wwPDB EM Validation Summary Report

Oct 19, 2026 – 01:17 pm BST

PDB ID	:	9SZ5 / pdb_00009sz5
EMDB ID	:	EMD-55360
Title	:	Structure of bacteriophage T5 L-shaped tail fiber : fiber domain
Authors	:	d'Acapito, A.; Linares, R.; Breyton, C.
Deposited on	:	2025-10-14
Resolution	:	3.59 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 ⓘ symbol.

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

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

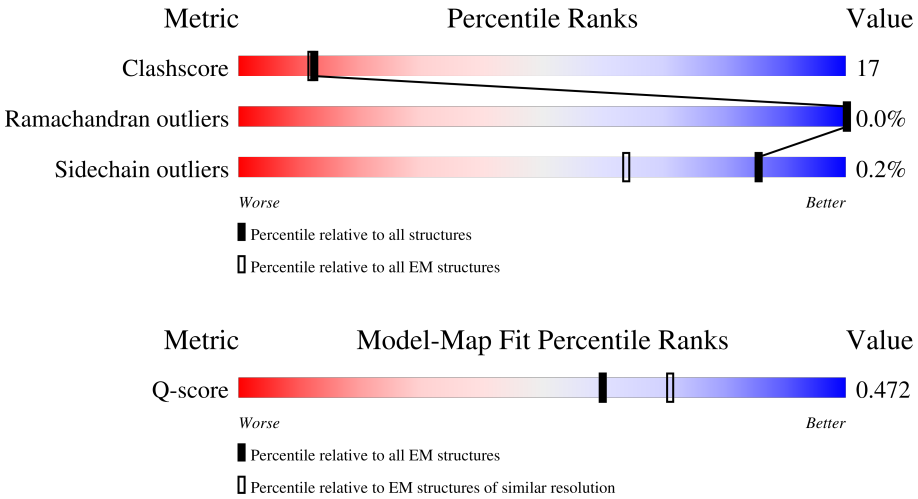
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 3.59 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12565 (3.09 - 4.09)

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	1396	7% 49% 26% 25%
1	B	1396	6% 48% 27% 25%
1	C	1396	7% 48% 27% 25%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 23484 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.

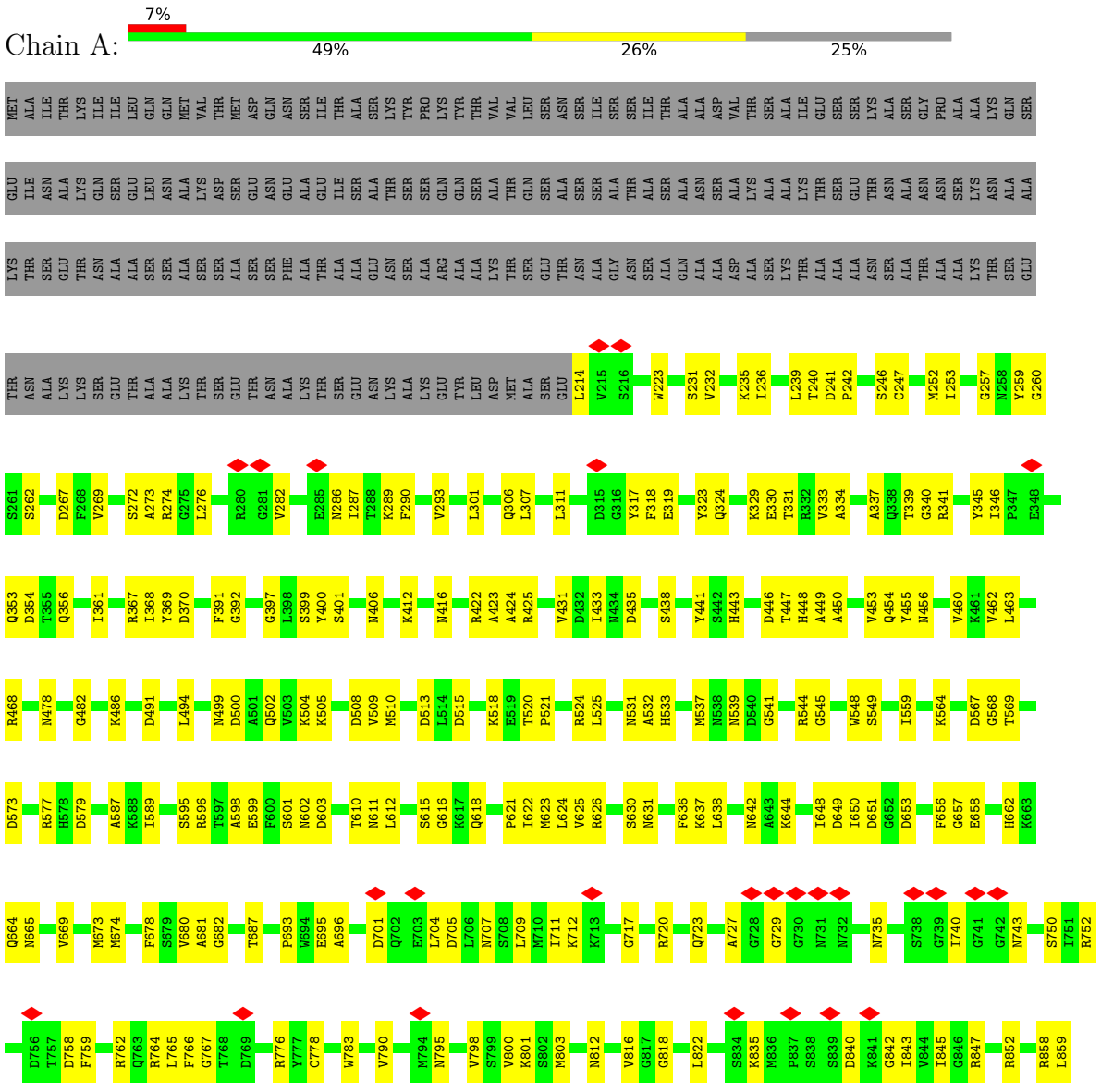
- Molecule 1 is a protein called Side tail fiber protein pb1.

