Full wwPDB EM Validation Report (i)

Mar 19, 2024 – 08:15 PM JST

PDB ID	:	6J9E
EMDB ID	:	EMD-9785
Title	:	Cryo-EM structure of Xanthomonos oryzae transcription elongation complex with NusA and the bacteriophage protein P7
Authors	:	You, L.L.; Zhang, Y.
Deposited on	:	2019-01-22
Resolution	:	3.41 Å(reported)
Based on initial models	:	2MC6, 6FLQ, 5UPC

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

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

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

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

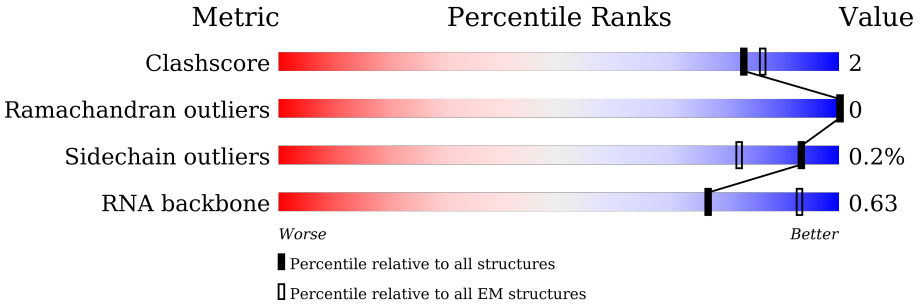
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.41 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 <=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	346	56% 5% 39%
1	B	346	58% • 40%
2	C	1383	5% 87% 6% 7%
3	D	1405	80% 5% 15%
4	E	99	64% • 34%
5	G	29	17% 83% 17%
6	H	29	21% 72% • 24%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	I	20	35% 25% 40%
8	J	77	5% 74% 12% 14%
9	F	507	16% 30% 67%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 24427 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	211	1543	968	273	298	4	0	0
1	B	208	1449	909	261	277	2	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP B2SQT4
A	-12	GLY	-	expression tag	UNP B2SQT4
A	-11	SER	-	expression tag	UNP B2SQT4
A	-10	SER	-	expression tag	UNP B2SQT4
A	-9	HIS	-	expression tag	UNP B2SQT4
A	-8	HIS	-	expression tag	UNP B2SQT4
A	-7	HIS	-	expression tag	UNP B2SQT4
A	-6	HIS	-	expression tag	UNP B2SQT4
A	-5	HIS	-	expression tag	UNP B2SQT4
A	-4	HIS	-	expression tag	UNP B2SQT4
A	-3	SER	-	expression tag	UNP B2SQT4
A	-2	GLN	-	expression tag	UNP B2SQT4
A	-1	ASP	-	expression tag	UNP B2SQT4
A	0	PRO	-	expression tag	UNP B2SQT4
B	-13	MET	-	initiating methionine	UNP B2SQT4
B	-12	GLY	-	expression tag	UNP B2SQT4
B	-11	SER	-	expression tag	UNP B2SQT4
B	-10	SER	-	expression tag	UNP B2SQT4
B	-9	HIS	-	expression tag	UNP B2SQT4
B	-8	HIS	-	expression tag	UNP B2SQT4
B	-7	HIS	-	expression tag	UNP B2SQT4
B	-6	HIS	-	expression tag	UNP B2SQT4
B	-5	HIS	-	expression tag	UNP B2SQT4
B	-4	HIS	-	expression tag	UNP B2SQT4
B	-3	SER	-	expression tag	UNP B2SQT4
B	-2	GLN	-	expression tag	UNP B2SQT4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	ASP	-	expression tag	UNP B2SQT4
B	0	PRO	-	expression tag	UNP B2SQT4

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	1288	9355	5904	1650	1773	28	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	1200	8733	5498	1555	1644	36	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	65	467	289	88	86	4	0	0

- Molecule 5 is a DNA chain called DNA (29-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	G	29	582	279	99	176	28	0	0

- Molecule 6 is a DNA chain called DNA (29-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	H	22	450	214	89	126	21	0	0

- Molecule 7 is a RNA chain called RNA (5'-R(*GP*CP*AP*UP*UP*CP*AP*AP*AP*GP*CP*GP*GP*AP*GP*AP*GP*GP*UP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	I	12	266	118	55	81	12	0	0

- Molecule 8 is a protein called 45L.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	J	66	488	308	78	102	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	-3	GLY	-	expression tag	UNP Q8LTJ5
J	-2	ALA	-	expression tag	UNP Q8LTJ5
J	-1	MET	-	expression tag	UNP Q8LTJ5
J	0	ALA	-	expression tag	UNP Q8LTJ5

- Molecule 9 is a protein called Transcription termination/antitermination protein NusA.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	F	165	1091	685	196	210	0	0

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
10	D	1	1	1	0

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

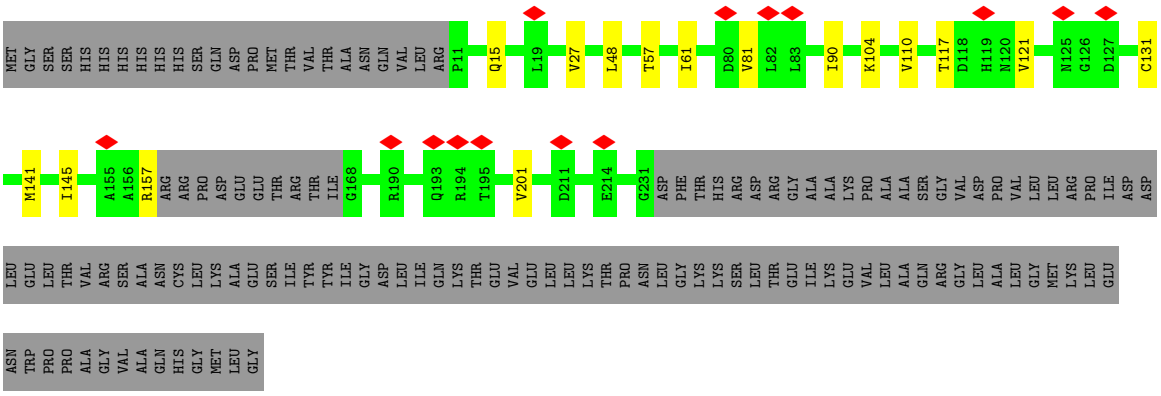
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
11	D	2	2	2	0

3 Residue-property plots (i)

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

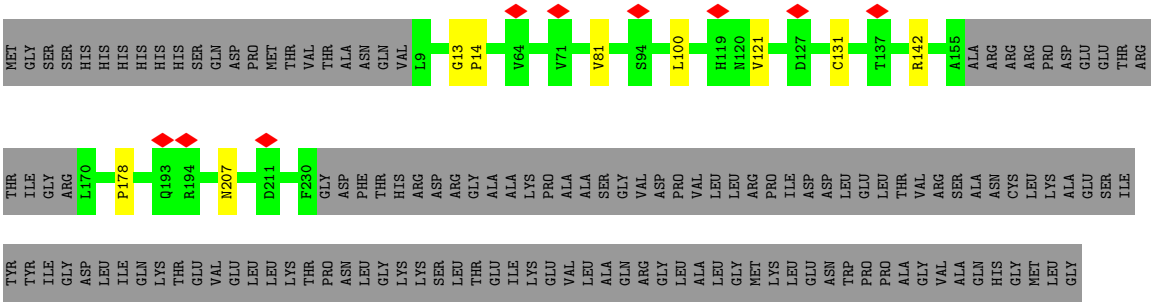
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



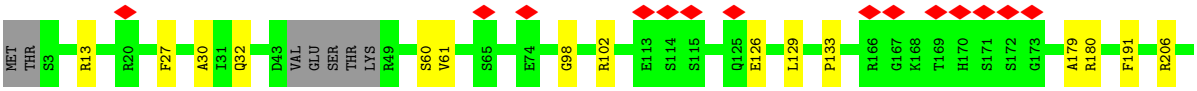
• Molecule 1: DNA-directed RNA polymerase subunit alpha

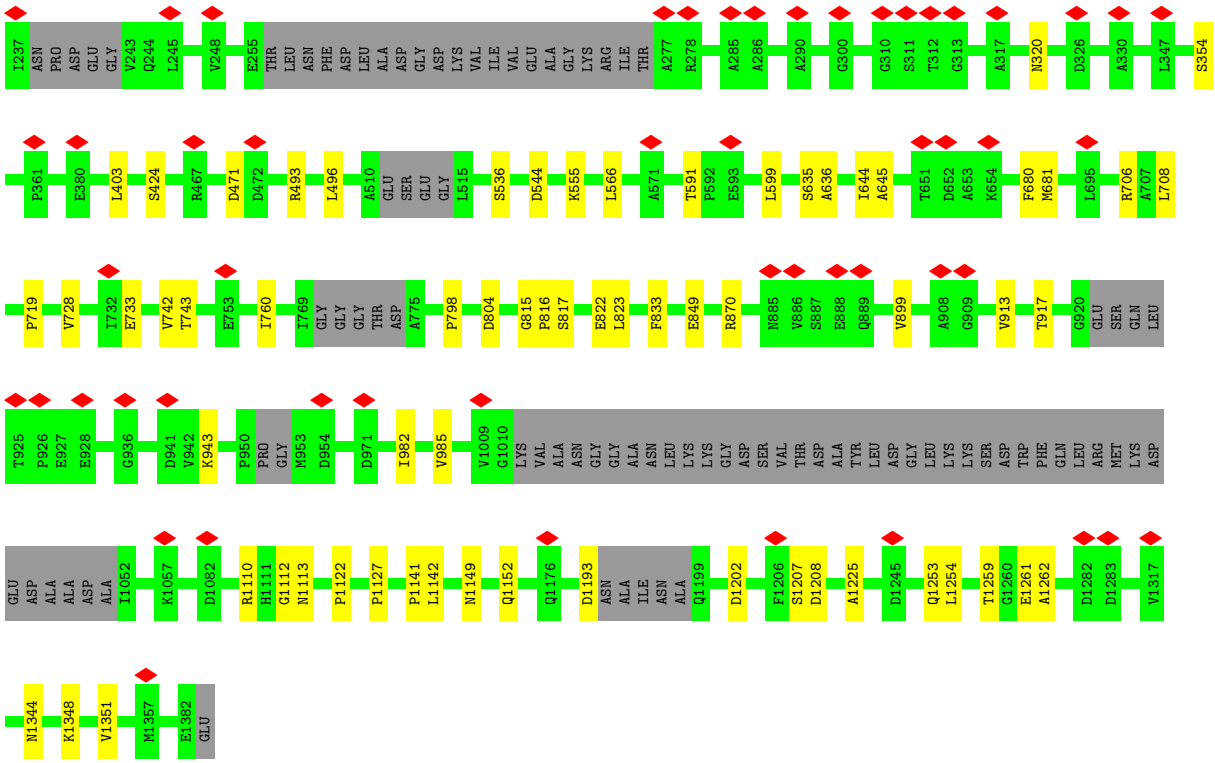
Chain B:



• Molecule 2: DNA-directed RNA polymerase subunit beta

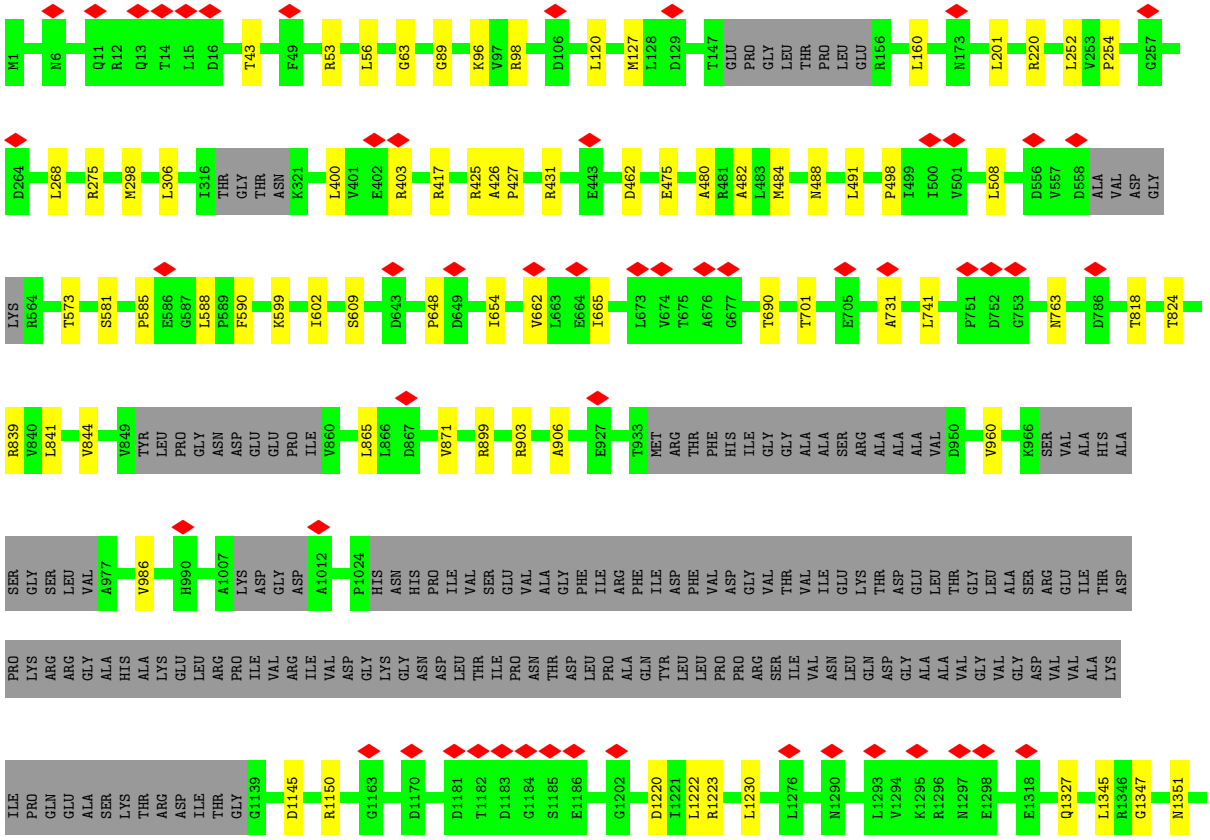
Chain C:

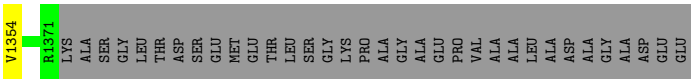




- Molecule 3: DNA-directed RNA polymerase subunit beta'

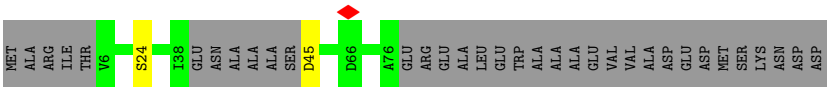
Chain D:





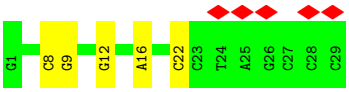
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:



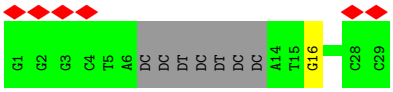
• Molecule 5: DNA (29-MER)

Chain G:



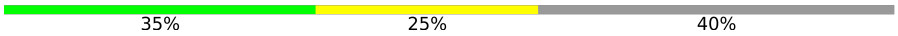
• Molecule 6: DNA (29-MER)

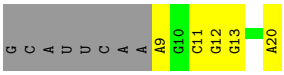
Chain H:



• Molecule 7: RNA (5'-R(*GP*CP*AP*UP*UP*CP*AP*AP*AP*GP*CP*GP*GP*AP*GP*AP *GP*GP*UP*A)-3')

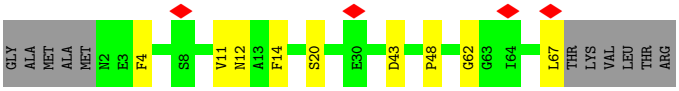
Chain I:





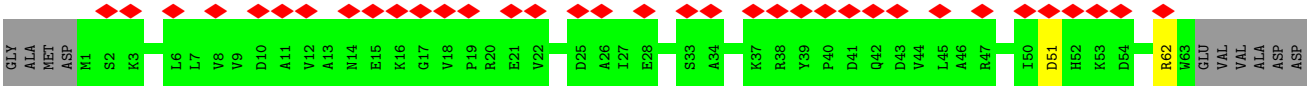
• Molecule 8: 45L

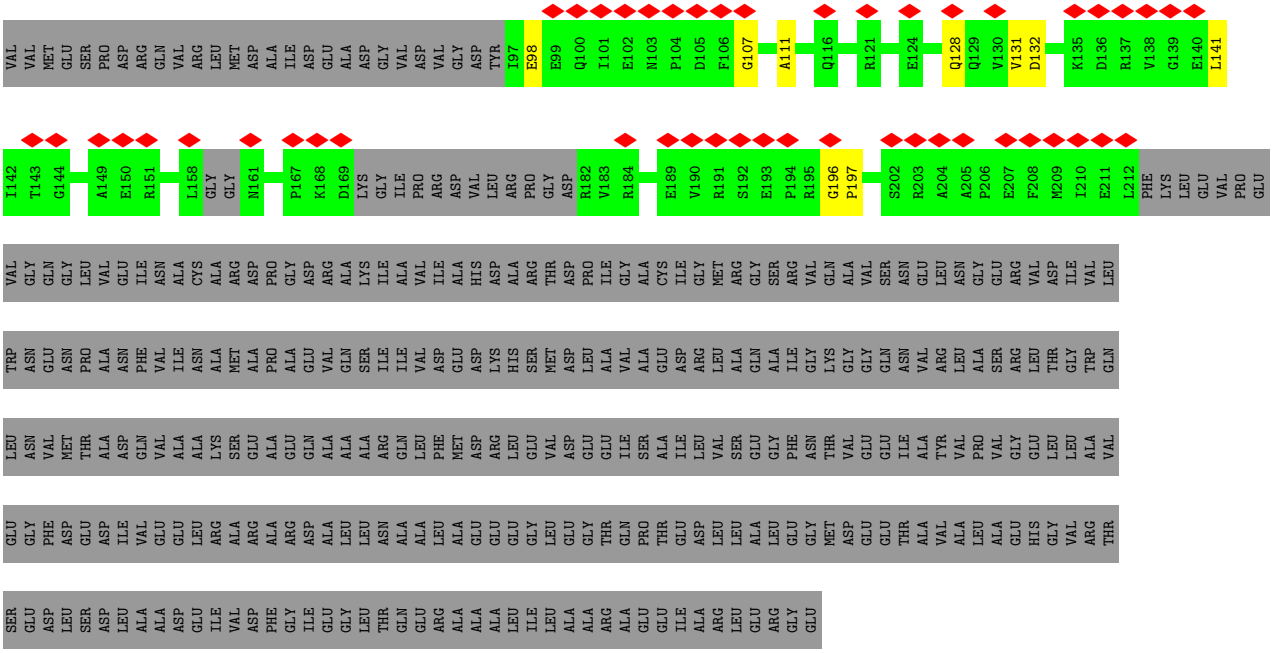
Chain J:



