Full wwPDB EM Validation Report ⓘ

Oct 15, 2024 – 12:34 AM JST

PDB ID	:	8I4E
EMDB ID	:	EMD-35170
Title	:	Omicron spike variant XBB with Bn03
Authors	:	Hao, A.H.; Zhang, X.; Chen, Z.G.; Sun, L.
Deposited on	:	2023-01-19
Resolution	:	3.98 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:

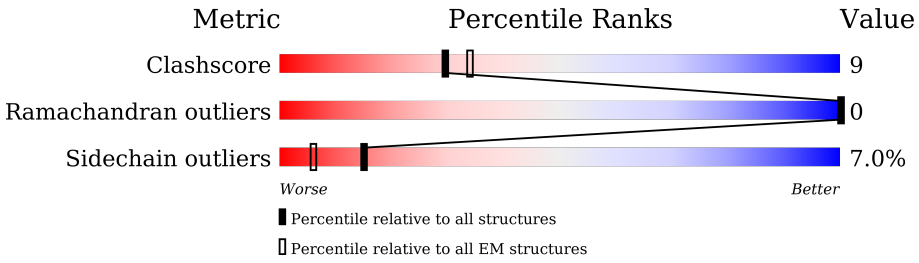
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.98 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1295	35% 11% 52%
2	C	258	32% 14% 54%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5824 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	619	4902	3148	813	920	21	0	0

