wwPDB EM Validation Summary Report

Oct 13, 2024 – 07:28 am BST

PDB ID	:	7OMM
EMDB ID	:	EMD-12990
Title	:	Cryo-EM structure of N. gonorhoeae LptDE in complex with ProMacrobodies (MBPs have not been built de novo)
Authors	:	Botte, M.; Ni, D.; Schenck, S.; Zimmermann, I.; Chami, M.; Bocquet, N.; Egloff, P.; Bucher, D.; Trabuco, M.; Cheng, R.K.Y.; Brunner, J.D.; Seeger, M.A.; Stahlberg, H.; Hennig, M.
Deposited on	:	2021-05-24
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 ⓘ 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:

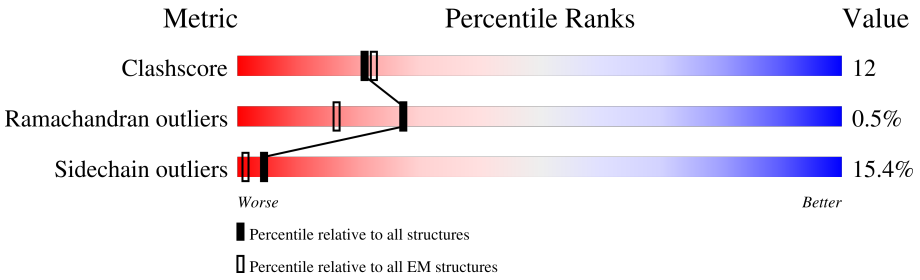
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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	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 <=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	801	8% 60% 25% • 13%
2	B	165	5% 61% 16% 22%
3	C	520	69% 80% 11% • 8%
4	D	526	69% 45% 35% 13% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13981 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 LPS-assembly protein LptD.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	698	Total	C	N	O	S	0	0
			5462	3430	985	1038	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	SER	ALA	conflict	UNP Q5F651

- Molecule 2 is a protein called LPS-assembly lipoprotein LptE.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	128	Total	C	N	O	S	0	0
			1020	640	179	198	3		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	160	HIS	-	expression tag	UNP A0A5K1Q6A7
B	161	HIS	-	expression tag	UNP A0A5K1Q6A7
B	162	HIS	-	expression tag	UNP A0A5K1Q6A7
B	163	HIS	-	expression tag	UNP A0A5K1Q6A7
B	164	HIS	-	expression tag	UNP A0A5K1Q6A7
B	165	HIS	-	expression tag	UNP A0A5K1Q6A7

- Molecule 3 is a protein called ProMacrobody 21,Maltodextrin-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	479	Total	C	N	O	S	0	0
			3731	2397	614	710	10		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	484	PRO	-	expression tag	UNP A0A0F8L1I7
C	485	GLY	-	expression tag	UNP A0A0F8L1I7
C	486	SER	-	expression tag	UNP A0A0F8L1I7
C	487	GLY	-	expression tag	UNP A0A0F8L1I7
C	488	GLY	-	expression tag	UNP A0A0F8L1I7
C	489	GLY	-	expression tag	UNP A0A0F8L1I7
C	490	SER	-	expression tag	UNP A0A0F8L1I7
C	491	ALA	-	expression tag	UNP A0A0F8L1I7
C	492	TRP	-	expression tag	UNP A0A0F8L1I7
C	493	SER	-	expression tag	UNP A0A0F8L1I7
C	494	HIS	-	expression tag	UNP A0A0F8L1I7
C	495	PRO	-	expression tag	UNP A0A0F8L1I7
C	496	GLN	-	expression tag	UNP A0A0F8L1I7
C	497	PHE	-	expression tag	UNP A0A0F8L1I7
C	498	GLU	-	expression tag	UNP A0A0F8L1I7
C	499	LYS	-	expression tag	UNP A0A0F8L1I7
C	500	GLY	-	expression tag	UNP A0A0F8L1I7
C	501	GLY	-	expression tag	UNP A0A0F8L1I7
C	502	GLY	-	expression tag	UNP A0A0F8L1I7
C	503	SER	-	expression tag	UNP A0A0F8L1I7
C	504	GLY	-	expression tag	UNP A0A0F8L1I7
C	505	GLY	-	expression tag	UNP A0A0F8L1I7
C	506	GLY	-	expression tag	UNP A0A0F8L1I7
C	507	SER	-	expression tag	UNP A0A0F8L1I7
C	508	GLY	-	expression tag	UNP A0A0F8L1I7
C	509	GLY	-	expression tag	UNP A0A0F8L1I7
C	510	SER	-	expression tag	UNP A0A0F8L1I7
C	511	ALA	-	expression tag	UNP A0A0F8L1I7
C	512	TRP	-	expression tag	UNP A0A0F8L1I7
C	513	SER	-	expression tag	UNP A0A0F8L1I7
C	514	HIS	-	expression tag	UNP A0A0F8L1I7
C	515	PRO	-	expression tag	UNP A0A0F8L1I7
C	516	GLN	-	expression tag	UNP A0A0F8L1I7
C	517	PHE	-	expression tag	UNP A0A0F8L1I7
C	518	GLU	-	expression tag	UNP A0A0F8L1I7
C	519	LYS	-	expression tag	UNP A0A0F8L1I7
C	520	ALA	-	expression tag	UNP A0A0F8L1I7

- Molecule 4 is a protein called ProMacrobody 51,Maltodextrin-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	489	Total	C	N	O	S	0	0
			3768	2422	614	723	9		

