W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB EM Validation Report (i)

Nov 19, 2022 – 09:51 pm GMT

PDB ID	:	6EYD
EMDB ID	:	EMD-3983
Title	:	Structure of Mycobacterium smegmatis RNA polymerase Sigma-A holoenzyme
Authors	:	Kouba, T.; Barvik, I.; Krasny, L.
Deposited on	:	2017-11-11
Resolution	:	4.20 Å(reported)

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

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

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

The following versions of software and data (see references (i)) were used in the production of this report:
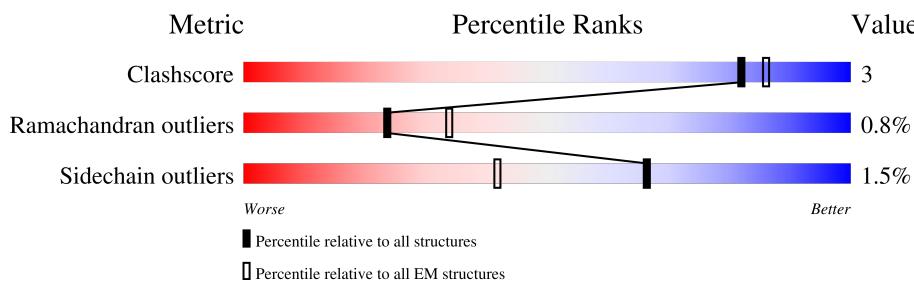
|		
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1   Overall quality at a glance   ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY
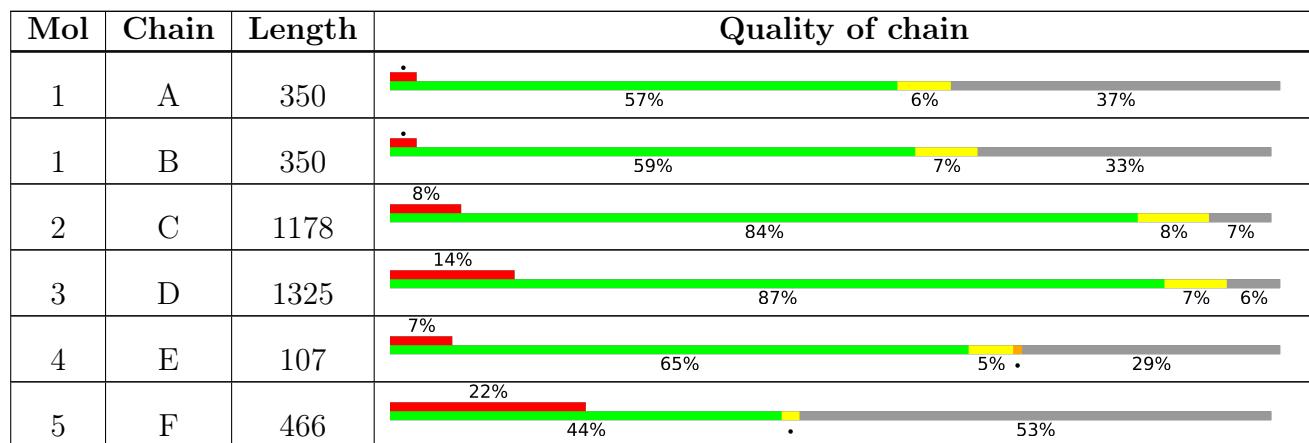
The reported resolution of this entry is 4.20 Å.

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	Percentile Ranks	Value
Clashscore		3
Ramachandran outliers		0.8%
Sidechain outliers		1.5%

Worse   *Better*

▌ Percentile relative to all structures

▯ Percentile relative to all EM structures

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	350	• 57% 6% 37%
1	B	350	• 59% 7% 33%
2	C	1178	8% 84% 8% 7%
3	D	1325	14% 87% 7% 6%
4	E	107	7% 65% 5% • 29%
5	F	466	22% 44% • 53%

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 22931 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
1	A	220	Total 1617	C 1022	N 278	O 315	S 2	0	0
1	B	233	Total 1660	C 1050	N 287	O 321	S 2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1092	Total 7982	C 5009	N 1395	O 1542	S 36	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	VAL	-	expression tag	UNP P60281
C	1170	LEU	-	expression tag	UNP P60281
C	1171	ALA	-	expression tag	UNP P60281
C	1172	ARG	-	expression tag	UNP P60281
C	1173	HIS	-	expression tag	UNP P60281
C	1174	GLY	-	expression tag	UNP P60281
C	1175	GLY	-	expression tag	UNP P60281
C	1176	SER	-	expression tag	UNP P60281
C	1177	GLY	-	expression tag	UNP P60281
C	1178	ALA	-	expression tag	UNP P60281

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1241	Total 9399	C 5890	N 1702	O 1767	S 40	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	VAL	-	expression tag	UNP A0QS66
D	1318	HIS	-	expression tag	UNP A0QS66
D	1319	HIS	-	expression tag	UNP A0QS66
D	1320	HIS	-	expression tag	UNP A0QS66
D	1321	HIS	-	expression tag	UNP A0QS66
D	1322	HIS	-	expression tag	UNP A0QS66
D	1323	HIS	-	expression tag	UNP A0QS66
D	1324	HIS	-	expression tag	UNP A0QS66
D	1325	HIS	-	expression tag	UNP A0QS66

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	76	Total 592	C 378	N 100	O 114	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	VAL	-	expression tag	UNP A0QWT1

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	217	Total 1678	C 1060	N 300	O 312	S 6	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
6	D	2	Total 2	Zn 2	0
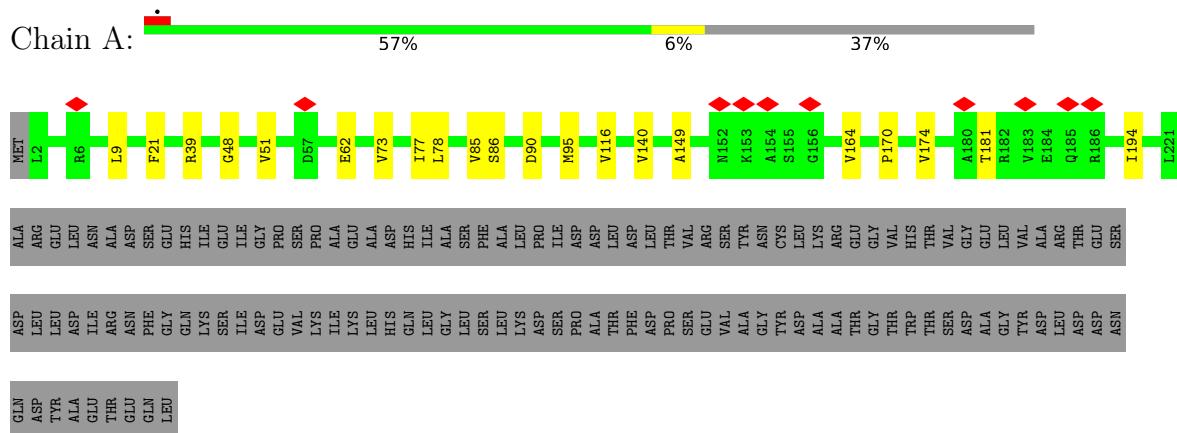
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
7	D	1	Total 1	Mg 1	0
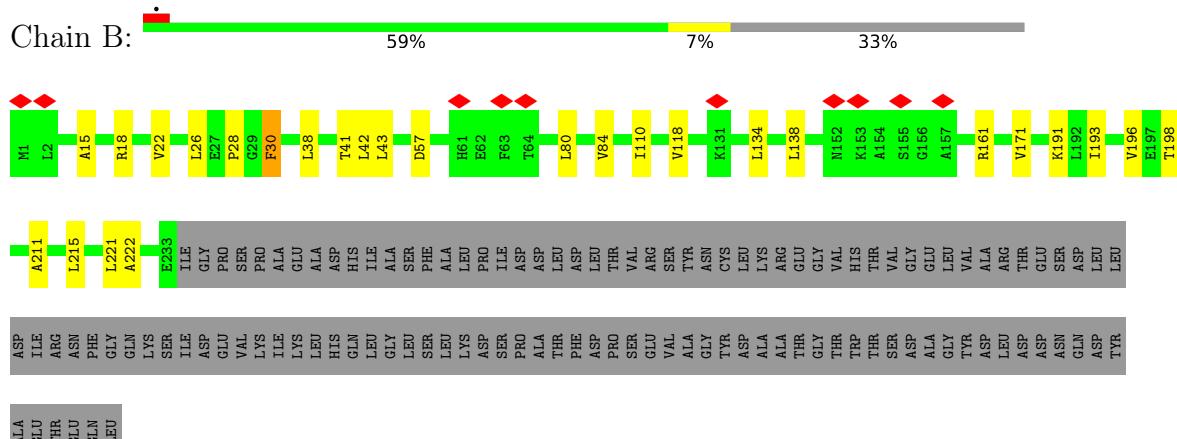
3 Residue-property plots ⓘ