• Molecule 9: Transcription termination/antitermination protein NusA

Chain F:




VAL VAL MET GLU SER PRO ASP ARG GLN VAL ARG LEU MET ASP ALA ILE ASP GLU ALA ASP GLY VAL ASP VAL GLY ASP TYR
I97 E98 E99 Q100 I101 E102 N103 P104 D105 F106 G107 A111 Q116 R121 E124 Q128 Q129 V130 V131 D132 K135 D136 R137 V138 G139 E140 L141
I142 T143 G144 A149 E150 R151 L158 GLY GLY N161 P167 K168 D169 LYS GLY ILE PRO ARG ASP VAL LEU ARG PRO GLY ASP R182 V183 R184 E189 V190 R191 S192 E193 P194 R195 G196 P197 S202 R203 A204 A205 P206 E207 F208 M209 I210 E211 L212 PHE LYS LEU GLU VAL PRO GLU
VAL GLY GLN GLY LEU VAL GLU ILE ASN ALA CYS ALA ARG ASP PRO GLY ASP ARG ALA LYS ILE ALA VAL ILE ALA HIS ASP ALA ARG THR ASP PRO ILE GLY ALA CYS ILE GLY MET ARG GLY SER ARG VAL GLN ALA VAL SER ASN GLU LEU ASN GLY GLU ARG VAL ASP ILE LEU LEU
TRP ASN GLU ASN PRO ALA ASN PHE VAL ILE ASN ALA MET ALA PRO ALA GLU VAL GLN SER ILE ILE VAL ASP GLU ASP LYS HIS SER MET ASP LEU ALA VAL ALA GLU ASP ARG LEU ALA GLN ALA ILE GLY LYS GLY GLY GLN ASN GLU VAL ARG LEU ALA SER ARG LEU THR GLY TRP GLN
LEU ASN VAL MET THR ALA ASP GLN VAL ALA ALA LYS SER GLU ALA GLU GLN ALA ALA ALA ARG GLN LEU PHE MET ASP ARG LEU GLU VAL ASP GLU GLU ILE SER ALA ILE LEU VAL SER GLU GLY PHE ASN THR VAL GLU GLU ILE ALA TYR VAL PRO VAL GLY GLU LEU LEU ALA VAL
GLU GLY PHE ASP GLU ASP ILE VAL GLU GLU LEU ARG ALA ARG ALA ARG ASP ALA LEU LEU ASN ALA ALA LEU ALA GLU GLU GLU GLY LEU GLU GLY THR GLN PRO THR GLU ASP LEU LEU ALA LEU GLU GLY MET ASP GLU GLU THR ALA VAL ALA LEU ALA GLU HIS GLY VAL ARG THR
SER GLU ASP LEU SER ASP LEU ALA ALA ASP GLU ILE VAL ASP PHE GLY ILE GLU GLY LEU THR GLN GLU ARG ALA ALA ALA LEU ILE LEU ALA ALA ARG ALA GLU GLU ILE ALA ARG LEU GLU ARG GLY GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	204450	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.56	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.114	Depositor
Minimum map value	-0.059	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	304.2, 304.2, 304.2	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.014, 1.014, 1.014	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.24	0/1562	0.46	0/2126
1	B	0.24	0/1466	0.47	0/2005
2	C	0.26	0/9510	0.46	1/12948 (0.0%)
3	D	0.25	0/8849	0.46	0/12033
4	E	0.24	0/468	0.38	0/635
5	G	0.54	0/649	1.01	0/999
6	H	0.53	0/505	0.82	0/776
7	I	0.25	0/299	0.84	0/466
8	J	0.29	0/497	0.46	0/676
9	F	0.26	0/1100	0.53	1/1506 (0.1%)
All	All	0.27	0/24905	0.51	2/34170 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	129	LEU	CA-CB-CG	5.13	127.09	115.30
9	F	141	LEU	CA-CB-CG	5.11	127.06	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1543	0	1516	9	0
1	B	1449	0	1360	4	0
2	C	9355	0	8763	45	0
3	D	8733	0	8464	46	0
4	E	467	0	452	2	0
5	G	582	0	326	4	0
6	H	450	0	245	1	0
7	I	266	0	131	4	0
8	J	488	0	432	6	0
9	F	1091	0	944	5	0
10	D	1	0	0	0	0
11	D	2	0	0	0	0
All	All	24427	0	22633	114	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 (114) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:61:VAL:HG11	2:C:496:LEU:HB3	1.84	0.59
2:C:719:PRO:HB3	2:C:817:SER:HB2	1.86	0.58
2:C:733:GLU:HB3	2:C:823:LEU:H	1.70	0.56
3:D:201:LEU:HD11	3:D:220:ARG:HH11	1.69	0.56
3:D:599:LYS:HE3	3:D:731:ALA:HB2	1.85	0.56
1:A:27:VAL:HG22	1:A:201:VAL:HG12	1.90	0.54
3:D:254:PRO:HD3	7:I:11:C:H41	1.73	0.54
1:A:57:THR:HB	1:A:157:ARG:HH12	1.73	0.53
3:D:648:PRO:HG3	3:D:701:THR:HG21	1.91	0.53
1:B:178:PRO:O	1:B:207:ASN:ND2	2.41	0.53
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.89	0.53
2:C:179:ALA:HB3	2:C:191:PHE:HB2	1.91	0.53
3:D:491:LEU:HA	3:D:498:PRO:HA	1.90	0.53
2:C:870:ARG:NH1	7:I:9:A:OP2	2.42	0.53
2:C:706:ARG:NH2	2:C:1112:GLY:O	2.42	0.53
3:D:43:THR:HG22	3:D:56:LEU:HB2	1.90	0.52
3:D:63:GLY:O	3:D:98:ARG:NH1	2.43	0.51
3:D:824:THR:O	3:D:839:ARG:NH1	2.44	0.51
3:D:1347:GLY:O	3:D:1351:ASN:ND2	2.43	0.51
2:C:1344:ASN:HD22	8:J:48:PRO:HB3	1.75	0.51
3:D:1222:LEU:HB2	3:D:1230:LEU:HD22	1.93	0.51
3:D:588:LEU:HD21	3:D:609:SER:HB2	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:536:SER:HB2	5:G:22:DC:H4'	1.92	0.50
2:C:1127:PRO:HB2	2:C:1254:LEU:HD13	1.94	0.50
2:C:102:ARG:HB3	2:C:126:GLU:HA	1.93	0.50
3:D:425:ARG:NH2	7:I:20:A:O2'	2.44	0.49
9:F:62:ARG:HA	9:F:98:GLU:HA	1.94	0.49
3:D:654:ILE:HG22	3:D:690:THR:HG23	1.94	0.49
2:C:1142:LEU:HD21	3:D:508:LEU:HD22	1.94	0.49
3:D:252:LEU:O	7:I:11:C:N4	2.45	0.49
2:C:13:ARG:HD3	2:C:1225:ALA:HB2	1.94	0.49
2:C:728:VAL:O	2:C:1110:ARG:NH1	2.46	0.49
2:C:760:ILE:HD11	2:C:798:PRO:HB3	1.95	0.48
3:D:1220:ASP:HA	3:D:1223:ARG:HG2	1.95	0.48
2:C:27:PHE:HB3	2:C:30:ALA:HB2	1.95	0.48
3:D:426:ALA:HB1	5:G:16:DA:H1'	1.94	0.48
3:D:1220:ASP:N	3:D:1220:ASP:OD1	2.44	0.48
2:C:833:PHE:HB3	2:C:1141:PRO:HB3	1.96	0.48
2:C:471:ASP:N	2:C:471:ASP:OD1	2.47	0.48
2:C:1207:SER:OG	2:C:1208:ASP:N	2.45	0.48
3:D:425:ARG:HG3	3:D:427:PRO:HD2	1.95	0.47
8:J:12:ASN:ND2	8:J:62:GLY:O	2.46	0.47
2:C:804:ASP:N	2:C:804:ASP:OD1	2.47	0.47
9:F:107:GLY:O	9:F:111:ALA:N	2.47	0.47
2:C:917:THR:HG23	2:C:943:LYS:HB3	1.96	0.47
3:D:127:MET:O	3:D:220:ARG:NH2	2.48	0.47
2:C:544:ASP:OD1	2:C:544:ASP:N	2.43	0.47
2:C:1193:ASP:N	2:C:1193:ASP:OD1	2.47	0.47
3:D:841:LEU:HB2	3:D:871:VAL:HG21	1.97	0.47
2:C:320:ASN:HD21	2:C:354:SER:HA	1.80	0.47
2:C:1259:THR:HG23	2:C:1261:GLU:H	1.80	0.46
2:C:742:VAL:HB	2:C:816:PRO:HD2	1.96	0.46
2:C:1113:ASN:ND2	2:C:1152:GLN:OE1	2.48	0.46
2:C:1348:LYS:HA	2:C:1351:VAL:HG22	1.96	0.46
3:D:462:ASP:N	3:D:462:ASP:OD1	2.48	0.46
1:A:15:GLN:HB2	1:A:27:VAL:HB	1.98	0.46
2:C:60:SER:OG	2:C:493:ARG:NH2	2.46	0.46
3:D:1145:ASP:OD2	3:D:1150:ARG:NH2	2.48	0.46
2:C:849:GLU:HB2	2:C:1122:PRO:HA	1.97	0.46
3:D:1345:LEU:HD21	3:D:1354:VAL:HG21	1.97	0.45
2:C:591:THR:HB	2:C:708:LEU:HD11	1.98	0.45
3:D:585:PRO:HD2	3:D:588:LEU:HD13	1.97	0.45
5:G:8:DC:H2"	5:G:9:DG:H5"	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:43:ASP:OD2	8:J:43:ASP:N	2.47	0.45
2:C:13:ARG:NH2	2:C:822:GLU:OE2	2.49	0.45
9:F:51:ASP:OD1	9:F:51:ASP:N	2.48	0.44
1:A:81:VAL:HG22	1:A:131:CYS:HB3	1.99	0.44
1:B:81:VAL:HG22	1:B:131:CYS:HB3	1.99	0.44
3:D:1327:GLN:HG2	5:G:12:DG:H5'	1.99	0.44
3:D:865:LEU:HD11	3:D:903:ARG:HB3	1.99	0.44
1:A:117:THR:OG1	1:A:121:VAL:O	2.36	0.44
2:C:644:ILE:HG12	2:C:680:PHE:HB2	2.00	0.43
8:J:11:VAL:HB	8:J:67:LEU:HB3	2.00	0.43
1:A:104:LYS:HG2	1:A:110:VAL:HG22	2.00	0.43
2:C:180:ARG:NH1	6:H:16:DG:OP1	2.51	0.43
1:A:90:ILE:HG21	1:A:145:ILE:HD13	1.99	0.43
1:B:13:GLY:HA3	1:B:14:PRO:HA	1.85	0.43
2:C:1253:GLN:HE21	2:C:1262:ALA:HB1	1.82	0.43
3:D:475:GLU:HG3	4:E:24:SER:HB2	2.00	0.43
3:D:400:LEU:HD12	3:D:403:ARG:HE	1.83	0.43
2:C:982:ILE:HA	2:C:985:VAL:HG22	2.01	0.43
2:C:1202:ASP:OD1	2:C:1202:ASP:N	2.46	0.43
3:D:275:ARG:NH1	3:D:298:MET:O	2.45	0.43
2:C:403:LEU:O	2:C:424:SER:OG	2.35	0.42
3:D:573:THR:HG21	3:D:590:PHE:HE2	1.84	0.42
3:D:160:LEU:HD23	3:D:160:LEU:HA	1.93	0.42
2:C:566:LEU:HD21	2:C:599:LEU:HD22	2.00	0.42
3:D:581:SER:HB2	3:D:590:PHE:HE1	1.85	0.42
2:C:98:GLY:HA2	2:C:133:PRO:HA	2.00	0.42
3:D:662:VAL:HA	3:D:665:ILE:HG22	2.01	0.42
3:D:844:VAL:HG21	3:D:899:ARG:HG3	2.02	0.42
2:C:899:VAL:HG12	2:C:913:VAL:HG13	2.00	0.42
3:D:480:ALA:HA	3:D:484:MET:HB2	2.02	0.42
2:C:635:SER:OG	2:C:636:ALA:N	2.53	0.42
2:C:743:THR:HG22	2:C:815:GLY:H	1.85	0.41
3:D:96:LYS:HA	3:D:96:LYS:HD3	1.93	0.41
3:D:120:LEU:HD12	3:D:120:LEU:HA	1.96	0.41
3:D:417:ARG:NH1	4:E:45:ASP:OD2	2.52	0.41
3:D:602:ILE:HD12	3:D:602:ILE:HA	1.94	0.41
2:C:706:ARG:HG3	2:C:1149:ASN:HD22	1.85	0.41
1:B:100:LEU:HD21	1:B:121:VAL:HG11	2.02	0.41
8:J:20:SER:O	8:J:20:SER:OG	2.31	0.41
1:A:48:LEU:HD23	1:A:48:LEU:HA	1.94	0.41
2:C:32:GLN:NE2	2:C:555:LYS:O	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:482:ALA:O	3:D:488:ASN:ND2	2.53	0.41
3:D:431:ARG:HH22	3:D:906:ALA:HB2	1.86	0.41
3:D:741:LEU:O	3:D:763:ASN:ND2	2.54	0.41
1:A:61:ILE:HG12	1:A:141:MET:HG3	2.02	0.40
3:D:53:ARG:HH12	3:D:89:GLY:H	1.68	0.40
9:F:128:GLN:HA	9:F:131:VAL:HG12	2.04	0.40
3:D:960:VAL:HG22	3:D:986:VAL:HG12	2.02	0.40
8:J:4:PHE:HB3	8:J:14:PHE:HB3	2.03	0.40
9:F:196:GLY:HA2	9:F:197:PRO:HD3	1.97	0.40
2:C:645:ALA:HB3	2:C:681:MET:HG3	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	207/346 (60%)	202 (98%)	5 (2%)	0	100	100
1	B	204/346 (59%)	200 (98%)	4 (2%)	0	100	100
2	C	1268/1383 (92%)	1229 (97%)	39 (3%)	0	100	100
3	D	1182/1405 (84%)	1152 (98%)	30 (2%)	0	100	100
4	E	61/99 (62%)	61 (100%)	0	0	100	100
8	J	64/77 (83%)	61 (95%)	3 (5%)	0	100	100
9	F	157/507 (31%)	145 (92%)	12 (8%)	0	100	100
All	All	3143/4163 (76%)	3050 (97%)	93 (3%)	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	157/289 (54%)	157 (100%)	0	100	100
1	B	134/289 (46%)	133 (99%)	1 (1%)	84	93
2	C	895/1166 (77%)	894 (100%)	1 (0%)	93	98
3	D	854/1175 (73%)	853 (100%)	1 (0%)	93	98
4	E	44/80 (55%)	44 (100%)	0	100	100
8	J	49/64 (77%)	49 (100%)	0	100	100
9	F	82/400 (20%)	81 (99%)	1 (1%)	71	87
All	All	2215/3463 (64%)	2211 (100%)	4 (0%)	93	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	142	ARG
2	C	206	ARG
3	D	818	THR
9	F	132	ASP