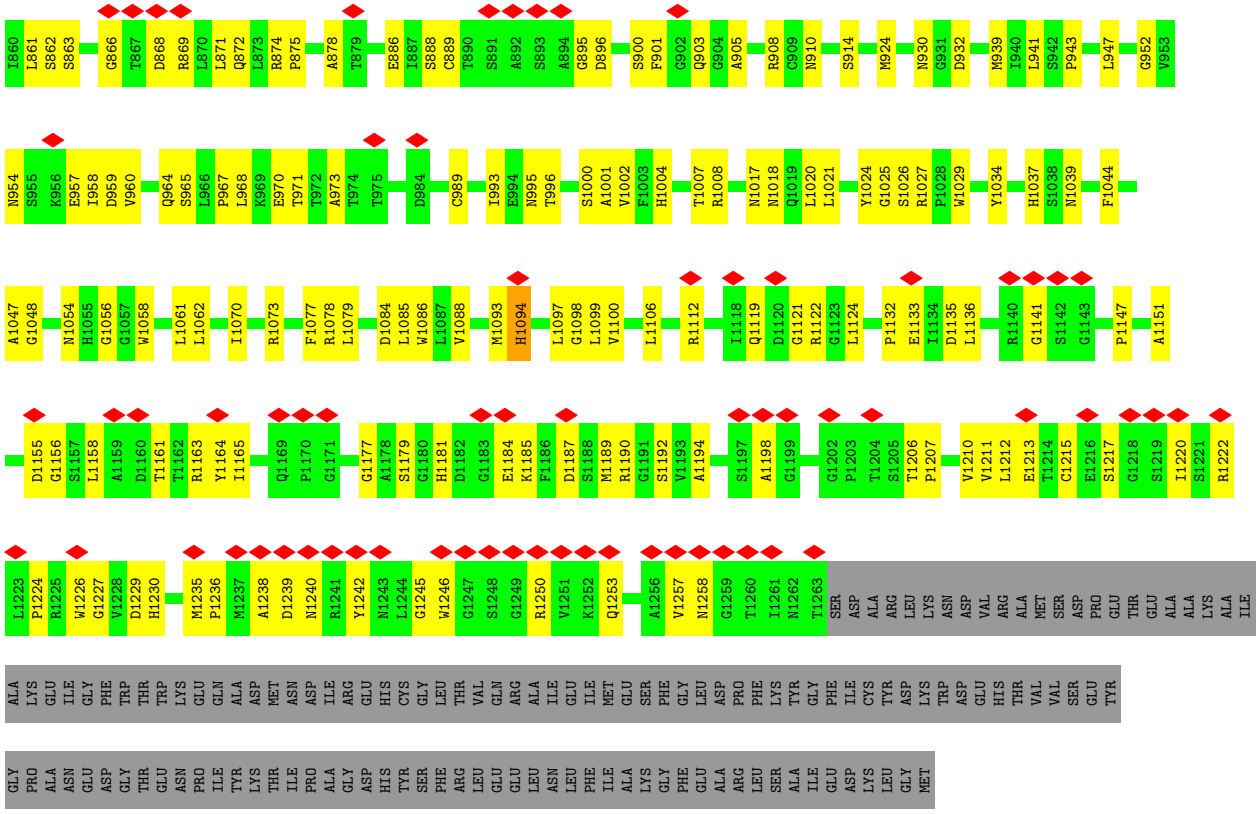
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1050	Total	C	N	O	S	0	0
			7828	4838	1407	1553	30		
1	B	1050	Total	C	N	O	S	0	0
			7828	4838	1407	1553	30		
1	C	1050	Total	C	N	O	S	0	0
			7828	4838	1407	1553	30		

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.

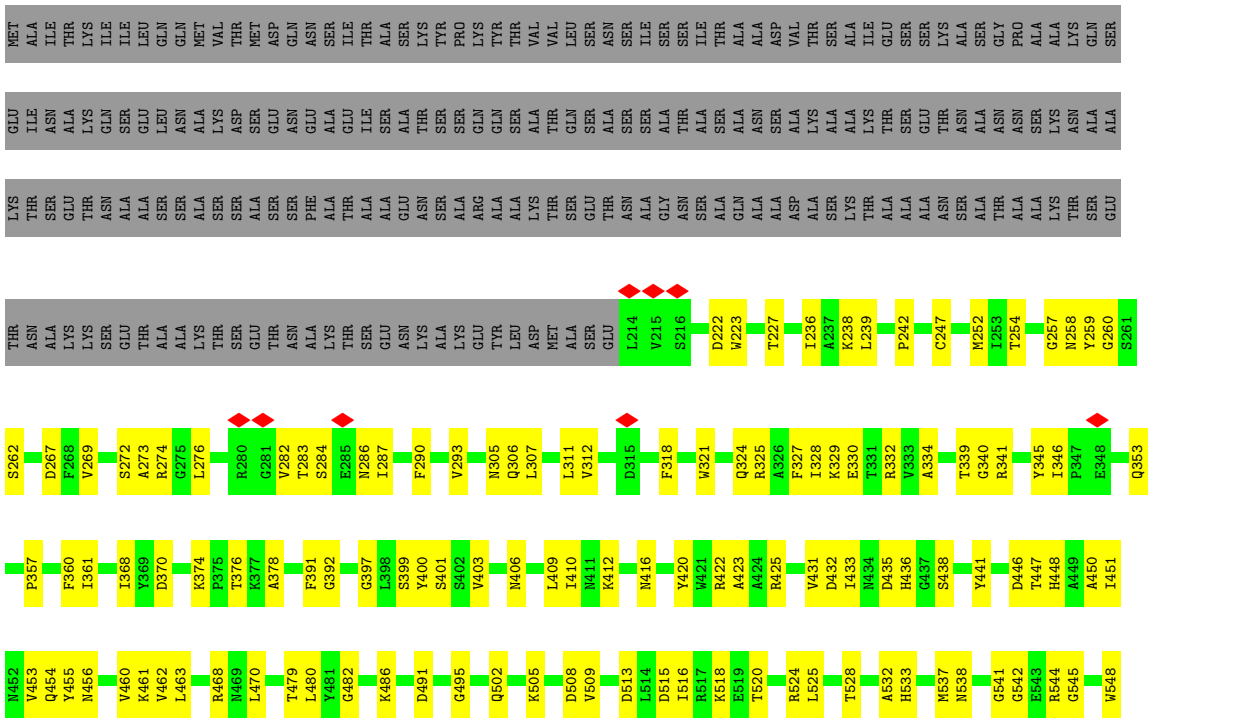
- Molecule 1: Side tail fiber protein pb1

