wwPDB EM Validation Summary Report (i)

May 18, 2024 – 07:22 pm BST

PDB ID	:	6Z7Q
EMDB ID	:	EMD-11112
Title	:	The atomic structure of the HAdVF-41 penton base in solution
Authors	:	Carlson, L.-A.; Rafie, K.
Deposited on	:	2020-06-01
Resolution	:	3.80 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:

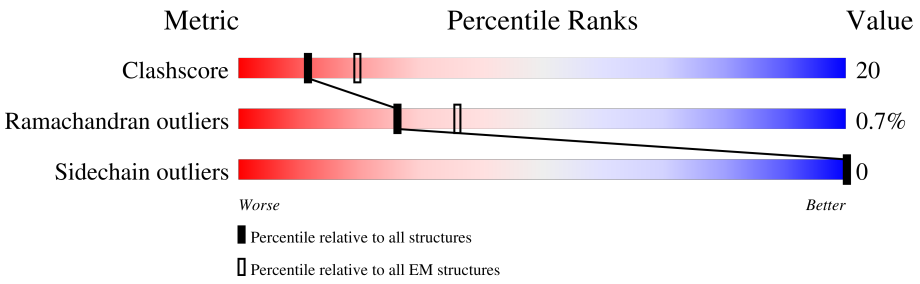
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	508	25% 46% 35% 18%
1	B	508	27% 47% 35% 18%
1	C	508	26% 46% 35% 18%
1	D	508	27% 47% 35% 18%
1	E	508	27% 47% 35% 18%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 16665 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 Penton protein.

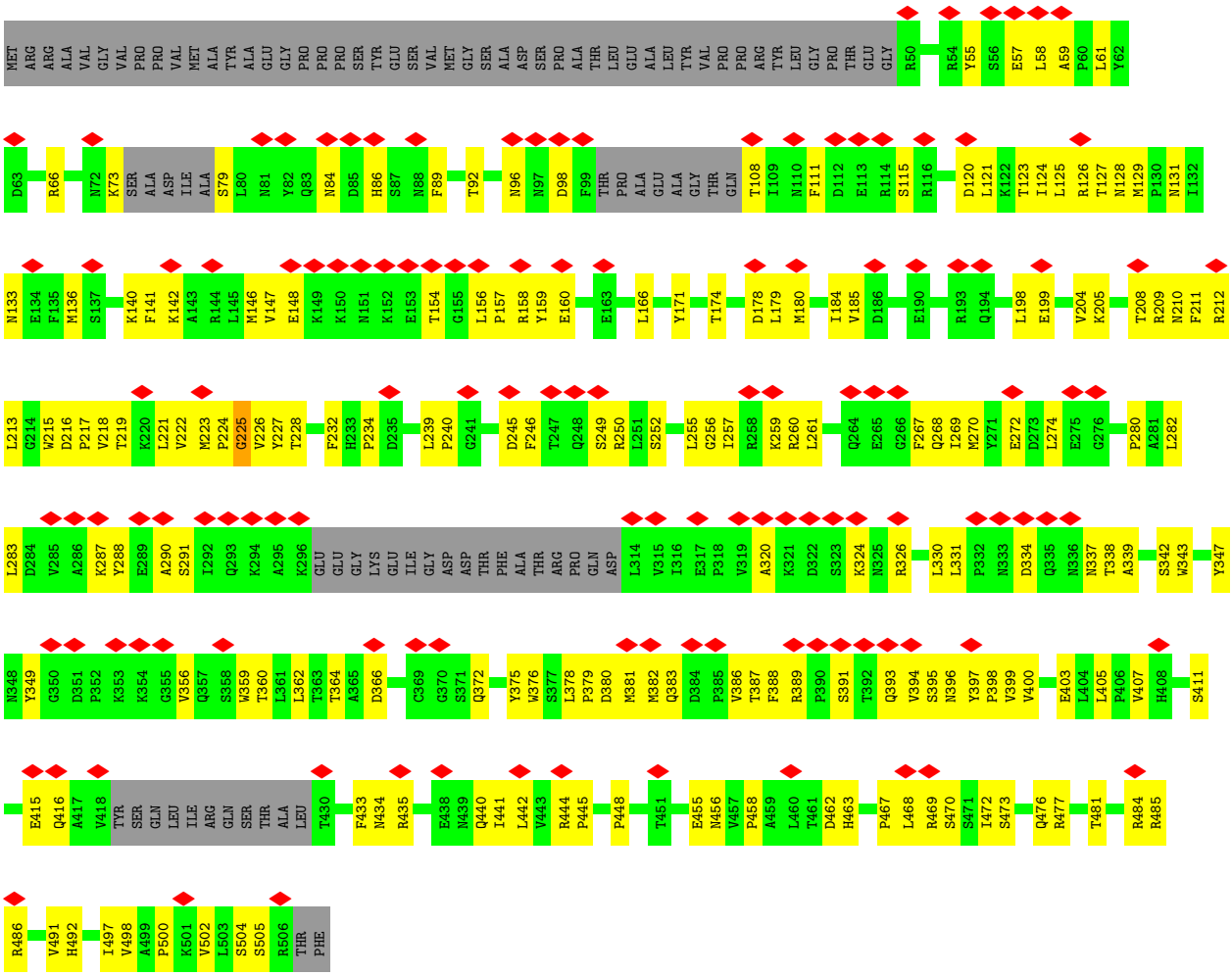
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	416	3333	2115	576	630	12	0	0
1	B	416	3333	2115	576	630	12	0	0
1	C	416	3333	2115	576	630	12	0	0
1	D	416	3333	2115	576	630	12	0	0
1	E	416	3333	2115	576	630	12	0	0

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.