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	226	GLN
1	B	152	GLN
2	C	82	GLN
2	C	475	HIS
2	C	579	HIS
2	C	790	GLN
2	C	1079	GLN
2	C	1149	ASN
2	C	1205	GLN
2	C	1248	GLN
2	C	1344	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	1349	ASN
3	D	9	ASN
3	D	113	HIS
3	D	170	GLN
3	D	340	GLN
3	D	1260	GLN
8	J	6	GLN
8	J	17	GLN
9	F	103	ASN
9	F	128	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	I	11/20 (55%)	2 (18%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	I	12	G
7	I	13	G

There are no RNA pucker outliers to report.

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)

Of 3 ligands modelled in this entry, 3 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

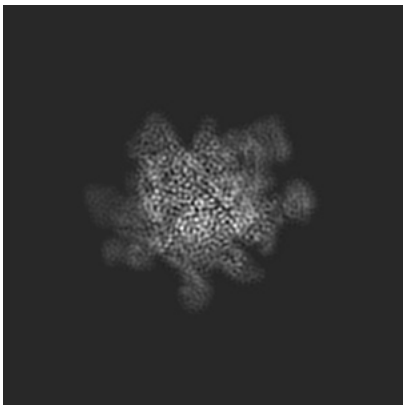
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9785. These allow visual inspection of the internal detail of the map and identification of artifacts.

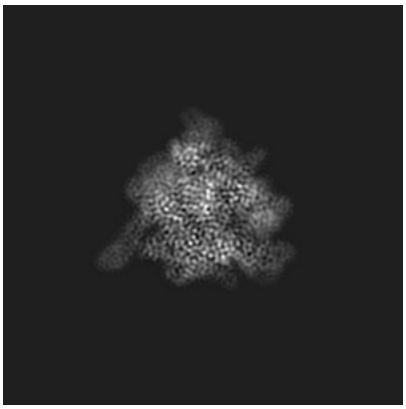
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

