



Full wwPDB EM Validation Report ⓘ

Nov 12, 2022 – 09:27 AM EST

PDB ID : 6PIG
EMDB ID : EMD-20350
Title : V. cholerae ThiQ-Cascade complex, closed conformation
Authors : Halpin-Healy, T.; Klompe, S.; Sternberg, S.H.
Deposited on : 2019-06-26
Resolution : 3.50 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:

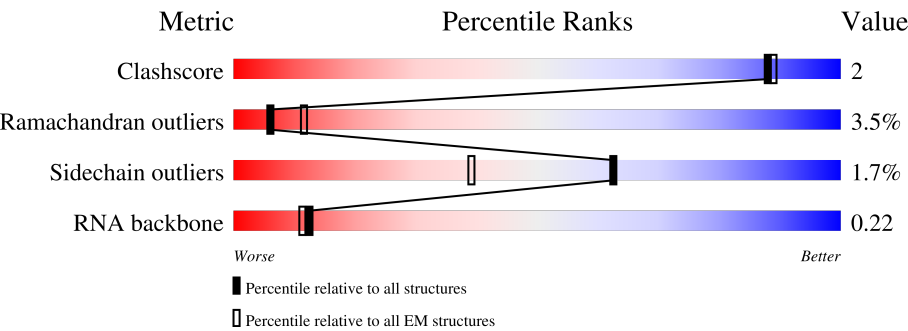
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 3.50 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
RNA backbone	4643	859

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	1	60	<div><div>7%</div><div>52%</div><div>47%</div><div>.</div></div>
2	A	343	<div><div>11%</div><div>88%</div><div>9%</div><div>.</div></div>
2	B	343	<div><div>7%</div><div>90%</div><div>8%</div><div>..</div></div>
2	C	343	<div><div>5%</div><div>92%</div><div>6%</div><div>.</div></div>
2	D	343	<div><div>5%</div><div>90%</div><div>8%</div><div>..</div></div>
2	E	343	<div><div>6%</div><div>90%</div><div>9%</div><div>.</div></div>
2	F	343	<div><div>5%</div><div>84%</div><div>6%</div><div>10%</div></div>

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Mol	Chain	Length	Quality of chain
3	G	511	<div><div></div><div>37%</div><div></div><div>86%</div><div></div><div>13%</div><div>..</div></div>
4	H	198	<div><div></div><div>59%</div><div></div><div>83%</div><div></div><div>15%</div><div>..</div></div>
5	I	358	<div><div></div><div>80%</div><div></div><div>88%</div><div></div><div>10%</div><div>.</div></div>
6	J	369	<div><div></div><div>79%</div><div></div><div>86%</div><div></div><div>11%</div><div>.</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 28867 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 RNA chain called RNA (60-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	60	Total	C	N	O	P	0	0
			1271	569	219	424	59		

- Molecule 2 is a protein called cas7 type I-F CRISPR-associated protein Csy3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	343	Total	C	N	O	S	0	0
			2742	1742	471	515	14		
2	B	339	Total	C	N	O	S	0	0
			2714	1727	467	506	14		
2	C	338	Total	C	N	O	S	0	0
			2705	1721	465	505	14		
2	D	338	Total	C	N	O	S	0	0
			2705	1721	465	505	14		
2	E	338	Total	C	N	O	S	0	0
			2705	1721	465	505	14		
2	F	310	Total	C	N	O	S	0	0
			2509	1603	431	461	14		

- Molecule 3 is a protein called cas5_8 naturally occurring fusion protein from *Vibrio cholerae* transposon Tn6677.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	511	Total	C	N	O	S	0	0
			4009	2533	699	757	20		

- Molecule 4 is a protein called type I-F CRISPR-associated endoribonuclease Cas6/Csy4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	197	Total	C	N	O	S	0	0
			1606	1022	285	292	7		

- Molecule 5 is a protein called TniQ monomer 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	357	Total	C	N	O	S	0	0
			2923	1875	508	525	15		

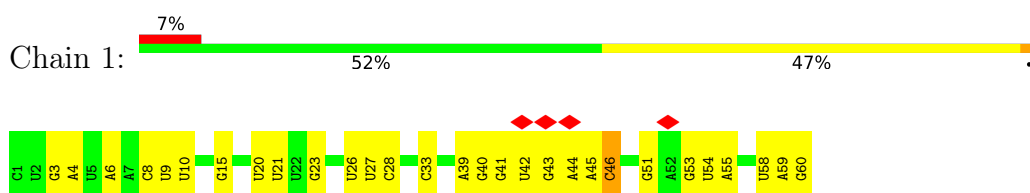
- Molecule 6 is a protein called TniQ monomer 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	368	Total	C	N	O	S	0	0
			2978	1909	515	538	16		

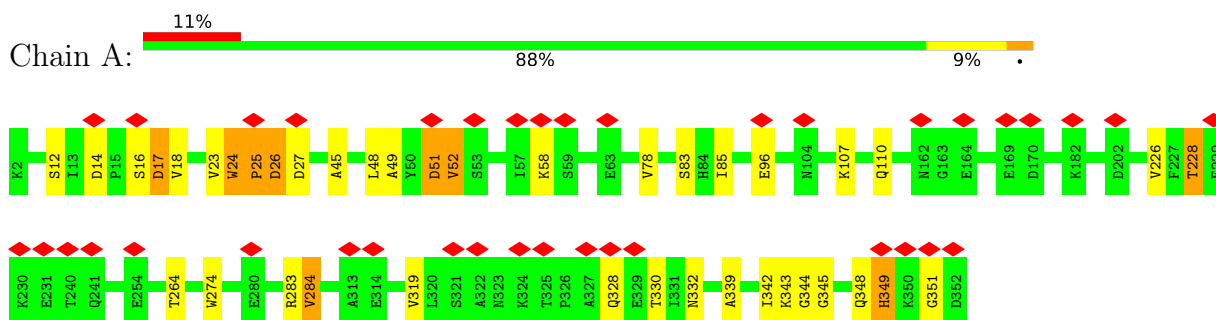
3 Residue-property plots

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

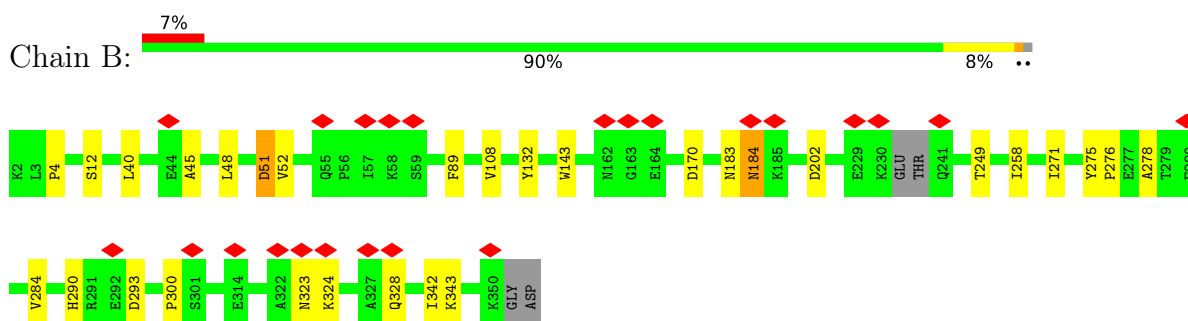
- Molecule 1: RNA (60-MER)



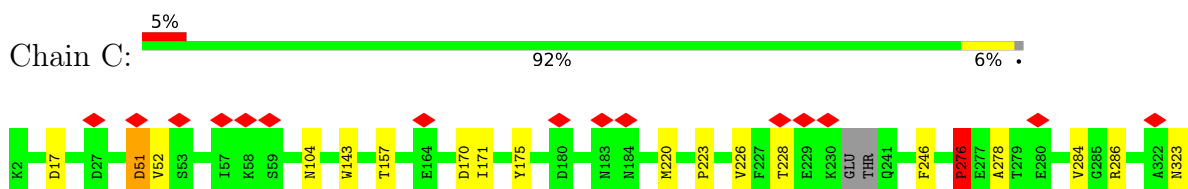
- Molecule 2: cas7 type I-F CRISPR-associated protein Csy3

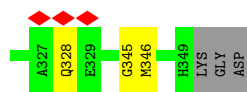


- Molecule 2: cas7 type I-F CRISPR-associated protein Csy3

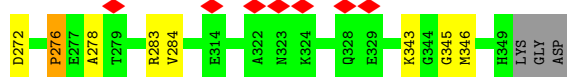
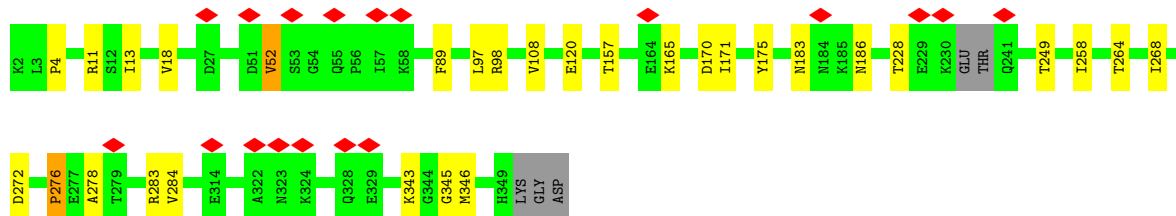
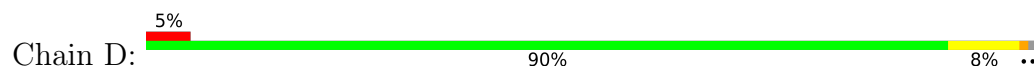


- Molecule 2: cas7 type I-F CRISPR-associated protein Csy3

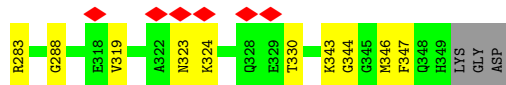
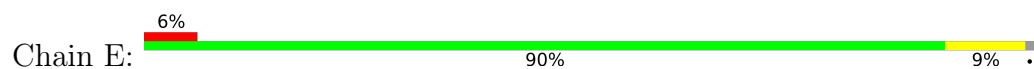




