Full wwPDB EM Validation Report

May 10, 2023 – 10:23 pm BST

PDB ID	:	8C7G
EMDB ID	:	EMD-16457
Title	:	Drosophila melanogaster Rab7 GEF complex Mon1-Ccz1-Bulli
Authors	:	Schaefer, J.; Herrmann, E.; Kuemmel, D.; Moeller, A.
Deposited on	:	2023-01-15
Resolution	:	3.20 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:

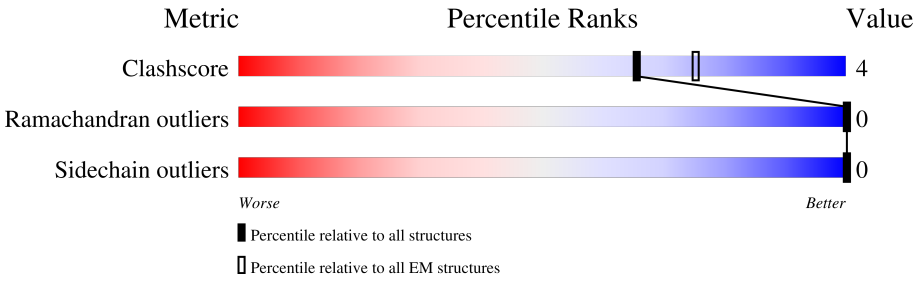
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 3.20 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	642	6% 82% 13% 5%
2	B	507	5% 72% 7% 21%
3	C	528	71% 8% 20%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11525 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 Mic1 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	607	4802	3086	822	870	24	0	0

- Molecule 2 is a protein called Caffeine, calcium, zinc sensitivity 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	402	3311	2119	560	615	17	1	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	486	ASP	-	expression tag	UNP Q9VZL5
B	487	TYR	-	expression tag	UNP Q9VZL5
B	488	LYS	-	expression tag	UNP Q9VZL5
B	489	ASP	-	expression tag	UNP Q9VZL5
B	490	HIS	-	expression tag	UNP Q9VZL5
B	491	ASP	-	expression tag	UNP Q9VZL5
B	492	GLY	-	expression tag	UNP Q9VZL5
B	493	ASP	-	expression tag	UNP Q9VZL5
B	494	TYR	-	expression tag	UNP Q9VZL5
B	495	LYS	-	expression tag	UNP Q9VZL5
B	496	ASP	-	expression tag	UNP Q9VZL5
B	497	HIS	-	expression tag	UNP Q9VZL5
B	498	ASP	-	expression tag	UNP Q9VZL5
B	499	ILE	-	expression tag	UNP Q9VZL5
B	500	ASP	-	expression tag	UNP Q9VZL5
B	501	TYR	-	expression tag	UNP Q9VZL5
B	502	LYS	-	expression tag	UNP Q9VZL5
B	503	ASP	-	expression tag	UNP Q9VZL5
B	504	ASP	-	expression tag	UNP Q9VZL5
B	505	ASP	-	expression tag	UNP Q9VZL5
B	506	ASP	-	expression tag	UNP Q9VZL5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	507	LYS	-	expression tag	UNP Q9VZL5

- Molecule 3 is a protein called Vacuolar fusion protein MON1 homolog.

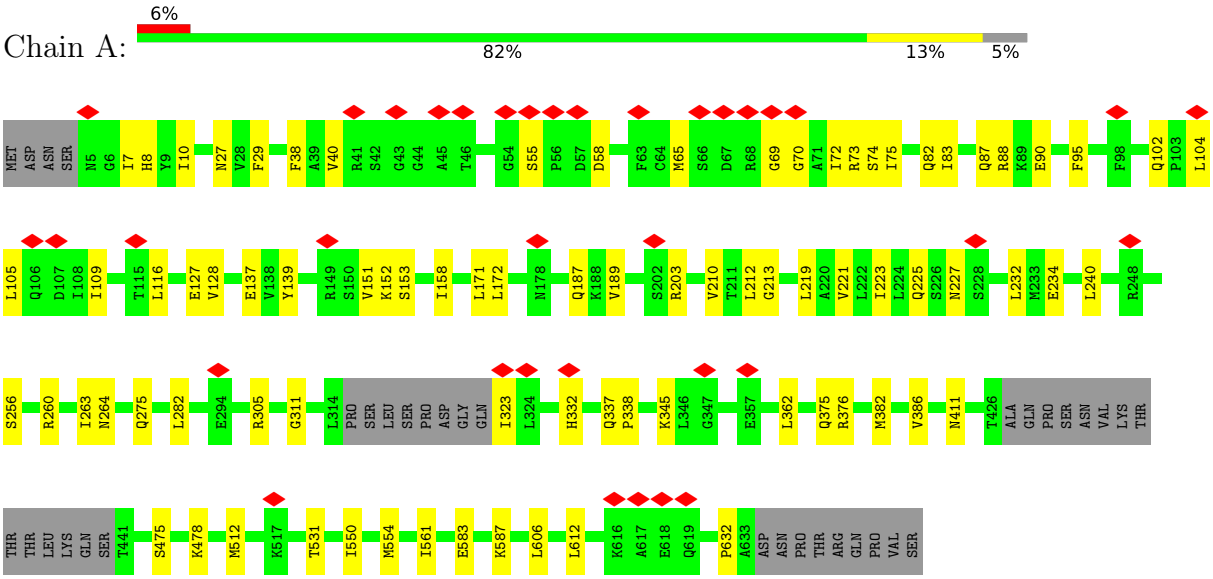
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	420	Total	C	N	O	S	0	0
			3412	2205	581	610	16		

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.

