wwPDB EM Validation Summary Report (i)

Nov 20, 2022 – 06:47 am GMT

PDB ID	:	6HDD
EMDB ID	:	EMD-0204
Title	:	OBP chaperonin in the nucleotide-free state
Authors	:	Semenyuk, P.I.; Stanishneva-Konovalova, T.B.; Sokolova, O.S.
Deposited on	:	2018-08-17
Resolution	:	4.50 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:

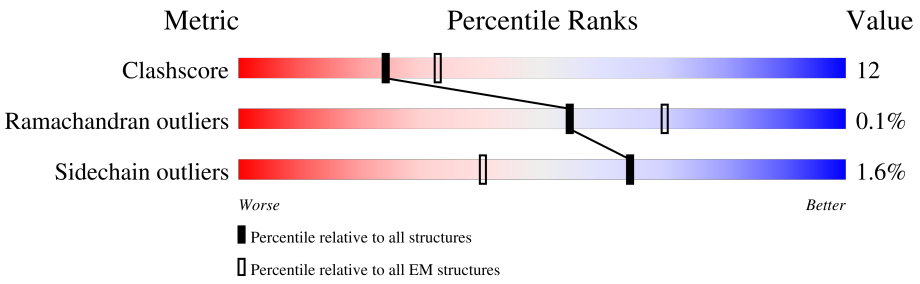
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.50 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	515	30% 70% 28% •
1	B	515	32% 69% 30% •
1	C	515	23% 70% 29% •
1	D	515	28% 66% 32% •
1	E	515	68% 74% 25% •
1	F	515	44% 69% 30% •
1	G	515	35% 66% 33% •

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 28154 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 Putative chaperonin GroEL.

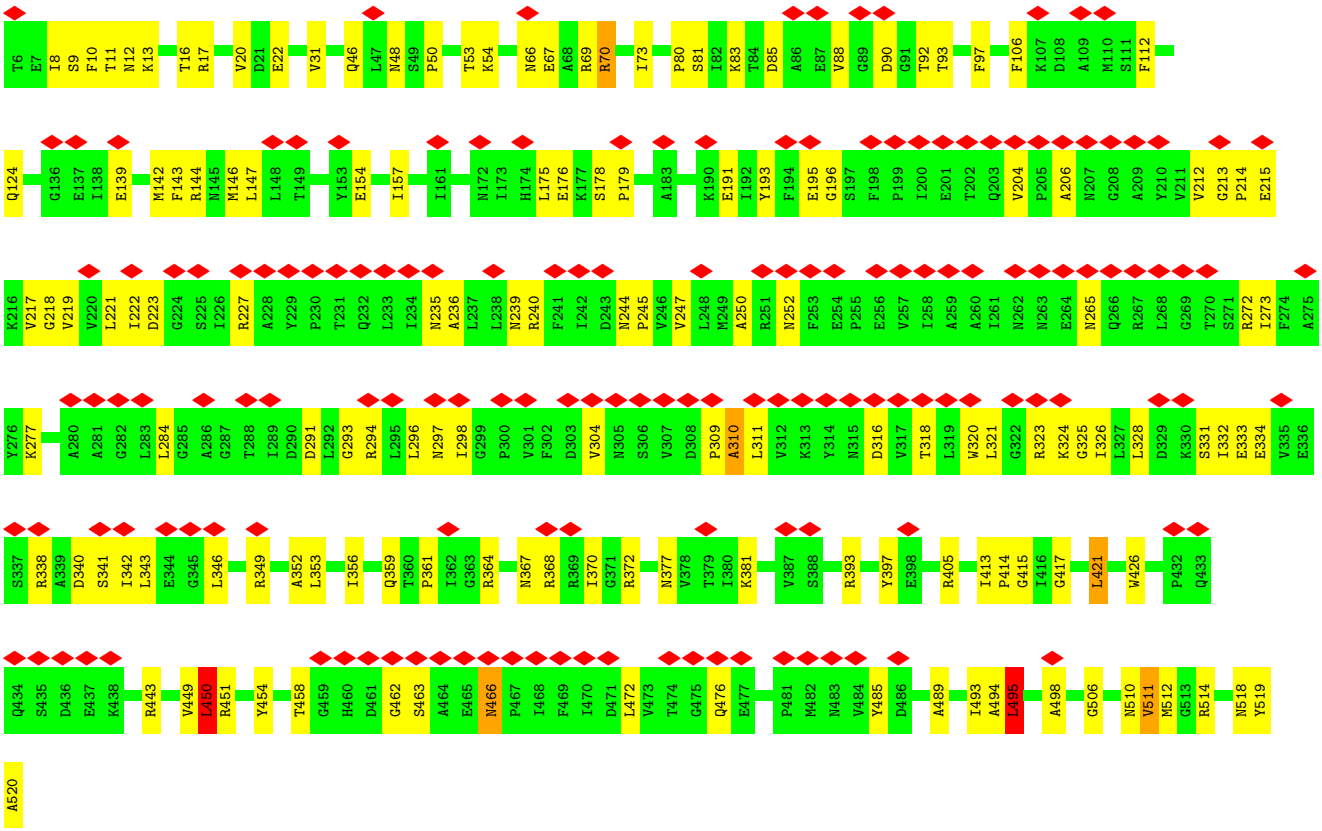
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	515	4022	2532	691	784	15	0	0
1	B	515	4022	2532	691	784	15	0	0
1	C	515	4022	2532	691	784	15	0	0
1	D	515	4022	2532	691	784	15	0	0
1	E	515	4022	2532	691	784	15	0	0
1	F	515	4022	2532	691	784	15	0	0
1	G	515	4022	2532	691	784	15	0	0

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.

