



wwPDB EM Validation Summary Report ⓘ

May 12, 2025 – 08:00 PM EDT

PDB ID : 8EAP / pdb_00008eap
EMDB ID : EMD-27790
Title : Cryo-EM structure of the in-situ gp10-gp26 from bacteriophage P22
Authors : Wang, C.; Liu, J.; Molineux, I.J.
Deposited on : 2022-08-29
Resolution : 3.30 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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

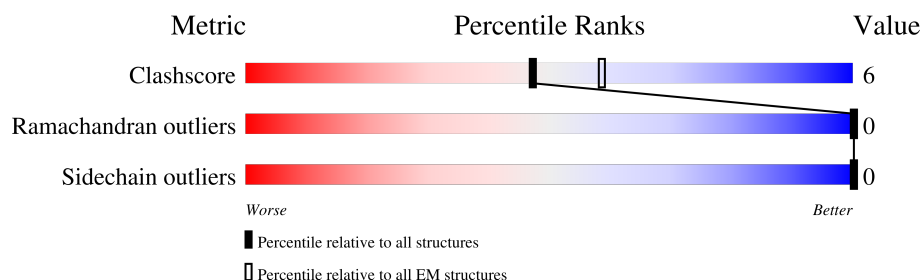
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

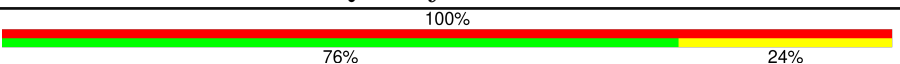
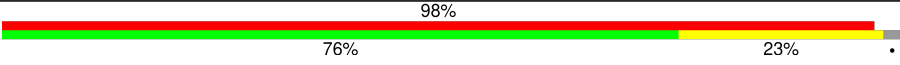
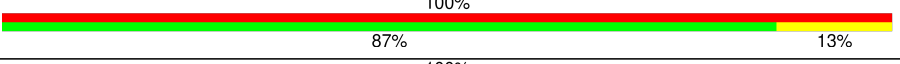

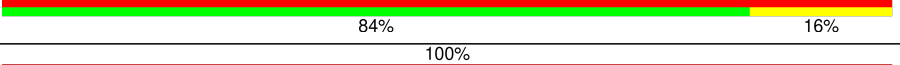

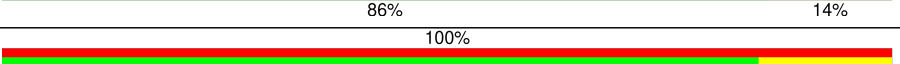
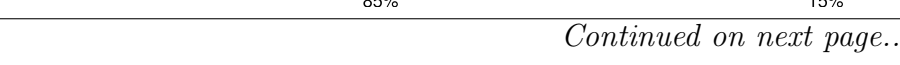
The reported resolution of this entry is 3.30 Å.

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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$. 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	62	
1	B	62	
1	C	62	
2	D	471	
2	E	471	
2	F	471	
2	G	471	
2	H	471	

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Mol	Chain	Length	Quality of chain
2	I	471	<div><div></div><div>100%</div><div>86%</div><div>14%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23485 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 Tail needle protein gp26.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	B	61	Total	C	N	O	0	0
			451	283	79	89		
1	A	62	Total	C	N	O	0	0
			459	287	80	92		
1	C	62	Total	C	N	O	0	0
			459	287	80	92		

- Molecule 2 is a protein called Packaged DNA stabilization protein gp10.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	471	Total	C	N	O	S	0	0
			3686	2326	631	711	18		
2	H	471	Total	C	N	O	S	0	0
			3686	2326	631	711	18		
2	I	471	Total	C	N	O	S	0	0
			3686	2326	631	711	18		
2	E	471	Total	C	N	O	S	0	0
			3686	2326	631	711	18		
2	D	471	Total	C	N	O	S	0	0
			3686	2326	631	711	18		
2	F	471	Total	C	N	O	S	0	0
			3686	2326	631	711	18		

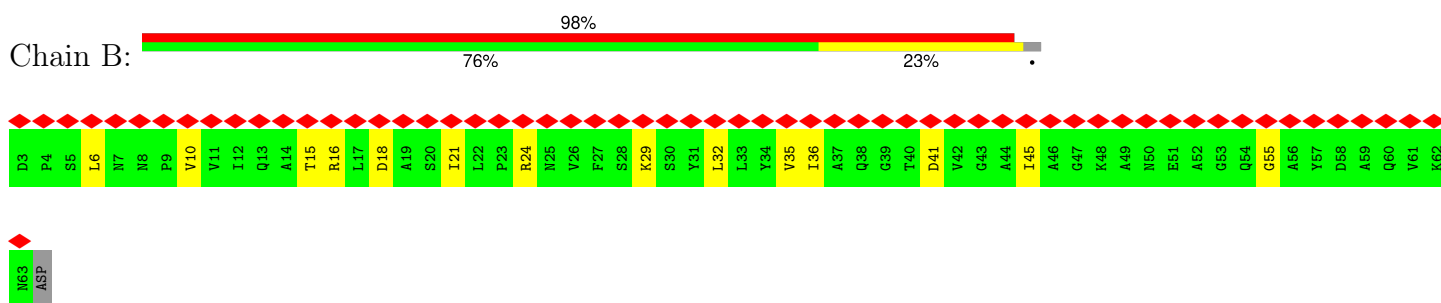
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	233	SER	GLY	conflict	UNP P26749
H	233	SER	GLY	conflict	UNP P26749
I	233	SER	GLY	conflict	UNP P26749
E	233	SER	GLY	conflict	UNP P26749
D	233	SER	GLY	conflict	UNP P26749
F	233	SER	GLY	conflict	UNP P26749

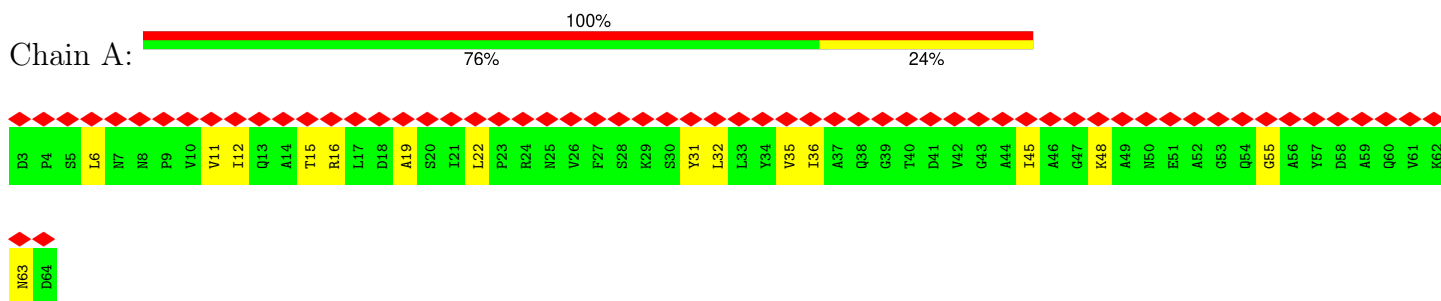
3 Residue-property plots

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.