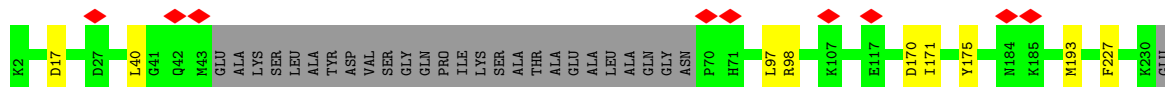
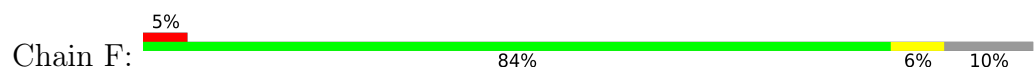
- Molecule 2: cas7 type I-F CRISPR-associated protein Csy3



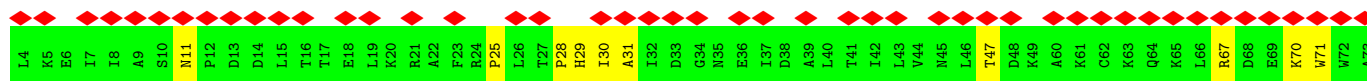
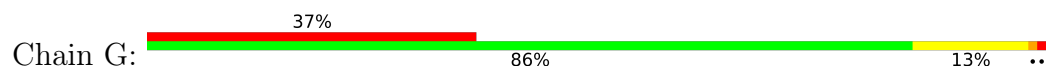
- Molecule 2: cas7 type I-F CRISPR-associated protein Csy3

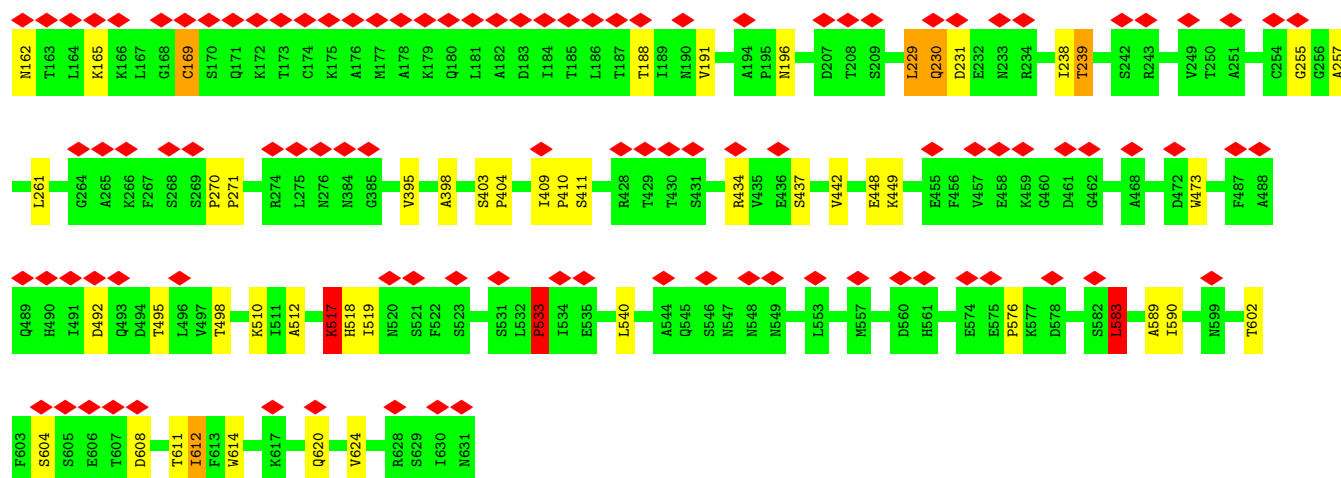


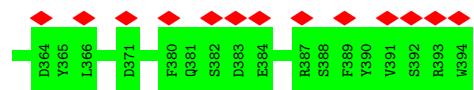
- Molecule 2: cas7 type I-F CRISPR-associated protein Csy3



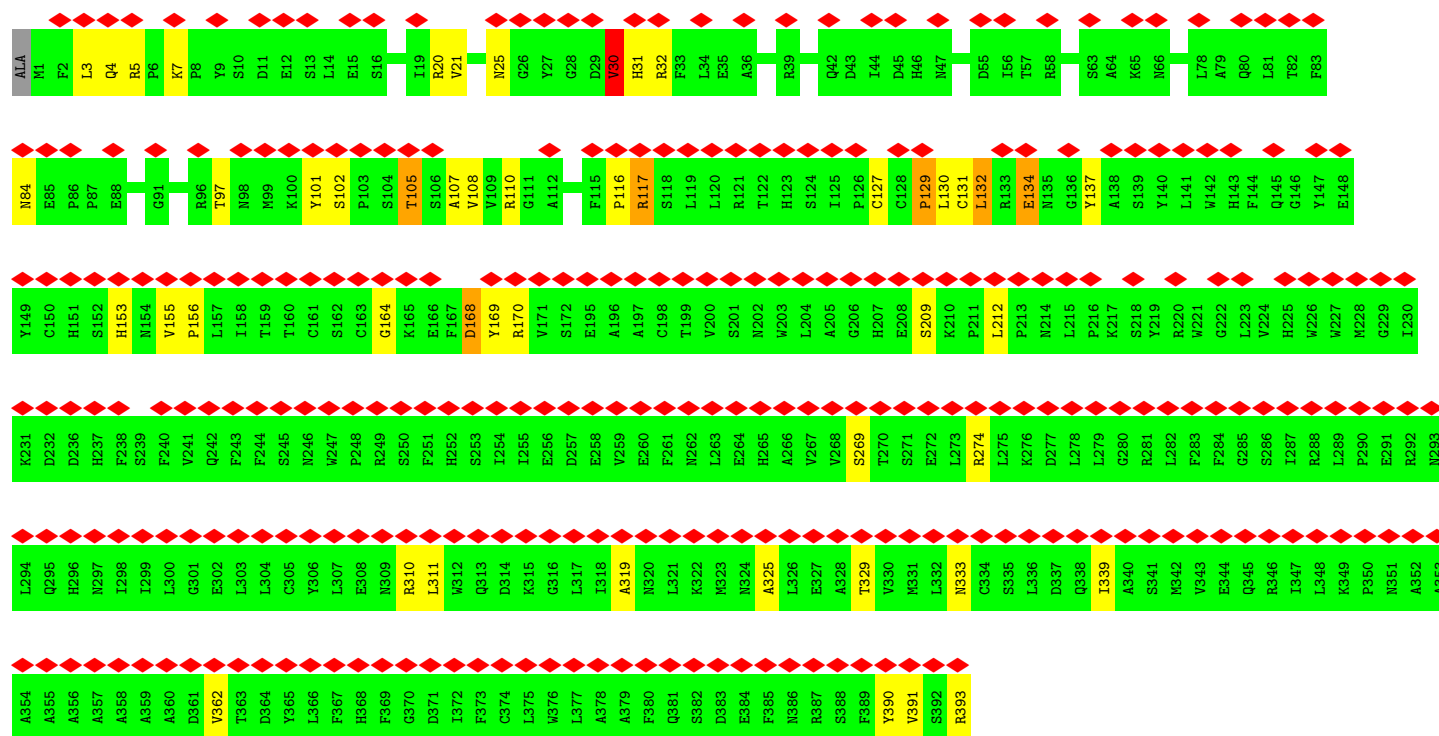
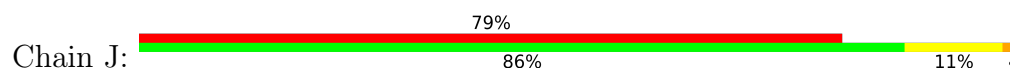
- Molecule 3: cas5_8 naturally occurring fusion protein from Vibrio cholerae transposon Tn6677







• Molecule 6: ThiQ monomer 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.130	Depositor
Minimum map value	-0.085	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	285.0, 285.0, 285.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	Depositor

5 Model quality

5.1 Standard geometry

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	1	0.24	0/1419	0.67	0/2209
2	A	0.69	0/2813	0.79	0/3821
2	B	0.68	0/2785	0.78	0/3783
2	C	0.68	0/2776	0.78	1/3772 (0.0%)
2	D	0.68	0/2776	0.78	0/3772
2	E	0.68	0/2776	0.78	0/3772
2	F	0.68	0/2577	0.78	0/3498
3	G	0.70	0/4098	0.81	1/5563 (0.0%)
4	H	0.69	0/1643	0.82	0/2216
5	I	0.69	0/3005	0.81	0/4071
6	J	0.69	0/3060	0.81	0/4150
All	All	0.67	0/29728	0.79	2/40627 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	3
2	B	0	4
2	D	0	3
2	E	0	4
2	F	0	1
3	G	0	13
4	H	0	4
5	I	0	13
6	J	0	9
All	All	0	54

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	533	PRO	N-CA-CB	-5.54	96.50	102.60
2	C	276	PRO	N-CA-CB	-5.20	96.88	102.60

There are no chirality outliers.

