



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 05:24 PM UTC

PDB ID : 9QX5 / pdb_00009qx5
EMDB ID : EMD-53435
Title : Cryo-EM structure of the C. elegans UBR4/KCMF1 complex (side focused refinement)
Authors : Grabarczyk, D.B.; Clausen, T.
Deposited on : 2025-04-15
Resolution : 3.50 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 ⓘ 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

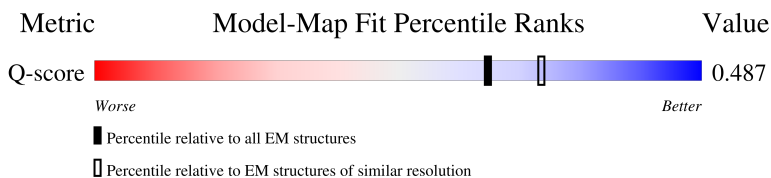
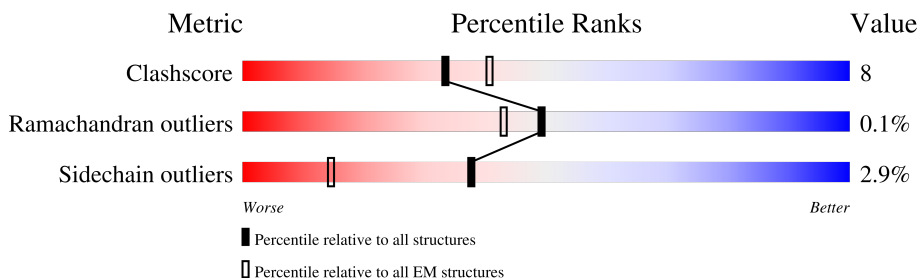
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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 $\leq 5\%$. 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	4284	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11554 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 UBR-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1435	Total	C	N	O	S	0	0
			11554	7416	1956	2116	66		

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4212	GLY	-	expression tag	UNP A0A0S4XR36
A	4213	SER	-	expression tag	UNP A0A0S4XR36
A	4214	LEU	-	expression tag	UNP A0A0S4XR36
A	4215	GLU	-	expression tag	UNP A0A0S4XR36
A	4216	VAL	-	expression tag	UNP A0A0S4XR36
A	4217	LEU	-	expression tag	UNP A0A0S4XR36
A	4218	PHE	-	expression tag	UNP A0A0S4XR36
A	4219	GLN	-	expression tag	UNP A0A0S4XR36
A	4220	GLY	-	expression tag	UNP A0A0S4XR36
A	4221	PRO	-	expression tag	UNP A0A0S4XR36
A	4222	ALA	-	expression tag	UNP A0A0S4XR36
A	4223	GLU	-	expression tag	UNP A0A0S4XR36
A	4224	ALA	-	expression tag	UNP A0A0S4XR36
A	4225	ALA	-	expression tag	UNP A0A0S4XR36
A	4226	ALA	-	expression tag	UNP A0A0S4XR36
A	4227	LYS	-	expression tag	UNP A0A0S4XR36
A	4228	GLU	-	expression tag	UNP A0A0S4XR36
A	4229	ALA	-	expression tag	UNP A0A0S4XR36
A	4230	ALA	-	expression tag	UNP A0A0S4XR36
A	4231	ALA	-	expression tag	UNP A0A0S4XR36
A	4232	LYS	-	expression tag	UNP A0A0S4XR36
A	4233	GLU	-	expression tag	UNP A0A0S4XR36
A	4234	ALA	-	expression tag	UNP A0A0S4XR36
A	4235	ALA	-	expression tag	UNP A0A0S4XR36
A	4236	ALA	-	expression tag	UNP A0A0S4XR36
A	4237	LYS	-	expression tag	UNP A0A0S4XR36
A	4238	GLU	-	expression tag	UNP A0A0S4XR36
A	4239	ALA	-	expression tag	UNP A0A0S4XR36

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	4240	ALA	-	expression tag	UNP A0A0S4XR36
A	4241	ALA	-	expression tag	UNP A0A0S4XR36
A	4242	LYS	-	expression tag	UNP A0A0S4XR36
A	4243	ALA	-	expression tag	UNP A0A0S4XR36
A	4244	LEU	-	expression tag	UNP A0A0S4XR36
A	4245	GLU	-	expression tag	UNP A0A0S4XR36
A	4246	ALA	-	expression tag	UNP A0A0S4XR36
A	4247	GLU	-	expression tag	UNP A0A0S4XR36
A	4248	ALA	-	expression tag	UNP A0A0S4XR36
A	4249	ALA	-	expression tag	UNP A0A0S4XR36
A	4250	ALA	-	expression tag	UNP A0A0S4XR36
A	4251	LYS	-	expression tag	UNP A0A0S4XR36
A	4252	GLU	-	expression tag	UNP A0A0S4XR36
A	4253	ALA	-	expression tag	UNP A0A0S4XR36
A	4254	ALA	-	expression tag	UNP A0A0S4XR36
A	4255	ALA	-	expression tag	UNP A0A0S4XR36
A	4256	LYS	-	expression tag	UNP A0A0S4XR36
A	4257	GLU	-	expression tag	UNP A0A0S4XR36
A	4258	ALA	-	expression tag	UNP A0A0S4XR36
A	4259	ALA	-	expression tag	UNP A0A0S4XR36
A	4260	ALA	-	expression tag	UNP A0A0S4XR36
A	4261	LYS	-	expression tag	UNP A0A0S4XR36
A	4262	GLU	-	expression tag	UNP A0A0S4XR36
A	4263	ALA	-	expression tag	UNP A0A0S4XR36
A	4264	ALA	-	expression tag	UNP A0A0S4XR36
A	4265	ALA	-	expression tag	UNP A0A0S4XR36
A	4266	LYS	-	expression tag	UNP A0A0S4XR36
A	4267	ALA	-	expression tag	UNP A0A0S4XR36
A	4268	HIS	-	expression tag	UNP A0A0S4XR36
A	4269	HIS	-	expression tag	UNP A0A0S4XR36
A	4270	HIS	-	expression tag	UNP A0A0S4XR36
A	4271	HIS	-	expression tag	UNP A0A0S4XR36
A	4272	HIS	-	expression tag	UNP A0A0S4XR36
A	4273	HIS	-	expression tag	UNP A0A0S4XR36
A	4274	HIS	-	expression tag	UNP A0A0S4XR36
A	4275	HIS	-	expression tag	UNP A0A0S4XR36
A	4276	HIS	-	expression tag	UNP A0A0S4XR36
A	4277	HIS	-	expression tag	UNP A0A0S4XR36







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	168687	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.051	Depositor
Minimum map value	-0.024	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	486.912, 486.912, 486.912	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.268, 1.268, 1.268	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	0.18	0/11794	0.37	0/15957