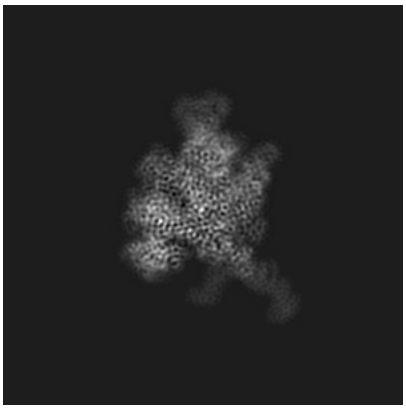
6.1.1 Primary map



X

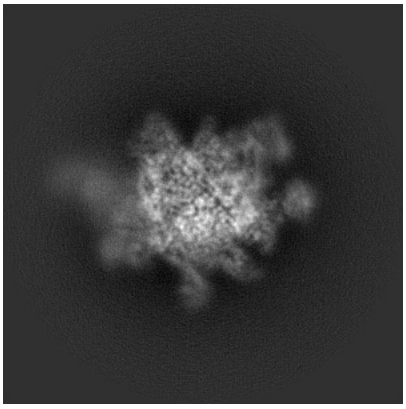


Y

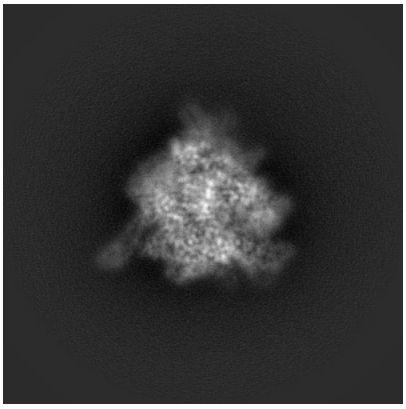


Z

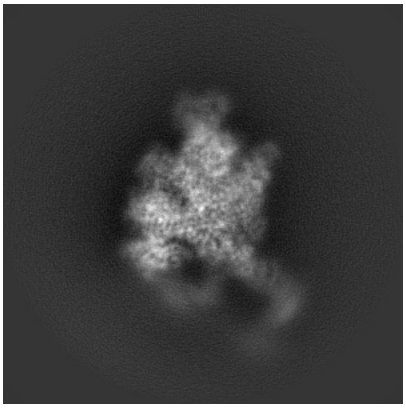
6.1.2 Raw map



X



Y

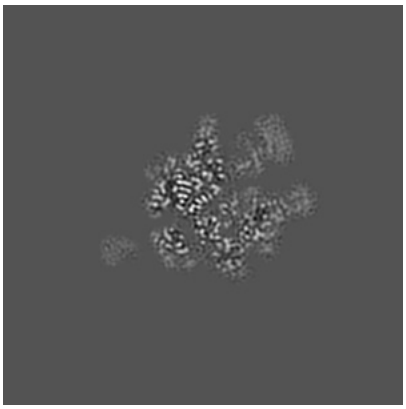


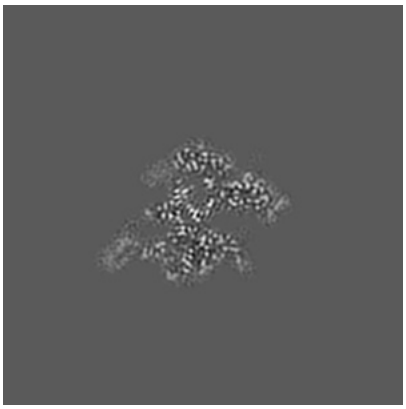
Z

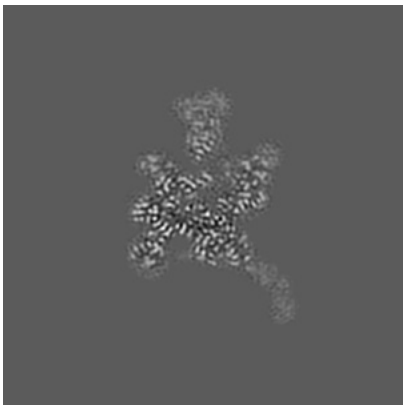
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

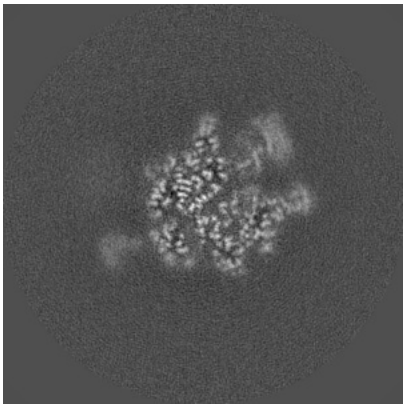
6.2.1 Primary map

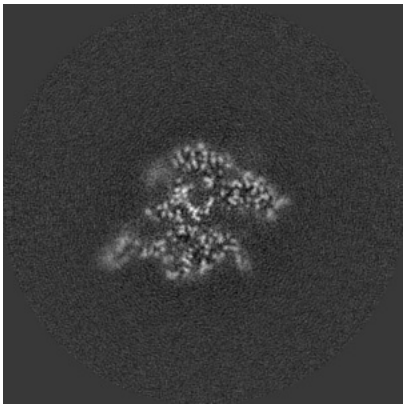

X Index: 150

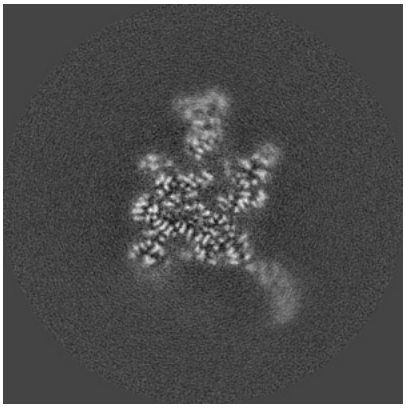

Y Index: 150


Z Index: 150

6.2.2 Raw map


X Index: 150

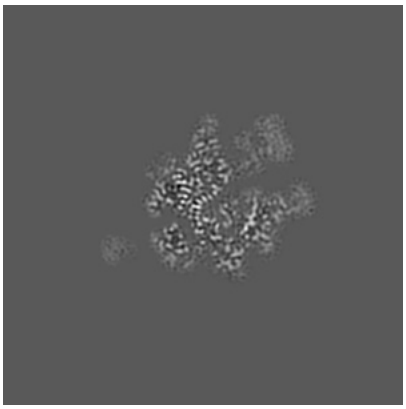

Y Index: 150

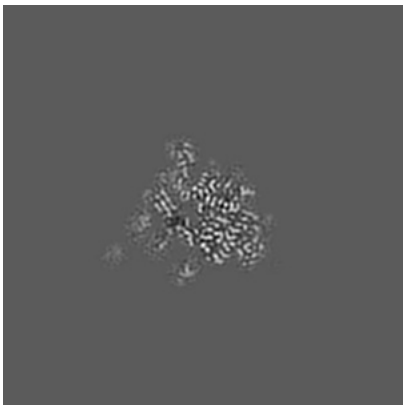

Z Index: 150

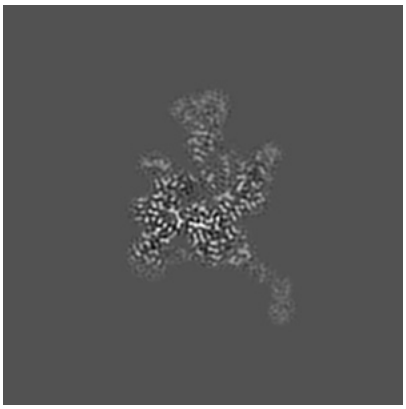
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

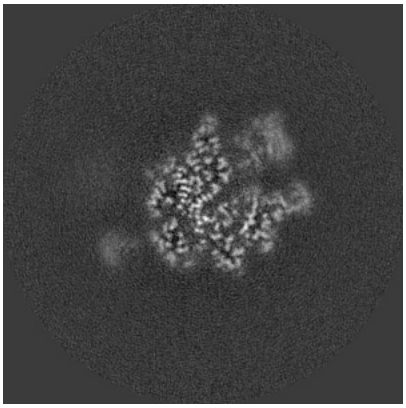
6.3.1 Primary map

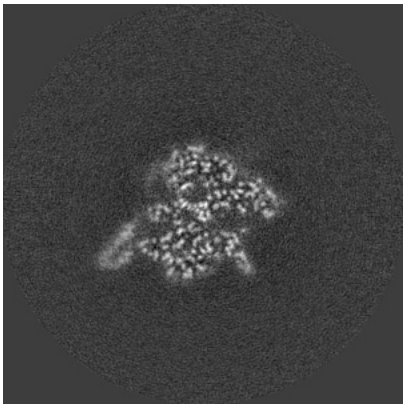

X Index: 149

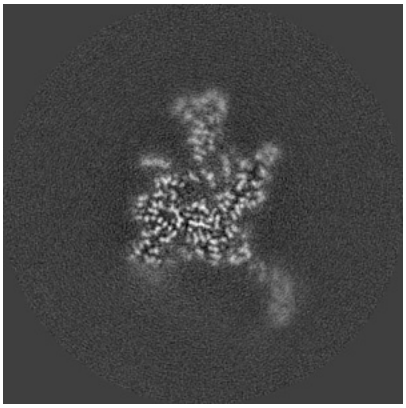

Y Index: 132


Z Index: 152

6.3.2 Raw map


X Index: 149

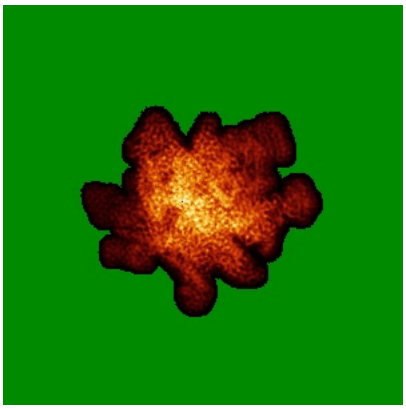

Y Index: 147


Z Index: 152

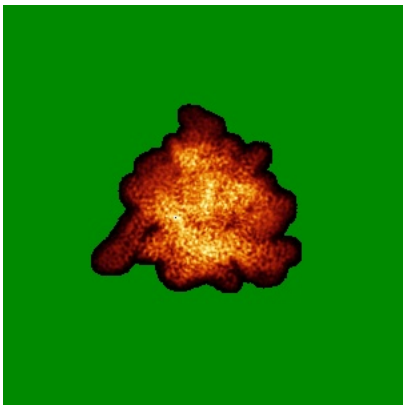
The images above show the largest variance slices of the map in three orthogonal directions.