There are 150 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P0DTC2
A	2	PRO	-	expression tag	UNP P0DTC2
A	3	MET	-	expression tag	UNP P0DTC2
A	4	GLY	-	expression tag	UNP P0DTC2
A	5	SER	-	expression tag	UNP P0DTC2
A	6	LEU	-	expression tag	UNP P0DTC2
A	7	GLN	-	expression tag	UNP P0DTC2
A	8	PRO	-	expression tag	UNP P0DTC2
A	9	LEU	-	expression tag	UNP P0DTC2
A	10	ALA	-	expression tag	UNP P0DTC2
A	11	THR	-	expression tag	UNP P0DTC2
A	12	LEU	-	expression tag	UNP P0DTC2
A	13	TYR	-	expression tag	UNP P0DTC2
A	14	LEU	-	expression tag	UNP P0DTC2
A	15	LEU	-	expression tag	UNP P0DTC2
A	16	GLY	-	expression tag	UNP P0DTC2
A	17	MET	-	expression tag	UNP P0DTC2
A	18	LEU	-	expression tag	UNP P0DTC2
A	19	VAL	-	expression tag	UNP P0DTC2
A	20	ALA	-	expression tag	UNP P0DTC2
A	21	SER	-	expression tag	UNP P0DTC2
A	22	VAL	-	expression tag	UNP P0DTC2
A	23	LEU	-	expression tag	UNP P0DTC2
A	24	ALA	-	expression tag	UNP P0DTC2
A	25	GLN	-	expression tag	UNP P0DTC2
A	26	CYS	-	expression tag	UNP P0DTC2
A	27	VAL	-	expression tag	UNP P0DTC2
A	28	ASN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	29	LEU	-	expression tag	UNP P0DTC2
A	30	ILE	-	expression tag	UNP P0DTC2
A	31	THR	-	expression tag	UNP P0DTC2
A	32	ARG	-	expression tag	UNP P0DTC2
A	33	THR	-	expression tag	UNP P0DTC2
A	34	GLN	-	expression tag	UNP P0DTC2
A	35	SER	-	expression tag	UNP P0DTC2
A	150	ASP	GLY	variant	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	153	GLN	HIS	variant	UNP P0DTC2
A	190	GLU	GLN	variant	UNP P0DTC2
A	220	GLU	VAL	variant	UNP P0DTC2
A	346	HIS	GLY	variant	UNP P0DTC2
A	353	THR	ARG	variant	UNP P0DTC2
A	375	ILE	LEU	variant	UNP P0DTC2
A	378	PHE	SER	variant	UNP P0DTC2
A	380	PRO	SER	variant	UNP P0DTC2
A	382	PHE	SER	variant	UNP P0DTC2
A	383	ALA	THR	variant	UNP P0DTC2
A	412	ASN	ASP	variant	UNP P0DTC2
A	415	SER	ARG	variant	UNP P0DTC2
A	424	ASN	LYS	variant	UNP P0DTC2
A	447	LYS	ASN	variant	UNP P0DTC2
A	452	PRO	VAL	variant	UNP P0DTC2
A	453	SER	GLY	variant	UNP P0DTC2
A	467	LYS	ASN	variant	UNP P0DTC2
A	484	ASN	SER	variant	UNP P0DTC2
A	485	LYS	THR	variant	UNP P0DTC2
A	491	ALA	GLU	variant	UNP P0DTC2
A	493	SER	PHE	variant	UNP P0DTC2
A	497	SER	PHE	variant	UNP P0DTC2
A	505	ARG	GLN	variant	UNP P0DTC2
A	508	TYR	ASN	variant	UNP P0DTC2
A	512	HIS	TYR	variant	UNP P0DTC2
A	621	GLY	ASP	variant	UNP P0DTC2
A	662	TYR	HIS	variant	UNP P0DTC2
A	686	LYS	ASN	variant	UNP P0DTC2
A	688	HIS	PRO	variant	UNP P0DTC2
A	771	LYS	ASN	variant	UNP P0DTC2
A	803	TYR	ASP	variant	UNP P0DTC2
A	961	HIS	GLN	variant	UNP P0DTC2
A	976	LYS	ASN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1216	GLY	-	expression tag	UNP P0DTC2
A	1217	SER	-	expression tag	UNP P0DTC2
A	1218	GLY	-	expression tag	UNP P0DTC2
A	1219	TYR	-	expression tag	UNP P0DTC2
A	1220	ILE	-	expression tag	UNP P0DTC2
A	1221	PRO	-	expression tag	UNP P0DTC2
A	1222	GLU	-	expression tag	UNP P0DTC2
A	1223	ALA	-	expression tag	UNP P0DTC2
A	1224	PRO	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	ASP	-	expression tag	UNP P0DTC2
A	1227	GLY	-	expression tag	UNP P0DTC2
A	1228	GLN	-	expression tag	UNP P0DTC2
A	1229	ALA	-	expression tag	UNP P0DTC2
A	1230	TYR	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	ARG	-	expression tag	UNP P0DTC2
A	1233	LYS	-	expression tag	UNP P0DTC2
A	1234	ASP	-	expression tag	UNP P0DTC2
A	1235	GLY	-	expression tag	UNP P0DTC2
A	1236	GLU	-	expression tag	UNP P0DTC2
A	1237	TRP	-	expression tag	UNP P0DTC2
A	1238	VAL	-	expression tag	UNP P0DTC2
A	1239	PHE	-	expression tag	UNP P0DTC2
A	1240	LEU	-	expression tag	UNP P0DTC2
A	1241	SER	-	expression tag	UNP P0DTC2
A	1242	THR	-	expression tag	UNP P0DTC2
A	1243	PHE	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	SER	-	expression tag	UNP P0DTC2
A	1246	GLY	-	expression tag	UNP P0DTC2
A	1247	LEU	-	expression tag	UNP P0DTC2
A	1248	GLU	-	expression tag	UNP P0DTC2
A	1249	VAL	-	expression tag	UNP P0DTC2
A	1250	LEU	-	expression tag	UNP P0DTC2
A	1251	PHE	-	expression tag	UNP P0DTC2
A	1252	GLN	-	expression tag	UNP P0DTC2
A	1253	GLY	-	expression tag	UNP P0DTC2
A	1254	PRO	-	expression tag	UNP P0DTC2
A	1255	GLY	-	expression tag	UNP P0DTC2
A	1256	GLY	-	expression tag	UNP P0DTC2
A	1257	TRP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	HIS	-	expression tag	UNP P0DTC2
A	1260	PRO	-	expression tag	UNP P0DTC2
A	1261	GLN	-	expression tag	UNP P0DTC2
A	1262	PHE	-	expression tag	UNP P0DTC2
A	1263	GLU	-	expression tag	UNP P0DTC2
A	1264	LYS	-	expression tag	UNP P0DTC2
A	1265	GLY	-	expression tag	UNP P0DTC2
A	1266	GLY	-	expression tag	UNP P0DTC2
A	1267	GLY	-	expression tag	UNP P0DTC2
A	1268	SER	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	GLY	-	expression tag	UNP P0DTC2
A	1272	SER	-	expression tag	UNP P0DTC2
A	1273	GLY	-	expression tag	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	SER	-	expression tag	UNP P0DTC2
A	1276	ALA	-	expression tag	UNP P0DTC2
A	1277	TRP	-	expression tag	UNP P0DTC2
A	1278	SER	-	expression tag	UNP P0DTC2
A	1279	HIS	-	expression tag	UNP P0DTC2
A	1280	PRO	-	expression tag	UNP P0DTC2
A	1281	GLN	-	expression tag	UNP P0DTC2
A	1282	PHE	-	expression tag	UNP P0DTC2
A	1283	GLU	-	expression tag	UNP P0DTC2
A	1284	LYS	-	expression tag	UNP P0DTC2
A	1285	GLY	-	expression tag	UNP P0DTC2
A	1286	GLY	-	expression tag	UNP P0DTC2
A	1287	SER	-	expression tag	UNP P0DTC2
A	1288	HIS	-	expression tag	UNP P0DTC2
A	1289	HIS	-	expression tag	UNP P0DTC2
A	1290	HIS	-	expression tag	UNP P0DTC2
A	1291	HIS	-	expression tag	UNP P0DTC2
A	1292	HIS	-	expression tag	UNP P0DTC2
A	1293	HIS	-	expression tag	UNP P0DTC2
A	1294	HIS	-	expression tag	UNP P0DTC2
A	1295	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Bn03.

