Full wwPDB EM Validation Report (i)

Nov 17, 2022 – 05:53 AM EST

PDB ID	:	7JR9
EMDB ID	:	EMD-22444
Title	:	Chlamydomonas reinhardtii radial spoke minimal head complex
Authors	:	Grossman-Haham, I.; Coudray, N.; Yu, Z.; Wang, F.; Bhabha, G.; Vale, R.D.
Deposited on	:	2020-08-11
Resolution	:	2.95 Å(reported)

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 (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:

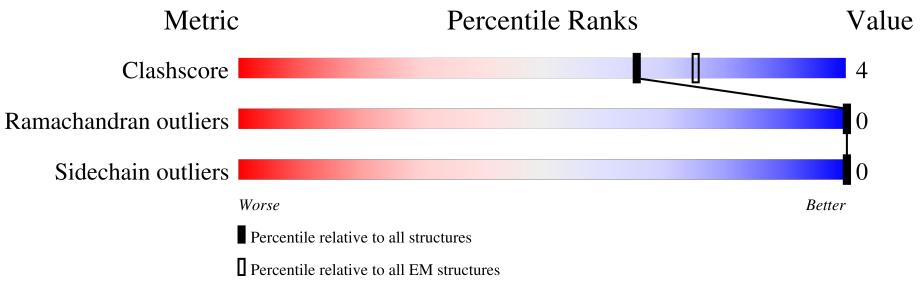
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.95 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	269	87% 8% 6%
1	B	269	82% 12% 7%
2	C	486	52% 6% 42%
3	D	459	66% 8% 26%
4	F	8	88% 12%
5	G	6	83% 17%
6	E	216	72% 10% 19%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10021 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 Radial spoke protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	254	1970	1258	333	374	5	0	0
1	B	251	1946	1243	329	369	5	0	0

- Molecule 2 is a protein called Flagellar radial spoke protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	280	2110	1349	362	393	6	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-20	MET	-	expression tag	UNP Q01656
C	-19	GLY	-	expression tag	UNP Q01656
C	-18	SER	-	expression tag	UNP Q01656
C	-17	SER	-	expression tag	UNP Q01656
C	-16	HIS	-	expression tag	UNP Q01656
C	-15	HIS	-	expression tag	UNP Q01656
C	-14	HIS	-	expression tag	UNP Q01656
C	-13	HIS	-	expression tag	UNP Q01656
C	-12	HIS	-	expression tag	UNP Q01656
C	-11	HIS	-	expression tag	UNP Q01656
C	-10	GLY	-	expression tag	UNP Q01656
C	-9	GLY	-	expression tag	UNP Q01656
C	-8	SER	-	expression tag	UNP Q01656
C	-7	ALA	-	expression tag	UNP Q01656
C	-6	GLU	-	expression tag	UNP Q01656
C	-5	ASN	-	expression tag	UNP Q01656
C	-4	LEU	-	expression tag	UNP Q01656
C	-3	TYR	-	expression tag	UNP Q01656
C	-2	PHE	-	expression tag	UNP Q01656

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLN	-	expression tag	UNP Q01656
C	0	GLY	-	expression tag	UNP Q01656

- Molecule 3 is a protein called Flagellar radial spoke protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	339	2574	1637	442	483	12	0	0

- Molecule 4 is a protein called Flagellar radial spoke protein 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	F	8	40	24	8	8	0	0

- Molecule 5 is a protein called Flagellar radial spoke protein 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	G	6	30	18	6	6	0	0

- Molecule 6 is a protein called Radial spoke protein 10.

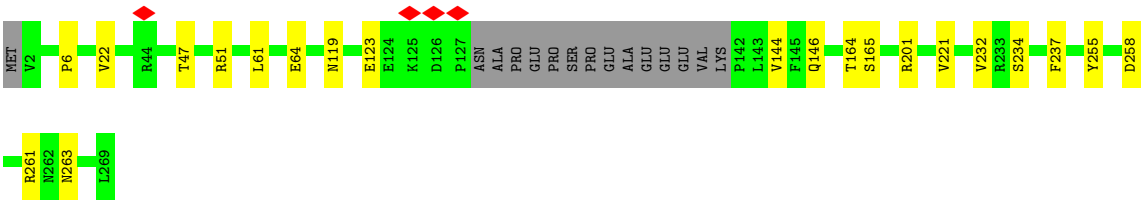
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	E	176	1351	862	226	254	9	0	0

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.

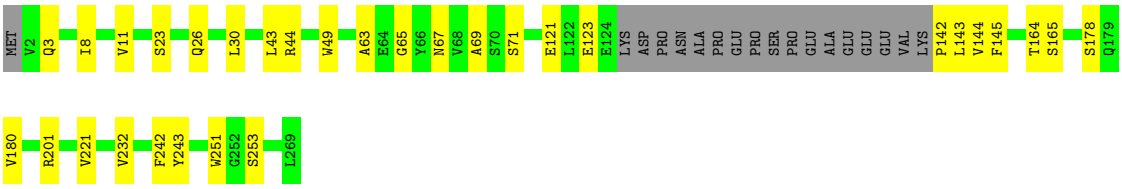
• Molecule 1: Radial spoke protein 9

Chain A:



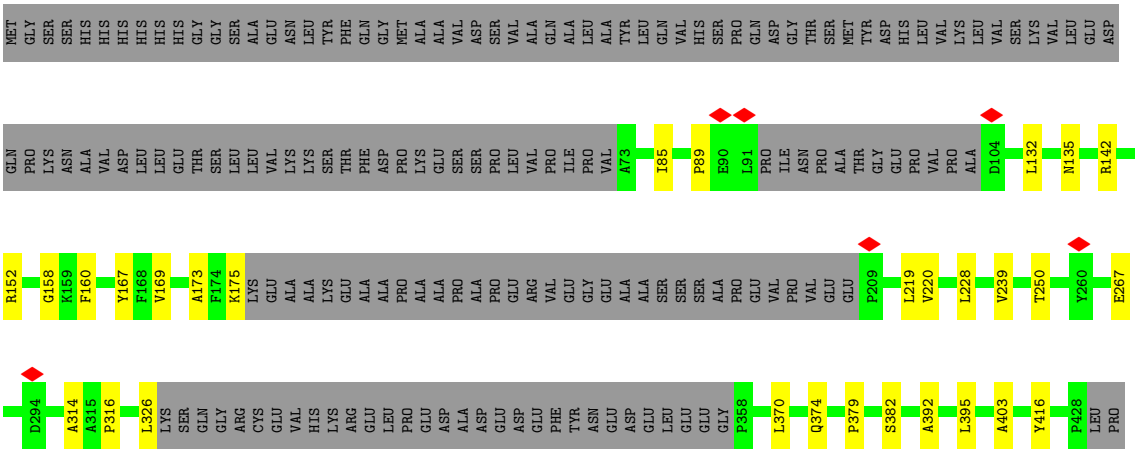
• Molecule 1: Radial spoke protein 9

Chain B:



• Molecule 2: Flagellar radial spoke protein 4

Chain C:



PRO PRO PRO VAL ALA GLN GLU PHE ALA TRP GLY GLU VAL GLU THR GLN GLU LEU GLU LEU LYS PRO ALA PRO PRO PRO PRO GLU GLU GLU ALA GLU ALA ASP GLU

- Molecule 3: Flagellar radial spoke protein 6

Chain D:

MET ALA ALA ASP VAL GLY GLN ALA LEU ALA PHE LEU GLN GLN VAL LYS THR THR GLN GLY ALA SER ILE ILE TYR GLU GLY LEU LYS ALA ALA LEU ALA LYS VAL LEU GLU ASP ARG PRO VAL ASN ALA VAL GLU ALA LEU GLU THR SER VAL LEU SER THR PRO PRO ALA ALA ASN LEU SER

VAL PRO LEU VAL PRO ALA ALA SER ALA ALA ALA A72 K78 A79 S80 P85 E86 P87 VAL LEU ASP PRO GLU SER GLY GLU PRO ILE ASP PRO D100 L116 R138 L139 R145 R151 F156 Y163 E167 A179 P180 E181 G182 L186 S201 L204

L208 T230 E247 D274 D275 S276 A277 D283 E292 M293 A294 N298 D318 P319 P320 ASP GLU GLU GLU GLU PRO GLU LYS N329 L346 A350 P353 P361 P362 W365 S373 T376 Q379 V380 A381 R387 T401 K410 E414 P430

ALA ALA GLY VAL GLU GLY GLY GLN GLN LEU LEU LEU GLU CYS ASN ASP LEU PRO PRO LYS PRO ALA PRO PRO GLU GLU GLU ASP GLU

- Molecule 4: Flagellar radial spoke protein 6

Chain F:

X500 X507

- Molecule 5: Flagellar radial spoke protein 10

Chain G:

X-5 X0

- Molecule 6: Radial spoke protein 10

Chain E:

MET ALA ASP ASP GLU LEU PRO PRO GLN PRO VAL TRP GLU GLY PRO LEU ASP GLU ASP GLY LYS PRO HIS GLY L25 G26 P31 PRO PRO PRO MET GLY GLU ASP ASP GLU GLU GLU LYS PRO G45 E53 R57 T64 A70 V71 G79 K80 K81 H82 G83 V88 Y89

P90 W99 V100 E101 D102 Q105 Y112 A124 R127 G169 K176 Y182 V190 K211 E212 F213 SER VAL ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	251088	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 ($e^-/Å^2$)	73.3	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.088	Depositor
Minimum map value	-0.041	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	273.6, 273.6, 273.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.855, 0.855, 0.855	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	0.42	0/2013	0.54	0/2738
1	B	0.44	0/1988	0.55	0/2704
2	C	0.41	0/2162	0.53	0/2944
3	D	0.42	0/2654	0.51	0/3630
6	E	0.39	0/1395	0.56	0/1877
All	All	0.42	0/10212	0.54	0/13893

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	1970	0	1948	12	0
1	B	1946	0	1926	17	0
2	C	2110	0	2087	17	0
3	D	2574	0	2467	21	0
4	F	40	0	10	1	0
5	G	30	0	8	1	0
6	E	1351	0	1235	13	0
All	All	10021	0	9681	80	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 4.