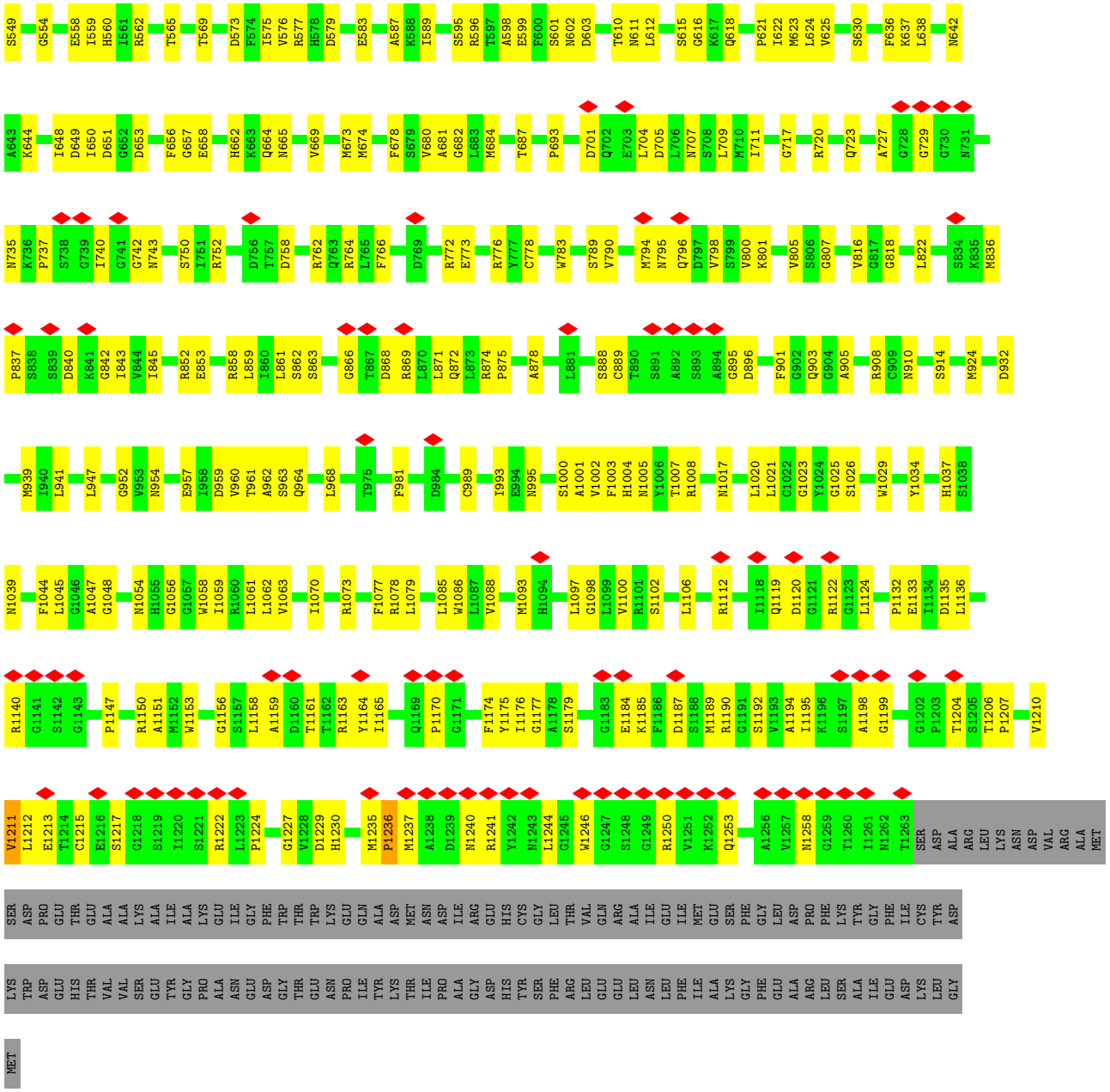




• Molecule 1: Side tail fiber protein pb1



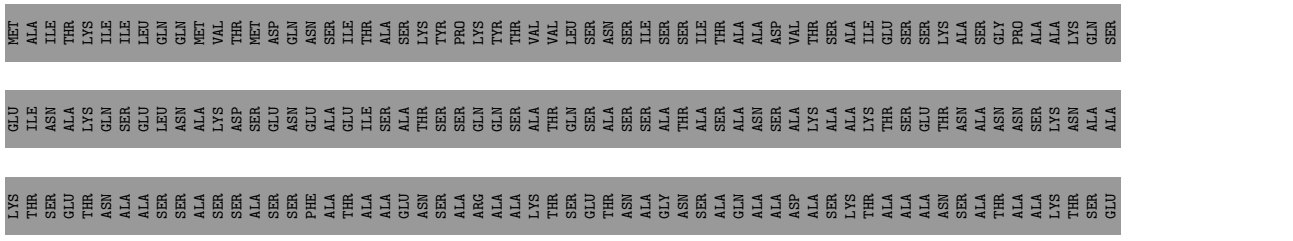


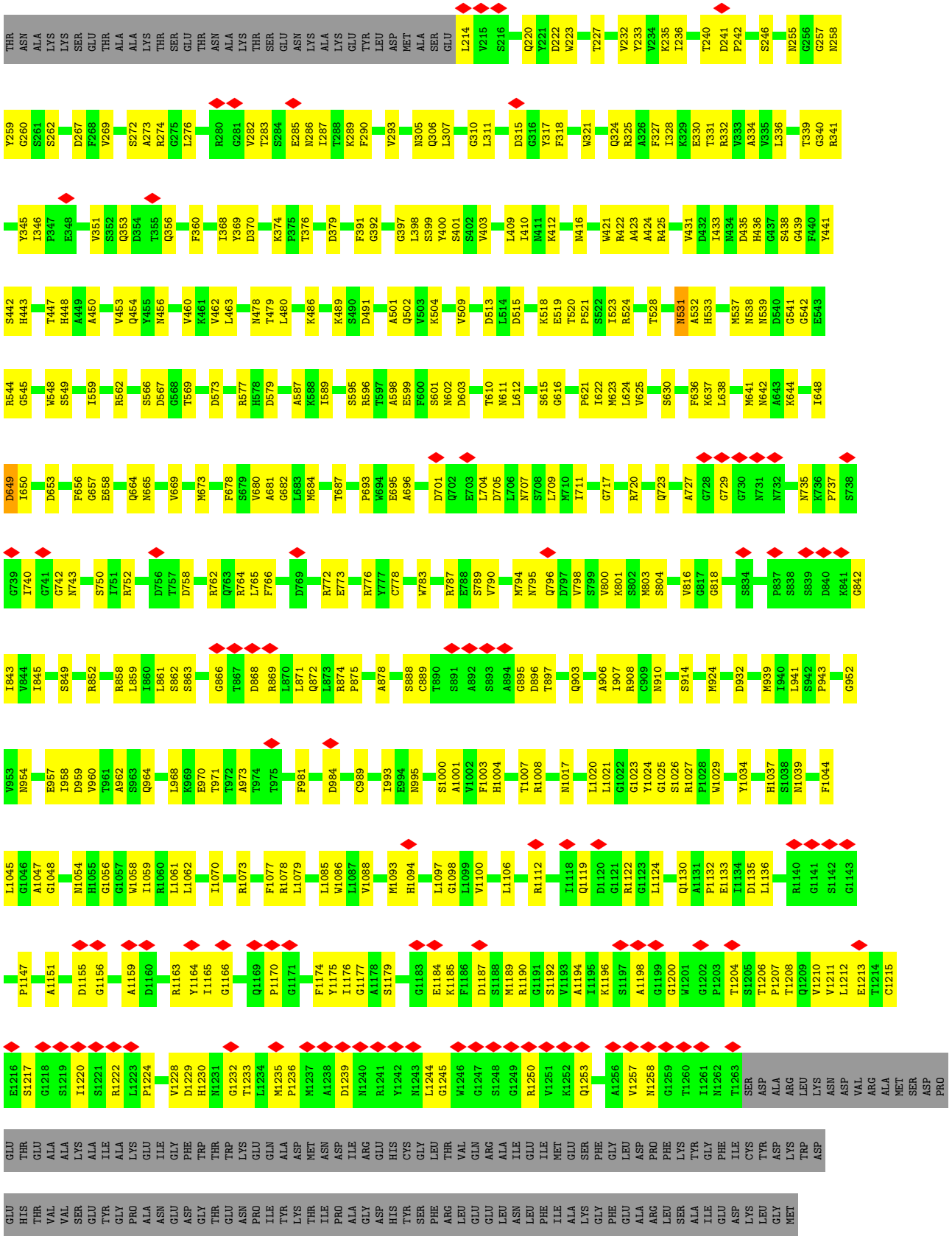


• Molecule 1: Side tail fiber protein pb1

Chain C:






THR ASN ALA LYS LYS SER GLU THR ALA ALA LYS THR SER GLU THR ASN ALA LYS THR SER GLU ASN LYS ALA LYS GLU TYR LEU ASP MET ALA SER GLU
L214 V215 S216 Q220 Y221 D222 W223 T227 V232 Y233 V234 K235 I236 T240 D241 P242 S246 N255 G256 G257 N258
Y259 G260 S261 S262 D267 F268 V269 S272 A273 R274 G275 L276 R280 G281 V282 T283 S284 E285 N286 I287 T288 K289 F290 V293 N305 Q306 L307 G310 L311 D315 G316 Y317 F318 W321 Q324 R325 A326 F327 I328 K329 E330 T331 R332 Y333 A334 V335 L336 T339 G340 R341
Y345 I346 P347 E348 V351 S352 Q353 D354 T355 Q356 F360 I368 Y369 D370 K374 P375 T376 D379 F391 G392 G397 L398 S399 Y400 S401 S402 V403 L409 I410 N411 K412 N416 W421 R422 A423 A424 R425 V431 D432 I433 N434 D435 H436 G437 S438 G439 F440 Y441
S442 H443 T447 H448 A449 A450 V453 Q454 Y455 N456 V460 K461 V462 L463 N478 T479 L480 K486 K489 S490 D491 A501 Q502 V503 K504 V509 D513 L514 D515 K518 E519 T520 P521 S522 I523 R524 T528 N531 A532 H533 M537 N538 N539 D540 G541 G542 E543
R544 G545 W548 S549 I559 R562 S566 D567 G568 T569 D573 R577 H578 D579 A587 K588 I589 S595 R596 T597 A598 E599 F600 S601 N602 D603 T610 N611 L612 S615 G616 P621 I622 M623 L624 V625 S630 F636 K637 L638 M641 N642 A643 K644 I648
D649 I650 D653 F656 G657 E658 Q664 N665 V669 M673 F678 S679 V680 A681 G682 L683 M684 T687 P693 W694 E695 A696 D701 Q702 E703 L704 D705 L706 N707 S708 L709 M710 I711 G717 R720 Q723 A727 G728 G729 G730 N731 N732 N735 K736 P737 S738
G739 I740 G741 G742 N743 S750 G751 R752 D756 T757 D758 R762 Q763 R764 L765 F766 D769 R772 E773 R776 Y777 C778 W783 R787 E788 S789 V790 M794 N795 Q796 D797 V798 S799 V800 K801 S802 M803 S804 V816 G817 G818 S834 P837 S838 S839 D840 K841 G842
I843 V844 I845 S849 R852 R858 L859 I860 L861 S862 S863 G866 T867 D868 R869 L870 L871 Q872 L873 R874 P875 A878 S888 C889 T890 S891 A892 S893 A894 G895 D896 T897 Q903 A906 I907 R908 C909 N910 S914 M924 D932 M939 I940 L941 S942 P943 G952
V953 N954 E957 I958 D959 V960 T961 A962 S963 Q964 L968 K969 E970 T971 T972 A973 T974 T975 F981 D984 C989 I993 E994 N995 S1000 A1001 V1002 F1003 H1004 T1007 R1008 N1017 L1020 L1021 G1022 G1023 Y1024 G1025 S1026 R1027 P1028 W1029 Y1034 H1037 S1038 N1039 F1044
L1045 G1046 A1047 G1048 N1054 H1055 G1056 G1057 W1058 I1059 R1060 L1061 L1062 I1070 R1073 F1077 R1078 L1079 L1085 W1086 L1087 V1088 M1093 H1094 L1097 G1098 L1099 V1100 L1106 R1112 I1118 Q1119 D1120 G1121 R1122 G1123 L1124 Q1130 A1131 P1132 E1133 I1134 D1135 L1136 R1140 G1141 S1142 G1143
P1147 A1151 D1155 G1156 A1159 D1160 R1163 Y1164 I1165 G1166 Q1169 P1170 G1171 F1174 Y1175 I1176 G1177 A1178 S1179 G1183 E1184 K1185 F1186 D1187 S1188 M1189 R1190 G1191 S1192 V1193 A1194 I1195 K1196 S1197 A1198 G1199 G1200 W1201 G1202 P1203 T1204 S1205 T1206 P1207 T1208 Q1209 V1210 V1211 L1212 E1213 T1214 C1215
E1216 S1217 G1218 S1219 I1220 S1221 R1222 L1223 P1224 V1228 D1229 H1230 N1231 G1232 T1233 L1234 M1235 P1236 M1237 A1238 D1239 N1240 R1241 Y1242 N1243 L1244 G1245 W1246 G1247 S1248 G1249 R1250 V1251 K1252 Q1253 A1256 V1257 N1258 G1259 T1260 L1261 N1262 T1263 SER ASP ALA ARG LEU LYS ASN ASP VAL ARG ALA MET SER ASP PRO
GLU THR GLU ALA ALA LYS GLU ILE ALA LYS GLU ILE GLY PHE TRP THR TRP LYS GLU GLN ALA ASP MET ASN ASP ILE ARG GLU HIS CYS GLY LEU THR VAL GLN ARG ALA ILE GLU LEU ASP PHE ILE MET GLU SER PHE GLY LEU ASP ALA ARG LEU SER ALA ILE GLU ASP
GLU HIS THR VAL VAL SER GLU TYR GLY PRO ALA ASN GLU ASP GLY THR GLU ASN PRO ILE TYR LYS THR ILE PRO ALA GLY ASP HIS TYR SER PHE ARG LEU GLU GLU LEU ASN LEU PHE ILE ALA LYS GLY PHE GLU ALA ARG LEU SER ALA ILE GLU ASP LYS LEU GLY MET

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39217	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	9.624	Depositor
Minimum map value	-6.174	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.110	Depositor
Recommended contour level	1.5	Depositor
Map size (Å)	691.712, 691.712, 691.712	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.351, 1.351, 1.351	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.15	0/7968	0.32	0/10794
1	B	0.14	0/7968	0.32	0/10794
1	C	0.14	0/7968	0.32	0/10794
All	All	0.14	0/23904	0.32	0/32382

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	7828	0	7645	339	0
1	B	7828	0	7645	353	0
1	C	7828	0	7645	360	0
All	All	23484	0	22935	783	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 17.

The worst 5 of 783 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:A:1242:TYR:HE1	1:C:1233:THR:HA	1.42	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1062:LEU:HD22	1:B:1073:ARG:HG2	1.63	0.81
1:A:704:LEU:HD21	1:A:709:LEU:HD21	1.65	0.79
1:C:1184:GLU:HG2	1:C:1185:LYS:HG3	1.65	0.78
1:C:704:LEU:HD21	1:C:709:LEU:HD21	1.64	0.78

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	1046/1396 (75%)	946 (90%)	100 (10%)	0	100	100
1	B	1046/1396 (75%)	949 (91%)	96 (9%)	1 (0%)	48	79
1	C	1046/1396 (75%)	944 (90%)	102 (10%)	0	100	100
All	All	3138/4188 (75%)	2839 (90%)	298 (10%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1236	PRO

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	838/1110 (76%)	836 (100%)	2 (0%)	87	85
1	B	838/1110 (76%)	836 (100%)	2 (0%)	87	85
1	C	838/1110 (76%)	836 (100%)	2 (0%)	87	85
All	All	2514/3330 (76%)	2508 (100%)	6 (0%)	85	85

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1211	VAL
1	C	531	ASN
1	C	649	ASP
1	A	1094	HIS
1	A	812	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	640	ASN
1	C	707	ASN
1	B	884	GLN
1	C	930	ASN
1	C	611	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	C	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1238:ALA	C	1239:ASP	N	5.82
1	C	1238:ALA	C	1239:ASP	N	4.49
1	A	1238:ALA	C	1239:ASP	N	3.14

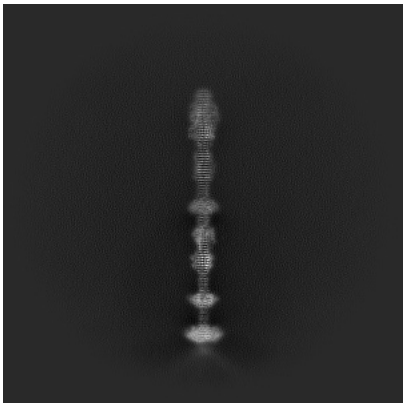
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-55360. These allow visual inspection of the internal detail of the map and identification of artifacts.

