Full wwPDB EM Validation Report ⓘ

Apr 25, 2022 – 10:42 am BST

PDB ID	:	7Z0O
EMDB ID	:	EMD-14428
Title	:	Structure of transcription factor UAF in complex with TBP and 35S rRNA promoter DNA
Authors	:	Baudin, F.; Murciano, B.; Fung, H.K.H.; Fromm, S.A.; Mueller, C.W.
Deposited on	:	2022-02-23
Resolution	:	2.80 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 following versions of software and data (see references ⓘ) were used in the production of this report:

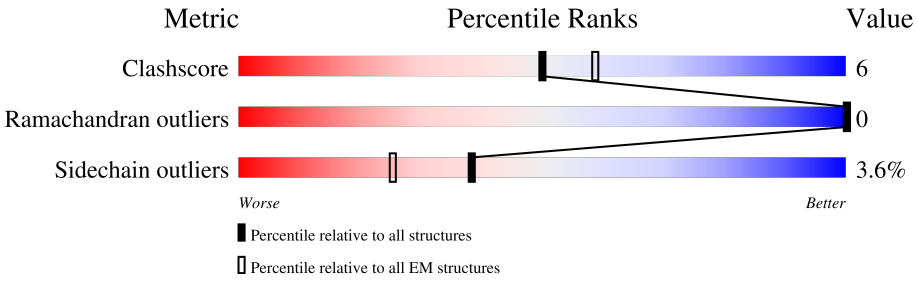
EMDB validation analysis	:	0.0.1.dev7
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	136	54% 15% 31%
1	C	136	62% 10% 29%
2	B	103	55% 18% 26%
3	D	364	5% 70% 11% 19%
4	E	366	10% 72% 10% 18%
5	F	145	15% 78% 14% 8%
6	G	228	8% 29% 7% 63%
7	H	242	52% 46% 25% 28%

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Mol	Chain	Length	Quality of chain
8	N	151	
9	T	151	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11864 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 Histone H3.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	94	Total 774	C 492	N 149	O 133	0	0
1	C	97	Total 799	C 508	N 153	O 138	0	0

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	76	Total 610	C 387	N 117	O 106	0	0

- Molecule 3 is a protein called RNA polymerase I-specific transcription initiation factor RRN5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	296	Total 2436	C 1535	N 450	O 441	S 10	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	SER	-	expression tag	UNP Q02983

- Molecule 4 is a protein called RNA polymerase I-specific transcription initiation factor RRN9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	301	Total 2518	C 1594	N 428	O 488	S 8	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	0	SER	-	expression tag	UNP P53437

- Molecule 5 is a protein called RNA polymerase I-specific transcription initiation factor RRN10.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	133	Total	C	N	O	S	0	0
			1067	678	179	207	3		

- Molecule 6 is a protein called Upstream activation factor subunit UAF30.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	84	Total	C	N	O	S	0	0
			681	430	114	134	3		

- Molecule 7 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	175	Total	C	N	O	S	0	0
			1380	899	236	240	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	GLY	-	expression tag	UNP P13393
H	0	HIS	-	expression tag	UNP P13393

- Molecule 8 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	39	Total	C	N	O	P	0	0
			820	390	162	229	39		

- Molecule 9 is a DNA chain called Template DNA.

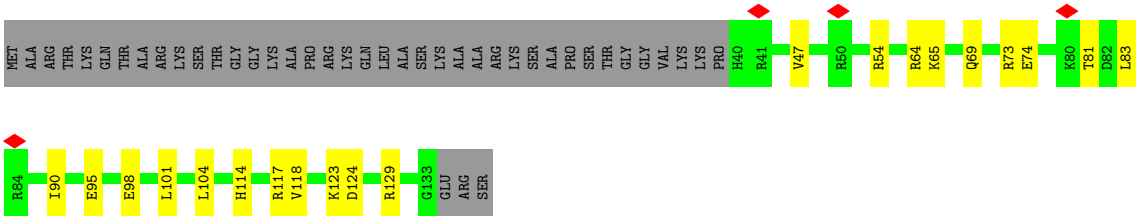
Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	39	Total	C	N	O	P	0	0
			779	378	123	239	39		

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.

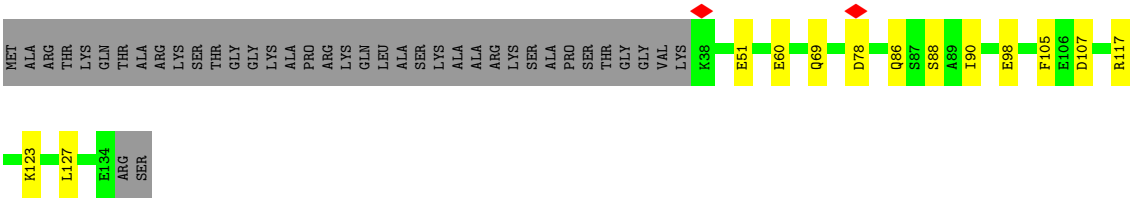
• Molecule 1: Histone H3

Chain A:



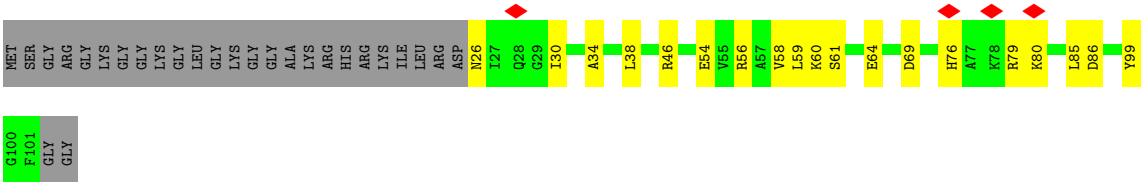
• Molecule 1: Histone H3

Chain C:



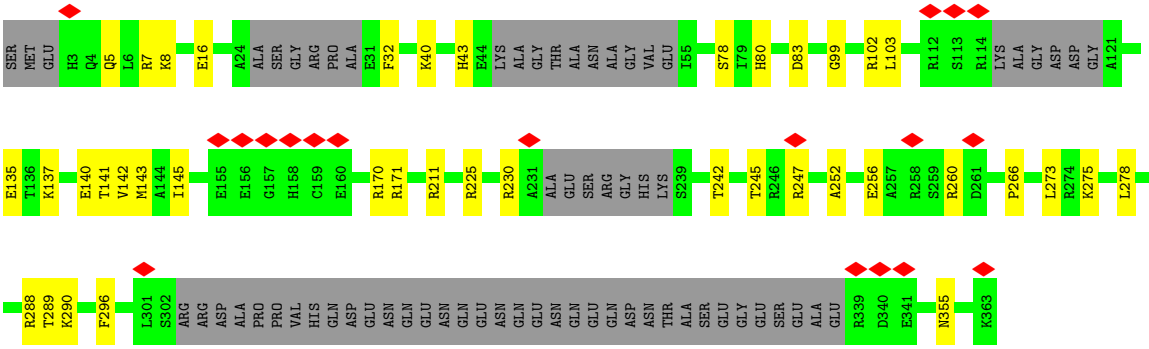
• Molecule 2: Histone H4

Chain B:



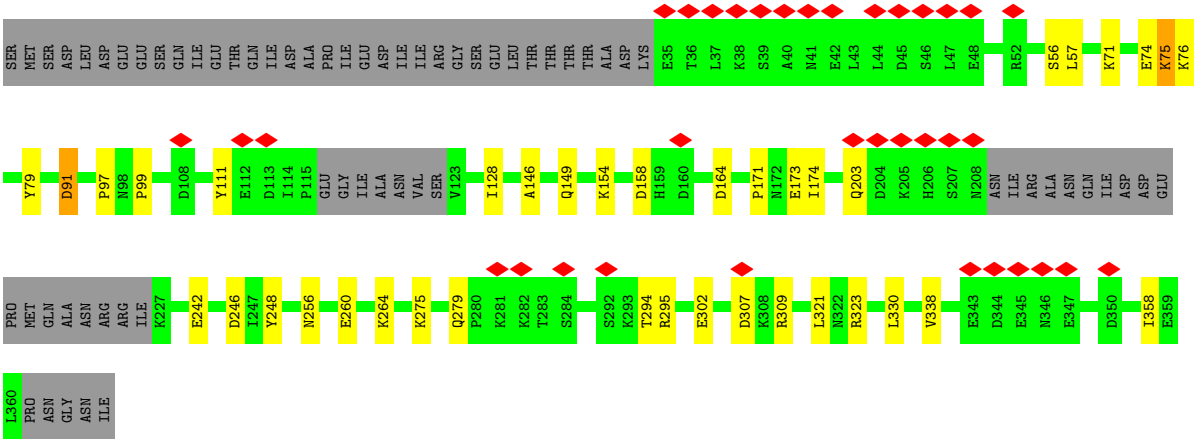
• Molecule 3: RNA polymerase I-specific transcription initiation factor RRN5

Chain D:



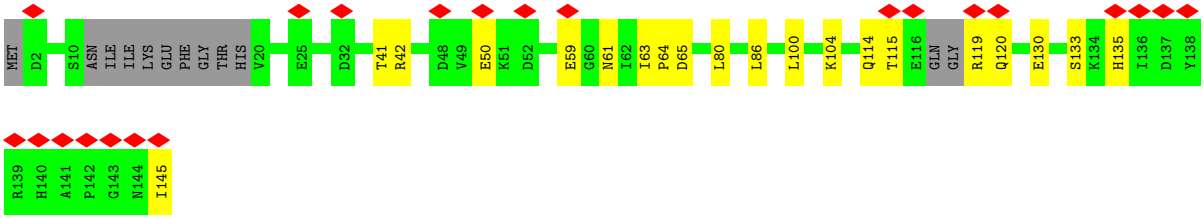
• Molecule 4: RNA polymerase I-specific transcription initiation factor RRN9

Chain E:



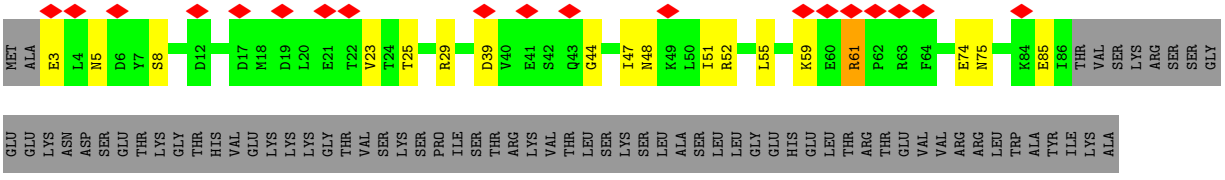
• Molecule 5: RNA polymerase I-specific transcription initiation factor RRN10

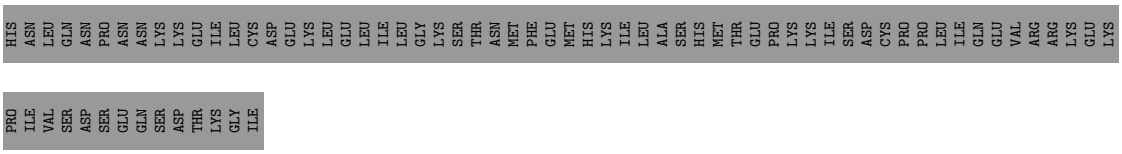
Chain F:



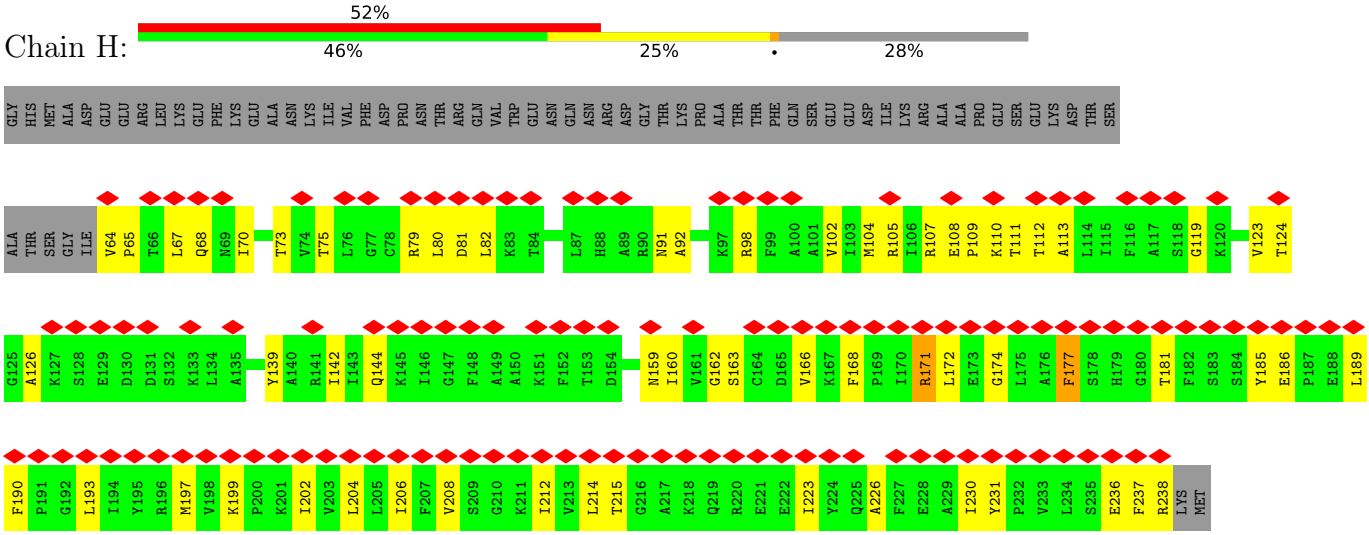
• Molecule 6: Upstream activation factor subunit UAF30

Chain G:

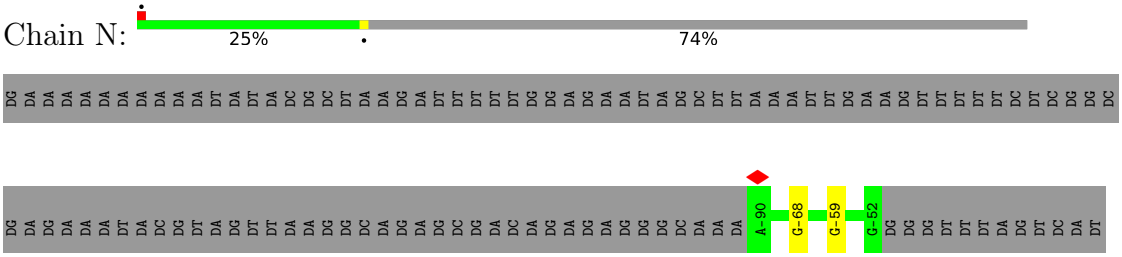




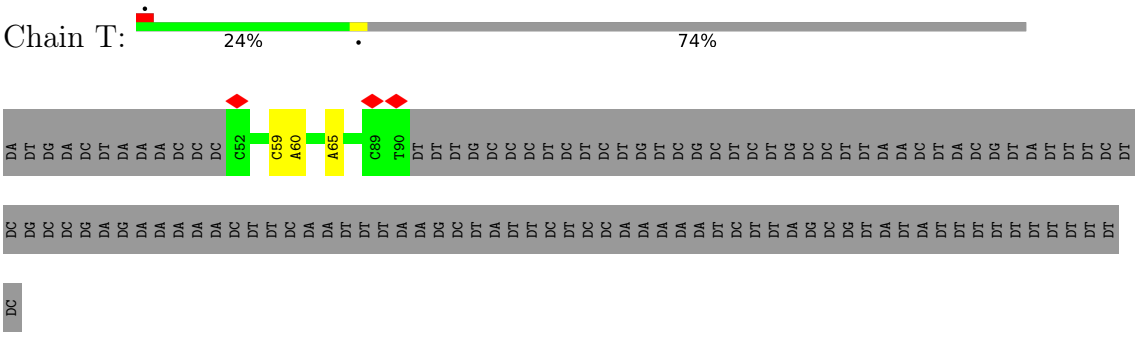
• Molecule 7: TATA-box-binding protein



• Molecule 8: Non-template DNA



• Molecule 9: Template DNA



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	193226	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 ($e^-/Å^2$)	49.4	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.961	Depositor
Minimum map value	-0.055	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	288.96, 288.96, 288.96	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.645, 0.645, 0.645	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	A	0.25	0/784	0.50	0/1049
1	C	0.25	0/810	0.51	0/1084
2	B	0.28	0/617	0.58	0/827
3	D	0.25	0/2486	0.50	0/3352
4	E	0.24	0/2564	0.43	0/3448
5	F	0.25	0/1086	0.46	0/1471
6	G	0.30	0/685	0.54	0/919
7	H	0.27	0/1407	0.52	0/1897
8	N	0.40	0/925	1.02	1/1430 (0.1%)
9	T	0.41	0/867	1.04	0/1331
All	All	0.28	0/12231	0.61	1/16808 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	N	-59	DG	C1'-O4'-C4'	-5.18	104.92	110.10

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	774	0	824	16	0
1	C	799	0	850	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	610	0	654	16	0
3	D	2436	0	2424	30	0
4	E	2518	0	2510	29	0
5	F	1067	0	1052	13	0
6	G	681	0	718	12	0
7	H	1380	0	1452	35	0
8	N	820	0	441	1	0
9	T	779	0	446	2	0
All	All	11864	0	11371	124	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 6.