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.
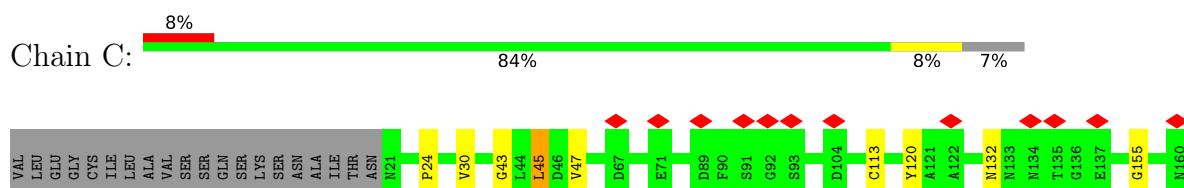
- Molecule 1: DNA-directed RNA polymerase subunit alpha
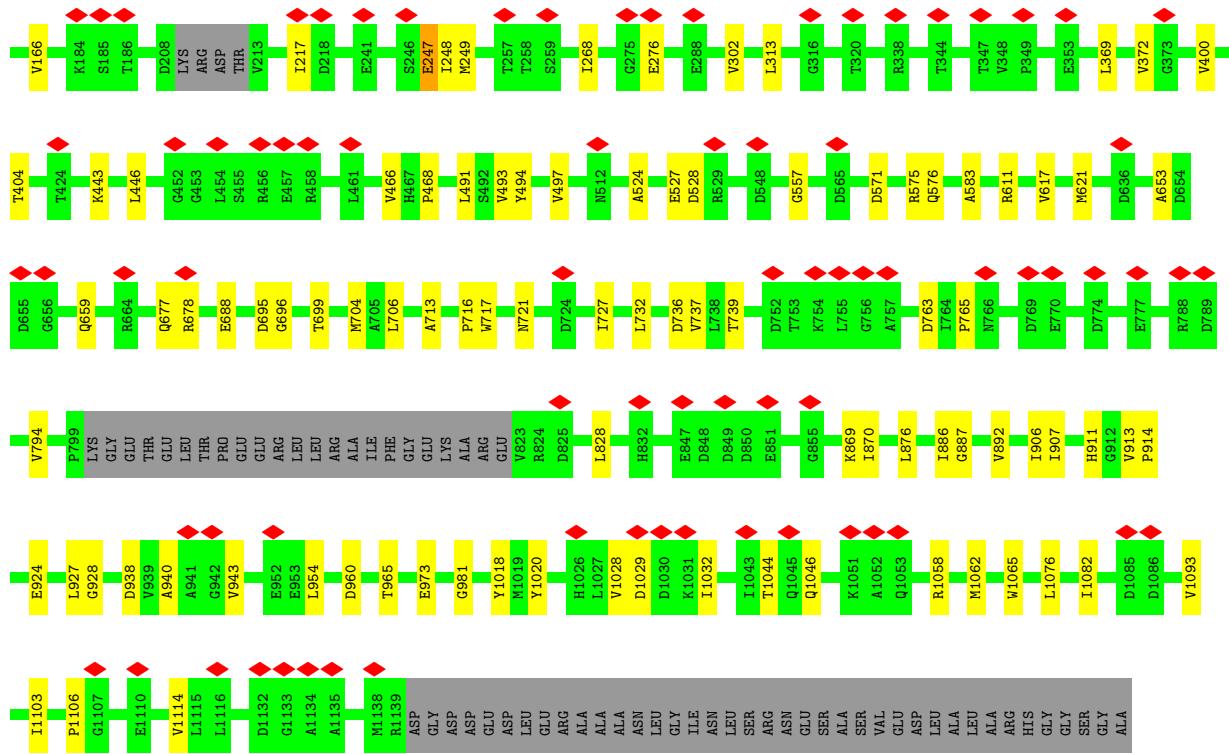
Chain A:

- Molecule 1: DNA-directed RNA polymerase subunit alpha
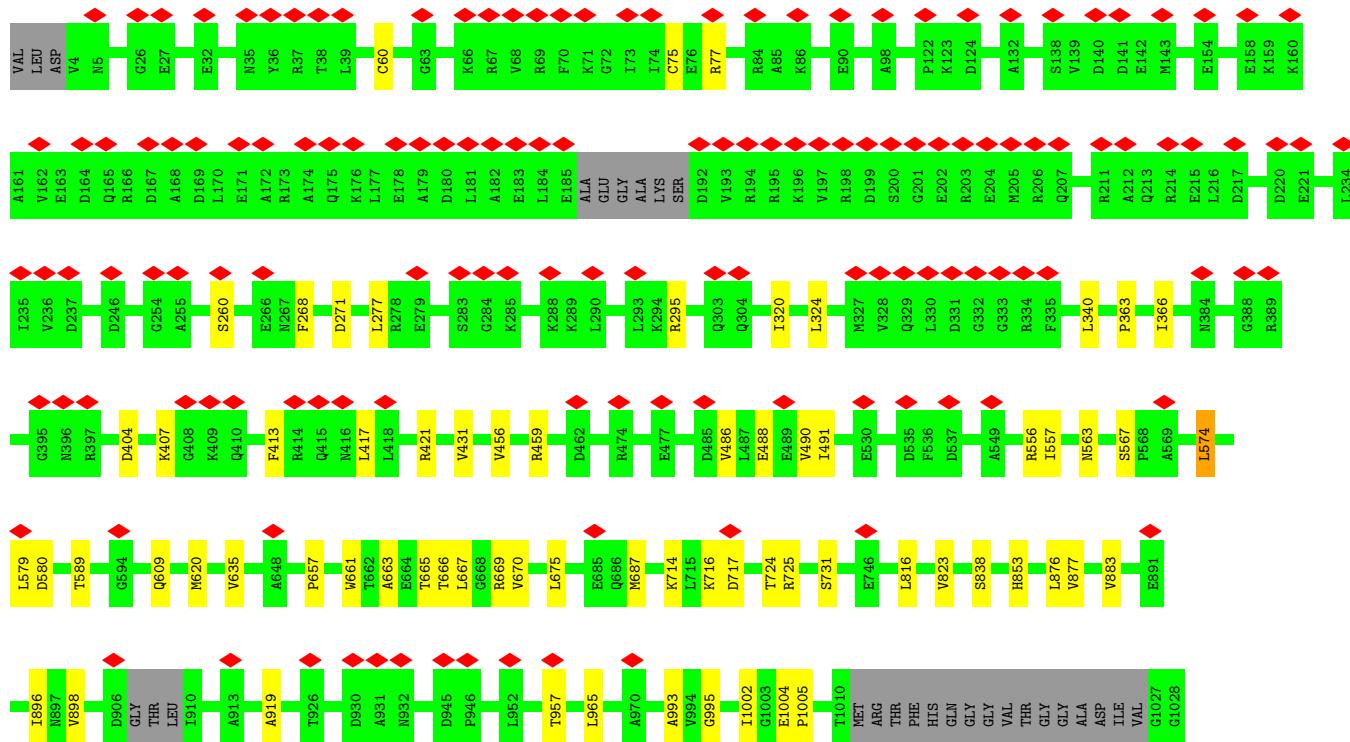
Chain B:

- Molecule 2: DNA-directed RNA polymerase subunit beta
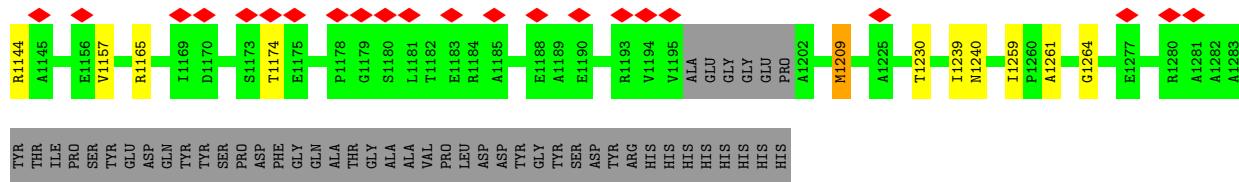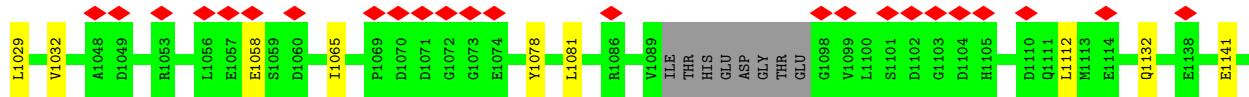
Chain C:

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

Chain D:

L1029 V1032 A1048 D1049 R1053 L1056 E1057 E1058 S1059 D1060 I1065 P1069 D1070 D1071 G1072 G1073 E1074 Y1078 L1081 R1086 V1089 ILE THR HIS GLU ASP GLY THR GLU G1098 V1099 L1100 S1101 D1102 G1103 D1104 H1105 D1110 Q1111 L1112 M1113 E1114 Q1132 E1138 E1141

R1144 A1145 E1156 V1157 R1165 I1169 D1170 S1173 T1174 E1175 P1178 G1179 S1180 L1181 T1182 E1183 R1184 A1185 E1188 A1189 E1190 R1193 V1194 V1195 ALA GLU GLY GLU GLU PRO A1202 M1209 A1225 T1230 I1239 N1240 I1259 P1260 A1261 G1264 E1277 R1280 A1281 A1282 A1283

TYR THR ILE PRO SER TYR GLU GLN ASP GLN TYR TYR SER PRO ASP PHE GLY GLN GLN ALA THR GLY ALA ALA VAL PRO LEU ASP ASP GLY TYR TYR THR TYR SER ASP TYR ARG HIS HIS HIS HIS HIS HIS HIS

● Molecule 4: DNA-directed RNA polymerase subunit omega

7%

Chain E:

65%   5% ●   29%

VAL SER THR PRO HIS ALA ASP ALA GLN LEU ASN ALA ALA ASP ASP LEU GLY ILE ILE ASP SER SER ALA ALA S24 A25 T33 L41 S42 R43 K47 N66 GLN LEU GLY ASP GLY ILE LEU LEU E74 E81 P82 G83 L84 Q85 E86 L89 D99 G106 GLU
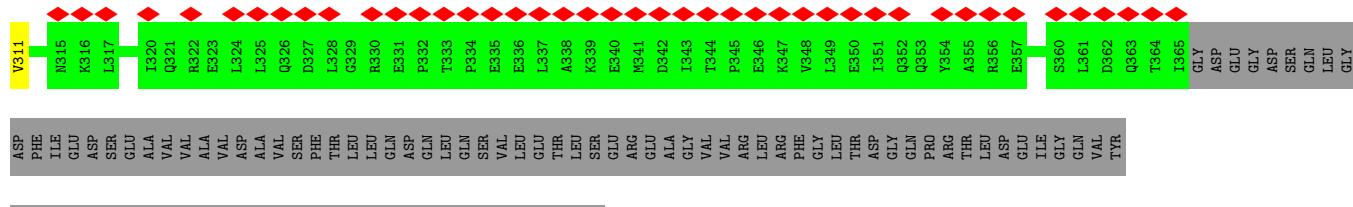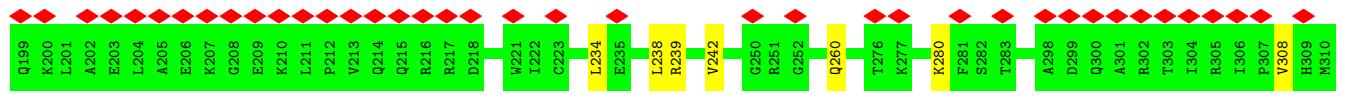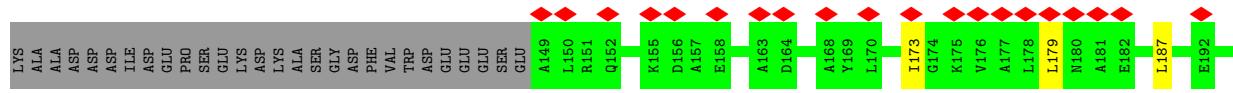
● Molecule 5: RNA polymerase sigma factor SigA

22%

Chain F:

44%   ●   53%

MET ALA ALA THR LYS ALA SER PRO ALA THR GLU GLU VAL LYS ARG THR ALA ALA THR LYS THR PRO ALA LYS LYS ALA PRO ALA LYS ARG ALA ALA ALA LYS SER ALA ALA LYS GLY GLY LYS SER ALA PRO LYS LYS SER ALA PRO ALA LYS ARG ALA ALA LYS GLY THR ALA ALA LYS

PRO GLU ASP GLY VAL THR ASP ASP LEU GLU VAL THR ASP ASP LEU GLU ALA GLU PRO GLY LEU ASP ASP LEU GLU ASP VAL GLU ASP THR ASP LEU GLU LEU ASP ASP SER ASP ASP THR ALA VAL GLU ASP GLU GLU ALA ASP ALA ALA THR PRO ALA VAL ALA THR ALA

LYS ALA ALA ASP ASP ILE ASP ASP GLU PRO SER GLU LYS ASP LYS SER ALA ASP PHE VAL TRP ASP GLU GLU GLU SER GLU A149 L150 R151 Q152 K155 D156 A157 E158 A163 D164 A168 Y169 L170 I173 G174 K175 V176 A177 L178 L179 N180 A181 E182 L187 E192

Q199 K200 L201 A202 E203 L204 A205 E206 K207 G208 E209 K210 L211 P212 V213 Q214 Q215 R216 R217 D218 W221 I222 C223 L234 E235 L238 R239 V242 G250 R251 G252 Q260 T276 K277 K280 F281 S282 T283 A298 D299 Q300 A301 R302 T303 I304 R305 I306 P307 V308 H309 M310

V311 N315 K316 L317 I320 Q321 R322 E323 L324 L325 Q326 D327 L328 G329 R330 E331 P332 T333 P334 E335 E336 L337 A338 K339 E340 M341 D342 I343 T344 P345 E346 K347 V348 L349 E350 I351 Q352 Q353 Y354 A355 R356 E357 S360 L361 D362 Q363 T364 I365 GLY ASP GLU GLY ASP SER GLN LEU GLY

ASP PHE ILE GLU ASP SER GLU ALA VAL VAL ALA VAL ASP ALA VAL SER PHE THR LEU LEU GLN ASP GLN GLN SER VAL LEU GLU THR LEU SER GLU ALA GLU ARG GLU VAL ARG LEU ARG PHE GLY LEU THR ASP GLY GLN PRO ARG THR LEU ASP GLU ILE GLY GLN VAL TYR

GLY VAL THR ARG GLU ARG ILE ARG GLN ILE GLU SER LYS THR MET SER LYS LEU ARG HIS PRO SER ARG SER GLN VAL LEU ARG ASP TYR LEU ASP

4　Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	42579	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	52	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	78000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.537	Depositor
Minimum map value	-0.227	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	278.72, 278.72, 278.72	wwPDB
Map dimensions	208, 208, 208	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5   Model quality ⓘ

5.1   Standard geometry ⓘ

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

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	0.72	0/1643	0.80	0/2242
1	B	0.73	0/1686	0.82	0/2308
2	C	0.72	0/8126	0.79	0/11071
3	D	0.74	0/9549	0.79	0/12947
4	E	0.71	0/604	0.78	0/822
5	F	0.75	0/1701	0.77	0/2301
All	All	0.73	0/23309	0.79	0/31691

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1617	0	1616	13	0
1	B	1660	0	1624	13	0
2	C	7982	0	7577	47	0
3	D	9399	0	9220	46	0
4	E	592	0	583	3	0
5	F	1678	0	1671	6	0
6	D	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	1	0	0	0	0
All	All	22931	0	22291	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 3.

