wwPDB EM Validation Summary Report (i)

Jun 27, 2024 – 05:50 AM JST

PDB ID	:	8HSH
EMDB ID	:	EMD-34997
Title	:	Thermus thermophilus RNA polymerase coreenzyme
Authors	:	Murayama, Y.; Ehara, H.; Sekine, S.
Deposited on	:	2022-12-19
Resolution	:	3.40 Å(reported)

This is a wwPDB EM Validation Summary 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:

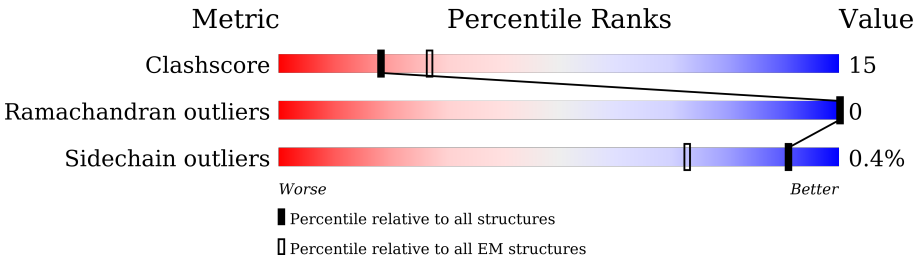
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.40 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	G	315	53% 20% 27%
1	H	315	47% 26% 27%
2	I	1119	66% 32%
3	J	1532	8% 56% 27% 17%
4	K	99	17% 55% 36% 8%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 23072 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	G	229	Total	C	N	O	S	0	0
			1806	1153	313	337	3		
1	H	229	Total	C	N	O	S	0	0
			1806	1153	313	337	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	1096	Total	C	N	O	S	0	0
			8644	5468	1543	1609	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	1278	Total	C	N	O	S	0	0
			10078	6384	1783	1883	28		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1525	ASP	-	expression tag	UNP Q8RQE8
J	1526	TYR	-	expression tag	UNP Q8RQE8
J	1527	LYS	-	expression tag	UNP Q8RQE8
J	1528	ASP	-	expression tag	UNP Q8RQE8
J	1529	ASP	-	expression tag	UNP Q8RQE8
J	1530	ASP	-	expression tag	UNP Q8RQE8
J	1531	ASP	-	expression tag	UNP Q8RQE8
J	1532	LYS	-	expression tag	UNP Q8RQE8

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	91	Total	C	N	O	S	0	0
			735	467	129	135	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	95	GLY	VAL	conflict	UNP Q8RQE7

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	J	2	Total	Zn	0
			2	2	

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

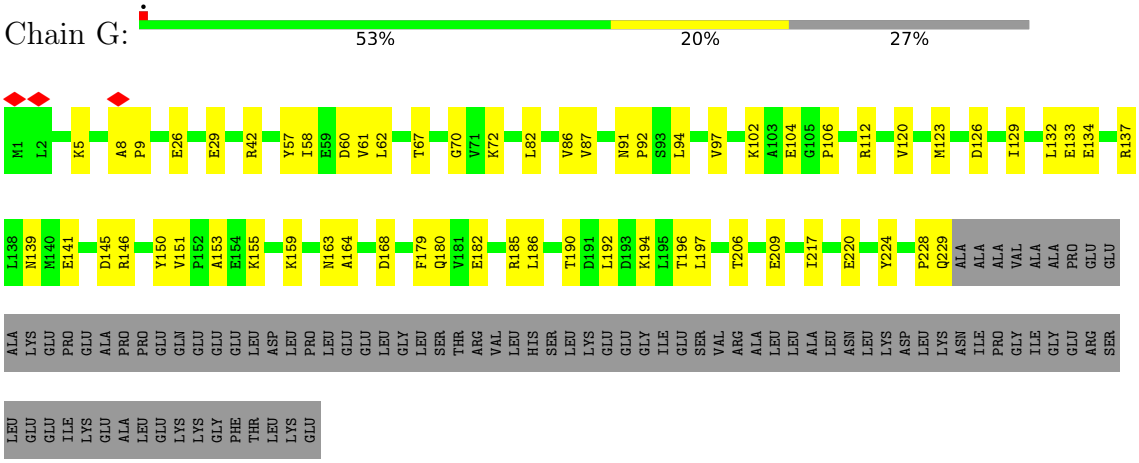
Mol	Chain	Residues	Atoms		AltConf
6	J	1	Total	Mg	0
			1	1	

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.

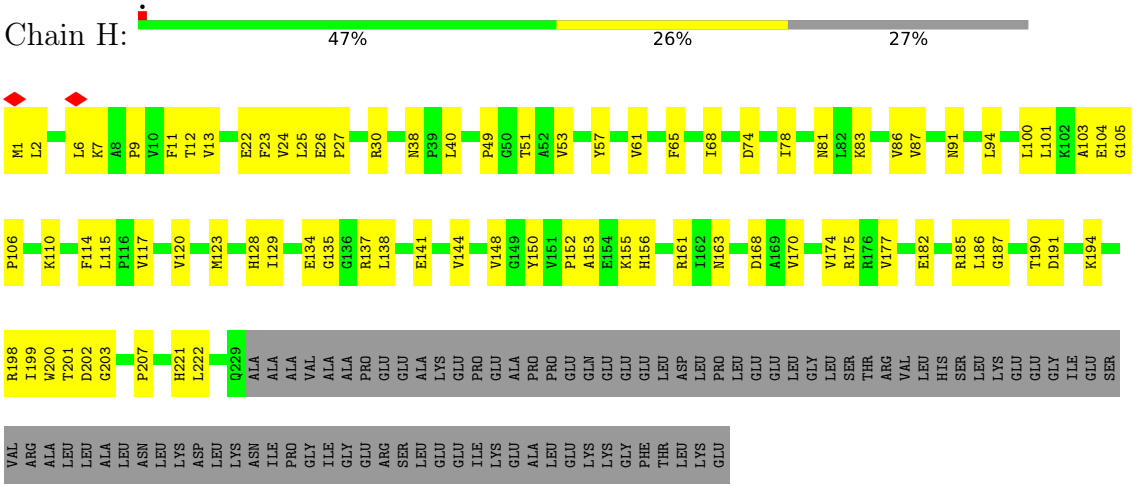
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain G:



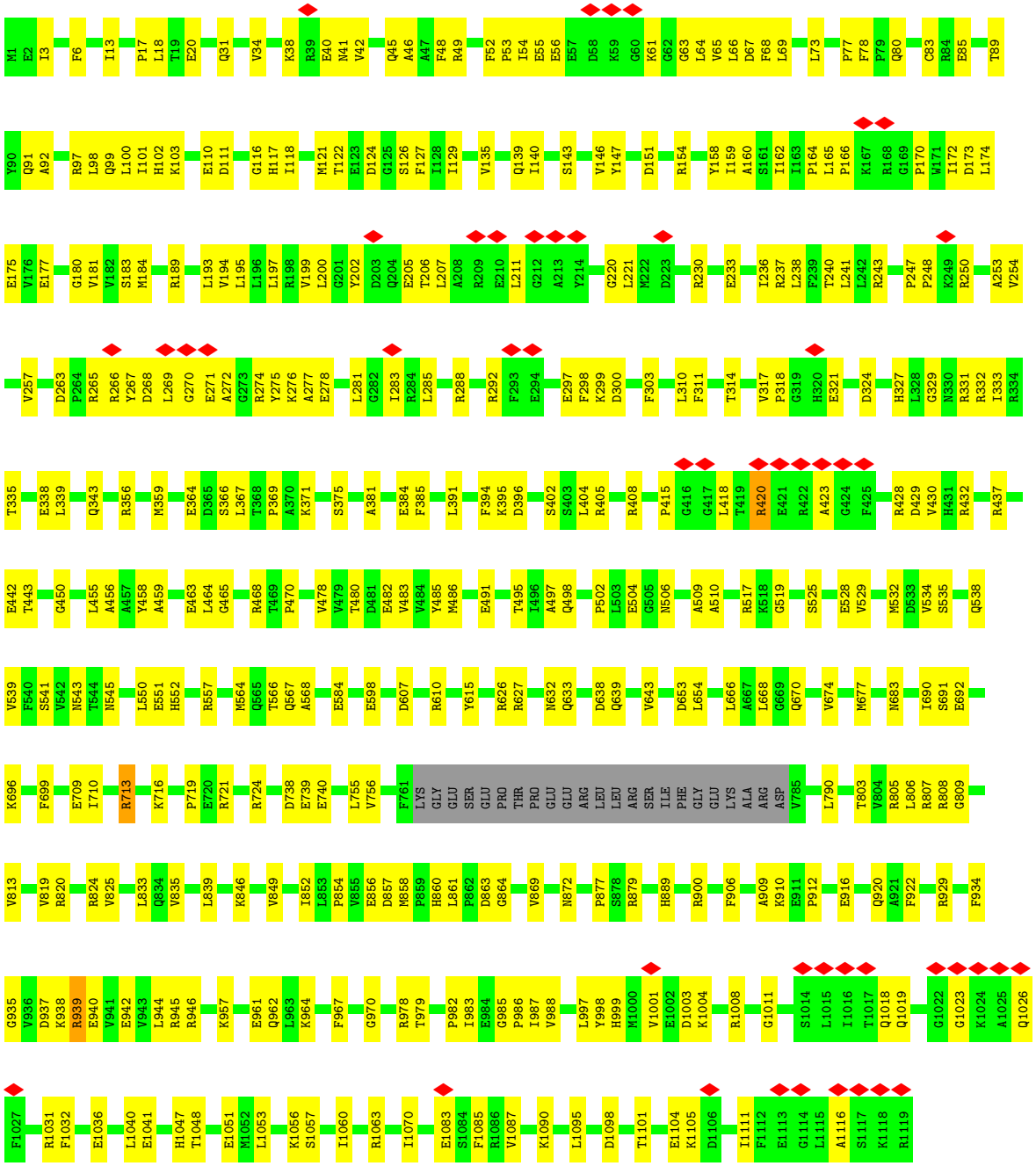
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain H:

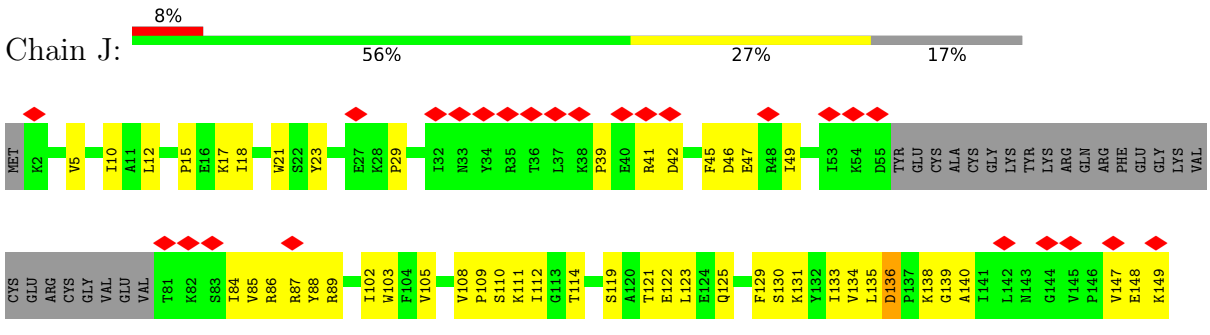


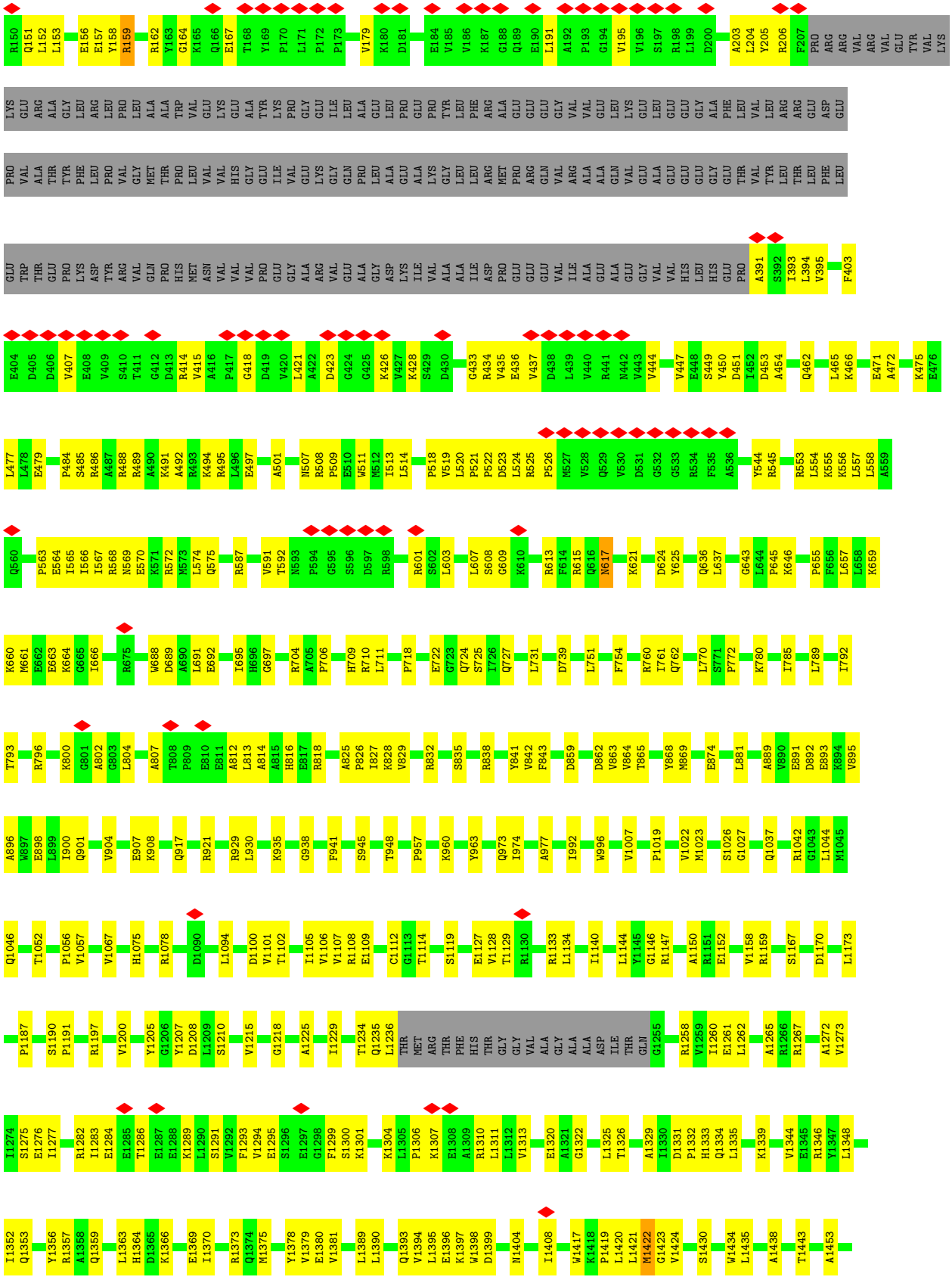
• Molecule 2: DNA-directed RNA polymerase subunit beta

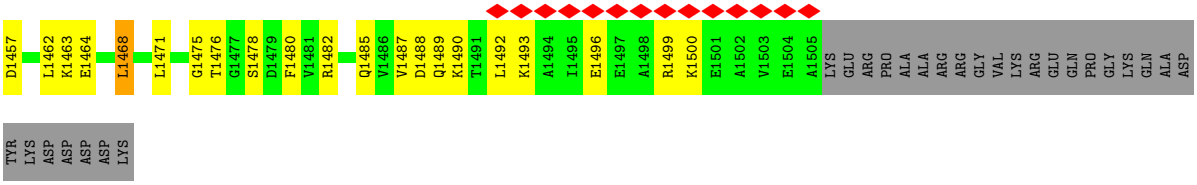
Chain I:



