Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 11:25 am GMT

PDB ID	:	6QD3
EMDB ID	:	EMD-4518
Title	:	MloK1 model from single particle analysis of 2D crystals, class 7 (intermediate conformation)
Authors	:	Righetto, R.; Biyani, N.; Kowal, J.; Chami, M.; Stahlberg, H.
Deposited on	:	2018-12-31
Resolution	:	5.00 Å(reported)
Based on initial model	:	6I9D

This is a Full wwPDB EM Validation 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:

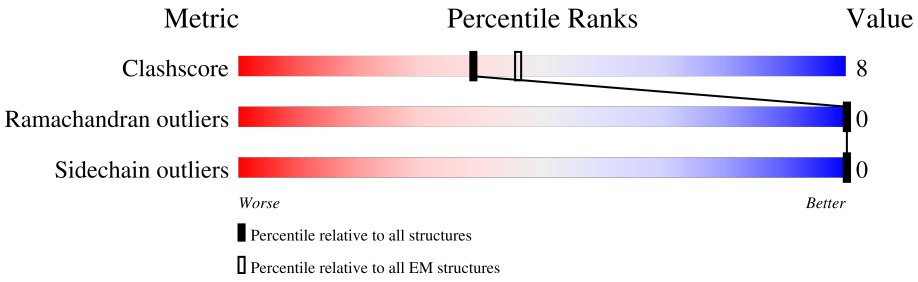
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 5.00 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	355	66% 80% 19%
1	B	355	67% 80% 19%
1	C	355	66% 81% 18%
1	D	355	66% 81% 18%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 21746 atoms, of which 11100 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 Cyclic nucleotide-gated potassium channel mll3241.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	355	Total	C	H	N	O	S	0	0
			5436	1734	2775	455	461	11		
1	B	355	Total	C	H	N	O	S	0	0
			5436	1734	2775	455	461	11		
1	C	355	Total	C	H	N	O	S	0	0
			5436	1734	2775	455	461	11		
1	D	355	Total	C	H	N	O	S	0	0
			5436	1734	2775	455	461	11		

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

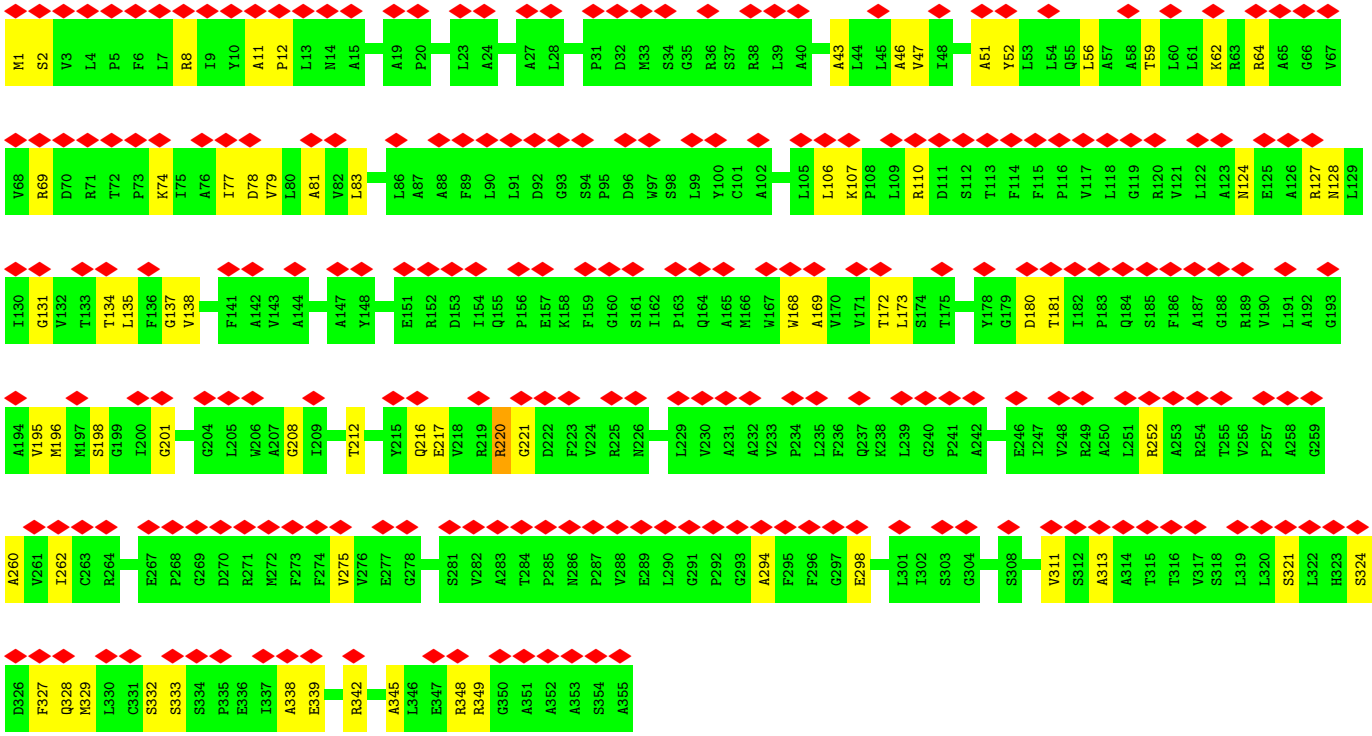
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	K	0
			1	1	
2	B	1	Total	K	0
			1	1	

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.

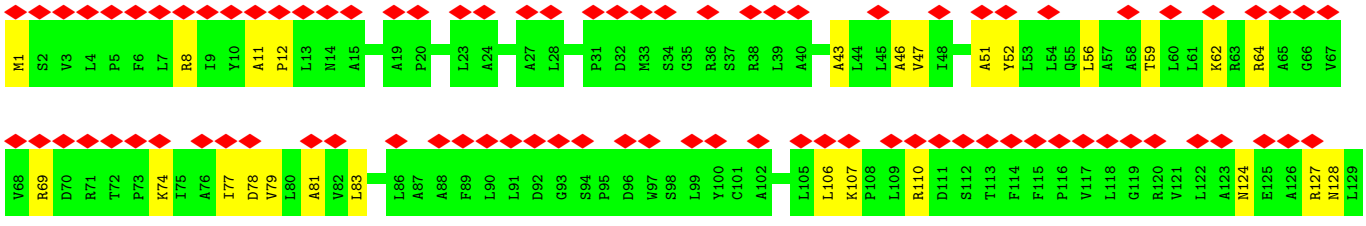
• Molecule 1: Cyclic nucleotide-gated potassium channel mll3241

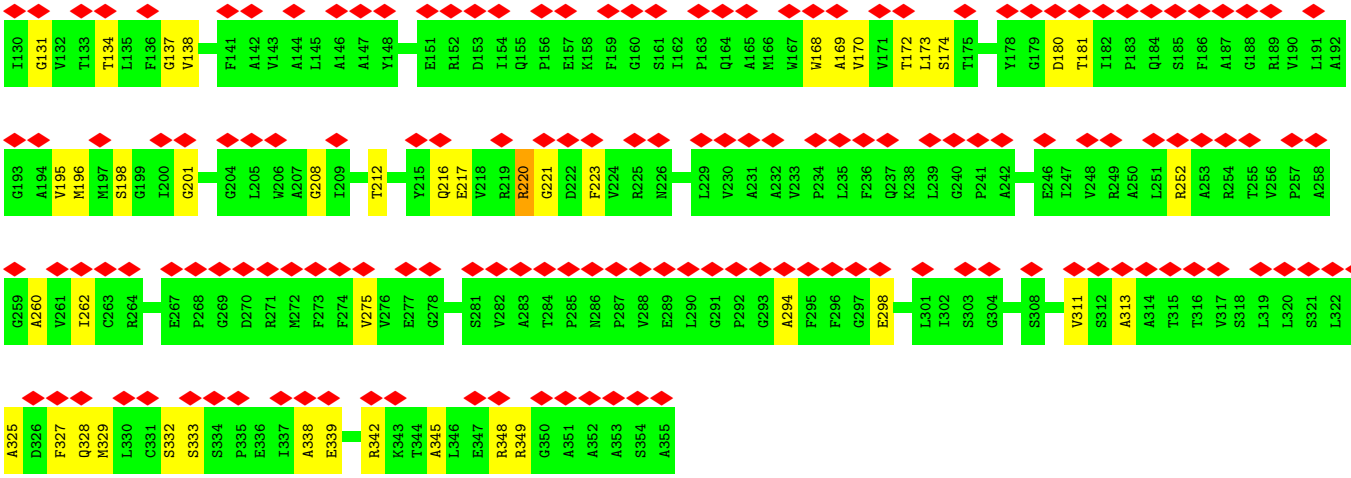
Chain A:



• Molecule 1: Cyclic nucleotide-gated potassium channel mll3241

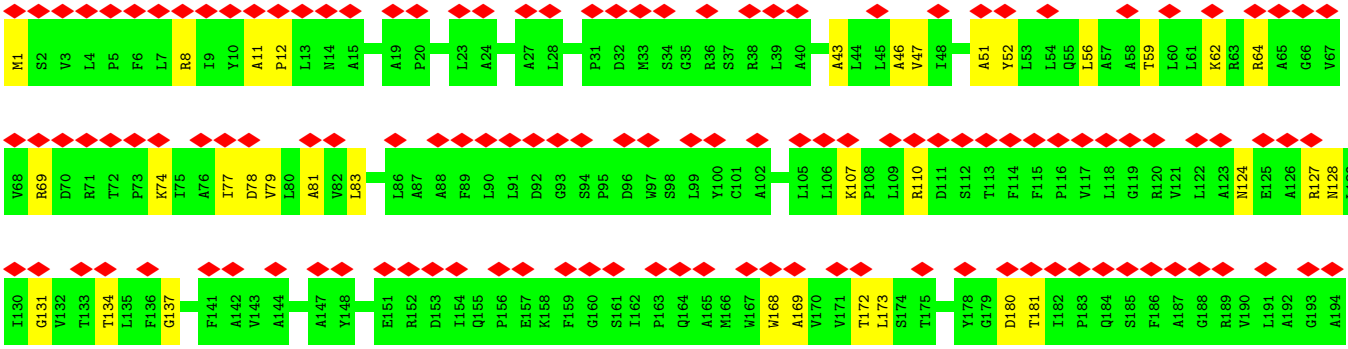
Chain B:





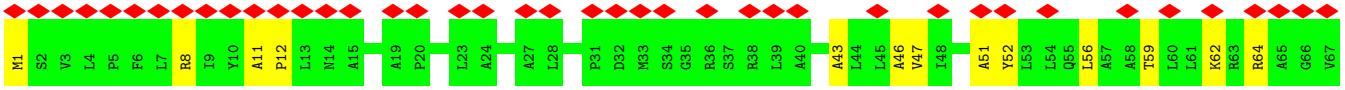
• Molecule 1: Cyclic nucleotide-gated potassium channel mll3241

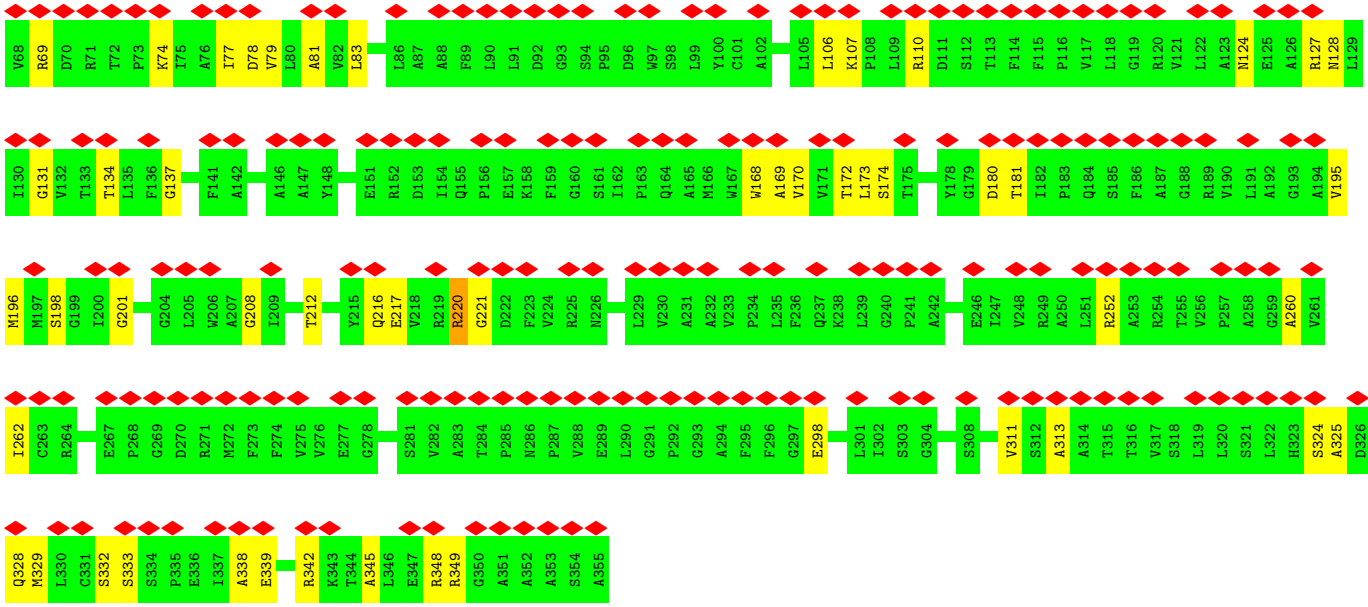
Chain C:



• Molecule 1: Cyclic nucleotide-gated potassium channel mll3241

Chain D:




V68 R69 D70 R71 T72 P73 K74 I75 A76 I77 D78 V79 L80 A81 V82 L83 L86 A87 A88 F89 L90 L91 D92 G93 S94 P95 D96 W97 S98 L99 Y100 C101 A102 L105 L106 K107 P108 L109 R110 D111 S112 T113 F114 F115 P116 V117 L118 G119 R120 V121 L122 A123 N124 E125 A126 R127 N128 L129
I130 G131 V132 T133 T134 L135 F136 G137 F141 A142 A146 A147 Y148 E151 R152 D153 I154 Q155 P156 E157 K158 F159 G160 S161 I162 P163 Q164 A165 M166 W167 W168 A169 V170 V171 T172 L173 S174 T175 Y178 G179 D180 T181 I182 P183 Q184 S185 F186 A187 G188 R189 V190 L191 A192 G193 A194 V195
M196 M197 S198 G199 I200 G201 G204 L205 W206 A207 G208 I209 T212 Y215 Q216 E217 V218 R219 R220 G221 D222 F223 V224 R225 N226 L229 V230 A231 A232 V233 P234 L235 F236 Q237 K238 L239 G240 P241 A242 E246 I247 V248 R249 A250 L251 R252 A253 R254 T255 V256 P257 A258 G259 A260 V261
I262 C263 R264 E267 P268 G269 D270 R271 M272 F273 F274 V275 V276 E277 G278 S281 V282 A283 T284 P285 N286 P287 V288 E289 L290 G291 P292 G293 A294 F295 F296 G297 E298 L301 I302 S303 G304 S308 V311 S312 A313 A314 T315 T316 V317 S318 L319 L320 S321 L322 H323 S324 A325 D326 F327
Q328 M329 L330 C331 S332 S333 S334 P335 E336 I337 A338 E339 R342 K343 T344 A345 L346 E347 R348 R349 G350 A351 A352 A353 S354 A355

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31417	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; The defocus at the center of each particle box was estimated based on the tilt geometry.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	4300	Depositor
Magnification	50000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	7.803	Depositor
Minimum map value	-6.595	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.0	Depositor
Map size (Å)	135.2, 135.2, 135.2	wwPDB
Map dimensions	104, 104, 104	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K

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	0.43	0/2720	0.63	1/3713 (0.0%)
1	B	0.43	0/2720	0.63	1/3713 (0.0%)
1	C	0.43	0/2720	0.63	1/3713 (0.0%)
1	D	0.43	0/2720	0.63	1/3713 (0.0%)
All	All	0.43	0/10880	0.63	4/14852 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	220	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	D	220	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	B	220	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	A	220	ARG	NE-CZ-NH2	-6.89	116.86	120.30

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	2661	2775	2775	49	0
1	B	2661	2775	2775	48	0
1	C	2661	2775	2775	45	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2661	2775	2775	46	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	10646	11100	11100	172	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 8.