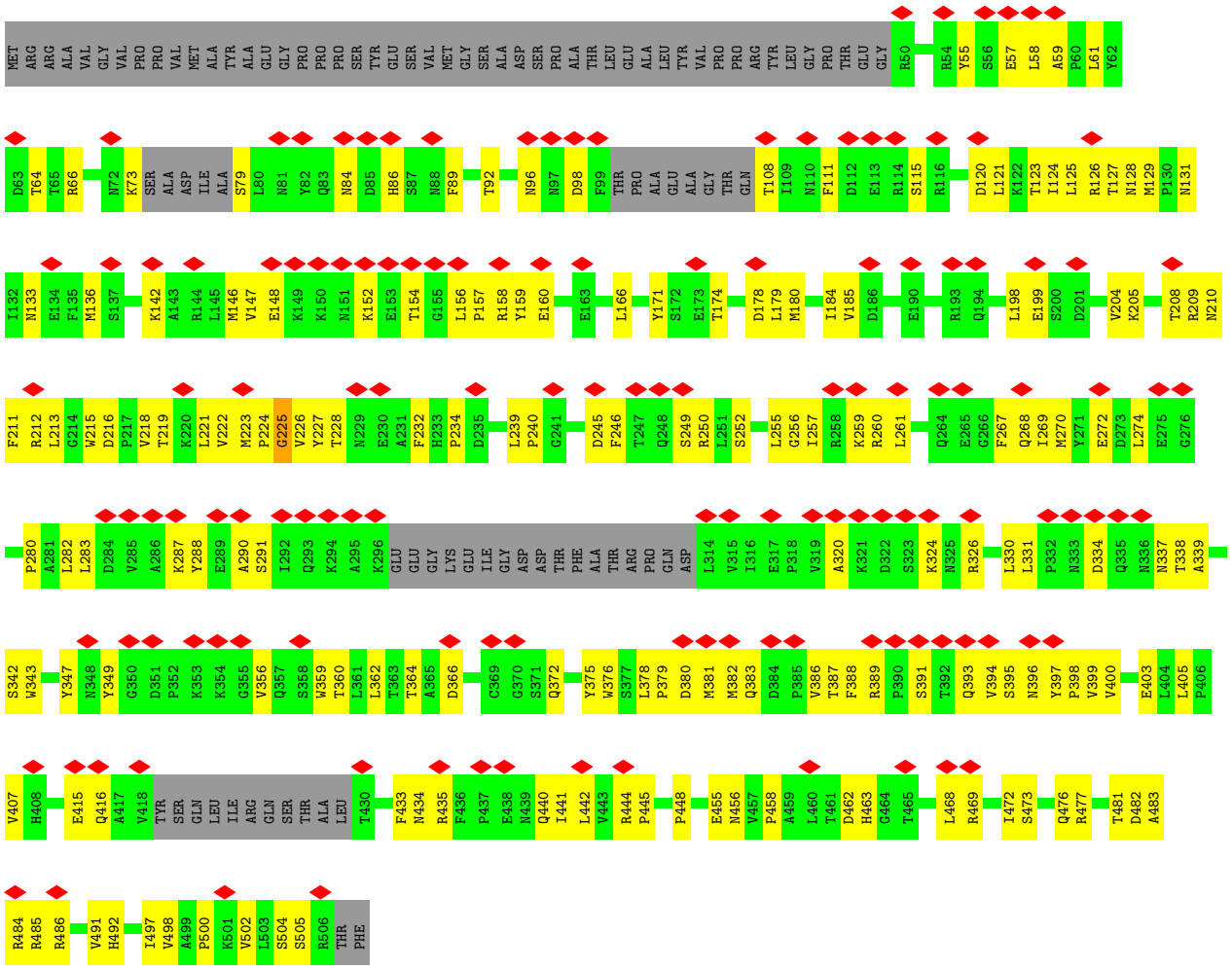
- Molecule 1: Penton protein

Chain A: 25% 46% 35% 18%



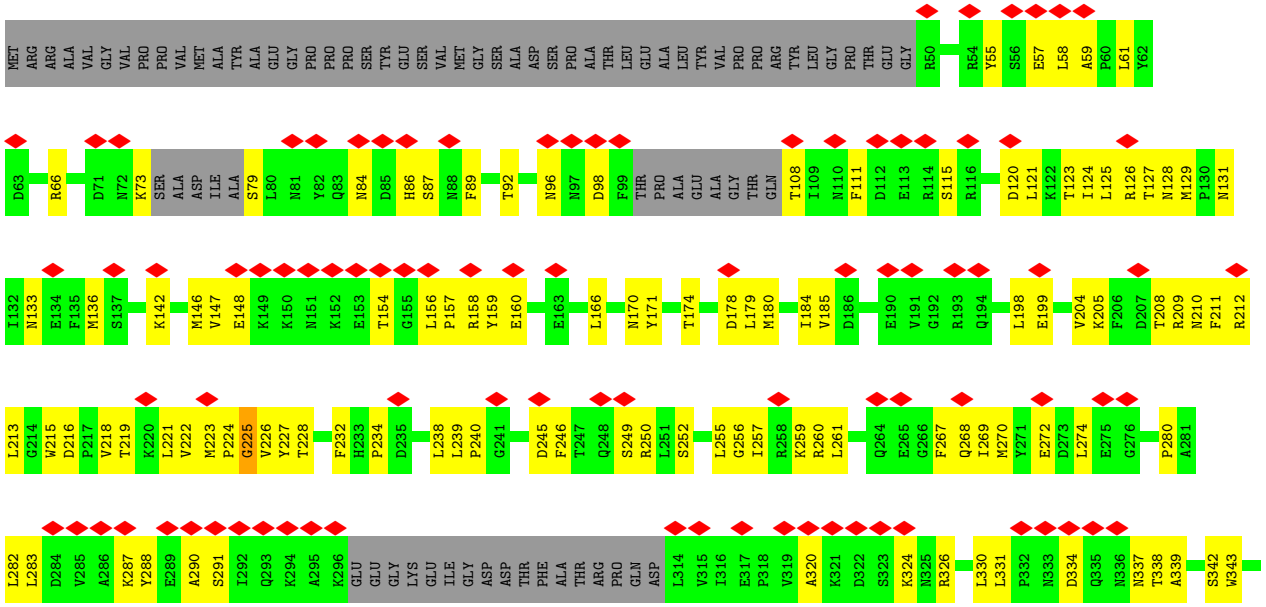
- Molecule 1: Penton protein

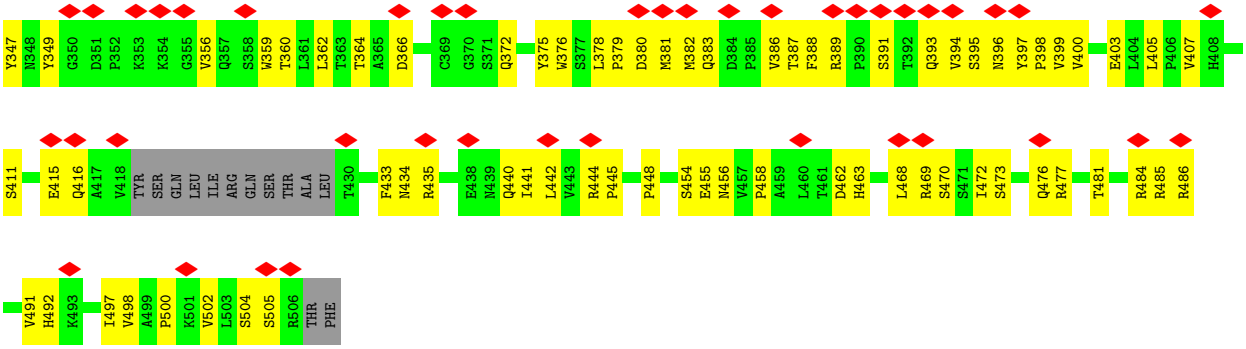
Chain B: 27% 47% 35% 18%



- Molecule 1: Penton protein

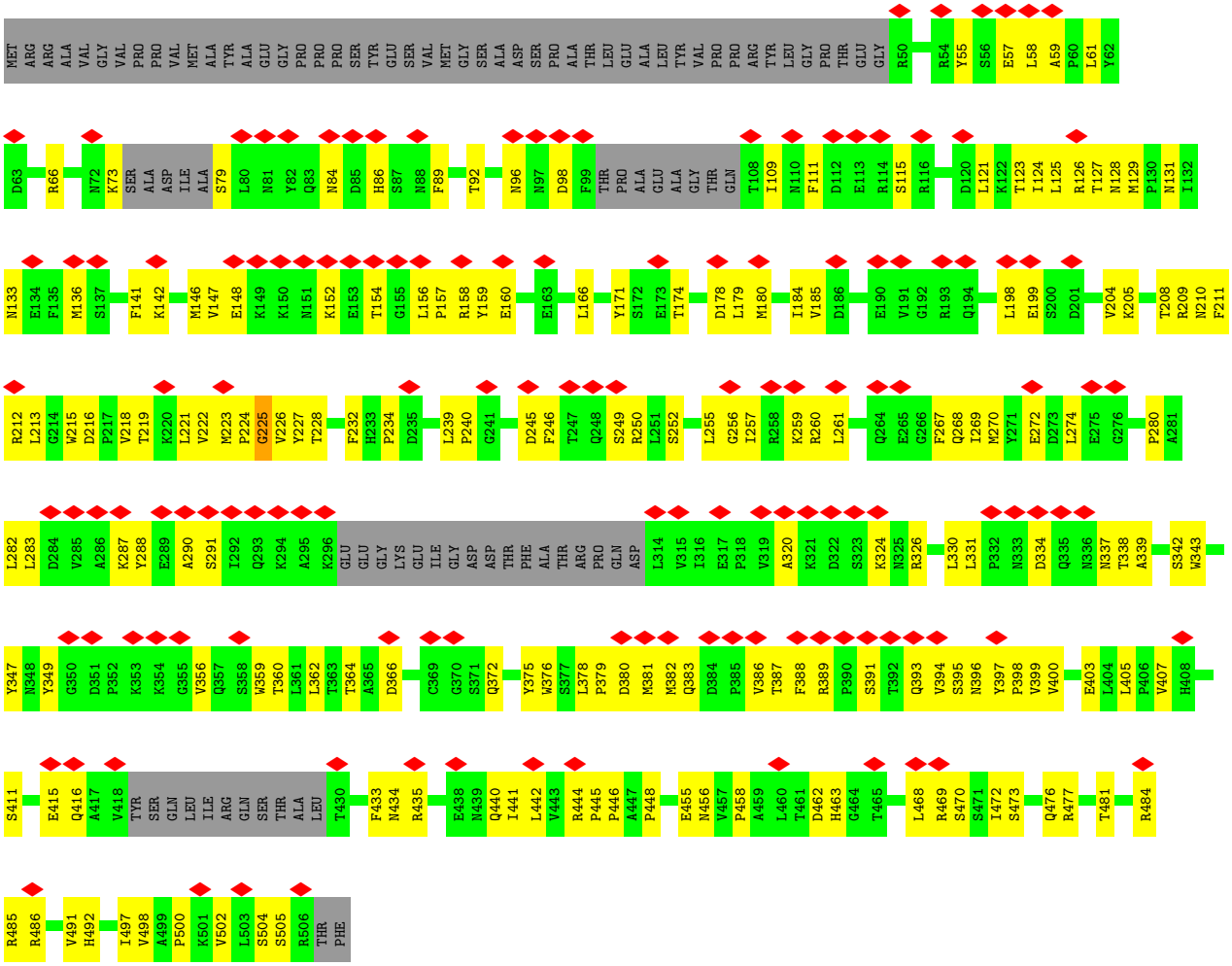
Chain C:





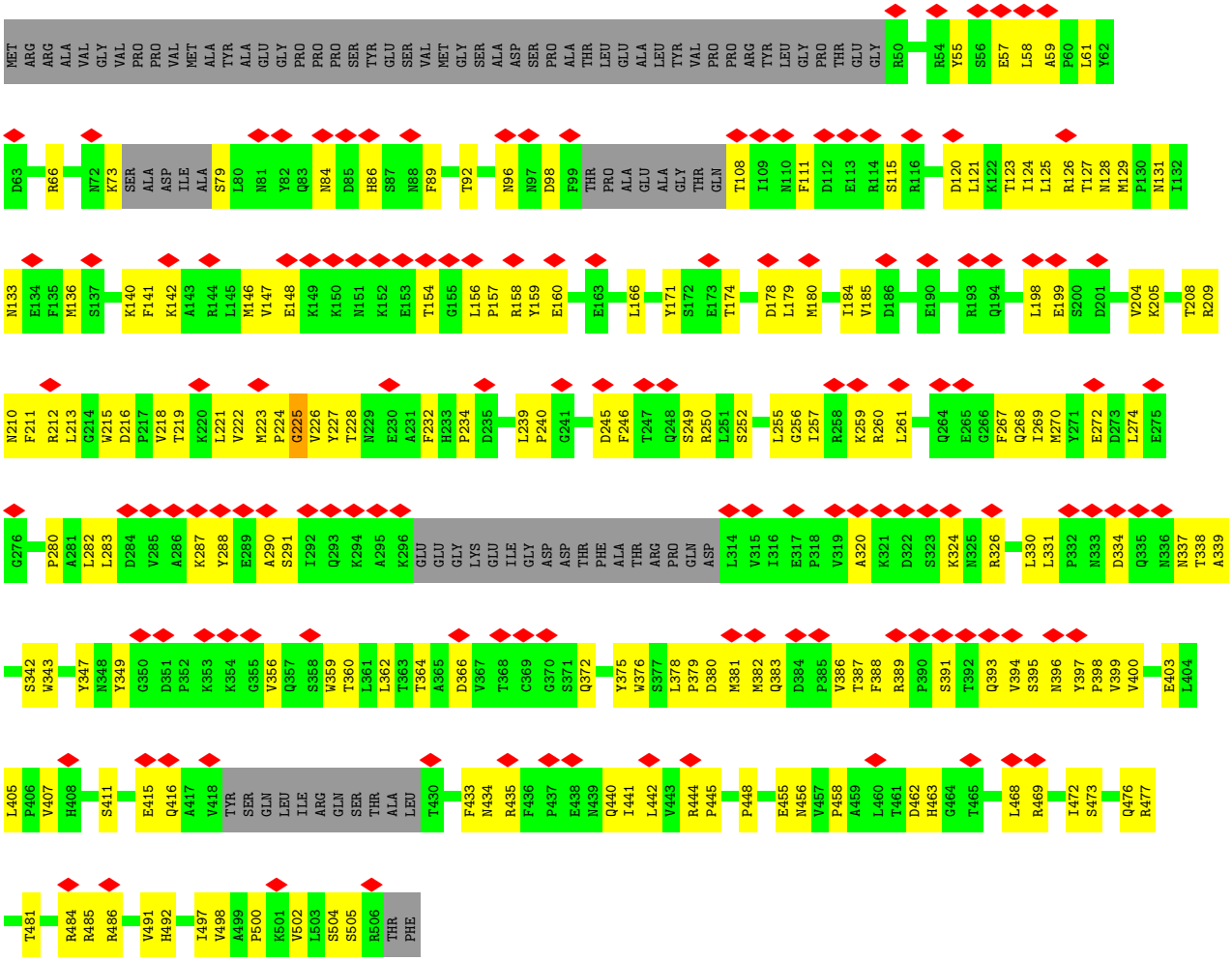
• Molecule 1: Penton protein

Chain D:



• Molecule 1: Penton protein

Chain E:


MET ARG ARG ALA VAL GLY VAL PRO PRO VAL MET ALA TYR ALA GLU GLY PRO PRO PRO SER TYR GLU SER VAL MET GLY SER ALA ASP SER PRO ALA THR LEU GLU GLU ALA LEU TYR VAL PRO PRO ARG TYR LEU GLY PRO THR GLU GLY R50 R54 Y55 S56 E57 L58 A59 P60 L61 Y62
D63 R66 N72 K73 SER ALA ASP ILE ALA S79 L80 N81 Y82 Q83 N84 D85 H86 S87 N88 F89 T92 N96 N97 D98 F99 THR PRO ALA GLU ALA GLY THR GLN T108 I109 N110 F111 D112 E113 R114 S115 R116 D120 L121 K122 T123 I124 L125 R126 T127 N128 M129 P130 N131 I132
N133 E134 F135 M136 S137 K140 F141 K142 A143 R144 L145 M146 V147 E148 K149 K150 N151 K152 E153 T154 G155 L156 P157 R158 Y159 E160 E163 L166 Y171 S172 E173 T174 D178 L179 M180 I184 V185 D186 E190 R193 Q194 L198 E199 S200 D201 V204 K205 T208 R209
N210 F211 R212 L213 G214 W215 D216 P217 V218 T219 K220 L221 V222 M223 P224 G225 V226 Y227 T228 N229 E230 A231 F232 H233 P234 D235 L239 P240 G241 D245 F246 T247 Q248 S249 R250 L251 S252 L255 G256 I257 R258 K259 R260 L261 Q264 E265 G266 F267 Q268 I269 M270 Y271 E272 D273 L274 E275
G276 P280 A281 L282 L283 D284 V285 A286 K287 Y288 E289 A290 S291 I292 Q293 K294 A295 K296 GLU GLU GLY LYS GLU ILE GLY ASP ASP THR PHE ALA THR ARG PRO GLN ASP L314 V315 I316 E317 P318 V319 A320 K321 D322 S323 K324 N325 R326 L330 L331 P332 N333 D334 Q335 N336 N337 T338 A339
S342 W343 Y347 N348 Y349 G350 D351 P352 K353 K354 G355 V356 Q357 S358 W359 T360 L361 L362 T363 T364 A365 D366 V367 T368 C369 G370 S371 Q372 Y375 W376 S377 L378 P379 D380 M381 M382 Q383 D384 P385 V386 T387 F388 R389 P390 S391 T392 Q393 V394 S395 N396 Y397 P398 V399 V400 E403 L404
L405 P406 V407 H408 S411 E415 Q416 A417 V418 TYR SER GLN LEU ILE ARG GLN SER THR ALA LEU T430 F433 N434 R435 F436 P437 E438 N439 Q440 I441 L442 V443 R444 P445 P448 E455 N456 V457 P458 A459 L460 T461 D462 H463 G464 T465 L468 R469 I472 S473 Q476 R477
T481 R484 R485 R486 V491 H492 I497 V498 A499 P500 K501 V502 L503 S504 S505 R506 THR PHE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	107110	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; per-micrograph CTF correction as well the initial per-particle CTF correction before 2D classification were performed in GCTF. Later per-particle CTF-refinement were performed in RELION 3.1-beta.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	0.93	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	16.641	Depositor
Minimum map value	-10.825	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.975	Depositor
Recommended contour level	5.0	Depositor
Map size (Å)	179.052, 179.052, 179.052	wwPDB
Map dimensions	172, 172, 172	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.041, 1.041, 1.041	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.34	0/3408	0.48	0/4635
1	B	0.34	0/3408	0.48	0/4635
1	C	0.35	0/3408	0.48	0/4635
1	D	0.34	0/3408	0.48	0/4635
1	E	0.34	0/3408	0.48	0/4635
All	All	0.34	0/17040	0.48	0/23175

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 (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	3333	0	3282	136	0
1	B	3333	0	3282	134	0
1	C	3333	0	3282	140	0
1	D	3333	0	3282	138	0
1	E	3333	0	3282	137	0
All	All	16665	0	16410	661	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 20.