All (80) 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:C:158:GLY:HA3	2:C:416:TYR:O	1.97	0.65
3:D:376:THR:HB	3:D:379:GLN:HE21	1.64	0.61
6:E:71:VAL:HG22	6:E:88:VAL:HG22	1.82	0.60
1:B:23:SER:HB3	1:B:26:GLN:HG2	1.84	0.60
6:E:112:TYR:OH	6:E:127:ARG:NH1	2.36	0.57
3:D:292:GLU:O	3:D:298:ASN:ND2	2.38	0.56
1:A:234:SER:OG	1:A:237:PHE:O	2.24	0.56
1:A:123:GLU:HG2	1:A:144:VAL:HG12	1.87	0.56
6:E:100:VAL:HB	6:E:105:GLN:HG3	1.87	0.56
3:D:78:LYS:HE3	3:D:204:LEU:HB2	1.89	0.55
2:C:85:ILE:HA	2:C:142:ARG:HE	1.71	0.54
2:C:152:ARG:HB3	2:C:173:ALA:HB3	1.89	0.54
3:D:350:ALA:O	3:D:387:ARG:NH2	2.37	0.54
6:E:182:TYR:O	6:E:190:VAL:HA	2.07	0.53
2:C:169:VAL:HG22	2:C:220:VAL:HG12	1.89	0.53
1:A:6:PRO:HG2	1:A:47:THR:HG21	1.91	0.53
1:B:44:ARG:NH2	1:B:67:ASN:O	2.43	0.52
1:B:123:GLU:HG2	1:B:144:VAL:HG12	1.92	0.52
1:B:8:ILE:HD11	1:B:30:LEU:HD13	1.91	0.52
3:D:151:ARG:HB3	3:D:167:GLU:HG2	1.92	0.51
6:E:57:ARG:HB2	6:E:79:GLY:HA2	1.92	0.51
1:B:221:VAL:HG22	1:B:232:VAL:HG22	1.92	0.51
3:D:201:SER:HB3	3:D:208:LEU:HD23	1.94	0.50
3:D:294:ALA:HB2	3:D:381:ALA:HB1	1.92	0.50
2:C:314:ALA:HB1	2:C:379:PRO:HB3	1.93	0.50
3:D:230:THR:OG1	3:D:247:GLU:OE1	2.30	0.50
1:A:22:VAL:HA	1:A:51:ARG:HH11	1.78	0.49
6:E:105:GLN:OE1	6:E:124:ALA:N	2.46	0.49
1:B:11:VAL:HG12	1:B:243:TYR:HE1	1.78	0.49
2:C:250:THR:N	2:C:267:GLU:OE2	2.46	0.49
6:E:81:LYS:HB2	6:E:102:ASP:HA	1.93	0.48
6:E:70:ALA:HB2	6:E:90:PRO:HD3	1.95	0.48
1:A:51:ARG:HB3	1:A:61:LEU:HD23	1.96	0.48
3:D:116:LEU:HD12	3:D:401:THR:HG23	1.96	0.48
3:D:353:PRO:HG3	3:D:414:GLU:HB3	1.95	0.48
1:A:164:THR:OG1	1:A:165:SER:N	2.47	0.47
1:B:43:LEU:HD13	1:B:65:GLY:HA3	1.95	0.47
1:B:242:PHE:HD1	1:B:253:SER:HB3	1.79	0.47
1:A:261:ARG:NH1	1:A:263:ASN:OD1	2.46	0.47
6:E:64:THR:HG23	6:E:71:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:89:PRO:HD3	2:C:142:ARG:HH22	1.80	0.47
6:E:169:GLY:N	6:E:176:LYS:O	2.46	0.47
1:B:71:SER:OG	1:B:178:SER:OG	2.34	0.46
2:C:219:LEU:HB3	2:C:228:LEU:HD23	1.98	0.46
3:D:387:ARG:HD3	3:D:410:LYS:HE3	1.98	0.45
1:A:255:TYR:OH	1:A:258:ASP:O	2.26	0.45
1:B:142:PRO:HB2	1:B:143:LEU:H	1.61	0.45
1:A:64:GLU:OE2	1:A:201:ARG:NH1	2.43	0.44
3:D:430:PRO:HG3	4:F:500:UNK:H2	1.82	0.44
2:C:132:LEU:HD23	2:C:135:ASN:HD22	1.83	0.44
1:B:3:GLN:NE2	1:B:251:TRP:O	2.40	0.44
6:E:83:GLY:O	6:E:99:TRP:N	2.47	0.44
1:B:164:THR:OG1	1:B:165:SER:N	2.49	0.44
6:E:112:TYR:HH	6:E:127:ARG:HH11	1.63	0.44
1:A:119:ASN:HB3	1:A:146:GLN:HB3	2.00	0.44
1:B:165:SER:O	1:B:201:ARG:N	2.51	0.44
1:A:221:VAL:HG22	1:A:232:VAL:HG22	1.99	0.44
3:D:156:PHE:HB2	3:D:163:TYR:HB2	2.00	0.44
1:B:8:ILE:HA	1:B:11:VAL:HG22	2.01	0.43
2:C:85:ILE:HG22	2:C:142:ARG:HG3	1.99	0.43
2:C:382:SER:HB2	2:C:392:ALA:HB3	2.00	0.43
1:B:121:GLU:HA	1:B:145:PHE:O	2.19	0.42
3:D:373:SER:OG	3:D:376:THR:OG1	2.33	0.42
5:G:0:UNK:HA	6:E:26:GLY:HA2	2.01	0.42
1:A:165:SER:O	1:A:201:ARG:N	2.49	0.42
1:B:69:ALA:O	1:B:180:VAL:N	2.45	0.42
3:D:319:PRO:HA	3:D:320:PRO:HD3	1.96	0.42
3:D:179:ALA:HB2	3:D:186:LEU:HG	2.02	0.42
1:B:49:TRP:H	1:B:63:ALA:HA	1.85	0.41
2:C:160:PHE:HB2	2:C:167:TYR:HB2	2.02	0.41
2:C:239:VAL:HG11	2:C:326:LEU:HD21	2.01	0.41
2:C:403:ALA:HB2	2:C:416:TYR:HD1	1.84	0.41
3:D:80:SER:OG	3:D:138:ARG:NH2	2.45	0.41
3:D:139:LEU:HD13	3:D:208:LEU:HD13	2.03	0.41
3:D:361:PRO:HA	3:D:362:PRO:HD3	1.95	0.41
2:C:152:ARG:HB2	2:C:175:LYS:H	1.85	0.41
2:C:316:PRO:HA	2:C:395:LEU:HD11	2.02	0.41
2:C:370:LEU:HB2	2:C:374:GLN:HB3	2.03	0.40
3:D:145:ARG:HH12	3:D:208:LEU:HB2	1.87	0.40
3:D:346:LEU:HD13	3:D:365:TRP:CD2	2.56	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	250/269 (93%)	243 (97%)	7 (3%)	0	100	100
1	B	247/269 (92%)	241 (98%)	6 (2%)	0	100	100
2	C	272/486 (56%)	259 (95%)	13 (5%)	0	100	100
3	D	333/459 (72%)	325 (98%)	8 (2%)	0	100	100
6	E	172/216 (80%)	167 (97%)	5 (3%)	0	100	100
All	All	1274/1699 (75%)	1235 (97%)	39 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	208/221 (94%)	208 (100%)	0	100	100
1	B	205/221 (93%)	205 (100%)	0	100	100
2	C	216/387 (56%)	216 (100%)	0	100	100
3	D	264/357 (74%)	264 (100%)	0	100	100
6	E	129/164 (79%)	129 (100%)	0	100	100
All	All	1022/1350 (76%)	1022 (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 (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	262	ASN
2	C	135	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