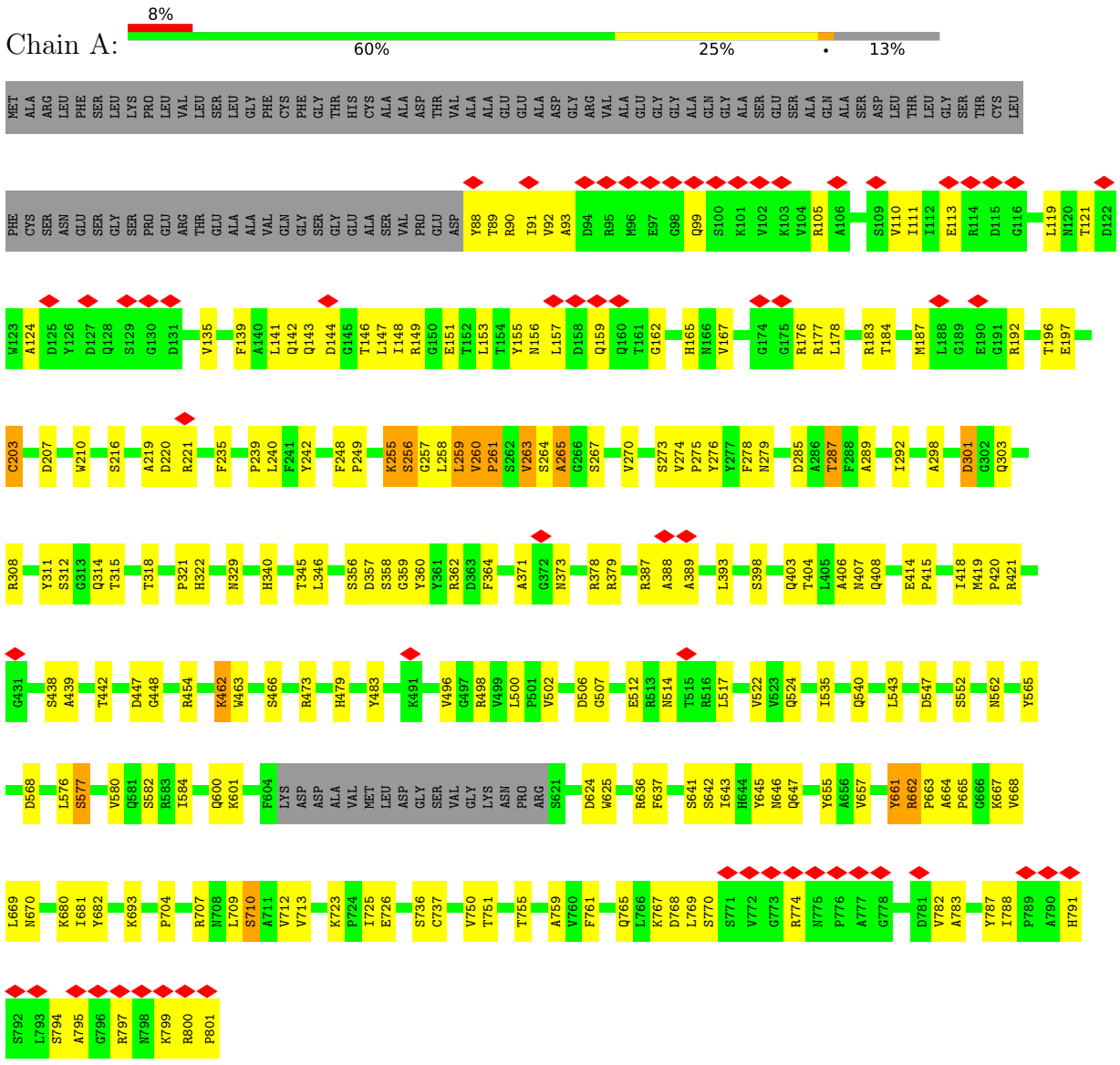
There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	490	PRO	-	expression tag	UNP A0A0F8L1I7
D	491	GLY	-	expression tag	UNP A0A0F8L1I7
D	492	SER	-	expression tag	UNP A0A0F8L1I7
D	493	GLY	-	expression tag	UNP A0A0F8L1I7
D	494	GLY	-	expression tag	UNP A0A0F8L1I7
D	495	GLY	-	expression tag	UNP A0A0F8L1I7
D	496	SER	-	expression tag	UNP A0A0F8L1I7
D	497	ALA	-	expression tag	UNP A0A0F8L1I7
D	498	TRP	-	expression tag	UNP A0A0F8L1I7
D	499	SER	-	expression tag	UNP A0A0F8L1I7
D	500	HIS	-	expression tag	UNP A0A0F8L1I7
D	501	PRO	-	expression tag	UNP A0A0F8L1I7
D	502	GLN	-	expression tag	UNP A0A0F8L1I7
D	503	PHE	-	expression tag	UNP A0A0F8L1I7
D	504	GLU	-	expression tag	UNP A0A0F8L1I7
D	505	LYS	-	expression tag	UNP A0A0F8L1I7
D	506	GLY	-	expression tag	UNP A0A0F8L1I7
D	507	GLY	-	expression tag	UNP A0A0F8L1I7
D	508	GLY	-	expression tag	UNP A0A0F8L1I7
D	509	SER	-	expression tag	UNP A0A0F8L1I7
D	510	GLY	-	expression tag	UNP A0A0F8L1I7
D	511	GLY	-	expression tag	UNP A0A0F8L1I7
D	512	GLY	-	expression tag	UNP A0A0F8L1I7
D	513	SER	-	expression tag	UNP A0A0F8L1I7
D	514	GLY	-	expression tag	UNP A0A0F8L1I7
D	515	GLY	-	expression tag	UNP A0A0F8L1I7
D	516	SER	-	expression tag	UNP A0A0F8L1I7
D	517	ALA	-	expression tag	UNP A0A0F8L1I7
D	518	TRP	-	expression tag	UNP A0A0F8L1I7
D	519	SER	-	expression tag	UNP A0A0F8L1I7
D	520	HIS	-	expression tag	UNP A0A0F8L1I7
D	521	PRO	-	expression tag	UNP A0A0F8L1I7
D	522	GLN	-	expression tag	UNP A0A0F8L1I7
D	523	PHE	-	expression tag	UNP A0A0F8L1I7
D	524	GLU	-	expression tag	UNP A0A0F8L1I7
D	525	LYS	-	expression tag	UNP A0A0F8L1I7
D	526	ALA	-	expression tag	UNP A0A0F8L1I7