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)
1:B:26:LEU:HB3	1:B:30:PHE:HB3	1.60	0.82
1:A:48:GLY:HA2	1:A:170:PRO:HG3	1.77	0.66
1:B:110:ILE:HD11	1:B:118:VAL:HG21	1.83	0.60
2:C:678:ARG:O	2:C:695:ASP:N	2.33	0.60
2:C:876:LEU:HD13	2:C:886:ILE:HD11	1.85	0.59
1:A:21:PHE:HB2	1:A:194:ILE:HG23	1.85	0.57
2:C:247:GLU:O	2:C:249:MET:N	2.37	0.57
3:D:883:VAL:HG11	3:D:1157:VAL:HG13	1.87	0.56
2:C:713:ALA:O	2:C:907:ILE:HA	2.06	0.55
5:F:173:ILE:HG22	5:F:238:LEU:HD13	1.90	0.54
1:B:15:ALA:HB3	1:B:18:ARG:HG2	1.90	0.53
3:D:589:THR:HG21	3:D:687:MET:HG2	1.89	0.53
2:C:739:THR:HG22	2:C:869:LYS:HA	1.91	0.53
2:C:1082:ILE:HG23	2:C:1106:PRO:HB3	1.91	0.53
3:D:407:LYS:HA	3:D:1230:THR:HG21	1.90	0.52
1:B:221:LEU:HD12	1:B:222:ALA:N	2.24	0.52
3:D:898:VAL:HG11	3:D:919:ALA:HB2	1.91	0.52
5:F:308:VAL:HA	5:F:311:VAL:HG12	1.92	0.52
1:A:9:LEU:HB3	1:B:221:LEU:HD13	1.92	0.52
2:C:696:GLY:N	2:C:699:THR:OG1	2.43	0.52
2:C:717:TRP:HA	3:D:724:THR:HG22	1.93	0.51
2:C:653:ALA:HB2	2:C:659:GLN:HE22	1.76	0.51
2:C:716:PRO:HA	2:C:721:ASN:HD21	1.75	0.51
2:C:913:VAL:HB	2:C:914:PRO:HD3	1.92	0.51
2:C:1028:VAL:O	2:C:1032:ILE:HG22	2.11	0.51
5:F:179:LEU:HD11	5:F:187:LEU:HD12	1.92	0.51
2:C:1093:VAL:HG23	2:C:1103:ILE:HG23	1.93	0.50
3:D:993:ALA:HB2	3:D:1261:ALA:HB1	1.93	0.50
2:C:1114:VAL:HG22	3:D:324:LEU:HD11	1.94	0.50
1:A:51:VAL:HG23	1:A:164:VAL:HG11	1.93	0.49
2:C:727:ILE:O	2:C:906:ILE:HA	2.12	0.49
3:D:567:SER:HB3	3:D:574:LEU:HD23	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:456:VAL:HA	3:D:490:VAL:HG11	1.94	0.49
2:C:369:LEU:HD11	2:C:446:LEU:HD22	1.94	0.49
3:D:459:ARG:HG3	3:D:490:VAL:HG12	1.94	0.49
2:C:113:CYS:SG	2:C:120:TYR:N	2.86	0.49
1:B:22:VAL:HG12	1:B:193:ILE:HG22	1.93	0.48
3:D:675:LEU:HD22	3:D:714:LYS:HB3	1.96	0.48
2:C:30:VAL:HB	2:C:954:LEU:HD13	1.95	0.48
1:A:77:ILE:HG23	1:A:164:VAL:HG23	1.96	0.48
2:C:493:VAL:HG13	2:C:494:TYR:CD1	2.49	0.48
2:C:571:ASP:HA	2:C:576:GLN:HE22	1.78	0.48
1:A:85:VAL:HG21	1:A:140:VAL:HG21	1.96	0.47
1:B:43:LEU:HD11	3:D:620:MET:HG2	1.96	0.47
2:C:217:ILE:HD11	2:C:268:ILE:HD11	1.97	0.47
2:C:446:LEU:HD21	2:C:491:LEU:HD12	1.97	0.47
3:D:995:GLY:HA2	3:D:1157:VAL:HG11	1.97	0.47
2:C:45:LEU:HD21	2:C:155:GLY:HA3	1.97	0.46
2:C:887:GLY:HA2	3:D:431:VAL:HB	1.97	0.46
2:C:24:PRO:HB3	2:C:688:GLU:HB3	1.97	0.46
2:C:1058:ARG:HA	3:D:421:ARG:HA	1.98	0.45
3:D:75:CYS:SG	3:D:77:ARG:HB2	2.57	0.45
3:D:663:ALA:HB1	3:D:665:THR:HG23	1.97	0.45
3:D:965:LEU:HD13	3:D:1132:GLN:HB3	1.98	0.45
1:B:26:LEU:HB3	1:B:30:PHE:CB	2.38	0.45
2:C:1065:TRP:CD1	3:D:877:VAL:HG11	2.51	0.45
3:D:320:ILE:HG21	3:D:340:LEU:HD23	1.97	0.45
3:D:486:VAL:O	3:D:490:VAL:HG13	2.17	0.45
3:D:1239:ILE:HG13	3:D:1240:ASN:HD22	1.82	0.45
3:D:556:ARG:HD3	4:E:89:LEU:HD13	1.99	0.45
5:F:239:ARG:HA	5:F:242:VAL:HG12	1.99	0.45
3:D:404:ASP:HA	3:D:407:LYS:HG2	1.99	0.44
4:E:41:LEU:HD21	4:E:47:LYS:HB3	1.99	0.44
1:A:95:MET:SD	1:A:95:MET:N	2.90	0.44
1:B:38:LEU:O	1:B:42:LEU:HD23	2.16	0.44
2:C:617:VAL:HG13	2:C:927:LEU:HD23	2.00	0.44
3:D:488:GLU:HA	3:D:491:ILE:HG22	1.99	0.44
1:A:78:LEU:HD21	2:C:611:ARG:HD3	2.00	0.43
2:C:1044:THR:HG21	2:C:1046:GLN:HE21	1.83	0.43
3:D:666:THR:HG22	3:D:669:ARG:HD2	2.00	0.43
3:D:366:ILE:HG23	5:F:260:GLN:HE22	1.83	0.43
2:C:794:VAL:HB	2:C:828:LEU:HB3	1.99	0.43
2:C:911:HIS:CE1	3:D:580:ASP:HA	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:45:LEU:HD11	2:C:443:LYS:HD2	2.01	0.43
3:D:277:LEU:HD11	3:D:295:ARG:HG2	2.00	0.43
3:D:1078:TYR:HB2	3:D:1081:LEU:HD21	2.00	0.43
2:C:468:PRO:HB2	2:C:557:GLY:HA3	2.00	0.43
2:C:575:ARG:O	2:C:575:ARG:HG3	2.19	0.43
1:B:41:THR:HG21	1:B:215:LEU:HG	2.01	0.42
3:D:1141:GLU:HA	3:D:1144:ARG:HD2	2.01	0.42
1:A:86:SER:O	1:A:116:VAL:HA	2.20	0.42
3:D:557:ILE:O	3:D:563:ASN:ND2	2.52	0.42
3:D:661:TRP:CZ3	3:D:663:ALA:HB2	2.55	0.42
3:D:876:LEU:HD23	3:D:1002:ILE:HG23	2.02	0.42
1:B:171:VAL:HA	1:B:198:THR:HA	2.01	0.42
2:C:166:VAL:HB	2:C:372:VAL:HG22	2.02	0.42
3:D:413:PHE:HA	3:D:417:LEU:HB2	2.01	0.42
3:D:896:ILE:HG21	3:D:965:LEU:HD12	2.01	0.42
3:D:1004:GLU:HG3	3:D:1005:PRO:HD3	2.00	0.42
1:A:39:ARG:HA	1:A:174:VAL:HG11	2.02	0.42
1:B:42:LEU:HD22	1:B:211:ALA:CB	2.50	0.42
3:D:1029:LEU:HA	3:D:1032:VAL:HG22	2.02	0.41
1:A:48:GLY:CA	1:A:170:PRO:HG3	2.47	0.41
3:D:1259:ILE:O	3:D:1264:GLY:HA3	2.21	0.41
2:C:583:ALA:HB1	2:C:621:MET:HG3	2.03	0.41
2:C:677:GLN:HA	2:C:695:ASP:O	2.21	0.41
1:B:80:LEU:HD22	1:B:138:LEU:HD21	2.03	0.41
2:C:466:VAL:HG23	3:D:853:HIS:ND1	2.35	0.41
2:C:736:ASP:HA	2:C:739:THR:HG23	2.03	0.41
2:C:1062:MET:SD	2:C:1062:MET:N	2.92	0.41
3:D:1165:ARG:NH1	3:D:1209:MET:SD	2.94	0.41
2:C:1076:LEU:HD23	3:D:1259:ILE:HG13	2.03	0.41
3:D:1065:ILE:HD12	3:D:1112:LEU:HD13	2.03	0.41
1:A:62:GLU:O	1:A:73:VAL:HG13	2.21	0.40
2:C:132:ASN:HD21	2:C:400:VAL:HG13	1.86	0.40
2:C:732:LEU:HD22	2:C:737:VAL:HG21	2.03	0.40
2:C:928:GLY:HA3	2:C:1018:TYR:O	2.21	0.40
1:A:95:MET:CE	1:A:140:VAL:HG23	2.52	0.40
2:C:706:LEU:N	2:C:1020:TYR:OH	2.54	0.40
3:D:635:VAL:HG21	3:D:670:VAL:HG21	2.03	0.40
2:C:47:VAL:HG12	2:C:497:VAL:HG23	2.03	0.40
3:D:363:PRO:HD3	5:F:234:LEU:HD13	2.04	0.40
3:D:459:ARG:CG	3:D:490:VAL:HG12	2.51	0.40
4:E:43:ARG:NE	4:E:99:ASP:OD1	2.54	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	
1	A	218/350 (62%)	201 (92%)	15 (7%)	2 (1%)	17	56
1	B	231/350 (66%)	211 (91%)	17 (7%)	3 (1%)	12	48
2	C	1086/1178 (92%)	985 (91%)	86 (8%)	15 (1%)	11	47
3	D	1229/1325 (93%)	1141 (93%)	83 (7%)	5 (0%)	34	72
4	E	72/107 (67%)	67 (93%)	5 (7%)	0	100	100
5	F	215/466 (46%)	196 (91%)	19 (9%)	0	100	100
All	All	3051/3776 (81%)	2801 (92%)	225 (7%)	25 (1%)	24	60

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	248	ILE
2	C	940	ALA
1	A	149	ALA
1	B	161	ARG
2	C	524	ALA
2	C	704	MET
2	C	892	VAL
2	C	247	GLU
3	D	1174	THR
1	A	181	THR
1	B	57	ASP
2	C	404	THR
1	B	28	PRO
2	C	938	ASP
2	C	943	VAL
2	C	973	GLU
3	D	579	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	609	GLN
3	D	1058	GLU
2	C	276	GLU
2	C	765	PRO
2	C	981	GLY
2	C	870	ILE
2	C	43	GLY
3	D	657	PRO

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	
1	A	174/297 (59%)	173 (99%)	1 (1%)	86	92
1	B	170/297 (57%)	165 (97%)	5 (3%)	42	64
2	C	800/988 (81%)	790 (99%)	10 (1%)	69	82
3	D	951/1103 (86%)	936 (98%)	15 (2%)	62	79
4	E	62/86 (72%)	60 (97%)	2 (3%)	39	62
5	F	164/379 (43%)	163 (99%)	1 (1%)	86	92
All	All	2321/3150 (74%)	2287 (98%)	34 (2%)	66	80

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	ASP
1	B	30	PHE
1	B	84	VAL
1	B	134	LEU
1	B	191	LYS
1	B	196	VAL
2	C	45	LEU
2	C	302	VAL
2	C	313	LEU
2	C	527	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	528	ASP
2	C	763	ASP
2	C	924	GLU
2	C	960	ASP
2	C	965	THR
2	C	1029	ASP
3	D	60	CYS
3	D	260	SER
3	D	268	PHE
3	D	271	ASP
3	D	574	LEU
3	D	667	LEU
3	D	716	LYS
3	D	717	ASP
3	D	725	ARG
3	D	731	SER
3	D	816	LEU
3	D	823	VAL
3	D	838	SER
3	D	957	THR
3	D	1209	MET
4	E	33	THR
4	E	41	LEU
5	F	280	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
2	C	132	ASN
2	C	576	GLN
2	C	659	GLN
2	C	677	GLN
2	C	882	ASN
2	C	1068	GLN
3	D	368	ASN
3	D	1146	GLN
3	D	1240	ASN
3	D	1252	ASN
4	E	85	GLN
5	F	172	GLN
5	F	260	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.
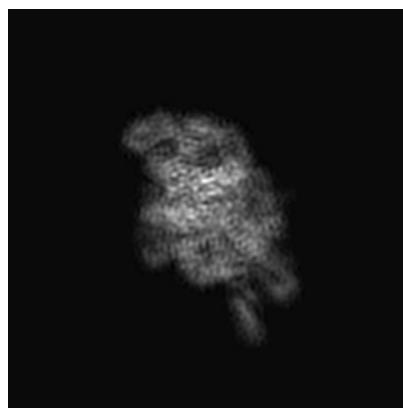
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-3983. These allow visual inspection of the internal detail of the map and identification of artifacts.
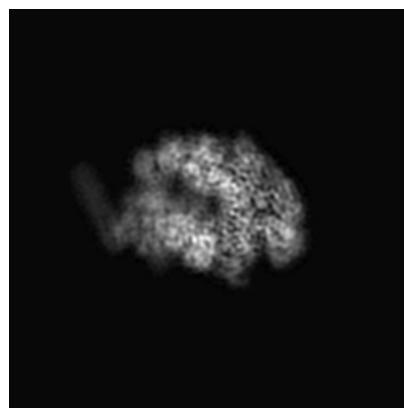
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections ⓘ
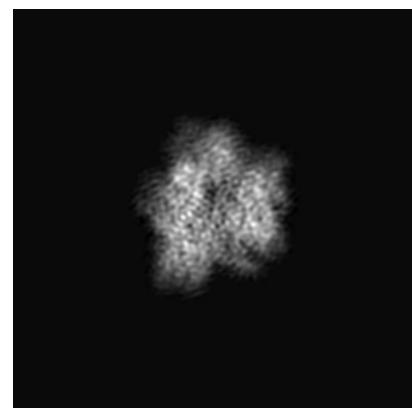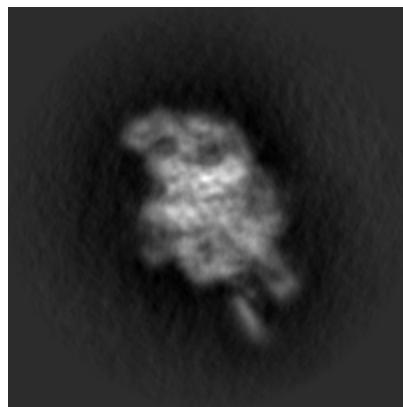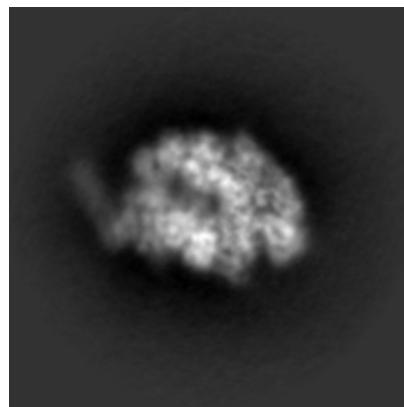
6.1.1 Primary map