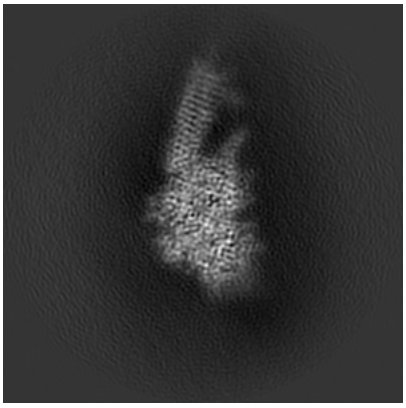
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-22444. These allow visual inspection of the internal detail of the map and identification of artifacts.

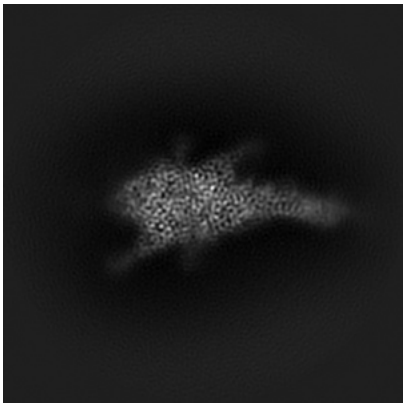
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

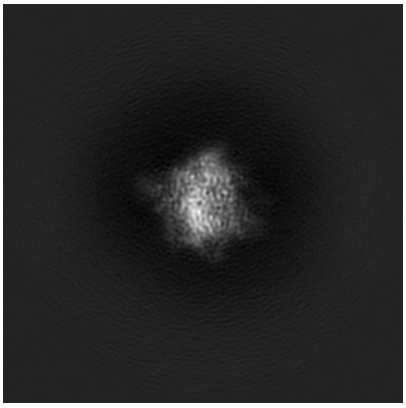
6.1.1 Primary map



X



Y

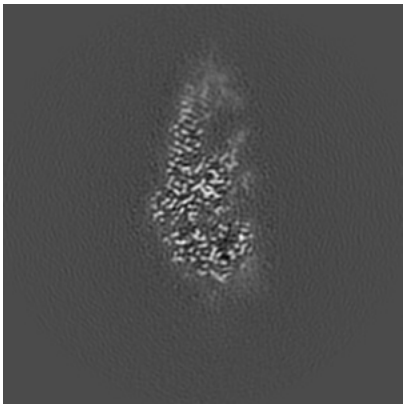


Z

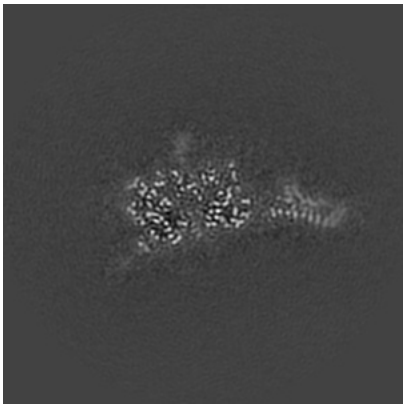
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