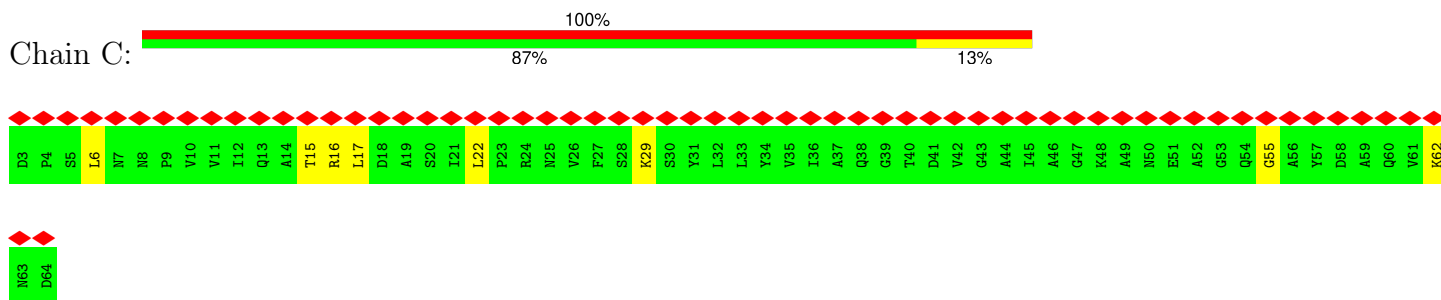
- Molecule 1: Tail needle protein gp26



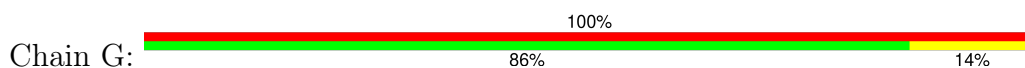
- Molecule 1: Tail needle protein gp26

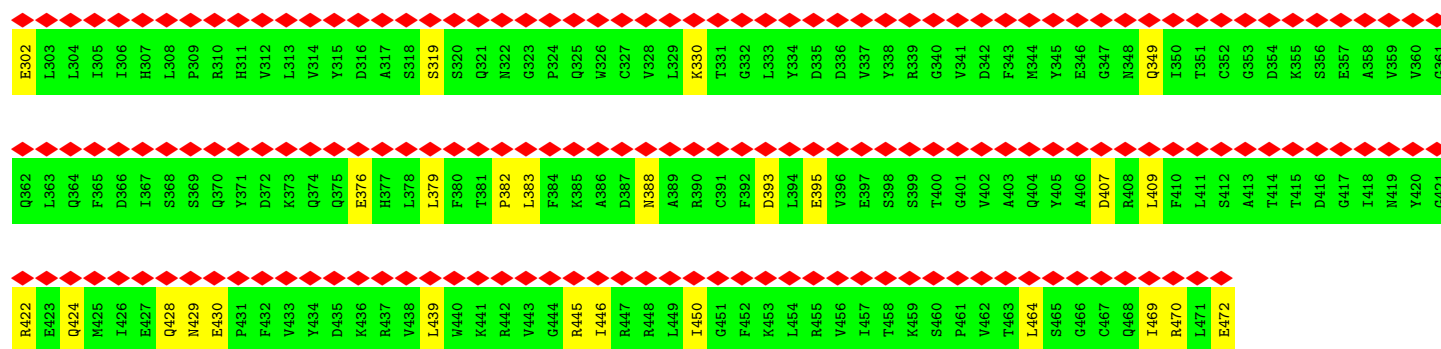


- Molecule 1: Tail needle protein gp26

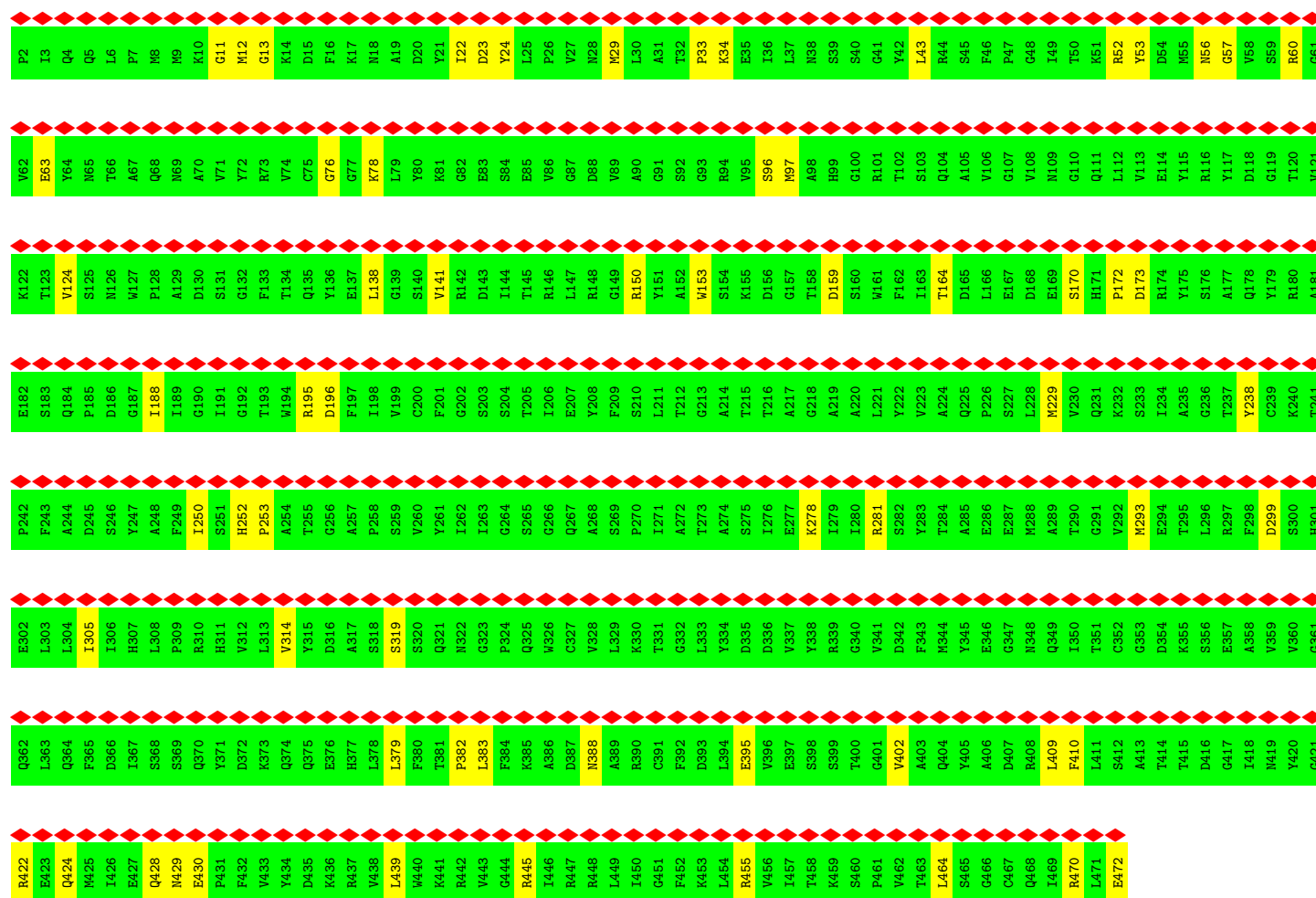
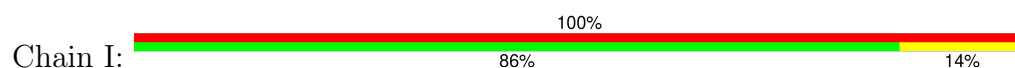


- Molecule 2: Packaged DNA stabilization protein gp10

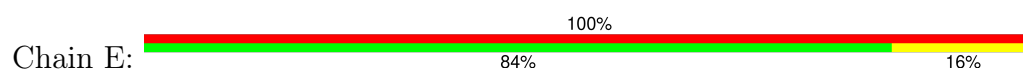




• Molecule 2: Packaged DNA stabilization protein gp10




• Molecule 2: Packaged DNA stabilization protein gp10



Q362 Q363 Q364 Q365 Q366 Q367 Q368 Q369 Q370 Q371 Q372 Q373 Q374 Q375 Q376 Q377 Q378 Q379 Q380 Q381 Q382 Q383 Q384 Q385 Q386 Q387 Q388 Q389 Q390 Q391 Q392 Q393 Q394 Q395 Q396 Q397 Q398 Q399 Q400 Q401 Q402 Q403 Q404 Q405 Q406 Q407 Q408 Q409 Q410 Q411 Q412 Q413 Q414 Q415 Q416 Q417 Q418 Q419 Q420 Q421

R422 R423 R424 R425 R426 R427 R428 R429 R430 R431 R432 R433 R434 R435 R436 R437 R438 R439 R440 R441 R442 R443 R444 R445 R446 R447 R448 R449 R450 R451 R452 R453 R454 R455 R456 R457 R458 R459 R460 R461 R462 R463 R464 R465 R466 R467 R468 R469 R470 R471 R472

• Molecule 2: Packaged DNA stabilization protein gp10

Chain F: 