All (54) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	24	TRP	Peptide
2	A	26	ASP	Peptide
2	A	348	GLN	Peptide
2	B	183	ASN	Peptide
2	B	184	ASN	Peptide
2	B	275	TYR	Peptide
2	B	343	LYS	Peptide
2	D	183	ASN	Peptide
2	D	186	ASN	Peptide
2	D	343	LYS	Peptide
2	E	183	ASN	Peptide
2	E	275	TYR	Peptide
2	E	343	LYS	Peptide
2	E	344	GLY	Peptide
2	F	275	TYR	Peptide
3	G	11	ASN	Peptide
3	G	188	THR	Peptide
3	G	229	LEU	Peptide
3	G	230	GLN	Peptide
3	G	231	ASP	Peptide
3	G	271	PRO	Peptide
3	G	28	PRO	Peptide
3	G	30	ILE	Peptide
3	G	448	GLU	Peptide
3	G	517	LYS	Peptide
3	G	583	LEU	Peptide
3	G	70	LYS	Peptide
3	G	96	GLY	Peptide
4	H	11	LEU	Peptide
4	H	140	GLN	Peptide
4	H	179	SER	Peptide
4	H	180	ILE	Peptide
5	I	100	LYS	Peptide
5	I	102	SER	Peptide
5	I	125	ILE	Peptide
5	I	130	LEU	Peptide

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Mol	Chain	Res	Type	Group
5	I	132	LEU	Peptide
5	I	143	HIS	Peptide
5	I	144	PHE	Peptide
5	I	145	GLN	Peptide
5	I	152	SER	Peptide
5	I	202	ASN	Peptide
5	I	238	PHE	Peptide
5	I	239	SER	Peptide
5	I	7	LYS	Peptide
6	J	129	PRO	Peptide
6	J	132	LEU	Peptide
6	J	153	HIS	Peptide
6	J	164	GLY	Peptide
6	J	168	ASP	Peptide
6	J	3	LEU	Peptide
6	J	30	VAL	Peptide
6	J	390	TYR	Peptide
6	J	7	LYS	Peptide

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	1	1271	0	643	3	0
2	A	2742	0	2663	16	0
2	B	2714	0	2643	10	0
2	C	2705	0	2630	7	0
2	D	2705	0	2630	9	0
2	E	2705	0	2630	9	0
2	F	2509	0	2447	7	0
3	G	4009	0	3977	21	0
4	H	1606	0	1594	13	0
5	I	2923	0	2837	4	0
6	J	2978	0	2889	14	0
All	All	28867	0	27583	106	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 2.

All (106) 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:H:152:LEU:O	4:H:164:ARG:NH1	2.33	0.62
4:H:154:GLU:O	4:H:163:PHE:O	2.17	0.62
6:J:20:ARG:HD2	6:J:132:LEU:HD13	1.82	0.62
6:J:132:LEU:O	6:J:132:LEU:HD12	1.98	0.62
2:D:249:THR:HG23	2:D:258:ILE:HD12	1.83	0.59
5:I:155:VAL:HB	5:I:156:PRO:HD3	1.85	0.59
2:A:14:ASP:O	3:G:510:LYS:NZ	2.35	0.57
2:A:319:VAL:HG21	2:A:330:THR:HG21	1.87	0.57
3:G:517:LYS:O	3:G:519:ILE:N	2.36	0.57
6:J:155:VAL:N	6:J:156:PRO:HD2	2.21	0.56
2:B:4:PRO:HG3	2:B:108:VAL:HG21	1.87	0.56
3:G:25:PRO:HG3	3:G:122:SER:HB3	1.88	0.55
4:H:104:CYS:SG	4:H:168:ARG:NH2	2.81	0.54
4:H:59:VAL:HG11	4:H:197:PRO:HD2	1.91	0.53
3:G:82:ARG:HB3	3:G:99:ARG:HD3	1.90	0.53
4:H:162:ASN:HD22	4:H:162:ASN:N	2.06	0.53
3:G:576:PRO:HB3	3:G:589:ALA:HB2	1.91	0.52
5:I:18:PHE:HA	5:I:21:VAL:HG12	1.93	0.51
4:H:156:SER:HA	4:H:163:PHE:HE2	1.76	0.51
1:1:4:A:C2	3:G:583:LEU:HD21	2.46	0.50
2:B:132:TYR:CE1	2:B:271:ILE:HD11	2.46	0.50
2:B:51:ASP:O	2:B:52:VAL:HG23	2.12	0.50
3:G:270:PRO:HG2	3:G:602:THR:HG21	1.93	0.50
3:G:540:LEU:O	3:G:612:ILE:HG22	2.11	0.50
3:G:159:PRO:O	3:G:160:LEU:HG	2.12	0.49
2:A:274:TRP:HB3	2:A:332:ASN:HB3	1.95	0.49
3:G:495:THR:HA	3:G:498:THR:HG22	1.95	0.49
2:D:98:ARG:NH1	2:D:120:GLU:OE1	2.46	0.49
2:C:220:MET:SD	2:D:11:ARG:NH2	2.87	0.48
2:B:132:TYR:CZ	2:B:271:ILE:HD11	2.48	0.48
2:A:25:PRO:HD3	2:A:83:SER:HB2	1.95	0.48
6:J:101:TYR:HB2	6:J:105:THR:HB	1.94	0.48
3:G:492:ASP:HB2	3:G:495:THR:HG22	1.95	0.48
2:E:17:ASP:HB3	2:E:258:ILE:HG12	1.95	0.47
6:J:30:VAL:O	6:J:32:ARG:N	2.47	0.47
3:G:67:ARG:NH1	3:G:169:CYS:SG	2.79	0.47
6:J:129:PRO:O	6:J:130:LEU:HG	2.13	0.47
6:J:127:CYS:HB3	6:J:169:TYR:HB2	1.96	0.47
2:A:284:VAL:HG11	2:A:339:ALA:HB1	1.96	0.47
2:D:13:ILE:HG21	2:D:268:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:171:ILE:HG23	2:C:175:TYR:HB2	1.96	0.47
5:I:279:LEU:HD12	5:I:279:LEU:O	2.14	0.47
6:J:325:ALA:HB3	6:J:362:VAL:HA	1.98	0.46
1:1:6:A:H4'	2:A:344:GLY:HA2	1.97	0.46
2:F:346:MET:N	2:F:346:MET:SD	2.89	0.46
3:G:395:VAL:HG21	3:G:398:ALA:HB2	1.98	0.46
6:J:134:GLU:HB2	6:J:137:TYR:CZ	2.51	0.46
2:B:249:THR:HB	2:B:258:ILE:HD12	1.96	0.46
2:A:107:LYS:HA	2:A:110:GLN:HE21	1.82	0.45
6:J:329:THR:HG22	6:J:339:ILE:HD13	1.97	0.45
2:A:18:VAL:HG23	2:A:264:THR:HG21	1.98	0.45
3:G:47:THR:HG22	3:G:134:ALA:HB3	1.98	0.45
4:H:184:TYR:O	4:H:186:LEU:HB2	2.15	0.45
2:D:157:THR:HG22	2:D:165:LYS:HG2	1.97	0.45
3:G:239:THR:HG22	3:G:473:TRP:HE1	1.82	0.45
3:G:230:GLN:HE22	3:G:238:ILE:HD11	1.82	0.45
6:J:311:LEU:O	6:J:319:ALA:HB2	2.17	0.45
2:A:51:ASP:O	2:A:52:VAL:HG23	2.16	0.44
2:A:12:SER:HB2	2:A:342:ILE:HG23	1.99	0.44
2:E:18:VAL:HG22	2:E:89:PHE:HB3	2.00	0.44
2:C:51:ASP:O	2:C:52:VAL:HG23	2.18	0.43
2:E:152:TRP:HA	2:E:212:THR:O	2.18	0.43
1:1:46:C:O2'	4:H:161:ARG:NH1	2.52	0.43
2:A:78:VAL:HG22	2:A:85:ILE:HD11	2.00	0.43
2:A:45:ALA:HB3	2:A:48:LEU:HD12	2.01	0.43
2:D:4:PRO:HG3	2:D:108:VAL:HG21	1.99	0.43
4:H:46:LEU:HG	4:H:53:GLY:HA3	1.99	0.43
4:H:154:GLU:HG3	4:H:163:PHE:CZ	2.53	0.43
2:A:49:ALA:HB1	2:B:300:PRO:HG3	2.00	0.43
2:E:346:MET:SD	2:E:346:MET:N	2.89	0.43
2:E:323:ASN:HA	2:E:324:LYS:HA	1.85	0.42
2:B:290:HIS:ND1	2:B:293:ASP:OD1	2.52	0.42
3:G:95:GLU:HB2	3:G:196:ASN:HD21	1.85	0.42
3:G:608:ASP:O	3:G:611:THR:OG1	2.38	0.42
2:D:345:GLY:HA2	2:D:346:MET:HA	1.87	0.42
3:G:162:ASN:HA	3:G:165:LYS:HG2	2.00	0.42
4:H:156:SER:CA	4:H:163:PHE:HE2	2.32	0.42
6:J:105:THR:HG23	6:J:117:ARG:HB2	2.02	0.42
2:F:171:ILE:HG23	2:F:175:TYR:HB2	2.02	0.42
4:H:147:ALA:HA	4:H:148:HIS:HA	1.90	0.42
2:E:226:VAL:HG23	2:E:228:THR:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:409:ILE:HG13	3:G:410:PRO:HD2	2.01	0.42
2:A:226:VAL:HG23	2:A:228:THR:HG22	2.02	0.41
2:C:345:GLY:HA2	2:C:346:MET:HA	1.85	0.41
2:F:40:LEU:HD11	4:H:145:ALA:HB1	2.02	0.41
3:G:191:VAL:HG21	3:G:590:ILE:HD11	2.03	0.41
2:D:171:ILE:HG23	2:D:175:TYR:HB2	2.02	0.41
2:F:315:HIS:O	2:F:318:GLU:HB3	2.20	0.41
2:C:226:VAL:HG13	2:C:228:THR:HG23	2.02	0.41
2:F:17:ASP:HB3	2:F:258:ILE:HG12	2.01	0.41
6:J:209:SER:HB3	6:J:212:LEU:HD13	2.01	0.41
2:D:18:VAL:HG23	2:D:264:THR:HG21	2.03	0.41
6:J:4:GLN:NE2	6:J:21:VAL:O	2.52	0.41
2:E:171:ILE:HG23	2:E:175:TYR:HB2	2.02	0.41
2:F:345:GLY:HA2	2:F:346:MET:HA	1.84	0.41
5:I:120:LEU:H	5:I:120:LEU:HD23	1.86	0.41
2:C:323:ASN:HA	2:C:324:LYS:HA	1.87	0.41
2:B:45:ALA:HB3	2:B:48:LEU:HD12	2.03	0.41
2:F:275:TYR:O	2:F:277:GLU:N	2.54	0.41
2:C:223:PRO:HG2	2:C:246:PHE:CD1	2.56	0.40
2:B:323:ASN:HA	2:B:324:LYS:HA	1.92	0.40
2:A:16:SER:O	2:A:17:ASP:HB2	2.21	0.40
2:B:12:SER:HB2	2:B:342:ILE:HG23	2.02	0.40
2:E:258:ILE:HG23	2:E:260:GLY:H	1.86	0.40
2:A:349:HIS:O	2:A:351:GLY:N	2.54	0.40
2:E:319:VAL:HG11	2:E:330:THR:HG21	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	339/343 (99%)	292 (86%)	34 (10%)	13 (4%)	3	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	335/343 (98%)	287 (86%)	41 (12%)	7 (2%)	7	38
2	C	334/343 (97%)	294 (88%)	32 (10%)	8 (2%)	6	35
2	D	334/343 (97%)	289 (86%)	38 (11%)	7 (2%)	7	38
2	E	334/343 (97%)	280 (84%)	48 (14%)	6 (2%)	8	41
2	F	304/343 (89%)	256 (84%)	41 (14%)	7 (2%)	6	36
3	G	505/511 (99%)	393 (78%)	89 (18%)	23 (5%)	2	21
4	H	195/198 (98%)	141 (72%)	45 (23%)	9 (5%)	2	21
5	I	349/358 (98%)	252 (72%)	74 (21%)	23 (7%)	1	13
6	J	362/369 (98%)	276 (76%)	72 (20%)	14 (4%)	3	25
All	All	3391/3494 (97%)	2760 (81%)	514 (15%)	117 (4%)	6	27