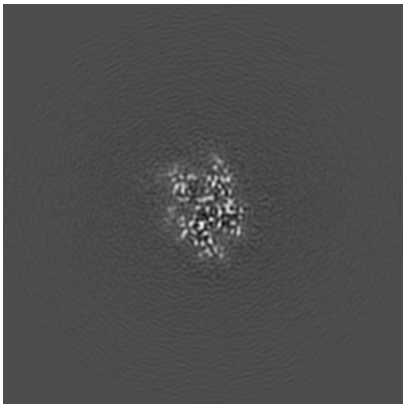
6.2.1 Primary map



X Index: 160



Y Index: 160

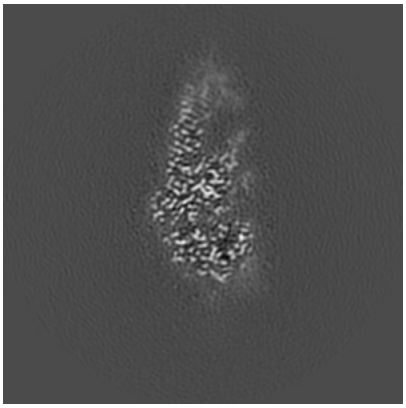


Z Index: 160

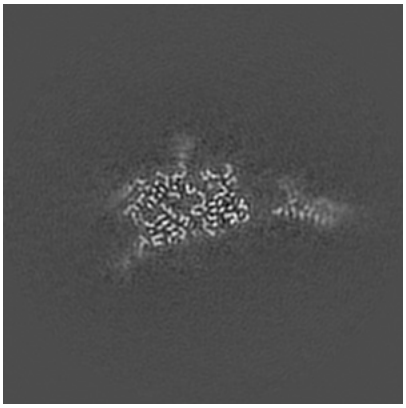
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

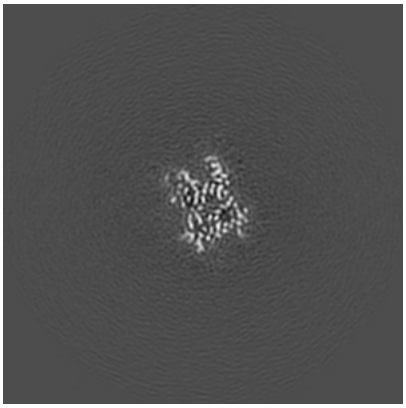
6.3.1 Primary map



X Index: 160



Y Index: 163



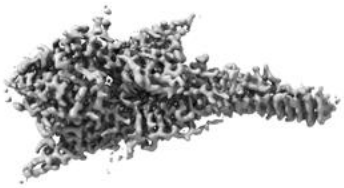
Z Index: 167

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

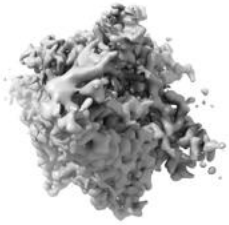
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

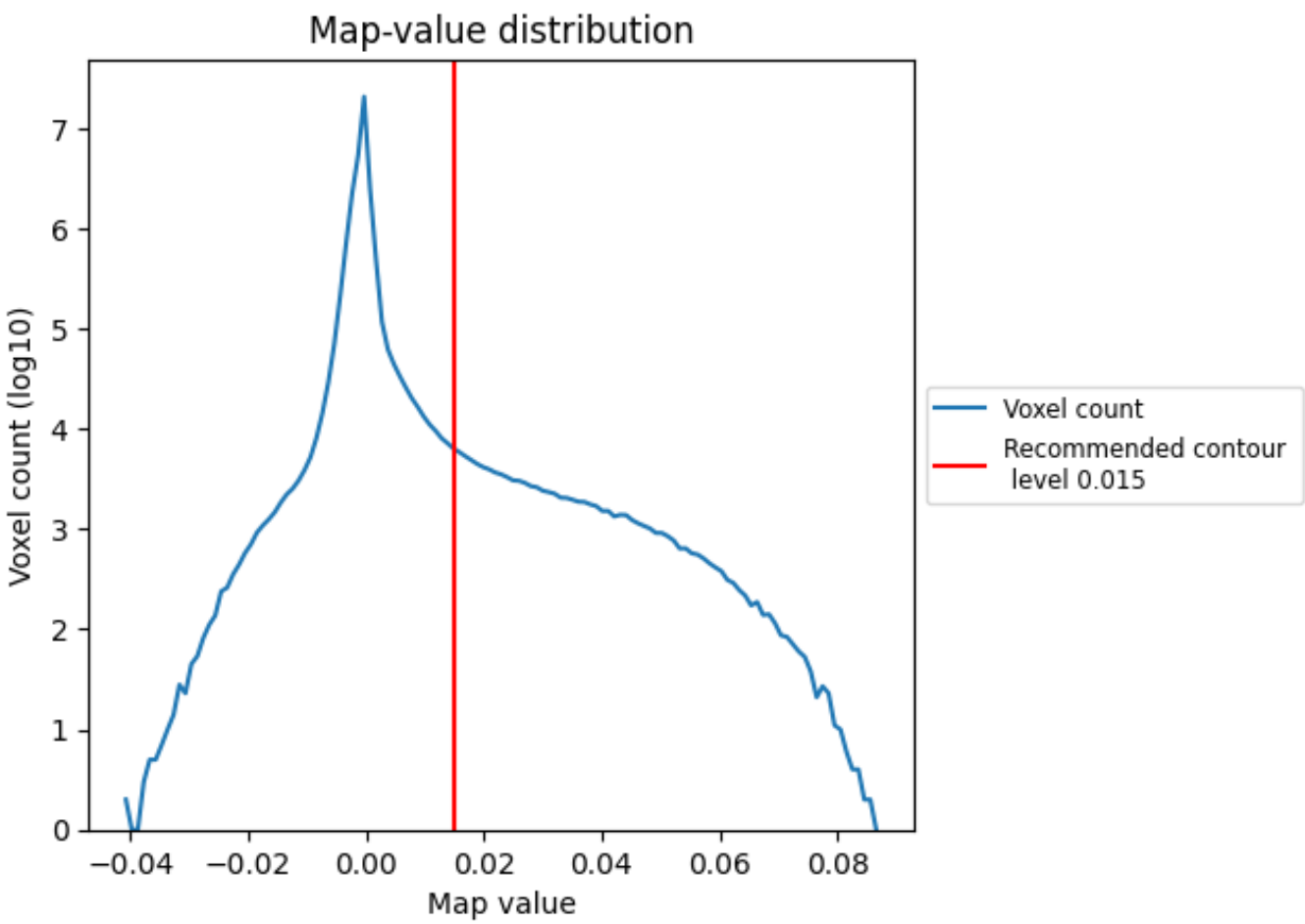
6.5 Mask visualisation (i)