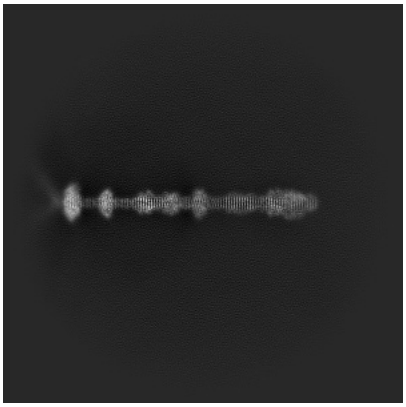
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

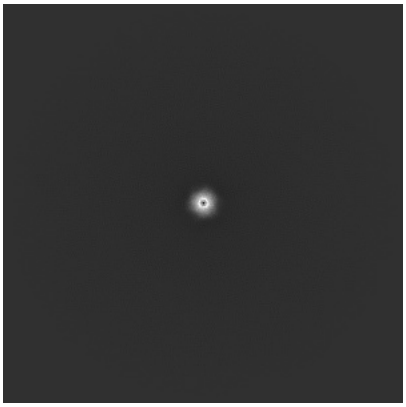
6.1.1 Primary map



X



Y

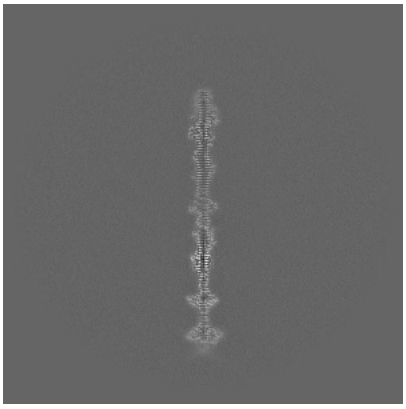


Z

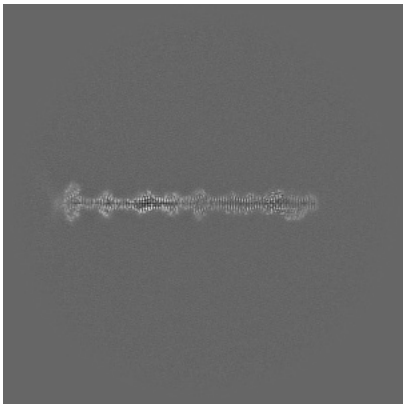
The images above show the map projected in three orthogonal directions.

6.2 Central slices

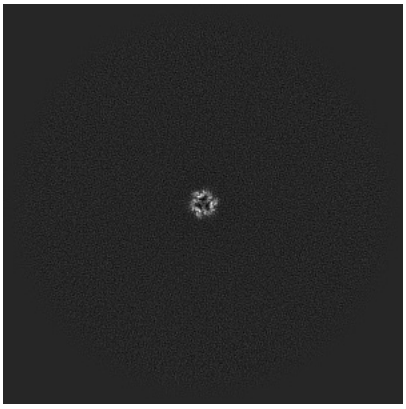
6.2.1 Primary map



X Index: 256



Y Index: 256

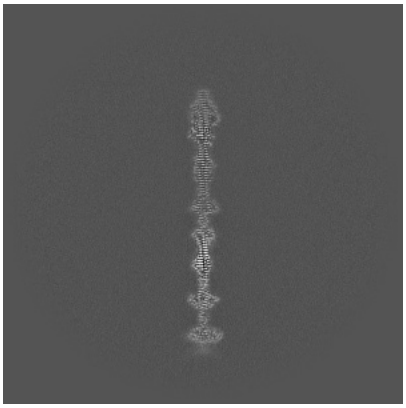


Z Index: 256

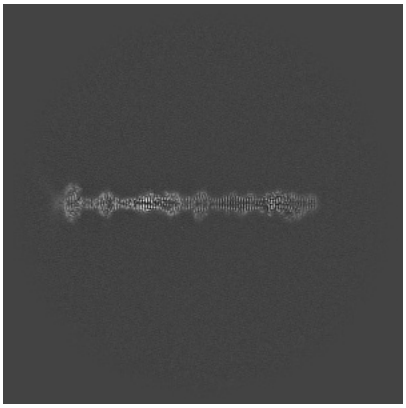
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

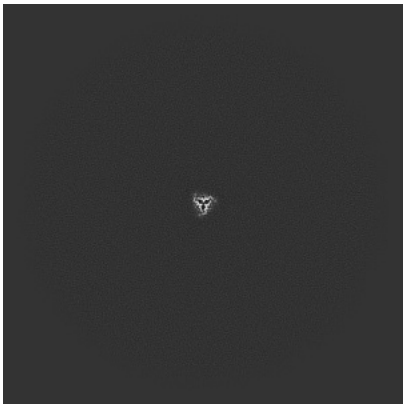
6.3.1 Primary map



X Index: 260



Y Index: 254

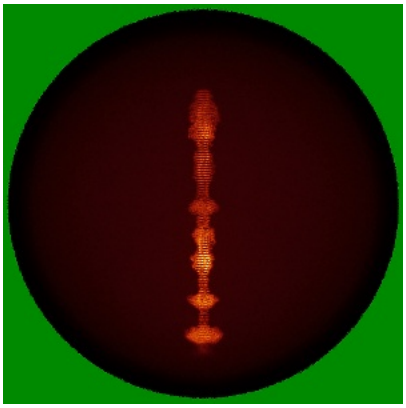


Z Index: 183

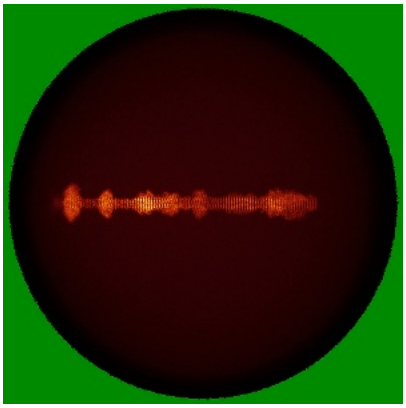
The images above show the largest variance slices of the map in three orthogonal directions.