All (172) 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:B:64:ARG:O	1:B:69:ARG:NH1	2.11	0.84
1:D:64:ARG:O	1:D:69:ARG:NH1	2.11	0.83
1:C:64:ARG:O	1:C:69:ARG:NH1	2.11	0.83
1:A:64:ARG:O	1:A:69:ARG:NH1	2.11	0.83
1:B:208:GLY:O	1:B:212:THR:OG1	1.98	0.82
1:C:208:GLY:O	1:C:212:THR:OG1	1.98	0.81
1:A:208:GLY:O	1:A:212:THR:OG1	1.98	0.81
1:D:208:GLY:O	1:D:212:THR:OG1	1.98	0.80
1:C:56:LEU:O	1:C:59:THR:OG1	1.99	0.79
1:A:56:LEU:O	1:A:59:THR:OG1	2.00	0.78
1:B:56:LEU:O	1:B:59:THR:OG1	2.00	0.77
1:D:56:LEU:O	1:D:59:THR:OG1	1.99	0.77
1:B:77:ILE:O	1:B:81:ALA:N	2.21	0.74
1:A:77:ILE:O	1:A:81:ALA:N	2.21	0.74
1:C:77:ILE:O	1:C:81:ALA:N	2.21	0.74
1:D:195:VAL:O	1:D:198:SER:OG	2.04	0.73
1:C:195:VAL:O	1:C:198:SER:OG	2.04	0.73
1:D:77:ILE:O	1:D:81:ALA:N	2.21	0.73
1:A:127:ARG:NH1	1:A:128:ASN:OD1	2.23	0.72
1:C:127:ARG:NH1	1:C:128:ASN:OD1	2.23	0.72
1:D:127:ARG:NH1	1:D:128:ASN:OD1	2.23	0.72
1:B:127:ARG:NH1	1:B:128:ASN:OD1	2.23	0.71
1:B:195:VAL:O	1:B:198:SER:OG	2.04	0.70
1:B:168:TRP:O	1:B:172:THR:OG1	2.06	0.69
1:C:124:ASN:OD1	1:D:252:ARG:NH1	2.26	0.69
1:D:168:TRP:O	1:D:172:THR:OG1	2.06	0.69
1:A:124:ASN:OD1	1:B:252:ARG:NH1	2.26	0.69
1:B:124:ASN:OD1	1:C:252:ARG:NH1	2.26	0.68
1:C:52:TYR:O	1:C:56:LEU:N	2.27	0.68
1:B:339:GLU:OE2	1:B:342:ARG:NH2	2.28	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:TYR:O	1:A:56:LEU:N	2.27	0.67
1:A:339:GLU:OE2	1:A:342:ARG:NH2	2.28	0.67
1:A:168:TRP:O	1:A:172:THR:OG1	2.06	0.67
1:B:52:TYR:O	1:B:56:LEU:N	2.27	0.67
1:A:195:VAL:O	1:A:198:SER:OG	2.04	0.67
1:C:339:GLU:OE2	1:C:342:ARG:NH2	2.28	0.67
1:C:168:TRP:O	1:C:172:THR:OG1	2.06	0.67
1:D:52:TYR:O	1:D:56:LEU:N	2.27	0.66
1:B:217:GLU:O	1:B:221:GLY:N	2.29	0.66
1:D:217:GLU:O	1:D:221:GLY:N	2.29	0.66
1:A:217:GLU:O	1:A:221:GLY:N	2.29	0.66
1:D:339:GLU:OE2	1:D:342:ARG:NH2	2.28	0.66
1:A:252:ARG:NH1	1:D:124:ASN:O	2.28	0.66
1:C:217:GLU:O	1:C:221:GLY:N	2.29	0.66
1:D:62:LYS:O	1:D:69:ARG:NH2	2.29	0.66
1:A:62:LYS:O	1:A:69:ARG:NH2	2.29	0.65
1:B:62:LYS:O	1:B:69:ARG:NH2	2.29	0.65
1:C:62:LYS:O	1:C:69:ARG:NH2	2.29	0.65
1:A:74:LYS:O	1:A:110:ARG:NE	2.30	0.64
1:B:74:LYS:O	1:B:110:ARG:NE	2.30	0.64
1:C:74:LYS:O	1:C:110:ARG:NE	2.30	0.64
1:D:74:LYS:O	1:D:110:ARG:NE	2.30	0.64
1:C:329:MET:O	1:C:332:SER:OG	2.11	0.64
1:A:252:ARG:NH1	1:D:124:ASN:OD1	2.31	0.63
1:A:298:GLU:OE2	1:A:348:ARG:NH1	2.33	0.62
1:D:47:VAL:O	1:D:51:ALA:N	2.33	0.62
1:D:298:GLU:OE2	1:D:348:ARG:NH1	2.33	0.62
1:A:47:VAL:O	1:A:51:ALA:N	2.33	0.62
1:B:298:GLU:OE2	1:B:348:ARG:NH1	2.33	0.61
1:C:298:GLU:OE2	1:C:348:ARG:NH1	2.33	0.61
1:B:47:VAL:O	1:B:51:ALA:N	2.33	0.61
1:C:47:VAL:O	1:C:51:ALA:N	2.33	0.61
1:C:124:ASN:O	1:D:252:ARG:NH1	2.35	0.60
1:B:124:ASN:O	1:C:252:ARG:NH1	2.35	0.60
1:A:329:MET:O	1:A:332:SER:OG	2.11	0.59
1:B:329:MET:O	1:B:332:SER:OG	2.11	0.59
1:D:329:MET:O	1:D:332:SER:OG	2.11	0.58
1:D:345:ALA:O	1:D:349:ARG:NE	2.36	0.58
1:A:78:ASP:OD1	1:A:107:LYS:NZ	2.36	0.58
1:A:124:ASN:O	1:B:252:ARG:NH1	2.37	0.58
1:B:78:ASP:OD1	1:B:107:LYS:NZ	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:ALA:O	1:B:349:ARG:NE	2.36	0.58
1:C:345:ALA:O	1:C:349:ARG:NE	2.36	0.58
1:D:78:ASP:OD1	1:D:107:LYS:NZ	2.36	0.58
1:C:78:ASP:OD1	1:C:107:LYS:NZ	2.36	0.57
1:A:345:ALA:O	1:A:349:ARG:NE	2.36	0.57
1:B:131:GLY:O	1:B:134:THR:OG1	2.22	0.57
1:C:298:GLU:N	1:C:298:GLU:OE1	2.37	0.57
1:A:131:GLY:O	1:A:134:THR:OG1	2.22	0.57
1:C:131:GLY:O	1:C:134:THR:OG1	2.22	0.56
1:D:131:GLY:O	1:D:134:THR:OG1	2.22	0.56
1:B:324:SER:O	1:B:327:PHE:N	2.39	0.56
1:D:298:GLU:OE1	1:D:298:GLU:N	2.37	0.55
1:A:324:SER:O	1:A:327:PHE:N	2.39	0.55
1:C:324:SER:O	1:C:327:PHE:N	2.39	0.55
1:A:298:GLU:OE1	1:A:298:GLU:N	2.37	0.55
1:D:169:ALA:O	1:D:173:LEU:N	2.40	0.54
1:D:324:SER:O	1:D:327:PHE:N	2.39	0.54
1:A:216:GLN:NE2	1:B:1:MET:SD	2.79	0.54
1:A:169:ALA:O	1:A:173:LEU:N	2.40	0.54
1:B:298:GLU:OE1	1:B:298:GLU:N	2.37	0.53
1:B:216:GLN:NE2	1:C:1:MET:SD	2.77	0.53
1:B:216:GLN:O	1:B:220:ARG:N	2.42	0.52
1:D:216:GLN:O	1:D:220:ARG:N	2.42	0.52
1:C:169:ALA:O	1:C:173:LEU:N	2.40	0.52
1:A:1:MET:SD	1:D:216:GLN:NE2	2.81	0.52
1:C:180:ASP:OD1	1:C:181:THR:N	2.43	0.52
1:B:169:ALA:O	1:B:173:LEU:N	2.40	0.52
1:C:216:GLN:NE2	1:D:1:MET:SD	2.80	0.51
1:C:260:ALA:O	1:C:313:ALA:N	2.42	0.51
1:C:216:GLN:O	1:C:220:ARG:N	2.42	0.51
1:B:260:ALA:O	1:B:313:ALA:N	2.42	0.51
1:D:324:SER:O	1:D:328:GLN:N	2.38	0.51
1:B:180:ASP:OD1	1:B:181:THR:N	2.43	0.51
1:C:324:SER:O	1:C:328:GLN:N	2.38	0.51
1:A:325:ALA:O	1:A:329:MET:N	2.42	0.51
1:D:180:ASP:OD1	1:D:181:THR:N	2.43	0.50
1:D:325:ALA:O	1:D:329:MET:N	2.42	0.50
1:A:324:SER:O	1:A:328:GLN:N	2.38	0.49
1:C:196:MET:SD	1:C:196:MET:N	2.86	0.49
1:A:216:GLN:O	1:A:220:ARG:N	2.42	0.49
1:A:180:ASP:OD1	1:A:181:THR:N	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:ALA:O	1:D:313:ALA:N	2.42	0.49
1:C:325:ALA:O	1:C:329:MET:N	2.42	0.49
1:A:260:ALA:O	1:A:313:ALA:N	2.42	0.48
1:C:338:ALA:O	1:C:342:ARG:N	2.45	0.48
1:B:325:ALA:O	1:B:329:MET:N	2.42	0.47
1:A:196:MET:N	1:A:196:MET:SD	2.86	0.47
1:D:338:ALA:O	1:D:342:ARG:N	2.45	0.47
1:D:196:MET:SD	1:D:196:MET:N	2.86	0.47
1:B:196:MET:SD	1:B:196:MET:N	2.86	0.46
1:B:324:SER:O	1:B:328:GLN:N	2.38	0.46
1:B:338:ALA:O	1:B:342:ARG:N	2.45	0.45
1:A:338:ALA:O	1:A:342:ARG:N	2.45	0.45
1:B:134:THR:O	1:B:137:GLY:N	2.50	0.45
1:C:134:THR:O	1:C:137:GLY:N	2.50	0.45
1:D:134:THR:O	1:D:137:GLY:N	2.50	0.45
1:D:198:SER:O	1:D:201:GLY:N	2.50	0.45
1:A:134:THR:O	1:A:137:GLY:N	2.50	0.45
1:B:134:THR:O	1:B:138:VAL:N	2.43	0.45
1:B:170:VAL:O	1:B:174:SER:OG	2.28	0.45
1:D:79:VAL:HG12	1:D:83:LEU:HD12	2.00	0.44
1:A:275:VAL:N	1:A:294:ALA:O	2.50	0.44
1:A:79:VAL:HG12	1:A:83:LEU:HD12	2.00	0.44
1:B:198:SER:O	1:B:201:GLY:N	2.50	0.44
1:D:329:MET:O	1:D:333:SER:N	2.51	0.44
1:B:329:MET:O	1:B:333:SER:N	2.51	0.44
1:A:329:MET:O	1:A:333:SER:N	2.51	0.44
1:C:79:VAL:HG12	1:C:83:LEU:HD12	2.00	0.44
1:B:275:VAL:N	1:B:294:ALA:O	2.50	0.43
1:A:8:ARG:O	1:A:11:ALA:HB2	2.18	0.43
1:A:198:SER:O	1:A:201:GLY:N	2.50	0.43
1:C:329:MET:O	1:C:333:SER:N	2.51	0.43
1:B:79:VAL:HG12	1:B:83:LEU:HD12	2.00	0.43
1:D:43:ALA:O	1:D:46:ALA:N	2.52	0.43
1:C:43:ALA:O	1:C:46:ALA:N	2.52	0.43
1:C:8:ARG:O	1:C:11:ALA:HB2	2.18	0.43
1:D:8:ARG:O	1:D:11:ALA:HB2	2.18	0.43
1:A:134:THR:O	1:A:138:VAL:N	2.43	0.42
1:B:8:ARG:O	1:B:11:ALA:HB2	2.18	0.42
1:A:325:ALA:HB3	1:D:220:ARG:CZ	2.49	0.42
1:B:43:ALA:O	1:B:46:ALA:N	2.52	0.42
1:C:262:ILE:HD12	1:C:311:VAL:HG12	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ALA:O	1:A:46:ALA:N	2.52	0.42
1:B:223:PHE:CD2	1:C:325:ALA:HB2	2.54	0.42
1:B:262:ILE:HD12	1:B:311:VAL:HG12	2.02	0.42
1:A:262:ILE:HD12	1:A:311:VAL:HG12	2.02	0.42
1:C:11:ALA:HB3	1:C:12:PRO:HD3	2.02	0.42
1:C:275:VAL:N	1:C:294:ALA:O	2.50	0.42
1:D:11:ALA:HB3	1:D:12:PRO:HD3	2.02	0.42
1:D:262:ILE:HD12	1:D:311:VAL:HG12	2.02	0.42
1:C:198:SER:O	1:C:201:GLY:N	2.50	0.41
1:A:325:ALA:H	1:D:220:ARG:HH21	1.68	0.41
1:B:106:LEU:O	1:B:110:ARG:N	2.54	0.41
1:A:11:ALA:HB3	1:A:12:PRO:HD3	2.02	0.41
1:A:2:SER:O	1:A:321:SER:OG	2.32	0.41
1:B:11:ALA:HB3	1:B:12:PRO:HD3	2.02	0.41
1:D:106:LEU:O	1:D:110:ARG:N	2.54	0.41
1:A:106:LEU:O	1:A:110:ARG:N	2.54	0.41
1:B:220:ARG:NH2	1:C:323:HIS:HB3	2.36	0.41
1:D:170:VAL:O	1:D:174:SER:OG	2.28	0.41
1:A:134:THR:HG1	1:A:135:LEU:H	1.69	0.40