All (117) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	17	ASP
2	A	25	PRO
2	A	58	LYS
2	A	349	HIS
2	B	184	ASN
2	B	278	ALA
2	C	276	PRO
2	C	278	ALA
2	D	278	ALA
2	E	278	ALA
2	F	278	ALA
3	G	97	VAL
3	G	403	SER
3	G	411	SER
3	G	449	LYS
3	G	518	HIS
4	H	141	LYS
4	H	180	ILE
4	H	181	PHE
4	H	189	SER
5	I	121	ARG
5	I	125	ILE
5	I	133	ARG
5	I	145	GLN
5	I	157	LEU

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Mol	Chain	Res	Type
6	J	107	ALA
6	J	168	ASP
6	J	391	VAL
2	A	228	THR
2	B	170	ASP
2	C	51	ASP
2	C	170	ASP
2	D	52	VAL
2	D	272	ASP
2	D	276	PRO
2	E	51	ASP
2	F	193	MET
2	F	288	GLY
2	F	307	PHE
3	G	29	HIS
3	G	31	ALA
3	G	71	TRP
3	G	255	GLY
3	G	533	PRO
3	G	614	TRP
3	G	624	VAL
4	H	185	GLY
4	H	186	LEU
5	I	104	SER
5	I	128	CYS
5	I	131	CYS
5	I	142	TRP
5	I	153	HIS
5	I	203	TRP
5	I	240	PHE
6	J	84	ASN
2	A	27	ASP
2	A	51	ASP
2	B	51	ASP
2	C	328	GLN
2	D	170	ASP
2	E	170	ASP
2	F	170	ASP
2	F	276	PRO
3	G	229	LEU
3	G	257	ALA
3	G	261	LEU

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Mol	Chain	Res	Type
3	G	512	ALA
3	G	604	SER
3	G	612	ILE
3	G	620	GLN
4	H	150	HIS
4	H	190	GLU
5	I	126	PRO
5	I	140	TYR
5	I	144	PHE
5	I	231	LYS
5	I	238	PHE
6	J	105	THR
6	J	110	ARG
6	J	116	PRO
6	J	117	ARG
6	J	134	GLU
6	J	269	SER
2	A	328	GLN
2	B	143	TRP
2	B	276	PRO
2	C	143	TRP
2	D	228	THR
2	E	276	PRO
5	I	136	GLY
5	I	147	TYR
6	J	25	ASN
6	J	131	CYS
2	A	284	VAL
2	B	328	GLN
2	F	227	PHE
3	G	517	LYS
5	I	202	ASN
6	J	31	HIS
2	A	26	ASP
2	C	104	ASN
2	D	284	VAL
2	E	193	MET
3	G	434	ARG
3	G	437	SER
4	H	197	PRO
5	I	156	PRO
6	J	5	ARG

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Mol	Chain	Res	Type
5	I	103	PRO
2	A	52	VAL
2	A	24	TRP
3	G	404	PRO
2	A	345	GLY
2	E	288	GLY
5	I	216	PRO
2	C	284	VAL

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	
2	A	300/301 (100%)	296 (99%)	4 (1%)	69	86
2	B	297/301 (99%)	293 (99%)	4 (1%)	69	86
2	C	296/301 (98%)	292 (99%)	4 (1%)	67	85
2	D	296/301 (98%)	291 (98%)	5 (2%)	60	82
2	E	296/301 (98%)	291 (98%)	5 (2%)	60	82
2	F	277/301 (92%)	274 (99%)	3 (1%)	73	88
3	G	451/451 (100%)	444 (98%)	7 (2%)	62	83
4	H	177/178 (99%)	173 (98%)	4 (2%)	50	77
5	I	322/322 (100%)	315 (98%)	7 (2%)	52	78
6	J	323/323 (100%)	314 (97%)	9 (3%)	43	72
All	All	3035/3080 (98%)	2983 (98%)	52 (2%)	62	82

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	23	VAL
2	A	96	GLU
2	A	283	ARG
2	A	343	LYS
2	B	40	LEU

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Mol	Chain	Res	Type
2	B	89	PHE
2	B	202	ASP
2	B	284	VAL
2	C	17	ASP
2	C	157	THR
2	C	276	PRO
2	C	286	ARG
2	D	52	VAL
2	D	89	PHE
2	D	97	LEU
2	D	276	PRO
2	D	283	ARG
2	E	5	THR
2	E	74	ASP
2	E	97	LEU
2	E	283	ARG
2	E	347	PHE
2	F	97	LEU
2	F	98	ARG
2	F	284	VAL
3	G	77	ASN
3	G	93	ARG
3	G	169	CYS
3	G	239	THR
3	G	442	VAL
3	G	533	PRO
3	G	583	LEU
4	H	14	LEU
4	H	142	GLU
4	H	149	TYR
4	H	159	THR
5	I	56	ILE
5	I	92	LEU
5	I	123	HIS
5	I	220	ARG
5	I	268	VAL
5	I	272	GLU
5	I	336	LEU
6	J	30	VAL
6	J	97	THR
6	J	102	SER
6	J	108	VAL

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Mol	Chain	Res	Type
6	J	170	ARG
6	J	274	ARG
6	J	310	ARG
6	J	333	ASN
6	J	393	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	110	GLN
2	A	174	ASN
2	A	312	GLN
2	B	145	ASN
2	B	174	ASN
2	B	183	ASN
2	B	218	ASN
2	C	174	ASN
2	C	311	GLN
2	D	135	ASN
2	E	99	GLN
2	E	241	GLN
2	F	174	ASN
2	F	183	ASN
2	F	311	GLN
3	G	196	ASN
3	G	230	GLN
3	G	246	ASN
4	H	17	ASN
4	H	162	ASN
4	H	178	ASN
5	I	60	ASN
5	I	154	ASN
5	I	368	HIS
6	J	23	ASN
6	J	95	ASN
6	J	202	ASN
6	J	345	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	59/60 (98%)	27 (45%)	0

All (27) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	3	G
1	1	8	C
1	1	9	U
1	1	10	U
1	1	15	G
1	1	20	U
1	1	21	U
1	1	23	G
1	1	26	U
1	1	27	U
1	1	28	C
1	1	33	C
1	1	39	A
1	1	40	G
1	1	41	G
1	1	42	U
1	1	43	G
1	1	44	A
1	1	45	A
1	1	46	C
1	1	51	G
1	1	53	G
1	1	54	U
1	1	55	A
1	1	58	U
1	1	59	A
1	1	60	G

There are no RNA pucker outliers to report.

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 [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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	I	3
6	J	2
3	G	2
2	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	172:SER	C	195:GLU	N	29.87
1	I	162:SER	C	193:GLY	N	29.40
1	G	276:ASN	C	384:ASN	N	23.55
1	A	231:GLU	C	240:THR	N	12.70
1	G	49:LYS	C	60:ALA	N	12.32
1	I	355:LYS	C	361:ASP	N	10.75
1	J	232:ASP	C	236:ASP	N	8.45
1	I	233:SER	C	236:ASP	N	7.81

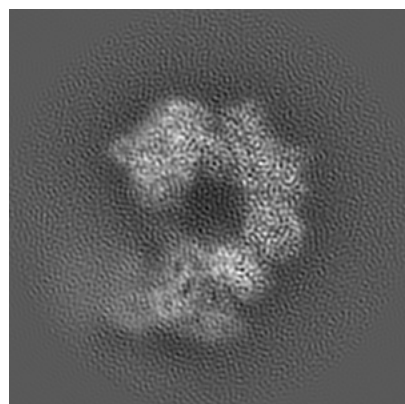
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20350. These allow visual inspection of the internal detail of the map and identification of artifacts.