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

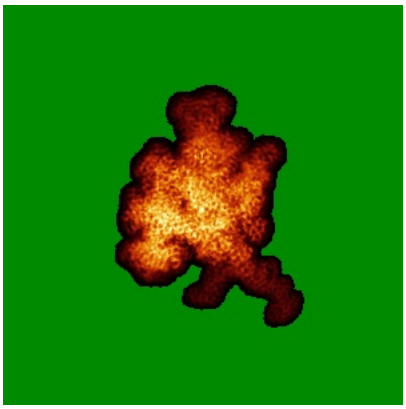
6.4.1 Primary map



X

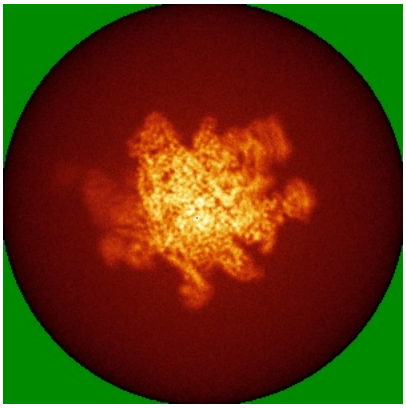


Y

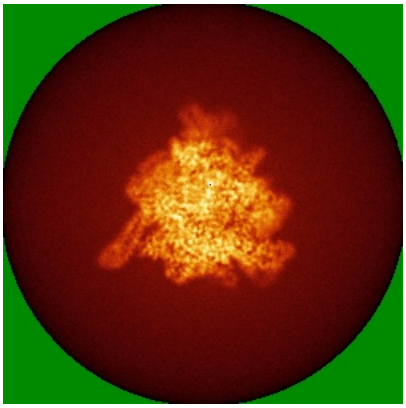


Z

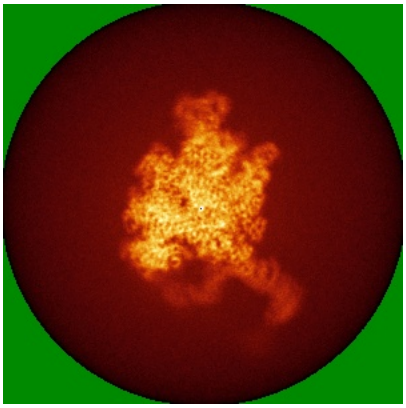
6.4.2 Raw map



X



Y

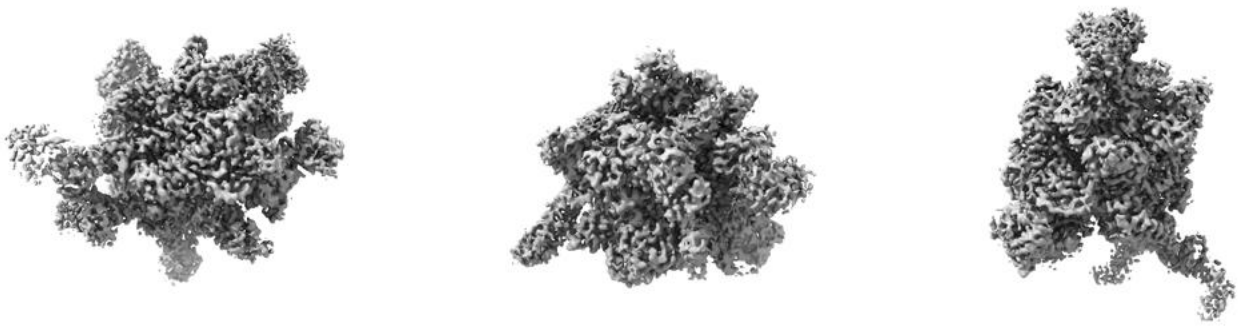


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

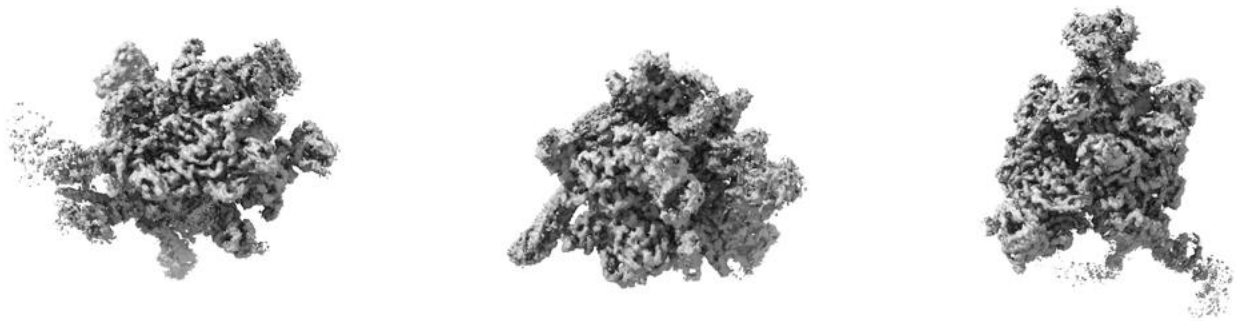
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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.

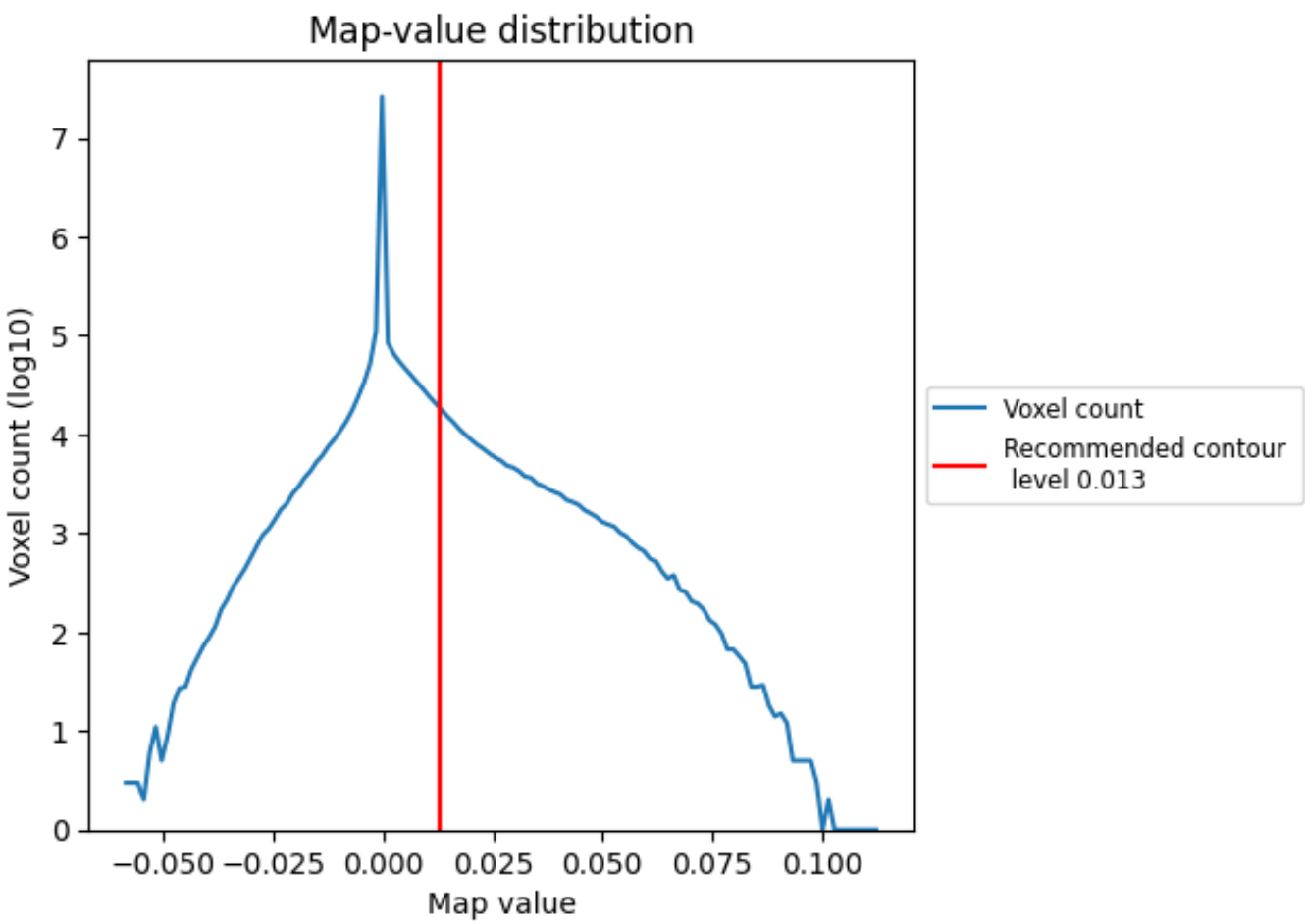
6.6 Mask visualisation (i)