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	353/355 (99%)	307 (87%)	46 (13%)	0	100	100
1	B	353/355 (99%)	307 (87%)	46 (13%)	0	100	100
1	C	353/355 (99%)	307 (87%)	46 (13%)	0	100	100
1	D	353/355 (99%)	307 (87%)	46 (13%)	0	100	100
All	All	1412/1420 (99%)	1228 (87%)	184 (13%)	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	273/273 (100%)	273 (100%)	0	100	100
1	B	273/273 (100%)	273 (100%)	0	100	100
1	C	273/273 (100%)	273 (100%)	0	100	100
1	D	273/273 (100%)	273 (100%)	0	100	100
All	All	1092/1092 (100%)	1092 (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 (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	328	GLN
1	B	328	GLN
1	C	328	GLN
1	D	328	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

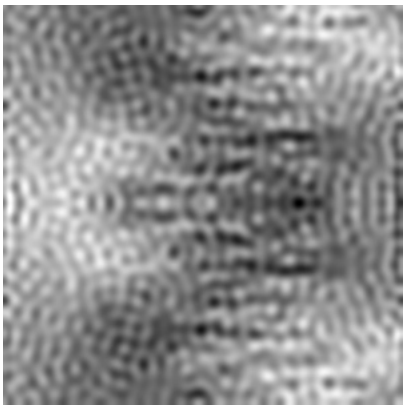
This section contains visualisations of the EMDB entry EMD-4518. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