All (124) 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:E:99:PRO:HA	5:F:80:LEU:HD21	1.74	0.69
1:C:107:ASP:OD1	3:D:275:LYS:NZ	2.25	0.69
1:A:98:GLU:HG3	2:B:38:LEU:HD21	1.75	0.68
5:F:61:ASN:ND2	5:F:65:ASP:OD2	2.28	0.65
1:C:117:ARG:HH22	1:C:123:LYS:HD2	1.61	0.65
7:H:80:LEU:HD23	7:H:119:GLY:HA2	1.79	0.65
2:B:30:ILE:O	2:B:56:ARG:NH1	2.30	0.65
1:A:101:LEU:HD11	2:B:59:LEU:HD23	1.78	0.64
2:B:46:ARG:NH1	3:D:16:GLU:OE2	2.30	0.64
5:F:42:ARG:NH2	5:F:65:ASP:OD1	2.32	0.63
7:H:174:GLY:HA2	7:H:177:PHE:HE1	1.64	0.63
1:A:74:GLU:OE1	2:B:60:LYS:NZ	2.31	0.63
7:H:168:PHE:HB3	7:H:238:ARG:HH22	1.63	0.63
7:H:202:ILE:HD13	7:H:226:ALA:HB2	1.82	0.62
4:E:111:TYR:O	7:H:91:ASN:ND2	2.28	0.62
1:A:129:ARG:NH1	2:B:54:GLU:OE1	2.34	0.60
3:D:355:ASN:ND2	6:G:75:ASN:OD1	2.35	0.58
2:B:79:ARG:NH2	2:B:86:ASP:OD1	2.37	0.58
3:D:355:ASN:ND2	6:G:74:GLU:OE2	2.33	0.58
6:G:44:GLY:O	6:G:48:ASN:ND2	2.37	0.57
7:H:193:LEU:HB3	7:H:206:ILE:HB	1.86	0.57
1:A:69:GLN:HG2	1:A:90:ILE:HG21	1.86	0.57
1:C:86:GLN:HG3	3:D:245:THR:HG22	1.85	0.57
5:F:130:GLU:HA	5:F:133:SER:HB3	1.86	0.57
3:D:247:ARG:NE	4:E:203:GLN:OE1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:266:PRO:HB2	3:D:296:PHE:HB2	1.86	0.56
3:D:140:GLU:HA	3:D:143:MET:HE2	1.86	0.56
7:H:111:THR:O	7:H:139:TYR:OH	2.23	0.56
7:H:70:ILE:HD11	7:H:160:ILE:HD12	1.88	0.55
3:D:288:ARG:HG3	3:D:289:THR:HG23	1.90	0.54
6:G:29:ARG:NH1	6:G:48:ASN:OD1	2.40	0.54
4:E:75:LYS:HE3	4:E:76:LYS:HG3	1.88	0.54
7:H:171:ARG:HH22	7:H:237:PHE:HB3	1.71	0.54
7:H:68:GLN:HE22	7:H:163:SER:HB3	1.73	0.54
1:A:81:THR:HG22	1:A:83:LEU:H	1.74	0.53
3:D:142:VAL:HG11	4:E:358:ILE:HD13	1.90	0.52
1:C:60:GLU:OE2	3:D:170:ARG:NH2	2.39	0.52
7:H:79:ARG:HH12	7:H:81:ASP:HB2	1.75	0.52
7:H:67:LEU:HA	7:H:162:GLY:HA2	1.90	0.52
7:H:204:LEU:HB2	7:H:212:ILE:HD11	1.92	0.51
1:C:69:GLN:HG3	1:C:90:ILE:HG21	1.93	0.51
3:D:5:GLN:NE2	6:G:85:GLU:OE1	2.41	0.51
7:H:108:GLU:HB3	7:H:109:PRO:HD3	1.93	0.51
7:H:171:ARG:CZ	7:H:174:GLY:HA3	2.41	0.50
1:A:114:HIS:CG	1:C:127:LEU:HD22	2.47	0.50
7:H:112:THR:O	7:H:124:THR:N	2.42	0.50
3:D:40:LYS:NZ	4:E:164:ASP:OD2	2.45	0.50
4:E:56:SER:HB3	5:F:63:ILE:HD11	1.93	0.50
1:C:78:ASP:OD2	3:D:211:ARG:NH2	2.42	0.50
4:E:149:GLN:HB2	7:H:108:GLU:HG3	1.94	0.49
1:A:104:LEU:HD22	2:B:58:VAL:HG11	1.95	0.48
1:A:129:ARG:HD3	2:B:58:VAL:HG22	1.96	0.48
4:E:246:ASP:N	4:E:246:ASP:OD1	2.47	0.48
7:H:186:GLU:HG3	7:H:189:LEU:HD12	1.96	0.48
1:A:118:VAL:N	3:D:135:GLU:OE2	2.46	0.48
3:D:290:LYS:NZ	8:N:-68:DG:OP2	2.37	0.47
4:E:295:ARG:NH2	9:T:65:DA:O4'	2.45	0.47
1:A:64:ARG:HH12	2:B:34:ALA:HB2	1.79	0.47
3:D:252:ALA:O	3:D:256:GLU:HB2	2.14	0.47
1:A:69:GLN:O	1:A:73:ARG:HG2	2.14	0.47
1:C:51:GLU:H	1:C:51:GLU:CD	2.17	0.47
3:D:225:ARG:NH1	3:D:242:THR:OG1	2.48	0.46
3:D:273:LEU:HA	3:D:278:LEU:HD12	1.97	0.46
7:H:113:ALA:HA	7:H:123:VAL:HA	1.97	0.46
3:D:230:ARG:NH2	4:E:294:THR:O	2.48	0.46
3:D:355:ASN:HD21	6:G:74:GLU:CD	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:115:THR:HB	5:F:120:GLN:HG2	1.98	0.46
7:H:159:ASN:OD1	7:H:160:ILE:N	2.49	0.46
4:E:71:LYS:HB3	4:E:264:LYS:HZ2	1.81	0.45
4:E:242:GLU:HB3	5:F:104:LYS:NZ	2.32	0.45
1:A:65:LYS:HB3	1:A:65:LYS:HE3	1.60	0.45
7:H:172:LEU:HD22	7:H:208:VAL:HG22	1.99	0.45
2:B:99:TYR:HD2	3:D:80:HIS:HA	1.82	0.45
4:E:74:GLU:OE2	4:E:323:ARG:NH1	2.50	0.45
1:C:98:GLU:OE2	3:D:171:ARG:NH2	2.50	0.45
3:D:141:THR:O	3:D:145:ILE:HD12	2.17	0.45
4:E:146:ALA:HB2	7:H:107:ARG:HG3	1.99	0.45
7:H:64:VAL:HB	7:H:65:PRO:HD3	1.99	0.45
7:H:177:PHE:H	7:H:177:PHE:HD1	1.64	0.45
2:B:85:LEU:HD23	2:B:85:LEU:HA	1.82	0.44
4:E:57:LEU:HD13	5:F:41:THR:HA	1.99	0.44
7:H:82:LEU:HD22	7:H:102:VAL:HG23	2.00	0.44
4:E:91:ASP:OD1	4:E:91:ASP:N	2.51	0.44
4:E:275:LYS:HA	4:E:275:LYS:HD3	1.80	0.44
5:F:64:PRO:HG3	5:F:100:LEU:HG	1.99	0.44
6:G:25:THR:HA	6:G:51:ILE:HG21	1.98	0.44
6:G:61:ARG:O	6:G:61:ARG:HD3	2.18	0.44
5:F:130:GLU:N	5:F:130:GLU:OE2	2.51	0.43
4:E:154:LYS:O	4:E:154:LYS:NZ	2.40	0.43
1:A:117:ARG:NH1	1:A:124:ASP:OD2	2.42	0.43
4:E:154:LYS:HA	4:E:154:LYS:HD2	1.89	0.43
4:E:256:ASN:O	4:E:260:GLU:HG2	2.19	0.43
7:H:171:ARG:NH2	7:H:237:PHE:HB3	2.33	0.43
7:H:204:LEU:HD22	7:H:230:ILE:HD13	1.99	0.43
1:A:74:GLU:OE2	2:B:26:ASN:HB3	2.19	0.42
7:H:92:ALA:HB2	7:H:104:MET:HB3	2.01	0.42
6:G:5:ASN:O	6:G:8:SER:OG	2.28	0.42
3:D:5:GLN:H	3:D:5:GLN:HG3	1.57	0.42
2:B:60:LYS:O	2:B:64:GLU:HG2	2.20	0.42
6:G:55:LEU:HA	6:G:55:LEU:HD23	1.82	0.42
7:H:110:LYS:HD2	7:H:110:LYS:HA	1.86	0.42
4:E:128:ILE:HG12	5:F:80:LEU:HD23	2.00	0.42
3:D:7:ARG:HG3	3:D:8:LYS:N	2.35	0.42
7:H:166:VAL:HG23	7:H:168:PHE:H	1.85	0.42
2:B:80:LYS:HA	2:B:80:LYS:HE2	2.02	0.41
4:E:171:PRO:HG2	4:E:174:ILE:HD12	2.02	0.41
7:H:174:GLY:HA2	7:H:177:PHE:CE1	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:23:VAL:HG11	6:G:55:LEU:HD21	2.02	0.41
6:G:47:ILE:O	6:G:51:ILE:HD12	2.20	0.41
7:H:70:ILE:HB	7:H:126:ALA:HB3	2.02	0.41
9:T:59:DC:H2"	9:T:60:DA:C8	2.56	0.41
7:H:142:ILE:HD13	7:H:142:ILE:HA	1.93	0.41
3:D:99:GLY:O	3:D:103:LEU:HG	2.20	0.41
5:F:145:ILE:HD12	7:H:144:GLN:NE2	2.35	0.41
4:E:97:PRO:HD2	5:F:86:LEU:O	2.21	0.41
4:E:307:ASP:OD2	4:E:309:ARG:NH2	2.41	0.41
4:E:330:LEU:HD23	4:E:330:LEU:HA	1.92	0.41
7:H:214:LEU:HB2	7:H:223:ILE:HD11	2.03	0.41
2:B:69:ASP:OD1	2:B:69:ASP:N	2.54	0.41
4:E:79:TYR:CE2	4:E:279:GLN:HB3	2.55	0.41
1:A:54:ARG:HG3	3:D:32:PHE:HZ	1.86	0.40
3:D:102:ARG:NH1	4:E:173:GLU:OE2	2.54	0.40
4:E:248:TYR:HB2	4:E:338:VAL:HG21	2.03	0.40
3:D:256:GLU:HG3	3:D:260:ARG:HG3	2.02	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	92/136 (68%)	92 (100%)	0	0	100	100
1	C	95/136 (70%)	93 (98%)	2 (2%)	0	100	100
2	B	74/103 (72%)	73 (99%)	1 (1%)	0	100	100
3	D	284/364 (78%)	279 (98%)	5 (2%)	0	100	100
4	E	295/366 (81%)	290 (98%)	5 (2%)	0	100	100
5	F	127/145 (88%)	124 (98%)	3 (2%)	0	100	100
6	G	82/228 (36%)	80 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	H	173/242 (72%)	170 (98%)	3 (2%)	0	100	100
All	All	1222/1720 (71%)	1201 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	82/113 (73%)	79 (96%)	3 (4%)	34	68
1	C	85/113 (75%)	83 (98%)	2 (2%)	49	81
2	B	65/81 (80%)	63 (97%)	2 (3%)	40	74
3	D	261/312 (84%)	257 (98%)	4 (2%)	65	89
4	E	288/345 (84%)	283 (98%)	5 (2%)	60	87
5	F	119/129 (92%)	114 (96%)	5 (4%)	30	63
6	G	78/211 (37%)	73 (94%)	5 (6%)	17	45
7	H	148/206 (72%)	134 (90%)	14 (10%)	8	25
All	All	1126/1510 (75%)	1086 (96%)	40 (4%)	38	69

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	VAL
1	A	95	GLU
1	A	123	LYS
2	B	61	SER
2	B	76	HIS
1	C	88	SER
1	C	105	PHE
3	D	43	HIS
3	D	78	SER
3	D	83	ASP

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Mol	Chain	Res	Type
3	D	137	LYS
4	E	75	LYS
4	E	91	ASP
4	E	158	ASP
4	E	302	GLU
4	E	321	LEU
5	F	50	GLU
5	F	59	GLU
5	F	114	GLN
5	F	119	ARG
5	F	135	HIS
6	G	3	GLU
6	G	39	ASP
6	G	52	ARG
6	G	59	LYS
6	G	61	ARG
7	H	73	THR
7	H	75	THR
7	H	98	ARG
7	H	105	ARG
7	H	171	ARG
7	H	177	PHE
7	H	181	THR
7	H	185	TYR
7	H	190	PHE
7	H	197	MET
7	H	199	LYS
7	H	215	THR
7	H	231	TYR
7	H	236	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	56	GLN
4	E	82	ASN

5.3.3 RNA

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 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)

There are no chain breaks in this entry.