The worst 5 of 661 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:213:LEU:HD12	1:A:228:THR:HG21	1.56	0.87
1:D:213:LEU:HD12	1:D:228:THR:HG21	1.56	0.87
1:C:213:LEU:HD12	1:C:228:THR:HG21	1.56	0.86
1:B:213:LEU:HD12	1:B:228:THR:HG21	1.56	0.85
1:E:213:LEU:HD12	1:E:228:THR:HG21	1.56	0.85

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	406/508 (80%)	287 (71%)	116 (29%)	3 (1%)	22	60
1	B	406/508 (80%)	287 (71%)	116 (29%)	3 (1%)	22	60
1	C	406/508 (80%)	287 (71%)	116 (29%)	3 (1%)	22	60
1	D	406/508 (80%)	287 (71%)	116 (29%)	3 (1%)	22	60
1	E	406/508 (80%)	287 (71%)	116 (29%)	3 (1%)	22	60
All	All	2030/2540 (80%)	1435 (71%)	580 (29%)	15 (1%)	26	60

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	383	GLN
1	B	383	GLN
1	C	383	GLN
1	D	383	GLN
1	E	383	GLN

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	374/447 (84%)	374 (100%)	0	100	100
1	B	374/447 (84%)	374 (100%)	0	100	100
1	C	374/447 (84%)	374 (100%)	0	100	100
1	D	374/447 (84%)	374 (100%)	0	100	100
1	E	374/447 (84%)	374 (100%)	0	100	100
All	All	1870/2235 (84%)	1870 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	ASN
1	B	133	ASN
1	C	133	ASN
1	D	133	ASN
1	E	133	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

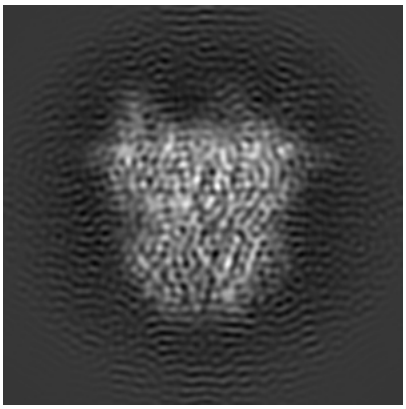
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11112. 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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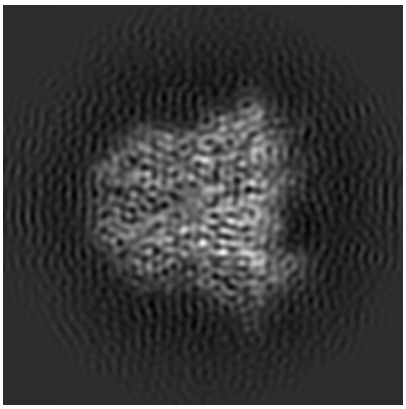
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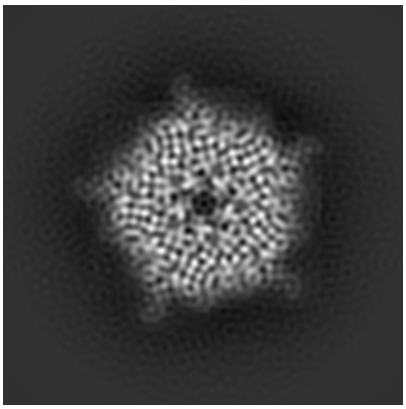
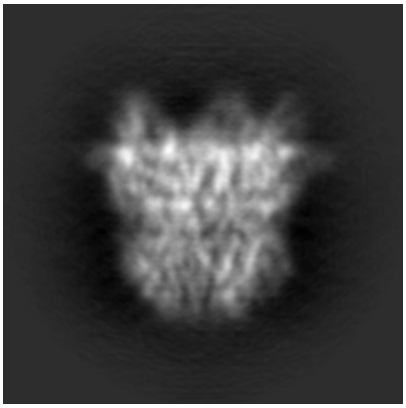

Z

6.1.2 Raw map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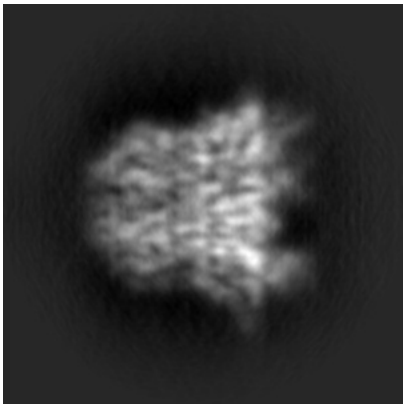
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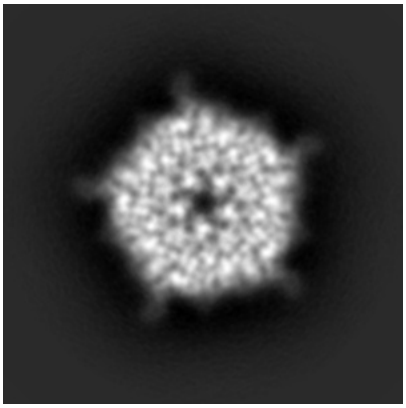
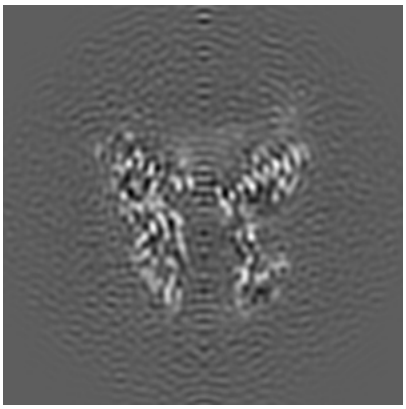

Z

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

6.2 Central slices (i)

6.2.1 Primary map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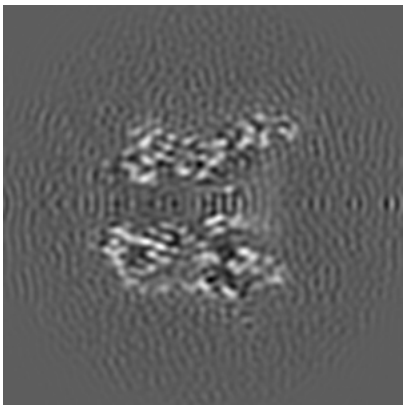
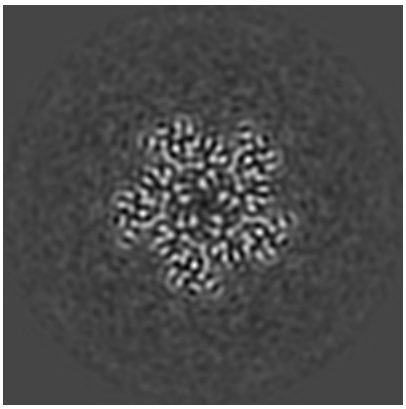

Y Index: 86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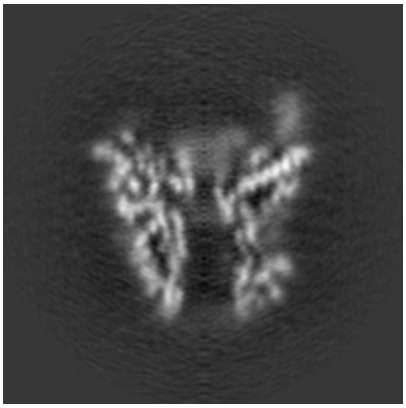
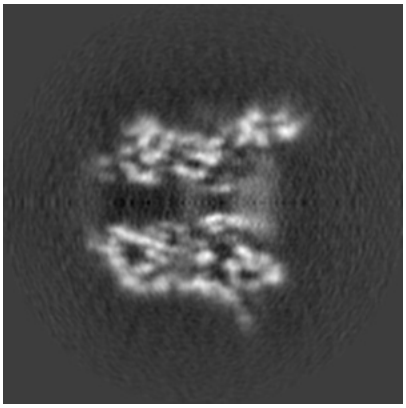
6.2.2 Raw map


X Index: 86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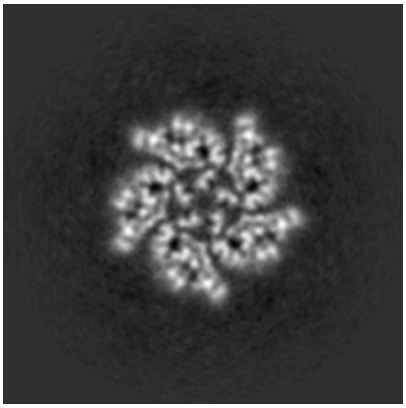
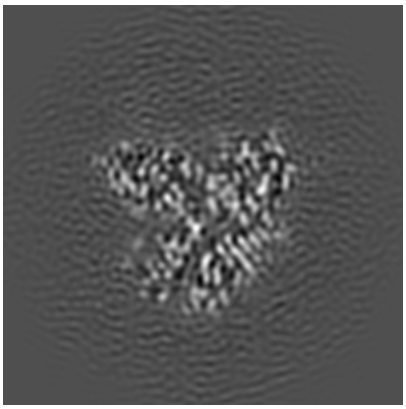
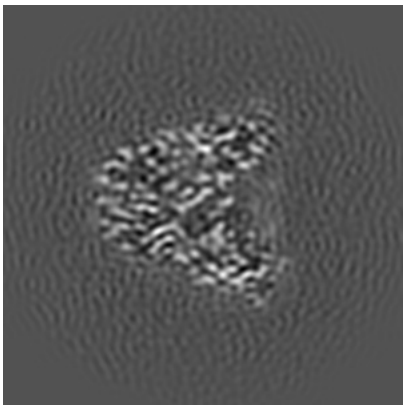