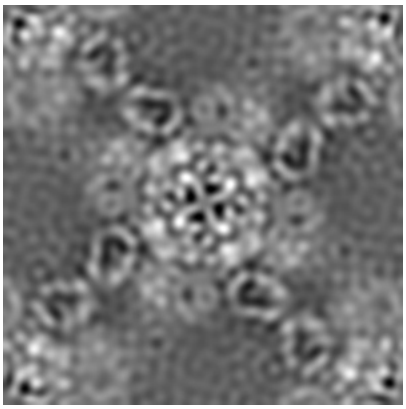
6.1 Orthogonal projections

6.1.1 Primary map

X

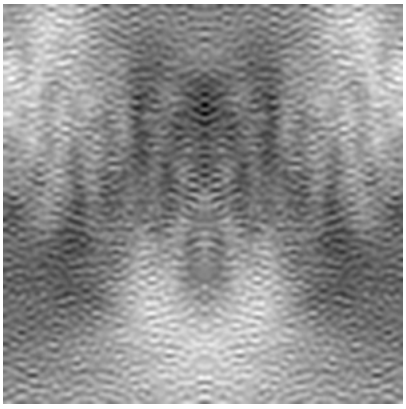


Y

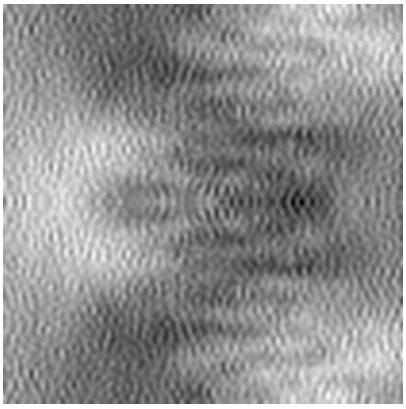


Z

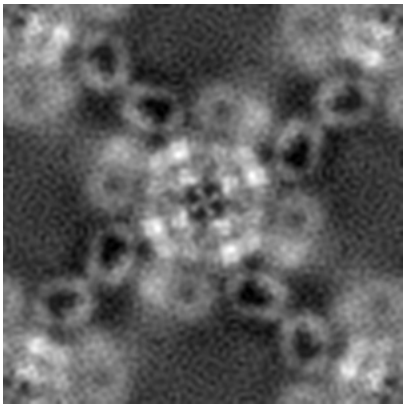
6.1.2 Raw map



X



Y



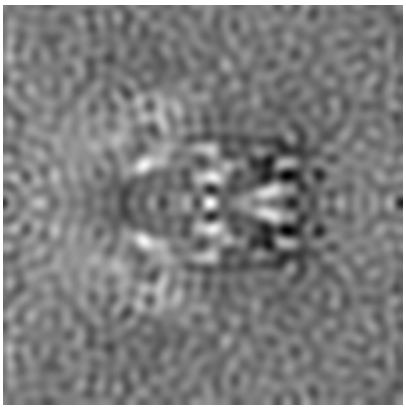
Z

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

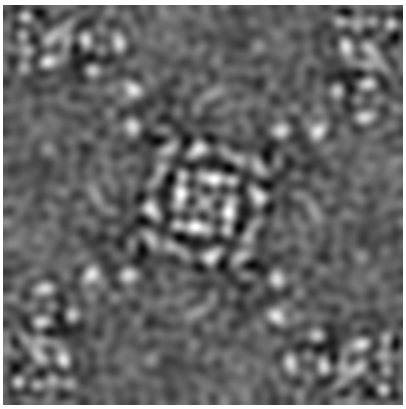
6.2 Central slices (i)

6.2.1 Primary map

X Index: 52

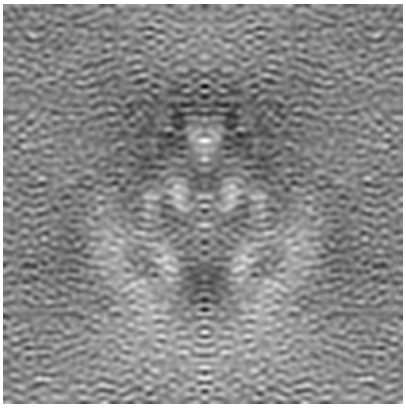


Y Index: 52

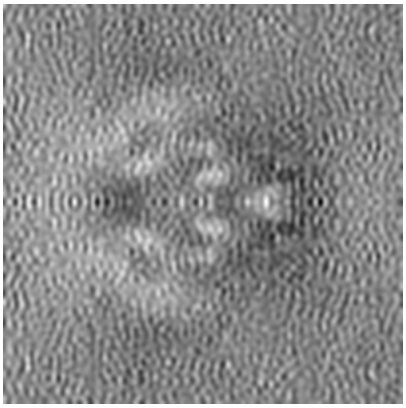


Z Index: 52

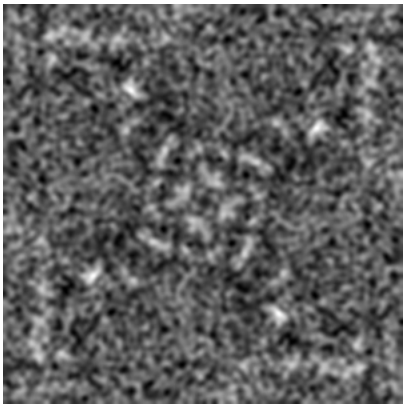
6.2.2 Raw map



X Index: 52



Y Index: 52

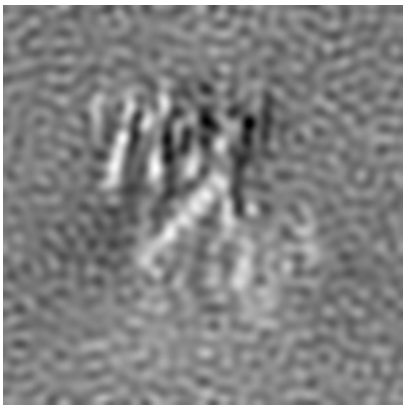


Z Index: 52

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

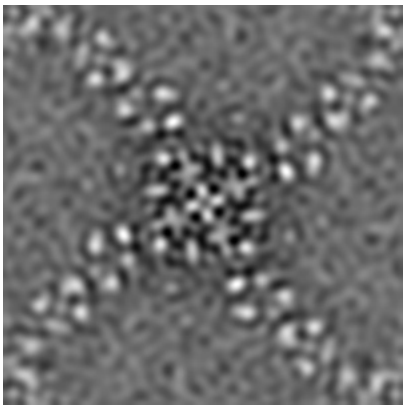
6.3 Largest variance slices (i)

6.3.1 Primary map



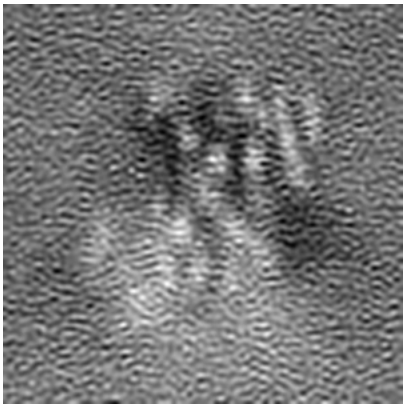
X Index: 59

Y Index: 45

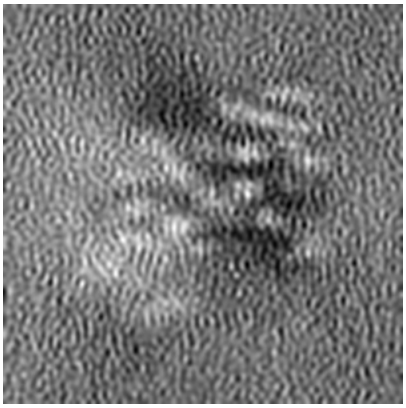


Z Index: 69

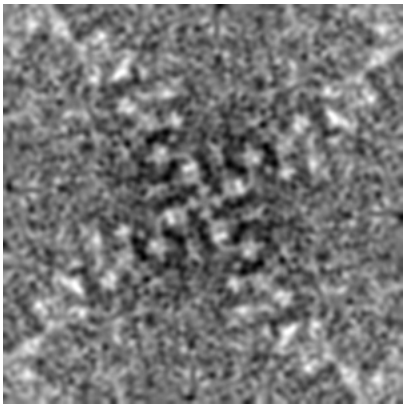
6.3.2 Raw map



X Index: 44



Y Index: 60



Z Index: 69

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

6.4.2 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.

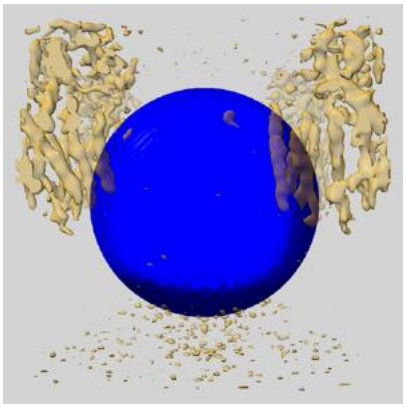
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

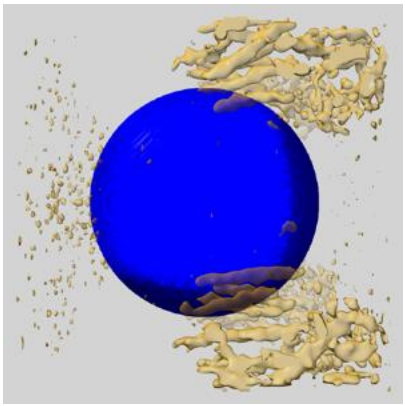
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

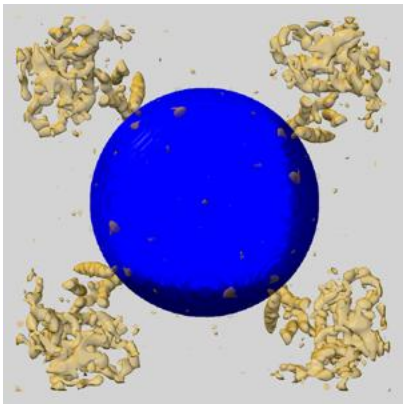
6.5.1 emd_4518_msk_1.map (i)