| X | Y | Z |
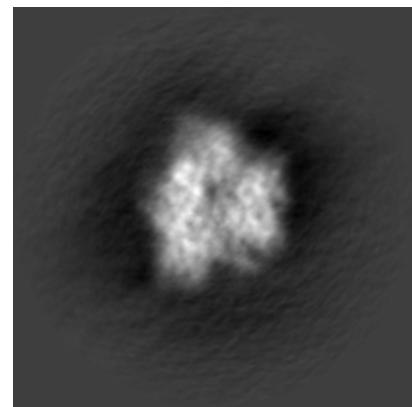
6.1.2 Raw map

| X | Y | Z |
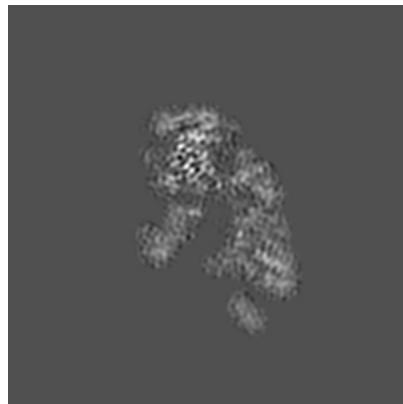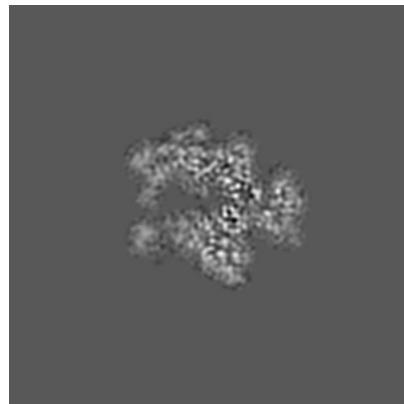
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
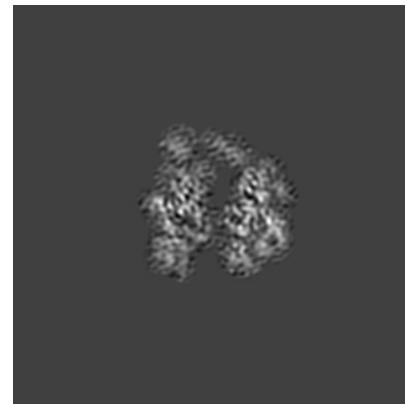
6.2.1 Primary map
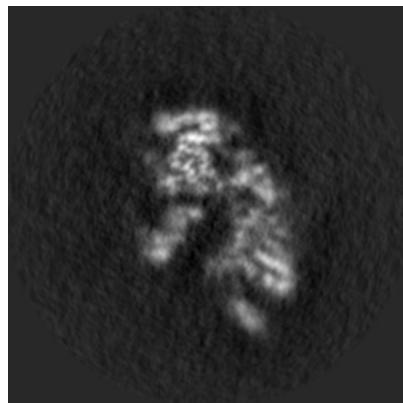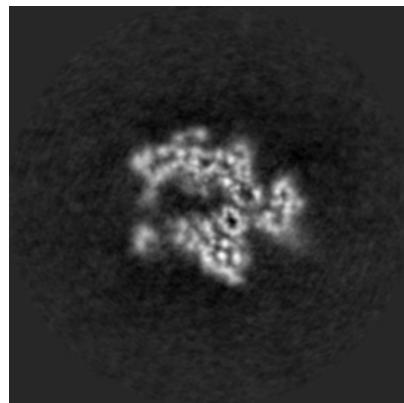
X Index: 104　　　　　　　Y Index: 104　　　　　　　Z Index: 104
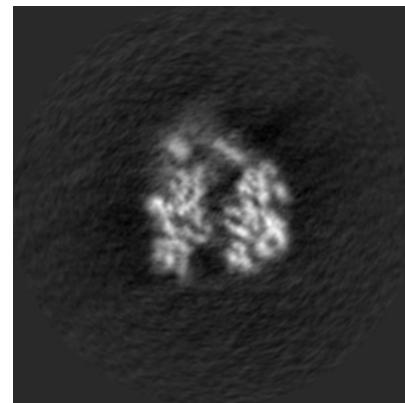
6.2.2 Raw map
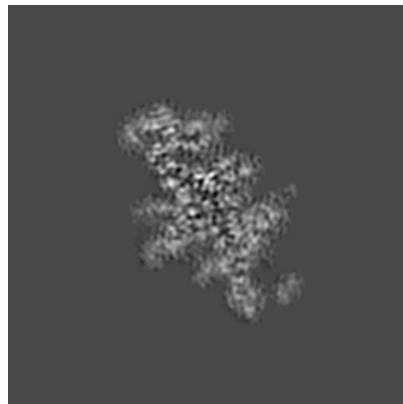
X Index: 104　　　　　　　Y Index: 104　　　　　　　Z Index: 104
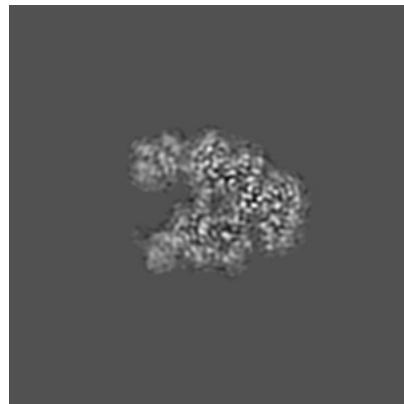
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ
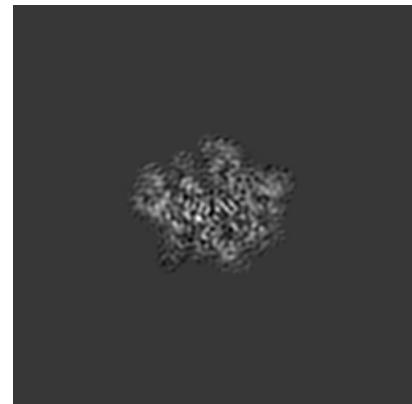
6.3.1 Primary map
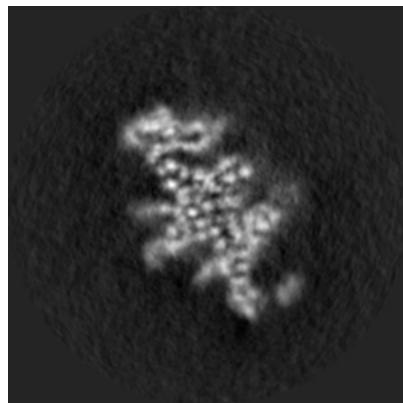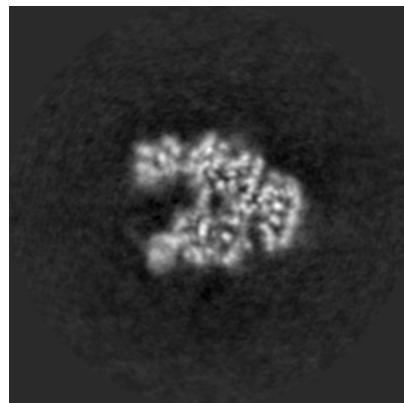
| X Index: 90 | Y Index: 95 | Z Index: 118 |
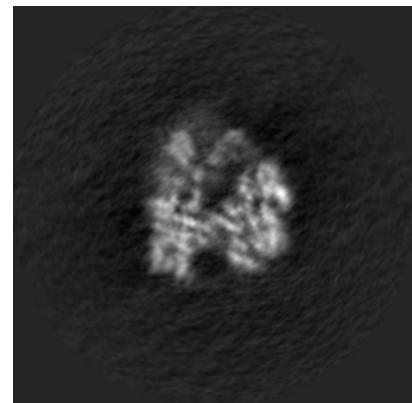
6.3.2 Raw map
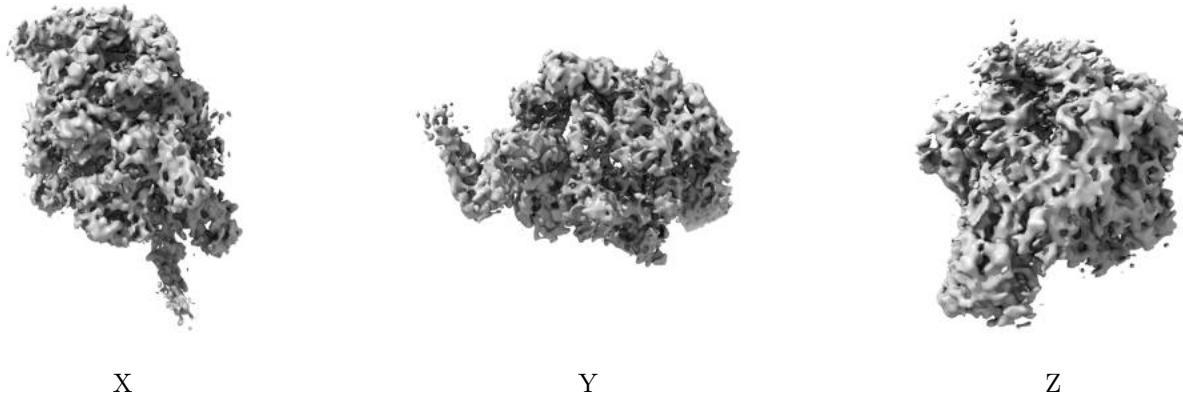
| X Index: 90 | Y Index: 95 | Z Index: 101 |