Z Index: 86

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: 70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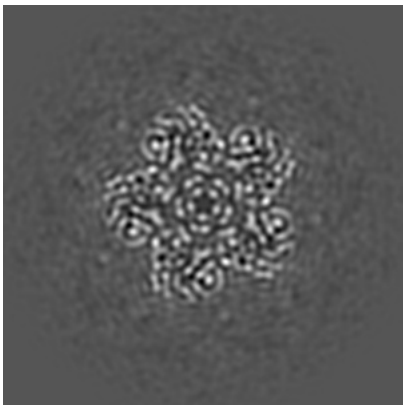
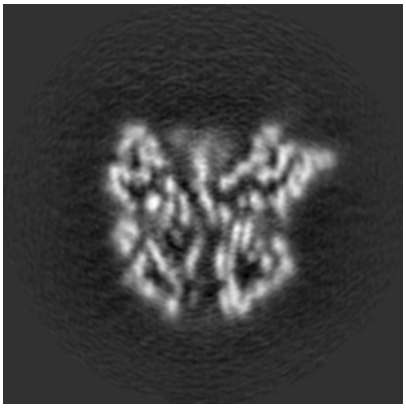
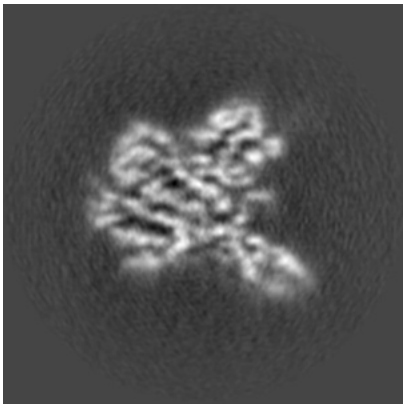

Z Index: 94

6.3.2 Raw map


X Index: 78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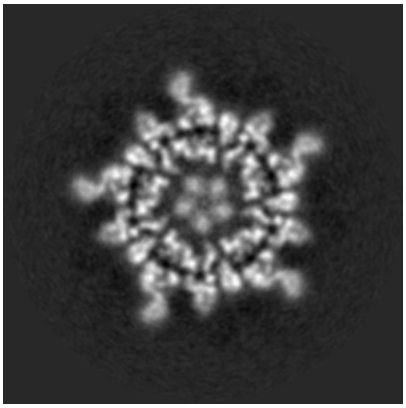
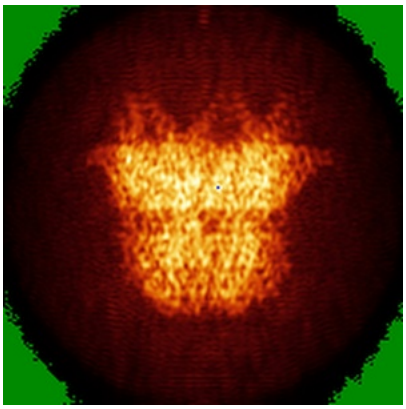
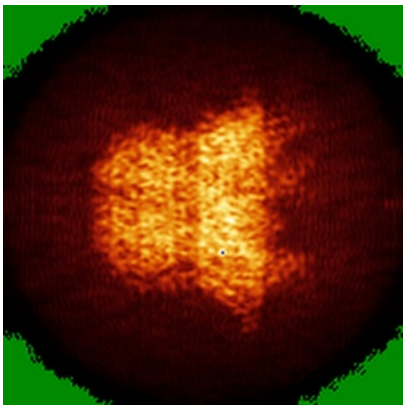

Z Index: 106

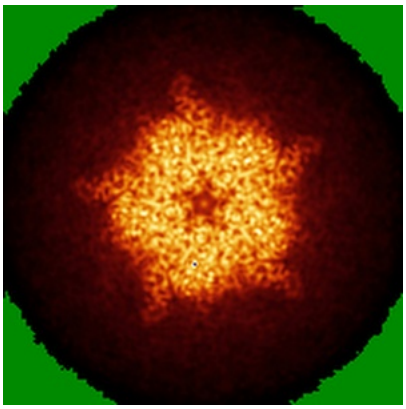
The images above show the largest variance slices of the map in three orthogonal directions.

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

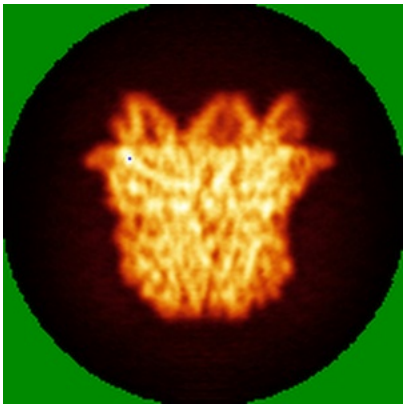
6.4.1 Primary map

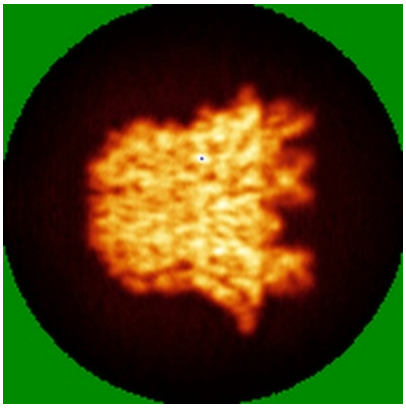

X

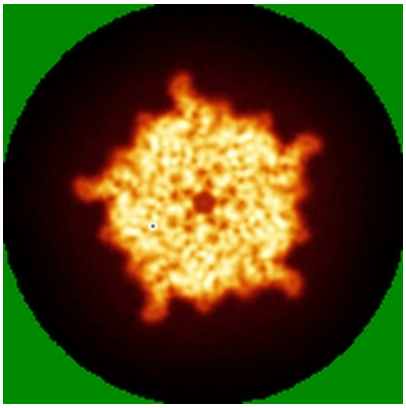

Y


Z

6.4.2 Raw map


X

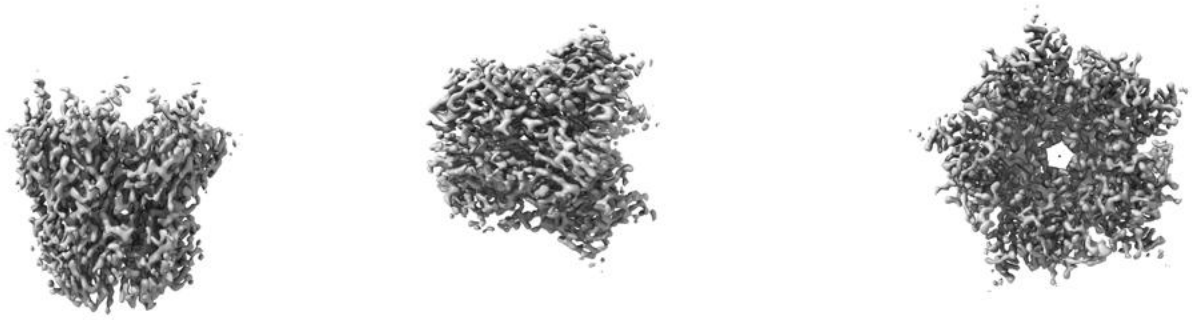

Y


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)

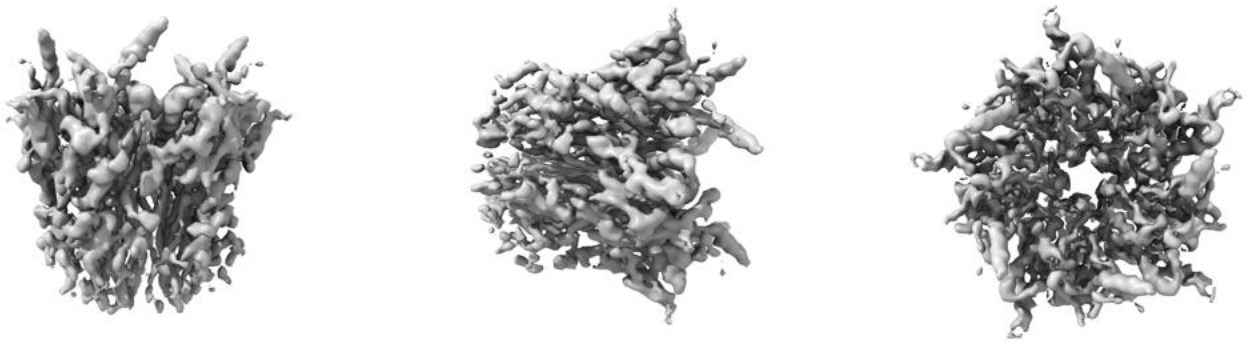
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 5.0. 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.