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

7 Map analysis (i)

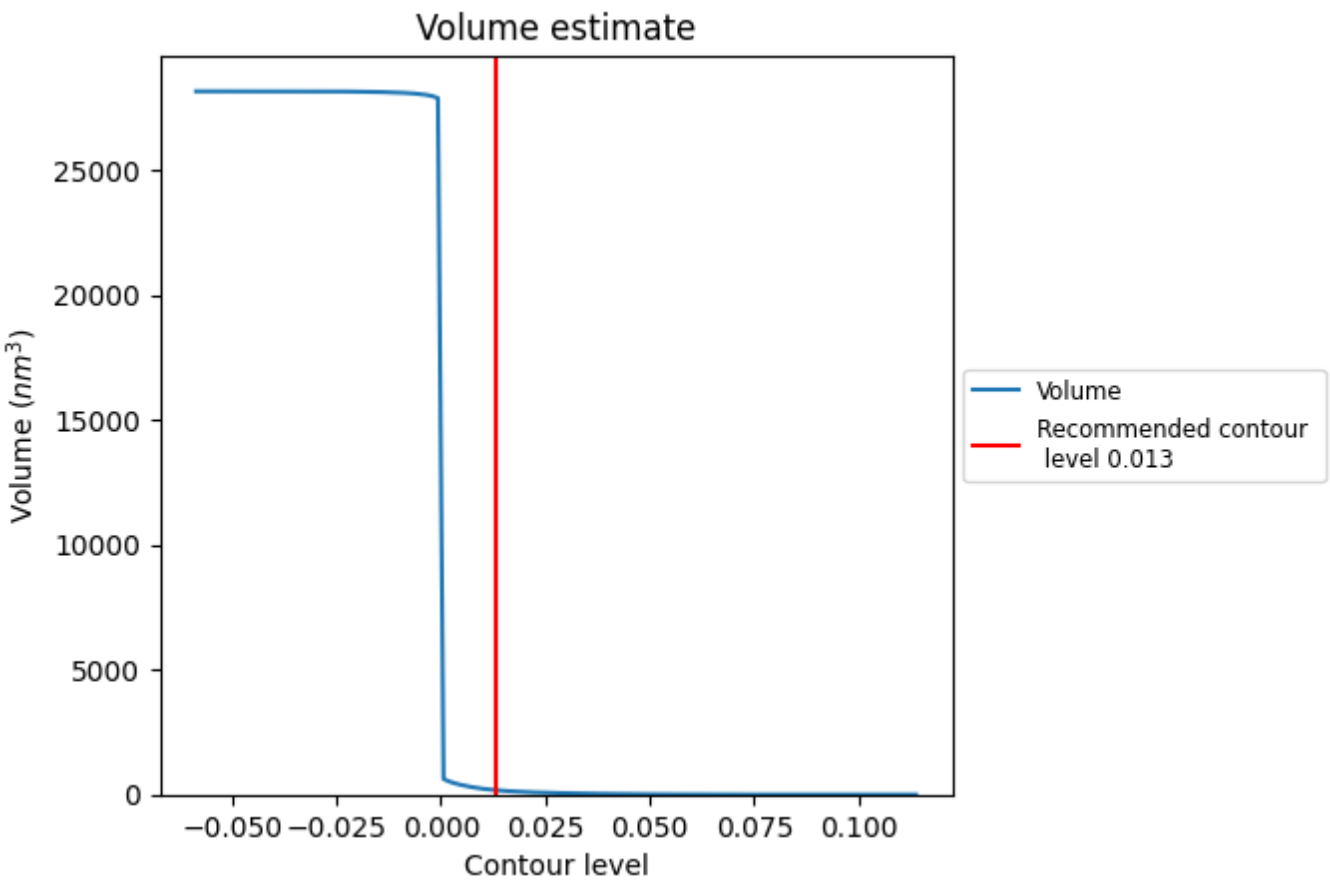
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

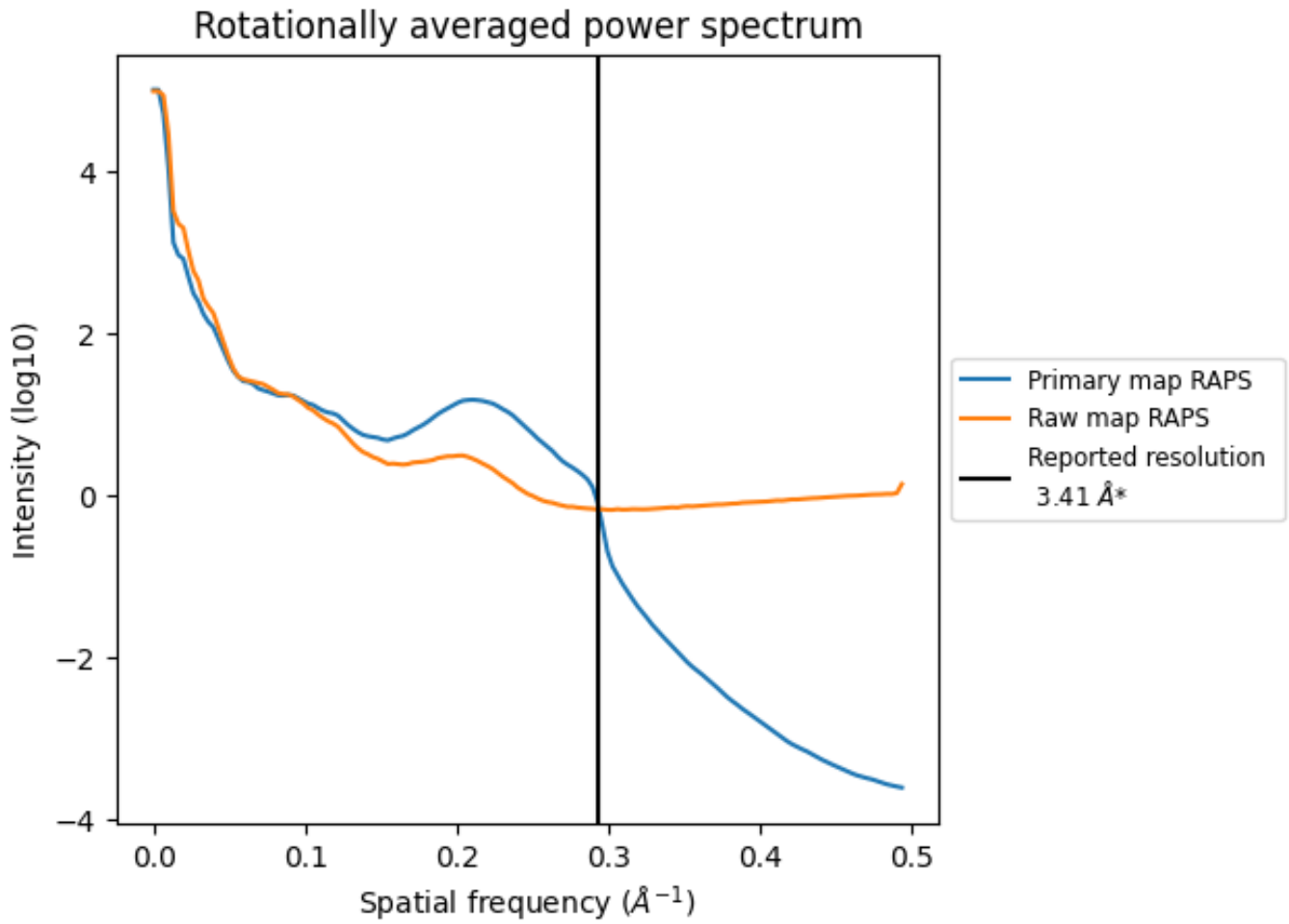
7.2 Volume estimate (i)



The volume at the recommended contour level is 179 nm^3; this corresponds to an approximate mass of 162 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)

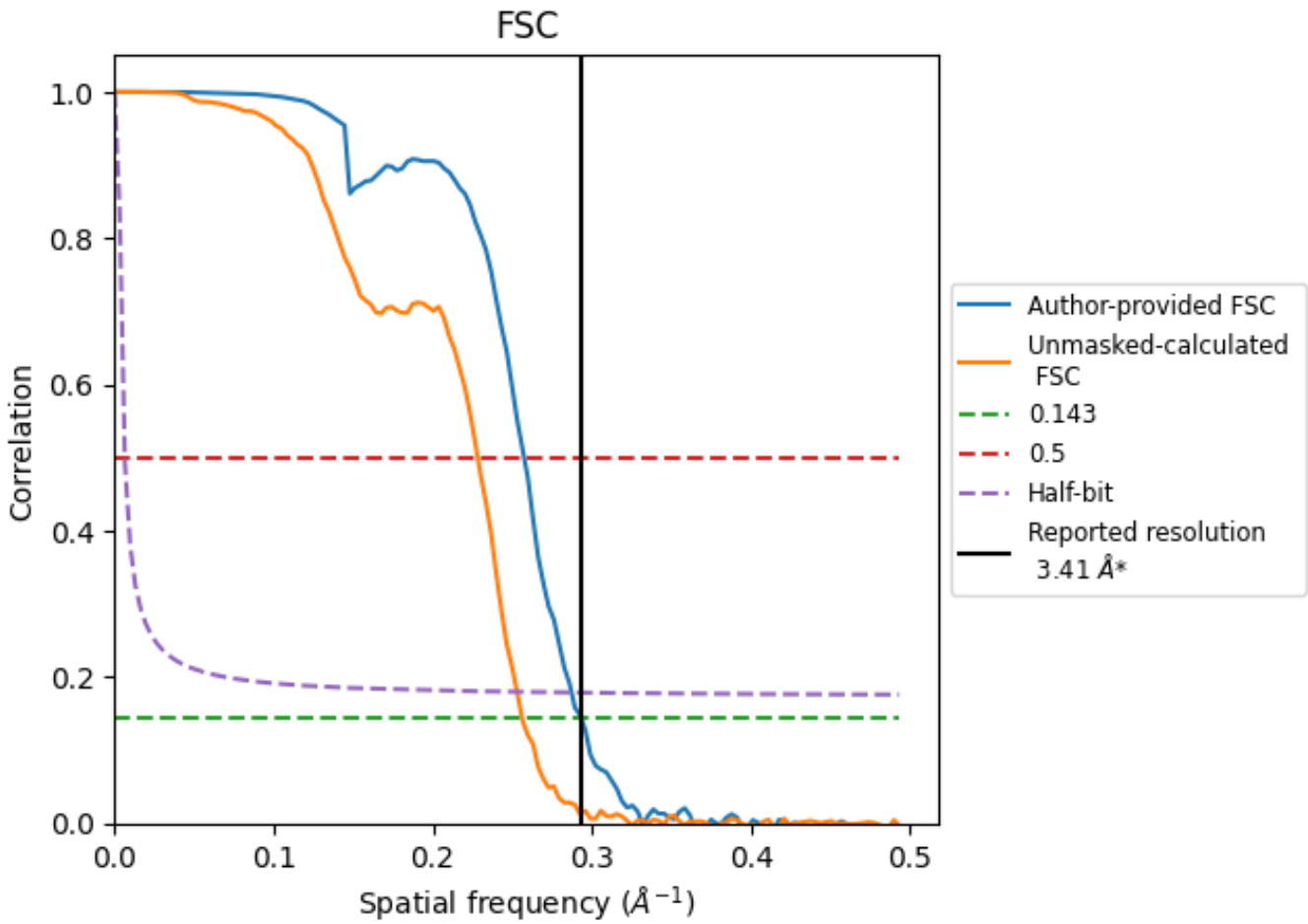


*Reported resolution corresponds to spatial frequency of 0.293 Å^{-1}

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 0.293 Å^{-1}

8.2 Resolution estimates (i)

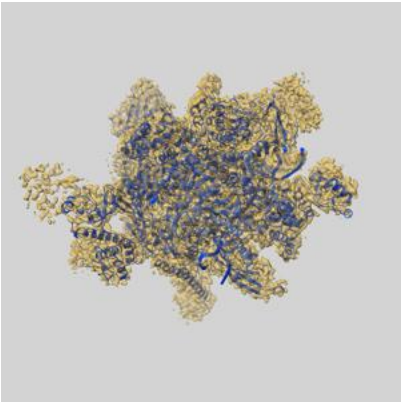
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.41	-	-
Author-provided FSC curve	3.41	3.89	3.48
Unmasked-calculated*	3.90	4.38	3.95