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	11554	0	11508	192	0
All	All	11554	0	11508	192	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 (192) 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:2335:ARG:HH22	1:A:2372:TRP:HE1	1.29	0.81
1:A:758:VAL:HG23	1:A:894:LEU:HD11	1.68	0.74
1:A:1175:ALA:HB2	1:A:2179:GLU:HB2	1.72	0.72
1:A:1107:MET:HE3	1:A:1107:MET:HA	1.73	0.71
1:A:2201:LEU:O	1:A:2205:ILE:HG12	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1060:THR:HG22	1:A:1756:VAL:HB	1.77	0.66
1:A:863:LYS:HD2	1:A:863:LYS:H	1.61	0.66
1:A:2179:GLU:HA	1:A:2182:LEU:HD12	1.78	0.65
1:A:806:HIS:CE1	1:A:842:TYR:HE1	2.13	0.65
1:A:758:VAL:O	1:A:762:MET:HG3	1.96	0.64
1:A:744:THR:HA	1:A:838:GLY:HA3	1.79	0.64
1:A:2414:LEU:HB3	1:A:2434:LEU:HD21	1.81	0.63
1:A:2321:CYS:HA	1:A:2388:ILE:HD11	1.80	0.63
1:A:1418:ARG:HH22	1:A:1696:ASN:HA	1.62	0.62
1:A:798:TRP:HA	1:A:801:GLN:HG3	1.81	0.62
1:A:938:ARG:HH21	1:A:997:PRO:HD3	1.65	0.62
1:A:1705:THR:HG22	1:A:1706:VAL:H	1.64	0.61
1:A:810:ALA:HA	1:A:813:LEU:HD12	1.83	0.61
1:A:716:VAL:HG23	1:A:735:LEU:HB3	1.83	0.61
1:A:2414:LEU:HD21	1:A:2433:LEU:HD23	1.83	0.60
1:A:1120:LEU:HD12	1:A:1123:GLU:HB3	1.83	0.60
1:A:773:GLN:NE2	1:A:777:ALA:HB3	2.16	0.60
1:A:2261:TYR:HD1	1:A:2320:LEU:HD22	1.67	0.59
1:A:1120:LEU:HD13	1:A:1347:ILE:HG22	1.84	0.59
1:A:2319:ASN:O	1:A:2323:LYS:HG2	2.04	0.58
1:A:1550:TYR:HB3	1:A:1568:VAL:HG12	1.85	0.57
1:A:2073:MET:HG3	1:A:2074:PRO:HD2	1.85	0.57
1:A:1037:PHE:HE2	1:A:1107:MET:HB2	1.70	0.57
1:A:1567:MET:HE1	1:A:1589:ILE:HD11	1.87	0.56
1:A:1125:ILE:HG13	1:A:1130:VAL:HG23	1.87	0.56
1:A:738:PHE:HD2	1:A:895:PHE:HZ	1.54	0.56
1:A:1720:ILE:HA	1:A:1740:TYR:HE2	1.71	0.56
1:A:2148:HIS:HE1	1:A:2153:LYS:HD2	1.71	0.55
1:A:805:MET:O	1:A:809:ILE:HG12	2.06	0.55
1:A:1475:SER:HB3	1:A:1486:CYS:HB2	1.87	0.55
1:A:2259:ILE:HD12	1:A:2280:LEU:HD23	1.89	0.55
1:A:753:LYS:HG3	1:A:754:MET:SD	2.47	0.55
1:A:741:PHE:HE1	1:A:898:ILE:HG21	1.71	0.55
1:A:2217:SER:HB3	1:A:2274:TYR:HB3	1.89	0.55
1:A:1952:LEU:O	1:A:1956:THR:HG23	2.07	0.54
1:A:2095:ASN:HD21	1:A:2163:GLY:H	1.54	0.54
1:A:1426:LEU:HD12	1:A:1430:THR:HB	1.89	0.54
1:A:1424:ILE:HD12	1:A:1432:LEU:HD23	1.90	0.54
1:A:2266:ILE:O	1:A:2273:SER:HB2	2.08	0.54
1:A:1469:ILE:HG13	1:A:1470:PRO:HD2	1.88	0.54
1:A:1526:ARG:HG3	1:A:1576:ASP:OD1	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2319:ASN:OD1	1:A:2323:LYS:HE3	2.07	0.53
1:A:2335:ARG:NH2	1:A:2372:TRP:HE1	2.02	0.53
1:A:869:TYR:O	1:A:873:VAL:HG23	2.09	0.53
1:A:989:ASP:HB3	1:A:1028:VAL:HG13	1.90	0.53
1:A:873:VAL:O	1:A:876:ILE:HG22	2.09	0.53
1:A:836:CYS:SG	1:A:854:LEU:HD22	2.50	0.52
1:A:668:PHE:O	1:A:672:ILE:HG22	2.09	0.52
1:A:1177:MET:HE3	1:A:2040:ALA:HA	1.92	0.52
1:A:896:MET:O	1:A:900:LEU:HG	2.08	0.52
1:A:2047:TYR:CE2	1:A:2186:ILE:HD12	2.45	0.52
1:A:809:ILE:HG22	1:A:813:LEU:HD11	1.91	0.52
1:A:679:LEU:HD12	1:A:679:LEU:H	1.75	0.52
1:A:938:ARG:HB2	1:A:993:PHE:CZ	2.44	0.52
1:A:1676:ASN:HB3	1:A:1694:ASN:HD21	1.76	0.51
1:A:983:VAL:O	1:A:987:ILE:HG23	2.10	0.51
1:A:1345:GLU:HB2	1:A:1962:TRP:HZ2	1.76	0.51
1:A:1720:ILE:HA	1:A:1740:TYR:CE2	2.45	0.50
1:A:686:GLU:HA	1:A:805:MET:HB3	1.92	0.50
1:A:1154:PHE:O	1:A:1157:ILE:HG22	2.12	0.50
1:A:2252:PHE:CE2	1:A:2286:LEU:HB3	2.47	0.49
1:A:717:TRP:HH2	1:A:799:GLU:HB3	1.77	0.49
1:A:975:LEU:O	1:A:979:LYS:HG2	2.11	0.49
1:A:882:ARG:HH11	1:A:883:PRO:HD2	1.77	0.49
1:A:904:GLN:HG2	1:A:955:TYR:CZ	2.48	0.49
1:A:1573:ASN:HB3	1:A:1594:SER:HB2	1.94	0.49
1:A:2157:LEU:HD23	1:A:2189:THR:HG21	1.95	0.49
1:A:960:LEU:HD13	1:A:977:ILE:HG21	1.94	0.49
1:A:928:GLU:HA	1:A:931:MET:HG2	1.95	0.49
1:A:2252:PHE:CD2	1:A:2308:ILE:HD11	2.48	0.49
1:A:704:THR:O	1:A:708:VAL:HG13	2.13	0.49
1:A:1543:ILE:HG23	1:A:1554:TYR:HB2	1.94	0.48
1:A:1106:LYS:O	1:A:1110:LYS:HG3	2.13	0.48
1:A:863:LYS:HD2	1:A:863:LYS:N	2.28	0.48
1:A:907:SER:HA	1:A:910:TRP:CE2	2.48	0.48
1:A:741:PHE:CE1	1:A:898:ILE:HD13	2.49	0.48
1:A:1055:LEU:HB2	1:A:1082:ILE:HD13	1.96	0.48
1:A:1495:ARG:HH21	1:A:2356:PRO:HD3	1.79	0.48
1:A:1504:ASP:HB3	1:A:2351:TRP:CE2	2.49	0.48
1:A:2329:ILE:HD12	1:A:2413:LYS:HG3	1.94	0.48
1:A:1525:VAL:HG12	1:A:1526:ARG:HG2	1.95	0.47
1:A:2269:MET:HA	1:A:2269:MET:HE2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1101:HIS:HD2	1:A:1318:LEU:HD21	1.79	0.47
1:A:2028:LEU:O	1:A:2032:GLU:HG3	2.14	0.47
1:A:687:ASN:O	1:A:690:ASP:HB3	2.14	0.47
1:A:1678:VAL:HG21	1:A:1690:CYS:SG	2.55	0.47
1:A:1680:ALA:O	1:A:1690:CYS:HA	2.15	0.47
1:A:1750:GLU:HG3	1:A:1751:THR:O	2.14	0.47
1:A:1098:GLU:H	1:A:1098:GLU:CD	2.23	0.47
1:A:1663:THR:HG22	1:A:1664:ALA:H	1.78	0.47
1:A:2428:ARG:H	1:A:2428:ARG:HG3	1.45	0.47
1:A:741:PHE:CZ	1:A:898:ILE:HD13	2.50	0.47
1:A:773:GLN:HG2	1:A:774:SER:H	1.79	0.47
1:A:2335:ARG:HH12	1:A:2372:TRP:CD1	2.33	0.47
1:A:1503:ILE:HG21	1:A:2356:PRO:HD2	1.97	0.46
1:A:1334:GLN:HG2	1:A:1958:SER:OG	2.15	0.46
1:A:757:LYS:O	1:A:761:LYS:HG2	2.16	0.46
1:A:695:ILE:H	1:A:695:ILE:HD12	1.81	0.46
1:A:984:LEU:HD23	1:A:984:LEU:HA	1.78	0.46
1:A:1721:MET:HB3	1:A:1739:ILE:O	2.16	0.46
1:A:2244:ASP:OD1	1:A:2245:PRO:HD2	2.15	0.46
1:A:1559:HIS:CG	1:A:1562:ASN:HB2	2.51	0.45
1:A:2198:PHE:O	1:A:2202:GLU:HG2	2.16	0.45
1:A:2236:LEU:HD23	1:A:2240:LEU:HD23	1.97	0.45
1:A:714:ILE:HD11	1:A:805:MET:HE3	1.97	0.45
1:A:762:MET:HA	1:A:765:ILE:HG12	1.98	0.45
1:A:2141:GLU:O	1:A:2145:MET:HG2	2.17	0.45
1:A:1455:LEU:HD22	1:A:1735:TYR:CE2	2.51	0.45
1:A:1483:LEU:HD11	1:A:1494:LEU:HD12	1.99	0.45
1:A:2110:ILE:HG21	1:A:2123:MET:SD	2.57	0.45
1:A:2127:VAL:HG11	1:A:2235:VAL:HG23	1.97	0.45
1:A:2268:PRO:O	1:A:2269:MET:HE2	2.16	0.45
1:A:1390:LEU:HD13	1:A:1750:GLU:OE1	2.17	0.45
1:A:1530:CYS:SG	1:A:1581:ASN:HB2	2.57	0.45
1:A:2137:ALA:O	1:A:2141:GLU:HG3	2.17	0.45
1:A:2208:ILE:HG22	1:A:2236:LEU:HD12	1.99	0.45
1:A:715:GLU:HG2	1:A:839:GLN:OE1	2.16	0.45
1:A:1495:ARG:HB3	1:A:1504:ASP:HB2	1.98	0.44
1:A:2305:LEU:O	1:A:2308:ILE:HG22	2.17	0.44
1:A:1684:THR:HG23	1:A:1685:SER:N	2.33	0.44
1:A:742:TRP:CH2	1:A:789:PHE:HZ	2.35	0.44
1:A:677:LYS:NZ	1:A:681:PHE:HB2	2.33	0.44
1:A:2209:LEU:O	1:A:2213:THR:HG23	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:815:LYS:HD2	1:A:815:LYS:HA	1.83	0.44
1:A:1027:LYS:H	1:A:1027:LYS:HG2	1.57	0.44
1:A:1974:LYS:HG3	1:A:1975:LEU:HG	1.99	0.44
1:A:918:LYS:O	1:A:922:ARG:HG2	2.18	0.44
1:A:1567:MET:HE2	1:A:1613:ILE:HD12	2.00	0.44
1:A:731:HIS:NE2	1:A:734:ASP:HB2	2.33	0.43
1:A:742:TRP:HA	1:A:742:TRP:CE3	2.52	0.43
1:A:1432:LEU:HD11	1:A:1446:LEU:HB3	2.00	0.43
1:A:751:ASP:OD1	1:A:754:MET:HG2	2.17	0.43
1:A:959:LEU:HD21	1:A:973:ALA:HB1	2.00	0.43
1:A:1559:HIS:CE1	1:A:1562:ASN:HD22	2.36	0.43
1:A:804:LEU:HD21	1:A:808:ARG:HH12	1.84	0.43
1:A:1990:LYS:HB2	1:A:1990:LYS:HE2	1.69	0.43
1:A:2200:TRP:H	1:A:2200:TRP:CD1	2.36	0.43
1:A:2244:ASP:O	1:A:2248:ILE:HG13	2.18	0.43
1:A:2389:LEU:CD2	1:A:2429:GLN:HB3	2.49	0.43
1:A:877:LEU:HD23	1:A:877:LEU:HA	1.84	0.43
1:A:1697:HIS:HB3	1:A:1716:VAL:O	2.18	0.43
1:A:2148:HIS:CE1	1:A:2153:LYS:HA	2.54	0.43
1:A:2332:TRP:HE1	1:A:2381:ILE:HG22	1.82	0.43
1:A:1432:LEU:HD13	1:A:1448:TYR:CE1	2.54	0.43
1:A:2073:MET:HE2	1:A:2073:MET:HB2	1.81	0.43
1:A:2205:ILE:HG21	1:A:2240:LEU:HD21	2.00	0.43
1:A:854:LEU:HD12	1:A:854:LEU:HA	1.74	0.43
1:A:1102:LEU:O	1:A:1106:LYS:HG3	2.18	0.43
1:A:2035:LEU:HD11	1:A:2081:MET:HB2	2.01	0.42
1:A:2390:LEU:HD23	1:A:2390:LEU:HA	1.92	0.42
1:A:738:PHE:O	1:A:741:PHE:HB3	2.19	0.42
1:A:705:GLU:O	1:A:708:VAL:HG22	2.20	0.42
1:A:882:ARG:NH1	1:A:883:PRO:HD2	2.33	0.42
1:A:703:ILE:HD12	1:A:703:ILE:HA	1.82	0.42
1:A:2045:TRP:CD1	1:A:2095:ASN:HD22	2.38	0.42
1:A:2064:GLU:HG2	1:A:2067:ARG:NH2	2.35	0.42
1:A:2294:ARG:HH12	1:A:2302:GLN:HE22	1.68	0.42
1:A:2312:LEU:HA	1:A:2312:LEU:HD23	1.76	0.42
1:A:2333:LYS:HB2	1:A:2420:LEU:HD21	2.01	0.42
1:A:706:LYS:HE2	1:A:706:LYS:HB2	1.82	0.42
1:A:1623:GLY:HA3	1:A:1626:MET:HE3	2.02	0.42
1:A:1174:LYS:HE2	1:A:1174:LYS:HB2	1.70	0.41
1:A:1632:SER:OG	1:A:1645:SER:HB3	2.20	0.41
1:A:2389:LEU:HD22	1:A:2429:GLN:HB3	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1004:TYR:HA	1:A:1007:GLN:HB2	2.01	0.41
1:A:741:PHE:CD1	1:A:895:PHE:HE1	2.38	0.41
1:A:2067:ARG:HG3	1:A:2110:ILE:HG12	2.03	0.41
1:A:2252:PHE:HE2	1:A:2286:LEU:HB3	1.84	0.41
1:A:719:VAL:HG12	1:A:735:LEU:HD12	2.02	0.41
1:A:754:MET:O	1:A:758:VAL:HG12	2.19	0.41
1:A:2249:ARG:HH21	1:A:2304:MET:HA	1.86	0.41
1:A:1997:GLU:O	1:A:2001:LYS:HB2	2.21	0.41
1:A:2389:LEU:HD23	1:A:2389:LEU:O	2.21	0.41
1:A:666:ASP:O	1:A:670:LYS:HG2	2.20	0.41
1:A:816:LYS:HD3	1:A:816:LYS:HA	1.97	0.41
1:A:992:THR:O	1:A:995:PRO:HD2	2.20	0.41
1:A:698:LEU:HG	1:A:812:HIS:NE2	2.35	0.41
1:A:754:MET:HE3	1:A:754:MET:HA	2.04	0.40
1:A:1441:GLN:O	1:A:1472:ASN:HA	2.21	0.40
1:A:2199:LYS:HA	1:A:2202:GLU:HG2	2.03	0.40
1:A:2429:GLN:O	1:A:2432:LYS:HG2	2.21	0.40
1:A:677:LYS:HA	1:A:677:LYS:HD2	1.85	0.40
1:A:998:LYS:HD2	1:A:998:LYS:HA	1.85	0.40
1:A:1510:LEU:HD11	1:A:1552:ARG:HD2	2.03	0.40
1:A:2335:ARG:O	1:A:2335:ARG:HG2	2.20	0.40
1:A:742:TRP:O	1:A:744:THR:HG22	2.21	0.40
1:A:1483:LEU:HG	1:A:1494:LEU:HB2	2.02	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	1415/4284 (33%)	1354 (96%)	60 (4%)	1 (0%)	48 79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2268	PRO