The images above show the largest variance slices of the map in three orthogonal directions.
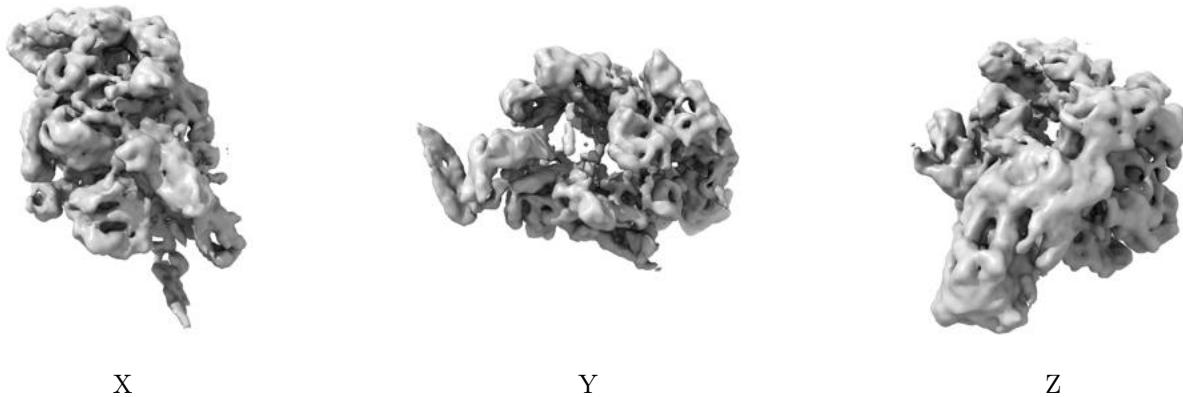
6.4   Orthogonal surface views (i)

6.4.1   Primary map

X   Y   Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.
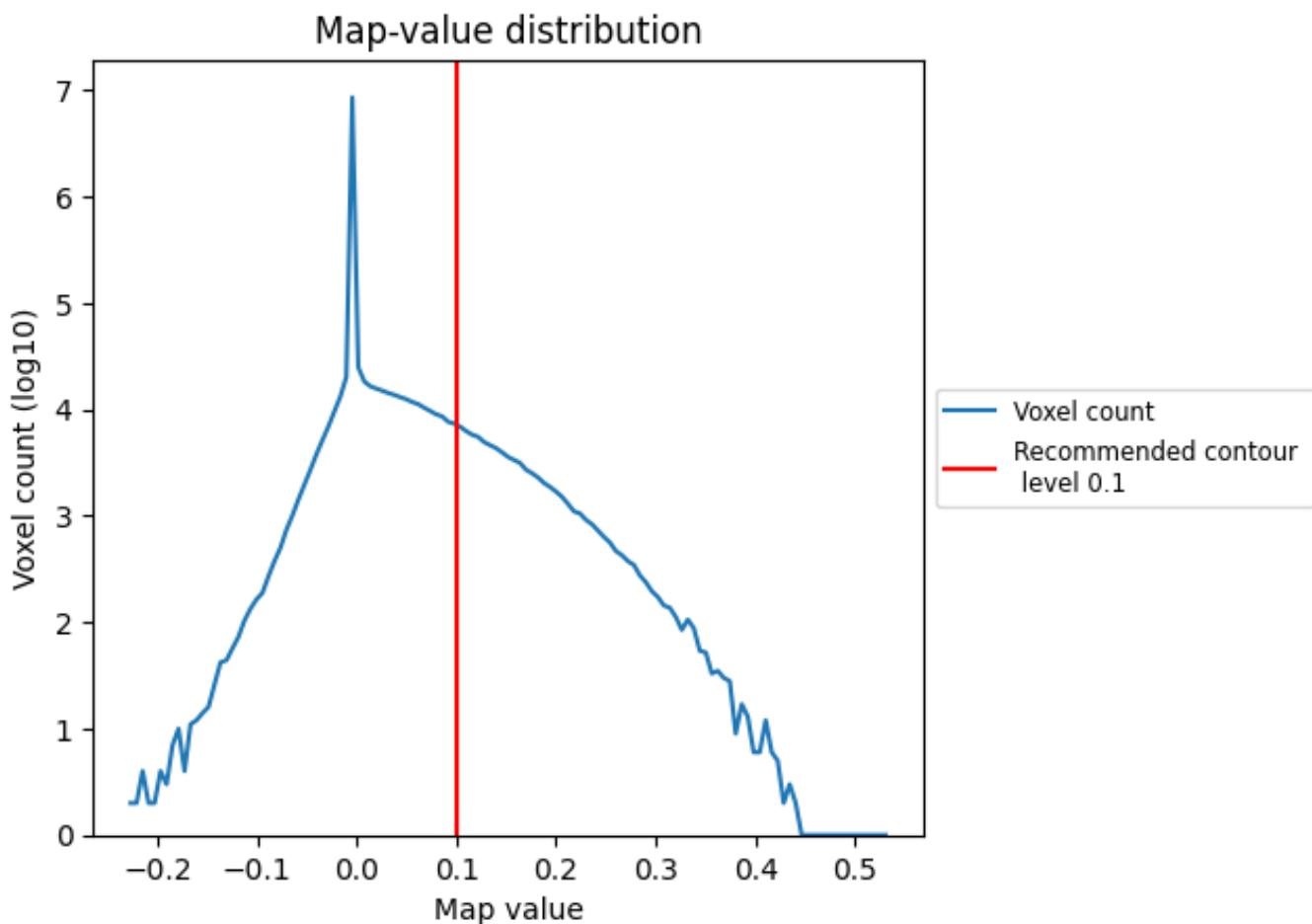
6.5   Mask visualisation (i)