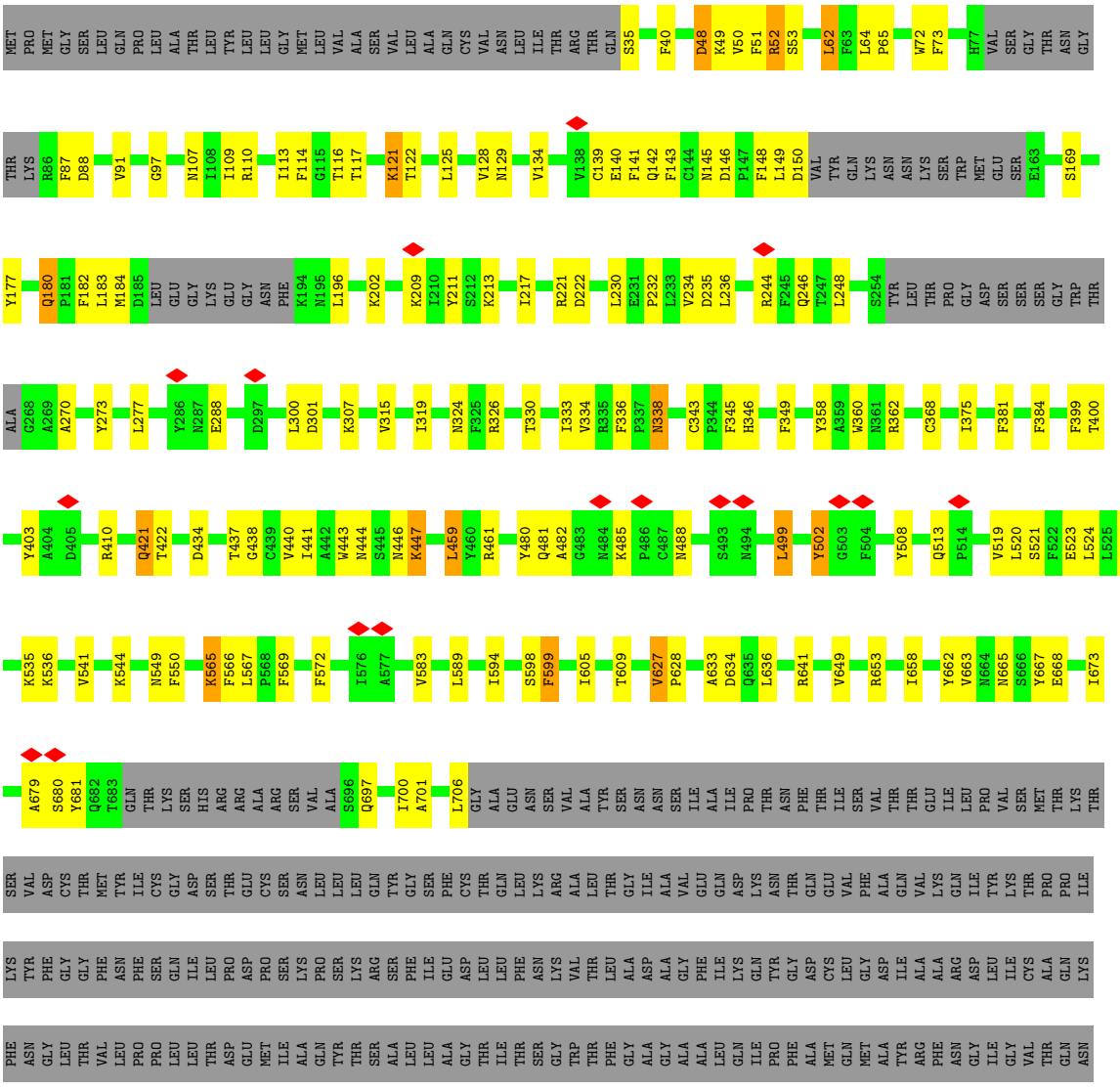
Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	119	Total	C	N	O	S	0	0
			922	585	151	182	4		

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.