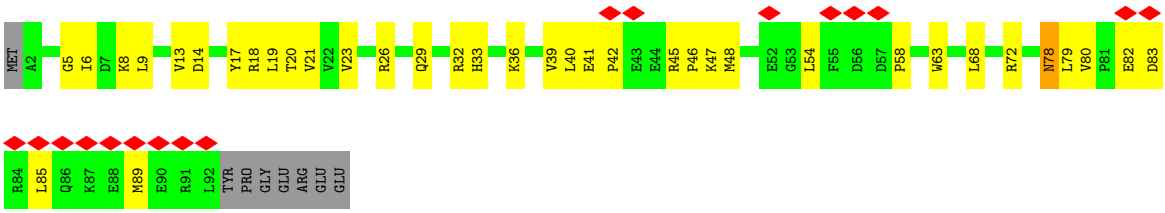
• Molecule 3: DNA-directed RNA polymerase subunit beta'




R150 Q151 L152 L153 E156 E157 Y158 R159 R162 Y163 G164 K165 Q166 E167 T168 Y169 P170 L171 P172 P173 V179 K180 D181 E184 V185 V186 K187 G188 Q189 E190 L191 A192 P193 G194 V195 V196 S197 R198 L199 D200 A203 L204 Y205 R206 F207 PRO ARG ARG VAL ARG VAL GLU TYR VAL LYS
LYS GLU ARG ALA GLY LEU ARG LEU PRO LEU ALA ALA TRP VAL GLU LYS GLU ALA TYR LYS PRO GLY GLU ILE LEU ALA GLU LEU PRO GLU PRO TYR LEU PHE ARG ALA GLU GLU GLU GLY VAL VAL GLU LEU LYS GLU LEU GLU GLU GLY ALA PHE LEU VAL LEU ARG ARG GLU ASP GLU
PRO VAL ALA THR TYR PHE LEU PRO VAL GLY MET THR PRO LEU VAL VAL HIS GLY GLU ILE VAL GLU LYS GLY GLN PRO LEU ALA GLU ALA LYS GLY GLU GLY ARG ALA ALA GLN VAL GLU ALA GLU GLU GLU GLY GLU THR VAL TYR LEU THR LEU PHE LEU
GLU TRP THR GLU PRO LYS ASP TYR ARG VAL GLN PRO HIS MET ASN VAL VAL VAL PRO GLU GLY ALA ARG VAL GLU ALA GLY ASP LYS ILE VAL ALA ALA ILE ASP PRO GLU GLU GLU VAL ILE ALA GLU ALA GLU GLY VAL VAL HIS LEU HIS GLU PRO A391 S392 I393 L394 V395 F403
E404 D405 D406 V407 E408 V409 S410 T411 G412 D413 R414 V415 A416 P417 G418 D419 V420 L421 A422 D423 G424 G425 K426 V427 K428 S429 D430 G433 R434 V435 E436 V437 D438 L439 V440 R441 N442 V443 V444 V447 E448 S449 Y450 D451 I452 D453 A454 Q462 L465 K466 E471 A472 K475 E476
L477 L478 E479 P484 S485 R486 A487 R488 R489 A490 K491 A492 R493 K494 R495 L496 E497 A501 N507 R508 P509 E510 W511 M512 I513 L514 P518 V519 L520 P521 P522 D523 L524 R525 P526 M527 V528 Q529 V530 D531 G532 G533 R534 F535 A536 Y544 R545 R553 L554 K555 K556 L557 L558 A559
Q560 P563 E564 I565 I566 I567 R568 N569 E570 K571 R572 M573 L574 Q575 R587 V591 T592 N593 P594 G595 S596 D597 R598 R601 S602 L603 L607 S608 G609 K610 R613 F614 R615 Q616 N617 K621 D624 Y625 Q636 L637 G643 L644 P645 K646 P655 F656 L657 L658 K659
K660 M661 E662 E663 K664 G665 I666 R675 W688 D689 A690 L691 E692 I695 H696 G697 R704 A705 P706 H709 R710 L711 P718 E722 G723 Q724 S725 I726 Q727 L731 D739 L751 F754 R760 I761 Q762 L770 S771 P772 K780 I785 L789 I792
T793 R796 K800 G801 A802 G803 L804 A807 T808 P809 E810 E811 A812 L813 A814 A815 H816 E817 R818 A825 P826 I827 K828 V829 R832 S835 R838 Y841 V842 F843 D859 D862 V863 V864 T865 Y868 M869 E874 L881 A889 V890 E891 D892 E893 K894 V895
A896 W897 E898 L899 I900 Q901 V904 E907 K908 Q917 R921 L930 K935 G938 F941 S945 T948 P957 K960 Y963 Q973 I974 A977 I992 W996 V1007 P1019 V1022 M1023 S1026 G1027 Q1037 R1042 G1043 L1044 M1045
Q1046 T1052 P1056 V1057 V1067 H1075 R1078 D1090 L1094 D1100 V1101 T1102 I1105 V1106 V1107 R1108 E1109 C1112 G1113 T1114 S1119 E1127 V1128 T1129 R1130 R1133 L1134 I1140 L1144 Y1145 G1146 R1147 A1150 R1151 E1152 V1158 R1159 S1167 D1170 L1173
P1187 S1190 P1191 R1197 V1200 Y1205 G1206 Y1207 D1208 L1209 S1210 V1215 G1218 A1225 I1229 T1234 Q1235 L1236 THR MET ARG THR PHE HIS THR GLY GLY VAL ALA GLY ALA ASP ILE THR GLN G1255 R1258 V1259 I1260 E1261 L1262 A1265 R1266 R1267 A1272 V1273
I1274 S1275 E1276 I1277 R1282 I1283 E1284 E1285 T1286 E1287 E1288 K1289 L1290 S1291 V1292 F1293 V1294 E1295 S1296 E1297 G1298 F1299 S1300 K1301 K1304 L1305 P1306 K1307 E1308 A1309 R1310 L1311 L1312 V1313 E1320 A1321 G1322 L1325 T1326 A1329 I1330 D1331 P1332 H1333 Q1334 L1335 K1339 V1344 E1345 R1346 Y1347 L1348
I1352 Q1353 Y1356 R1357 A1358 Q1359 L1363 H1364 D1365 K1366 E1369 I1370 R1373 Q1374 M1375 Y1378 V1379 E1380 V1381 L1389 L1390 Q1393 V1394 L1395 E1396 K1397 W1398 D1399 N1404 I1408 W1417 K1418 P1419 L1420 L1421 M1422 G1423 V1424 S1430 W1434 L1435 A1438 T1443 A1453



• Molecule 4: DNA-directed RNA polymerase subunit omega



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	392560	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.053	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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	G	0.29	0/1838	0.54	0/2498
1	H	0.28	0/1838	0.54	0/2498
2	I	0.29	0/8808	0.56	0/11910
3	J	0.28	0/10246	0.55	1/13842 (0.0%)
4	K	0.29	0/747	0.59	0/1005
All	All	0.29	0/23477	0.55	1/31753 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	J	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	1468	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	J	1109	GLU	Peptide
3	J	136	ASP	Peptide

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	G	1806	0	1861	43	0
1	H	1806	0	1861	60	0
2	I	8644	0	8749	263	0
3	J	10078	0	10315	325	0
4	K	735	0	753	33	0
5	J	2	0	0	0	0
6	J	1	0	0	0	0
All	All	23072	0	23539	684	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 15.