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

7 Map analysis (i)

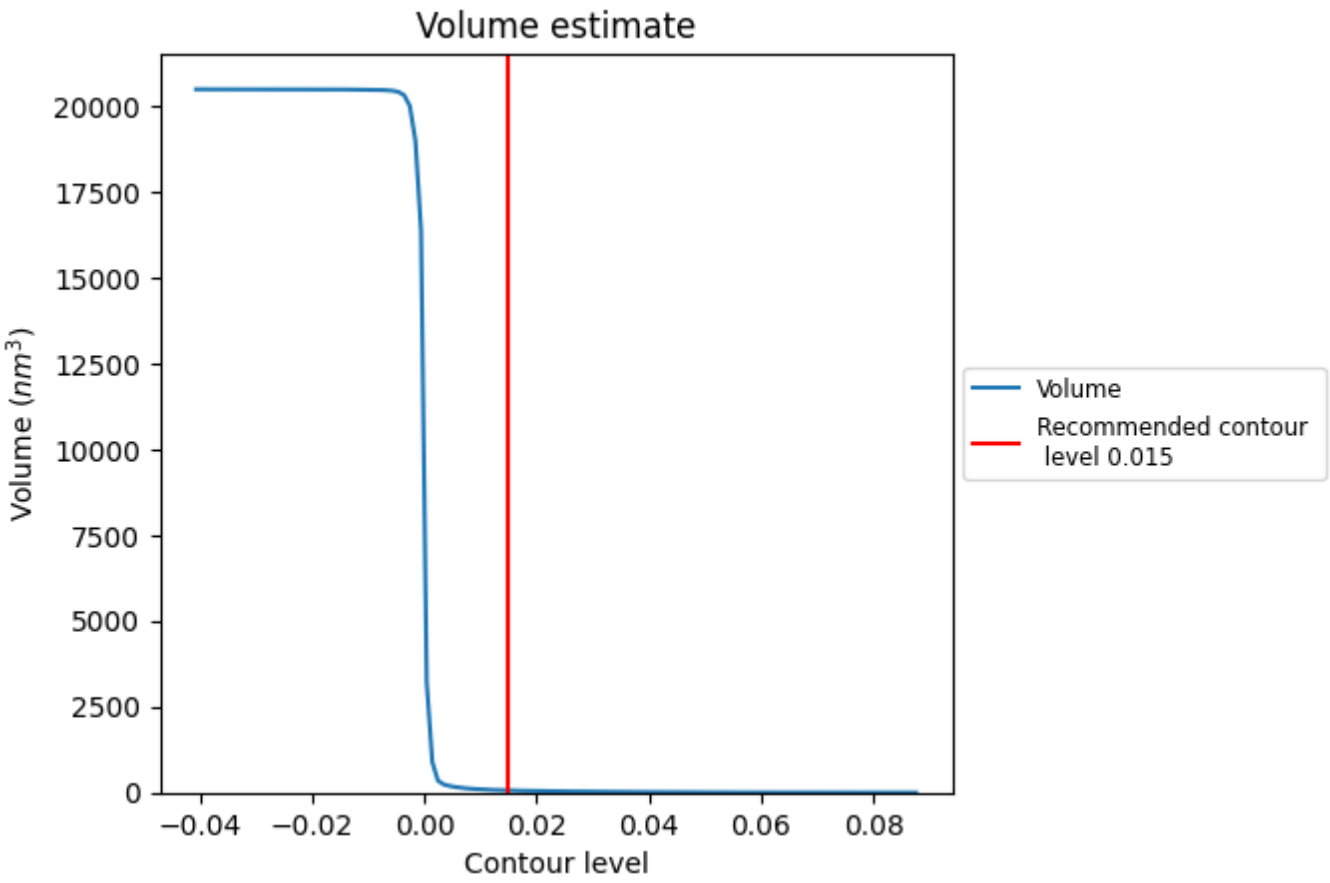
This section contains the results of statistical analysis of the map.

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.