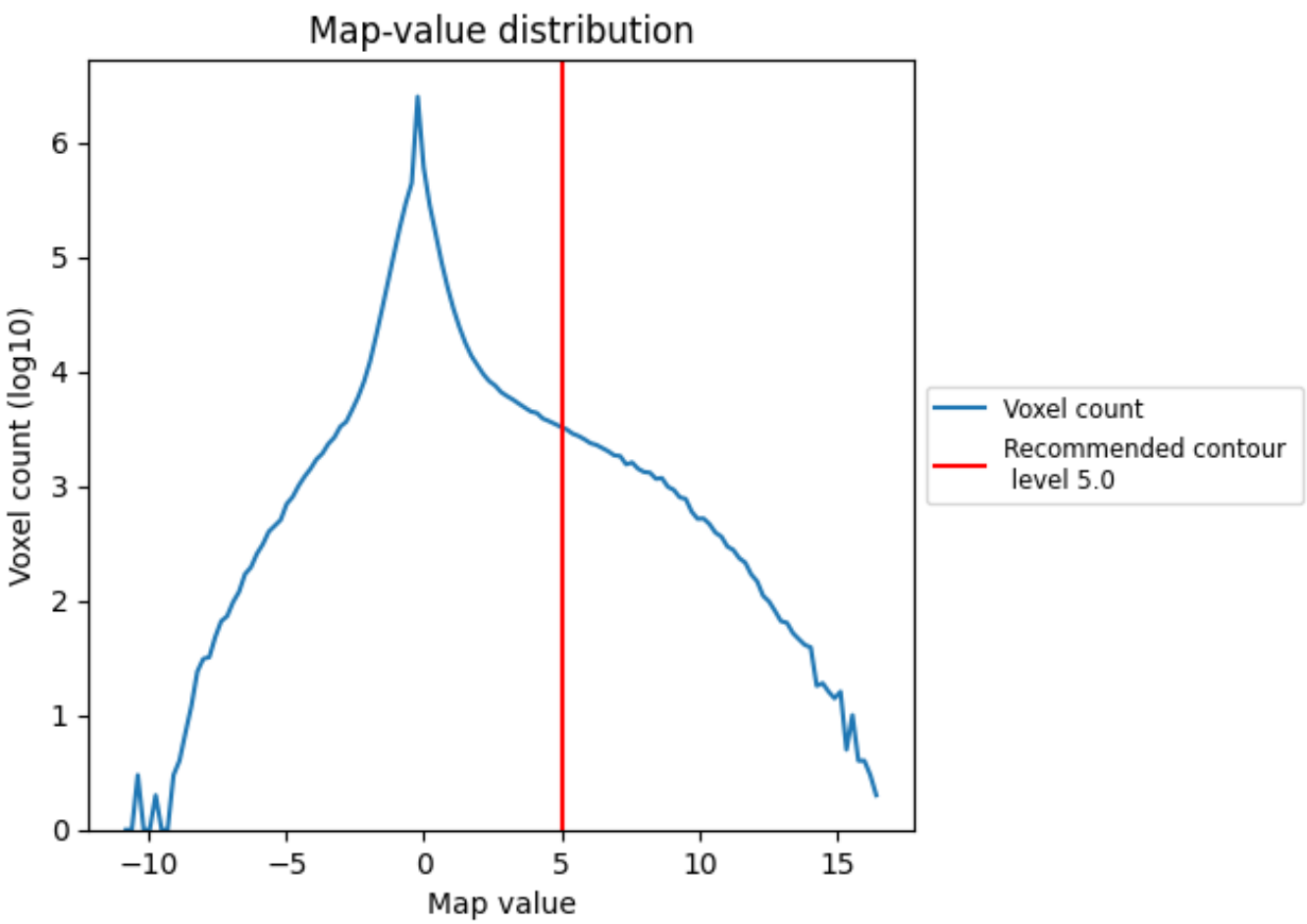
6.6 Mask visualisation (i)

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

7 Map analysis (i)

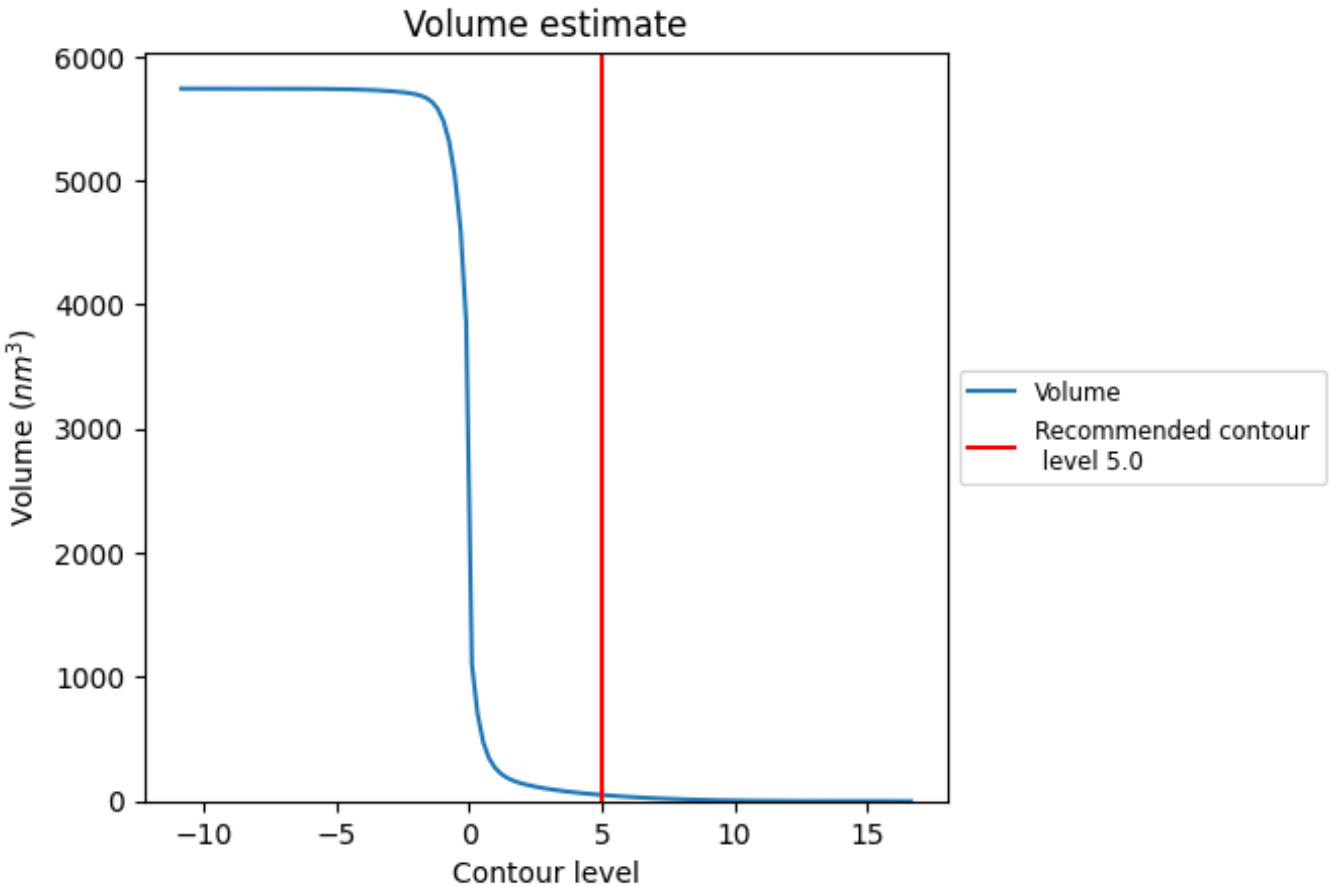
This section contains the results of statistical analysis of the map.