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	1278/3859 (33%)	1241 (97%)	37 (3%)	37 60

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	665	LEU
1	A	703	ILE
1	A	723	LEU
1	A	735	LEU
1	A	894	LEU
1	A	915	SER
1	A	919	LEU
1	A	926	PHE
1	A	1005	ILE
1	A	1036	LEU
1	A	1039	LYS
1	A	1063	TYR
1	A	1067	SER
1	A	1085	VAL
1	A	1362	THR
1	A	1366	LEU
1	A	1430	THR
1	A	1604	SER
1	A	1613	ILE
1	A	1663	THR
1	A	1676	ASN
1	A	1692	SER
1	A	1693	THR
1	A	1957	LEU
1	A	2041	VAL
1	A	2073	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2075	LEU
1	A	2081	MET
1	A	2192	ILE
1	A	2210	GLU
1	A	2224	LEU
1	A	2240	LEU
1	A	2259	ILE
1	A	2322	LEU
1	A	2384	CYS
1	A	2395	LEU
1	A	2428	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	687	ASN
1	A	724	GLN
1	A	806	HIS
1	A	1035	GLN
1	A	1522	ASN
1	A	1549	GLN
1	A	1562	ASN
1	A	1634	HIS
1	A	1754	ASN
1	A	2079	GLN
1	A	2083	GLN
1	A	2095	ASN
1	A	2105	HIS
1	A	2148	HIS
1	A	2251	HIS
1	A	2313	GLN
1	A	2429	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

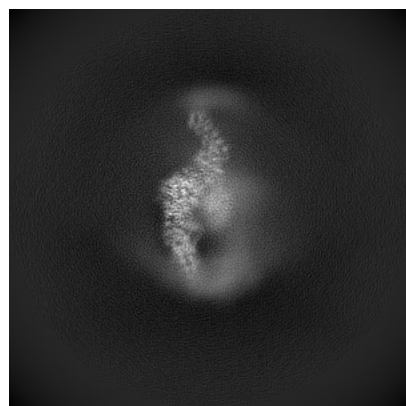
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53435. These allow visual inspection of the internal detail of the map and identification of artifacts.