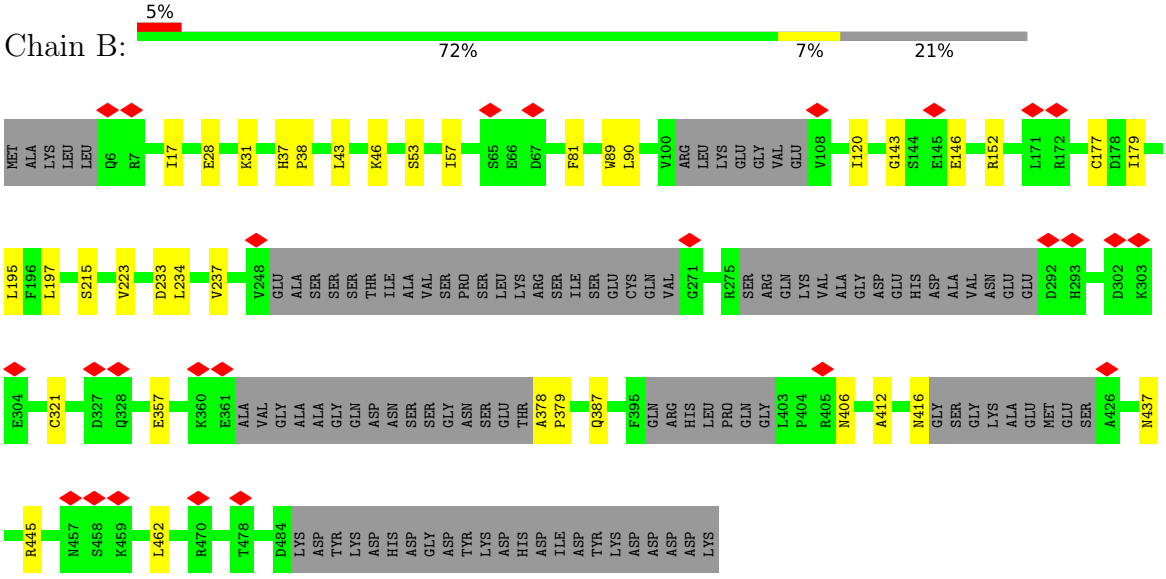
• Molecule 1: Mic1 domain-containing protein

Chain A:



• Molecule 2: Caffeine, calcium, zinc sensitivity 1

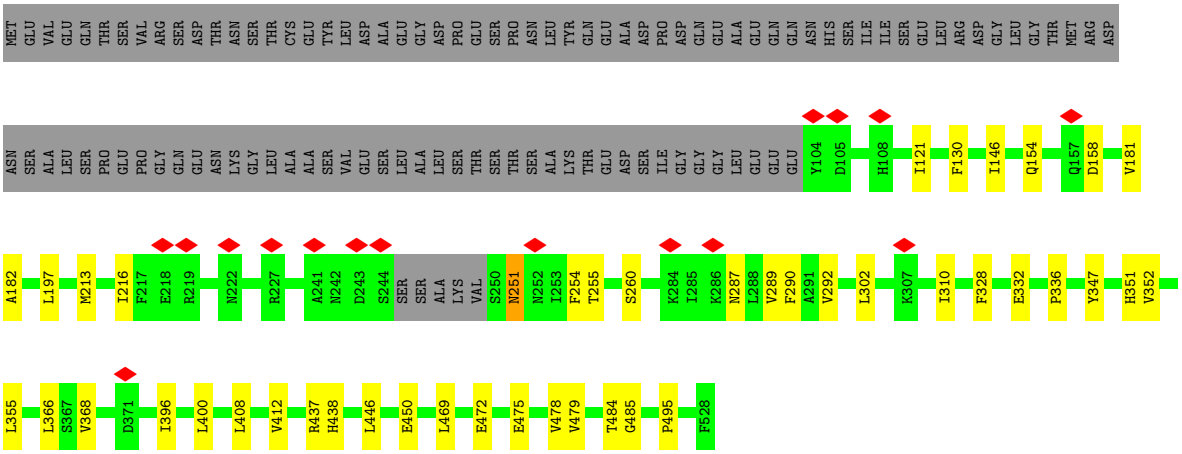
Chain B:



• Molecule 3: Vacuolar fusion protein MON1 homolog

Chain C:


71%
8%
20%


MET GLU VAL GLU GLN THR SER VAL ARG SER ASP THR ASN SER THR CYS GLU TYR LEU ASP ALA GLU GLY ASP PRO GLU SER PRO ASN LEU TYR GLN GLU ALA ASP PRO ASP GLN GLU ALA GLU GLN GLN ASN HIS SER ILE ILE SER GLU LEU ARG ASP GLY LEU GLY THR MET ARG ASP
ASN SER ALA LEU SER PRO GLU PRO GLY GLN GLU ASN LYS GLY LEU ALA ALA SER VAL GLU SER LEU ALA LEU SER THR SER THR SER ALA LYS THR GLU ASP SER ILE GLY GLY GLY LEU GLU GLU GLU Y104 D105 H108 I121 F130 I146 Q154 Q157 D158 V181
A182 L197 M213 I216 F217 E218 R219 N222 R227 A241 N242 D243 S244 SER SER ALA LYS VAL S250 N251 N252 I253 F254 T255 S260 K284 I285 K286 N287 L288 V289 F290 A291 V292 L302 K307 I310 F328 E332 P336 Y347 H351 V352
L355 L366 S367 V368 D371 I396 L400 L408 V412 R437 H438 L446 E450 L469 E472 E475 V478 V479 T484 G485 P495 F528

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	390520	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.356	Depositor
Minimum map value	-0.054	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	295.68, 295.68, 295.68	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.92399997, 0.92399997, 0.92399997	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	0.27	0/4892	0.51	0/6631
2	B	0.28	0/3382	0.50	0/4578
3	C	0.28	0/3486	0.51	2/4710 (0.0%)
All	All	0.27	0/11760	0.50	2/15919 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	251	ASN	N-CA-C	6.25	127.87	111.00
3	C	251	ASN	N-CA-CB	-5.57	100.57	110.60