The worst 5 of 684 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:206:ARG:O	3:J:391:ALA:HA	1.51	1.10
3:J:41:ARG:HG3	3:J:42:ASP:H	1.40	0.86
2:I:805:ARG:HH21	2:I:807:ARG:HH21	1.25	0.85
3:J:828:LYS:HZ3	3:J:863:VAL:H	1.29	0.80
3:J:957:PRO:HG2	3:J:1007:VAL:HG22	1.64	0.80

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	G	227/315 (72%)	221 (97%)	6 (3%)	0	100	100
1	H	227/315 (72%)	217 (96%)	10 (4%)	0	100	100
2	I	1092/1119 (98%)	1008 (92%)	84 (8%)	0	100	100
3	J	1270/1532 (83%)	1200 (94%)	70 (6%)	0	100	100
4	K	89/99 (90%)	81 (91%)	8 (9%)	0	100	100
All	All	2905/3380 (86%)	2727 (94%)	178 (6%)	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	G	202/273 (74%)	202 (100%)	0	100	100
1	H	202/273 (74%)	202 (100%)	0	100	100
2	I	921/941 (98%)	917 (100%)	4 (0%)	91	95
3	J	1079/1287 (84%)	1075 (100%)	4 (0%)	91	95
4	K	80/87 (92%)	77 (96%)	3 (4%)	33	61
All	All	2484/2861 (87%)	2473 (100%)	11 (0%)	91	95

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	1422	MET
4	K	36	LYS
4	K	78	ASN
4	K	72	ARG
3	J	159	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	I	139	GLN
3	J	1075	HIS
3	J	1364	HIS

5.3.3 RNA (i)

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)

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.

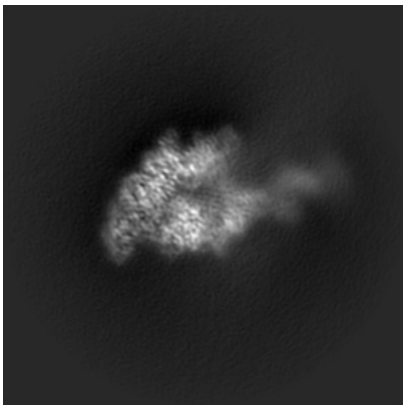
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-34997. These allow visual inspection of the internal detail of the map and identification of artifacts.

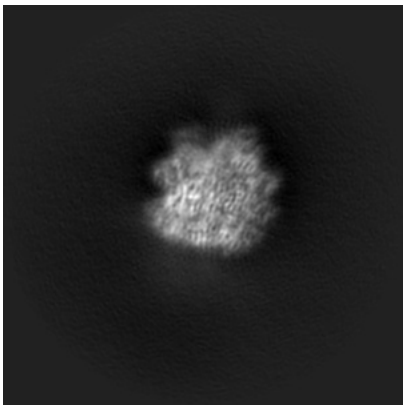
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

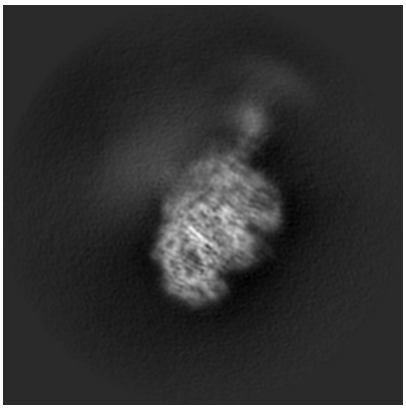
6.1.1 Primary map



X

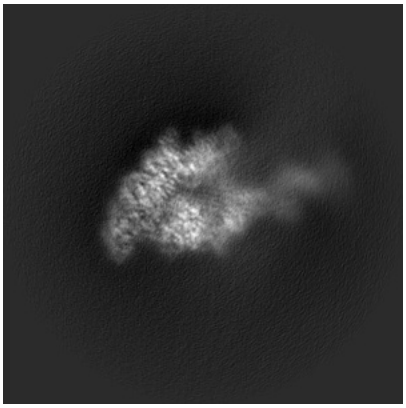


Y

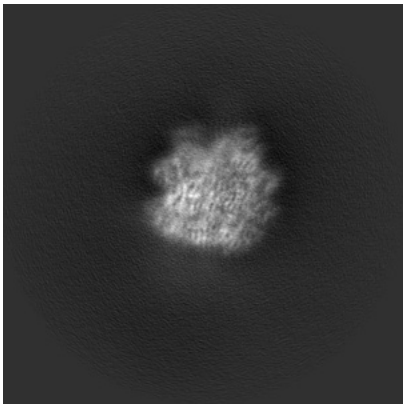


Z

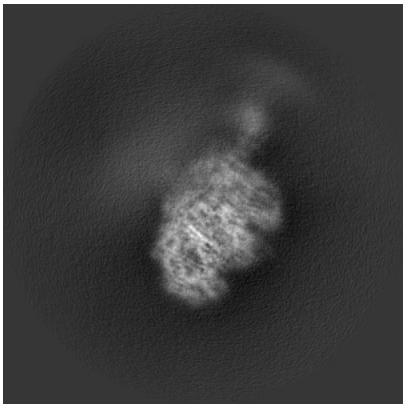
6.1.2 Raw map



X



Y

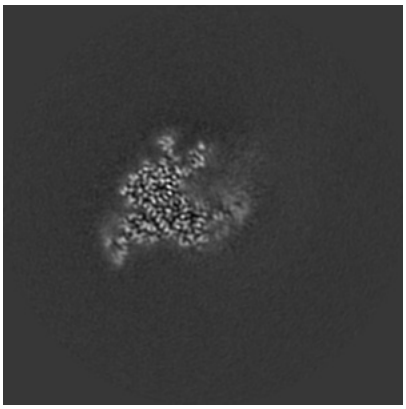


Z

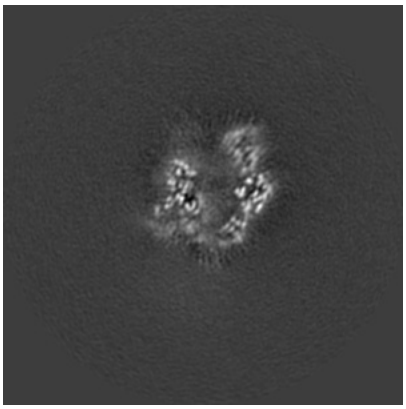
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