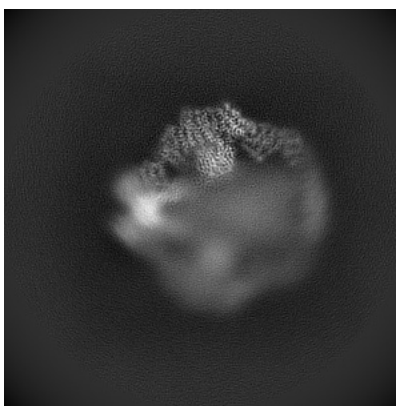
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

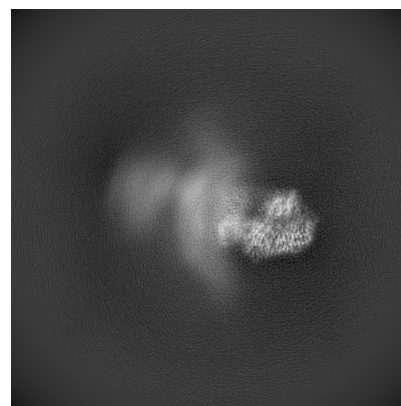
6.1.1 Primary map



X

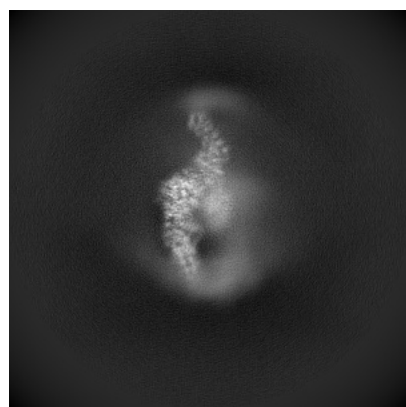


Y

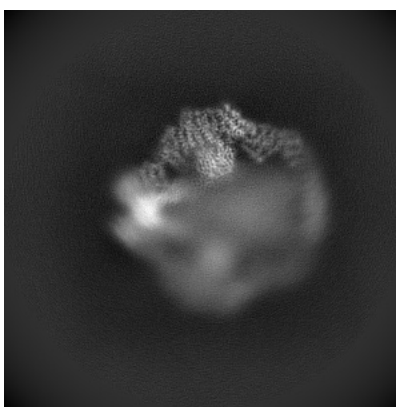


Z

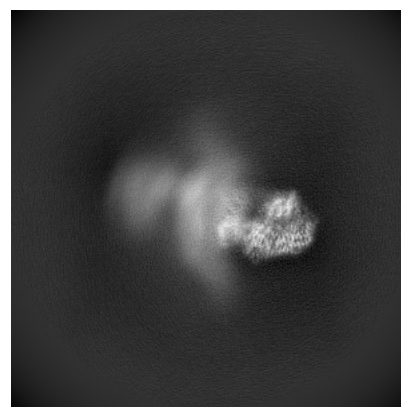
6.1.2 Raw map



X



Y

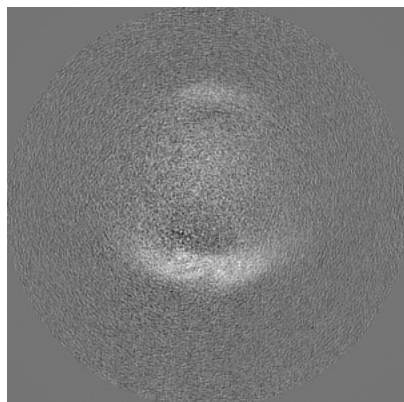


Z

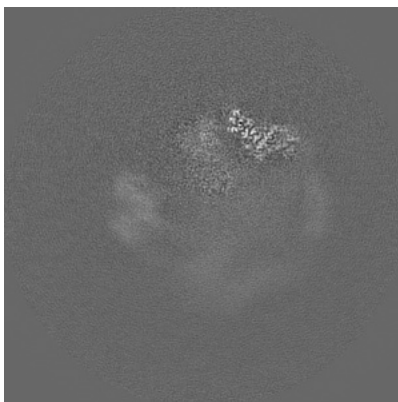
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

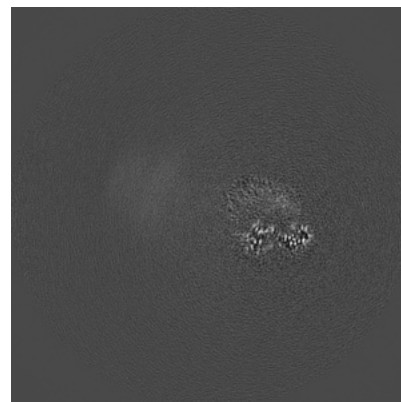
6.2.1 Primary map



X Index: 192

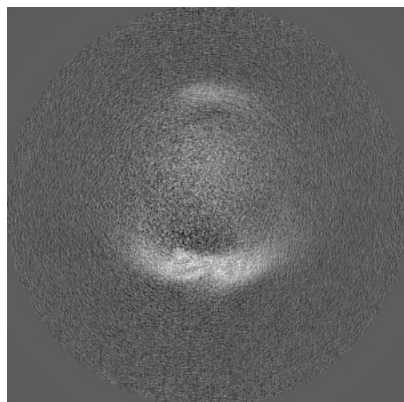


Y Index: 192

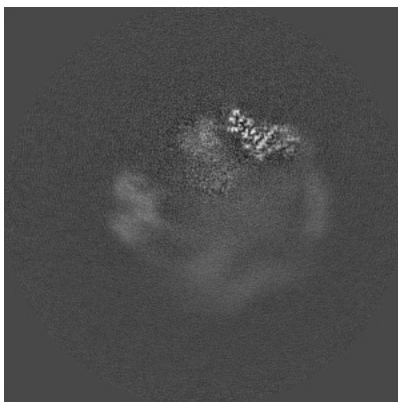


Z Index: 192

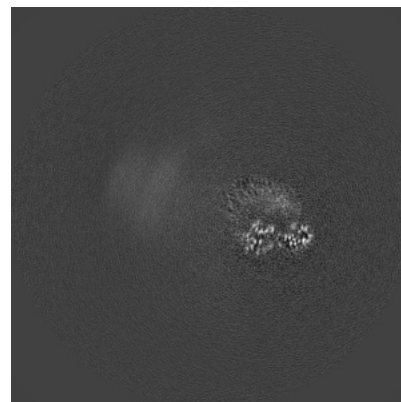
6.2.2 Raw map



X Index: 192



Y Index: 192

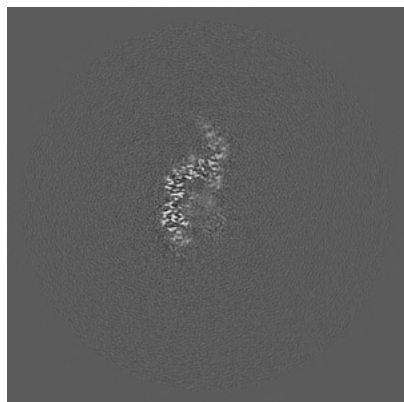


Z Index: 192

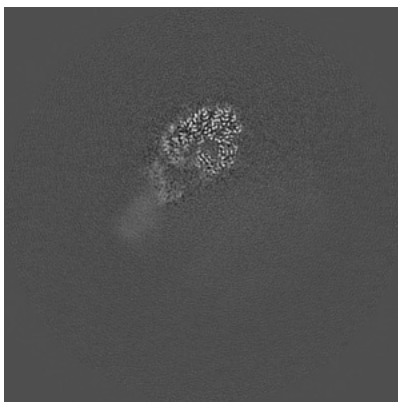
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