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

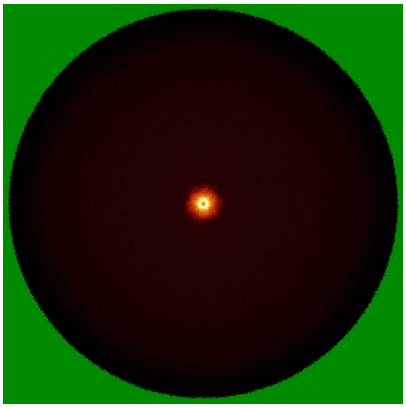
6.4.1 Primary map



X



Y

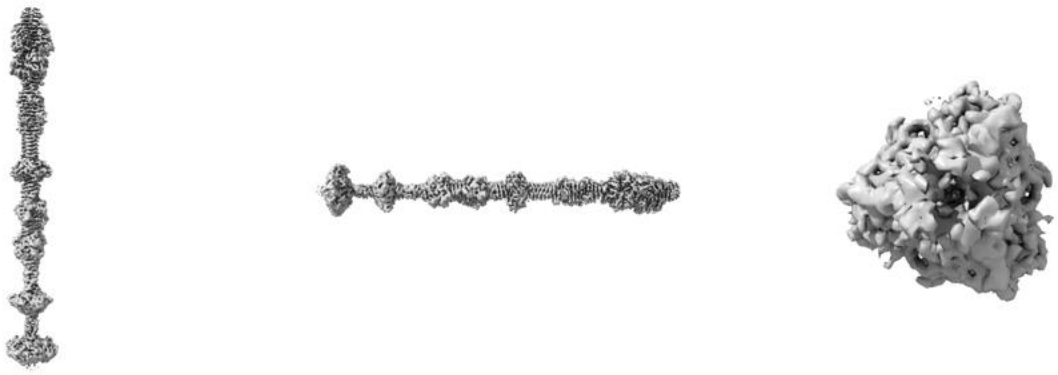


Z

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 1.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

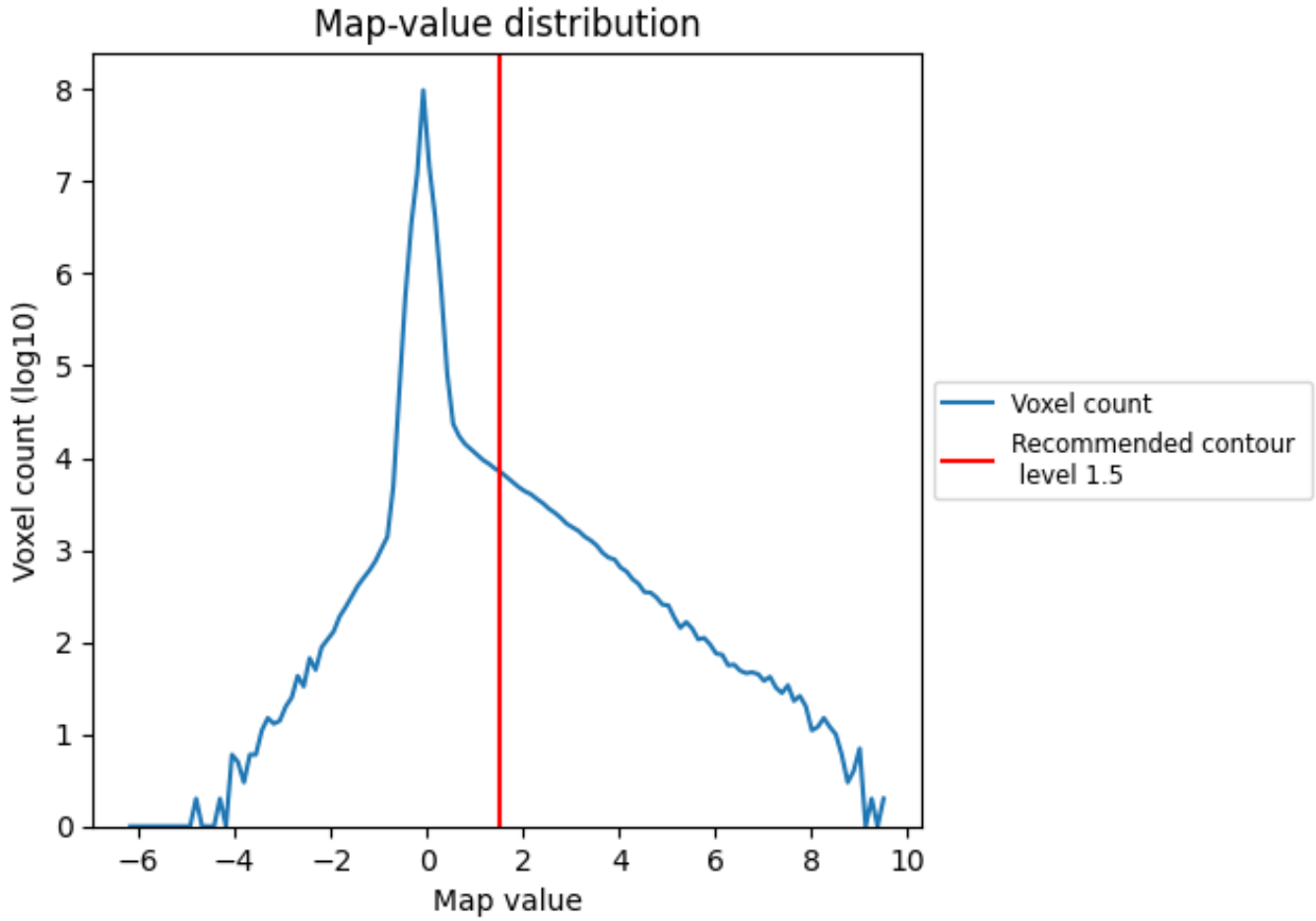
6.6 Mask visualisation (i)