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	4802	0	4947	50	0
2	B	3311	0	3253	22	0
3	C	3412	0	3472	28	0
All	All	11525	0	11672	95	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 (95) 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)
3:C:289:VAL:HG12	3:C:290:PHE:CD1	2.27	0.69
2:B:179:ILE:HD11	2:B:412:ALA:HA	1.74	0.69
3:C:251:ASN:O	3:C:251:ASN:OD1	2.11	0.69
1:A:73:ARG:NH1	1:A:90:GLU:OE1	2.26	0.68
1:A:260:ARG:NH1	1:A:275:GLN:OE1	2.28	0.66
2:B:416:ASN:HD21	2:B:445:ARG:HE	1.46	0.63
1:A:227:ASN:ND2	1:A:234:GLU:OE2	2.26	0.59
3:C:332:GLU:OE2	3:C:351:HIS:NE2	2.36	0.58
1:A:583:GLU:OE2	1:A:587:LYS:NZ	2.36	0.58
1:A:210:VAL:HG22	1:A:223:ILE:HG12	1.86	0.57
1:A:531:THR:OG1	2:B:387:GLN:OE1	2.23	0.56
3:C:290:PHE:HB2	3:C:366:LEU:HD12	1.87	0.55
1:A:69:GLY:HA3	1:A:88:ARG:HE	1.72	0.55
3:C:121:ILE:HB	3:C:130:PHE:HB3	1.88	0.55
2:B:53:SER:O	2:B:57:ILE:HD12	2.07	0.54
1:A:375:GLN:O	1:A:376:ARG:NH1	2.32	0.54
2:B:406:ASN:HD21	2:B:437:ASN:HD21	1.53	0.54
3:C:408:LEU:O	3:C:412:VAL:HG23	2.07	0.54
2:B:17:ILE:HG12	2:B:90:LEU:HG	1.89	0.54
3:C:290:PHE:HE2	3:C:310:ILE:HB	1.72	0.54
3:C:182:ALA:HB2	3:C:197:LEU:HD21	1.90	0.53
2:B:37:HIS:HB3	2:B:38:PRO:HD3	1.91	0.53
1:A:102:GLN:OE1	1:A:104:LEU:HG	2.09	0.53
2:B:28:GLU:HB2	2:B:31:LYS:HD2	1.91	0.53
1:A:10:ILE:HD11	1:A:282:LEU:HD21	1.90	0.52
3:C:289:VAL:HG12	3:C:290:PHE:HD1	1.74	0.52
2:B:146:GLU:O	2:B:152:ARG:NH1	2.42	0.51
1:A:332:HIS:HB2	1:A:345:LYS:HZ3	1.75	0.51
1:A:550:ILE:O	1:A:554:MET:HE2	2.11	0.51
1:A:95:PHE:HE1	1:A:128:VAL:HG21	1.77	0.50
3:C:251:ASN:HB2	3:C:254:PHE:CE2	2.46	0.50
1:A:74:SER:HB2	1:A:87:GLN:HB3	1.92	0.50
1:A:55:SER:HB2	1:A:58:ASP:HB2	1.93	0.50
3:C:287:ASN:HB3	3:C:368:VAL:HG12	1.93	0.50
3:C:255:THR:HG23	3:C:260:SER:O	2.12	0.49
1:A:512:MET:HE1	2:B:197:LEU:HD11	1.94	0.49
1:A:212:LEU:HD12	1:A:221:VAL:HG22	1.94	0.49
1:A:561:ILE:HG21	3:C:475:GLU:HG3	1.94	0.49
3:C:146:ILE:HD13	3:C:181:VAL:HG21	1.95	0.49
2:B:120:ILE:HG21	2:B:177:CYS:HB3	1.93	0.49
1:A:213:GLY:O	1:A:219:LEU:HD12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:GLN:HB3	1:A:338:PRO:HD3	1.94	0.48
2:B:43:LEU:HA	2:B:46:LYS:HD3	1.96	0.48
1:A:305:ARG:HH12	1:A:362:LEU:HD11	1.78	0.48
3:C:292:VAL:HG22	3:C:302:LEU:HD13	1.94	0.48
2:B:462:LEU:HD12	3:C:469:LEU:HD21	1.95	0.48
1:A:158:ILE:HD11	1:A:172:LEU:HD23	1.96	0.47
3:C:478:VAL:HG23	3:C:495:PRO:HA	1.95	0.47
1:A:203:ARG:HH12	1:A:225:GLN:CD	2.18	0.47
1:A:82:GLN:HB3	1:A:83:ILE:HD12	1.96	0.46
1:A:158:ILE:CD1	1:A:172:LEU:HD23	2.45	0.46
1:A:475:SER:HA	1:A:478:LYS:NZ	2.30	0.46
2:B:406:ASN:HD21	2:B:437:ASN:ND2	2.12	0.46
1:A:382:MET:N	1:A:382:MET:SD	2.89	0.45
2:B:215:SER:HA	2:B:321:CYS:O	2.16	0.45
1:A:72:ILE:HG21	1:A:75:ILE:HD11	1.98	0.45
1:A:382:MET:O	1:A:386:VAL:HG13	2.17	0.45
1:A:65:MET:HG2	1:A:105:LEU:HD11	1.99	0.45
3:C:446:LEU:O	3:C:450:GLU:HG2	2.16	0.45
2:B:195:LEU:HD12	2:B:357:GLU:OE1	2.17	0.45
2:B:81:PHE:HB3	2:B:89:TRP:HZ3	1.81	0.45
3:C:328:PHE:CE1	3:C:352:VAL:HG11	2.52	0.45
2:B:233:ASP:O	2:B:237:VAL:HG23	2.17	0.45
3:C:336:PRO:HB2	3:C:347:TYR:CD2	2.52	0.44
1:A:219:LEU:HD23	1:A:240:LEU:HD12	1.99	0.44
1:A:632:PRO:O	3:C:438:HIS:NE2	2.51	0.44
1:A:232:LEU:HD13	1:A:256:SER:HA	2.00	0.43
1:A:606:LEU:HD22	1:A:612:LEU:HD11	2.00	0.43
3:C:412:VAL:HG11	3:C:437:ARG:HH12	1.82	0.43
1:A:311:GLY:HA3	1:A:323:ILE:HD11	2.00	0.43
1:A:127:GLU:HB2	1:A:139:TYR:O	2.19	0.43
1:A:70:GLY:N	1:A:88:ARG:HH21	2.17	0.42
3:C:472:GLU:HB2	3:C:479:VAL:HG22	2.00	0.42
3:C:396:ILE:O	3:C:400:LEU:HD13	2.19	0.42
1:A:187:GLN:O	1:A:189:VAL:HG23	2.19	0.42
3:C:484:THR:OG1	3:C:485:GLY:N	2.52	0.42
1:A:65:MET:HG2	1:A:105:LEU:HD21	2.01	0.42
1:A:90:GLU:OE2	1:A:116:LEU:HB2	2.19	0.42
1:A:411:ASN:OD1	1:A:475:SER:OG	2.30	0.42
1:A:137:GLU:HG3	1:A:153:SER:HB2	2.01	0.42
1:A:212:LEU:HG	1:A:219:LEU:HD11	2.02	0.42
1:A:263:ILE:O	1:A:264:ASN:ND2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:PHE:HB3	2:B:89:TRP:CZ3	2.54	0.41
3:C:154:GLN:HA	3:C:158:ASP:O	2.21	0.41
1:A:7:ILE:O	1:A:8:HIS:ND1	2.53	0.41
1:A:151:VAL:HG23	1:A:152:LYS:N	2.36	0.41
2:B:143:GLY:O	2:B:152:ARG:HD3	2.21	0.40
2:B:378:ALA:HB3	2:B:379:PRO:HD3	2.03	0.40
3:C:355:LEU:HD23	3:C:355:LEU:HA	1.89	0.40
1:A:29:PHE:HB2	1:A:38:PHE:HB2	2.04	0.40
1:A:171:LEU:C	1:A:172:LEU:HD12	2.42	0.40
1:A:27:ASN:H	1:A:40:VAL:HG12	1.86	0.40
1:A:109:ILE:HD12	1:A:109:ILE:H	1.86	0.40
3:C:213:MET:O	3:C:216:ILE:HG22	2.21	0.40
2:B:223:VAL:HG21	2:B:234:LEU:HD21	2.03	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	601/642 (94%)	580 (96%)	21 (4%)	0	100	100
2	B	389/507 (77%)	375 (96%)	14 (4%)	0	100	100
3	C	416/528 (79%)	403 (97%)	13 (3%)	0	100	100
All	All	1406/1677 (84%)	1358 (97%)	48 (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	546/579 (94%)	546 (100%)	0	100	100
2	B	369/455 (81%)	369 (100%)	0	100	100
3	C	378/469 (81%)	378 (100%)	0	100	100
All	All	1293/1503 (86%)	1293 (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	187	GLN
1	A	264	ASN
2	B	416	ASN
2	B	437	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.