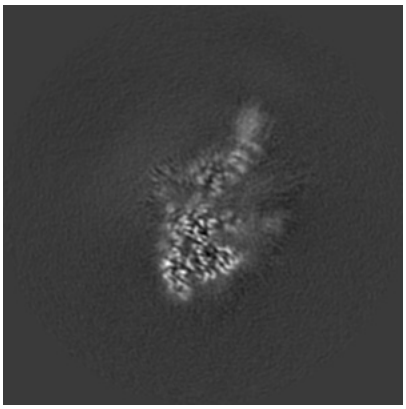
6.2.1 Primary map



X Index: 160

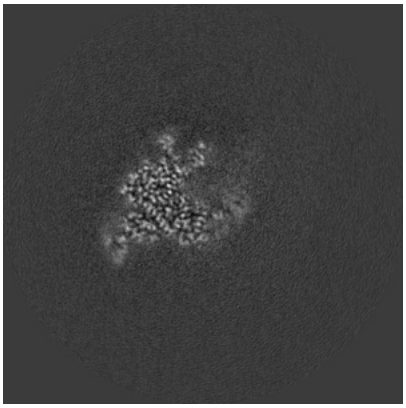


Y Index: 160

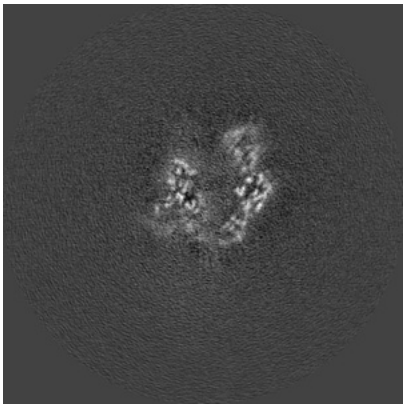


Z Index: 160

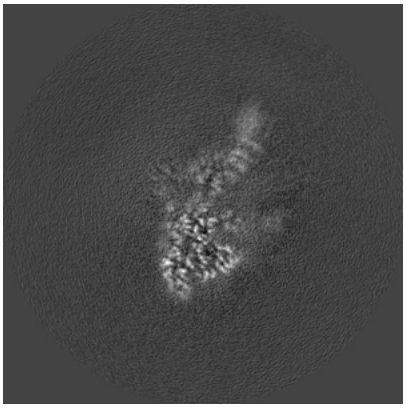
6.2.2 Raw map



X Index: 160



Y Index: 160

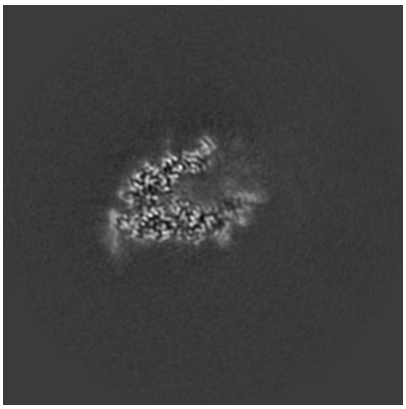


Z Index: 160

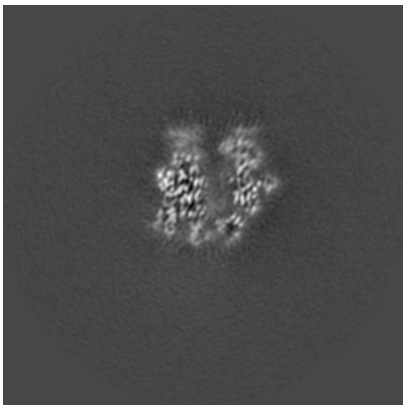
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

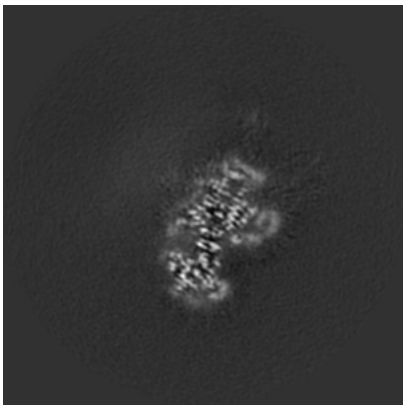
6.3.1 Primary map



X Index: 166

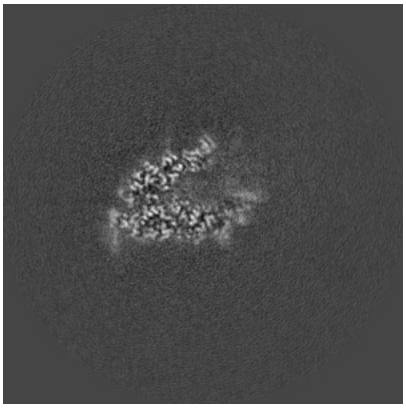


Y Index: 152

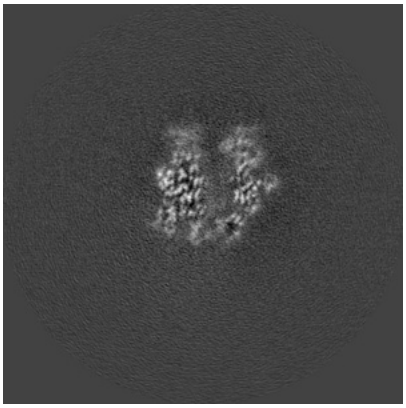


Z Index: 142

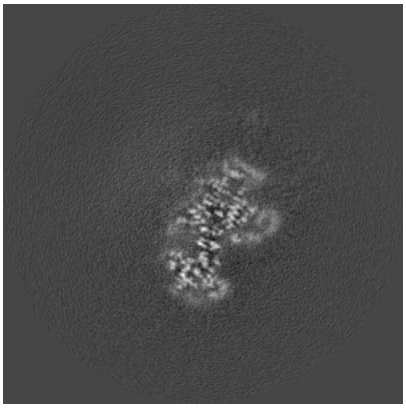
6.3.2 Raw map



X Index: 166



Y Index: 152

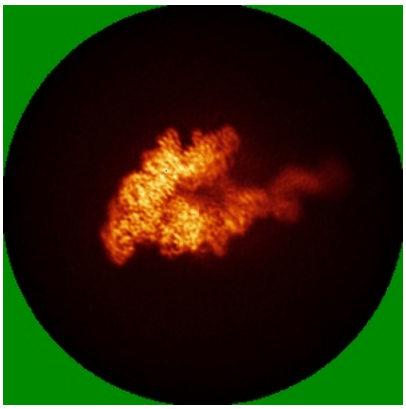


Z Index: 142

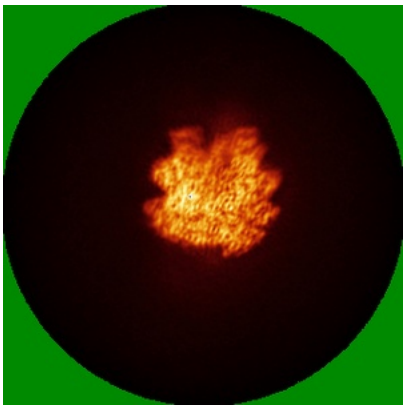
The images above show the largest variance slices of the map in three orthogonal directions.

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

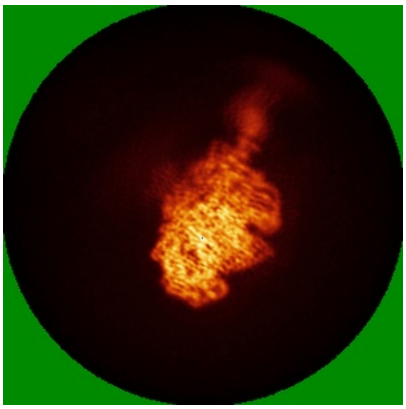
6.4.1 Primary map



X

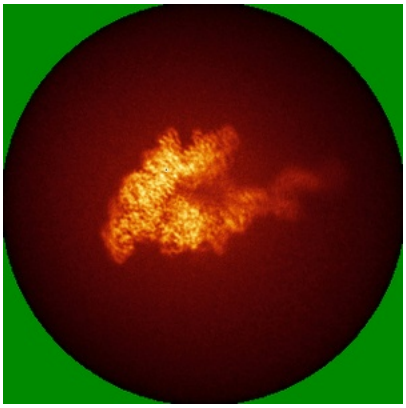


Y

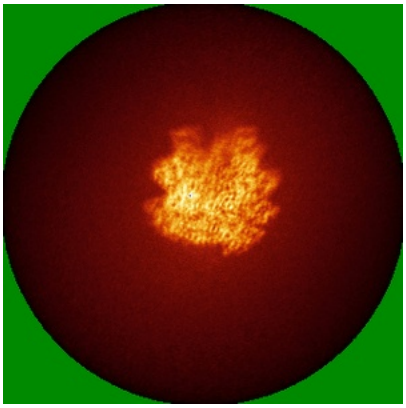


Z

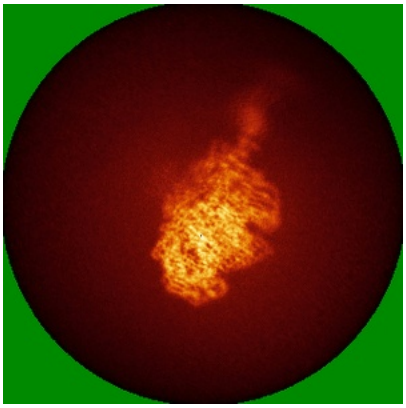
6.4.2 Raw map



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 0.008. 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.