X



Y

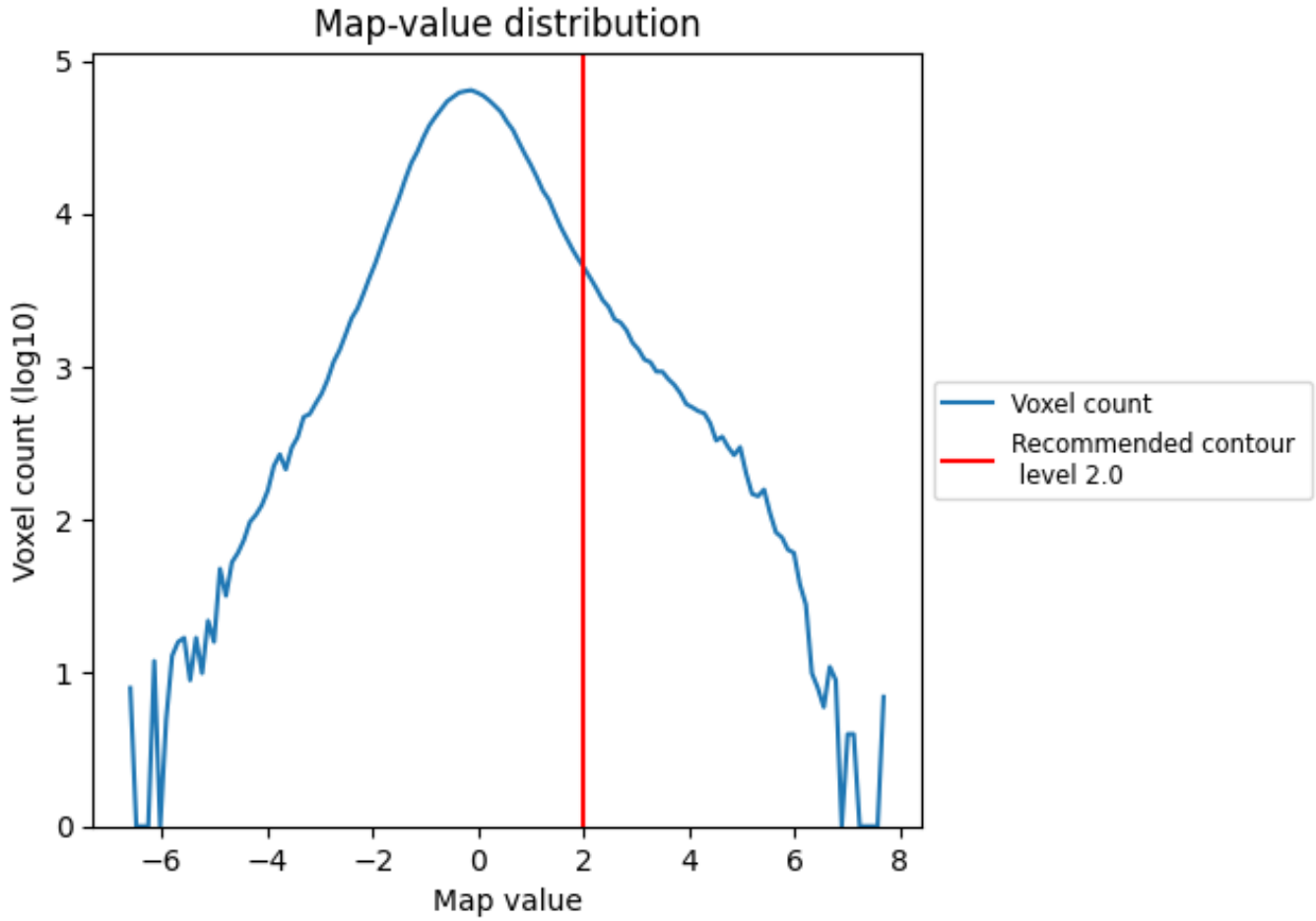


Z

7 Map analysis

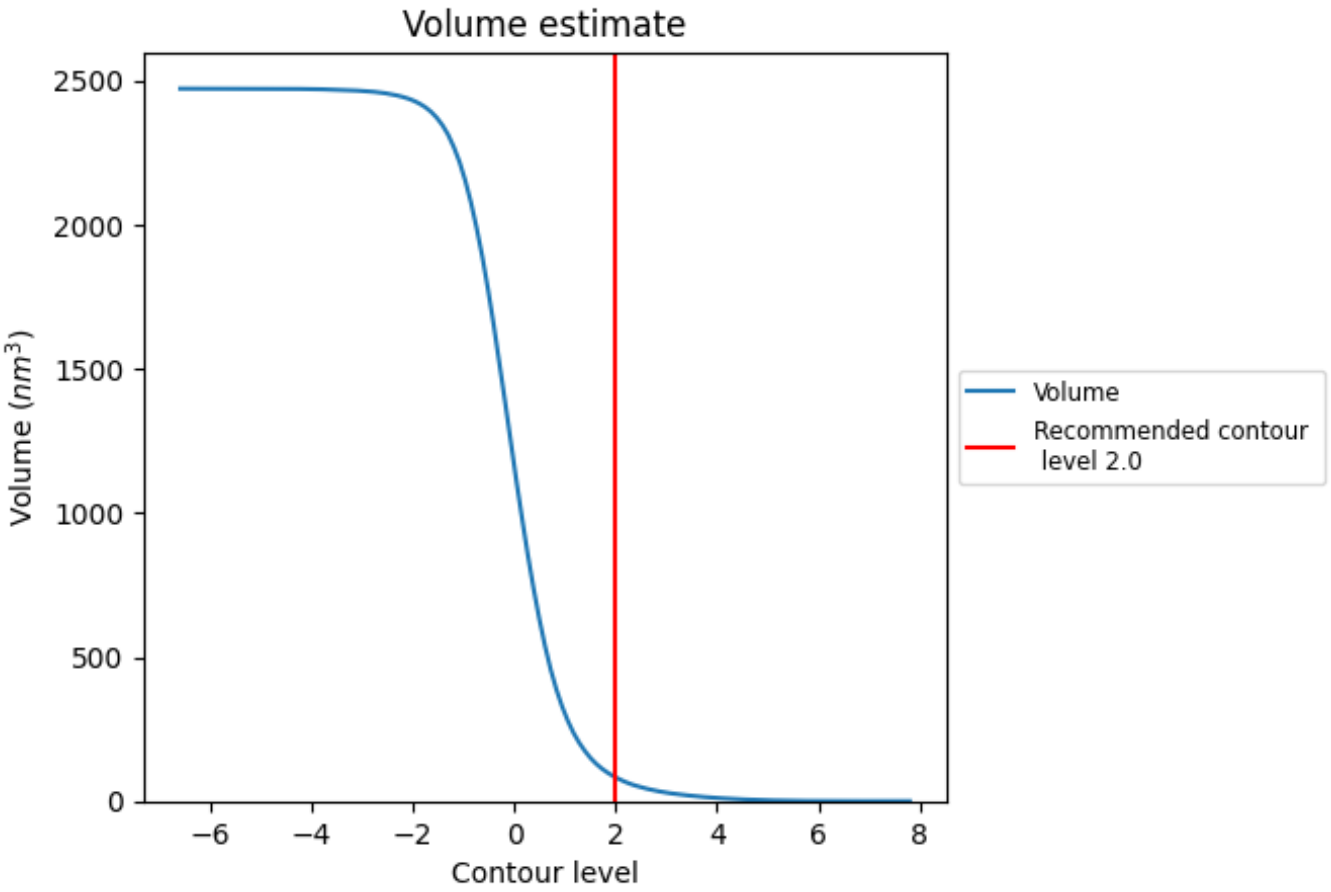
This section contains the results of statistical analysis of the map.

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.