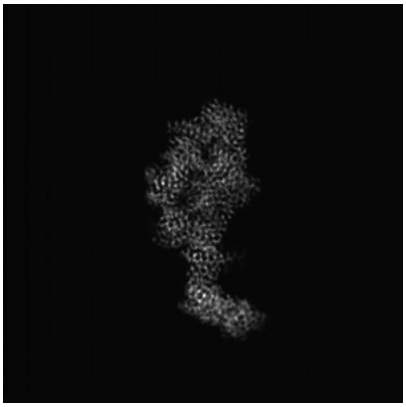
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16457. These allow visual inspection of the internal detail of the map and identification of artifacts.

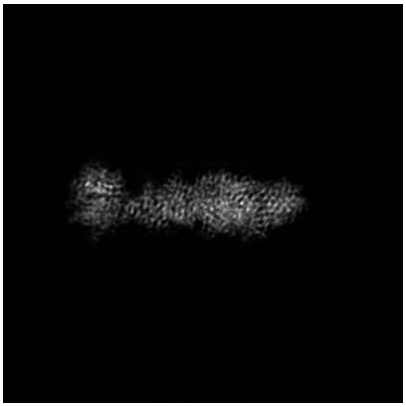
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

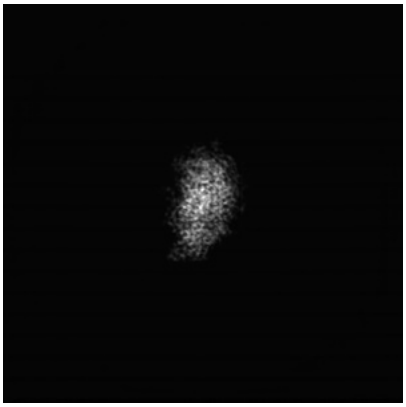
6.1.1 Primary map



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: 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: 159

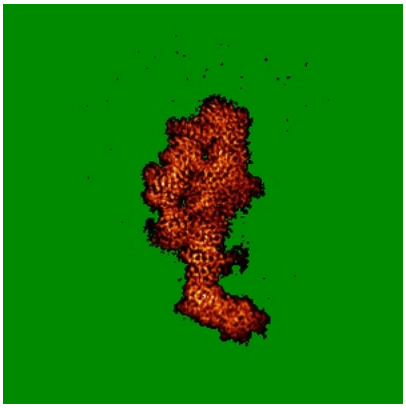
Y Index: 162

Z Index: 175

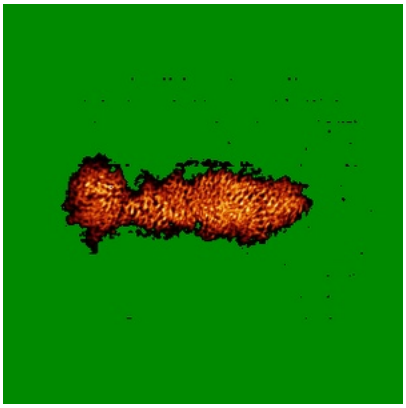
The images above show the largest variance slices of the map in three orthogonal directions.