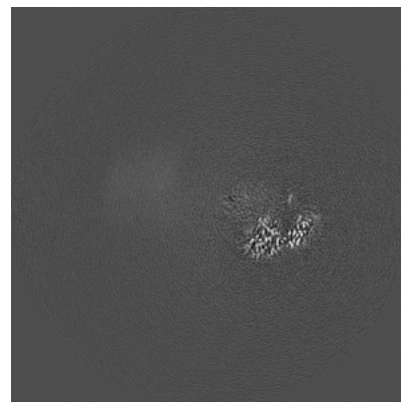
6.3.1 Primary map



X Index: 269

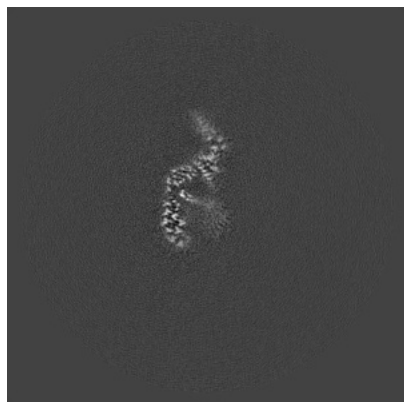


Y Index: 160

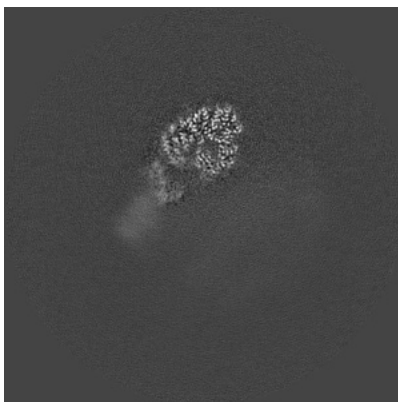


Z Index: 210

6.3.2 Raw map



X Index: 265



Y Index: 160

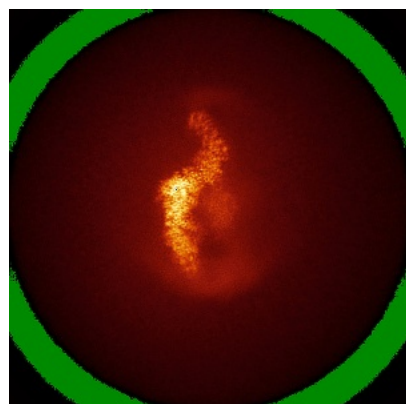


Z Index: 214

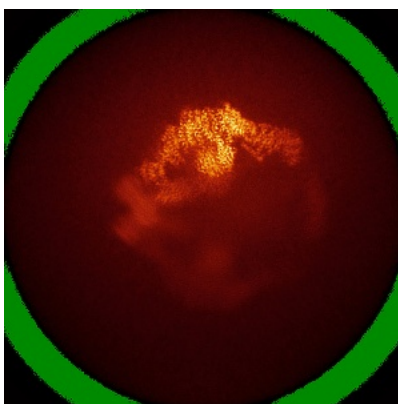
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

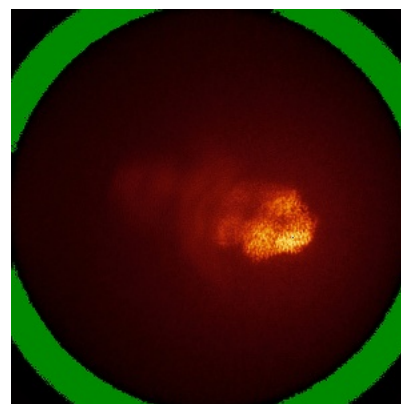
6.4.1 Primary map



X

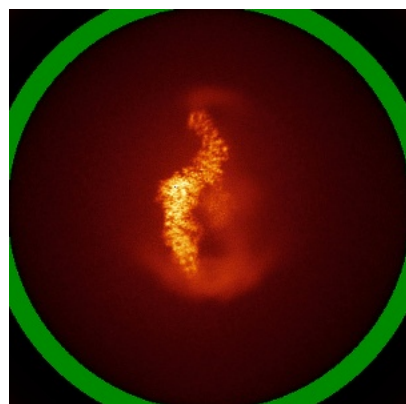


Y

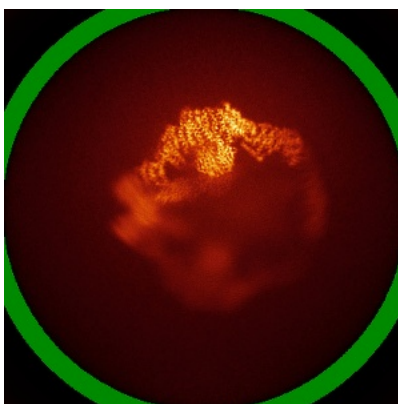


Z

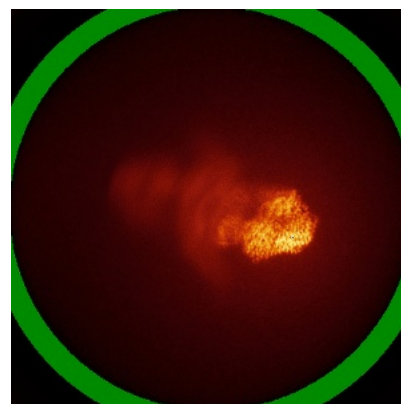
6.4.2 Raw map



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.

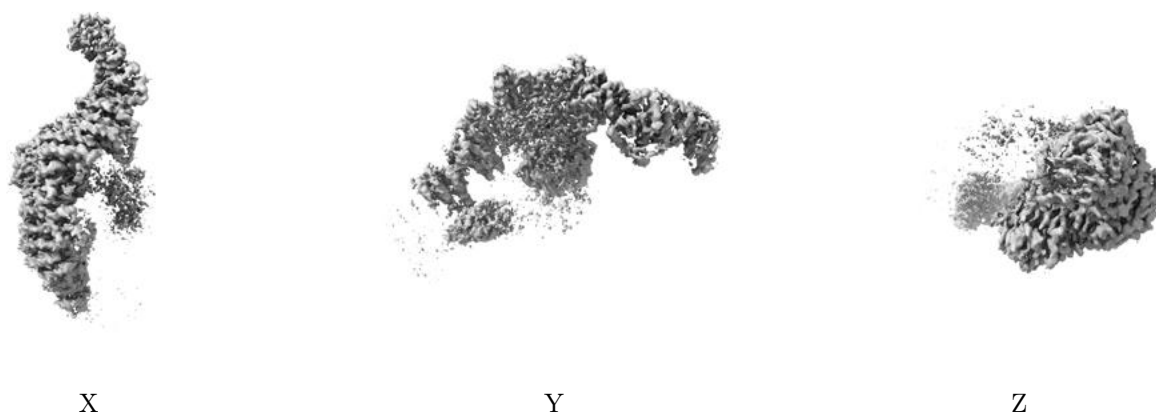
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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.

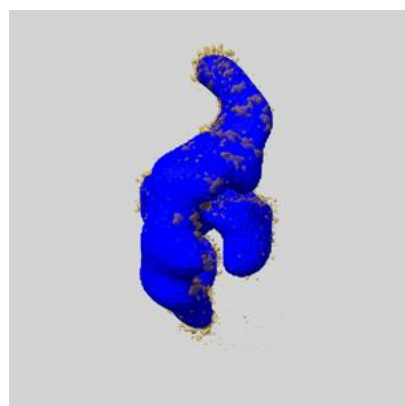
6.6 Mask visualisation [i](#)

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

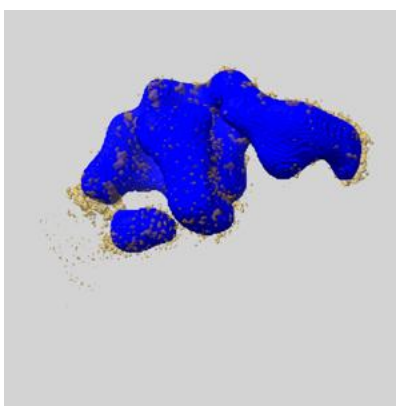
A mask typically either:

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

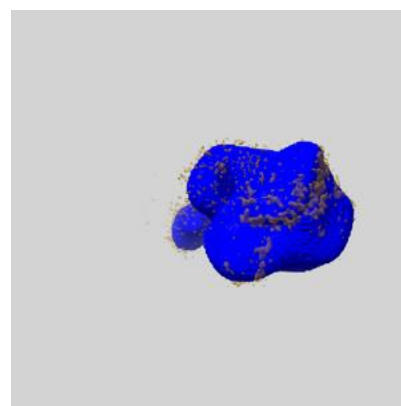
6.6.1 emd_53435_msk_1.map [i](#)