3 Residue-property plots (i)

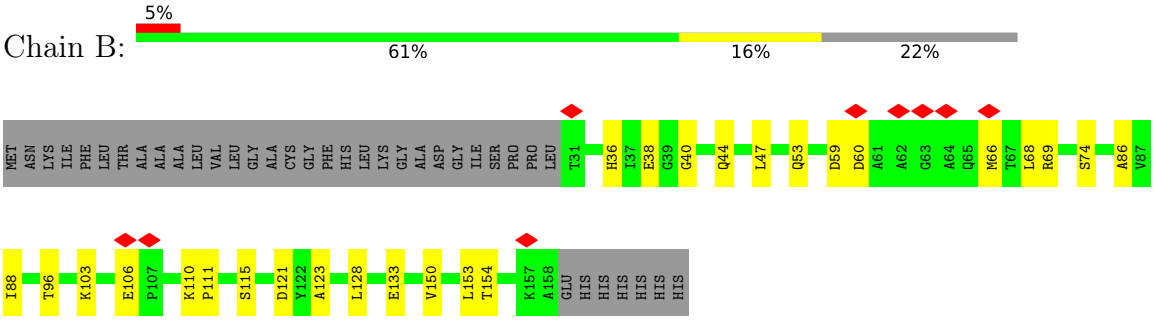
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: LPS-assembly protein LptD



• Molecule 2: LPS-assembly lipoprotein LptE

Chain B:

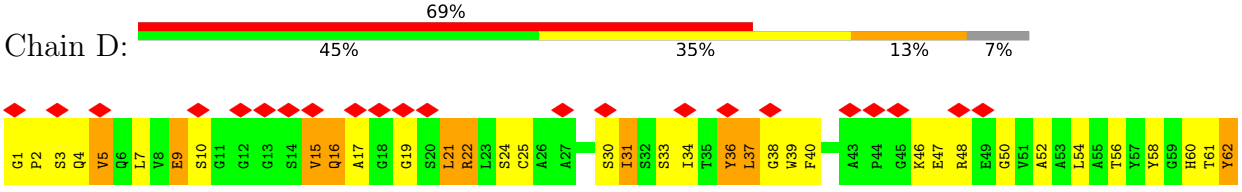


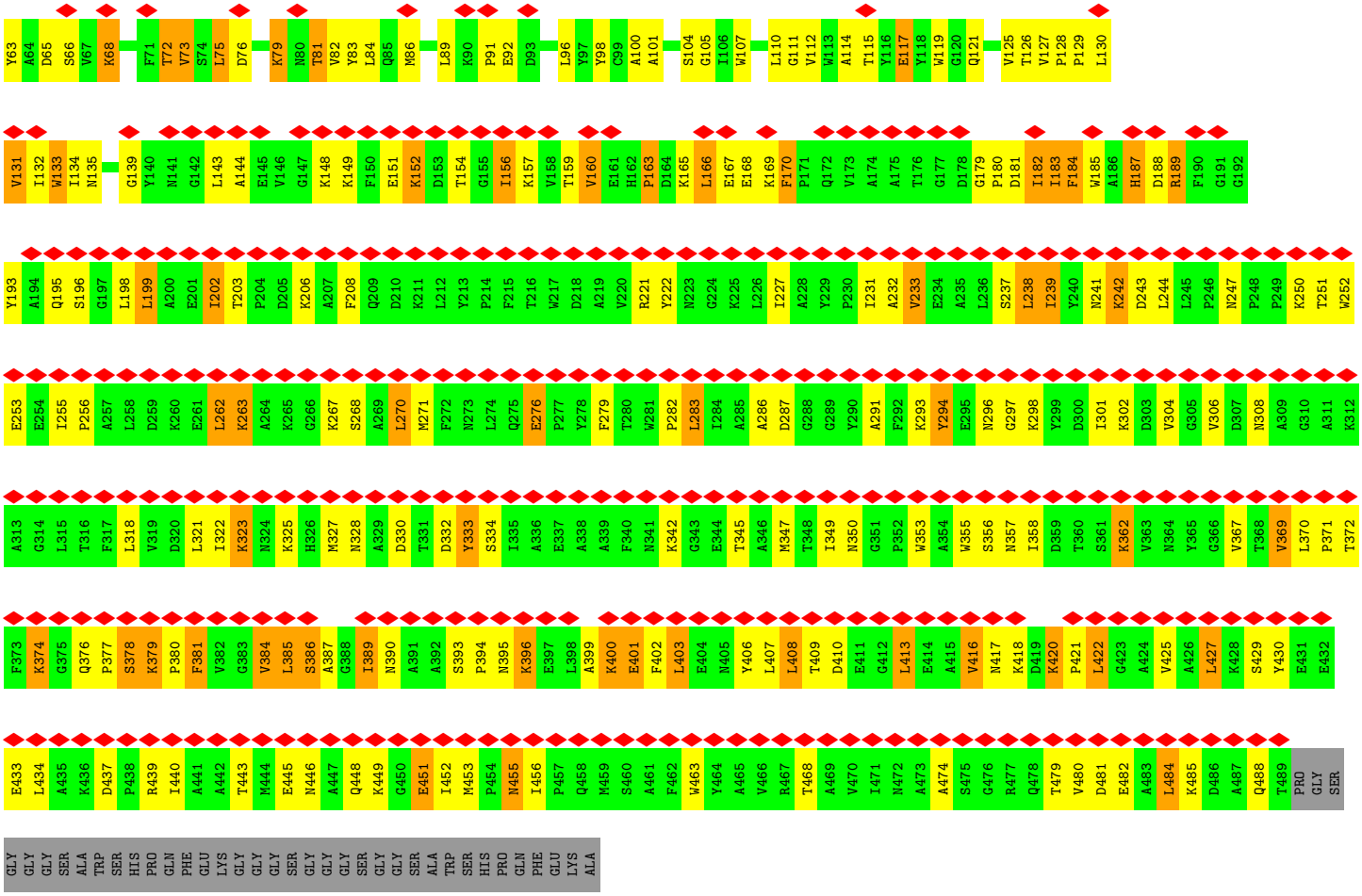
• Molecule 3: ProMacrobody 21,Maltodextrin-binding protein

Chain C:

• Molecule 4: ProMacrobody 51,Maltodextrin-binding protein

Chain D:




Y63 A64 D65 S66 V67 K68 F71 T72 V73 S74 L75 D76 K79 N80 T81 V82 Y83 L84 Q85 M86 L89 K90 P91 E92 D93 L96 Y97 Y98 C99 A100 A101 S104 G105 I106 W107 L110 G111 V112 W113 A114 T115 Y116 E117 Y118 W119 G120 Q121 V125 T126 V127 P128 P129 L130
V131 I132 W133 I134 N135 G139 Y140 N141 G142 L143 A144 E145 V146 G147 K148 K149 F150 E151 K152 D153 T154 G155 I156 K157 V158 T159 V160 E161 H162 P163 D164 K165 L166 E167 E168 K169 F170 P171 Q172 V173 A174 A175 T176 G177 D178 G179 P180 D181 I182 I183 F184 W185 A186 H187 D188 R189 F190 G191 G192
Y193 A194 Q195 S196 G197 L198 L199 A200 E201 I202 T203 P204 D205 K206 A207 F208 Q209 D210 K211 L212 Y213 P214 F215 T216 W217 D218 A219 V220 R221 Y222 N223 G224 K225 L226 I227 A228 Y229 P230 I231 A232 V233 E234 A235 L236 S237 L238 I239 Y240 N241 K242 D243 L244 L245 P246 N247 P248 P249 K250 T251 W252
E253 E254 I255 P256 A257 L258 D259 K260 E261 L262 K263 A264 K265 G266 K267 S268 A269 L270 M271 F272 N273 L274 Q275 E276 P277 Y278 P279 T280 W281 P282 L283 I284 A285 A286 D287 G288 G289 Y290 A291 P292 K293 Y294 E295 N296 G297 K298 Y299 D300 I301 K302 D303 V304 G305 V306 D307 N308 A309 G310 A311 K312
A313 G314 L315 T316 F317 L318 V319 D320 L321 I322 K323 N324 K325 H326 M327 N328 A329 D330 T331 D332 Y333 S334 I335 A336 E337 A338 A339 F340 N341 K342 G343 E344 T345 A346 M347 T348 I349 N350 G351 P352 W353 A354 W355 S356 N357 I358 D359 T360 S361 K362 V363 N364 Y365 G366 V367 T368 V369 L370 P371 T372
F373 K374 G375 Q376 P377 S378 K379 P380 F381 V382 G383 V384 L385 S386 A387 G388 I389 N390 A391 A392 S393 P394 N395 K396 E397 L398 A399 K400 E401 F402 L403 E404 N405 Y406 L407 L408 T409 D410 E411 G412 L413 E414 A415 V416 N417 K418 D419 K420 P421 L422 G423 A424 V425 A426 L427 K428 S429 Y430 E431 E432
E433 L434 A435 K436 D437 P438 R439 I440 A441 A442 T443 M444 E445 N446 A447 Q448 K449 G450 E451 I452 M453 P454 N455 I456 P457 Q458 M459 S460 A461 F462 W463 Y464 A465 V466 R467 T468 A469 V470 I471 N472 A473 A474 S475 G476 R477 Q478 T479 V480 D481 E482 A483 L484 K485 D486 A487 Q488 T489 PRO GLY SER
GLY GLY GLY SER ALA TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY GLY SER GLY GLY GLY SER GLY GLY SER ALA TRP SER HIS PRO GLN PHE GLU LYS ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	184206	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.965	Depositor
Minimum map value	-1.718	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	344.4, 344.4, 344.4	wwPDB
Map dimensions	390, 390, 390	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8830769, 0.8830769, 0.8830769	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	0.38	0/5594	0.59	0/7569
2	B	0.27	0/1034	0.44	0/1400
3	C	0.63	0/3829	0.87	0/5208
4	D	0.63	0/3865	0.74	0/5260
All	All	0.52	0/14322	0.71	0/19437

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	5462	0	5221	127	0
2	B	1020	0	1024	20	0
3	C	3731	0	3645	32	0
4	D	3768	0	3692	153	0
All	All	13981	0	13582	321	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 12.

The worst 5 of 321 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)
4:D:131:VAL:HB	4:D:180:PRO:HB3	1.36	1.07
4:D:333:TYR:O	4:D:333:TYR:HD1	1.40	1.04
4:D:401:GLU:OE1	4:D:401:GLU:O	1.82	0.97
4:D:333:TYR:O	4:D:333:TYR:CD1	2.28	0.87
4:D:333:TYR:CD1	4:D:333:TYR:C	2.43	0.86

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	694/801 (87%)	570 (82%)	120 (17%)	4 (1%)	22 50
2	B	126/165 (76%)	118 (94%)	8 (6%)	0	100 100
3	C	477/520 (92%)	457 (96%)	17 (4%)	3 (1%)	22 50
4	D	487/526 (93%)	464 (95%)	21 (4%)	2 (0%)	30 60
All	All	1784/2012 (89%)	1609 (90%)	166 (9%)	9 (0%)	27 54

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	PRO
3	C	390	LYS
4	D	163	PRO
1	A	207	ASP
1	A	265	ALA

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	556/632 (88%)	509 (92%)	47 (8%)	8 29
2	B	108/136 (79%)	108 (100%)	0	100 100
3	C	384/409 (94%)	361 (94%)	23 (6%)	16 41
4	D	387/409 (95%)	236 (61%)	151 (39%)	0 0
All	All	1435/1586 (90%)	1214 (85%)	221 (15%)	4 9

5 of 221 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	130	LEU
4	D	238	LEU
4	D	485	LYS
4	D	416	VAL
4	D	143	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	581	GLN
3	C	59	ASN
3	C	100	ASN
1	A	314	GLN
1	A	201	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)

There are no chain breaks in this entry.