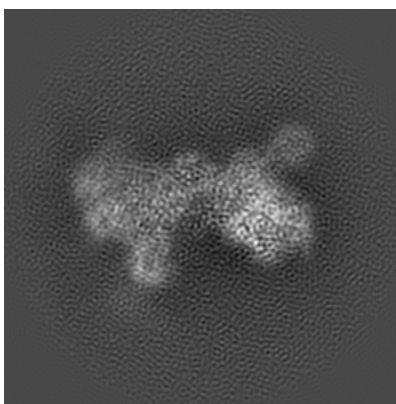
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

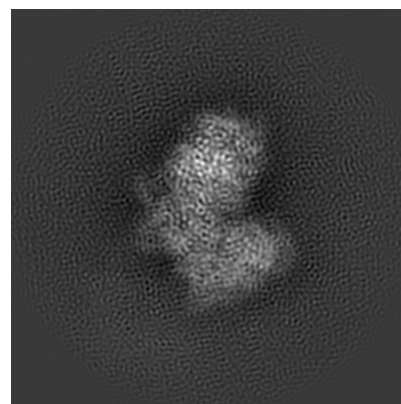
6.1.1 Primary map



X

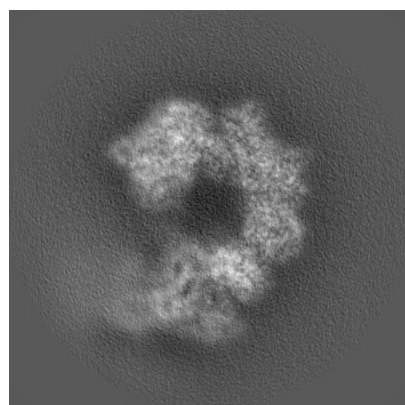


Y

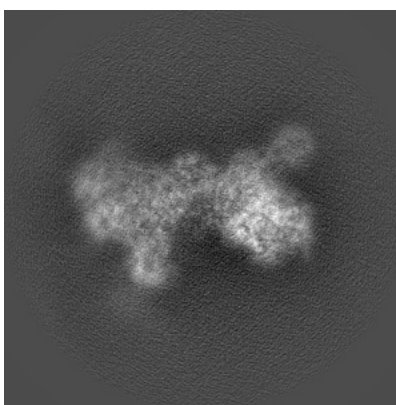


Z

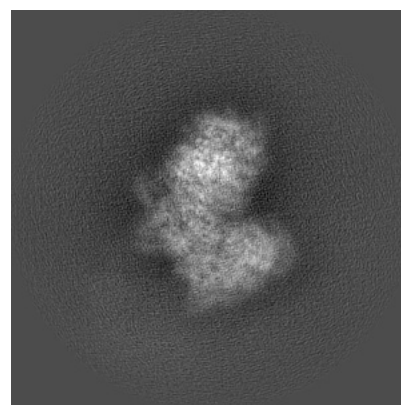
6.1.2 Raw map



X



Y

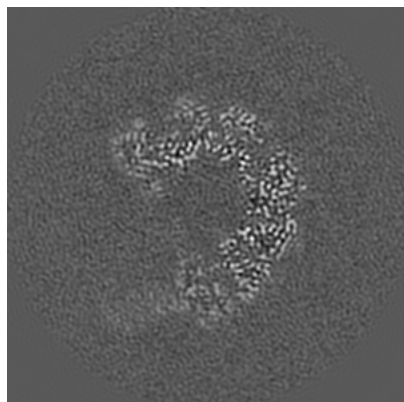


Z

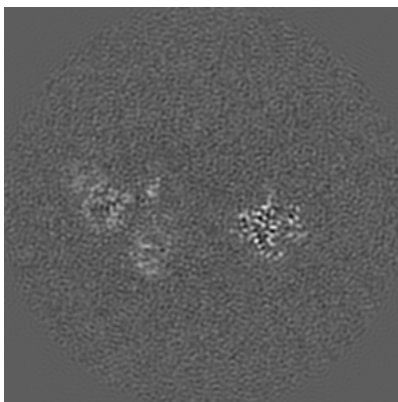
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

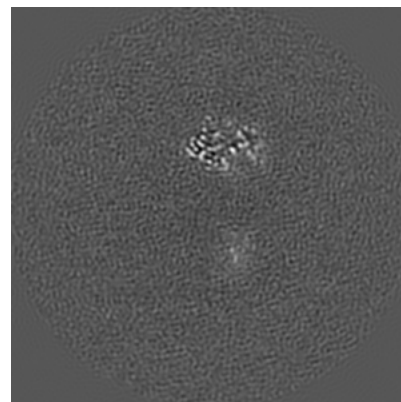
6.2.1 Primary map



X Index: 150

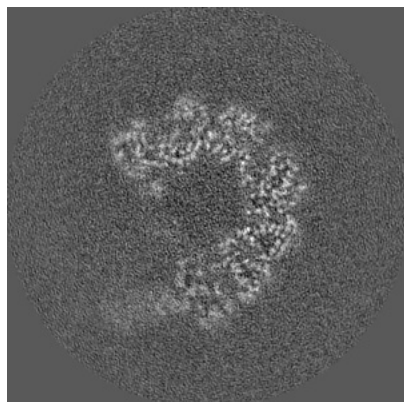


Y Index: 150

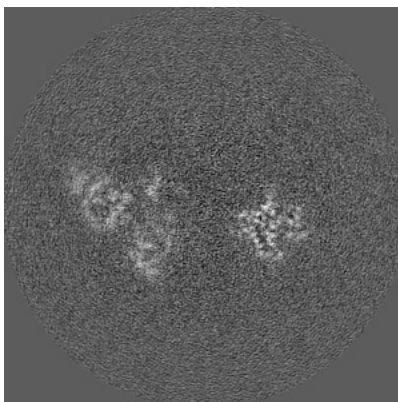


Z Index: 150

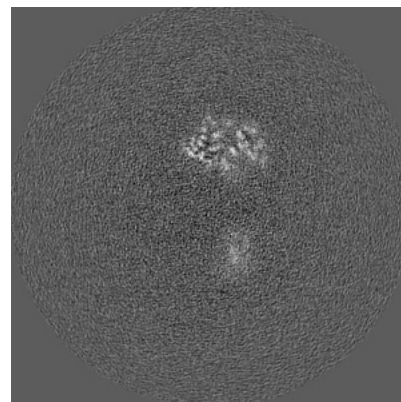
6.2.2 Raw map



X Index: 150



Y Index: 150

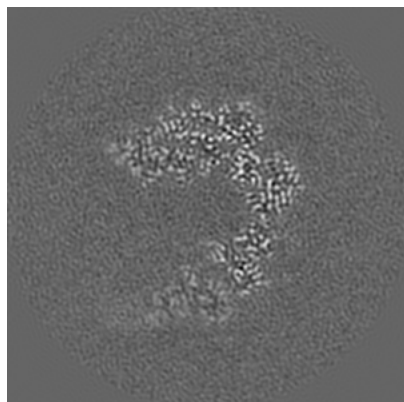


Z Index: 150

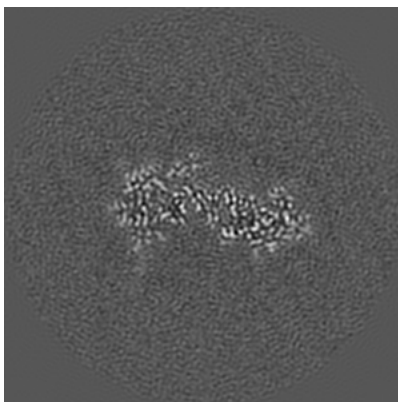
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