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

7 Map analysis ⓘ
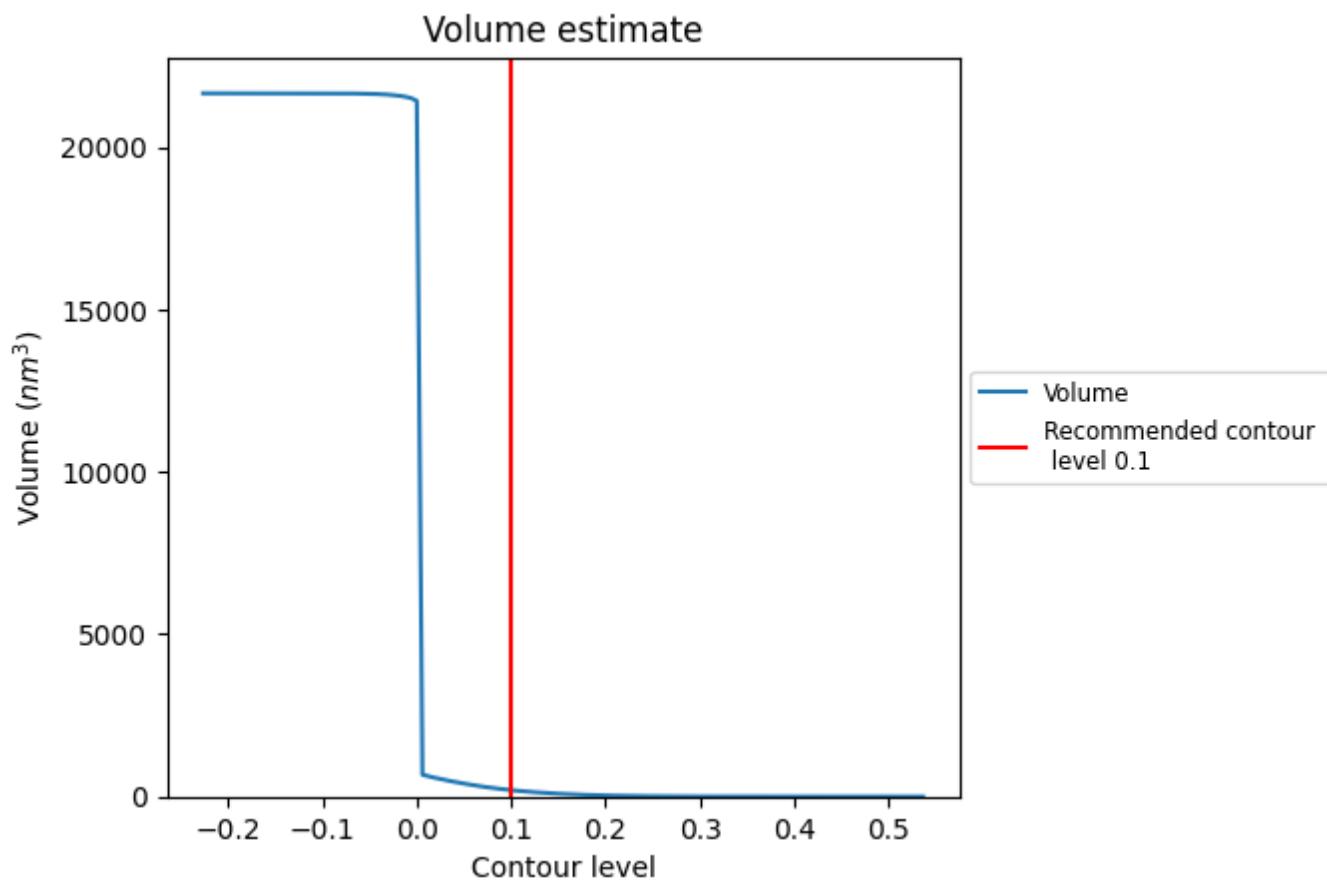
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

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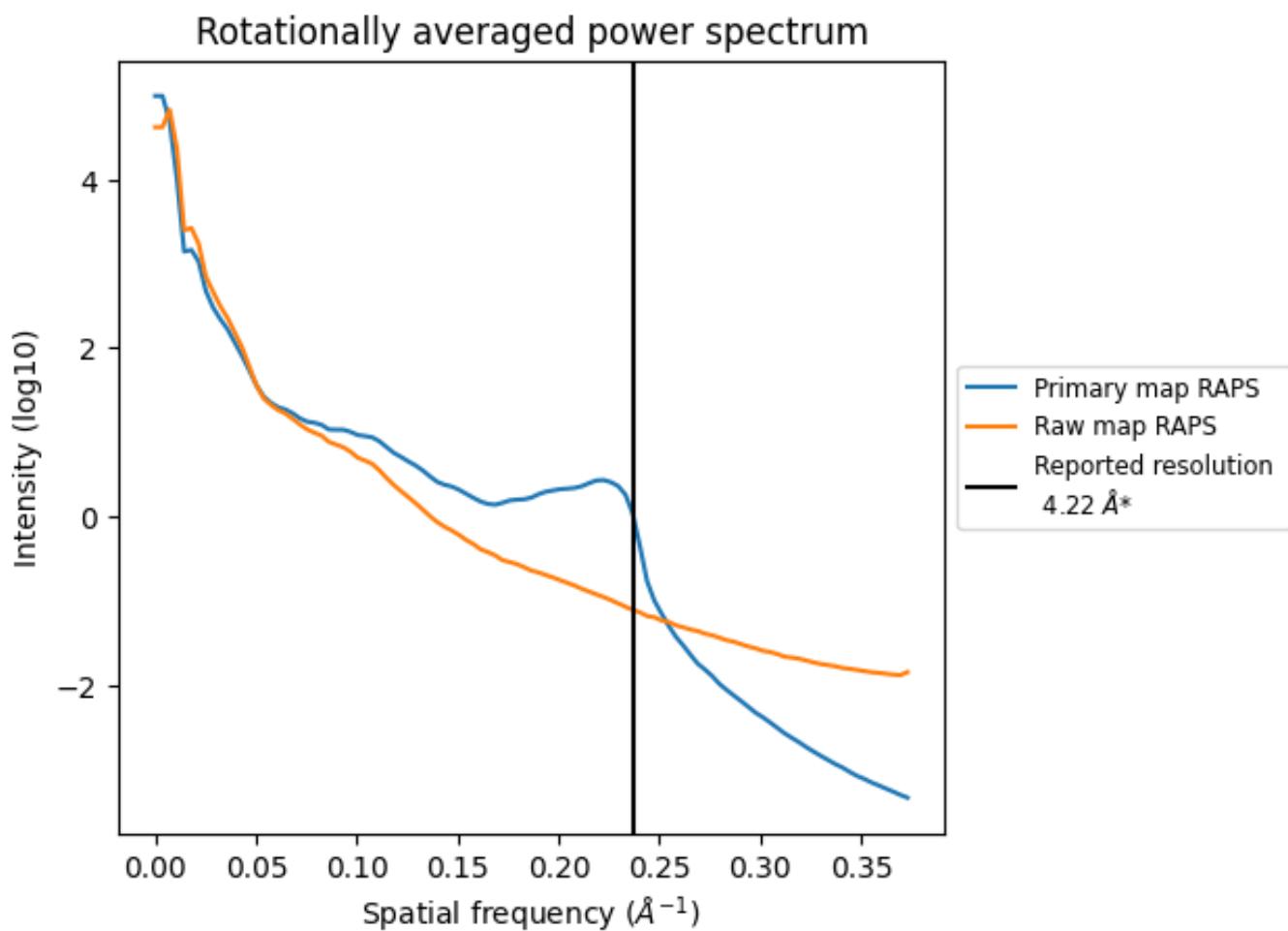
7.2   Volume estimate ⓘ

The volume at the recommended contour level is 199 nm^3; this corresponds to an approximate mass of 180 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)
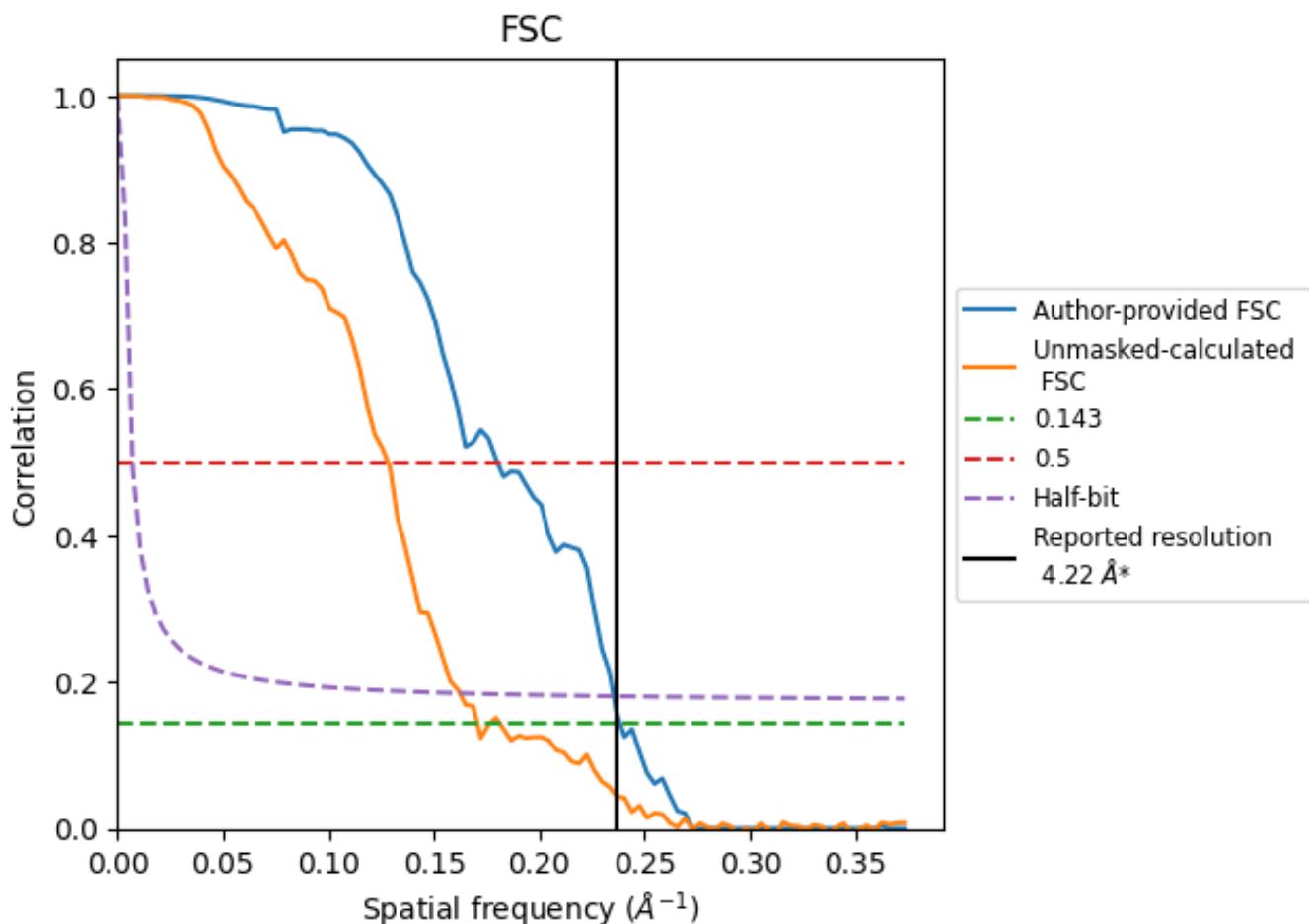
*Reported resolution corresponds to spatial frequency of 0.237 Å^{-1}