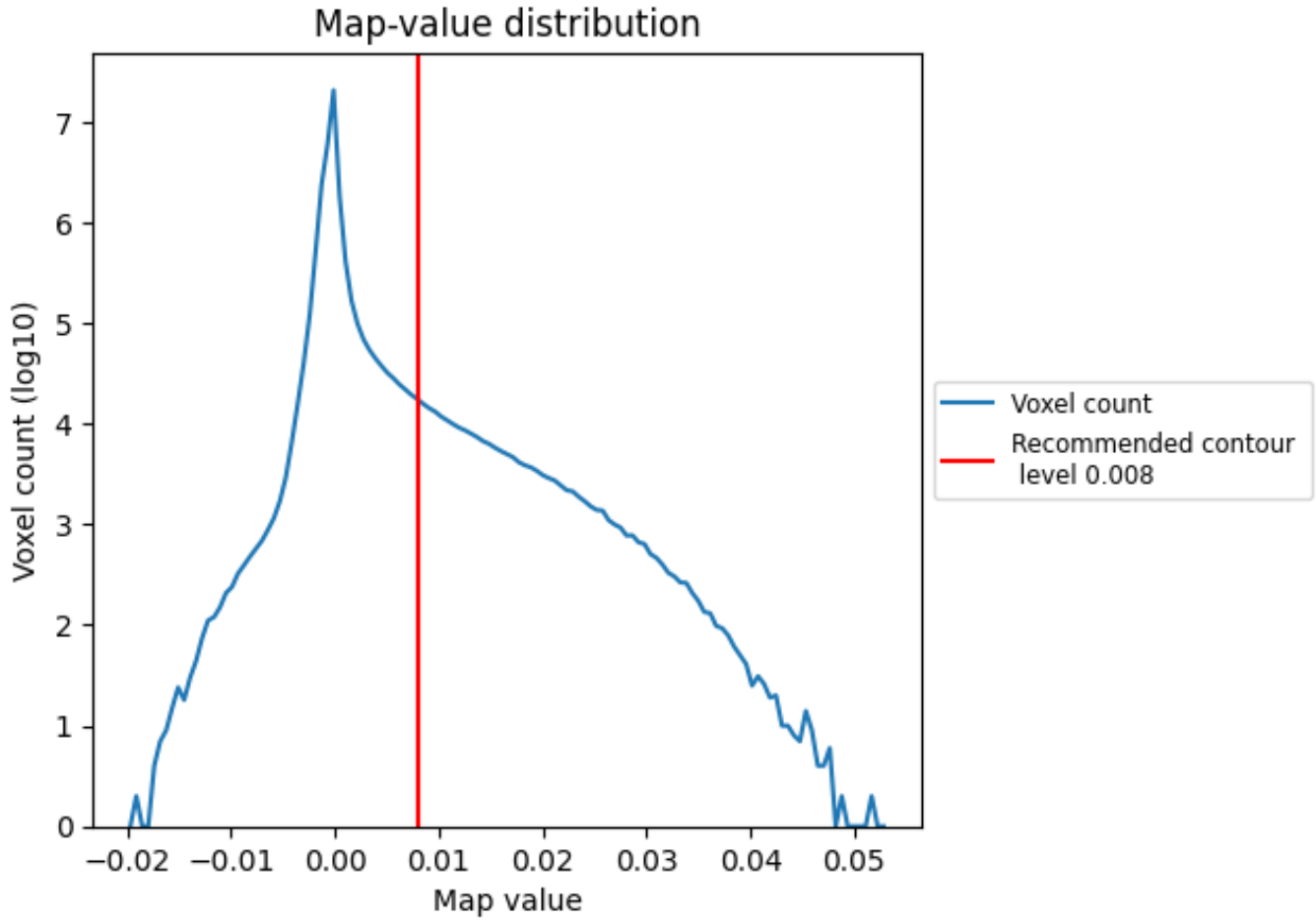
6.6 Mask visualisation (i)

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

7 Map analysis

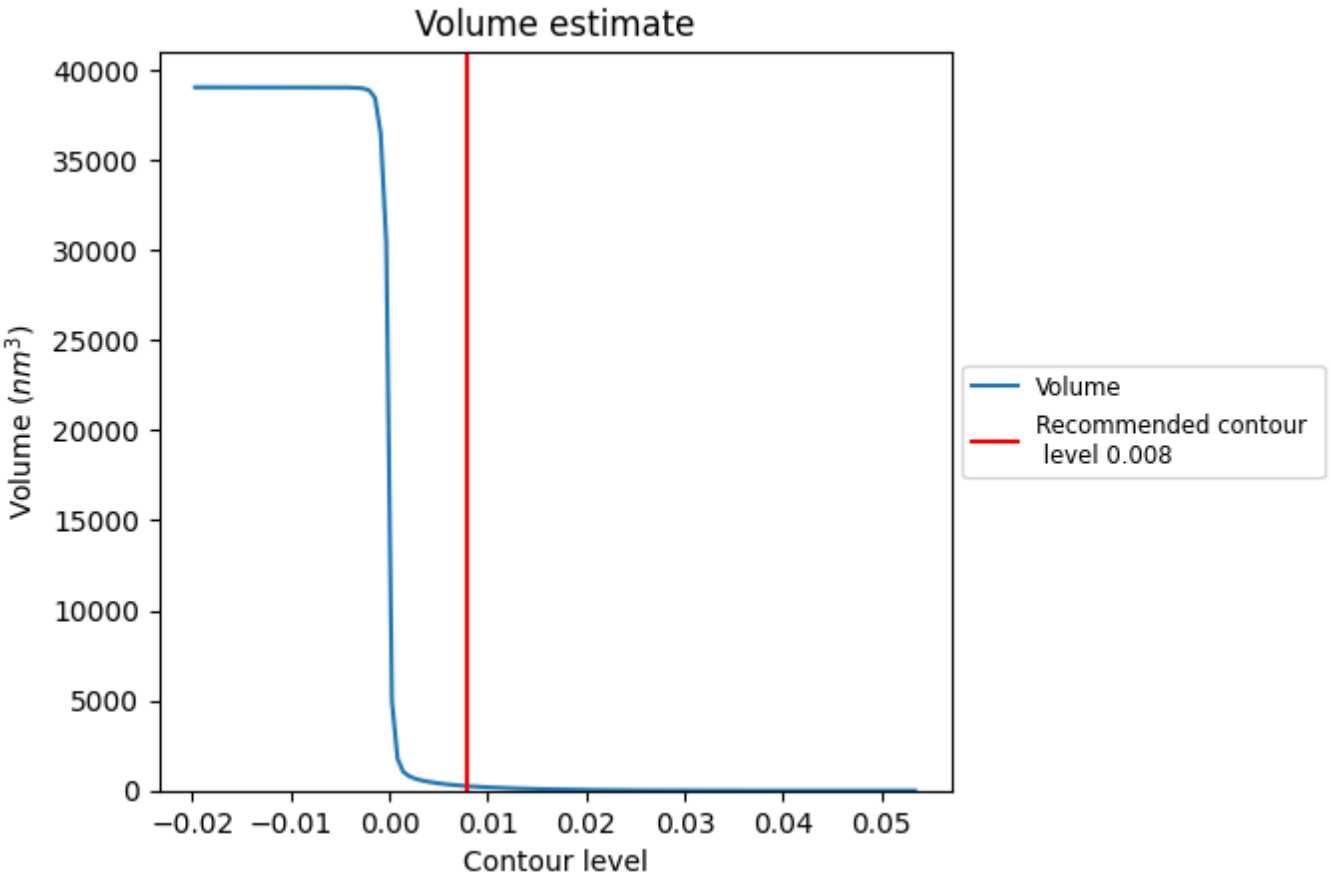
This section contains the results of statistical analysis of the map.

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.