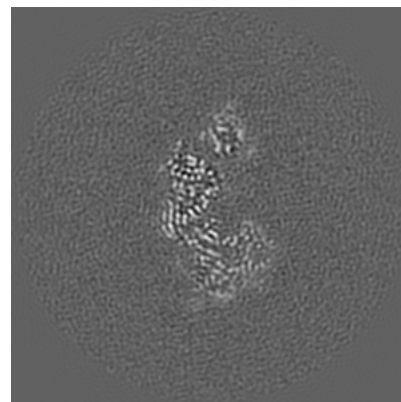
6.3.1 Primary map



X Index: 142

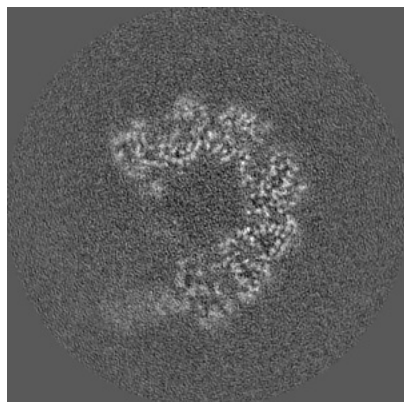


Y Index: 181

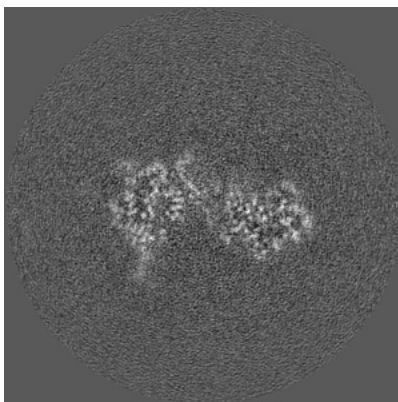


Z Index: 190

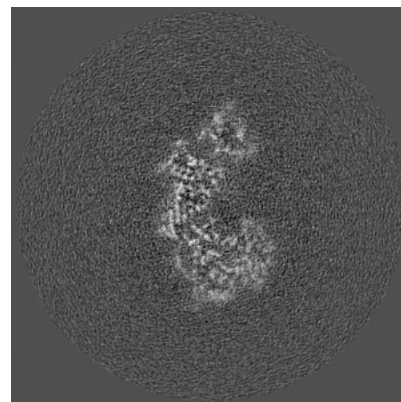
6.3.2 Raw map



X Index: 150



Y Index: 178

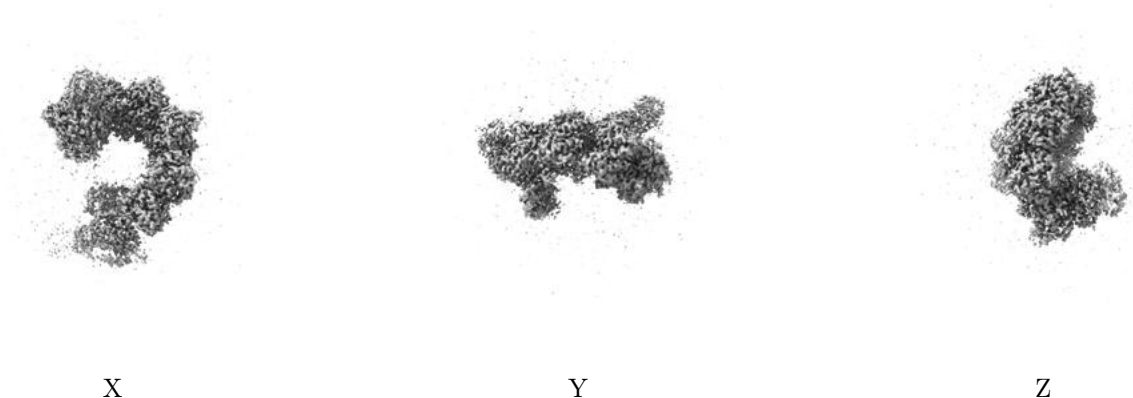


Z Index: 189

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

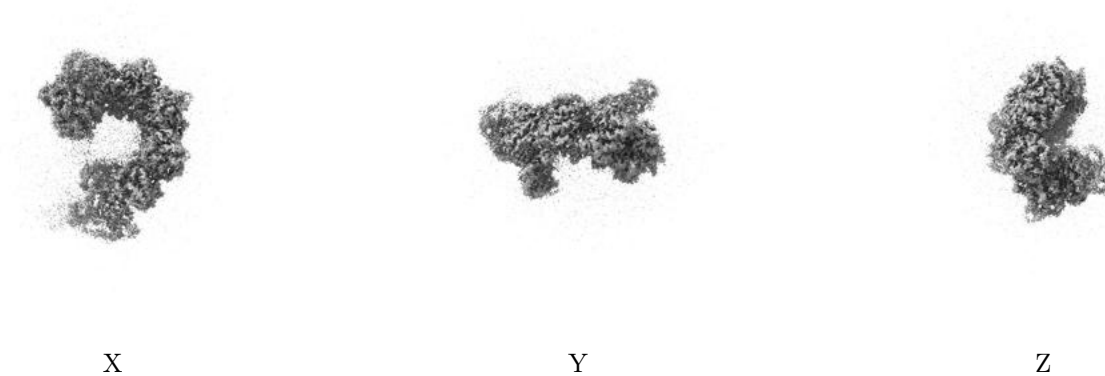
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

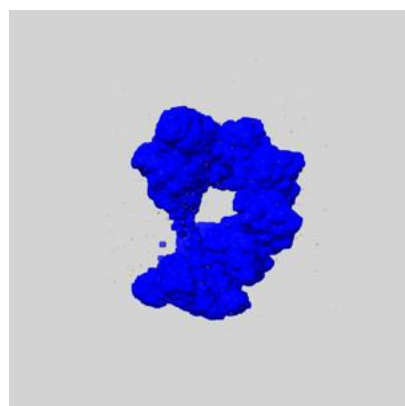
6.5 Mask visualisation [i](#)

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

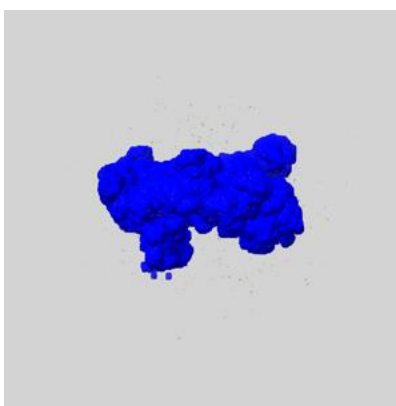
A mask typically either:

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

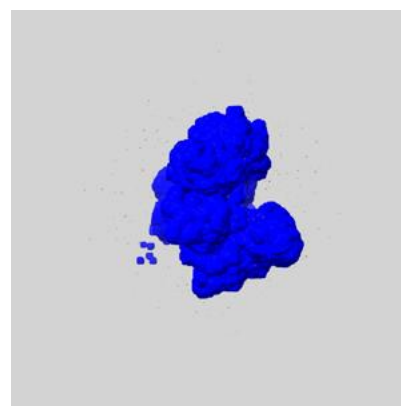
6.5.1 emd_20350_msk_1.map [i](#)