F2 F3 F4 F5 F6 F7 F8 F9 F10 F11 F12 F13 F14 F15 F16 F17 F18 F19 F20 F21 F22 F23 F24 F25 F26 F27 F28 F29 F30 F31 F32 F33 F34 F35 F36 F37 F38 F39 F40 F41 F42 F43 F44 F45 F46 F47 F48 F49 F50 F51 F52 F53 F54 F55 F56 F57 F58 F59 F60 F61

V62 V63 V64 V65 V66 V67 V68 V69 V70 V71 V72 V73 V74 V75 V76 V77 V78 V79 V80 V81 V82 V83 V84 V85 V86 V87 V88 V89 V90 V91 V92 V93 V94 V95 V96 V97 V98 V99 V100 V101 V102 V103 V104 V105 V106 V107 V108 V109 V110 V111 V112 V113 V114 V115 V116 V117 V118 V119 V120 V121

K122 T123 V124 S125 T126 W127 P128 A129 D130 S131 G132 F133 T134 Q135 Y136 E137 L138 G139 S140 V141 R142 D143 T144 L145 T146 R147 L148 G149 R150 Y151 A152 G153 S154 K155 D156 E157 T158 D159 S160 W161 F162 T163 T164 D165 L166 E167 D168 E169 S170 H171 P172 D173 R174 Y175 S176 A177 Q178 R180 A181

E182 S183 Q184 P185 D186 G187 T188 I189 G190 S191 G192 T193 W194 R195 D196 F197 L198 V199 C200 F201 G202 S203 S204 T205 T206 E207 Y208 F209 S210 L211 T212 G213 A214 T215 T216 A217 G218 A219 A220 L221 Y222 V223 A224 Q225 P226 S227 E228 L229 W229 V230 Q231 V232 S233 T234 A235 G236 T237 Y238 C239 K240 T241

F242 F243 A244 D245 S246 Y247 A248 F249 T250 S251 H252 P253 A254 T255 G256 A257 S258 L259 V260 Y261 T262 T263 G264 S265 G266 Q267 A268 S269 P270 L271 A272 T273 A274 S275 T276 E277 K278 S279 T279 L280 R281 S282 Y283 T284 A285 E286 H288 A289 T290 G291 V292 W293 E294 T295 L296 R297 F298 D299 S300 H301

E302 L303 L304 I305 I306 H307 L308 P309 R310 H311 S312 L313 W314 Y315 D316 A317 S318 S319 S320 Q321 R322 G323 P324 Q325 W326 Q327 V328 L329 R330 T331 G332 L333 Y334 D335 D336 V337 Y338 R339 G340 V341 D342 F343 H344 Y345 E346 G347 H348 Q349 T350 T351 C352 G353 D354 K355 S356 E357 A358 V359 W360 G361

Q362 Q363 Q364 Q365 Q366 Q367 Q368 Q369 Q370 Q371 Q372 Q373 Q374 Q375 Q376 Q377 Q378 Q379 Q380 Q381 Q382 Q383 Q384 Q385 Q386 Q387 Q388 Q389 Q390 Q391 Q392 Q393 Q394 Q395 Q396 Q397 Q398 Q399 Q400 Q401 Q402 Q403 Q404 Q405 Q406 Q407 Q408 Q409 Q410 Q411 Q412 Q413 Q414 Q415 Q416 Q417 Q418 Q419 Q420 Q421

R422 R423 R424 R425 R426 R427 R428 R429 R430 R431 R432 R433 R434 R435 R436 R437 R438 R439 R440 R441 R442 R443 R444 R445 R446 R447 R448 R449 R450 R451 R452 R453 R454 R455 R456 R457 R458 R459 R460 R461 R462 R463 R464 R465 R466 R467 R468 R469 R470 R471 R472

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	106070	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.032	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	512.63995, 512.63995, 512.63995	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.068, 1.068, 1.068	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	0.18	0/465	0.37	0/633
1	B	0.16	0/457	0.41	0/622
1	C	0.18	0/465	0.38	0/633
2	D	0.13	0/3767	0.26	0/5100
2	E	0.13	0/3767	0.27	0/5100
2	F	0.13	0/3767	0.27	0/5100
2	G	0.13	0/3767	0.26	0/5100
2	H	0.13	0/3767	0.26	0/5100
2	I	0.13	0/3767	0.26	0/5100
All	All	0.14	0/23989	0.27	0/32488

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	459	0	456	13	0
1	B	451	0	452	11	0
1	C	459	0	456	8	0
2	D	3686	0	3592	46	0
2	E	3686	0	3592	49	0
2	F	3686	0	3592	45	0
2	G	3686	0	3592	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	3686	0	3592	44	0
2	I	3686	0	3592	42	0
All	All	23485	0	22916	267	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 6.

The worst 5 of 267 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:12:MET:SD	2:I:34:LYS:NZ	2.53	0.82
2:D:12:MET:SD	2:F:34:LYS:NZ	2.53	0.79
1:A:15:THR:HG23	1:A:16:ARG:HG2	1.66	0.77
2:F:258:PRO:HG3	2:F:288:MET:HE1	1.74	0.70
2:F:422:ARG:NH2	2:F:424:GLN:OE1	2.27	0.68

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	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
1	B	59/62 (95%)	56 (95%)	3 (5%)	0	100	100
1	C	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
2	D	469/471 (100%)	450 (96%)	19 (4%)	0	100	100
2	E	469/471 (100%)	450 (96%)	19 (4%)	0	100	100
2	F	469/471 (100%)	451 (96%)	18 (4%)	0	100	100
2	G	469/471 (100%)	448 (96%)	21 (4%)	0	100	100
2	H	469/471 (100%)	451 (96%)	18 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	469/471 (100%)	448 (96%)	21 (4%)	0	100	100
All	All	2993/3012 (99%)	2868 (96%)	125 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	48/48 (100%)	48 (100%)	0	100	100
1	B	47/48 (98%)	47 (100%)	0	100	100
1	C	48/48 (100%)	48 (100%)	0	100	100
2	D	395/395 (100%)	395 (100%)	0	100	100
2	E	395/395 (100%)	395 (100%)	0	100	100
2	F	395/395 (100%)	395 (100%)	0	100	100
2	G	395/395 (100%)	395 (100%)	0	100	100
2	H	395/395 (100%)	395 (100%)	0	100	100
2	I	395/395 (100%)	395 (100%)	0	100	100
All	All	2513/2514 (100%)	2513 (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. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	18	ASN
2	D	225	GLN
2	F	419	ASN
2	D	362	GLN
2	I	362	GLN

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](#)

There are no chain breaks in this entry.

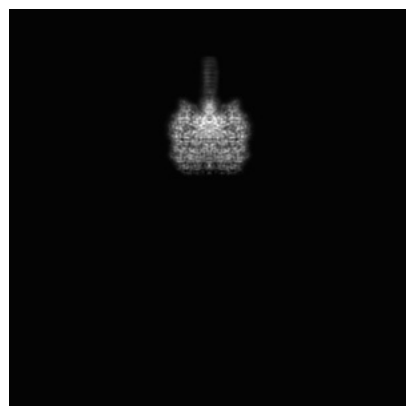
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27790. These allow visual inspection of the internal detail of the map and identification of artifacts.

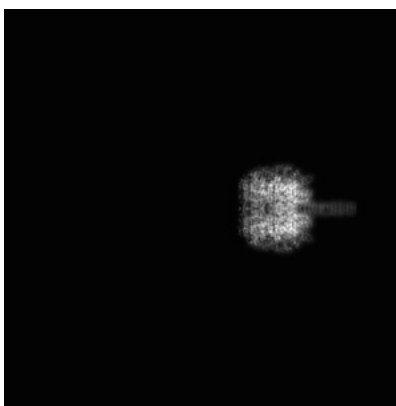
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

