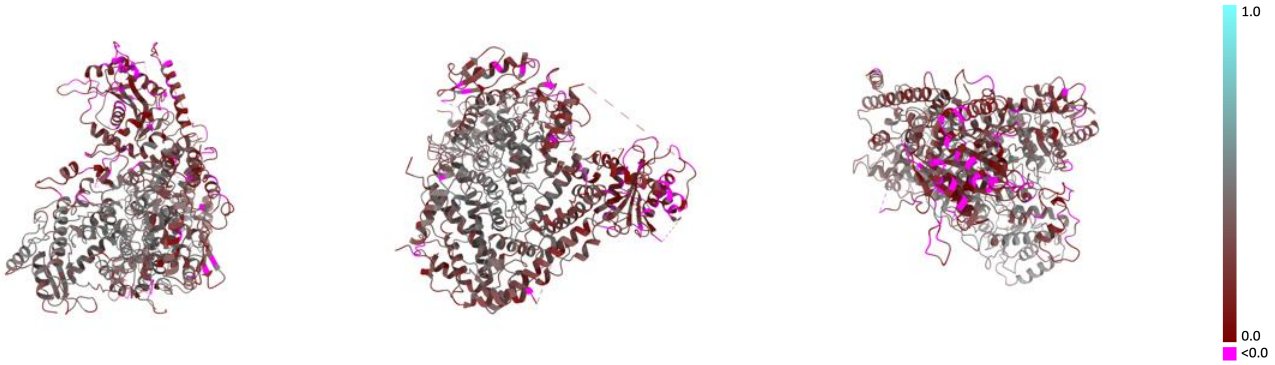
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0407 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.

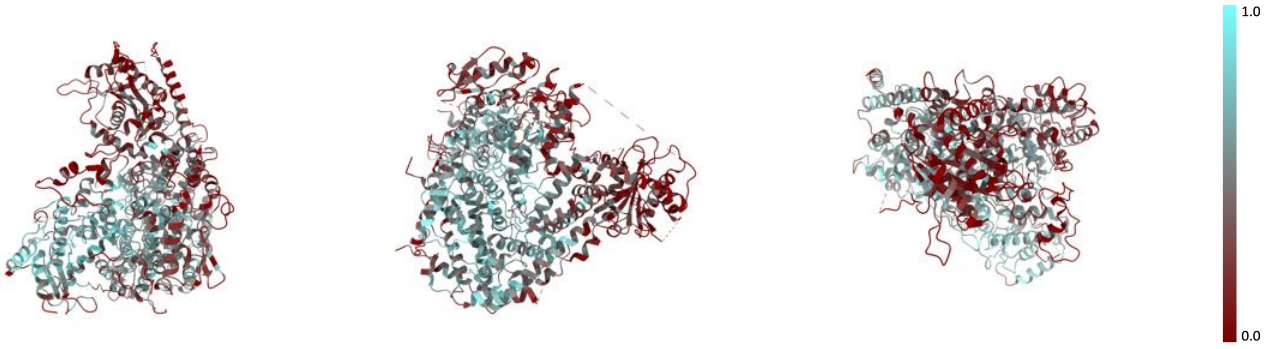
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

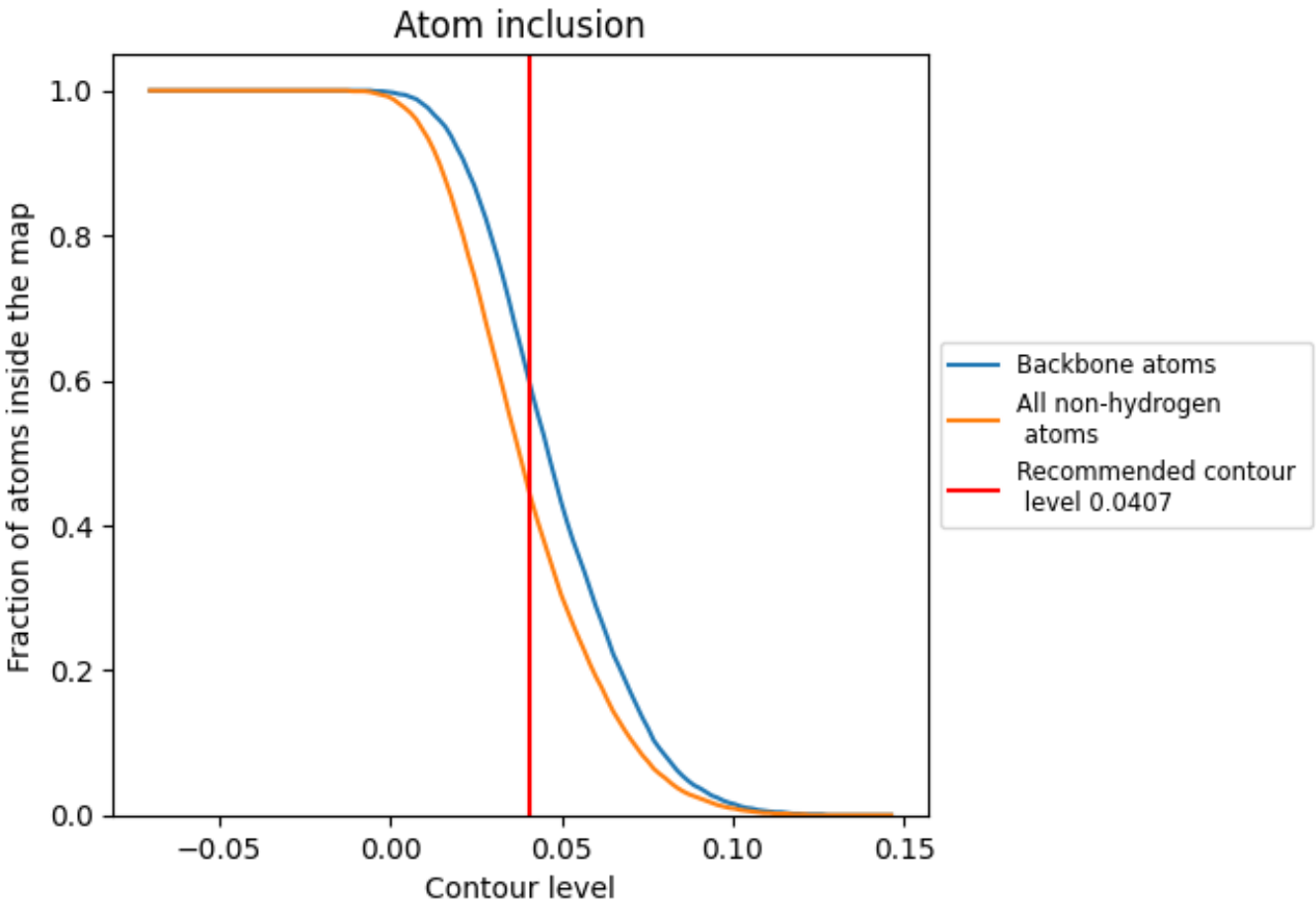
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0407).

9.4 Atom inclusion (i)



At the recommended contour level, 59% of all backbone atoms, 44% 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 (0.0407) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4420	0.3100
A	0.3140	0.2580
B	0.5540	0.3590
C	0.4930	0.3020