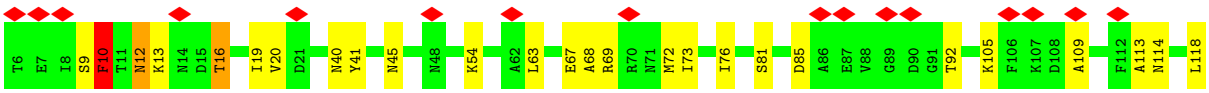
• Molecule 1: Putative chaperonin GroEL

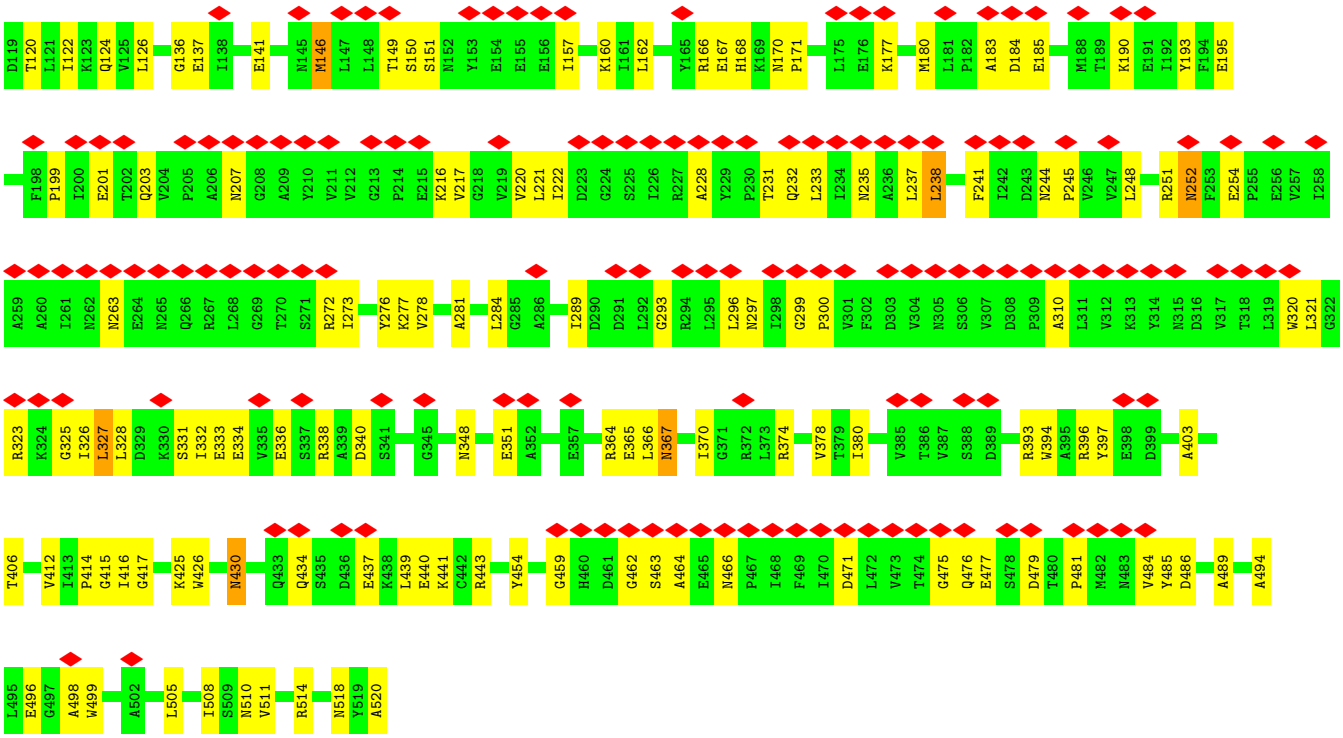
Chain A: 30% 70% 28%



• Molecule 1: Putative chaperonin GroEL

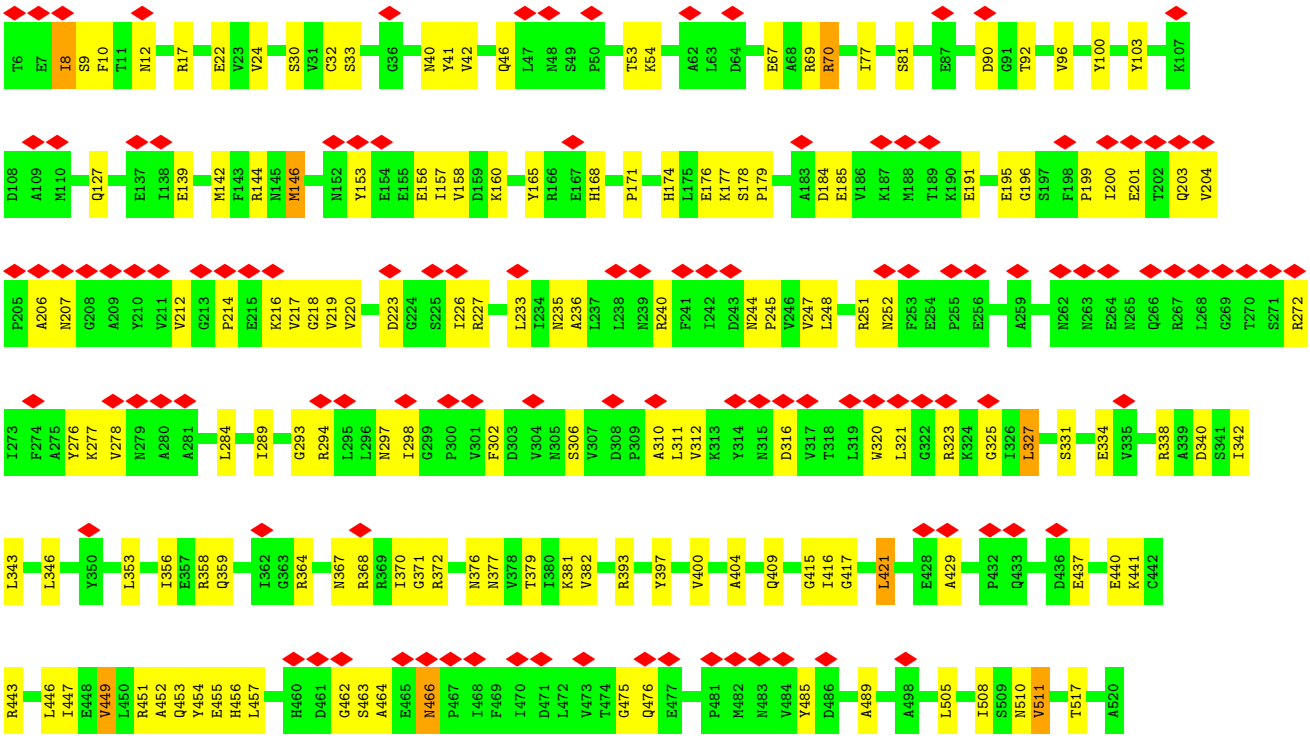
Chain B: 32% 69% 30%





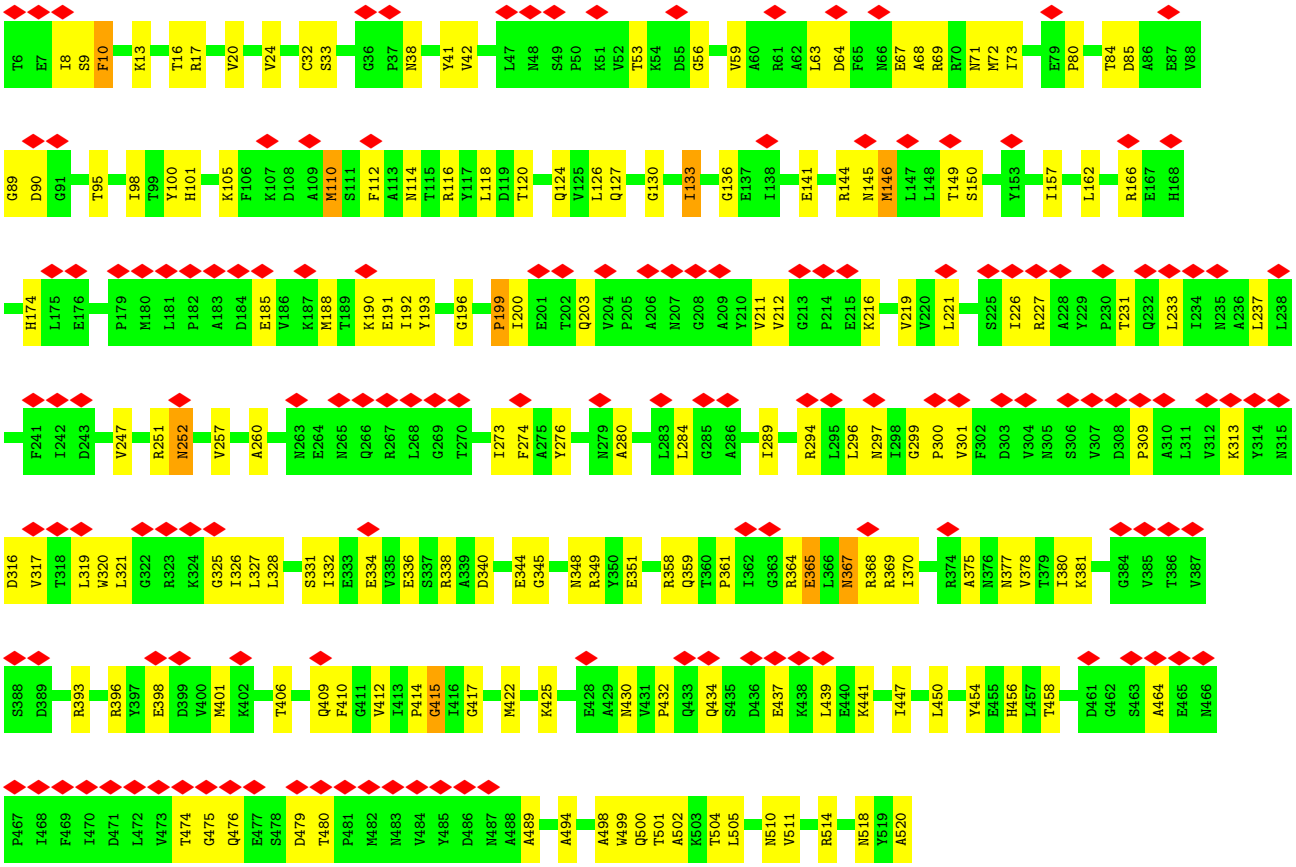
- Molecule 1: Putative chaperonin GroEL

Chain C:



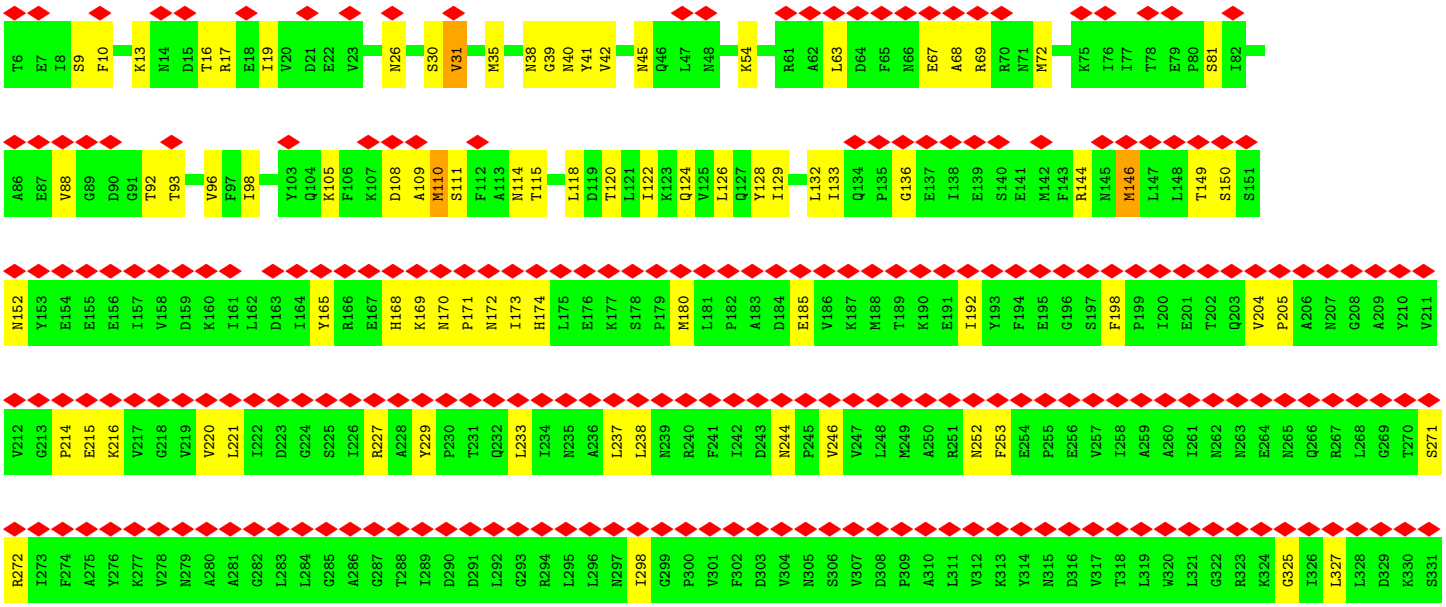
- Molecule 1: Putative chaperonin GroEL

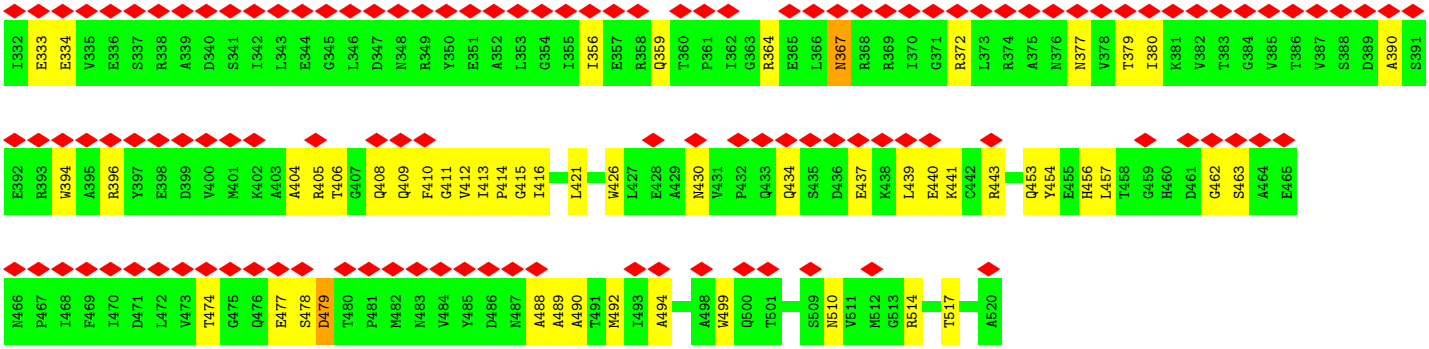
Chain D:



- Molecule 1: Putative chaperonin GroEL

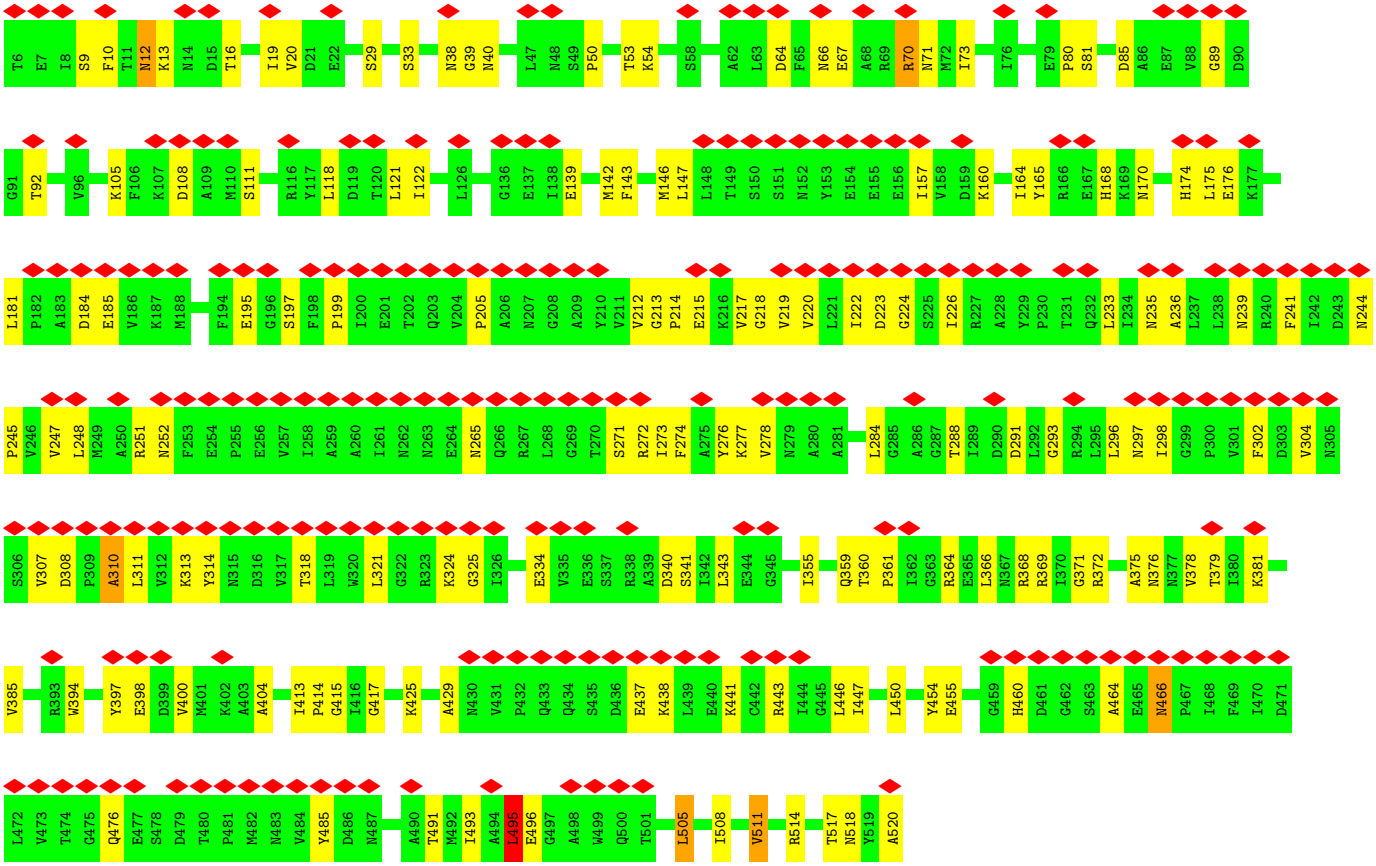
Chain E:





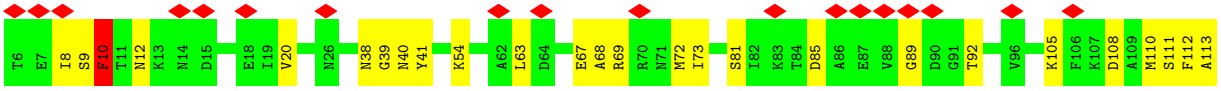
- Molecule 1: Putative chaperonin GroEL

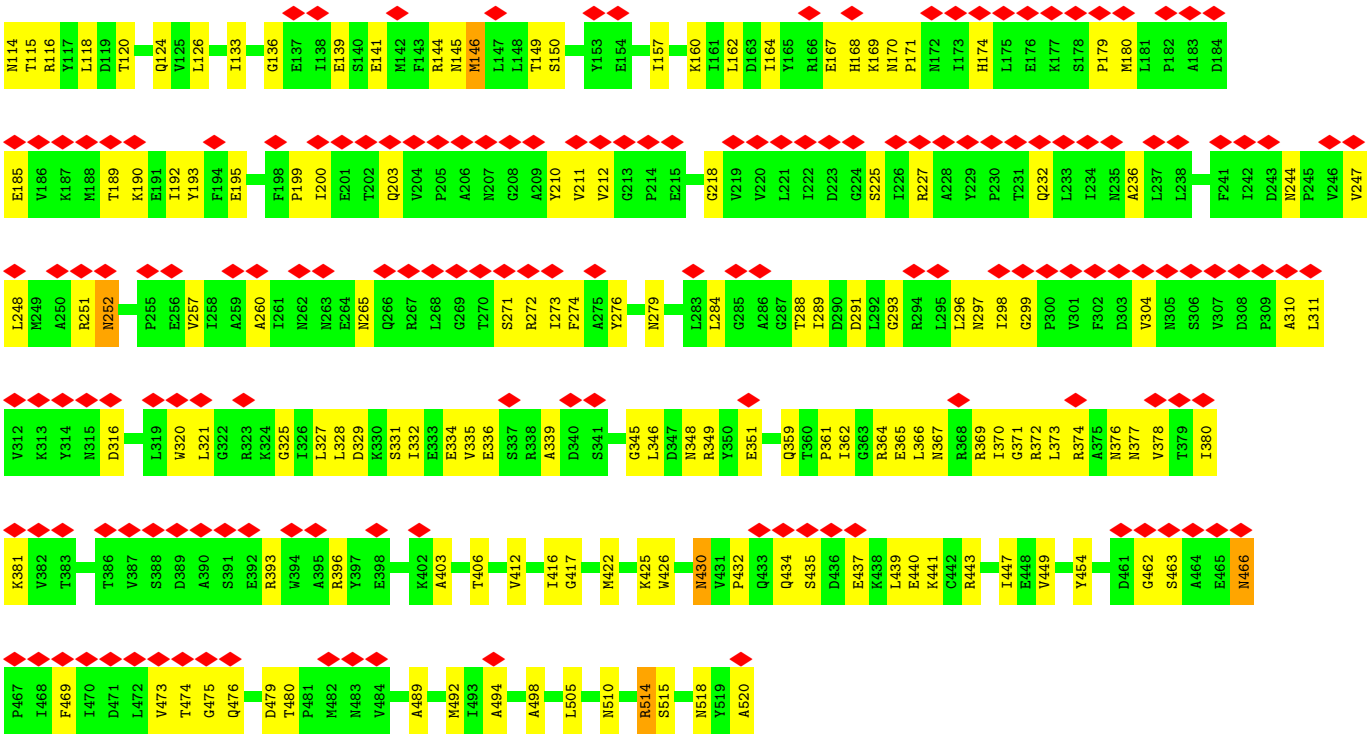
Chain F:



- Molecule 1: Putative chaperonin GroEL

Chain G:




N114 T115 R116 Y117 L118 D119 T120 Q124 V125 L126 I133 G136 E137 I138 E139 S140 E141 M142 F143 R144 N145 M146 L147 L148 T149 S150 Y153 E154 I157 K160 I161 L162 D163 I164 Y165 R166 E167 H168 K169 N170 P171 N172 I173 H174 L175 E176 K177 S178 P179 M180 L181 P182 A183 D184
E185 V186 K187 M188 T189 K190 E191 I192 Y193 F194 E195 F198 P199 I200 E201 T202 Q203 V204 P205 A206 N207 G208 A209 Y210 V211 V212 G213 P214 E215 G218 V219 V220 L221 I222 D223 G224 S225 I226 R227 A228 Y229 P230 T231 Q232 L233 I234 N235 A236 L237 L238 P241 I242 D243 N244 P245 V246 V247
L248 M249 A250 R251 N252 P255 E256 V257 I258 A259 A260 I261 N262 N263 E264 N265 Q266 R267 L268 G269 T270 S271 R272 I273 F274 A275 Y276 N279 L283 L284 G285 A286 G287 T288 I289 D290 D291 L292 G293 R294 L295 L296 N297 I298 G299 P300 V301 F302 D303 V304 N305 S306 V307 D308 P309 A310 L311
V312 K313 Y314 N315 D316 L319 W320 L321 G322 R323 K324 G325 I326 L327 L328 D329 K330 S331 I332 E333 E334 V335 E336 S337 R338 A339 D340 S341 G345 L346 D347 N348 R349 Y350 E351 Q359 T360 P361 I362 G363 R364 E365 L366 N367 R368 R369 I370 G371 R372 L373 R374 A375 N376 N377 V378 T379 I380
K381 V382 T383 T386 V387 S388 D389 A390 S391 E392 R393 W394 A395 R396 Y397 E398 K402 A403 T406 V412 I416 G417 M422 K425 W426 N430 V431 P432 Q433 Q434 S435 D436 E437 K438 L439 E440 K441 C442 R443 I447 E448 V449 Y454 D461 G462 S463 A464 E465 N466
P467 I468 F469 I470 D471 L472 V473 T474 G475 Q476 D479 T480 P481 M482 N483 V484 A489 M492 I493 A494 A498 L505 N510 R514 S515 N518 Y519 A520

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	127180	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 ($e^-/Å^2$)	100	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.228	Depositor
Minimum map value	-0.070	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	220.16, 220.16, 220.16	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	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	0.54	1/4088 (0.0%)	0.76	2/5545 (0.0%)
1	B	0.46	0/4088	0.72	3/5545 (0.1%)
1	C	0.48	0/4088	0.71	2/5545 (0.0%)
1	D	0.40	0/4088	0.70	1/5545 (0.0%)
1	E	0.38	0/4088	0.65	1/5545 (0.0%)
1	F	0.44	0/4088	0.70	2/5545 (0.0%)
1	G	0.47	0/4088	0.72	2/5545 (0.0%)
All	All	0.45	1/28616 (0.0%)	0.71	13/38815 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	8
1	C	0	7
1	D	0	4
1	E	0	5
1	F	0	5
1	G	0	5
All	All	0	42

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	31	VAL	CB-CG2	-5.03	1.42	1.52

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	505	LEU	CB-CG-CD1	-9.00	95.69	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	133	ILE	C-N-CA	7.90	141.46	121.70
1	G	505	LEU	CB-CG-CD1	-7.89	97.59	111.00
1	A	450	LEU	CA-CB-CG	-6.55	100.24	115.30
1	F	495	LEU	CB-CG-CD2	-6.21	100.44	111.00

There are no chirality outliers.