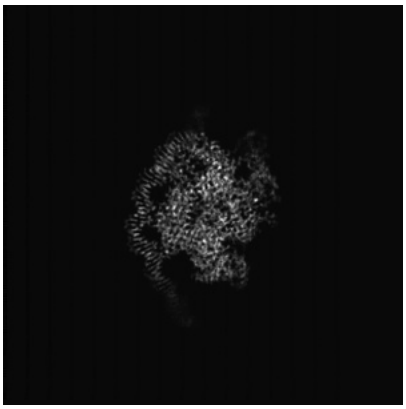
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14428. These allow visual inspection of the internal detail of the map and identification of artifacts.

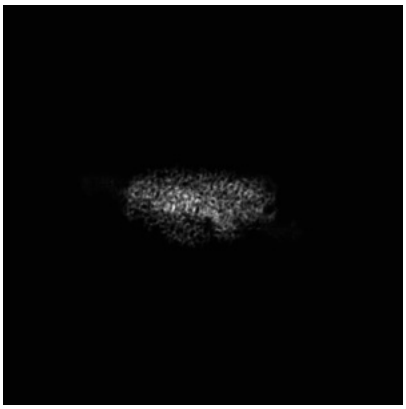
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

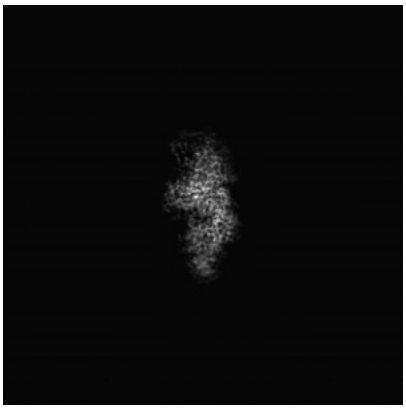
6.1.1 Primary map



X

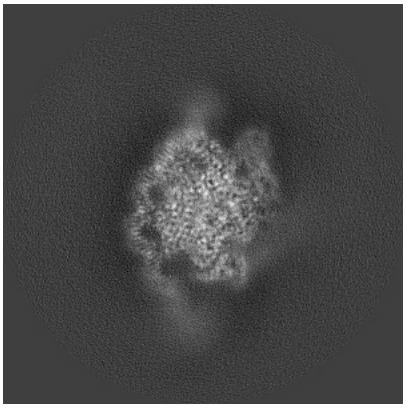


Y

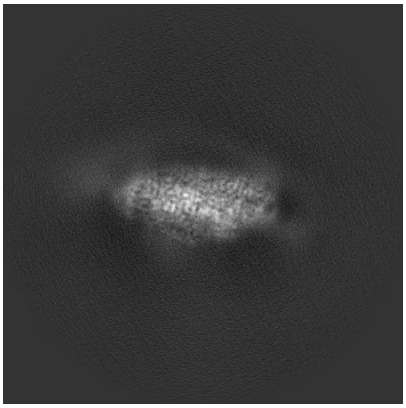


Z

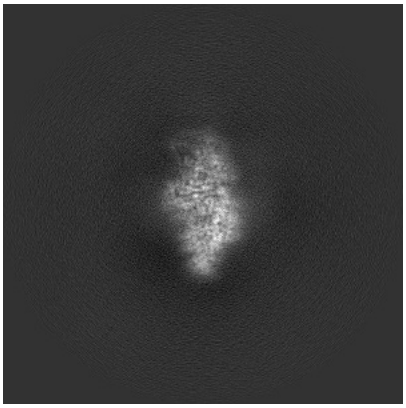
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

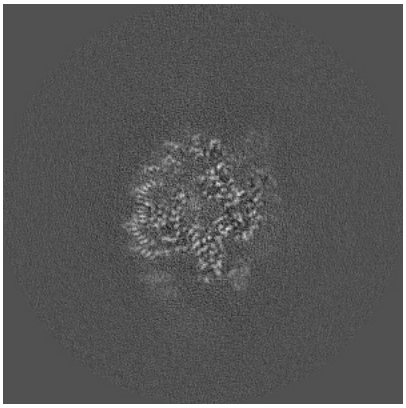
6.2.1 Primary map

X Index: 224

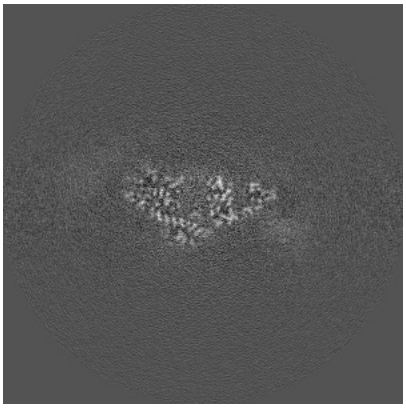
Y Index: 224

Z Index: 224

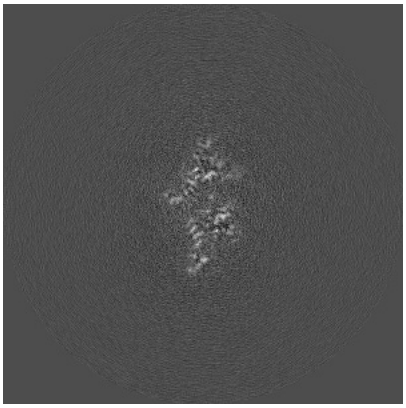
6.2.2 Raw map



X Index: 224



Y Index: 224



Z Index: 224

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

6.3 Largest variance slices (i)

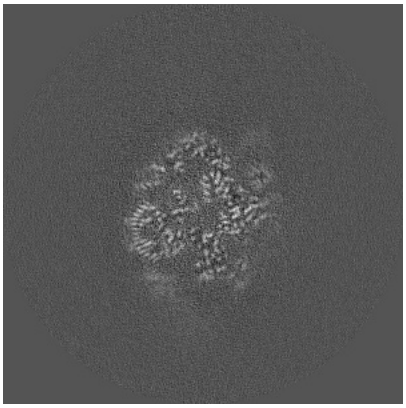
6.3.1 Primary map

X Index: 228

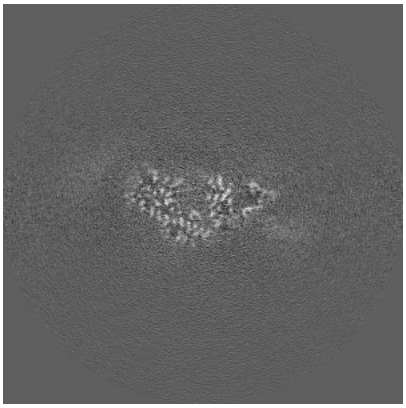
Y Index: 241

Z Index: 191

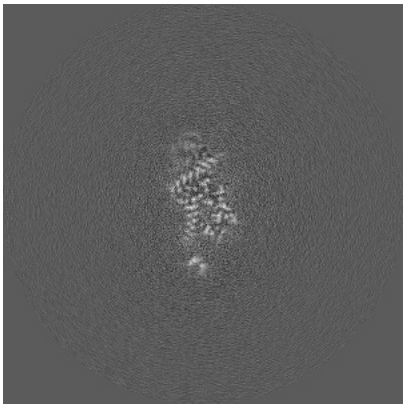
6.3.2 Raw map



X Index: 228



Y Index: 225



Z Index: 238

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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. 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

X Y Z

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.