6 Map visualisation

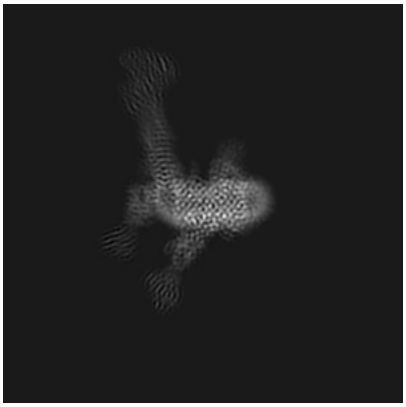
This section contains visualisations of the EMDB entry EMD-12990. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

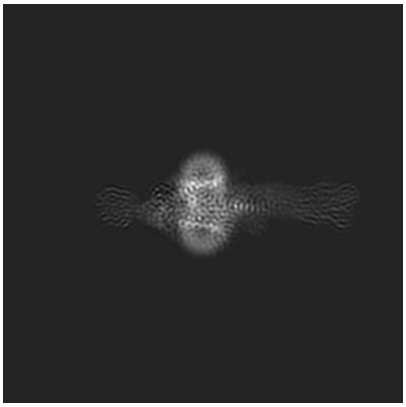
6.1 Orthogonal projections

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: 195

Y Index: 195

Z Index: 195

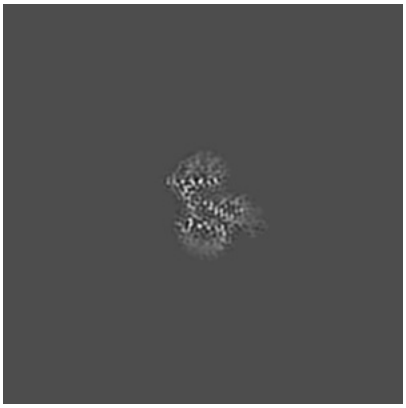
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 185

Y Index: 189

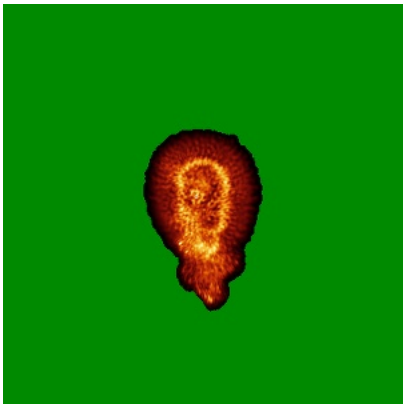


Z Index: 216

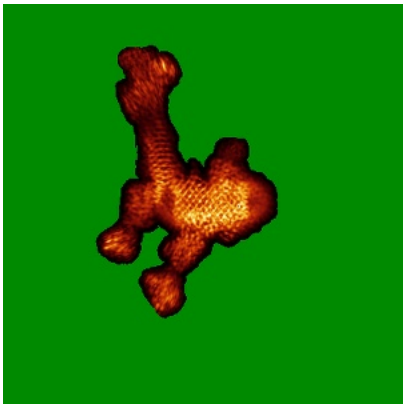
The images above show the largest variance slices of the map in three orthogonal directions.

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

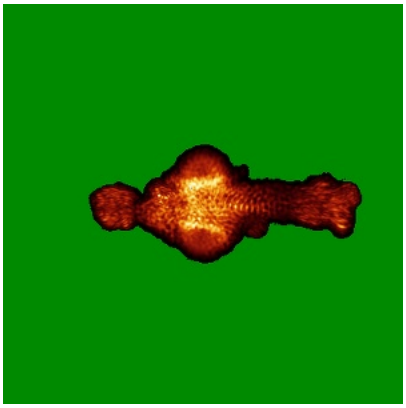
6.4.1 Primary map



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

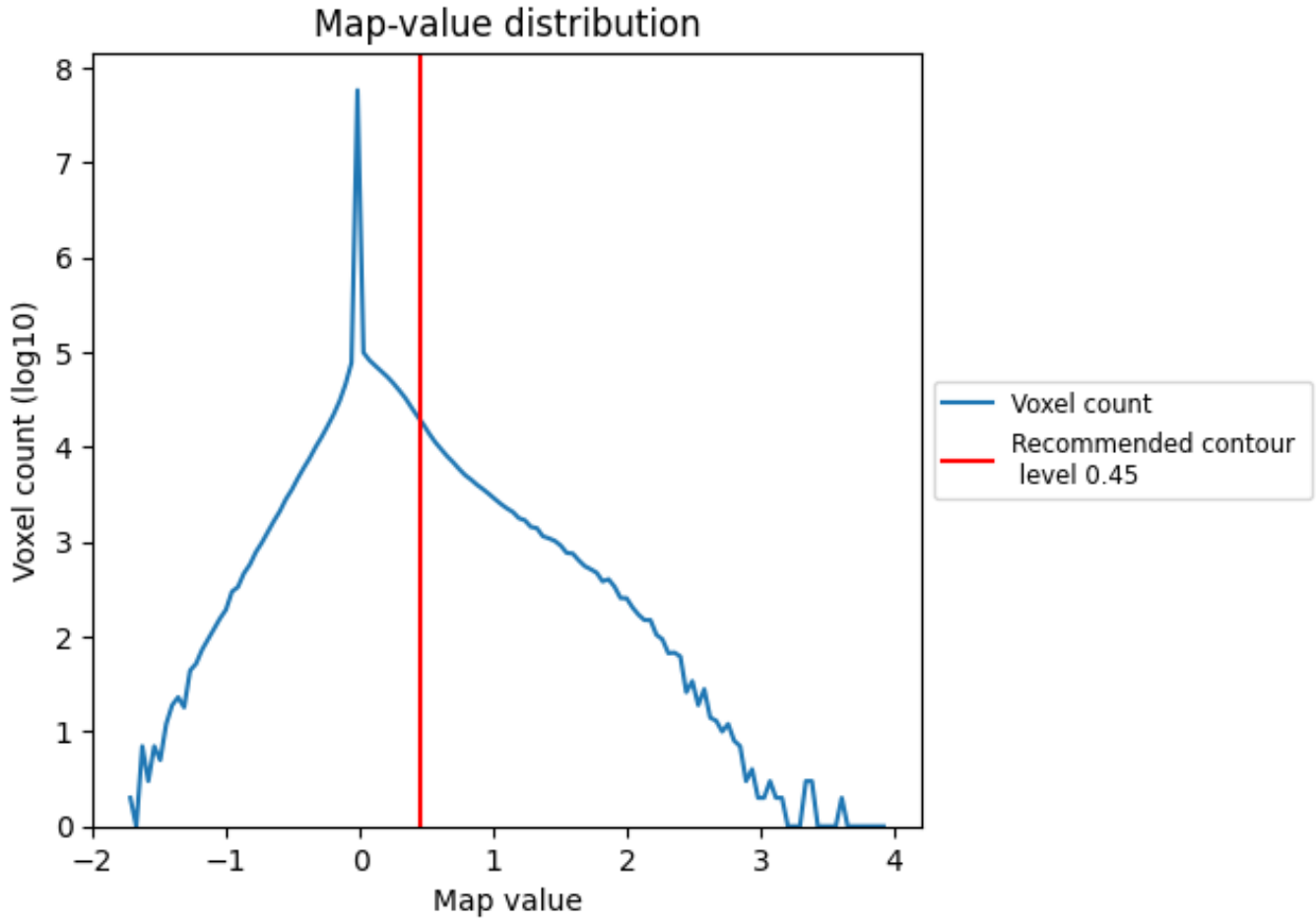
6.6 Mask visualisation (i)