X



Y

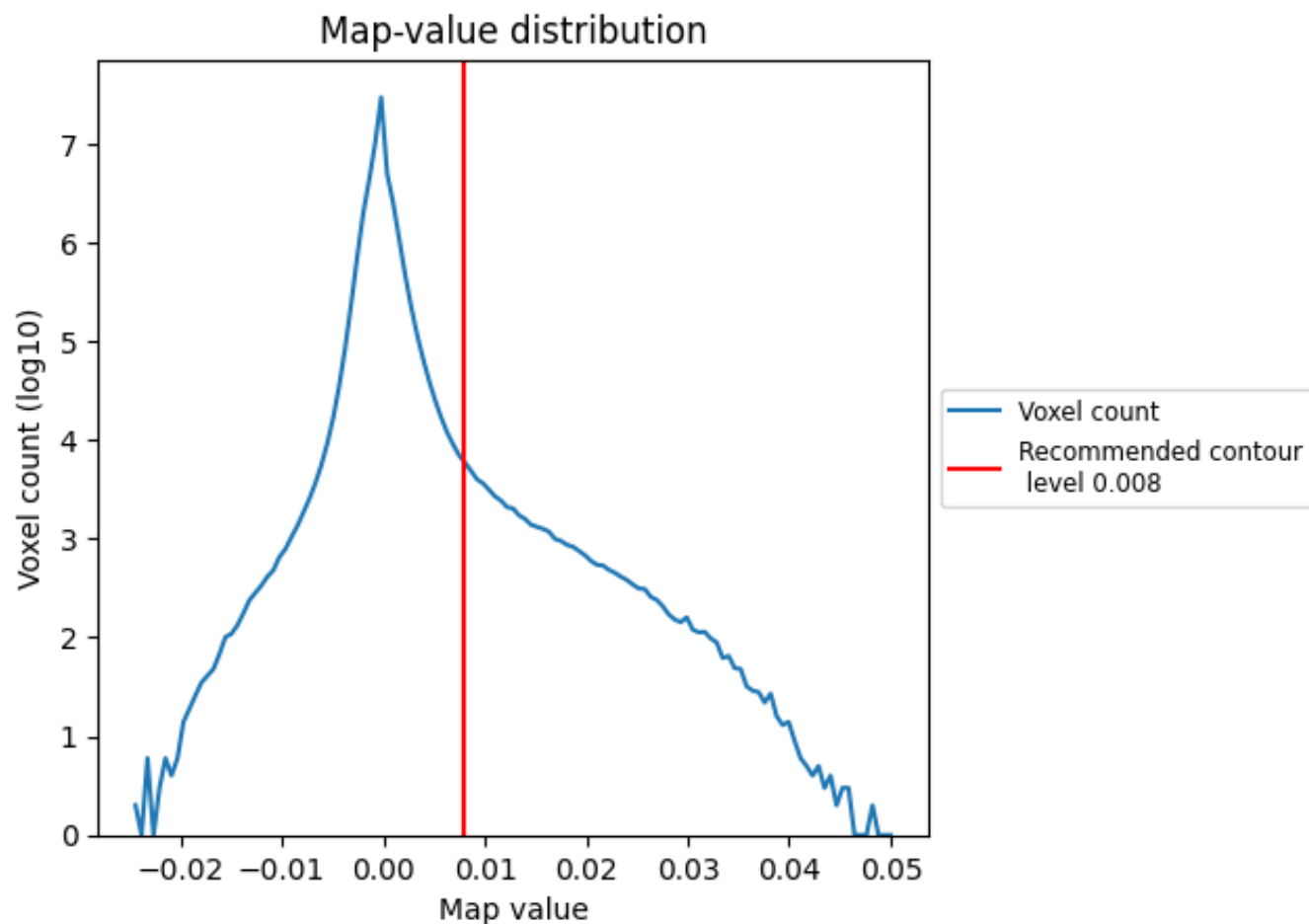


Z

7 Map analysis [i](#)

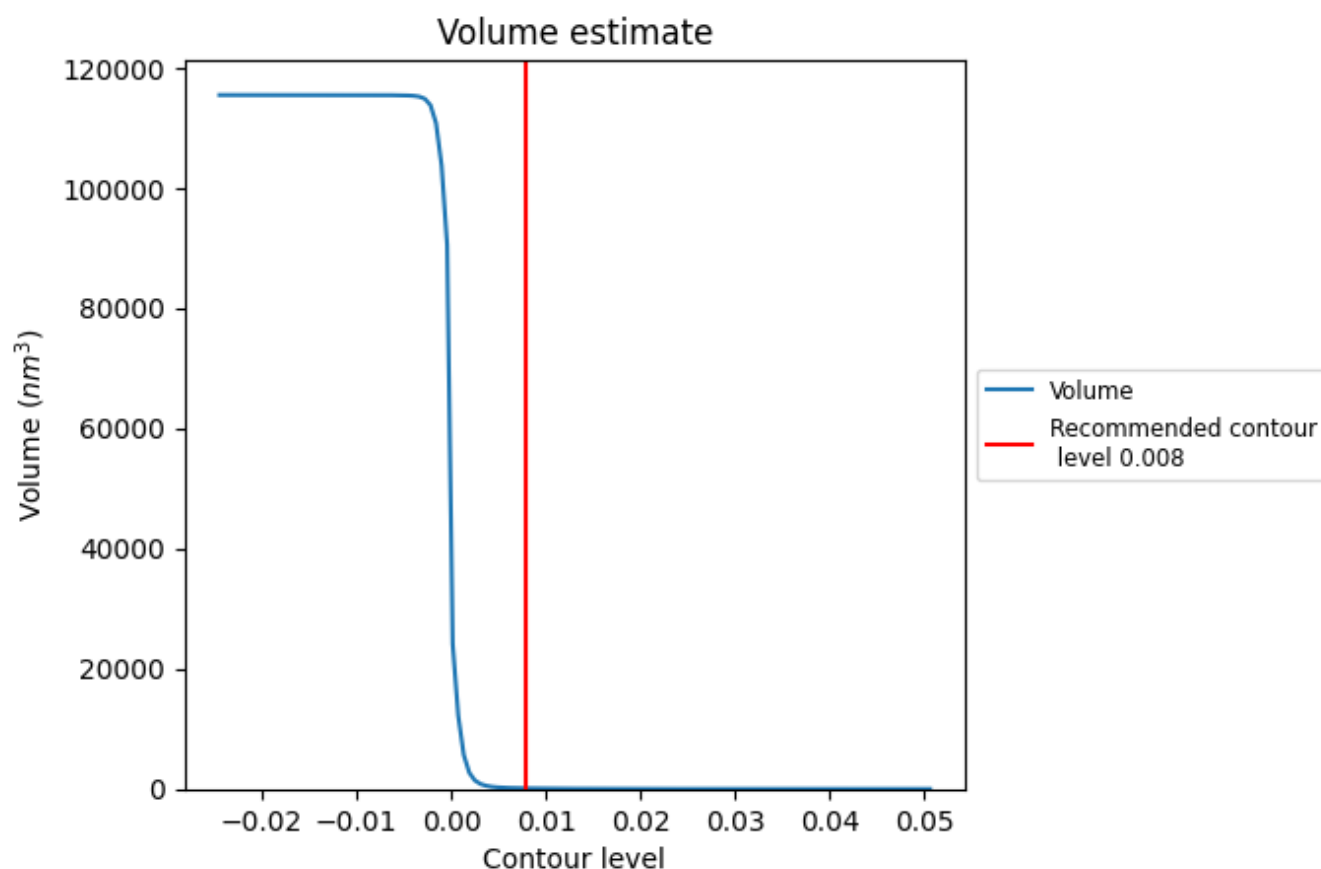
This section contains the results of statistical analysis of the map.

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.