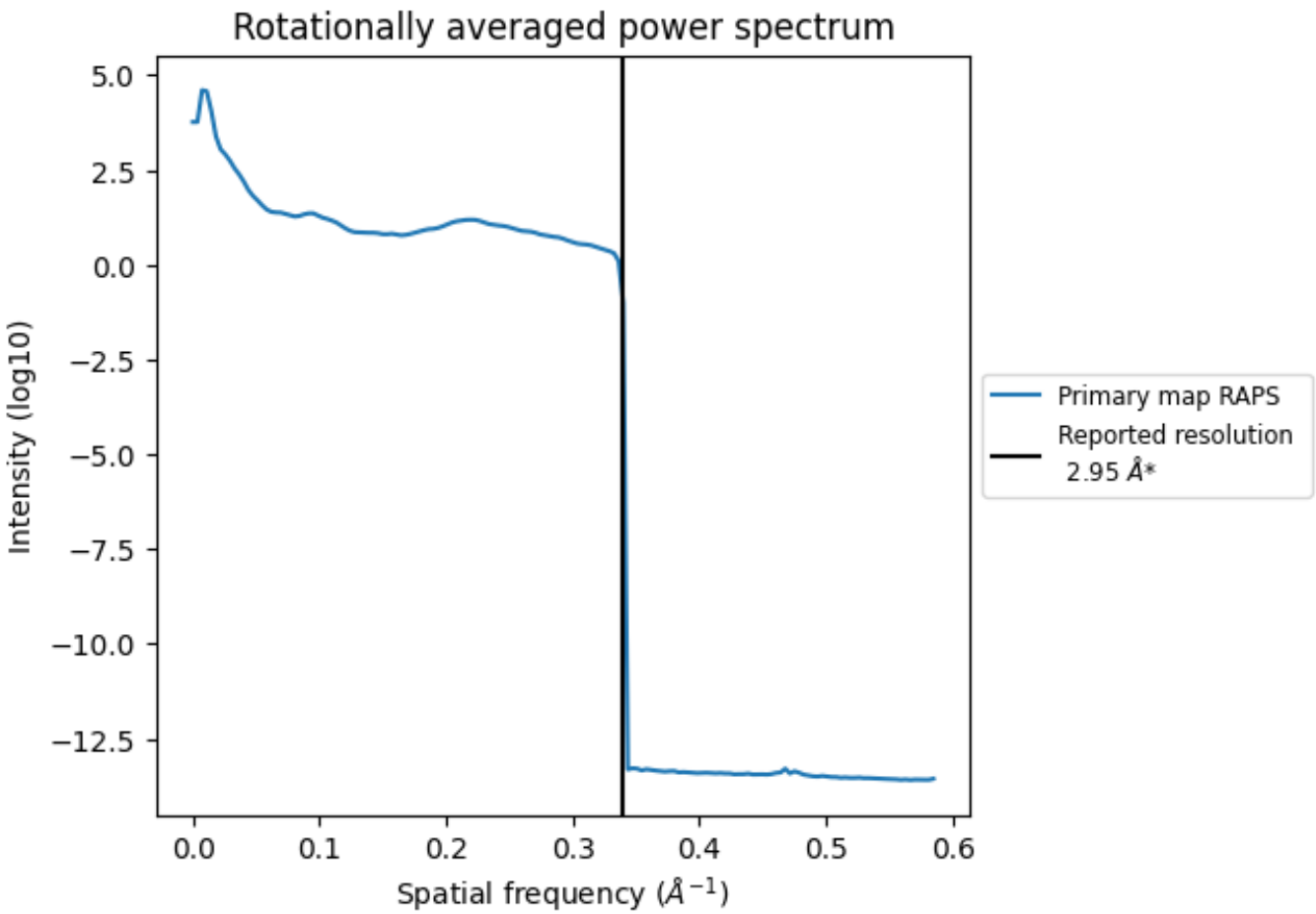
7.2 Volume estimate (i)



The volume at the recommended contour level is 63 nm^3; this corresponds to an approximate mass of 57 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 0.339 Å^{-1}

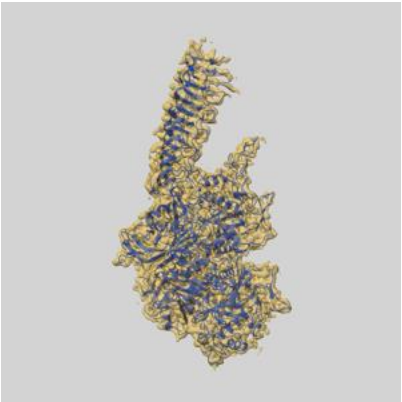
8 Fourier-Shell correlation (i)

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

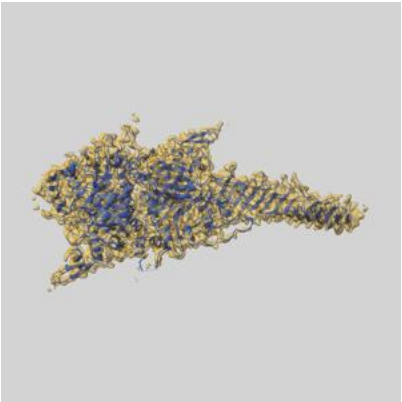
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-22444 and PDB model 7JR9. Per-residue inclusion information can be found in section 3 on page 5.