X



Y

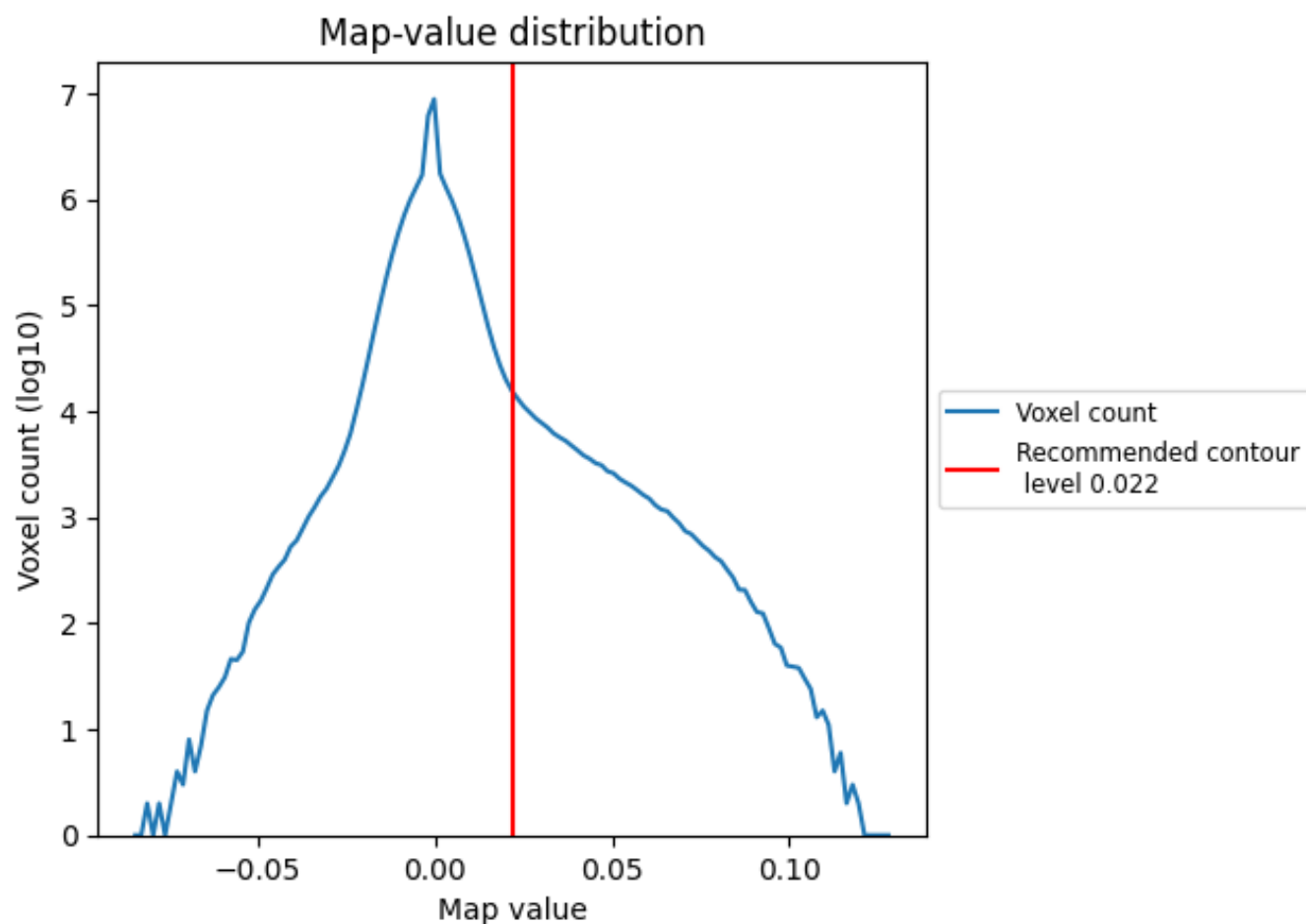


Z

7 Map analysis [i](#)

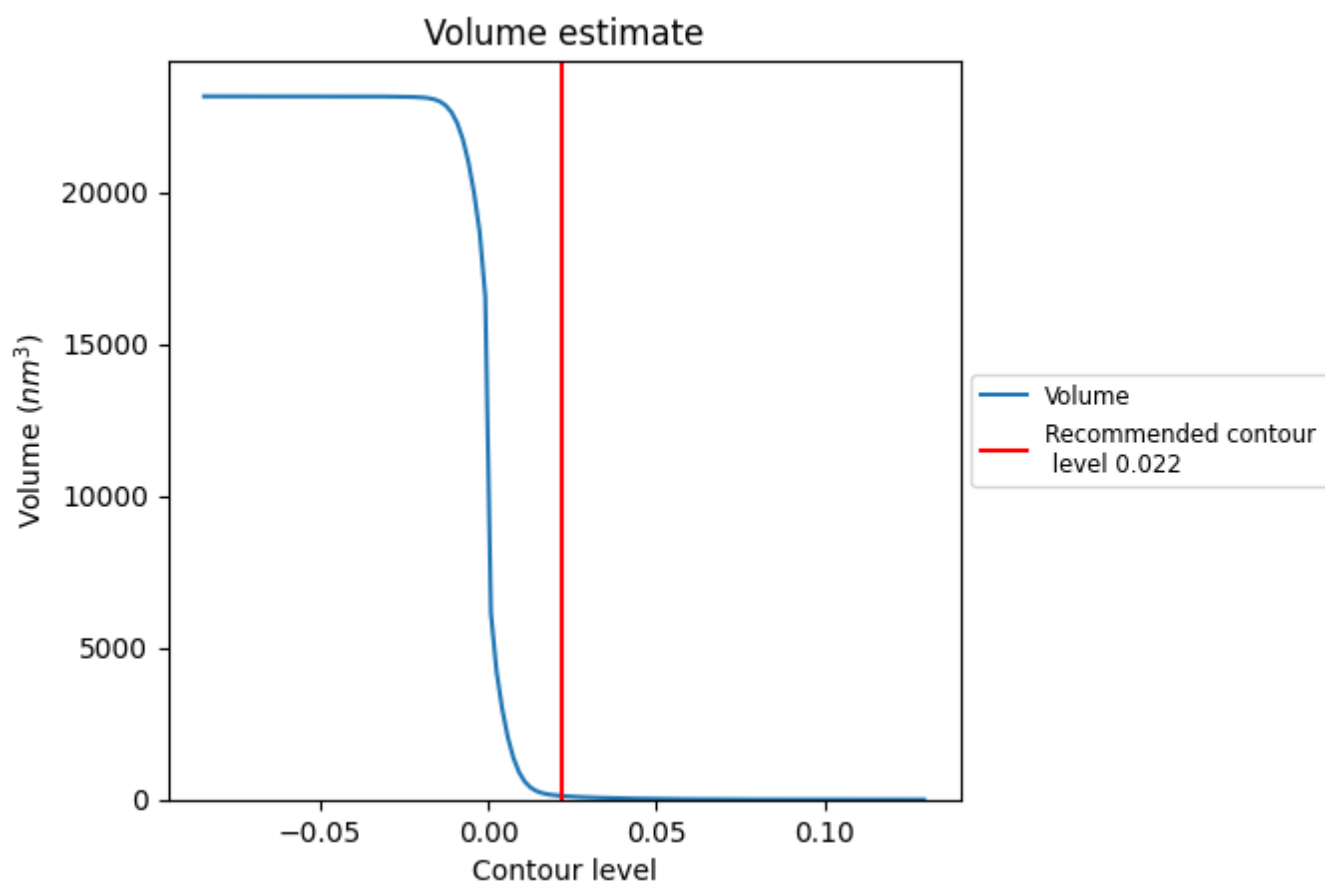
This section contains the results of statistical analysis of the map.

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.

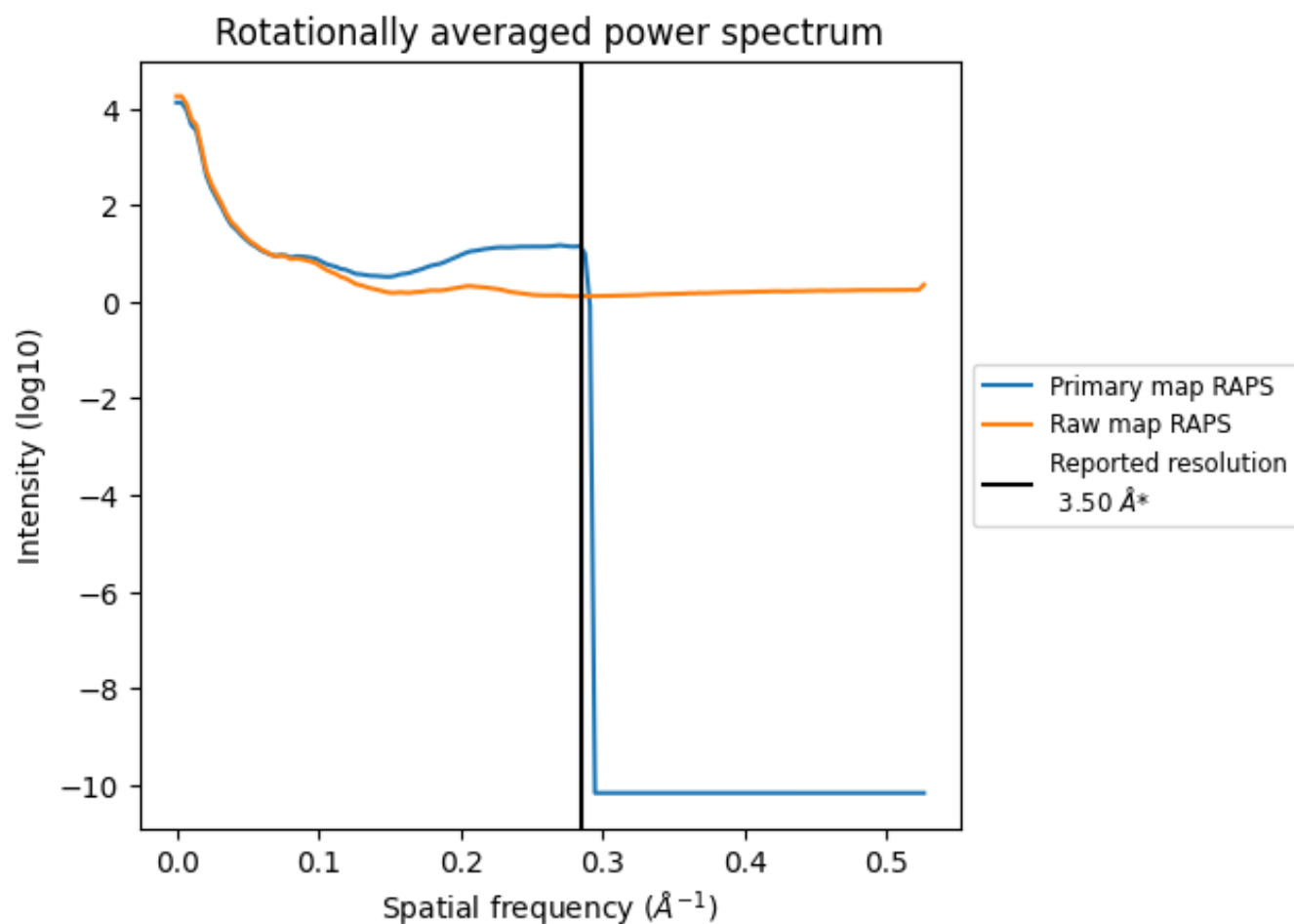
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 119 nm³; this corresponds to an approximate mass of 107 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 ⓘ