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 0.237 Å^{-1}

8.2   Resolution estimates   ⓘ
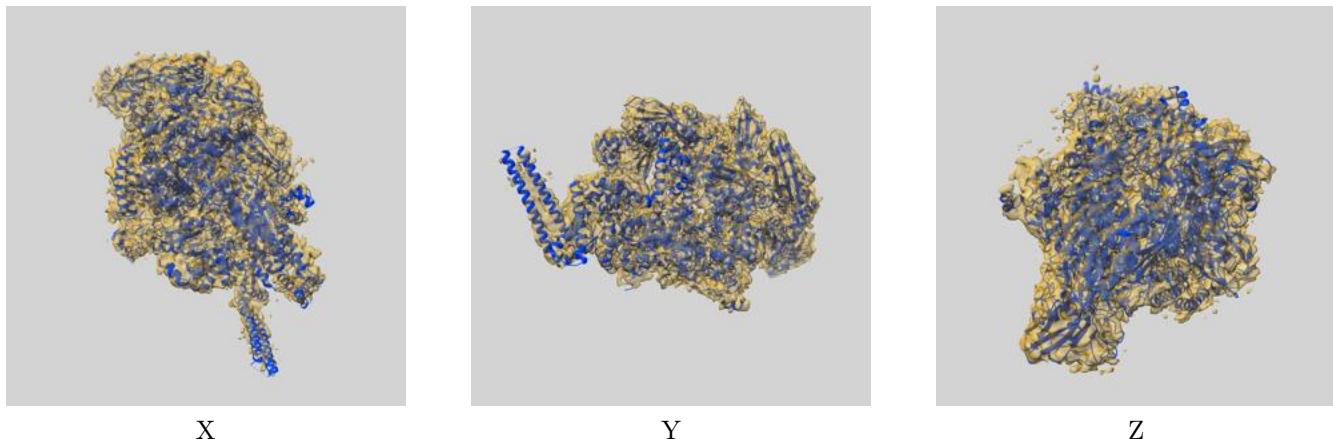
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.22	-	-
Author-provided FSC curve	4.20	5.56	4.25
Unmasked-calculated*	5.86	7.81	6.17

*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 5.86 differs from the reported value 4.22 by more than 10 %

9 Map-model fit ⓘ
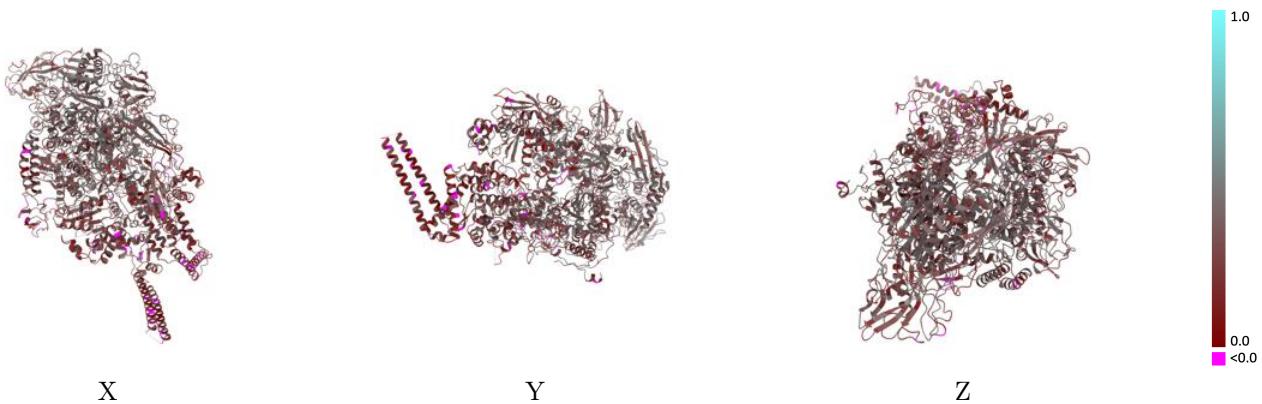
This section contains information regarding the fit between EMDB map EMD-3983 and PDB model 6EYD. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay ⓘ

| X | Y | Z |
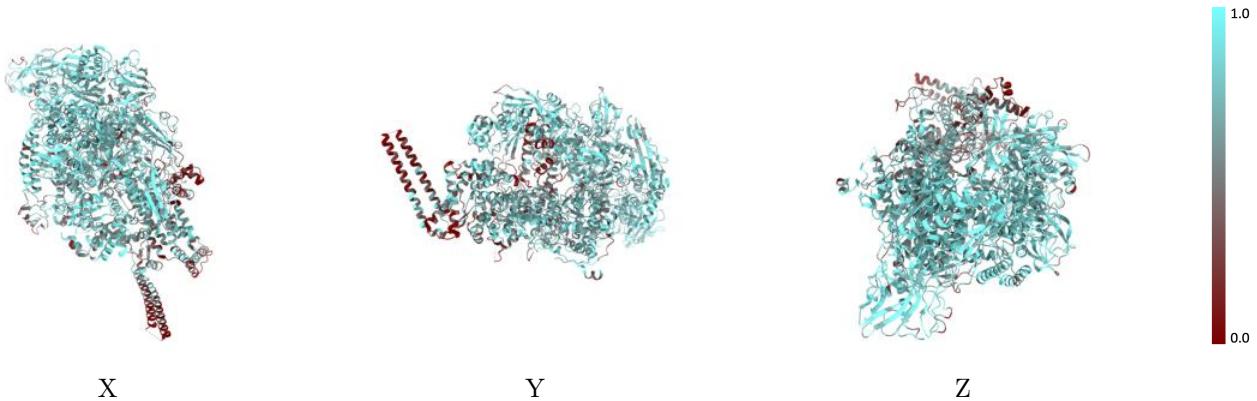
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ

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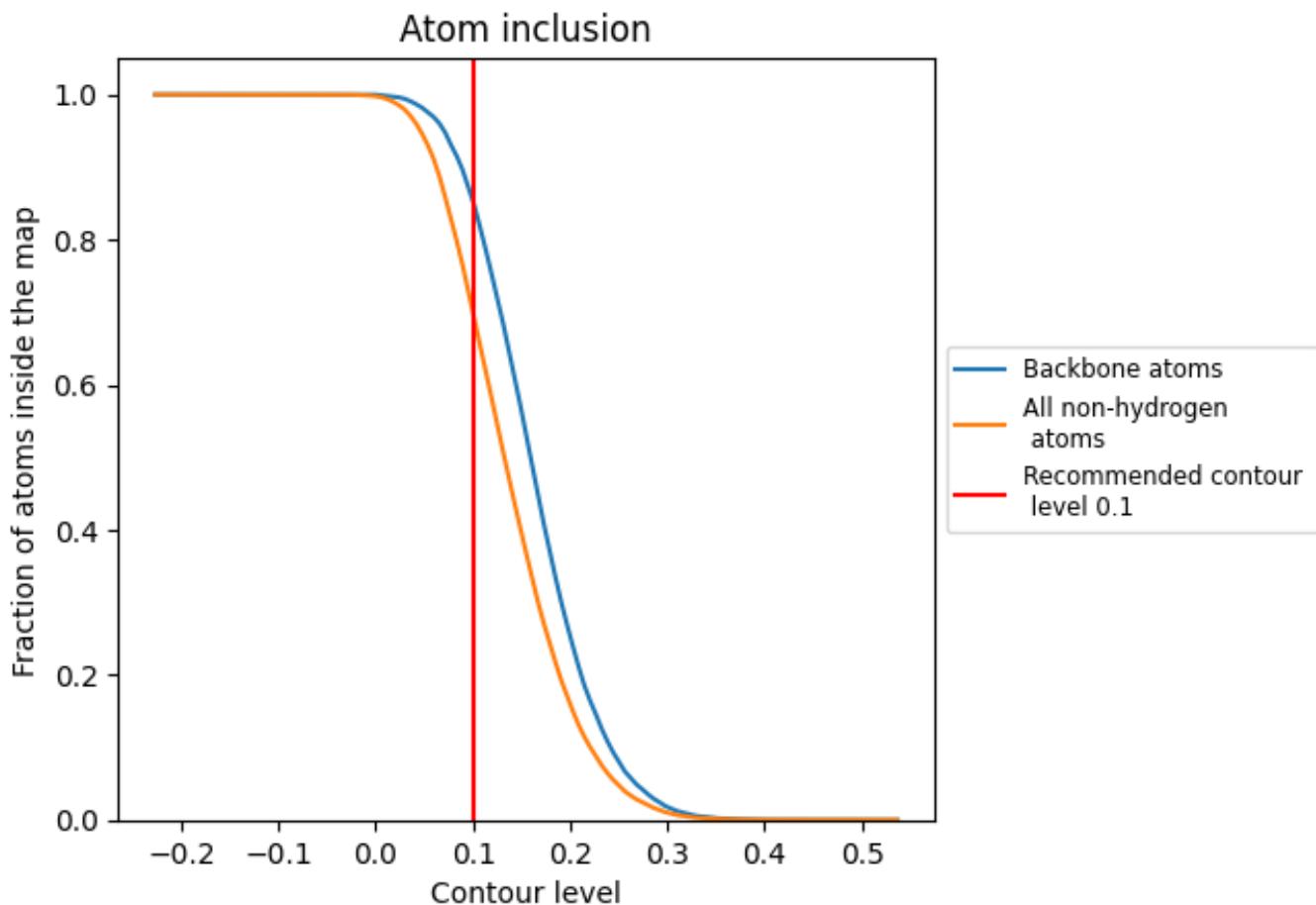
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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 (0.1).

9.4   Atom inclusion ⓘ

At the recommended contour level, 85% of all backbone atoms, 70% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7003	0.3140
A	0.7585	0.3570
B	0.7930	0.3420
C	0.7462	0.3350
D	0.6797	0.2980
E	0.7353	0.3230
F	0.4340	0.2260

1.0

0.0
<0.0