*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 3.90 differs from the reported value 3.41 by more than 10 %

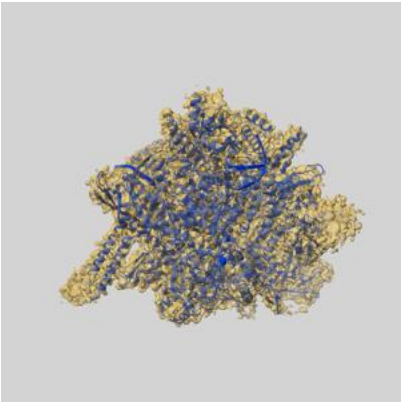
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-9785 and PDB model 6J9E. Per-residue inclusion information can be found in section 3 on page 7.

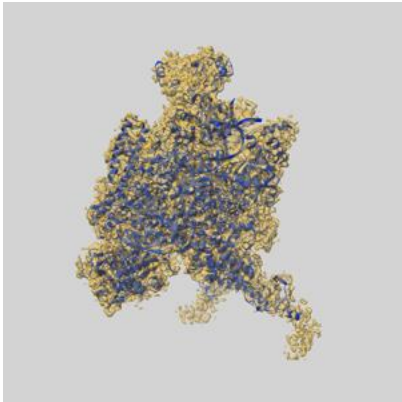
9.1 Map-model overlay (i)



X



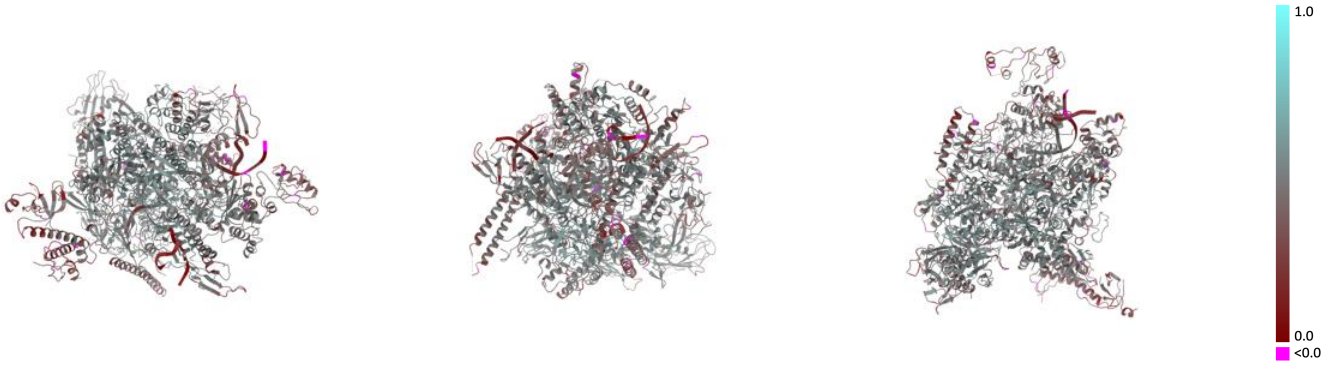
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.013 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.

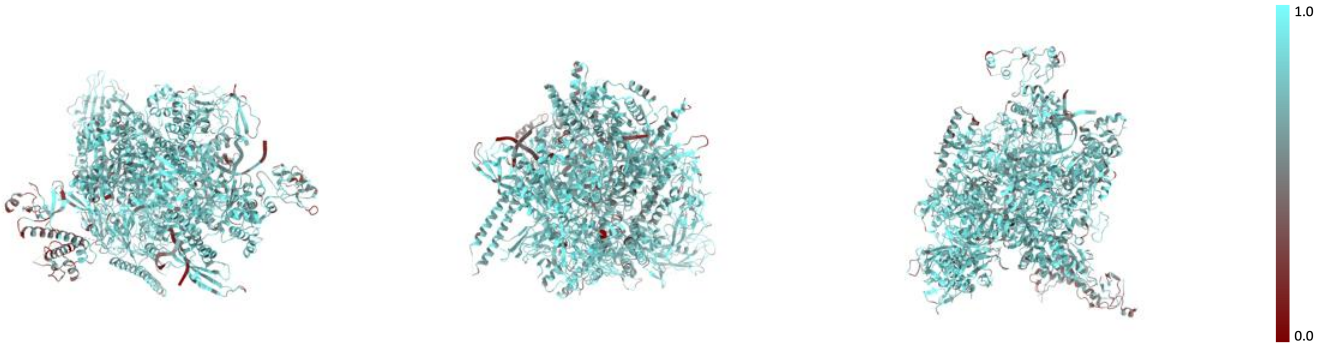
9.2 Q-score mapped to coordinate model (i)



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.

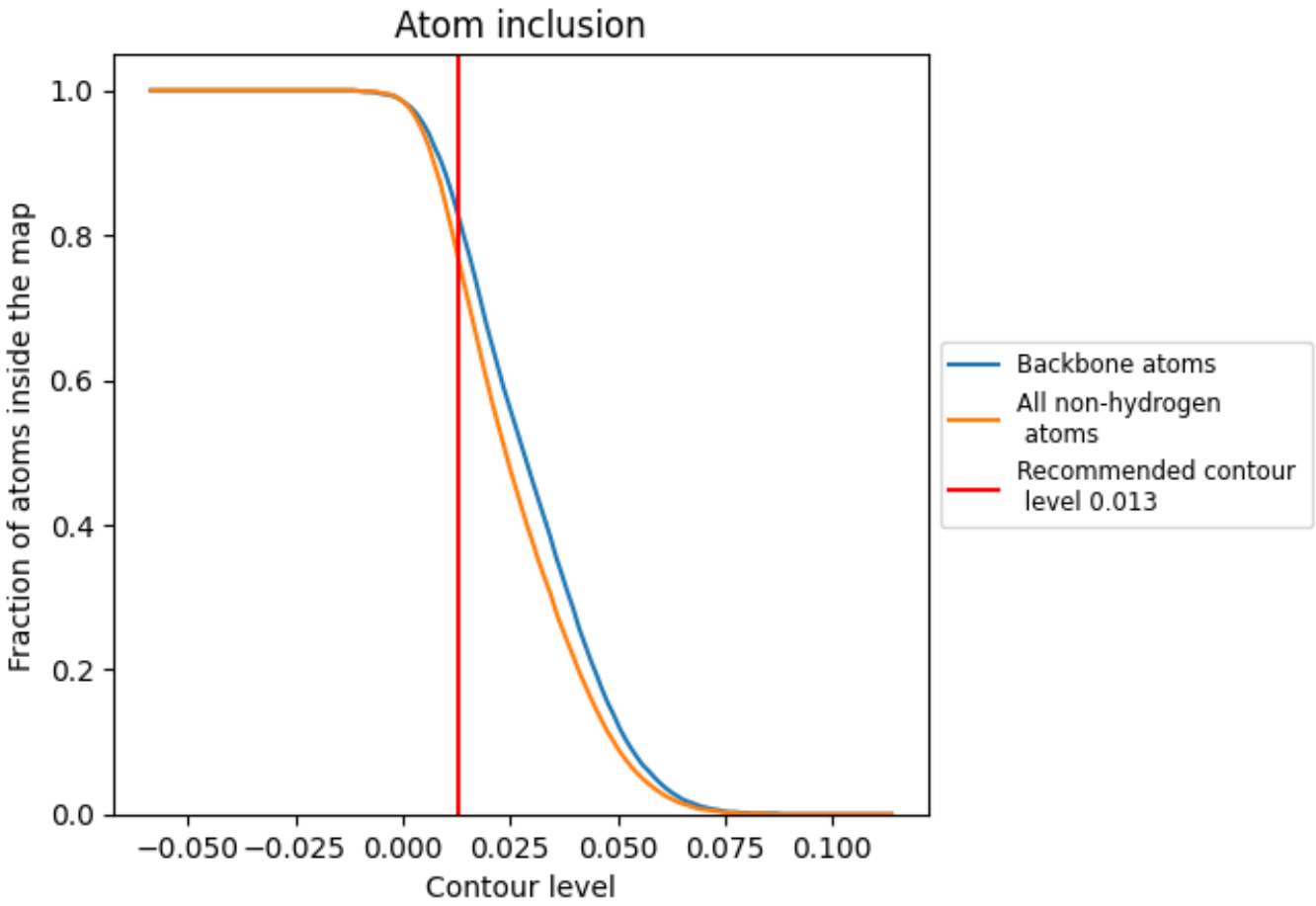
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.013).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7670	0.4510
A	0.7660	0.4720
B	0.7840	0.4500
C	0.7940	0.4690
D	0.7820	0.4620
E	0.7820	0.4600
F	0.4500	0.2840
G	0.7290	0.3590
H	0.6240	0.2770
I	0.8500	0.4640
J	0.7570	0.4580