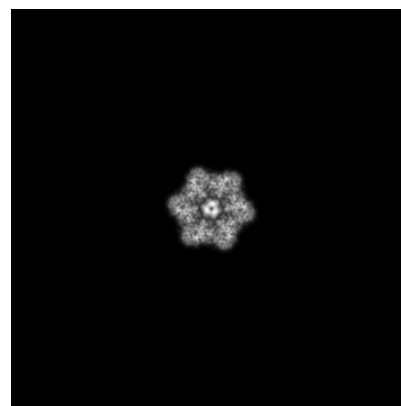
6.1.1 Primary map



X

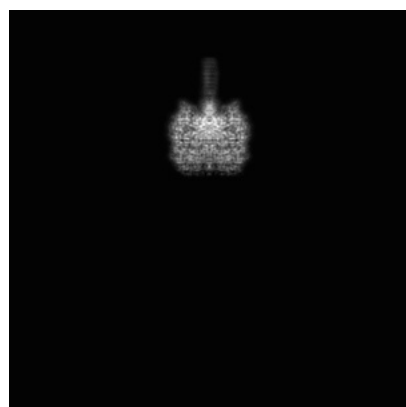


Y

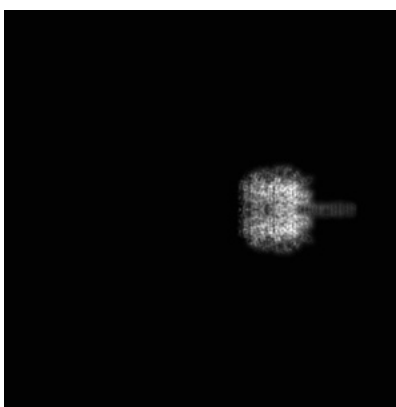


Z

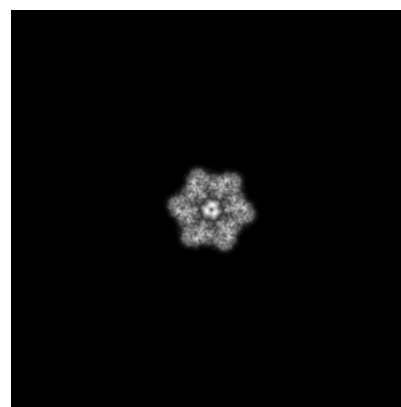
6.1.2 Raw map



X



Y

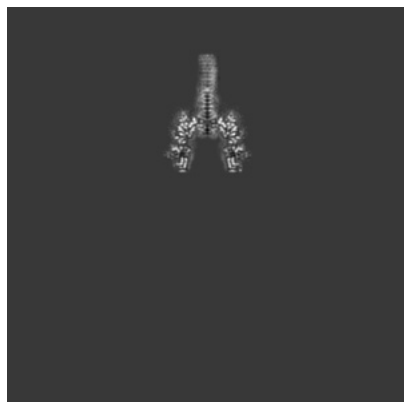


Z

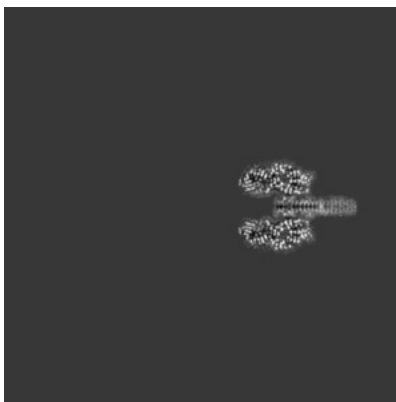
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

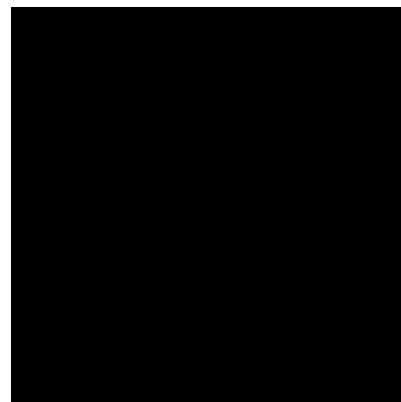
6.2.1 Primary map



X Index: 240

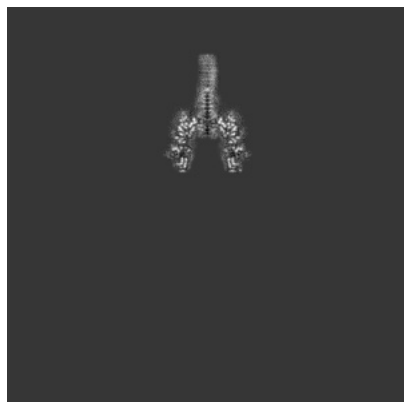


Y Index: 240

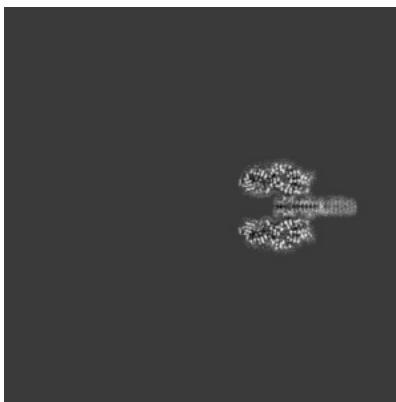


Z Index: 240

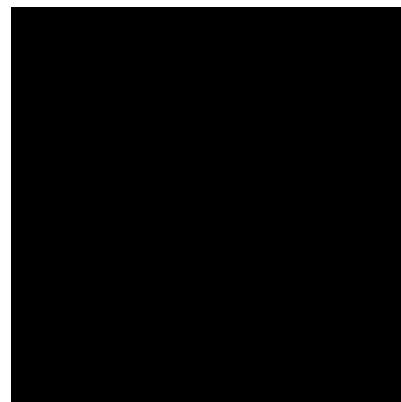
6.2.2 Raw map



X Index: 240



Y Index: 240

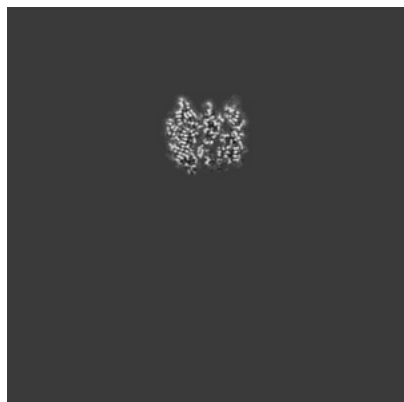


Z Index: 240

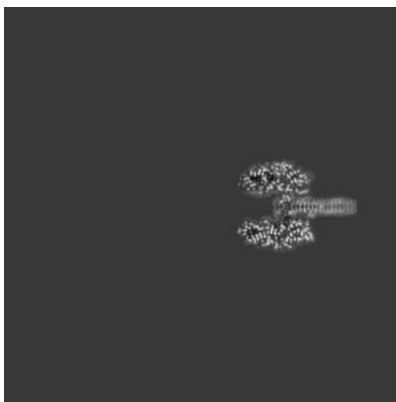
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