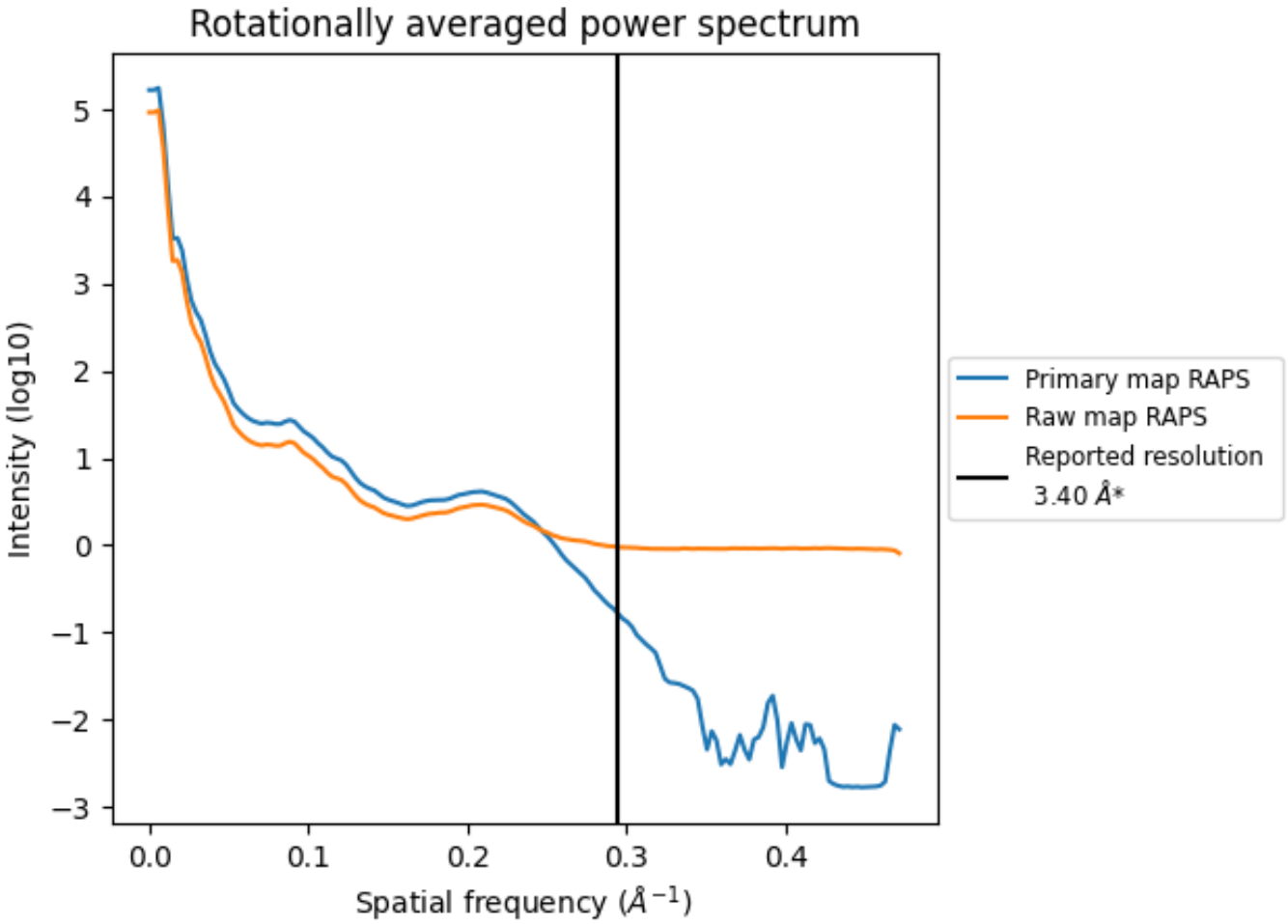
7.2 Volume estimate (i)



The volume at the recommended contour level is 246 nm^3; this corresponds to an approximate mass of 222 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)

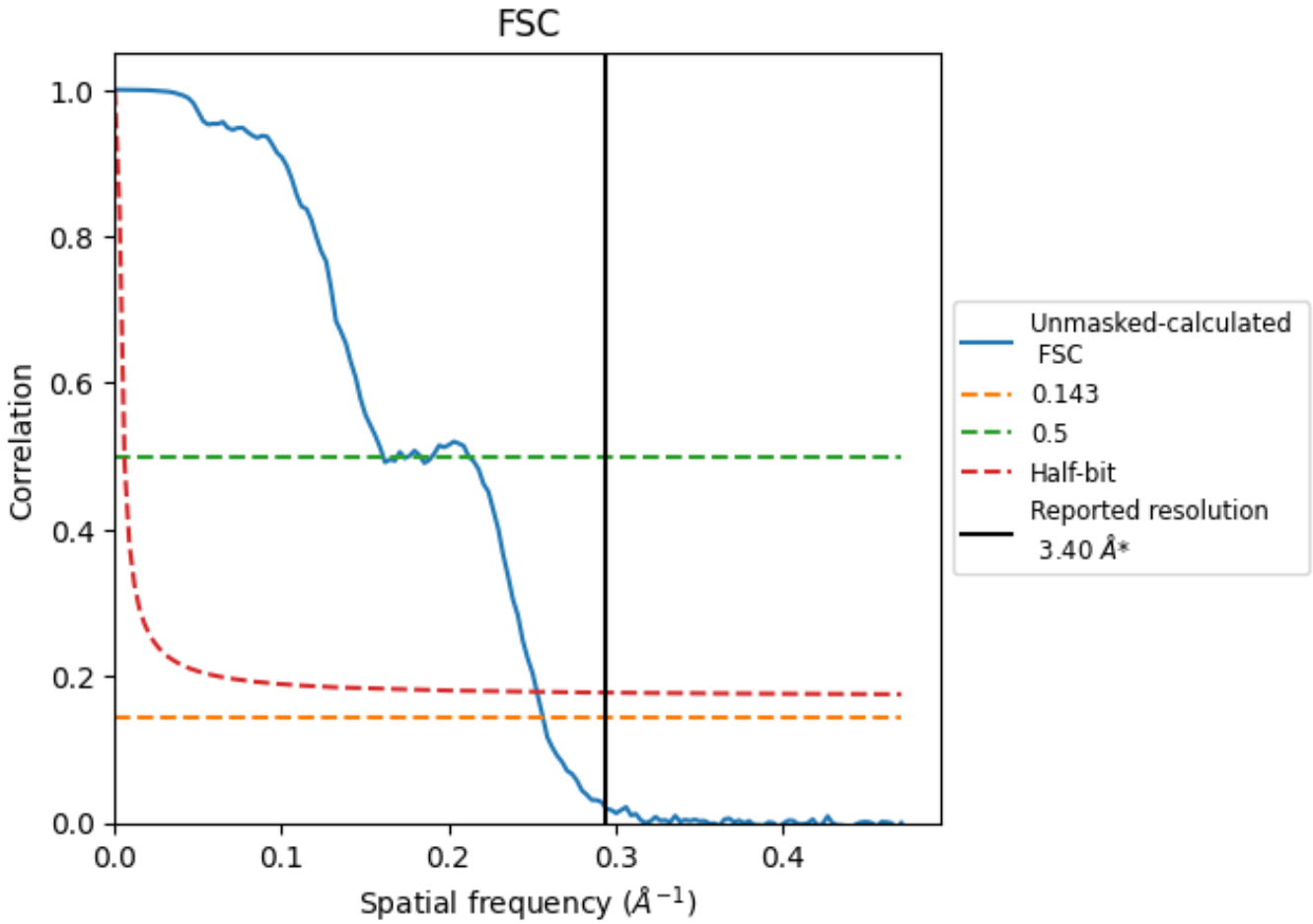


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

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 0.294 Å^{-1}

8.2 Resolution estimates (i)

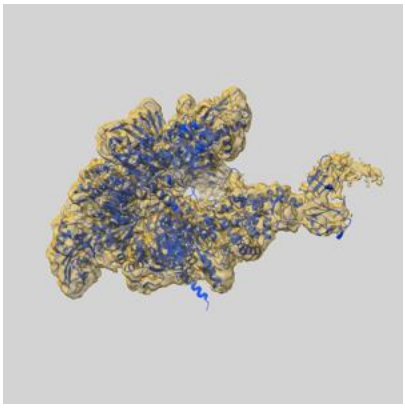
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.89	6.22	3.95

*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 3.89 differs from the reported value 3.4 by more than 10 %

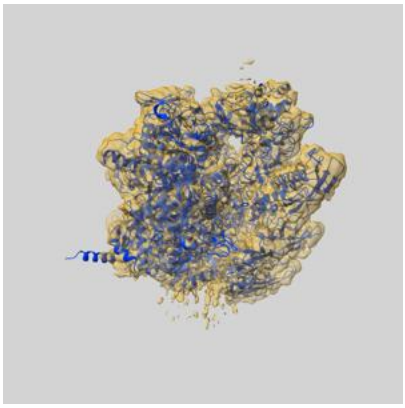
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-34997 and PDB model 8HSH. Per-residue inclusion information can be found in section 3 on page 5.