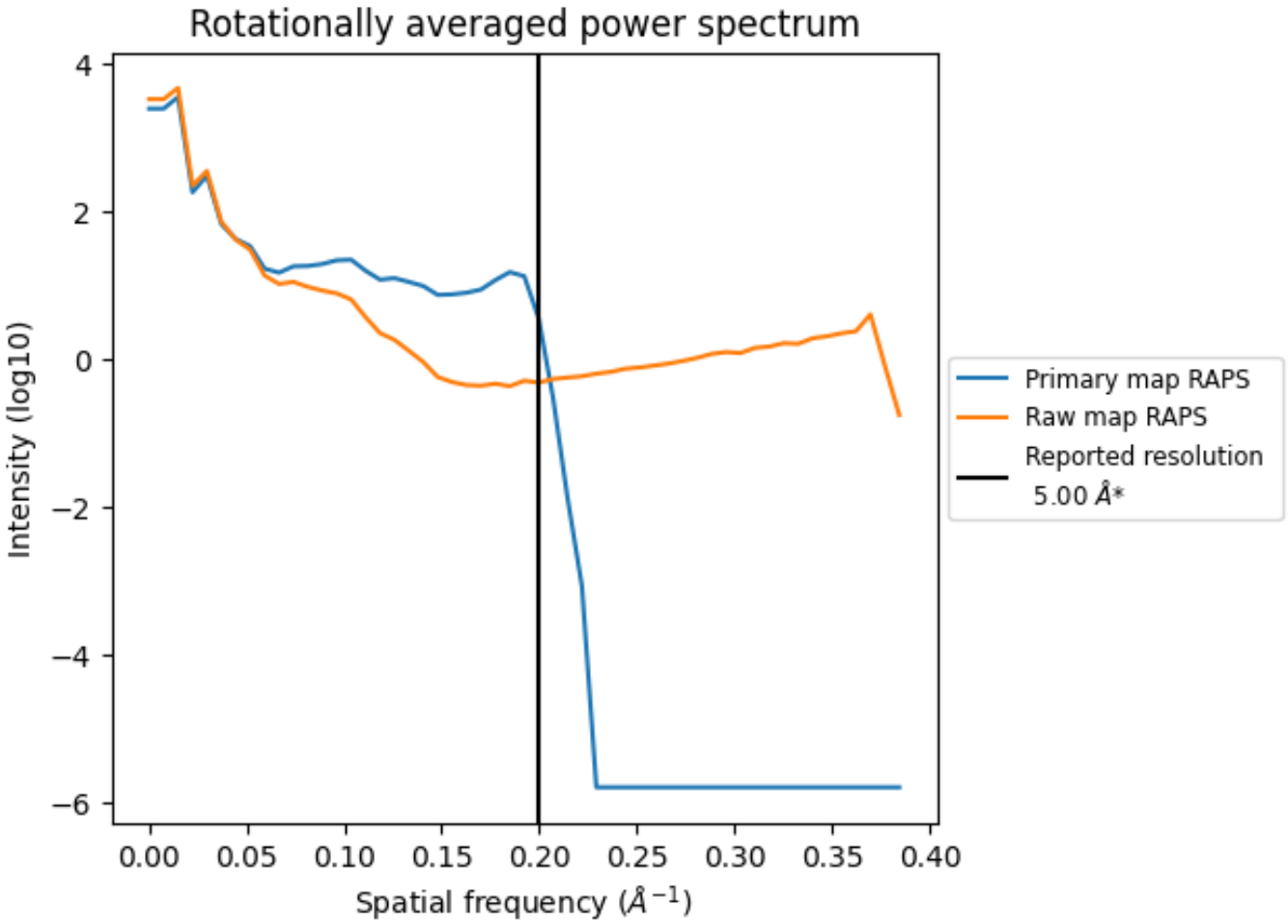
7.2 Volume estimate



The volume at the recommended contour level is 82 nm^3; this corresponds to an approximate mass of 74 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)

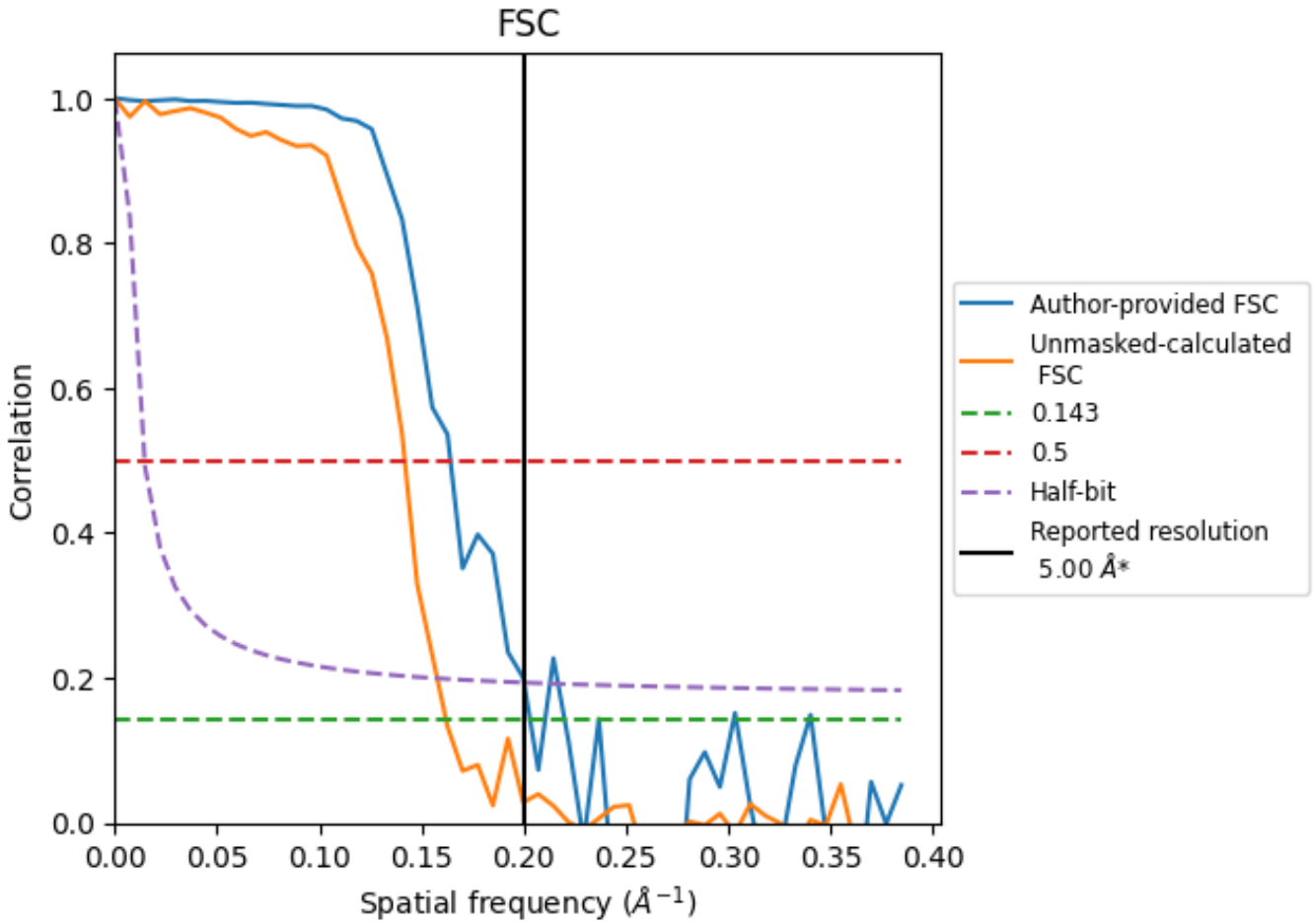


*Reported resolution corresponds to spatial frequency of 0.200 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.200 Å^{-1}

8.2 Resolution estimates (i)

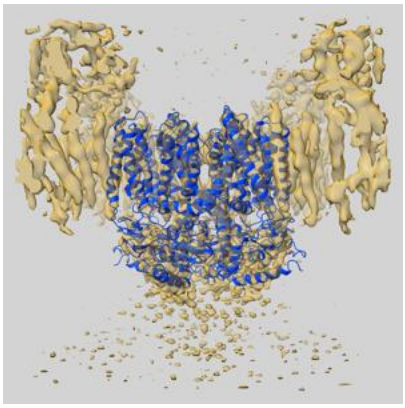
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.00	-	-
Author-provided FSC curve	4.93	6.09	5.00
Unmasked-calculated*	6.18	7.05	6.34

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.18 differs from the reported value 5.0 by more than 10 %

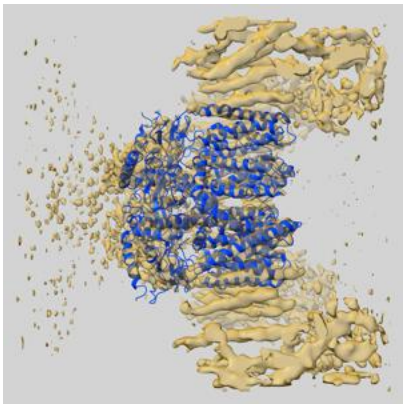
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4518 and PDB model 6QD3. Per-residue inclusion information can be found in section 3 on page 4.