5 of 42 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	ASN	Peptide
1	A	213	GLY	Peptide
1	A	310	ALA	Peptide
1	A	414	PRO	Peptide
1	A	415	GLY	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4022	0	4021	96	0
1	B	4022	0	4021	104	0
1	C	4022	0	4021	103	0
1	D	4022	0	4020	107	0
1	E	4022	0	4021	84	0
1	F	4022	0	4021	99	0
1	G	4022	0	4021	110	0
All	All	28154	0	28146	671	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 671 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:361:PRO:HG3	1:A:364:ARG:HH21	1.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:LEU:O	1:D:166:ARG:HB2	1.82	0.79
1:B:325:GLY:O	1:B:334:GLU:HA	1.86	0.75
1:C:293:GLY:HA2	1:C:298:ILE:HB	1.69	0.74
1:E:421:LEU:HD11	1:E:454:TYR:HB2	1.69	0.73

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	513/515 (100%)	411 (80%)	101 (20%)	1 (0%)	47	81
1	B	513/515 (100%)	420 (82%)	93 (18%)	0	100	100
1	C	513/515 (100%)	425 (83%)	87 (17%)	1 (0%)	47	81
1	D	513/515 (100%)	421 (82%)	89 (17%)	3 (1%)	25	65
1	E	513/515 (100%)	418 (82%)	95 (18%)	0	100	100
1	F	513/515 (100%)	426 (83%)	87 (17%)	0	100	100
1	G	513/515 (100%)	408 (80%)	105 (20%)	0	100	100
All	All	3591/3605 (100%)	2929 (82%)	657 (18%)	5 (0%)	54	85

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	PHE
1	D	414	PRO
1	D	415	GLY
1	C	416	ILE
1	D	199	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	439/439 (100%)	433 (99%)	6 (1%)	67	81
1	B	439/439 (100%)	432 (98%)	7 (2%)	62	79
1	C	439/439 (100%)	434 (99%)	5 (1%)	73	85
1	D	439/439 (100%)	432 (98%)	7 (2%)	62	79
1	E	439/439 (100%)	432 (98%)	7 (2%)	62	79
1	F	439/439 (100%)	431 (98%)	8 (2%)	59	77
1	G	439/439 (100%)	430 (98%)	9 (2%)	53	72
All	All	3073/3073 (100%)	3024 (98%)	49 (2%)	64	79

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	146	MET
1	F	252	ASN
1	E	252	ASN
1	F	70	ARG
1	F	491	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	252	ASN
1	G	38	ASN
1	E	367	ASN
1	F	101	HIS
1	G	174	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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.

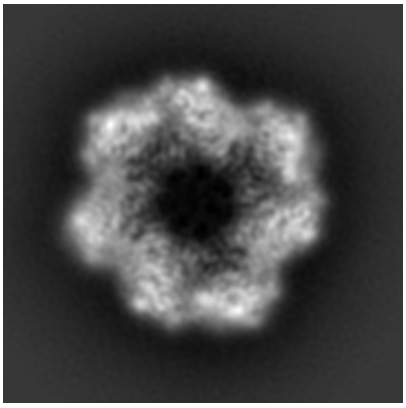
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0204. These allow visual inspection of the internal detail of the map and identification of artifacts.

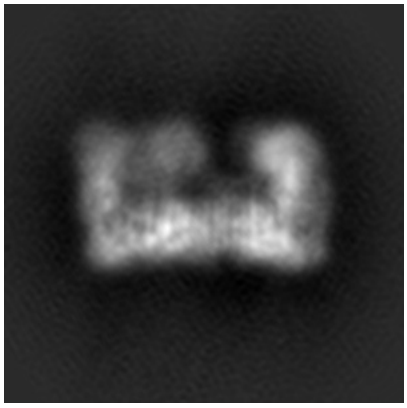
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

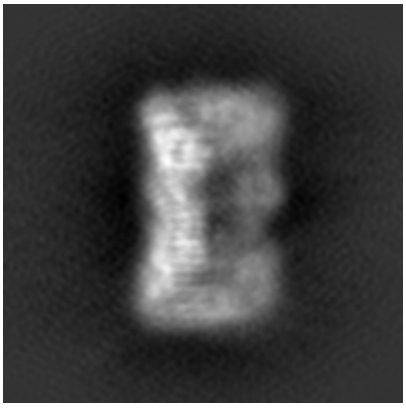
6.1.1 Primary map



X



Y

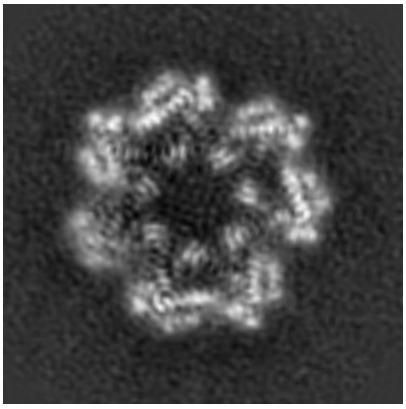


Z

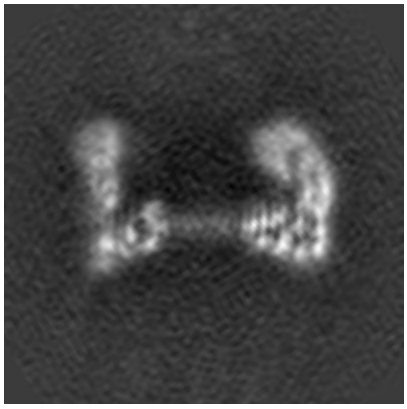
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 128



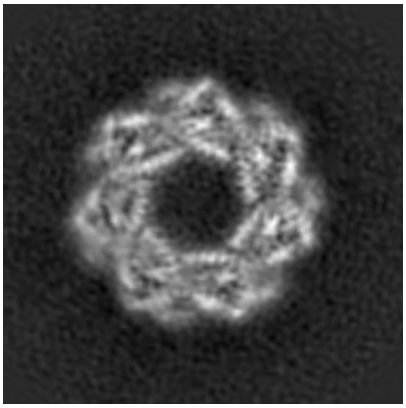
Y Index: 128

Z Index: 128

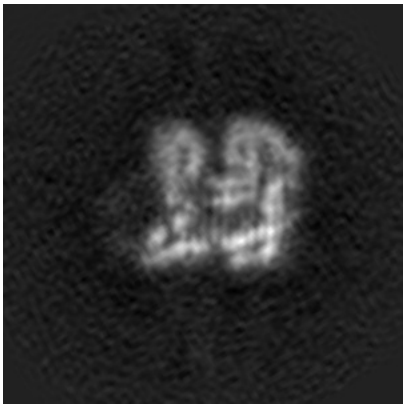
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