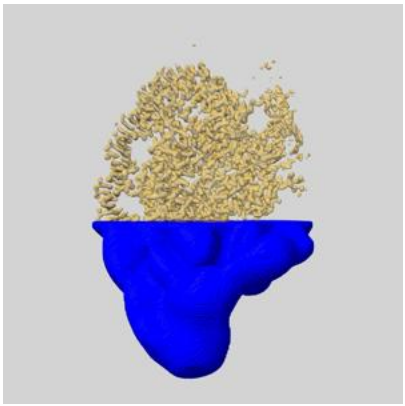
6.5 Mask visualisation (i)

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

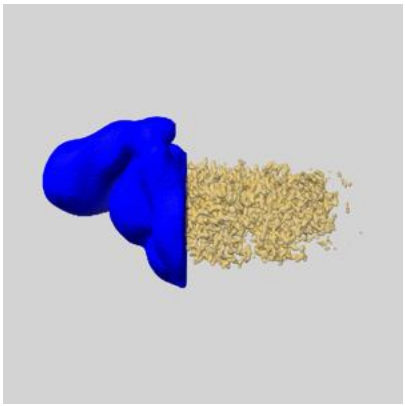
A mask typically either:

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

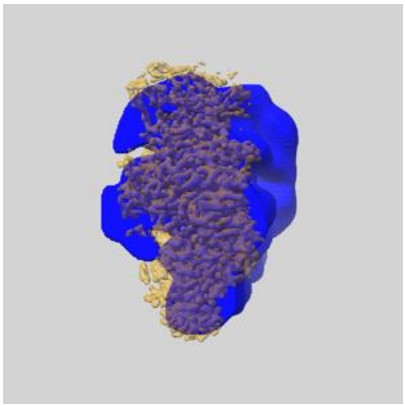
6.5.1 emd_14428_msk_1.map (i)



X



Y

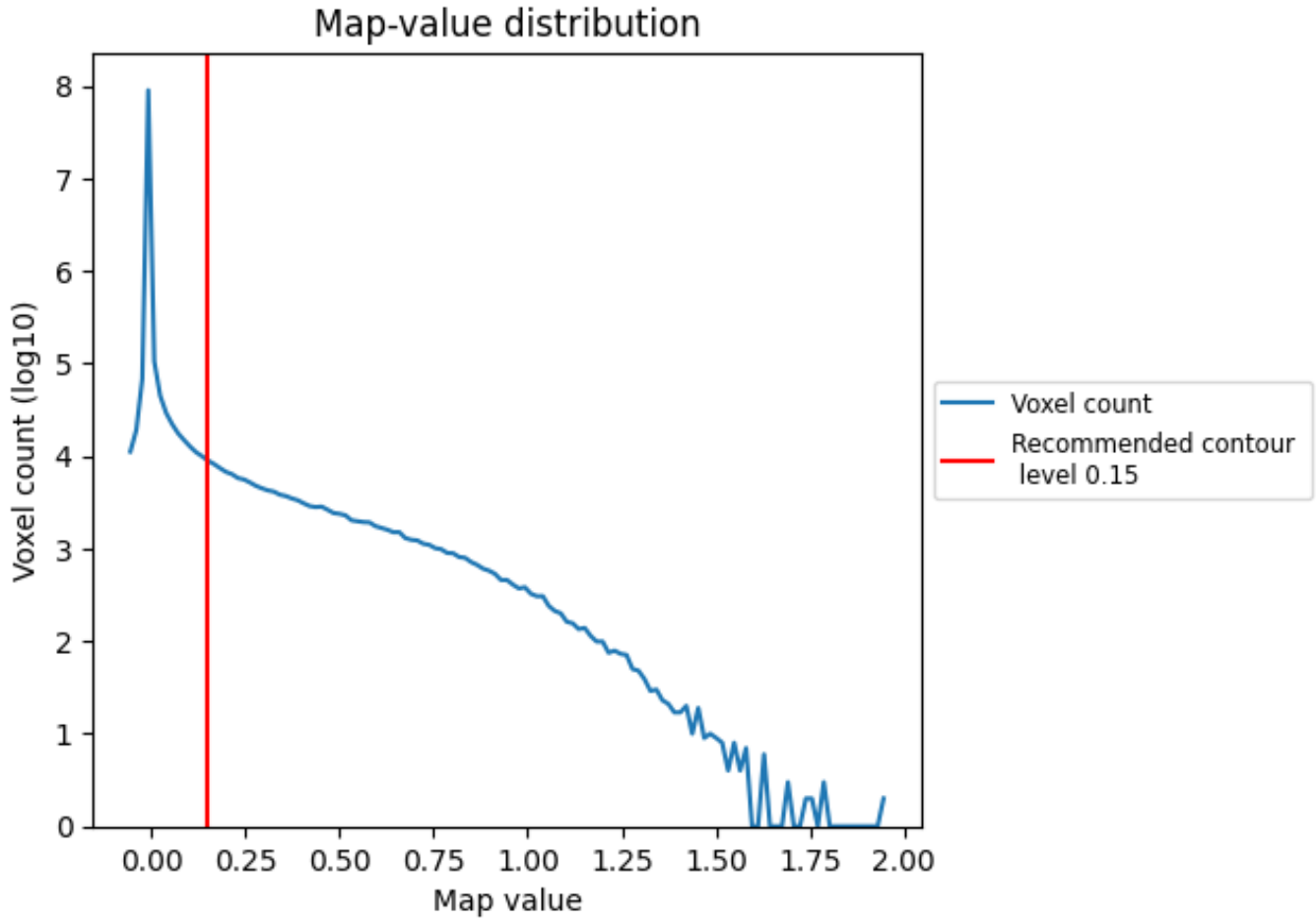


Z

7 Map analysis

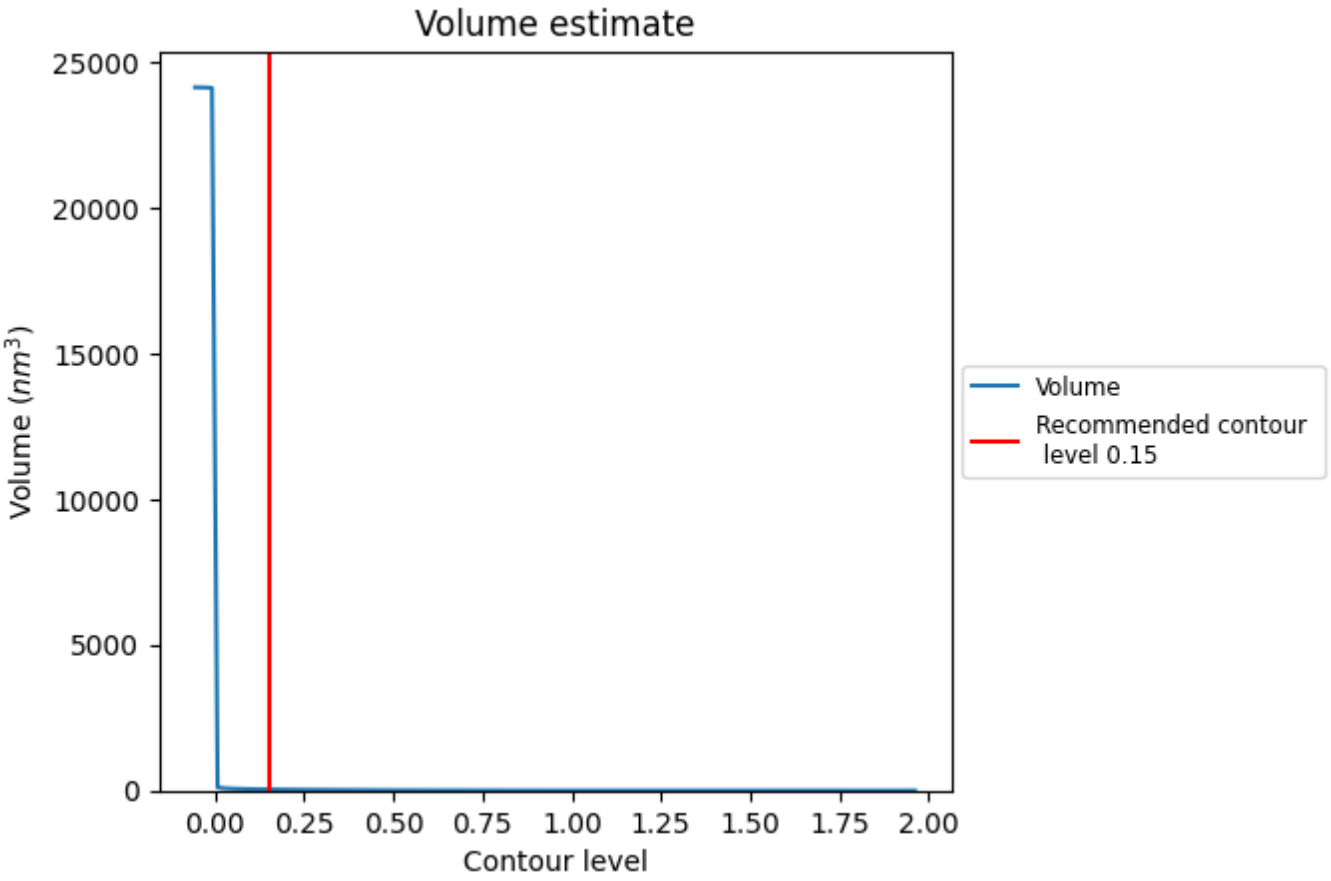
This section contains the results of statistical analysis of the map.