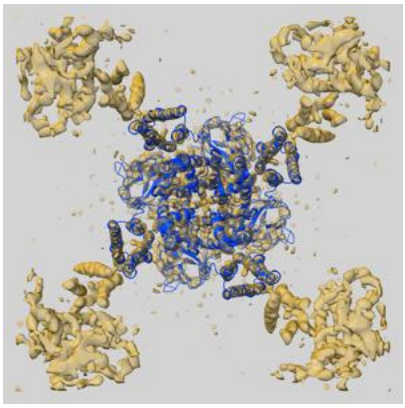
9.1 Map-model overlay



X



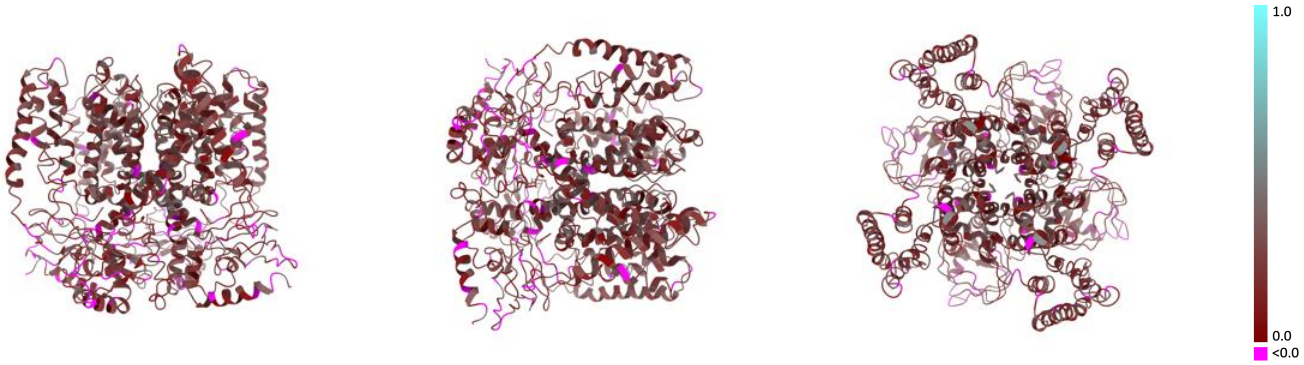
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0 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.

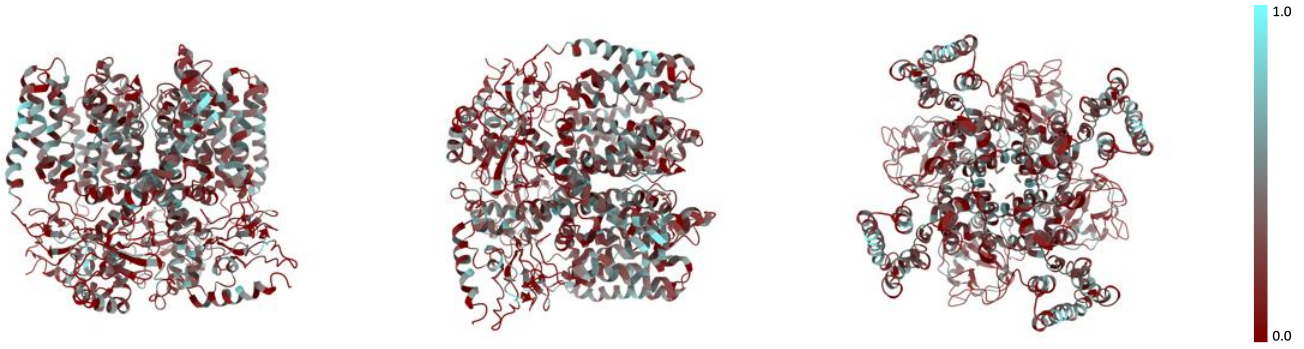
9.2 Q-score mapped to coordinate model



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.

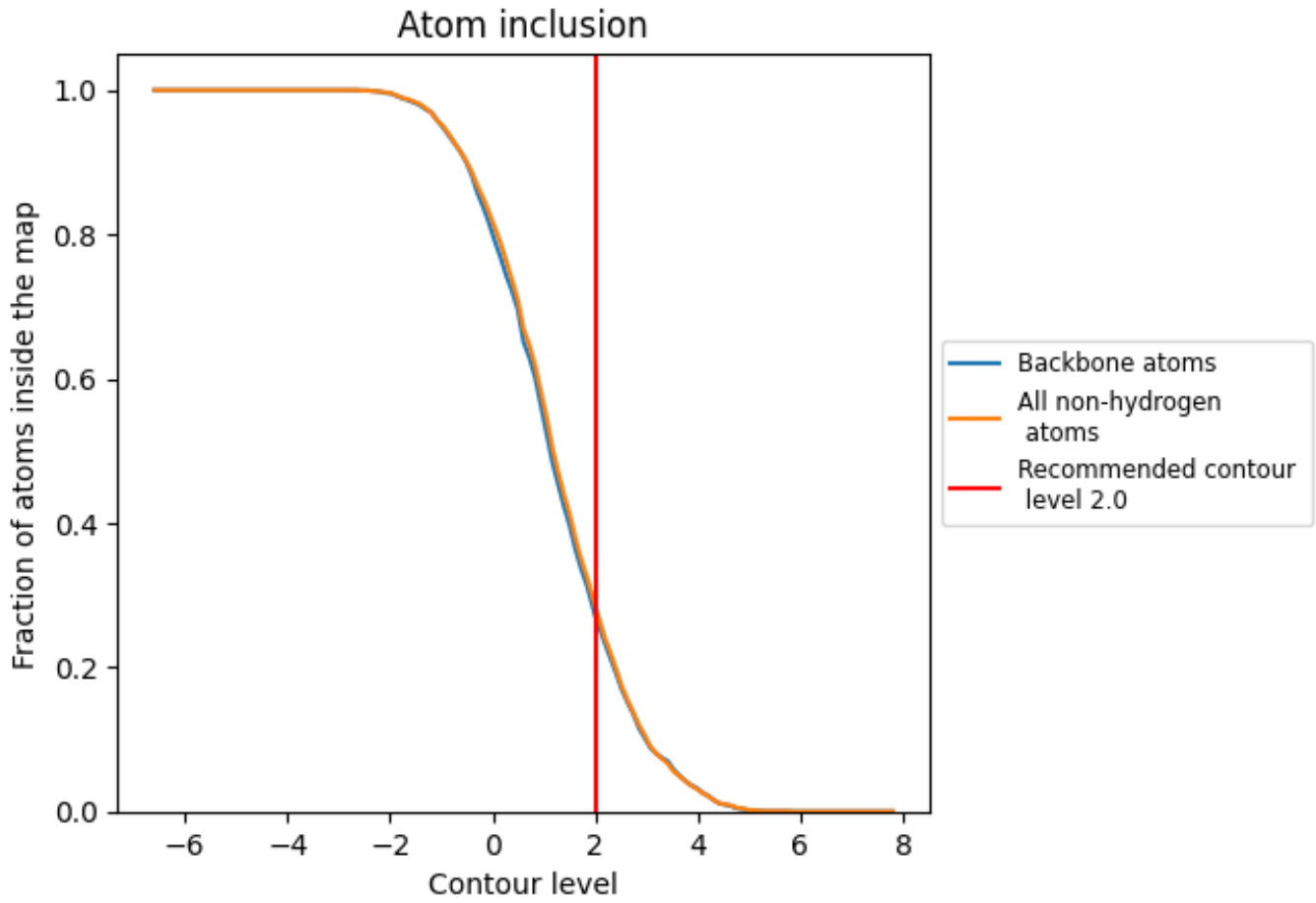
9.3 Atom inclusion mapped to coordinate model



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 (2.0).

9.4 Atom inclusion (i)



At the recommended contour level, 27% of all backbone atoms, 28% 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 (2.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2840	0.2040
A	0.2903	0.2040
B	0.2922	0.2040
C	0.2927	0.2050
D	0.2915	0.2040