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

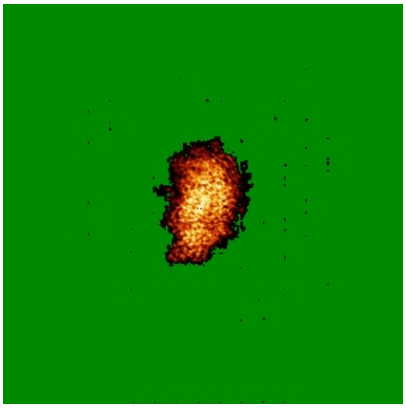
6.4.1 Primary map



X



Y

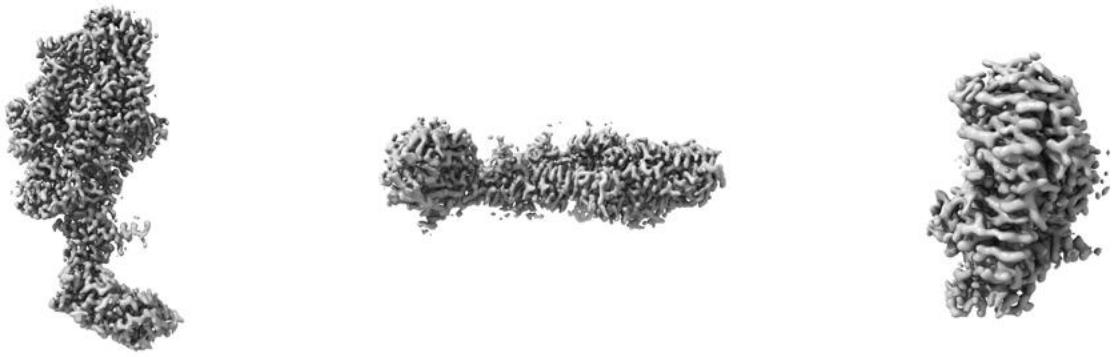


Z

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

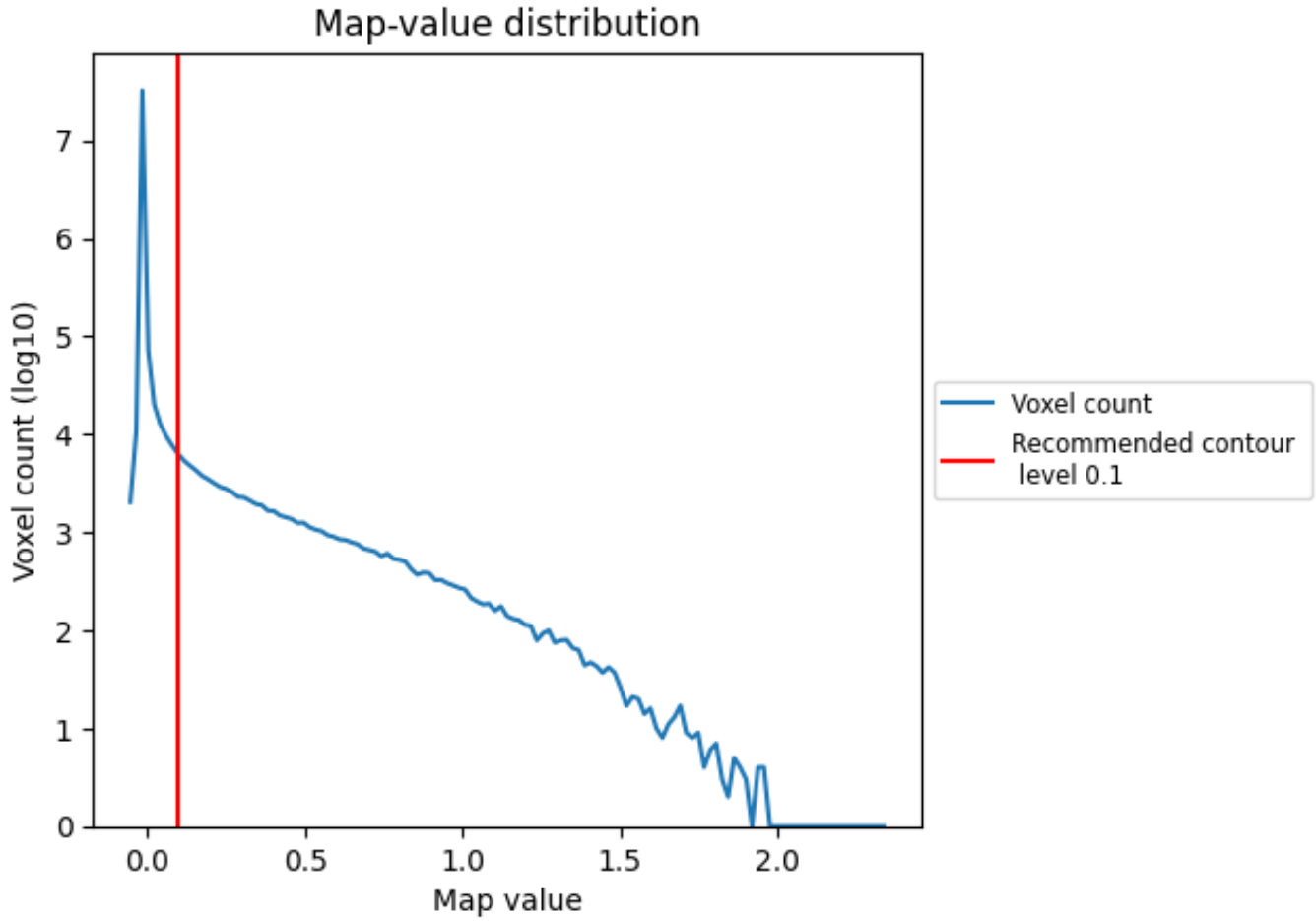
6.6 Mask visualisation (i)