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.

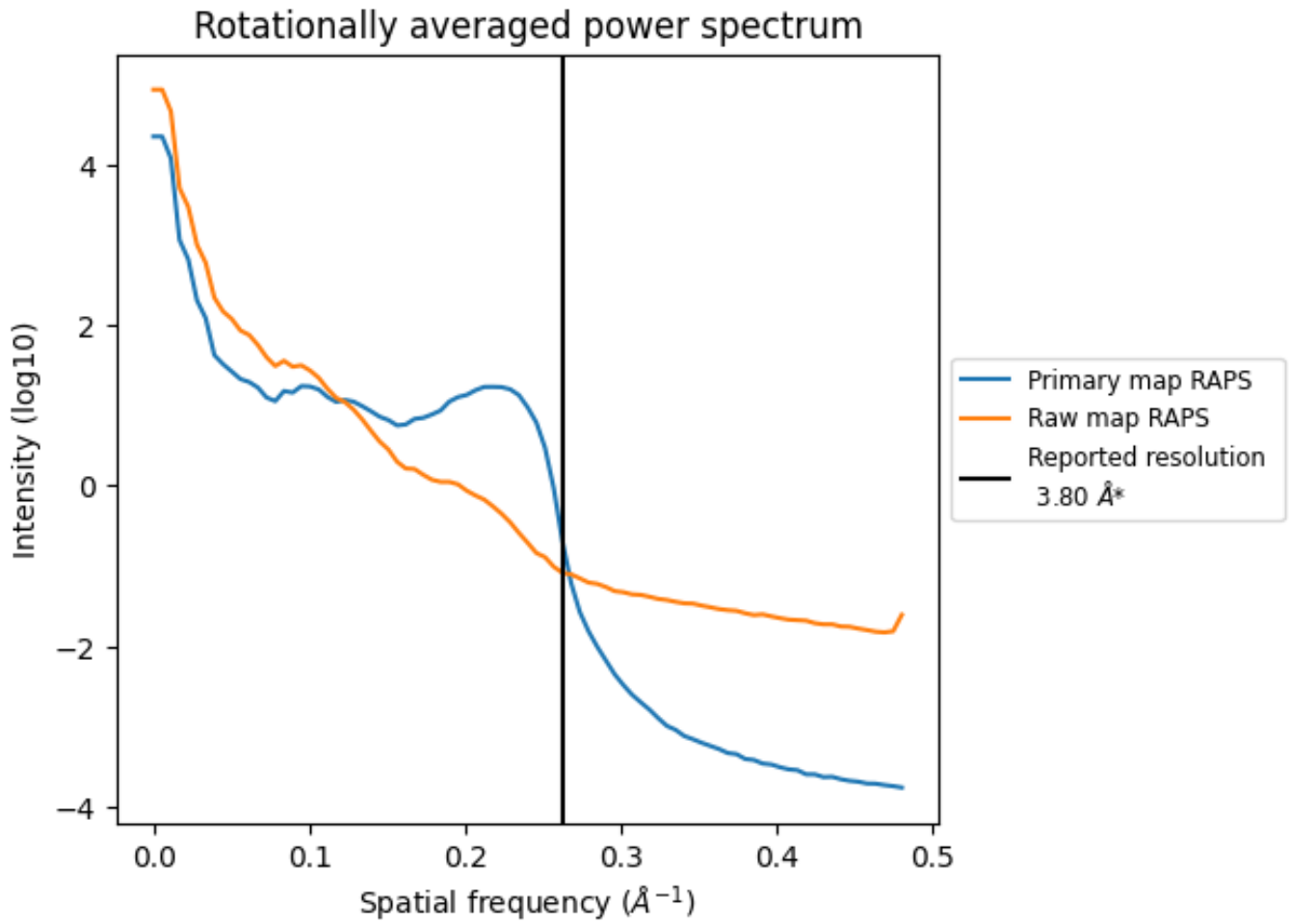
7.2 Volume estimate (i)



The volume at the recommended contour level is 50 nm^3; this corresponds to an approximate mass of 45 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)

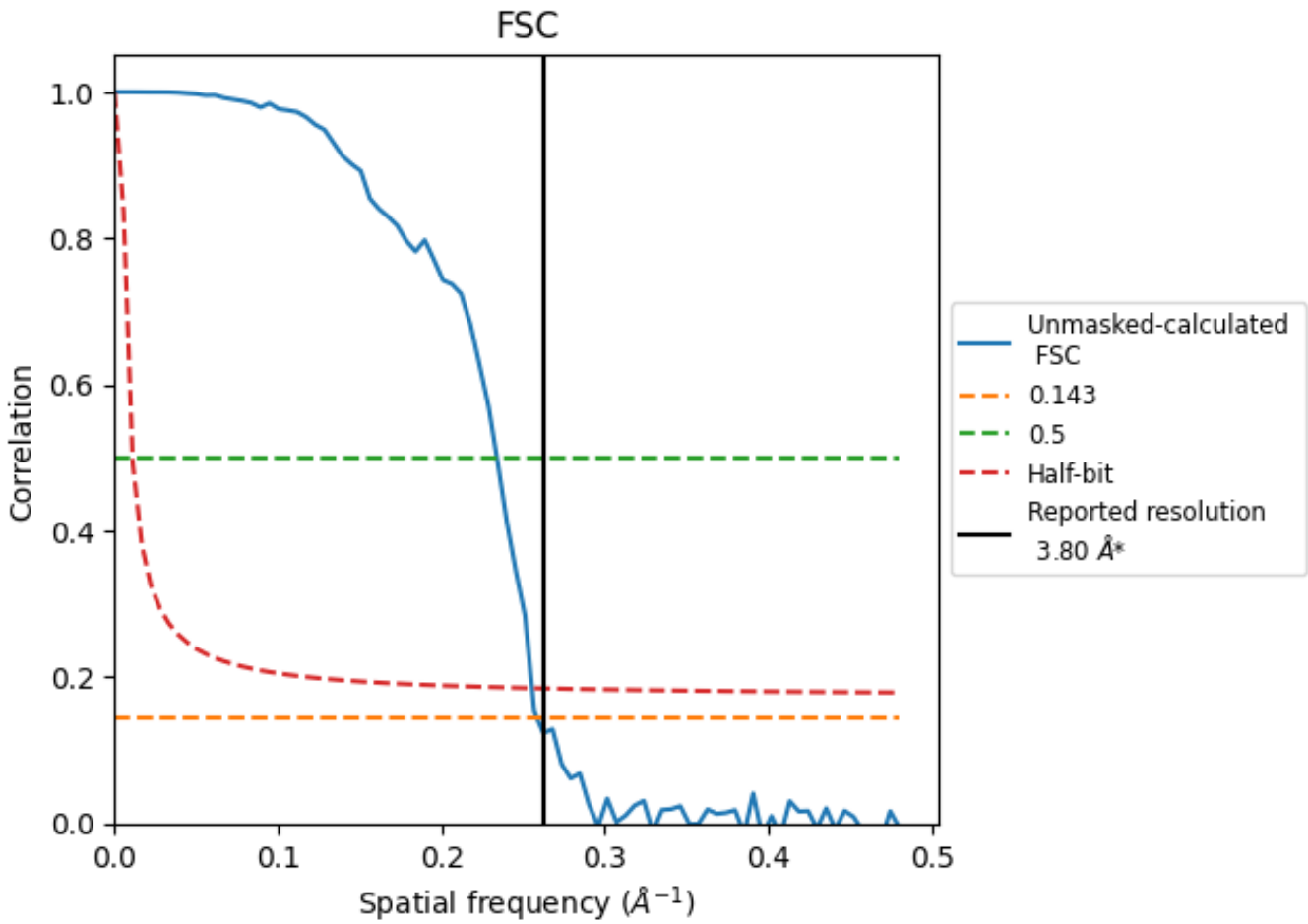


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

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 0.263 Å^{-1}

8.2 Resolution estimates (i)

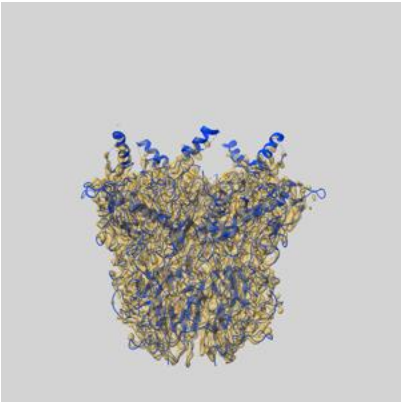
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.87	4.27	3.91

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

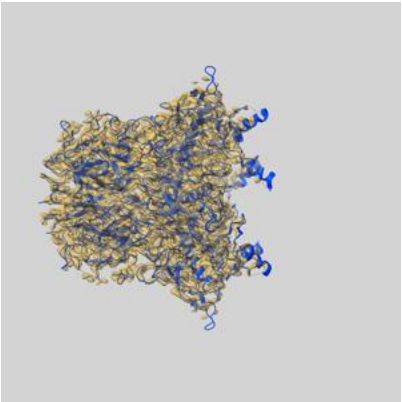
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11112 and PDB model 6Z7Q. Per-residue inclusion information can be found in section 3 on page 4.