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

7 Map analysis

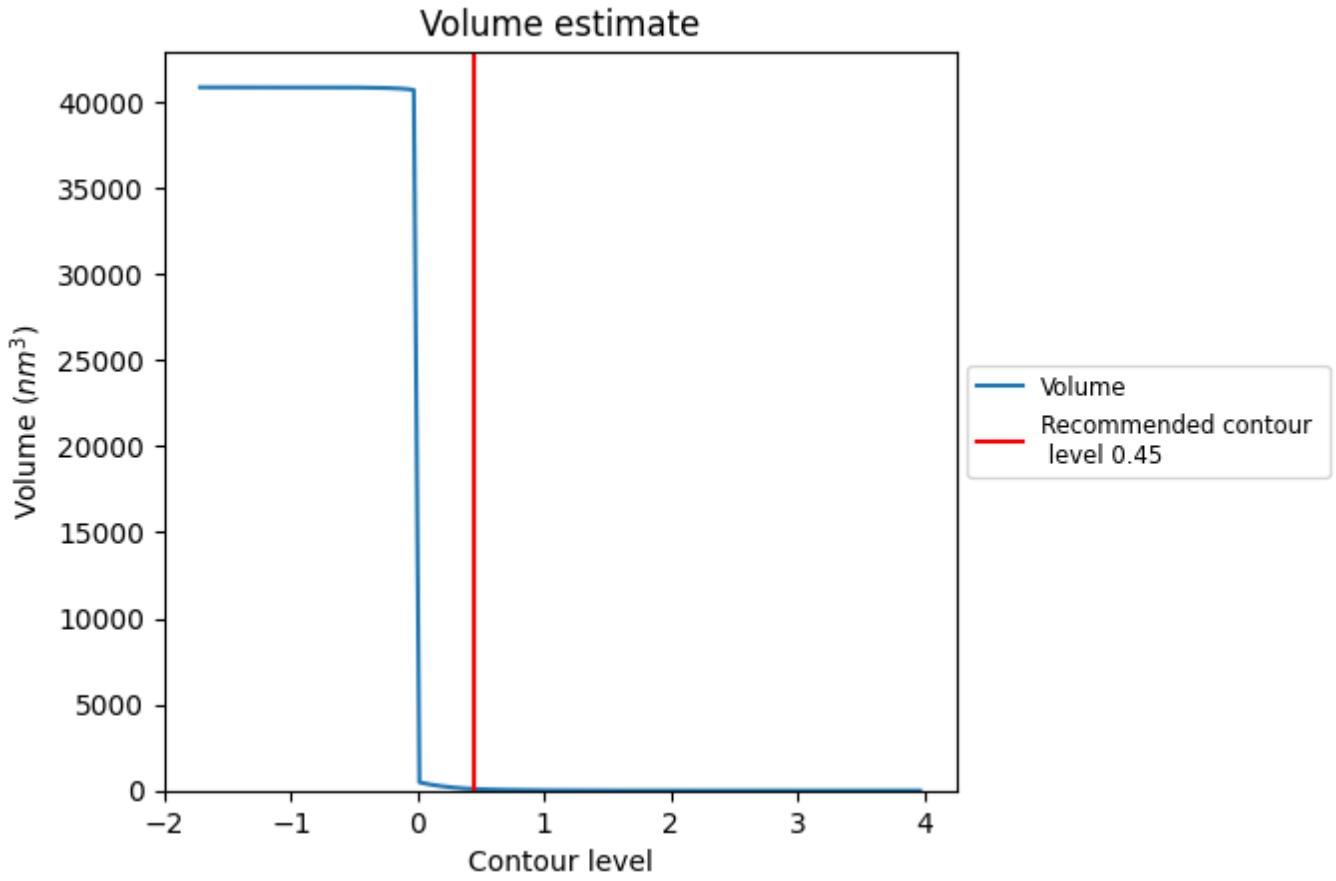
This section contains the results of statistical analysis of the map.

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.