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

7 Map analysis

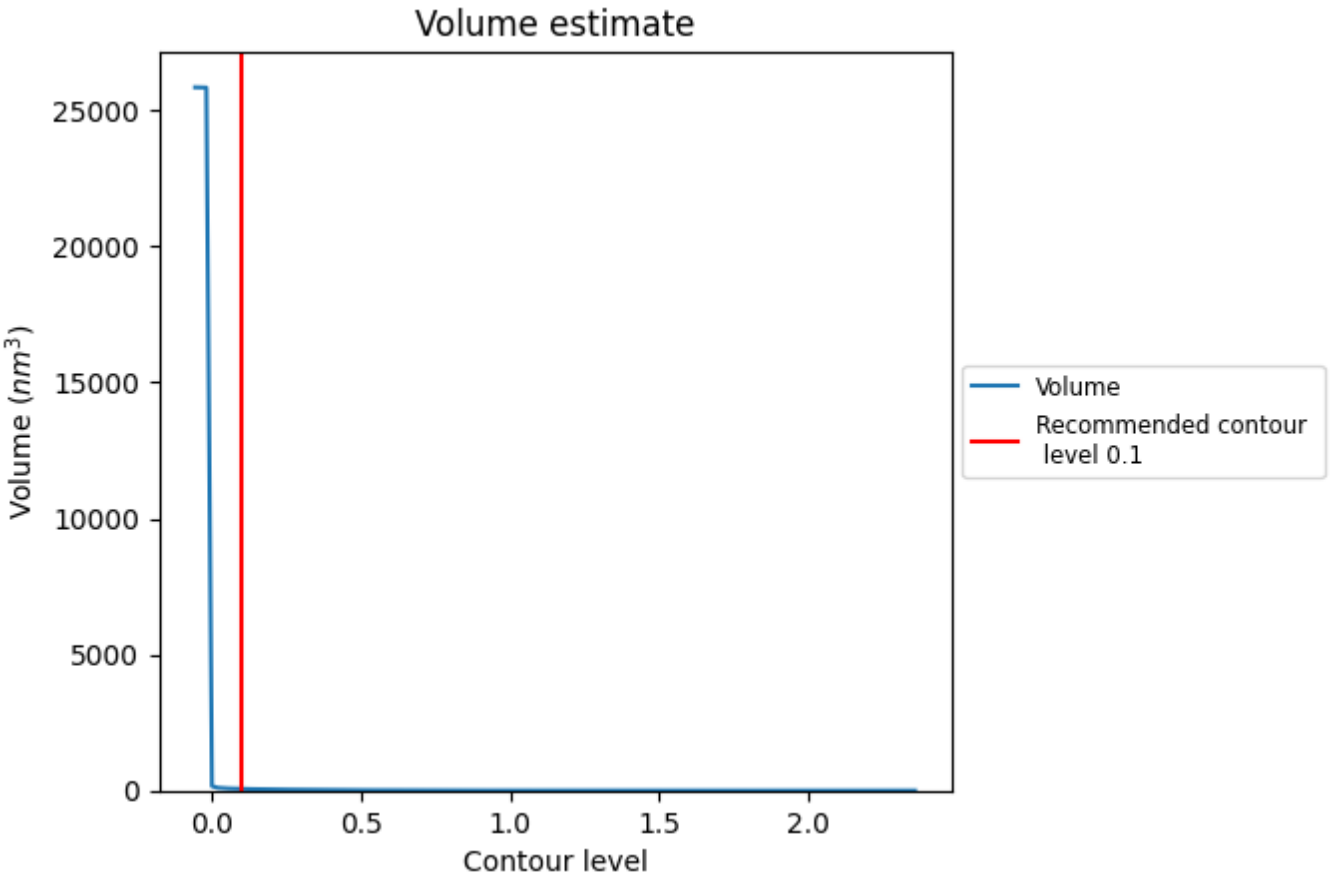
This section contains the results of statistical analysis of the map.

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.

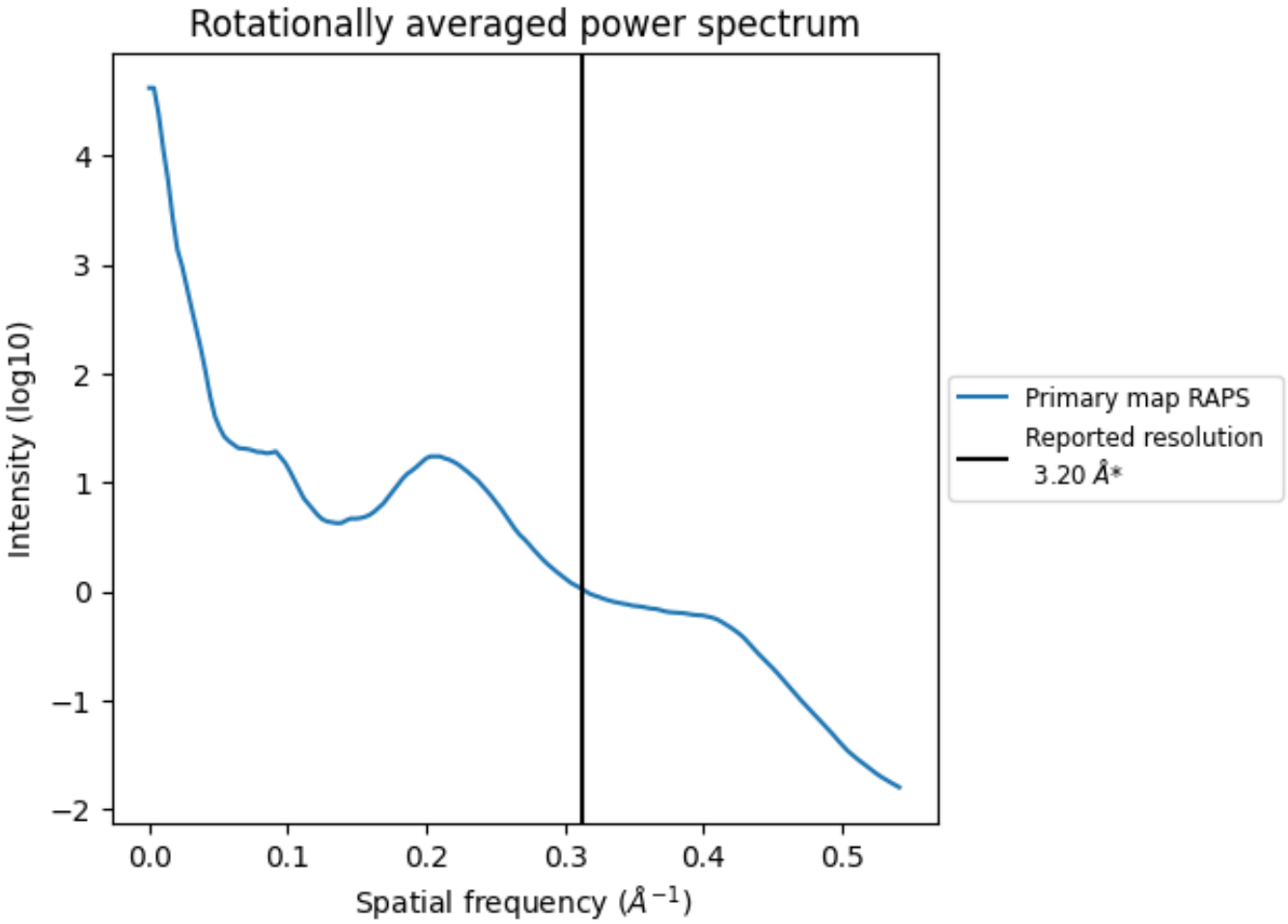
7.2 Volume estimate



The volume at the recommended contour level is 62 nm^3; this corresponds to an approximate mass of 56 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)