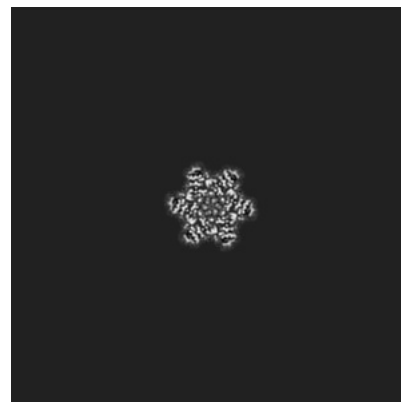
6.3.1 Primary map



X Index: 261

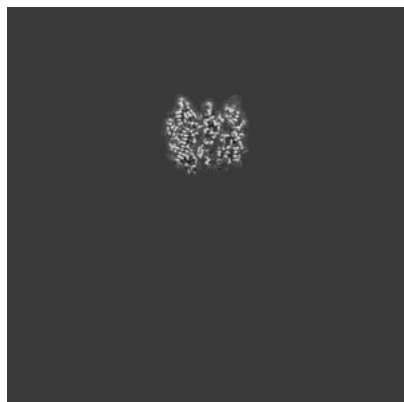


Y Index: 238

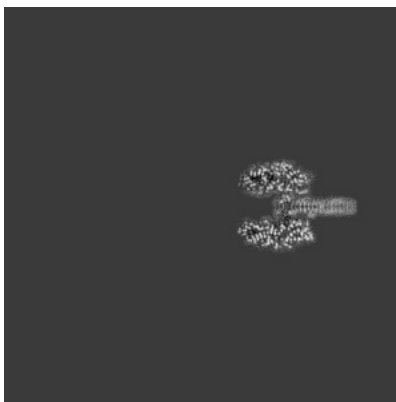


Z Index: 344

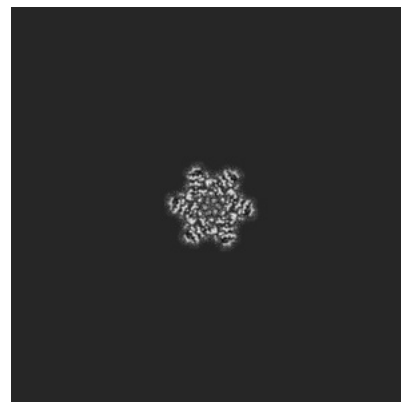
6.3.2 Raw map



X Index: 261



Y Index: 238

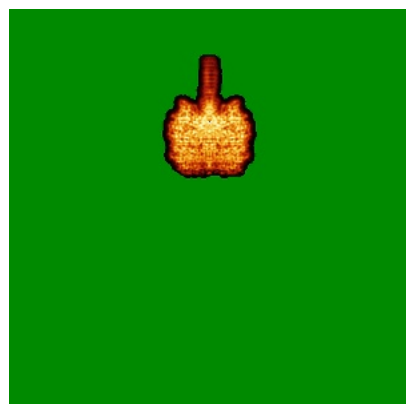


Z Index: 344

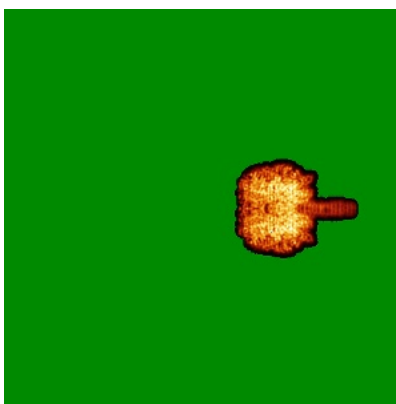
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

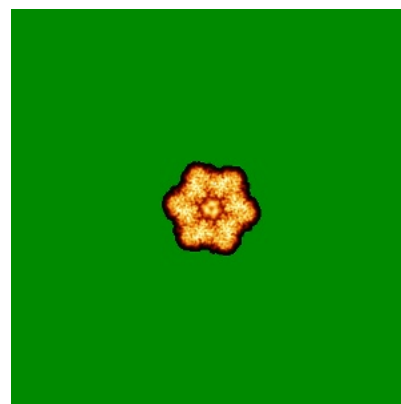
6.4.1 Primary map



X

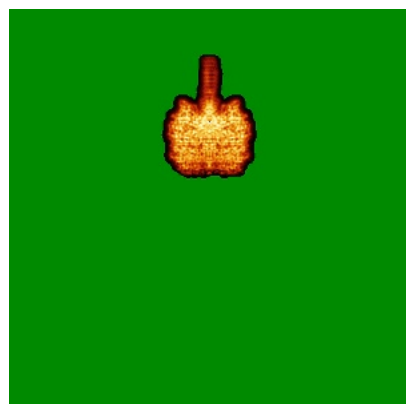


Y

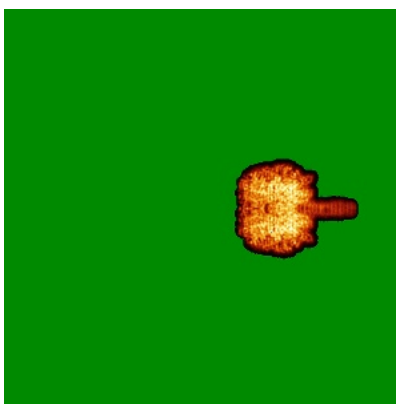


Z

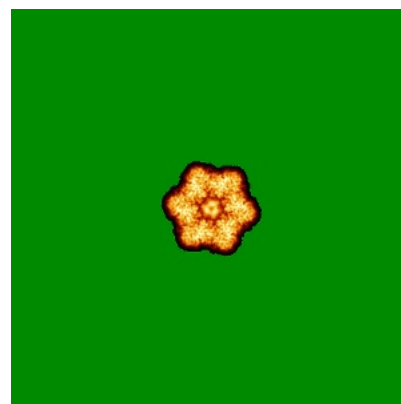
6.4.2 Raw map



X



Y

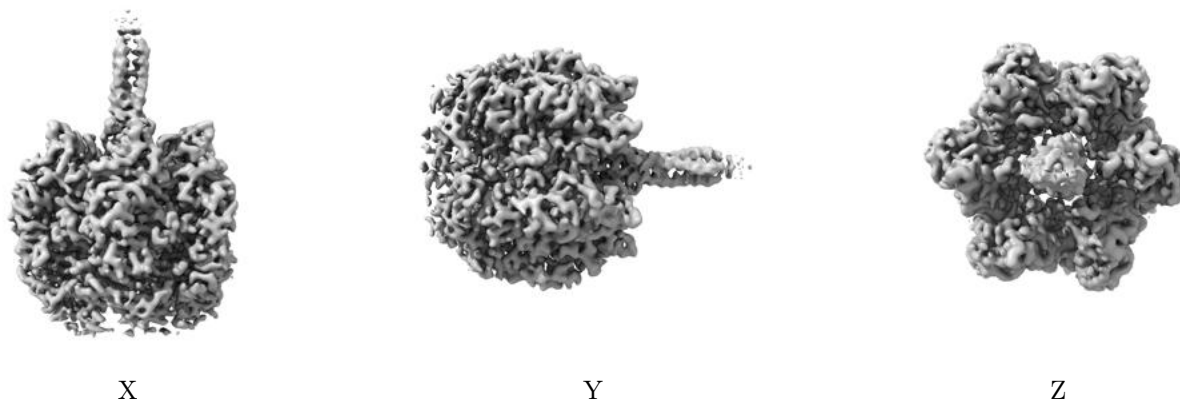


Z

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.

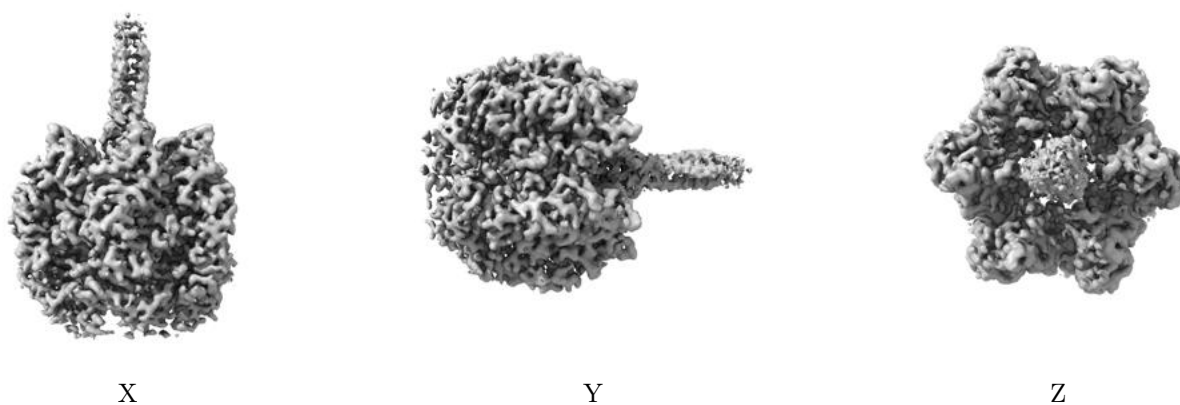
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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



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.