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.

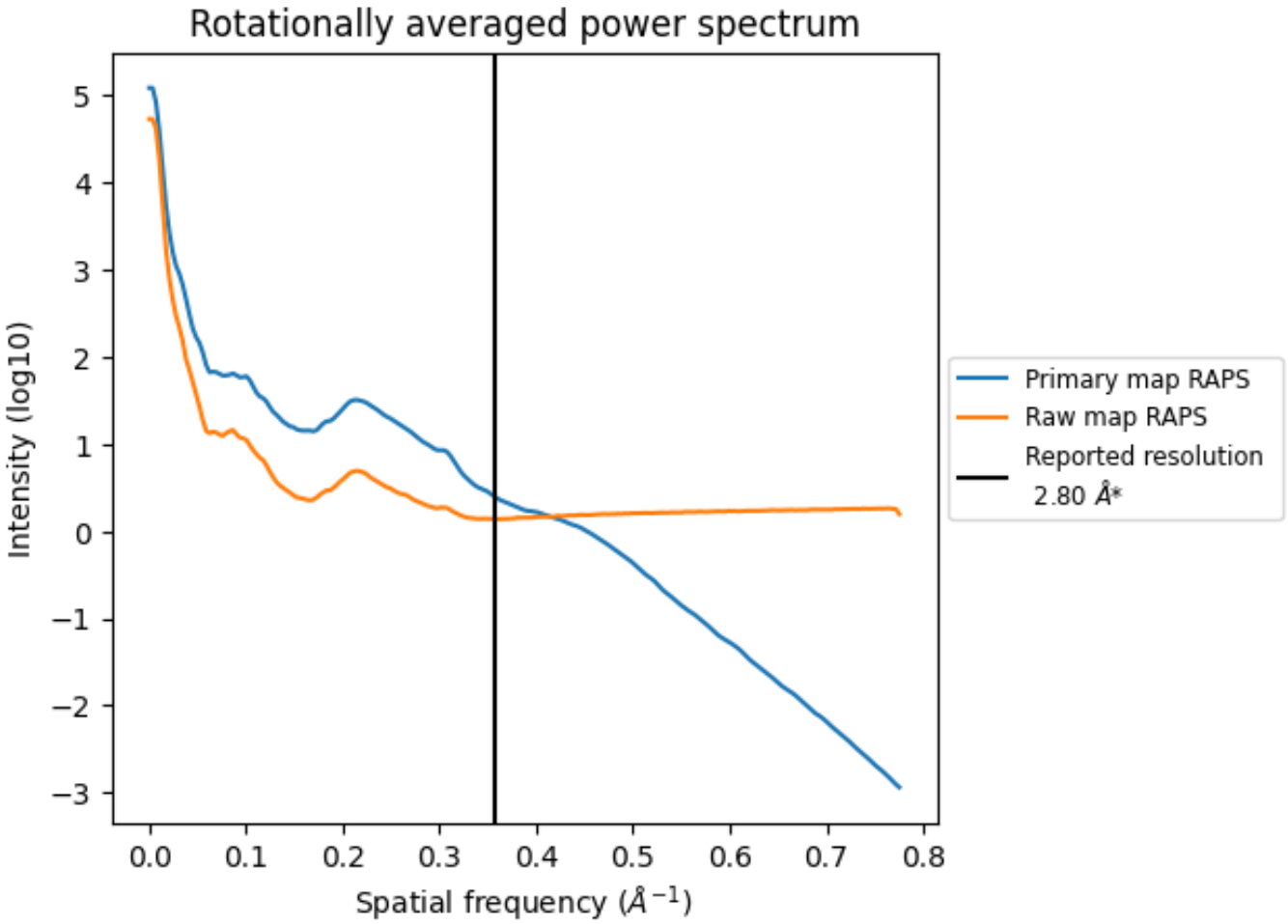
7.2 Volume estimate



The volume at the recommended contour level is 39 nm^3; this corresponds to an approximate mass of 35 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)