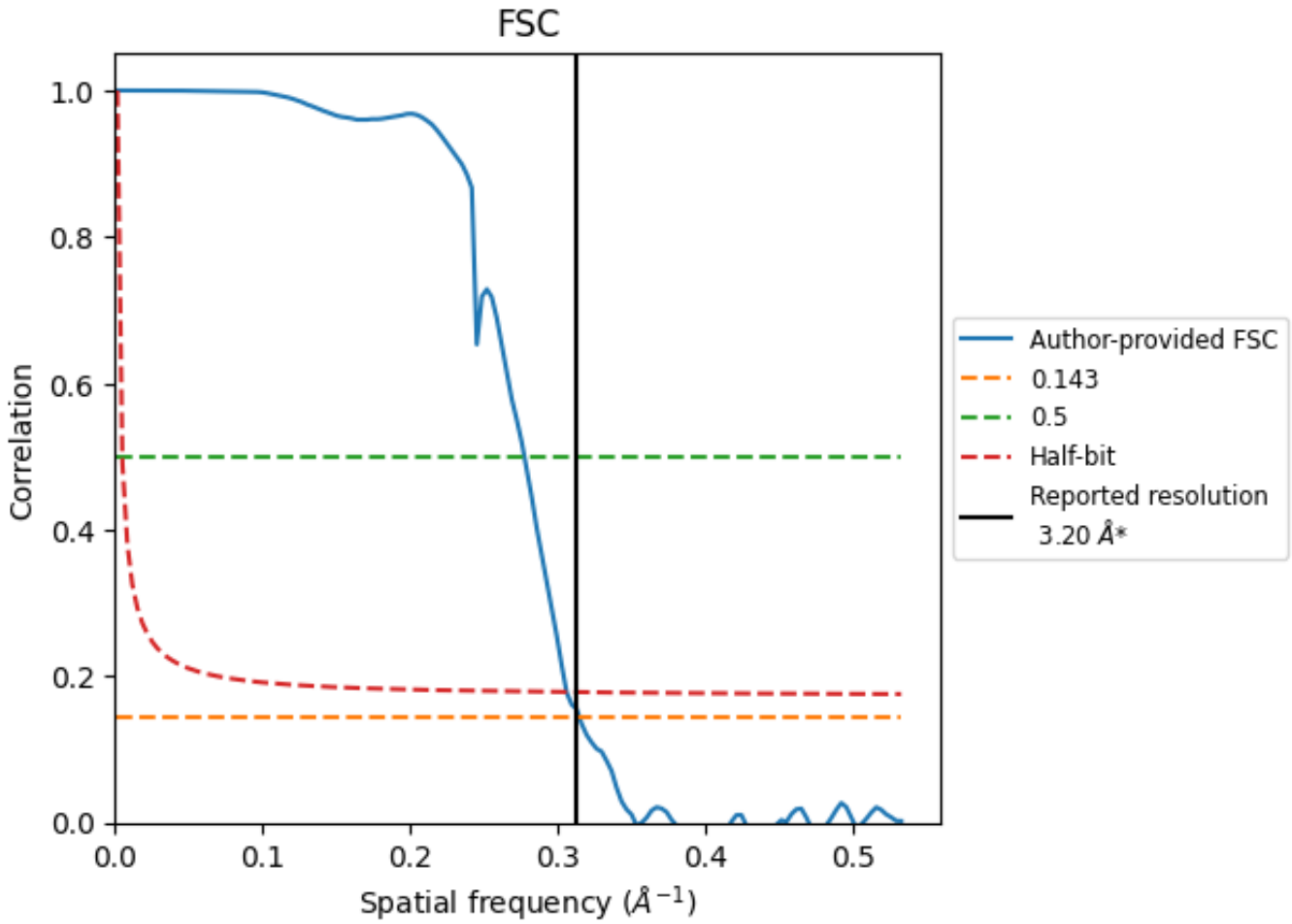


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

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 0.312 Å^{-1}

8.2 Resolution estimates (i)

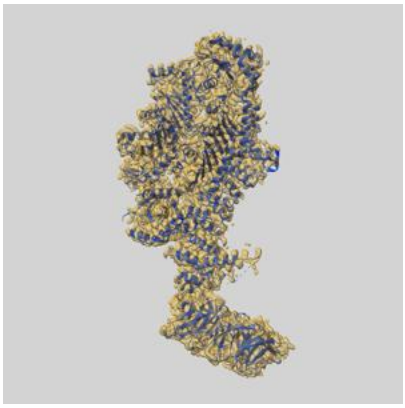
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.18	3.60	3.27
Unmasked-calculated*	-	-	-

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

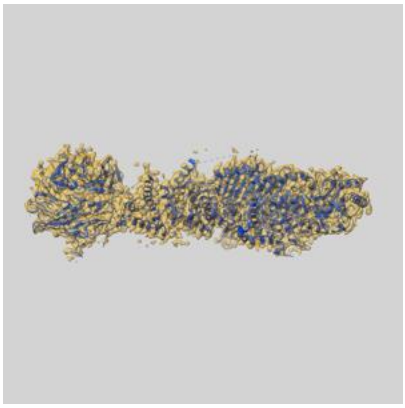
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16457 and PDB model 8C7G. Per-residue inclusion information can be found in section 3 on page 5.

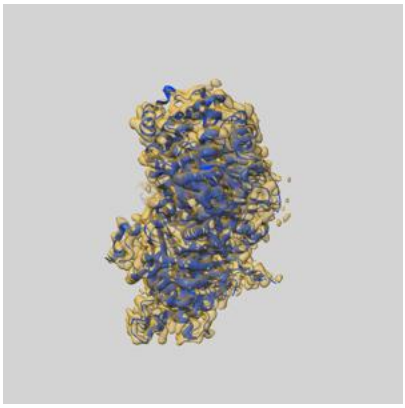
9.1 Map-model overlay



X



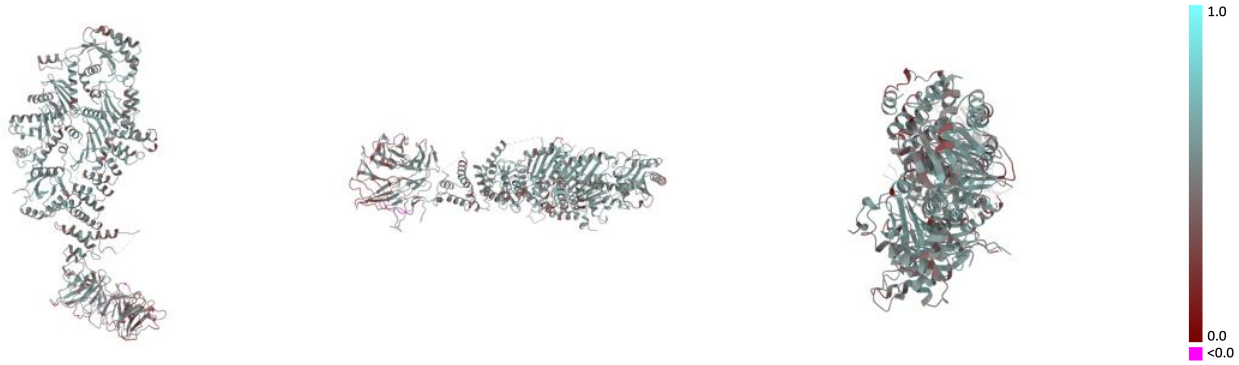
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