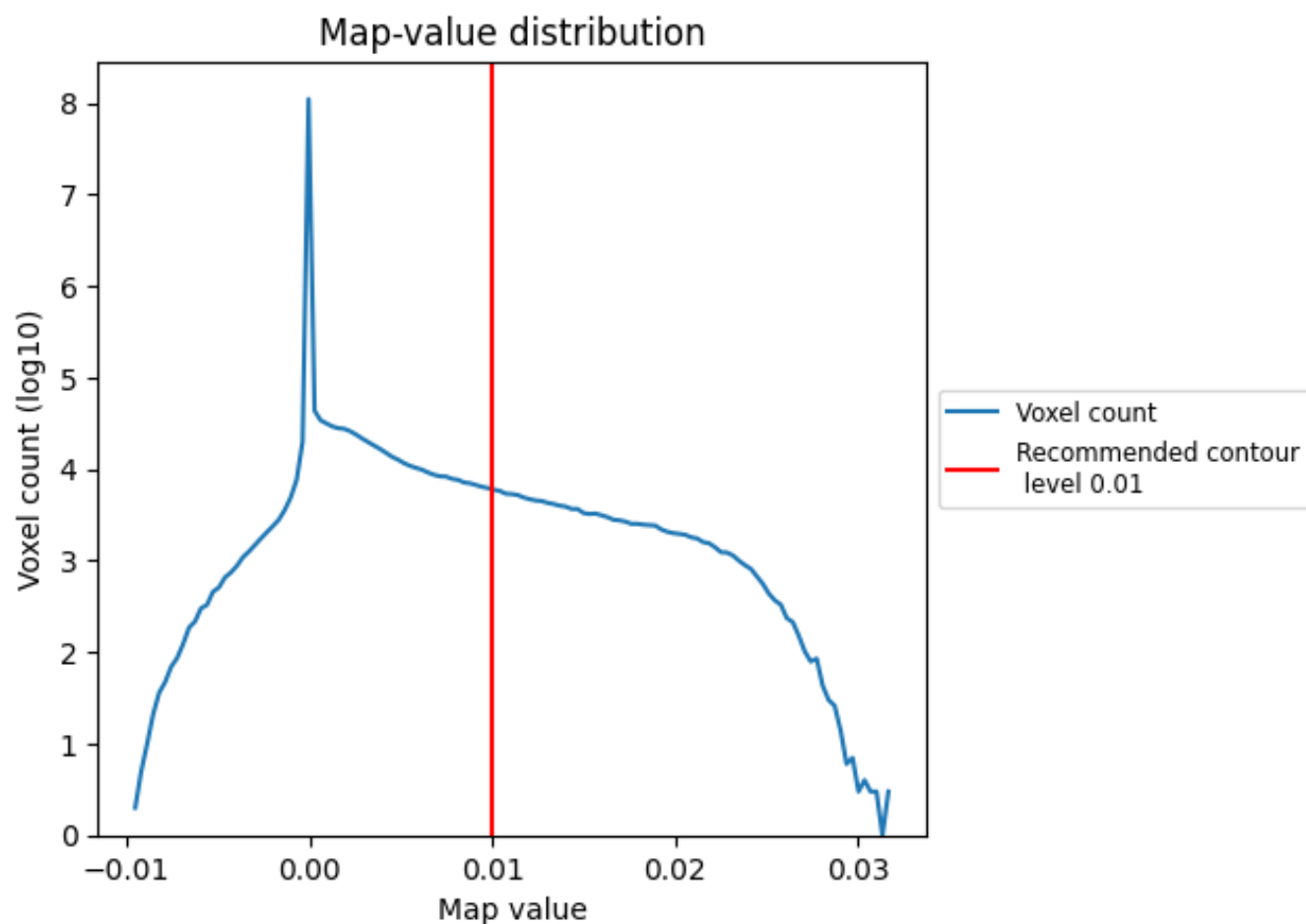
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

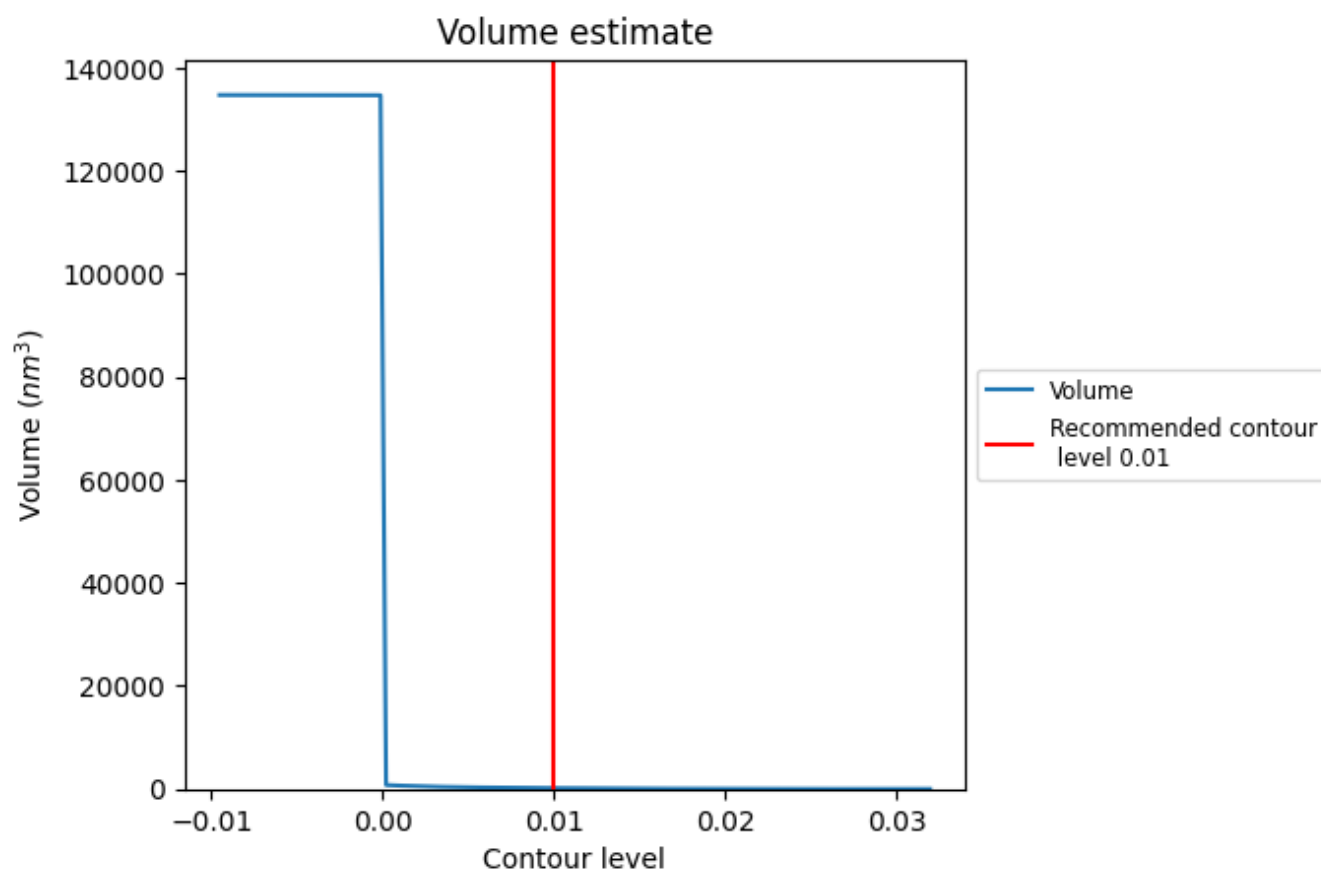
This section contains the results of statistical analysis of the map.

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.