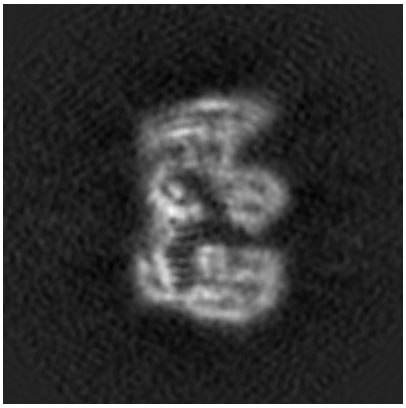
6.3.1 Primary map



X Index: 103



Y Index: 183



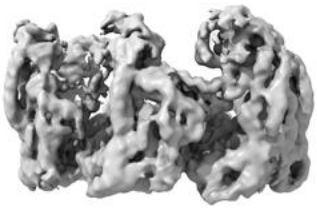
Z Index: 180

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

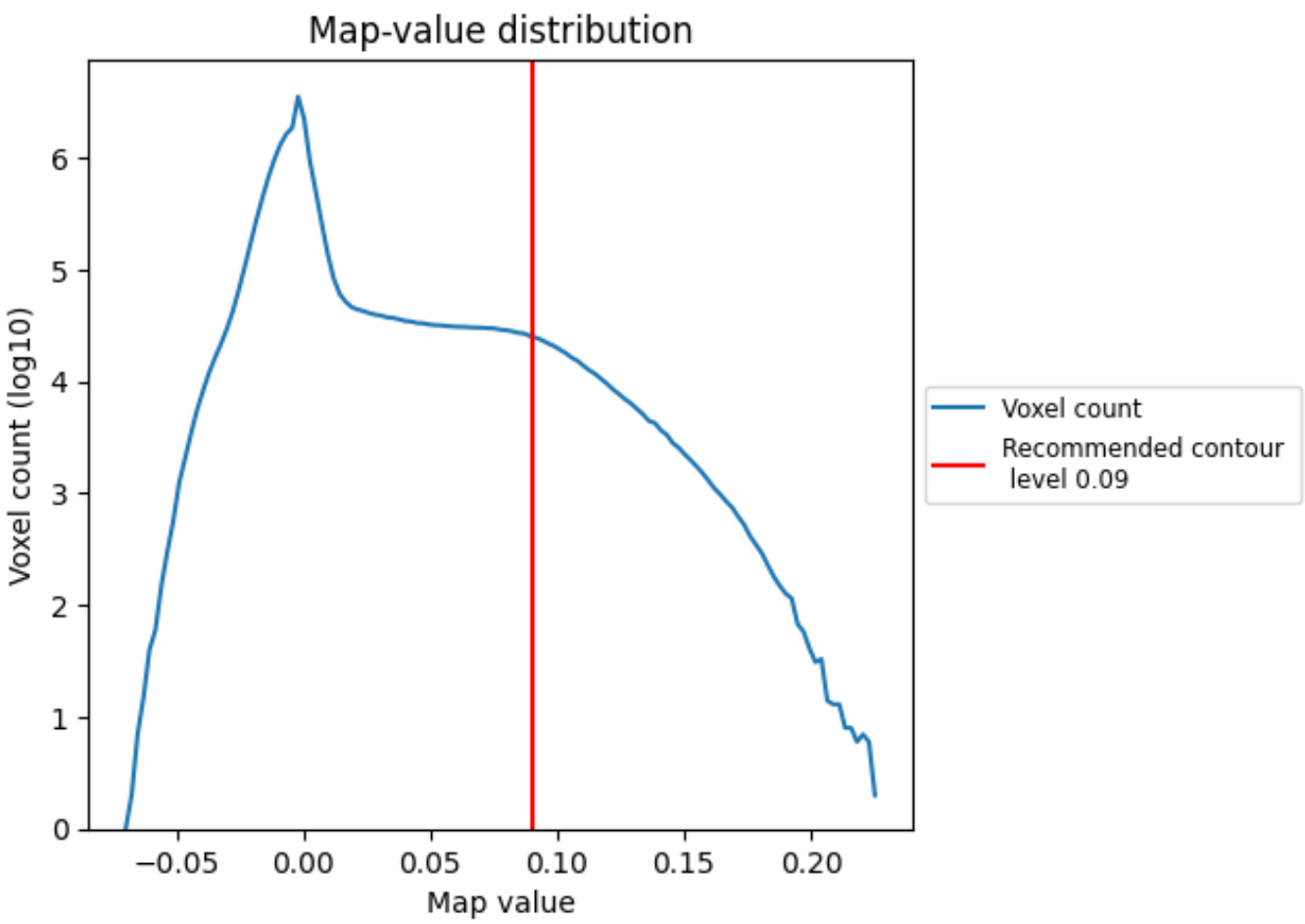
6.5 Mask visualisation (i)

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

7 Map analysis (i)

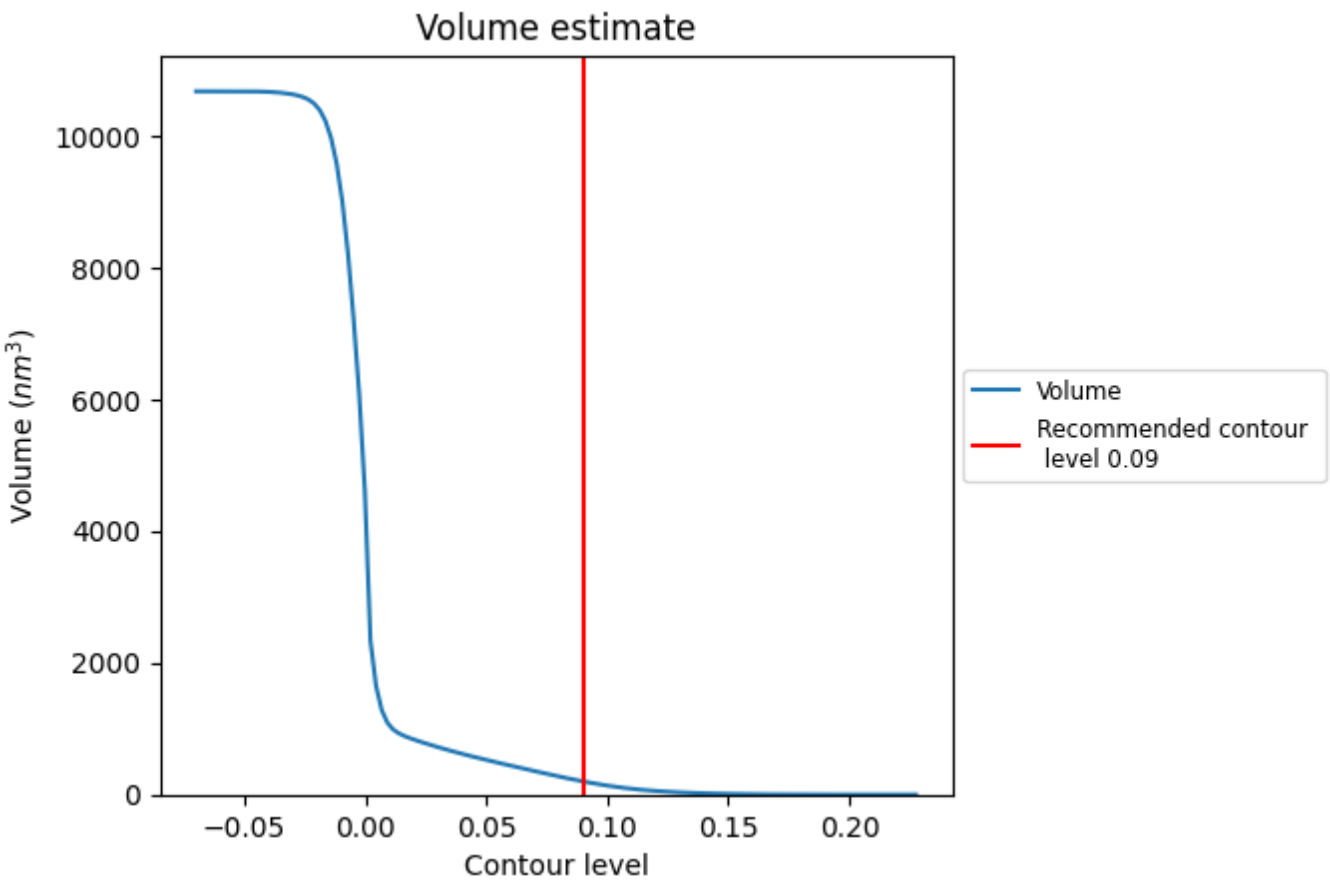
This section contains the results of statistical analysis of the map.

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.