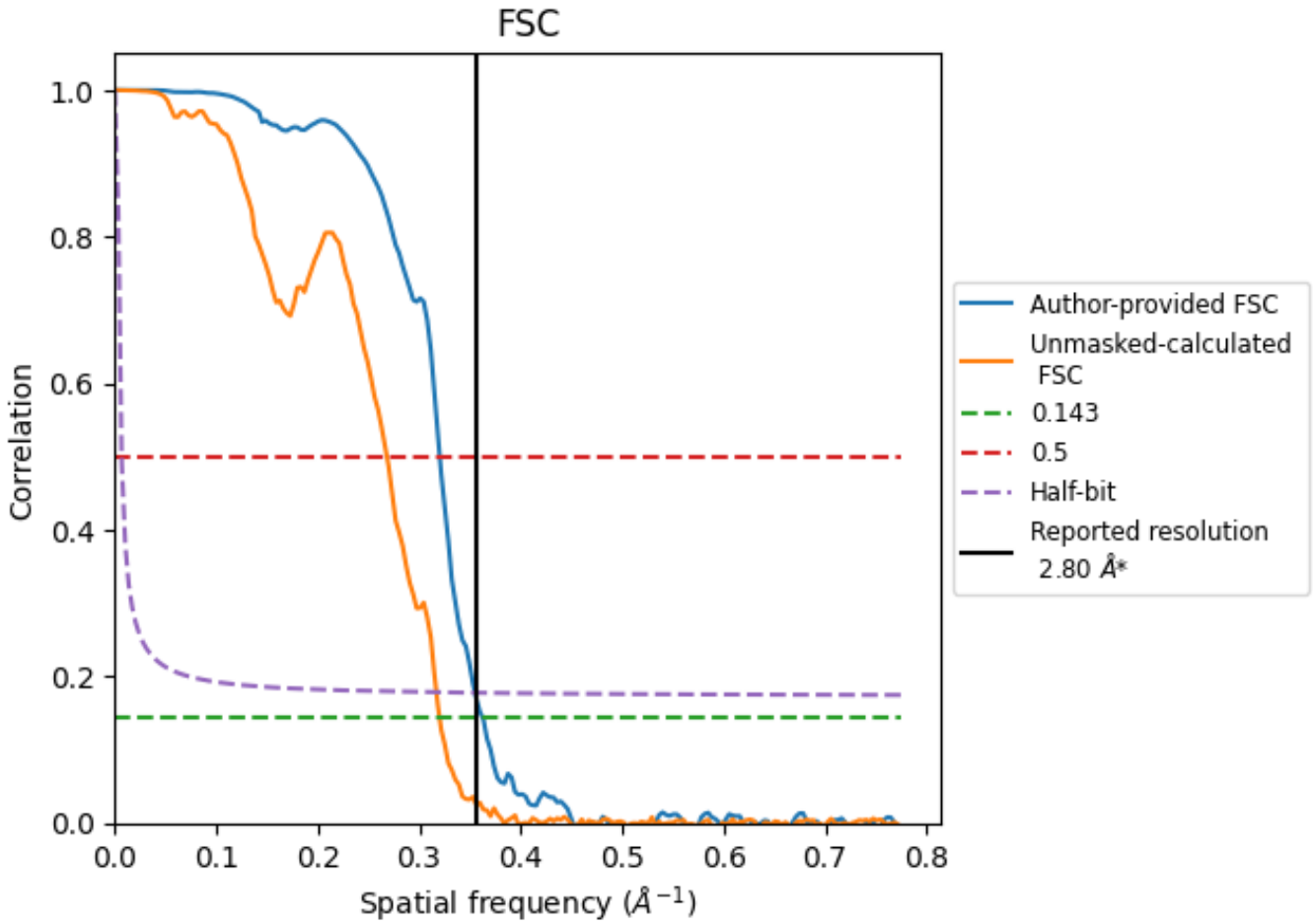


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8.2 Resolution estimates (i)

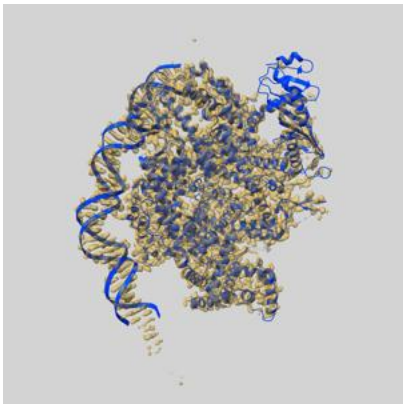
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.76	3.12	2.82
Unmasked-calculated*	3.12	3.73	3.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.12 differs from the reported value 2.8 by more than 10 %

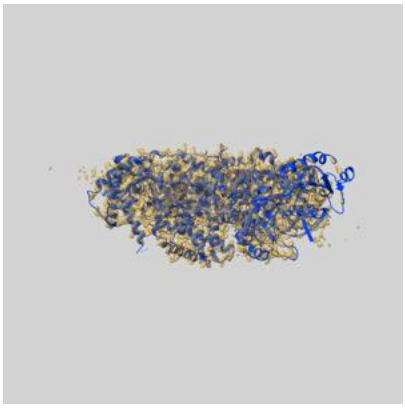
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14428 and PDB model 7Z0O. Per-residue inclusion information can be found in section 3 on page 6.

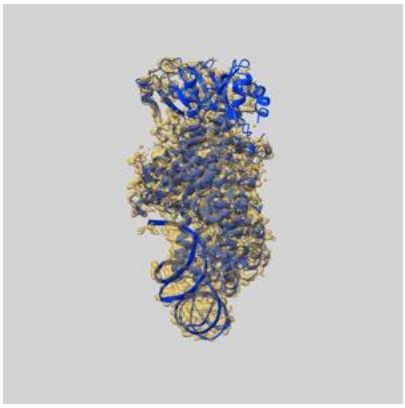
9.1 Map-model overlay



X



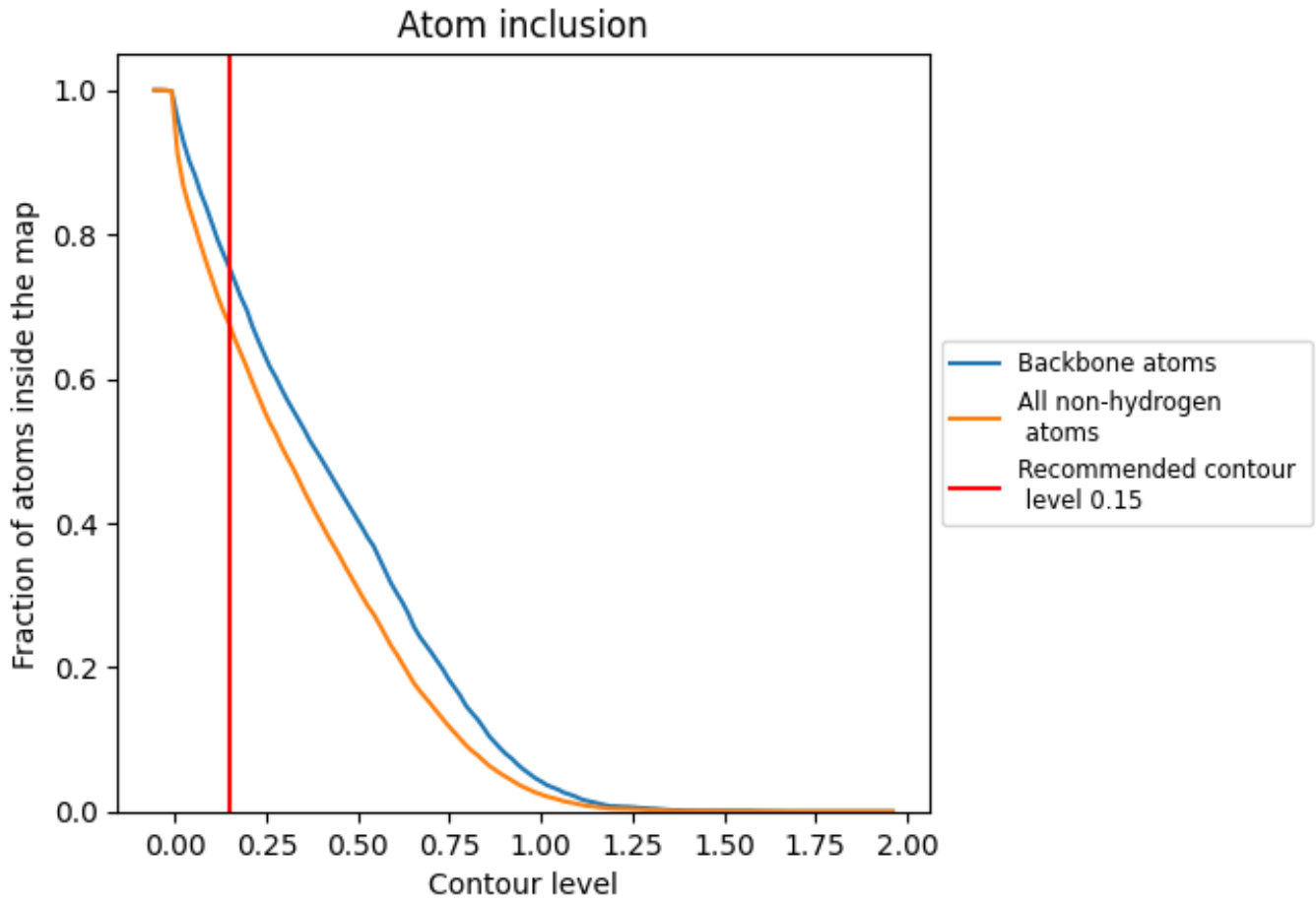
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.