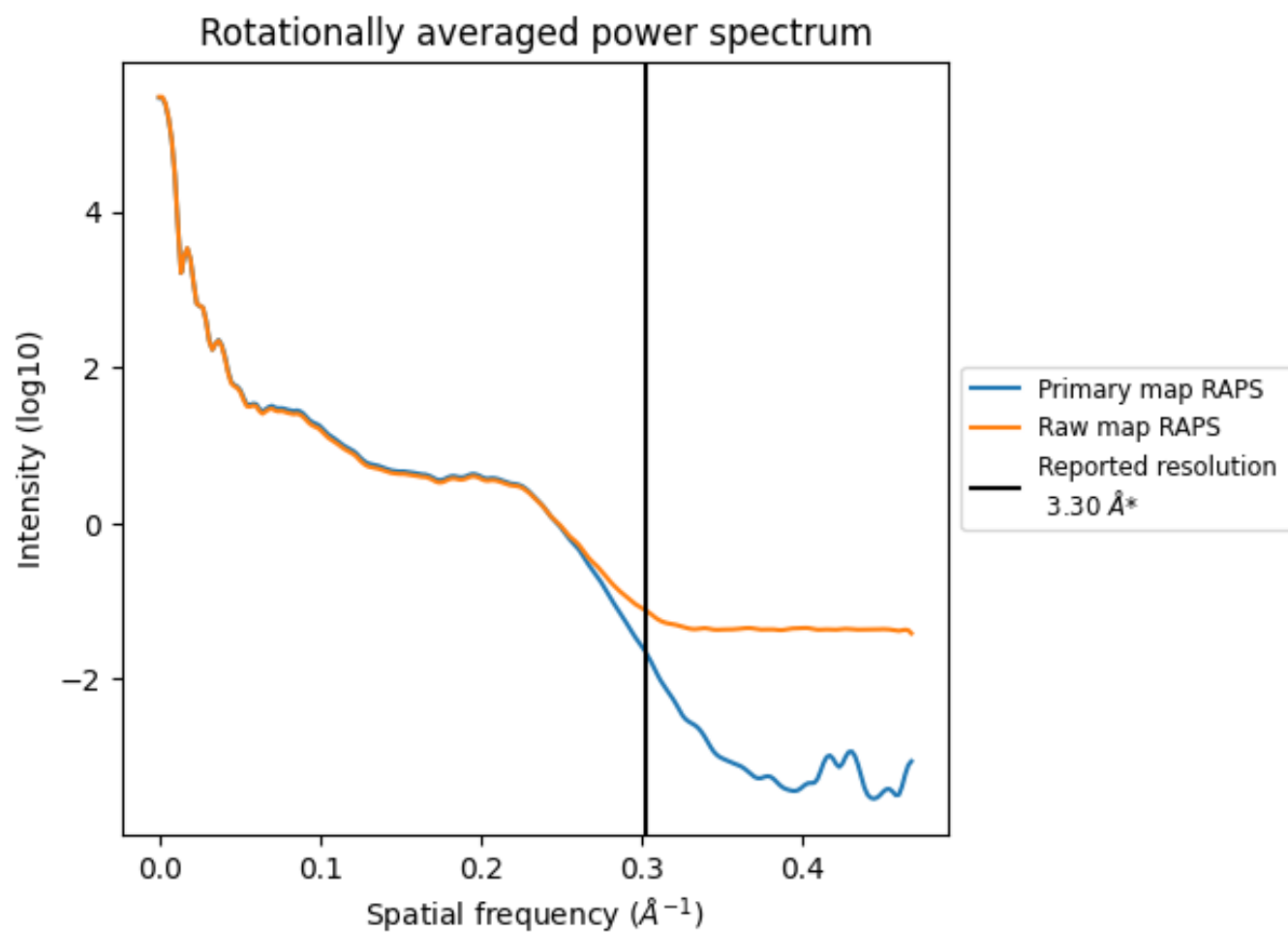
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 166 nm^3 ; this corresponds to an approximate mass of 150 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 ⓘ

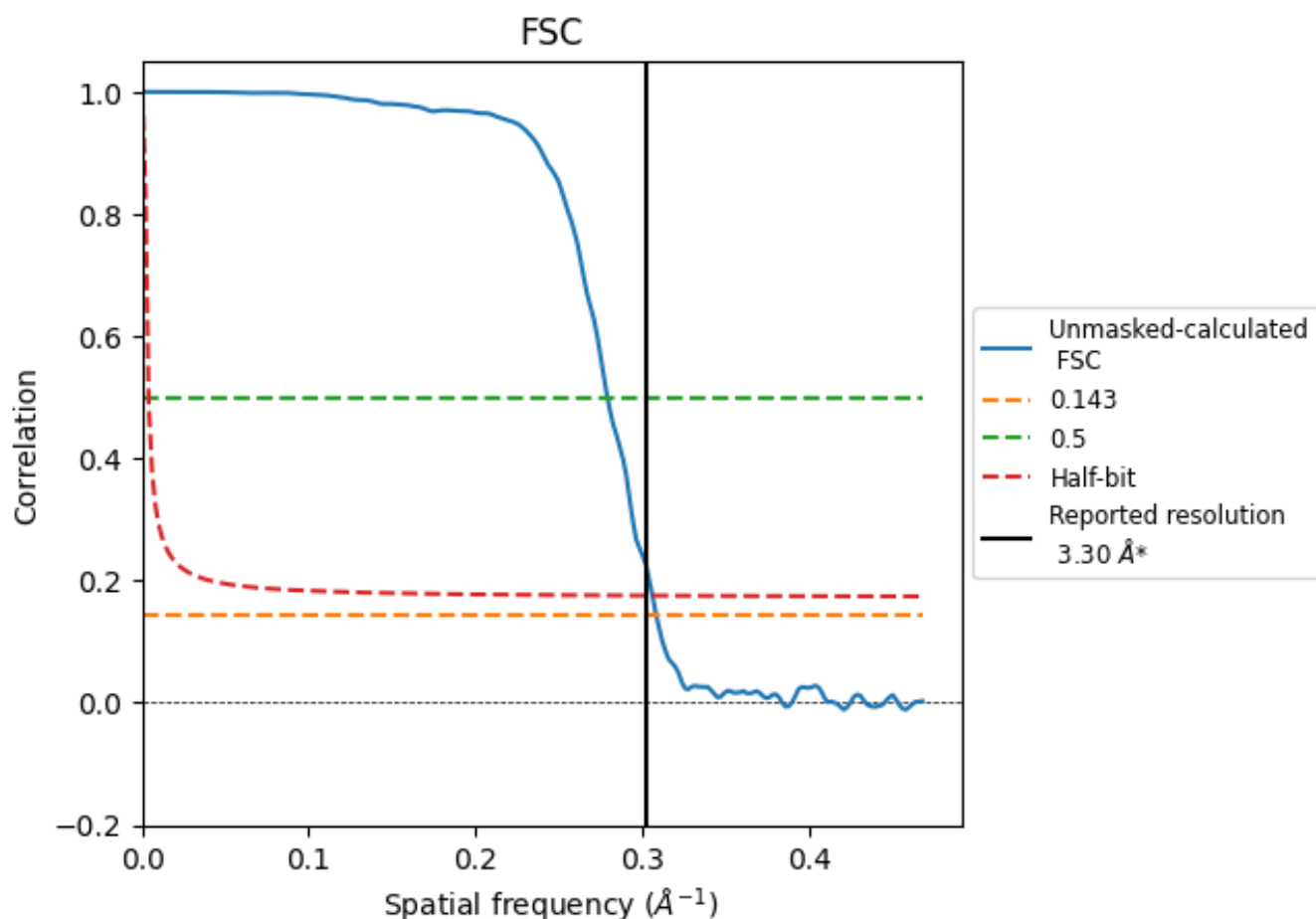


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

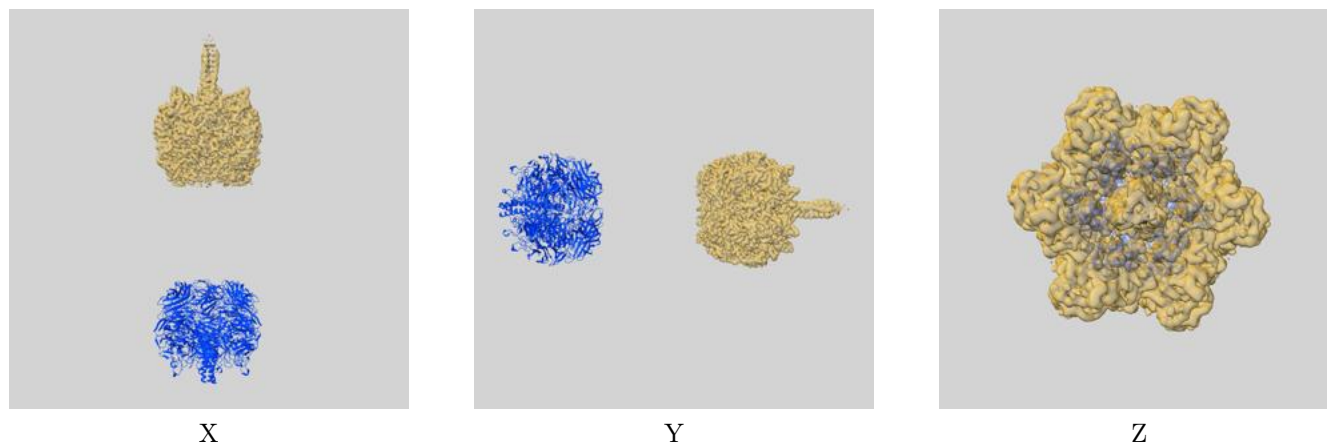
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.24	3.58	3.26