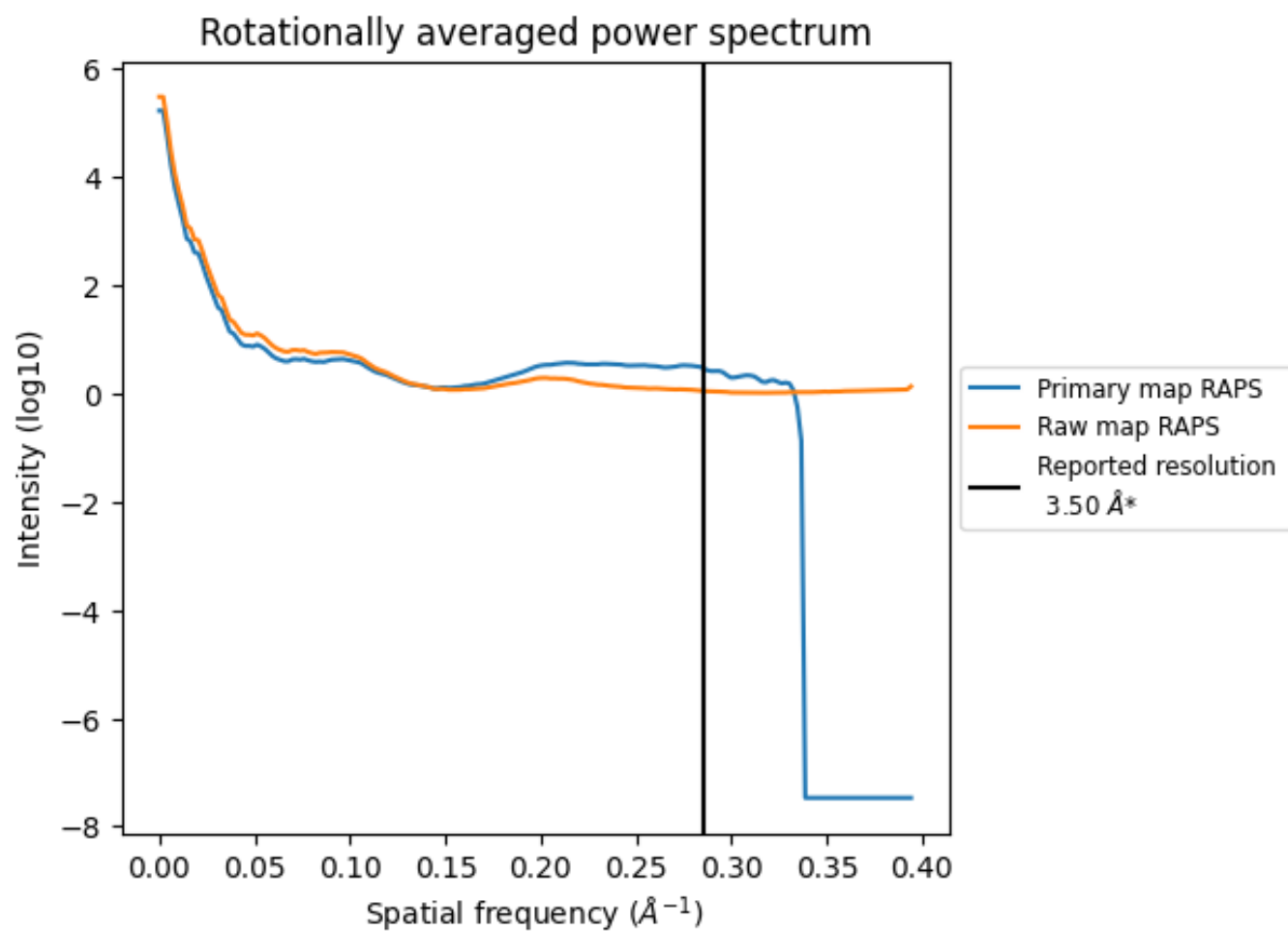
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 106 nm³; this corresponds to an approximate mass of 95 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 ⓘ

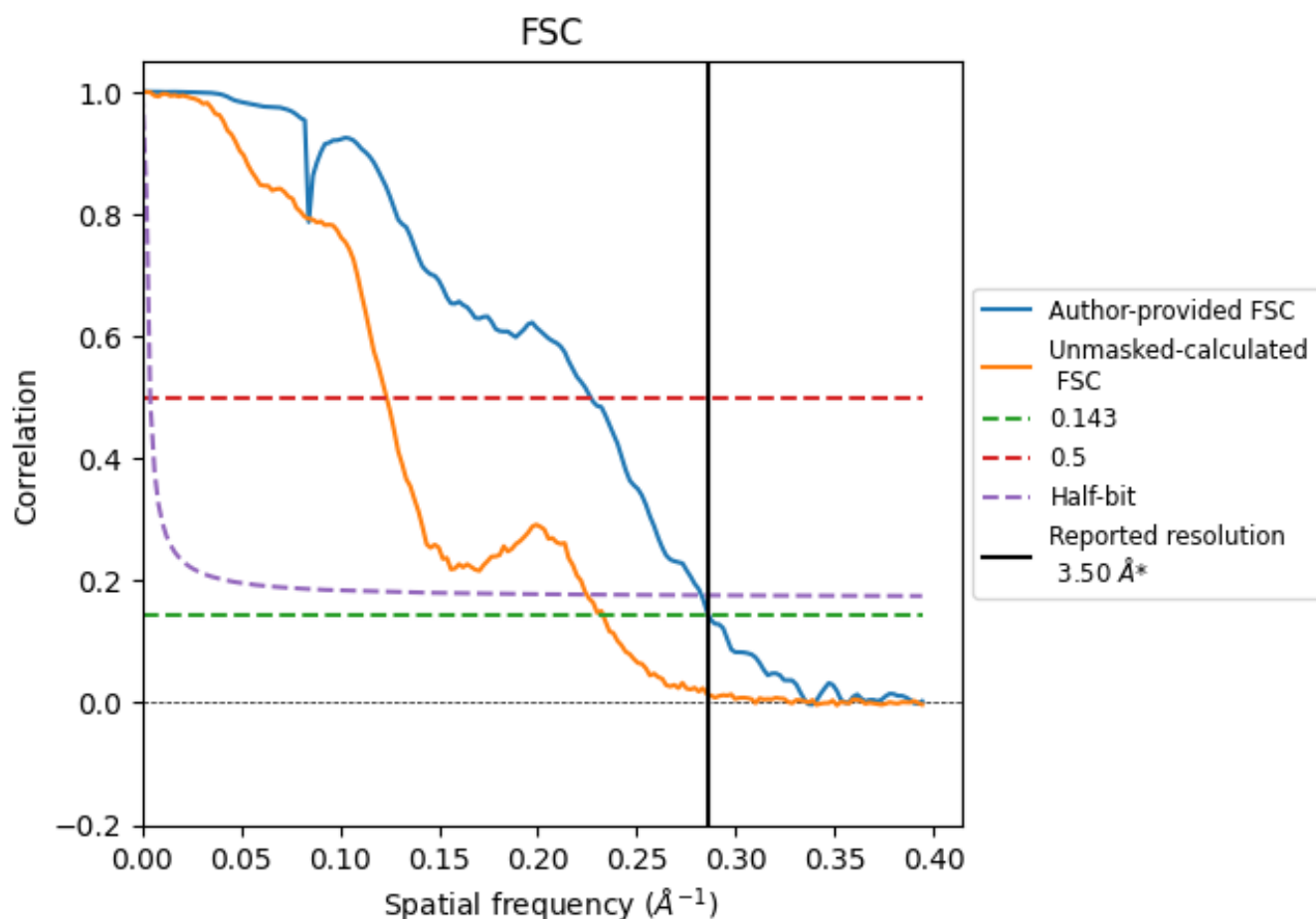


*Reported resolution corresponds to spatial frequency of 0.286 $\text{\AA}^{-1}$

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 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