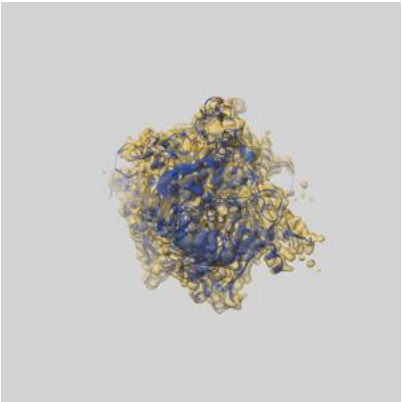
9.1 Map-model overlay (i)



X



Y



Z

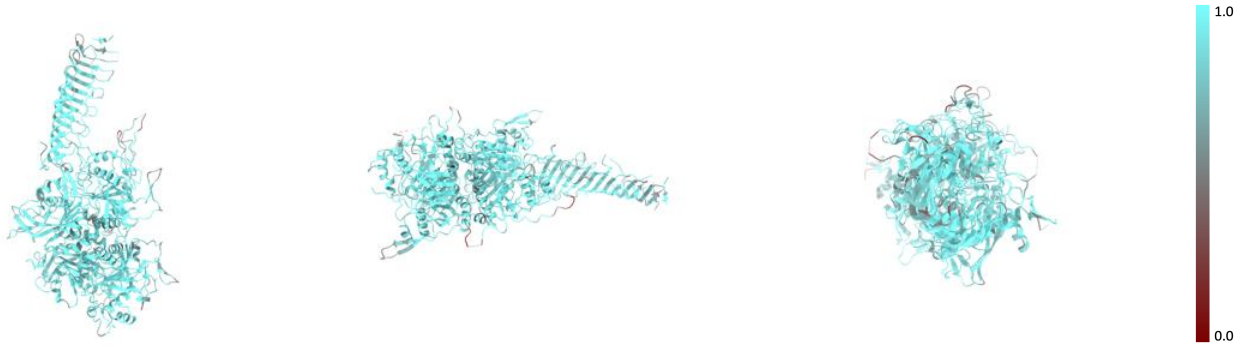
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

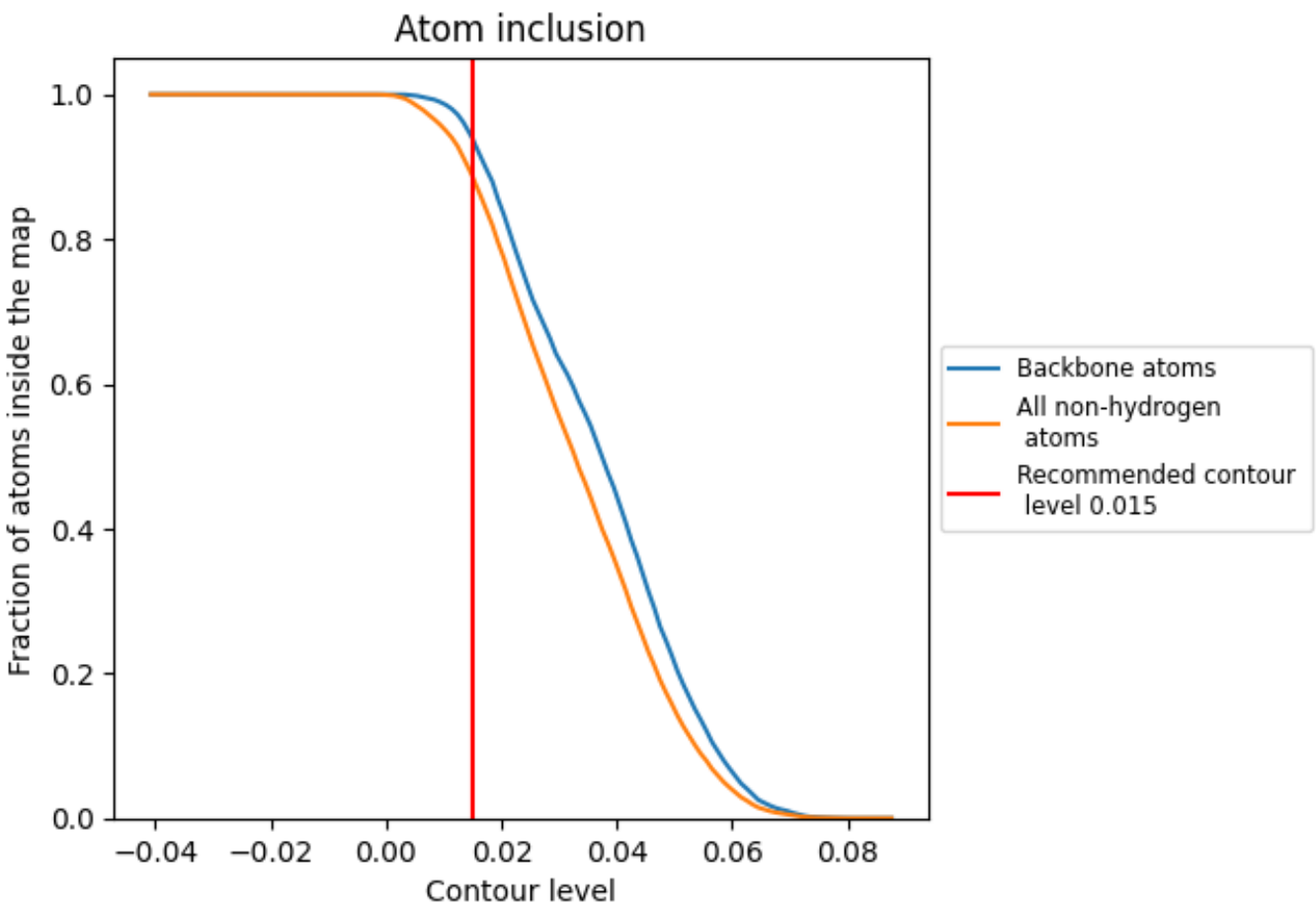
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 89% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8866	0.5750
A	0.8983	0.5840
B	0.9175	0.5930
C	0.8824	0.5710
D	0.8796	0.5770
E	0.8457	0.5400
F	0.9000	0.4750
G	0.8333	0.5180