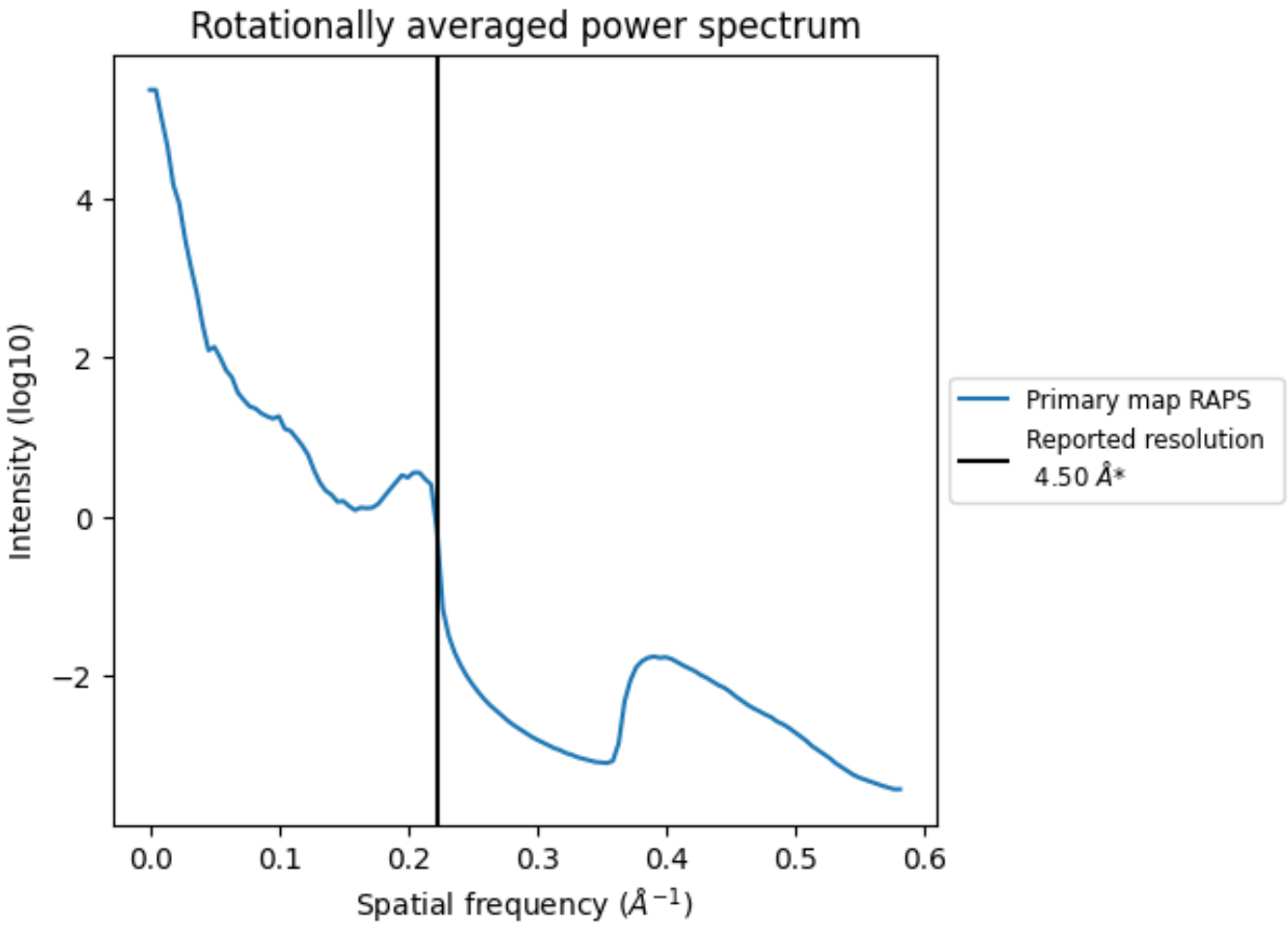
7.2 Volume estimate (i)



The volume at the recommended contour level is 200 nm^3; this corresponds to an approximate mass of 180 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)

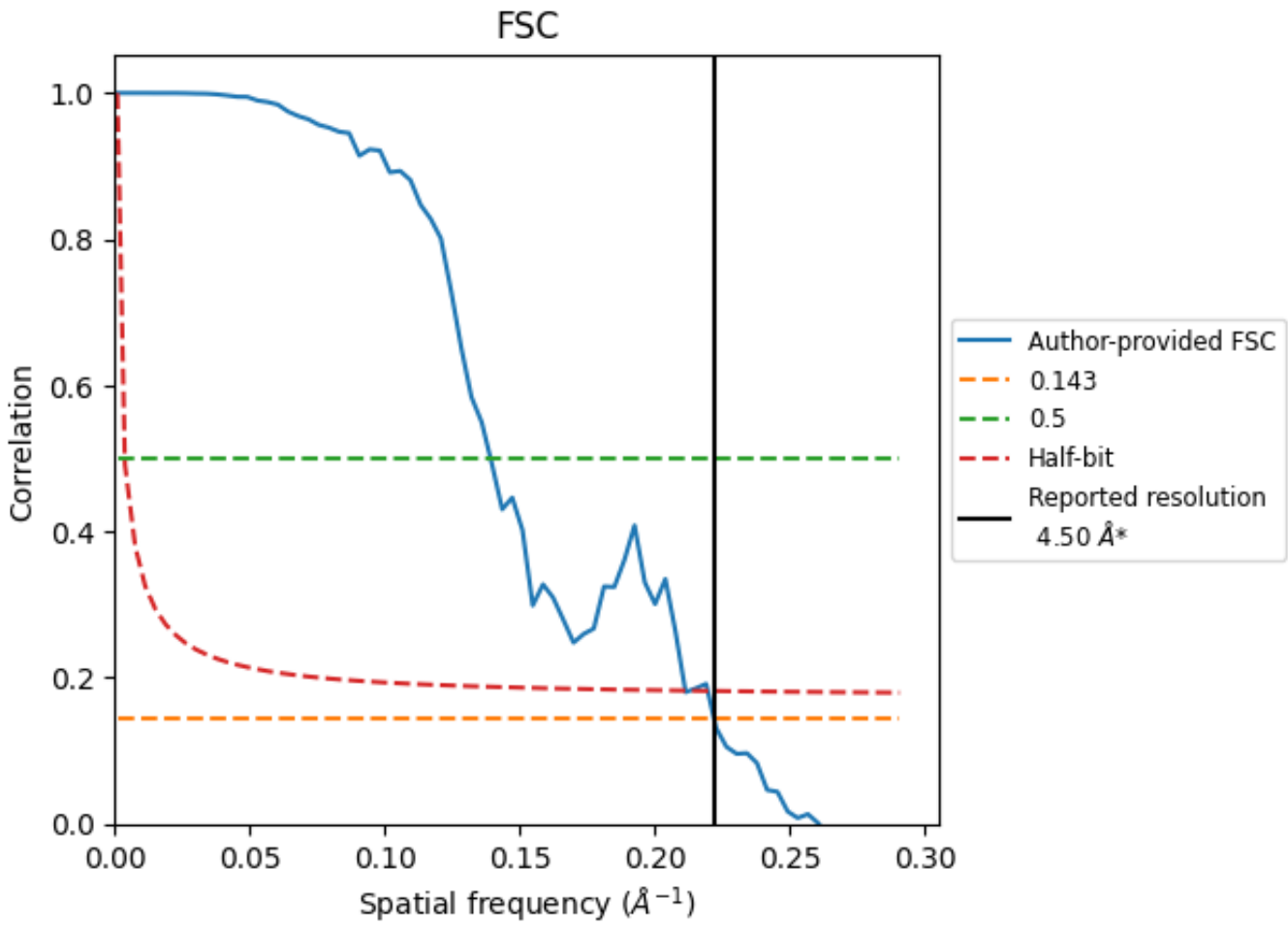


*Reported resolution corresponds to spatial frequency of 0.222 Å^{-1}

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 0.222 Å^{-1}

8.2 Resolution estimates (i)

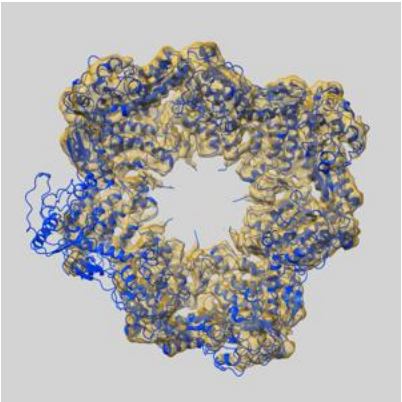
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.50	7.18	4.73
Unmasked-calculated*	-	-	-

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

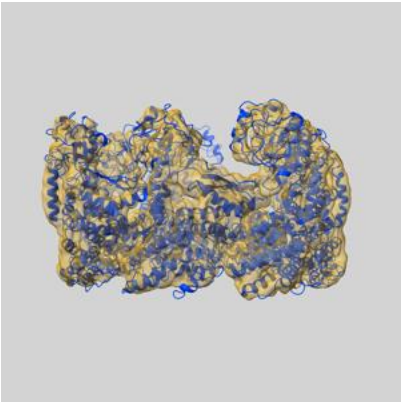
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0204 and PDB model 6HDD. Per-residue inclusion information can be found in section 3 on page 4.