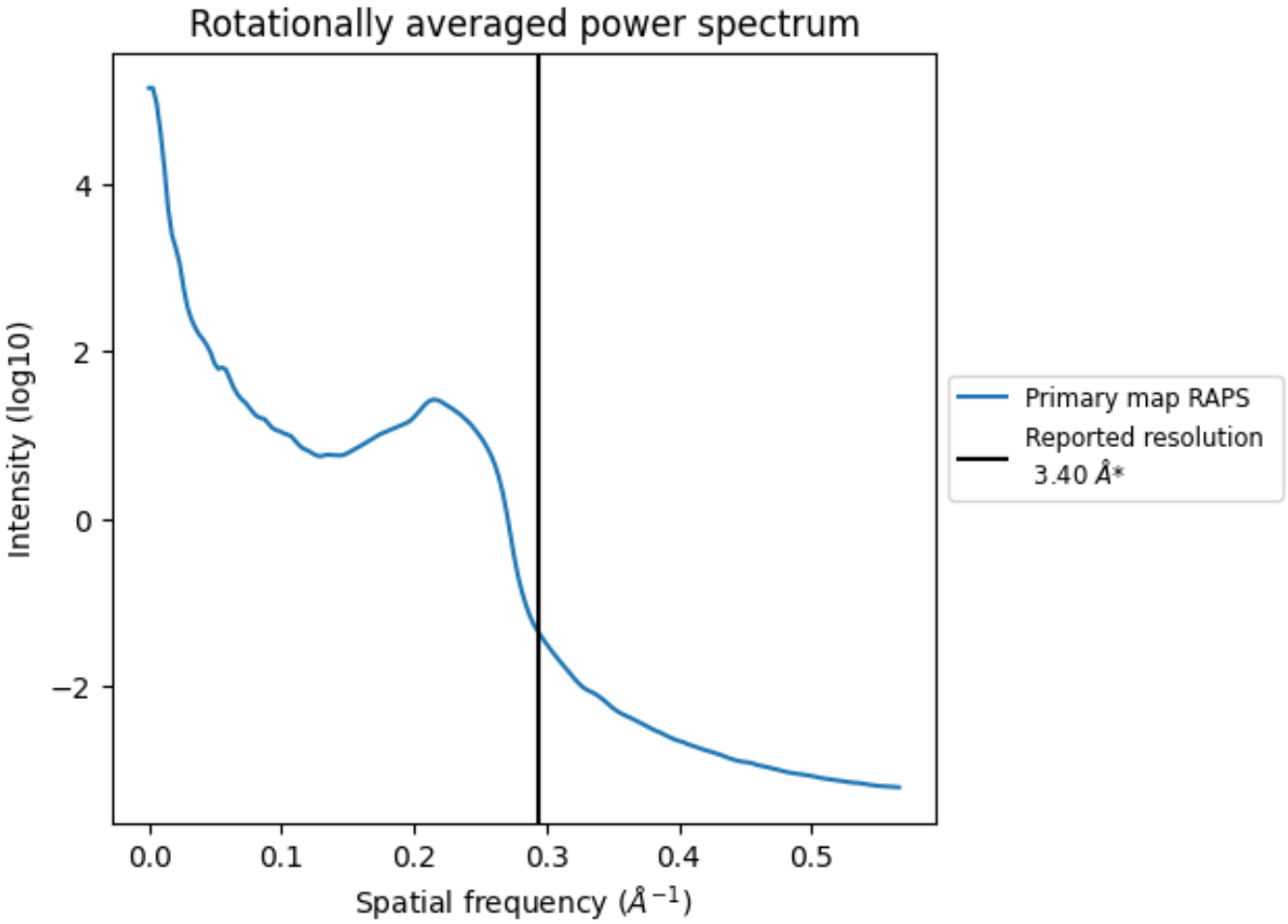
7.2 Volume estimate (i)



The volume at the recommended contour level is 91 nm^3; this corresponds to an approximate mass of 82 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 $Å^{-1}$

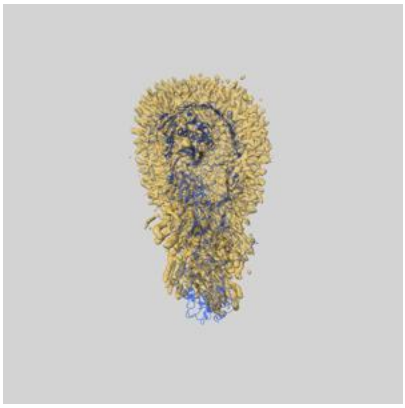
8 Fourier-Shell correlation

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

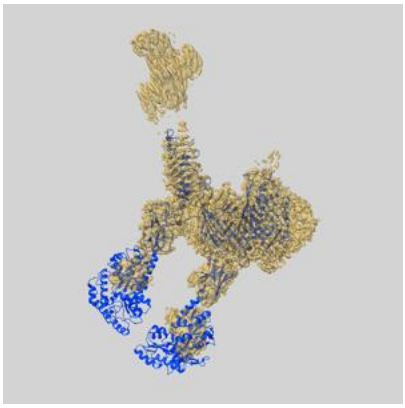
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12990 and PDB model 7OMM. Per-residue inclusion information can be found in section 3 on page 6.