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

9 Map-model fit [i](#)

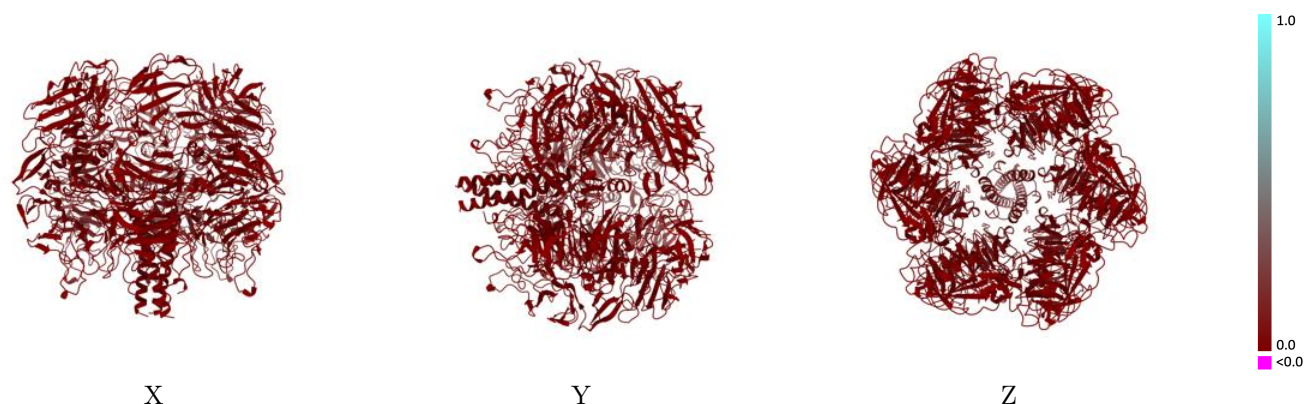
This section contains information regarding the fit between EMDB map EMD-27790 and PDB model 8EAP. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



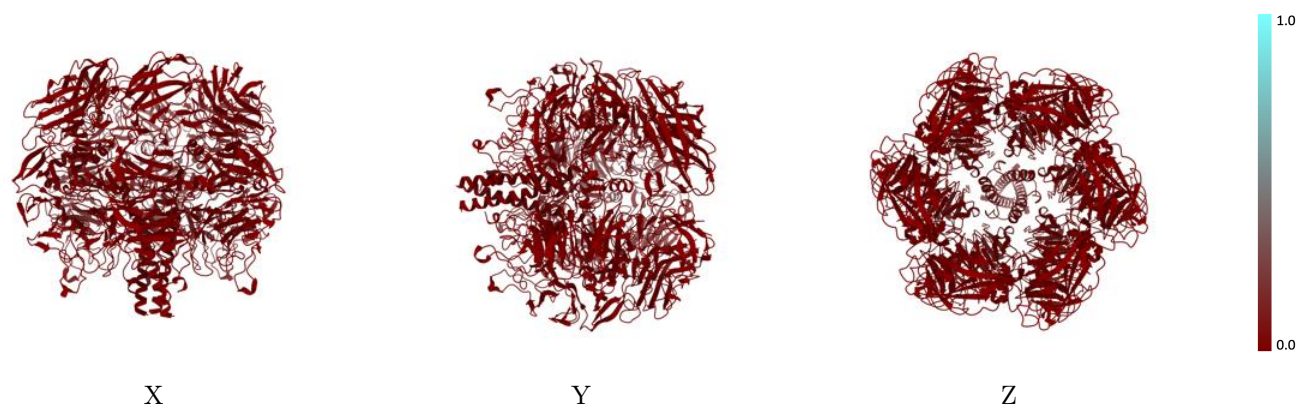
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



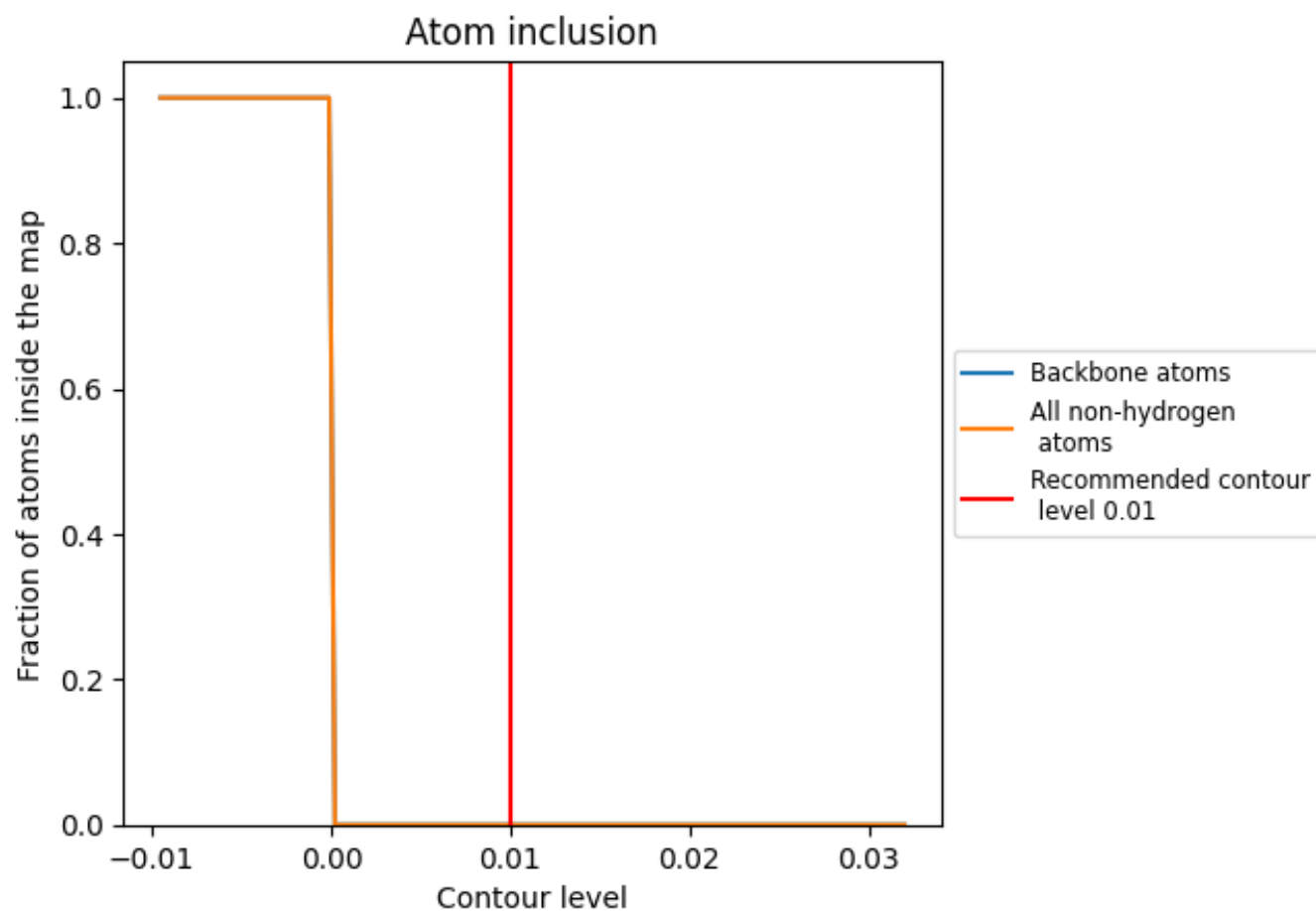
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 0% of all backbone atoms, 0% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.0000</div>	<div><div></div>0.0000</div>
A	<div><div></div>0.0000</div>	<div><div></div>0.0000</div>
B	<div><div></div>0.0000</div>	<div><div></div>0.0000</div>
C	<div><div></div>0.0000</div>	<div><div></div>0.0000</div>
D	<div><div></div>0.0000</div>	<div><div></div>0.0000</div>
E	<div><div></div>0.0000</div>	<div><div></div>0.0000</div>
F	<div><div></div>0.0000</div>	<div><div></div>0.0000</div>
G	<div><div></div>0.0000</div>	<div><div></div>0.0000</div>
H	<div><div></div>0.0000</div>	<div><div></div>0.0000</div>
I	<div><div></div>0.0000</div>	<div><div></div>0.0000</div>

1.0

0.0

<0.0