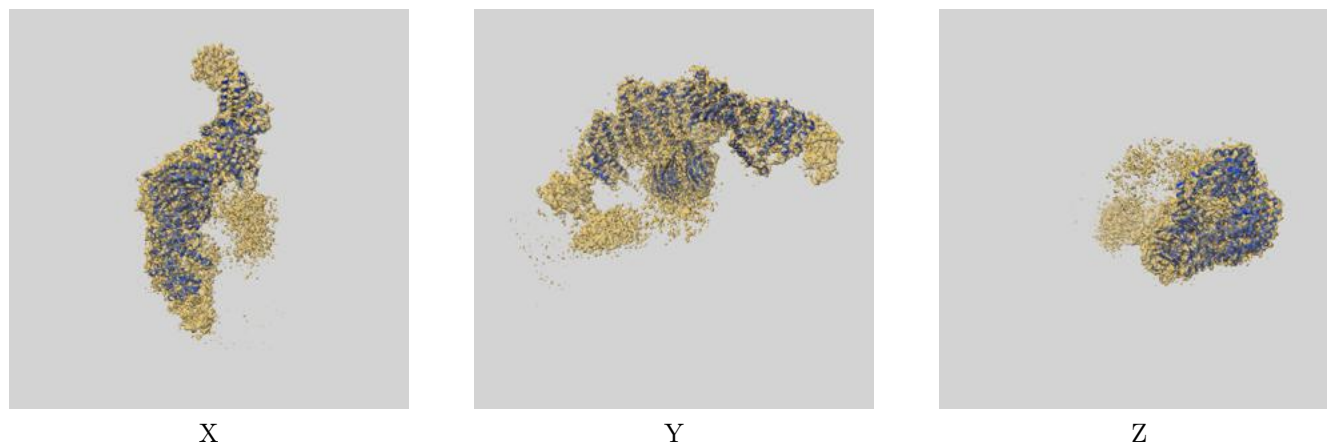
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.49	4.41	3.54
Unmasked-calculated*	4.29	8.10	4.45

*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 4.29 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

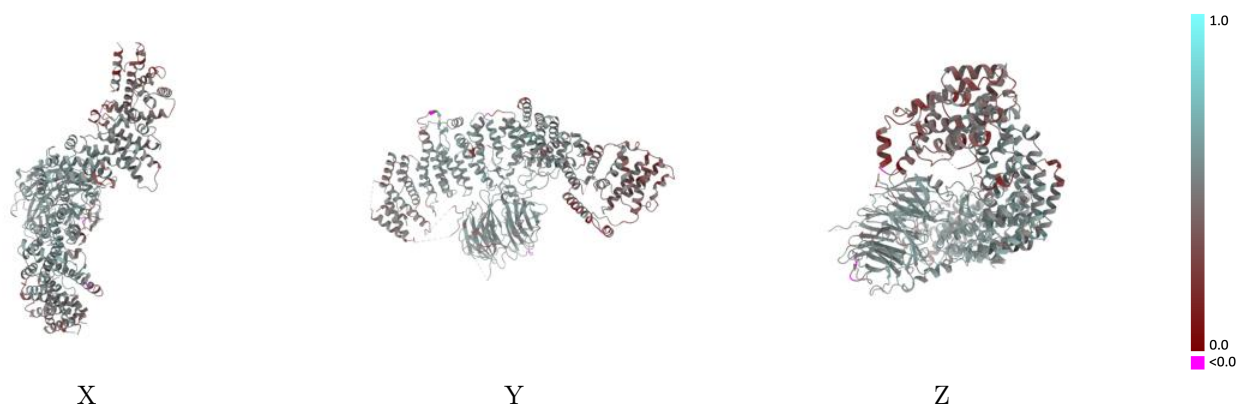
This section contains information regarding the fit between EMDB map EMD-53435 and PDB model 9QX5. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



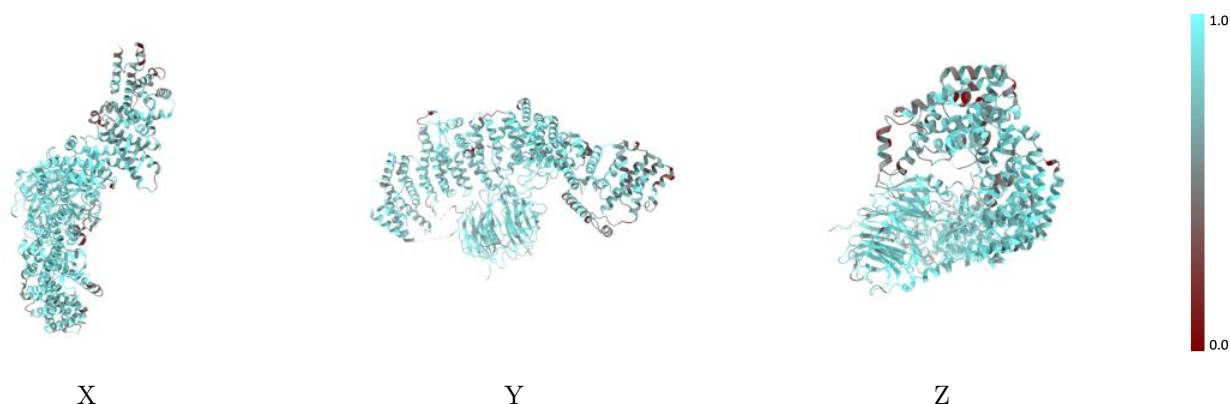
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



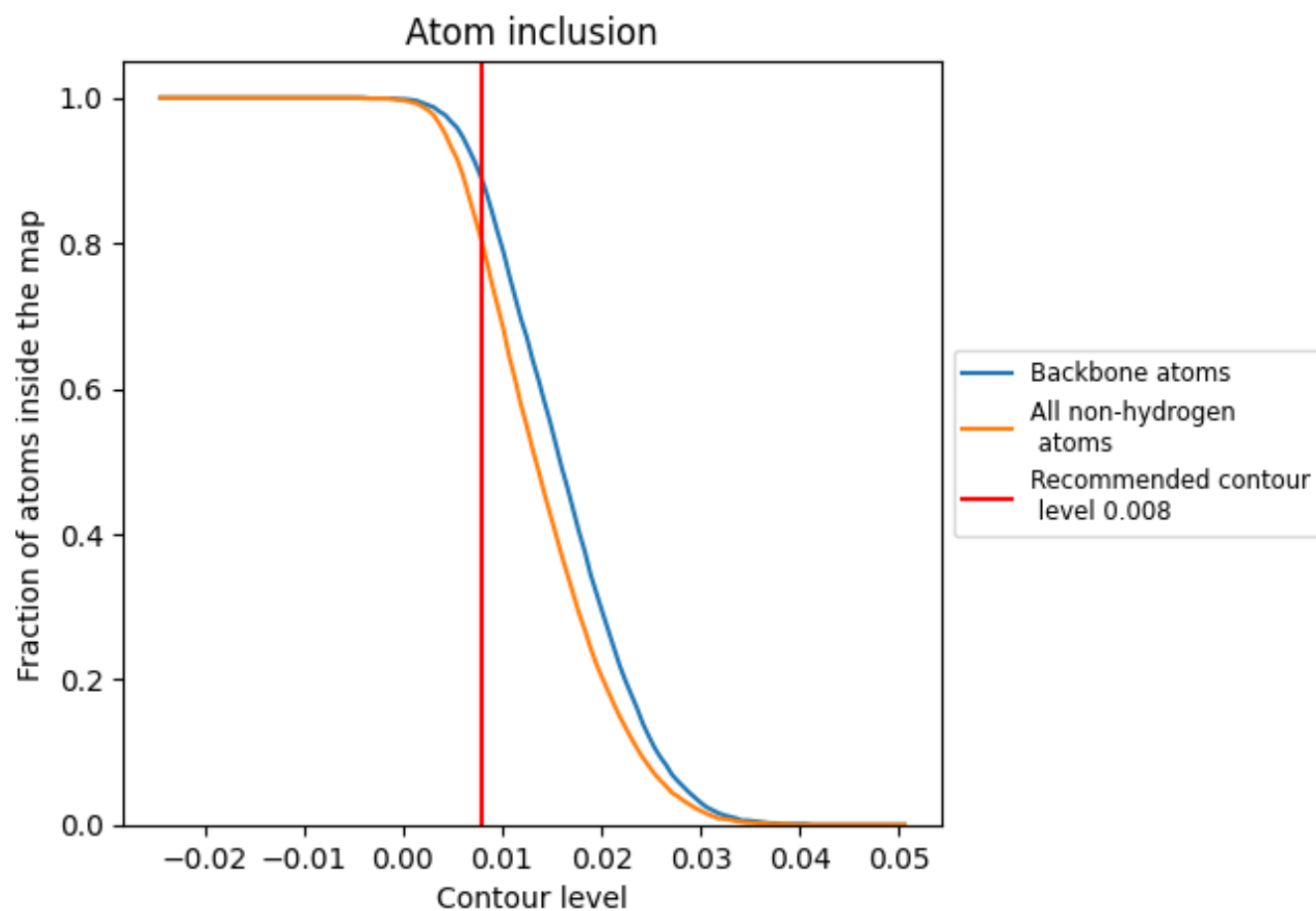
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.008).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 80% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8010	0.4870
A	0.8010	0.4870