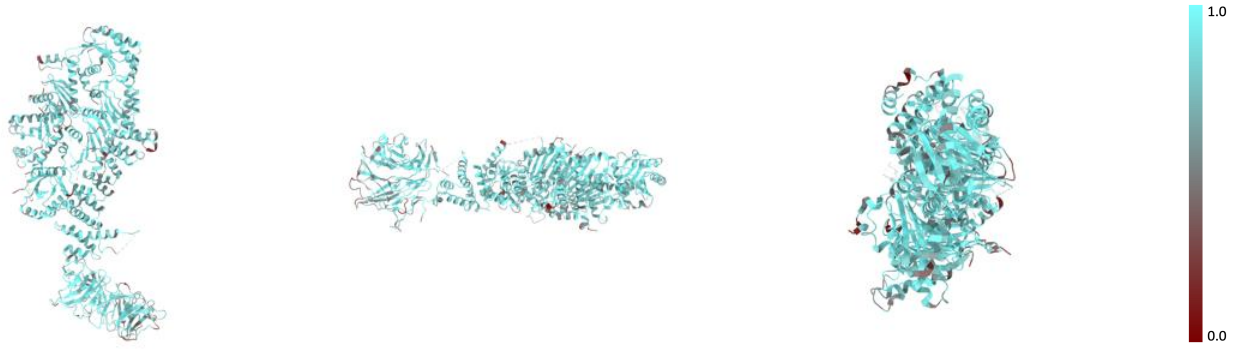
9.2 Q-score mapped to coordinate model (i)



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.

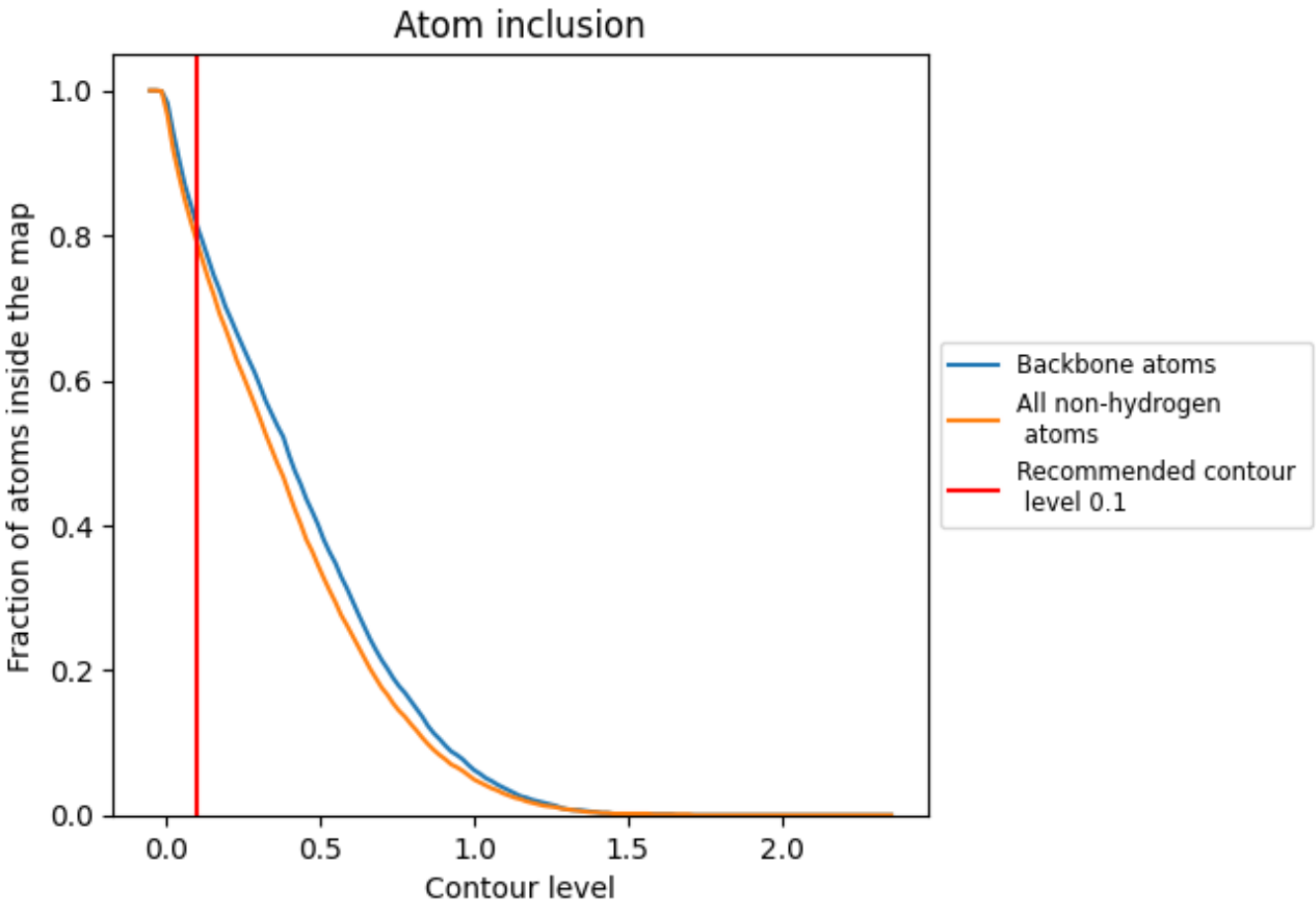
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 79% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7890	0.4900
A	0.7680	0.4520
B	0.7960	0.5240
C	0.8110	0.5110