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

7 Map analysis

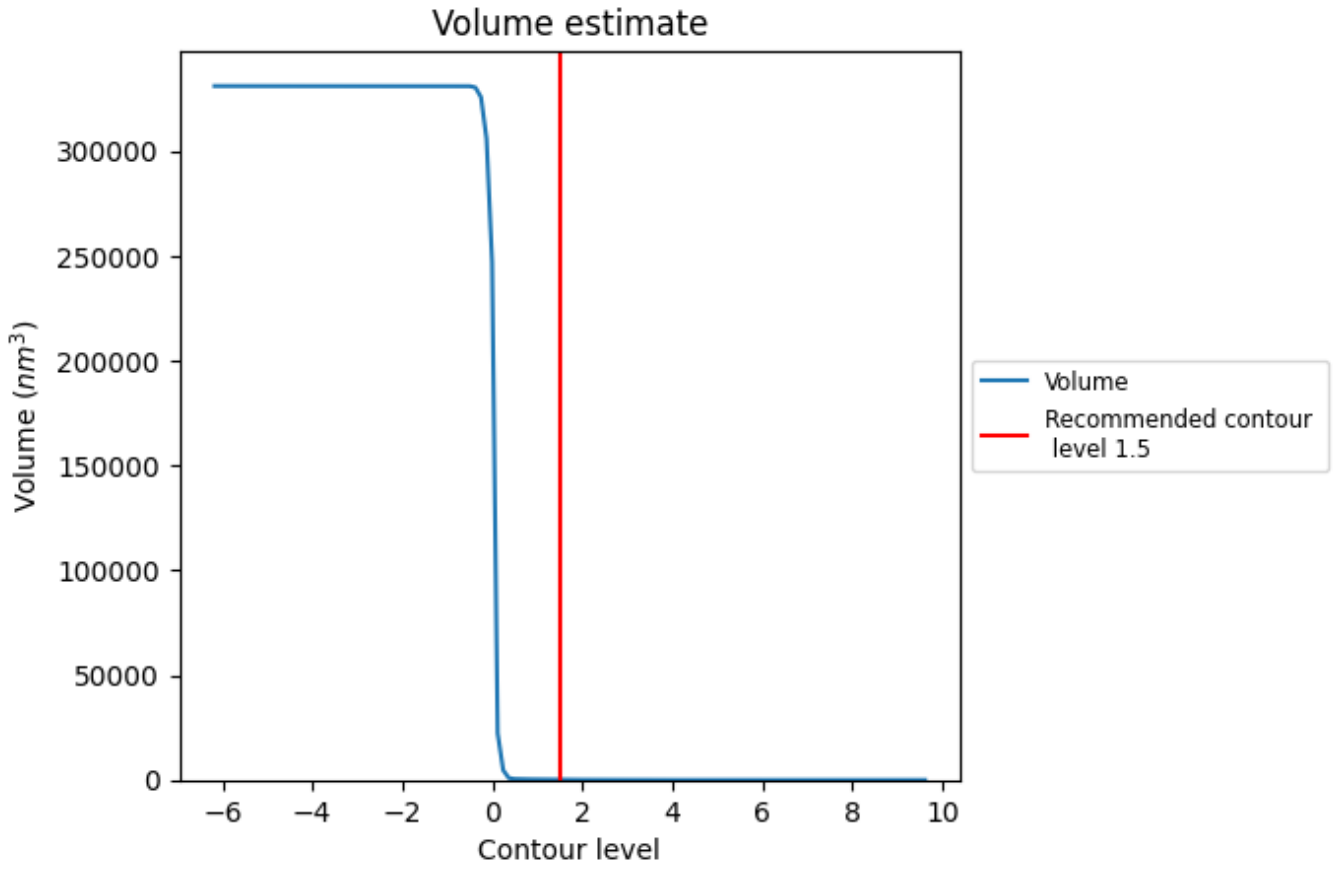
This section contains the results of statistical analysis of the map.

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.

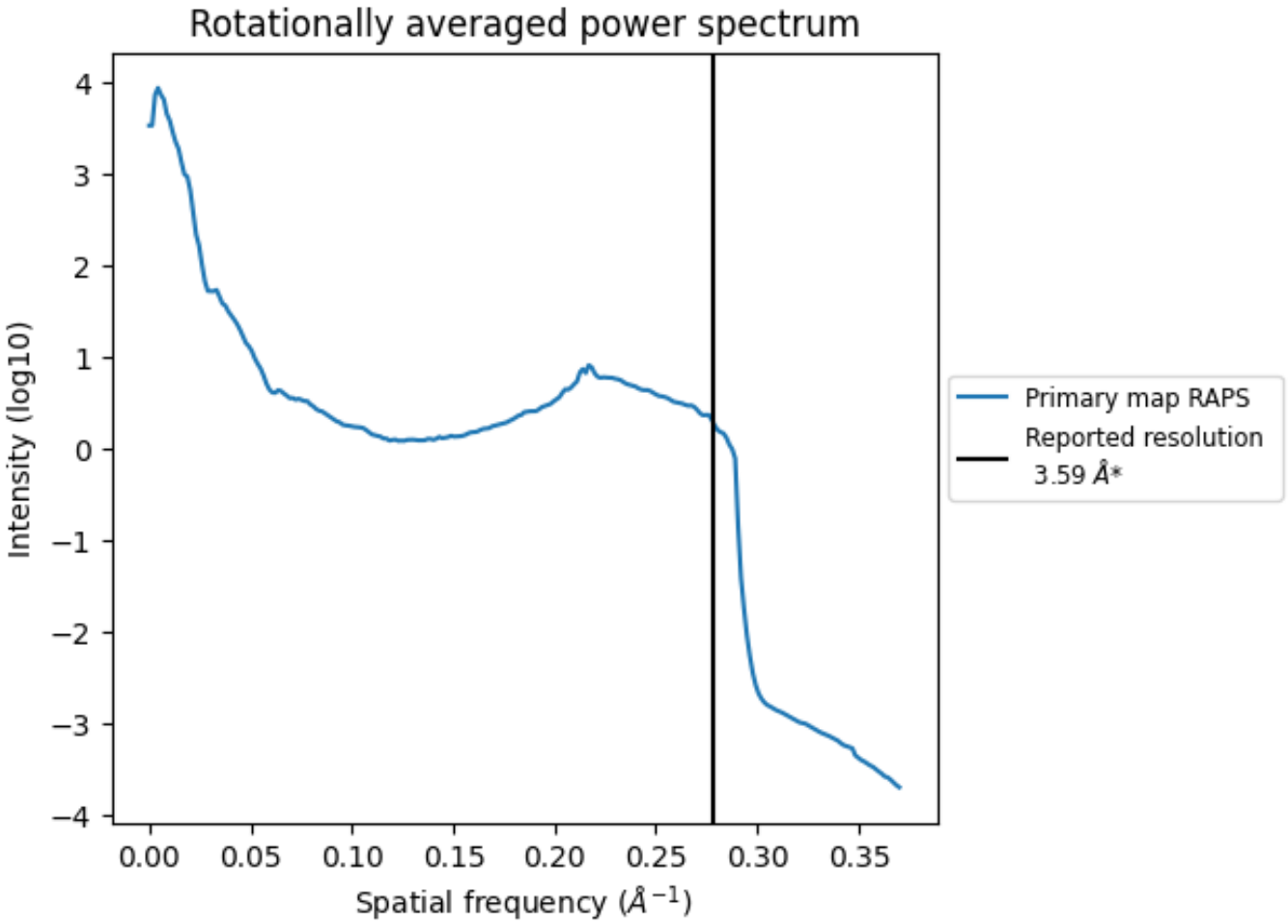
7.2 Volume estimate (i)



The volume at the recommended contour level is 161 nm^3; this corresponds to an approximate mass of 146 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 0.279 Å^{-1}

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

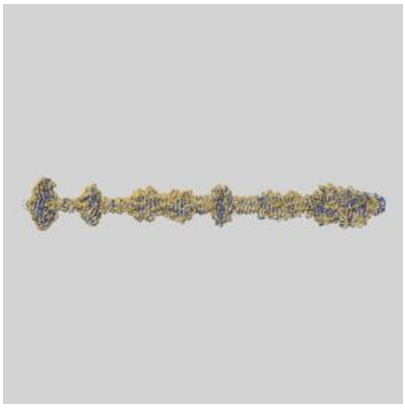
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-55360 and PDB model 9SZ5. Per-residue inclusion information can be found in section 3 on page 4.