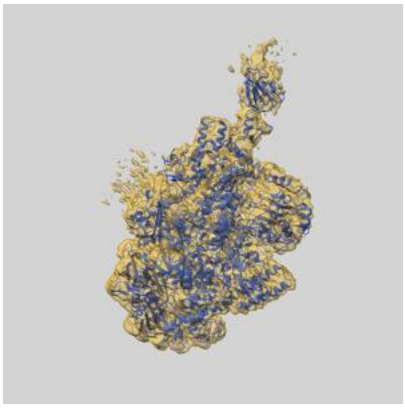
9.1 Map-model overlay



X



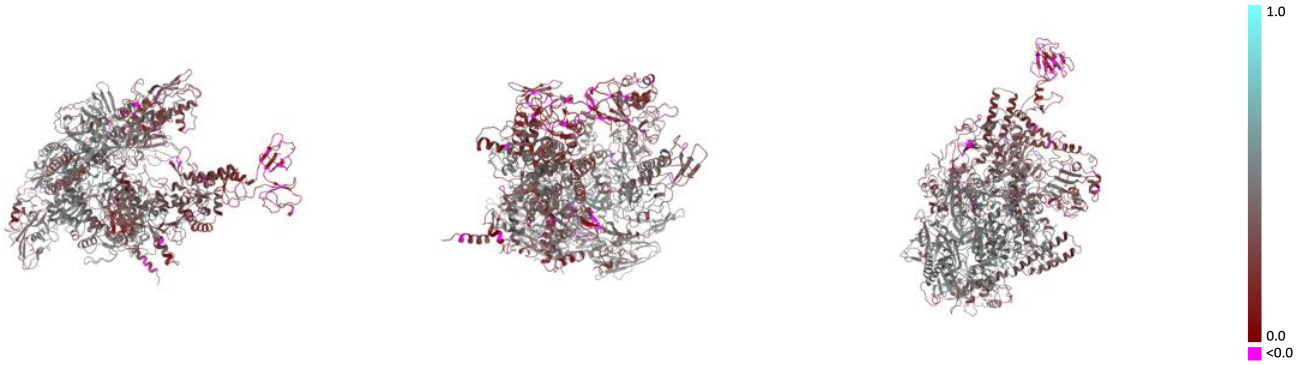
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.008 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.

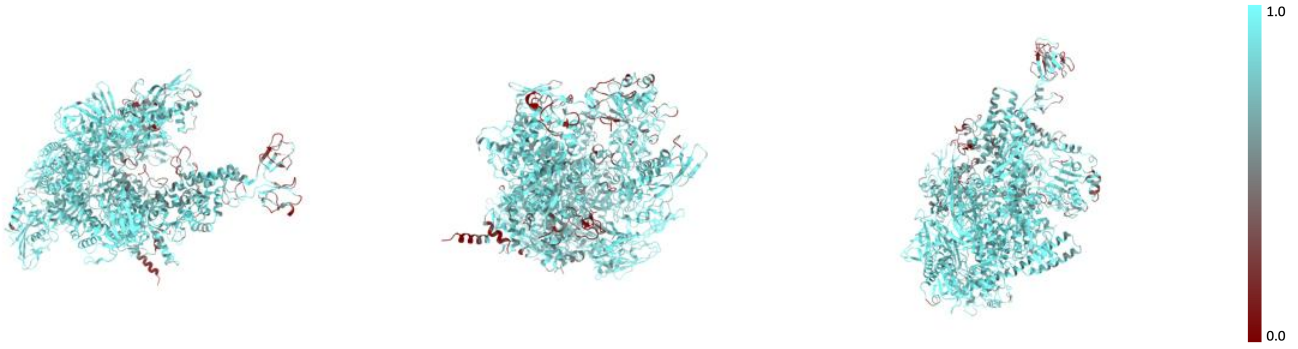
9.2 Q-score mapped to coordinate model (i)



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.

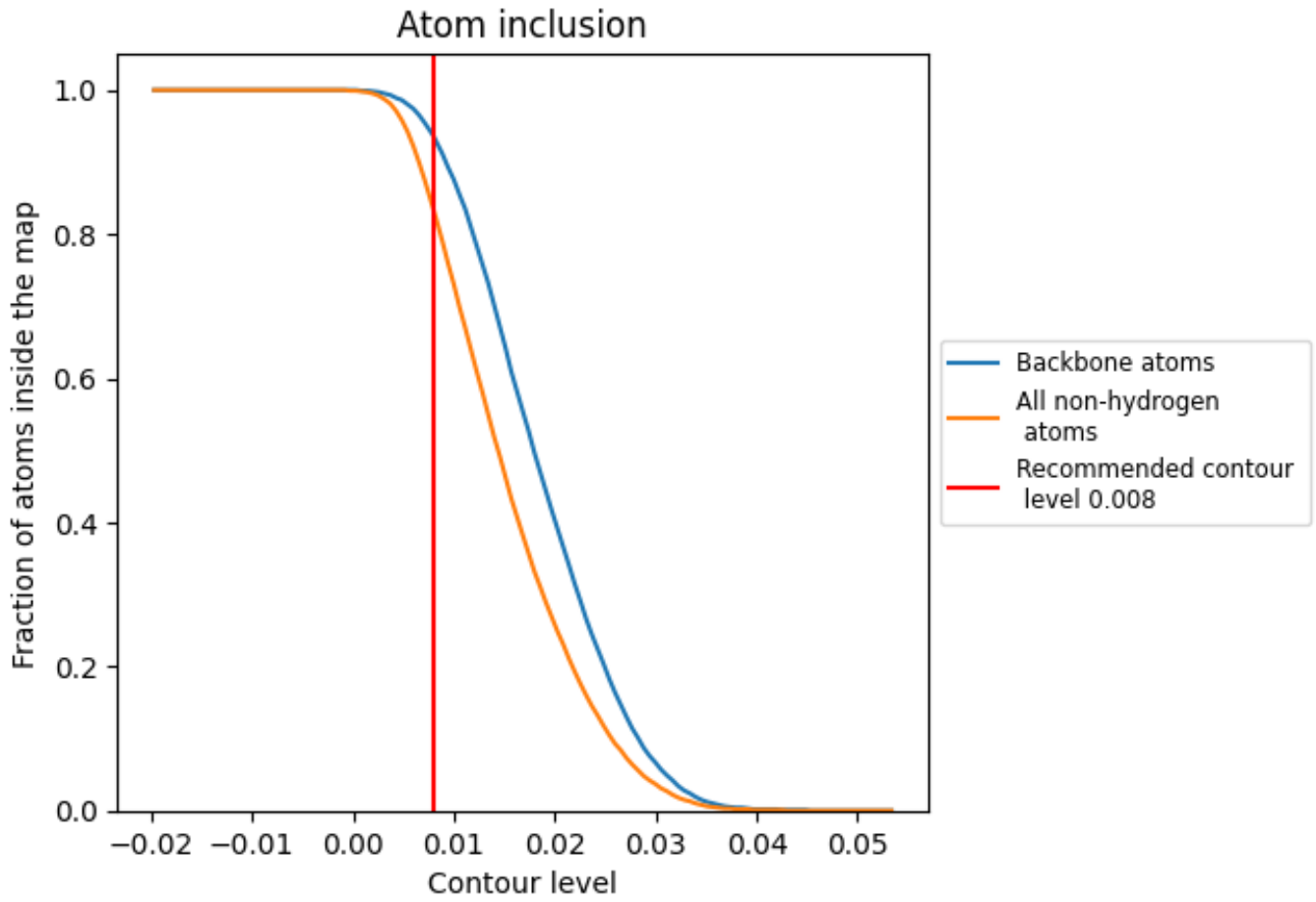
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.008).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 83% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8340	0.3740
G	0.9160	0.4390
H	0.9100	0.4120
I	0.8490	0.3980
J	0.7990	0.3380
K	0.7430	0.3250