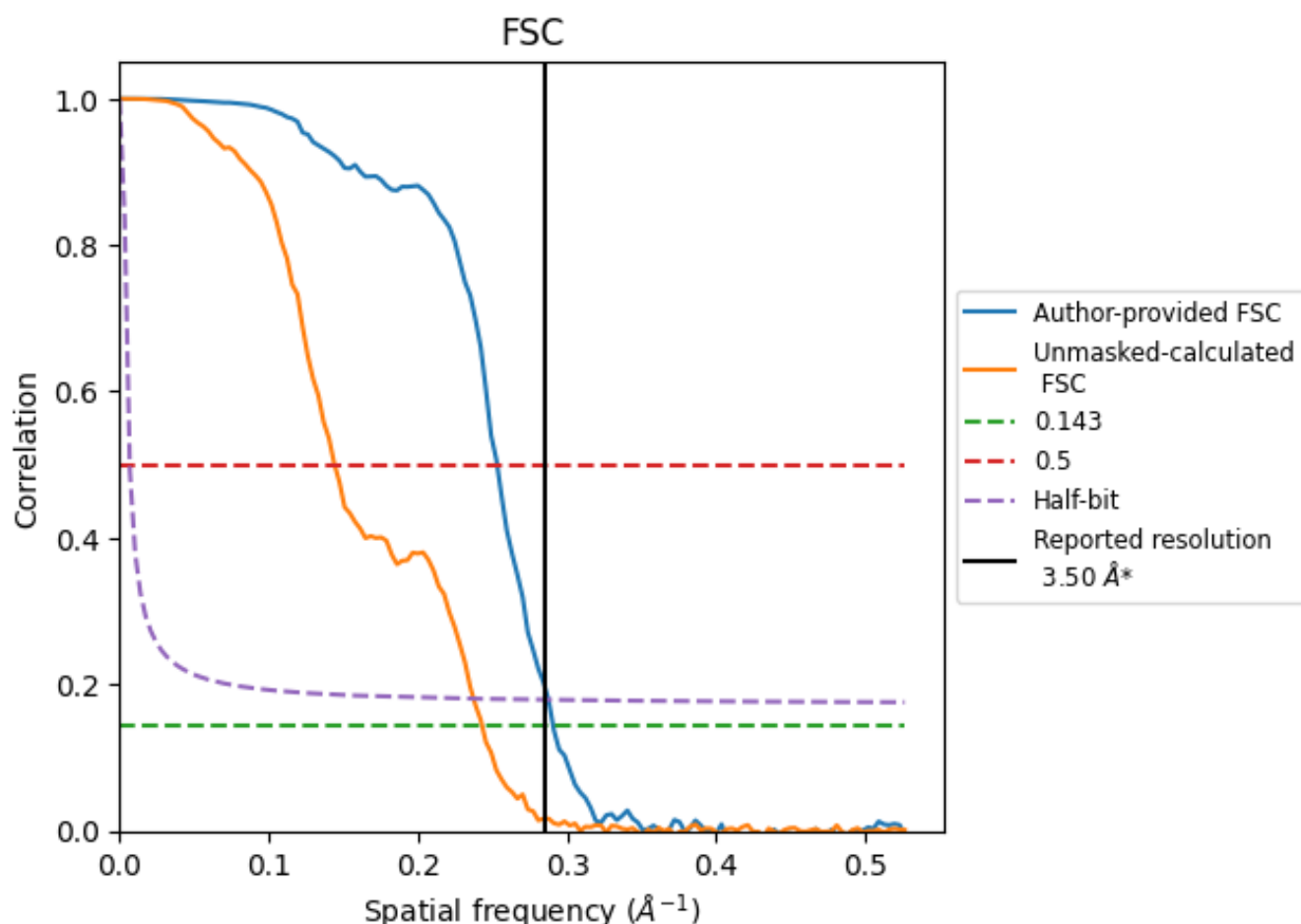


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

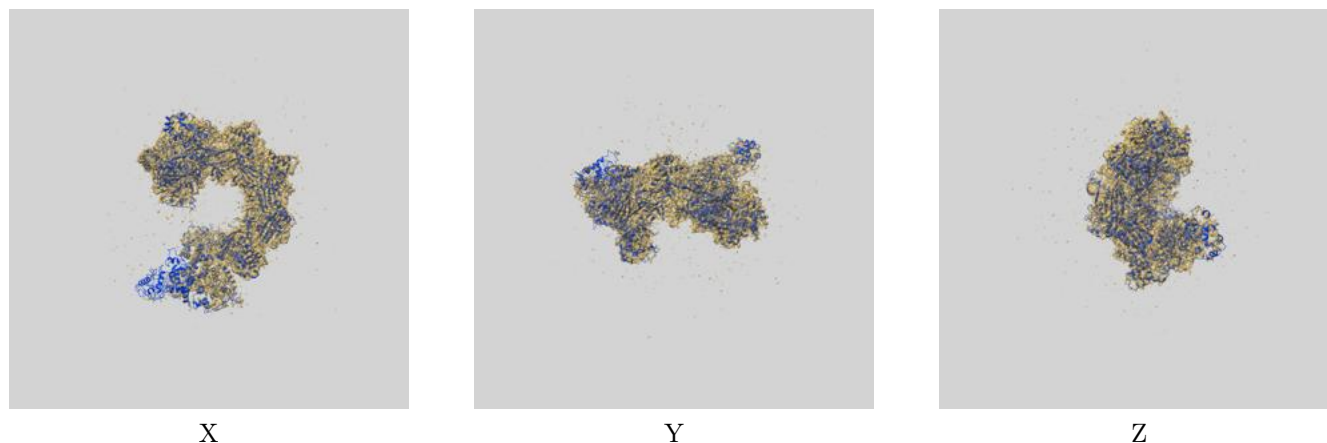
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.44	3.95	3.48
Unmasked-calculated*	4.11	6.94	4.21

*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 4.11 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

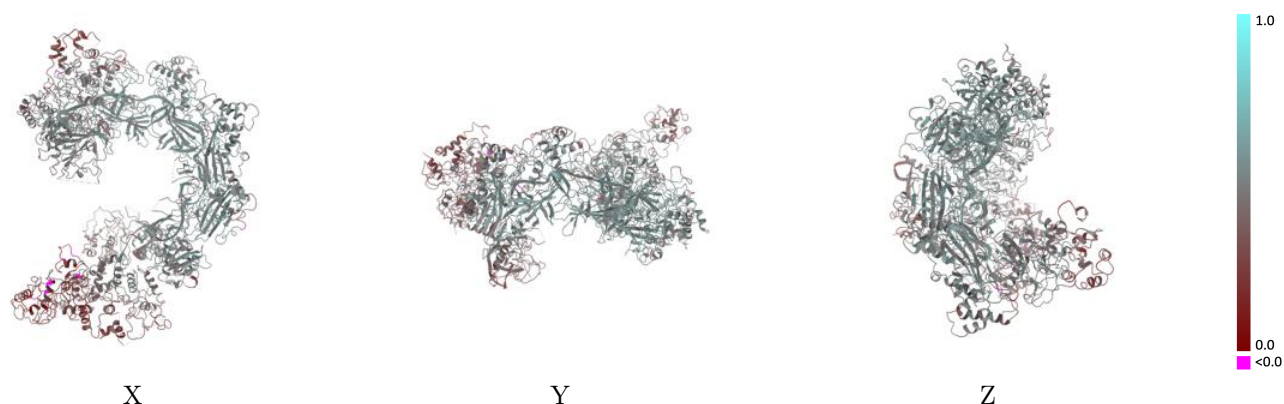
This section contains information regarding the fit between EMDB map EMD-20350 and PDB model 6PIG. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



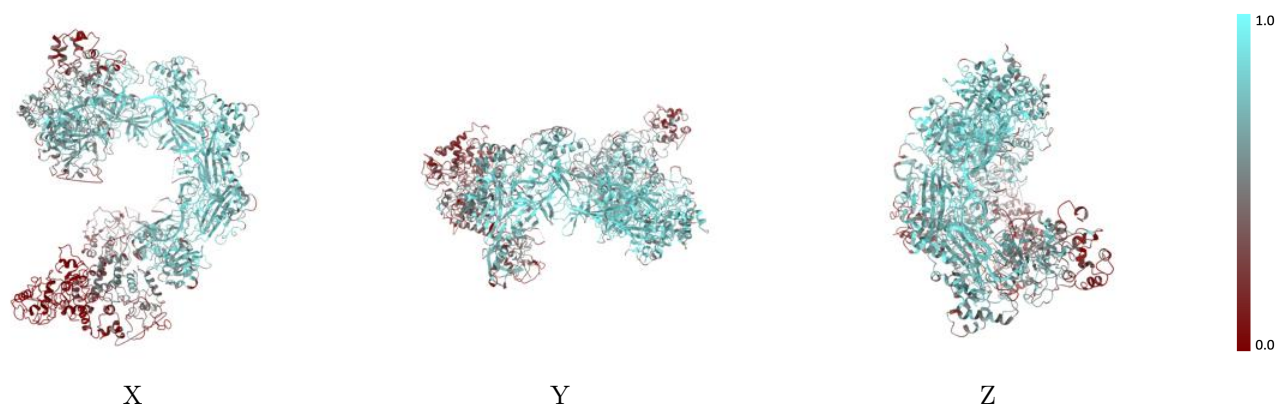
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



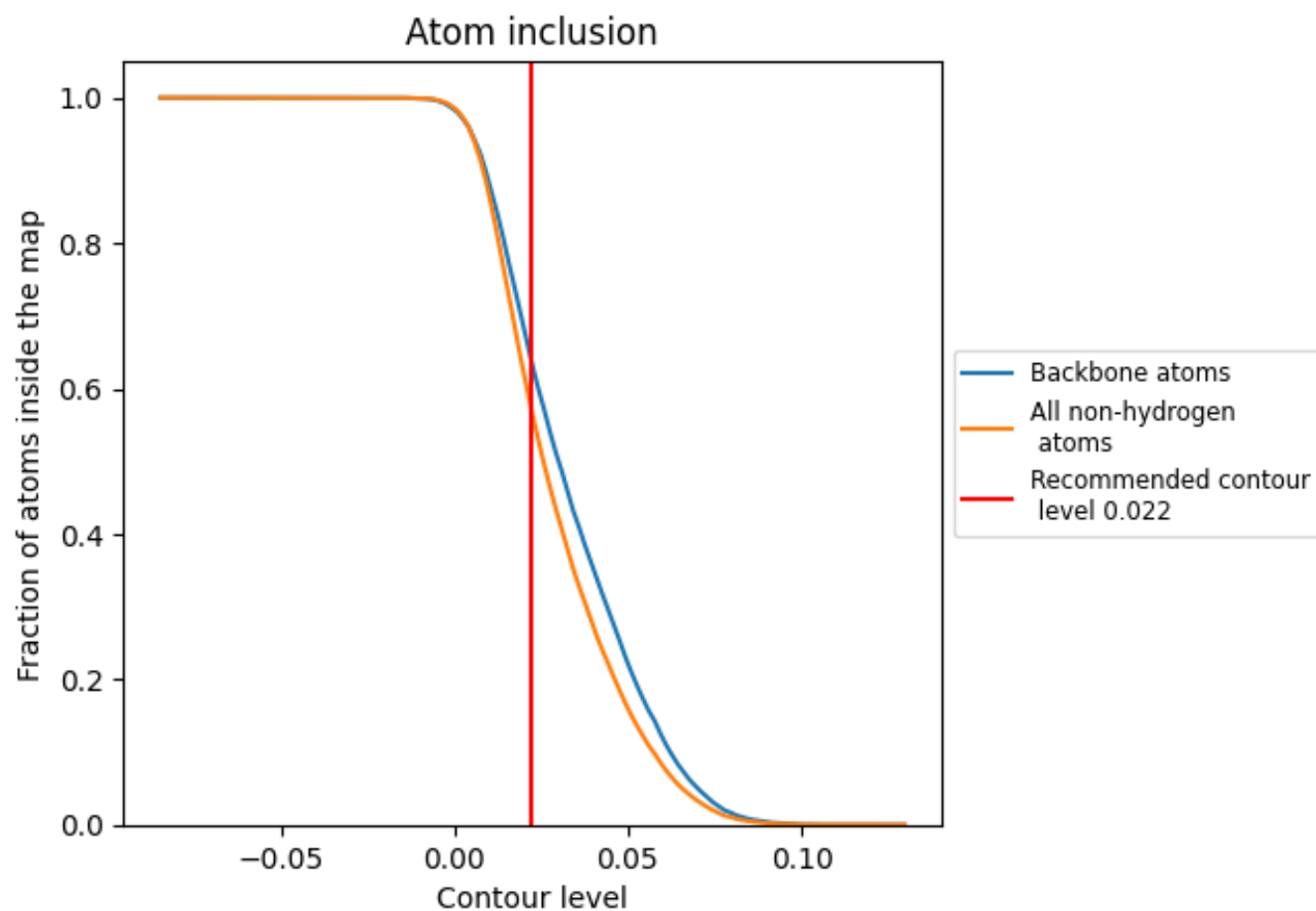
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.022).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 58% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5753	<div></div> 0.4590
1	<div></div> 0.7663	<div></div> 0.4890
A	<div></div> 0.6791	<div></div> 0.4950
B	<div></div> 0.7452	<div></div> 0.5170
C	<div></div> 0.7756	<div></div> 0.5290
D	<div></div> 0.7575	<div></div> 0.5250
E	<div></div> 0.7462	<div></div> 0.5170
F	<div></div> 0.7167	<div></div> 0.5080
G	<div></div> 0.4888	<div></div> 0.4360
H	<div></div> 0.3671	<div></div> 0.3800
I	<div></div> 0.1964	<div></div> 0.3360
J	<div></div> 0.2188	<div></div> 0.3400

1.0

0.0

<0.0