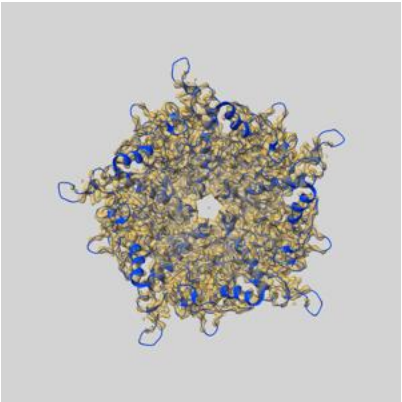
9.1 Map-model overlay (i)



X



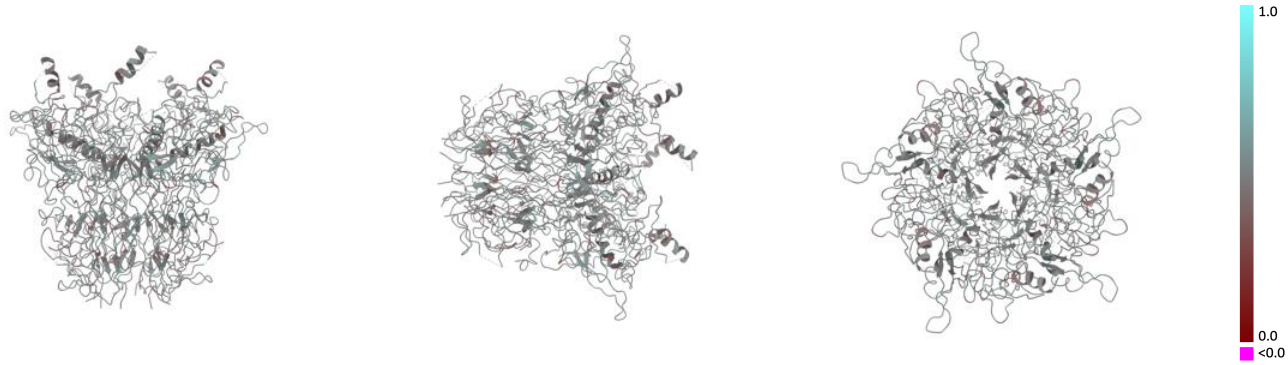
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.0 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.

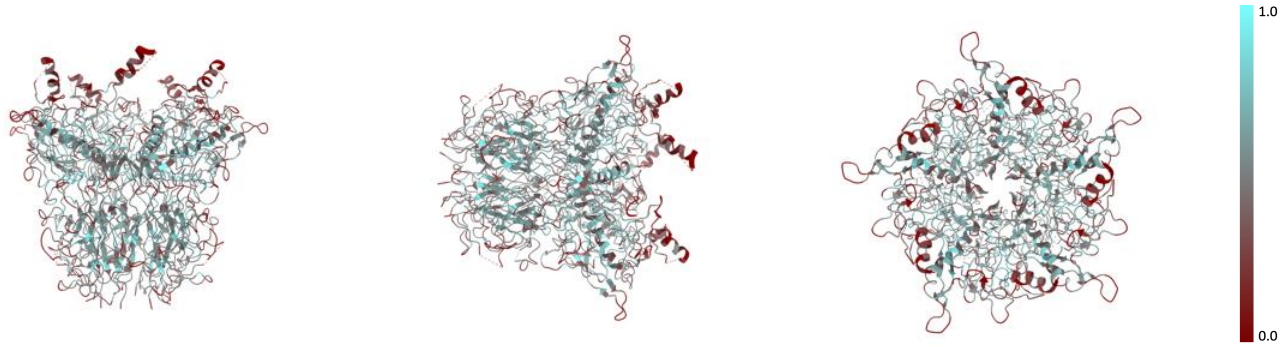
9.2 Q-score mapped to coordinate model (i)



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.

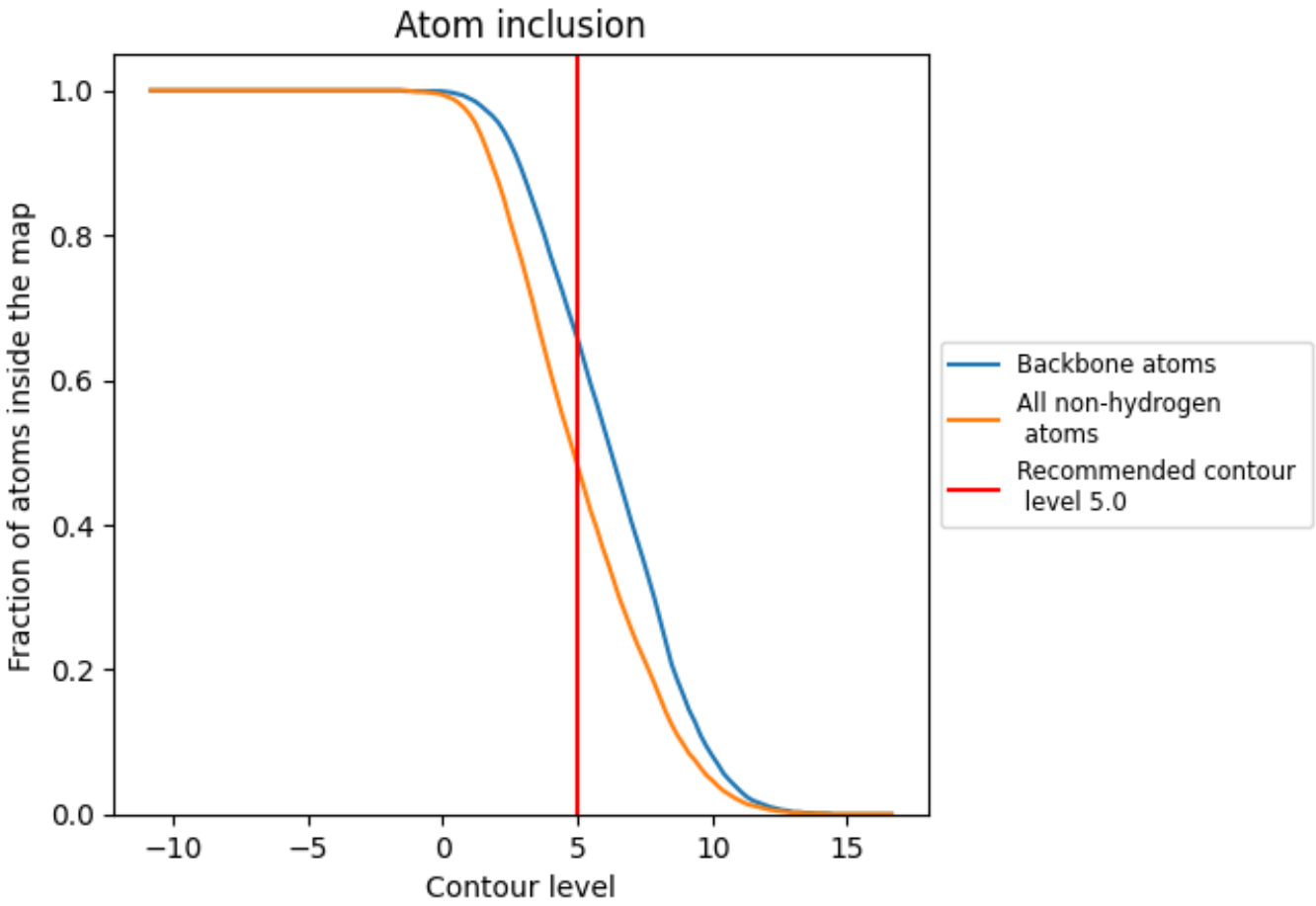
9.3 Atom inclusion mapped to coordinate model (i)



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 (5.0).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 48% 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 (5.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4810	0.4860
A	0.4790	0.4850
B	0.4860	0.4870
C	0.4800	0.4870
D	0.4790	0.4860
E	0.4820	0.4860