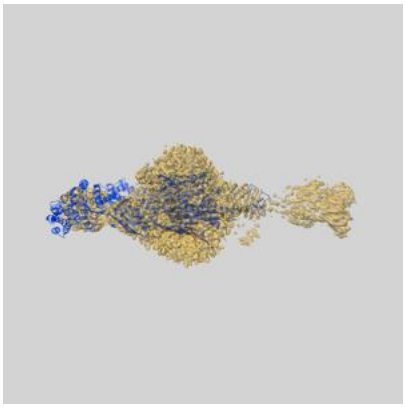
9.1 Map-model overlay



X



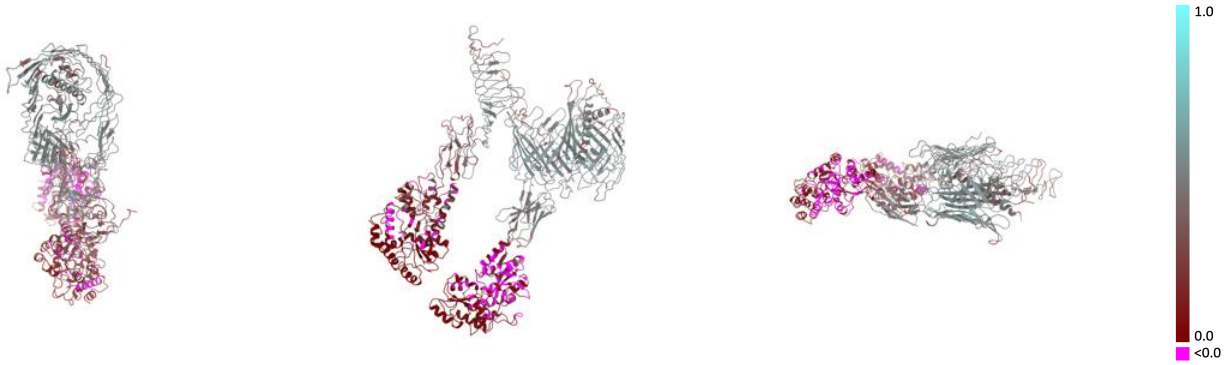
Y



Z

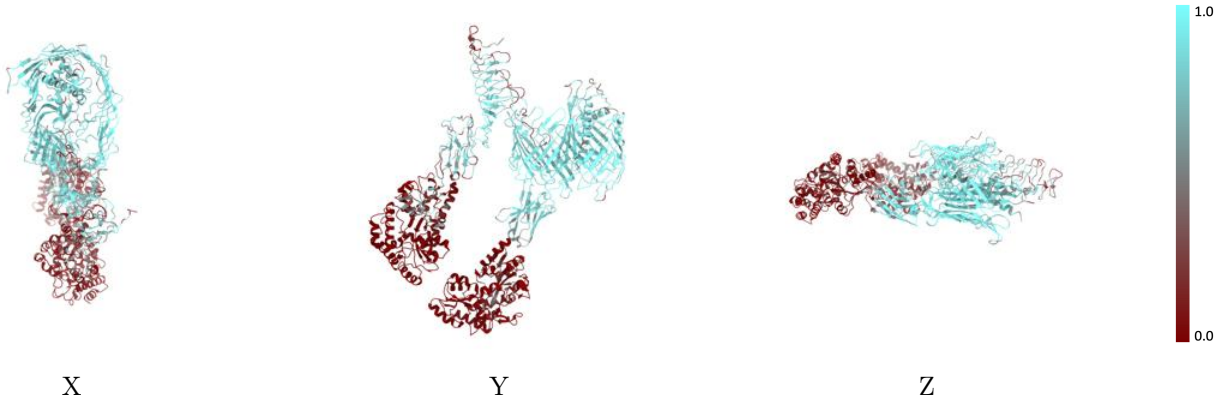
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



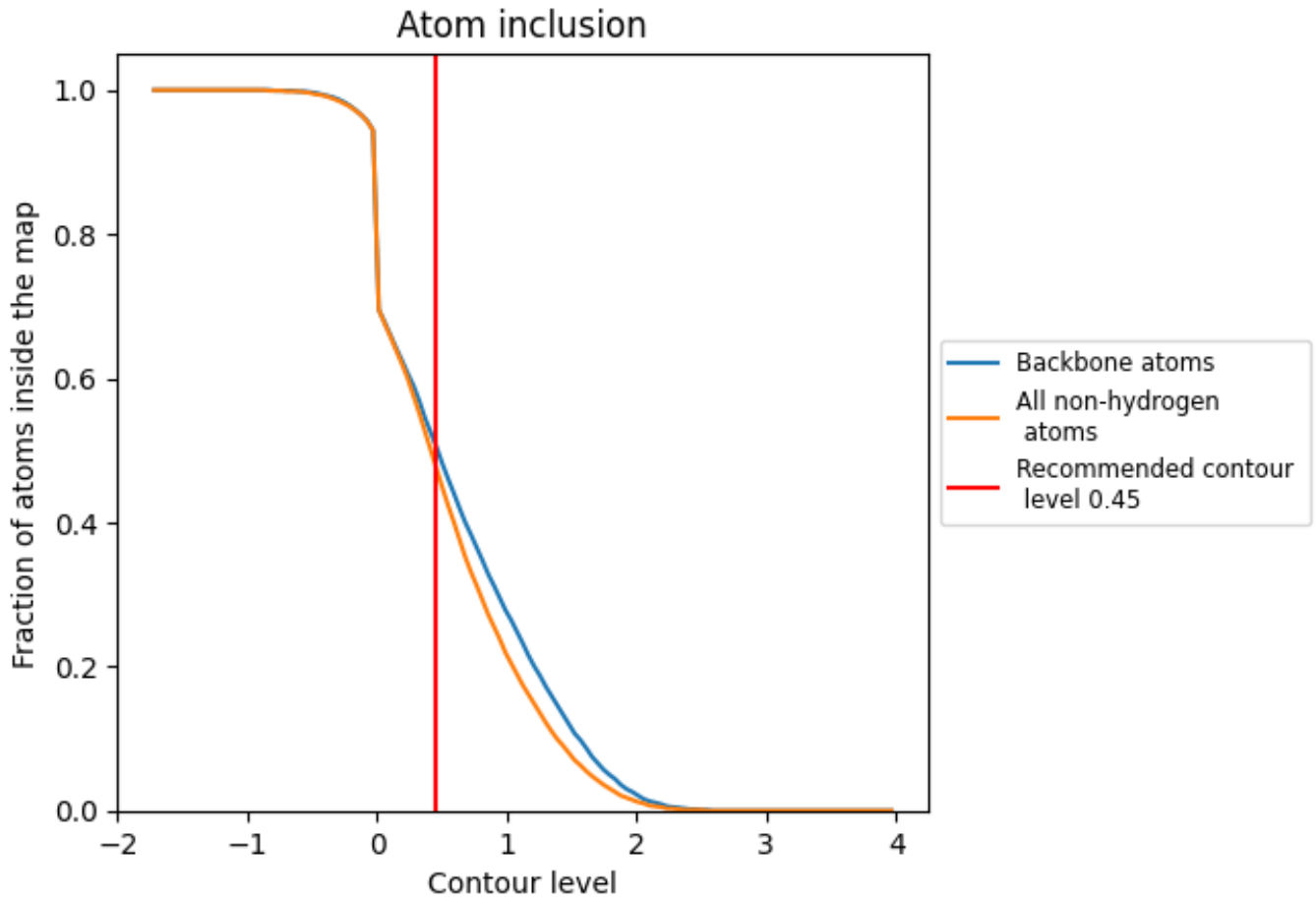
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.45).

9.4 Atom inclusion (i)



At the recommended contour level, 51% of all backbone atoms, 48% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4780	0.2830
A	0.7840	0.4720
B	0.7480	0.4570
C	0.2330	0.1050
D	0.2110	0.1380