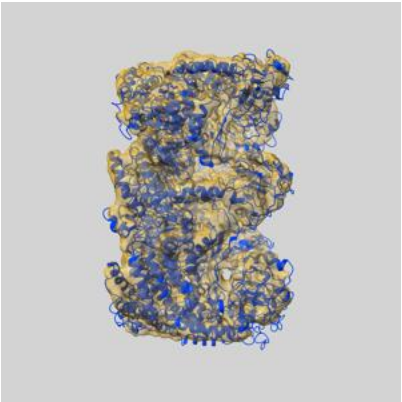
9.1 Map-model overlay (i)



X



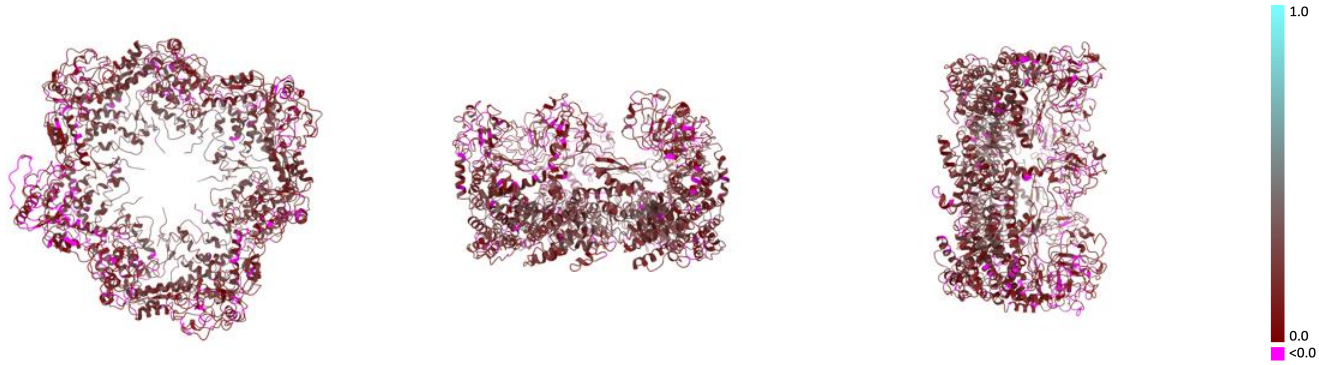
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

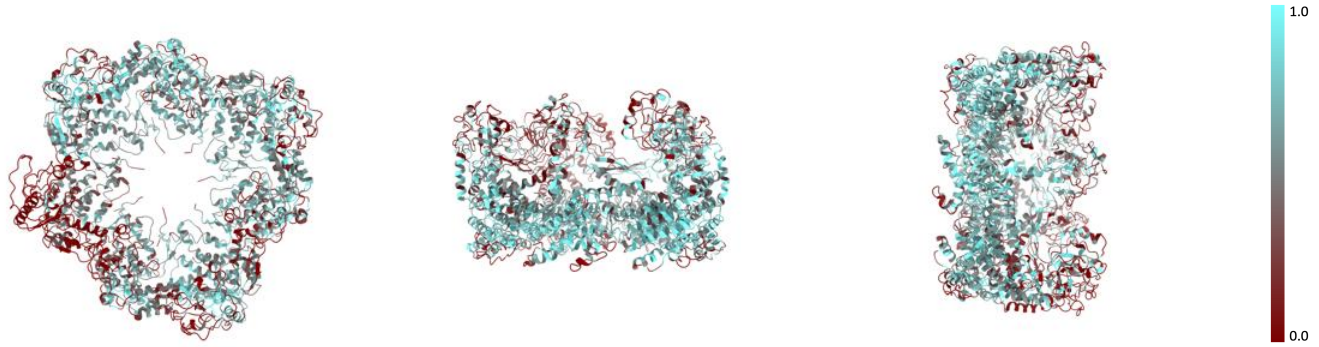
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

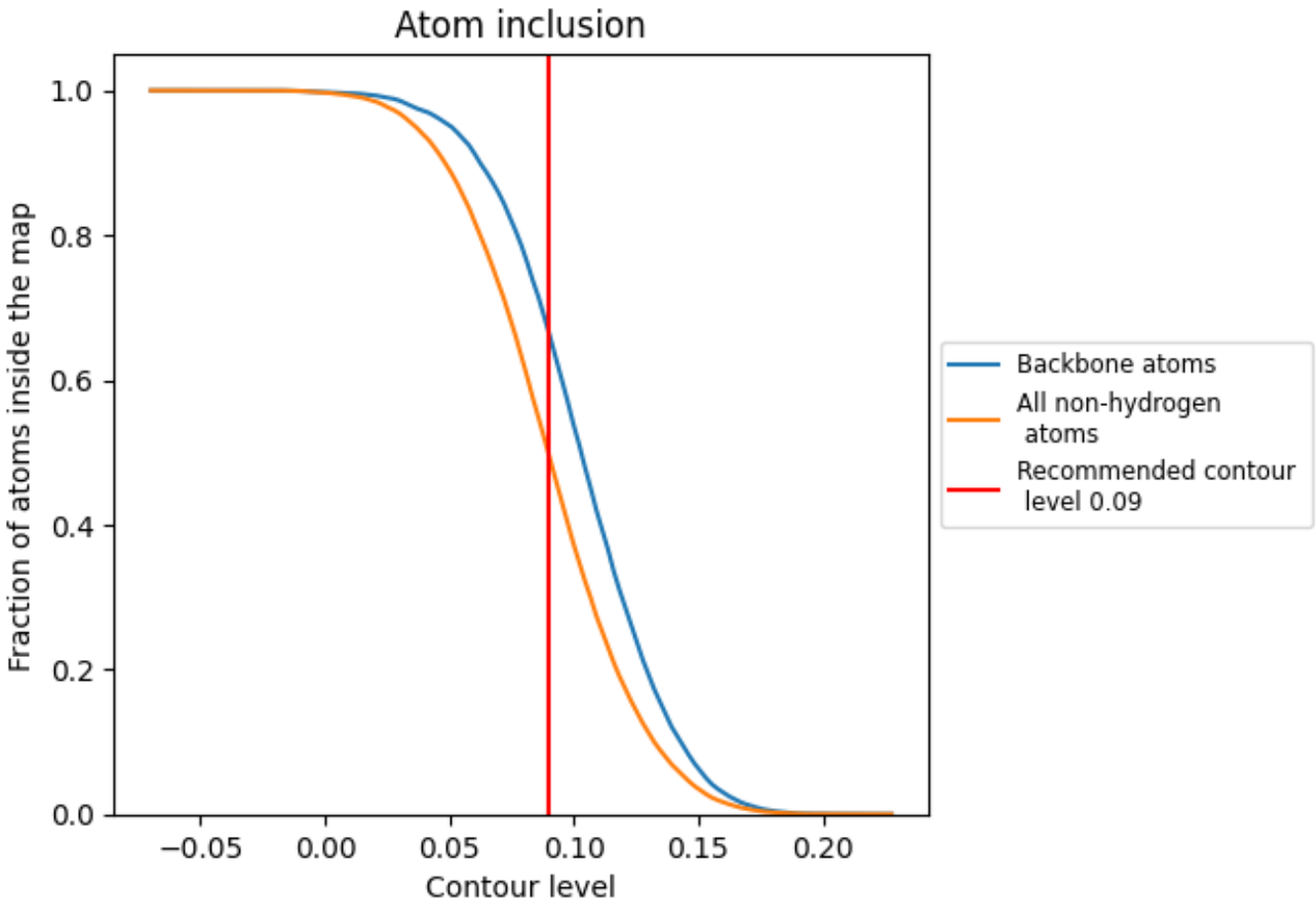
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.09).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 50% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4959	0.1640
A	0.5516	0.1870
B	0.5417	0.1820
C	0.6097	0.1880
D	0.5585	0.1580
E	0.2498	0.1040
F	0.4494	0.1610
G	0.5105	0.1680