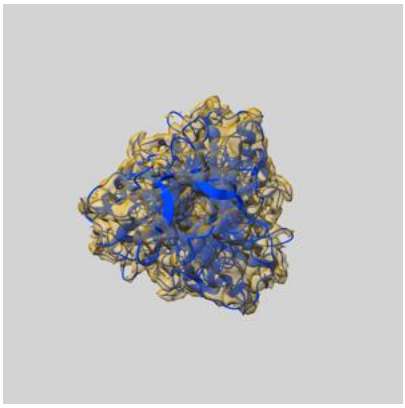
9.1 Map-model overlay



X



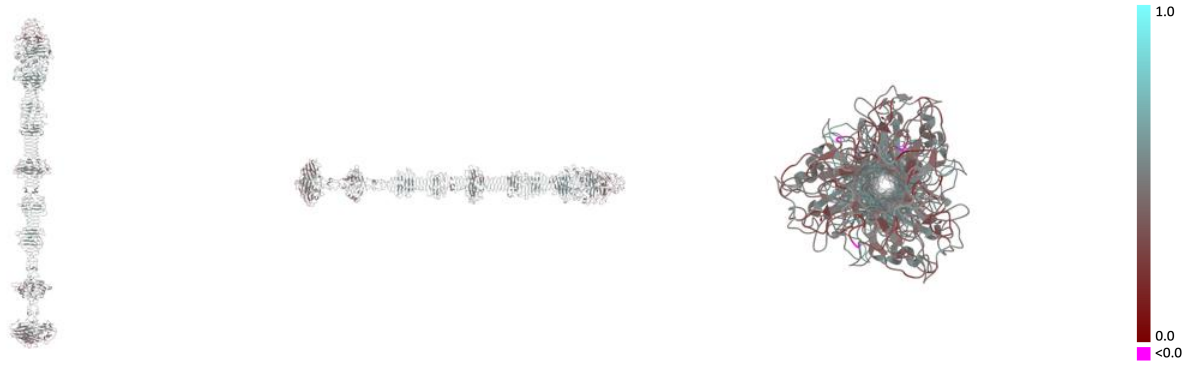
Y



Z

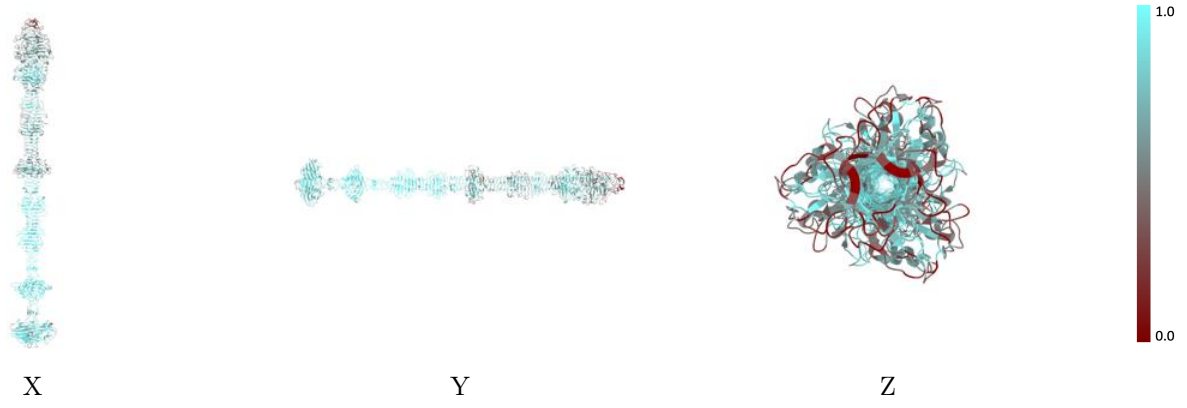
The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



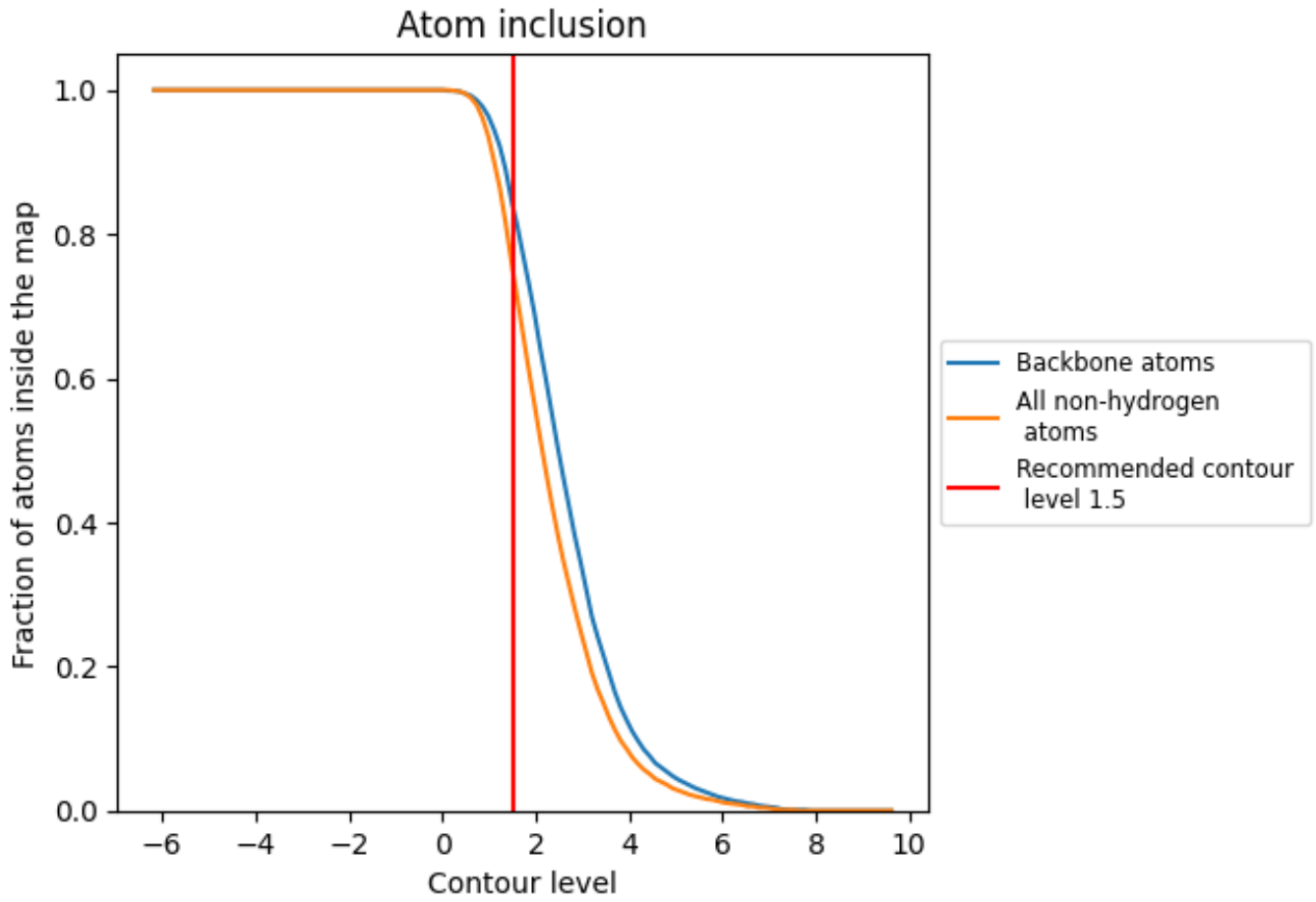
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.5).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 75% 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 (1.5) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.7530	0.4720
A	0.7540	0.4730
B	0.7520	0.4720
C	0.7530	0.4710