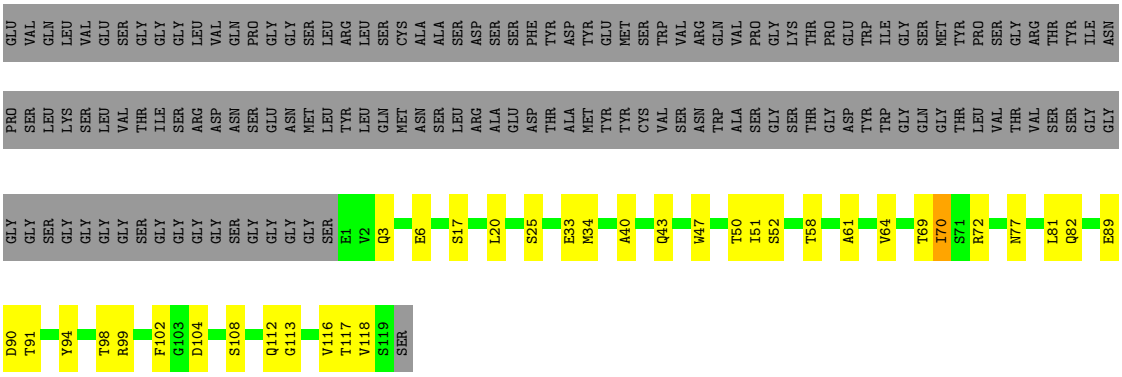
- Molecule 1: Spike glycoprotein

Chain A:



- Molecule 2: Bn03

Chain C:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	716985	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.672	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.028	Depositor
Map size (Å)	238.592, 238.592, 238.592	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.932, 0.932, 0.932	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	0.25	0/5029	0.43	0/6846
2	C	0.24	0/945	0.41	0/1283
All	All	0.25	0/5974	0.42	0/8129

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

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	4902	0	4737	83	0
2	C	922	0	866	23	0
All	All	5824	0	5603	103	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 9.

All (103) 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:91:THR:HA	2:C:116:VAL:O	1.68	0.91
2:C:94:TYR:O	2:C:113:GLY:HA2	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ARG:HE	1:A:52:ARG:H	1.41	0.68
1:A:110:ARG:HB2	1:A:129:ASN:HB2	1.76	0.67
1:A:91:VAL:HG21	1:A:244:ARG:HH21	1.61	0.65
1:A:49:LYS:HE3	1:A:232:PRO:HB3	1.80	0.64
1:A:627:VAL:HG13	1:A:628:PRO:HD3	1.81	0.63
2:C:17:SER:OG	2:C:82:GLN:NE2	2.32	0.62
1:A:48:ASP:OD1	1:A:52:ARG:NH1	2.34	0.61
1:A:91:VAL:HG11	1:A:244:ARG:HE	1.66	0.60
1:A:403:TYR:HB2	1:A:521:SER:HB2	1.83	0.59
1:A:114:PHE:HB2	1:A:125:LEU:HB3	1.85	0.59
1:A:196:LEU:HB2	1:A:217:ILE:HD12	1.85	0.58
1:A:53:SER:HB3	1:A:288:GLU:HA	1.87	0.56
1:A:358:TYR:HD1	1:A:461:ARG:HB2	1.71	0.56
1:A:381:PHE:HD1	1:A:443:TRP:HB3	1.70	0.55
1:A:481:GLN:HE22	1:A:488:ASN:H	1.54	0.55
2:C:51:ILE:HG12	2:C:58:THR:HG22	1.87	0.55
2:C:47:TRP:NE1	2:C:50:THR:OG1	2.40	0.55
1:A:421:GLN:NE2	1:A:422:THR:O	2.41	0.54
2:C:40:ALA:HB3	2:C:43:GLN:HE21	1.72	0.54
2:C:34:MET:HG3	2:C:72:ARG:HE	1.73	0.54
1:A:64:LEU:HD12	1:A:65:PRO:HD2	1.90	0.53
1:A:326:ARG:HH21	1:A:599:PHE:HA	1.73	0.53
1:A:149:LEU:HB2	1:A:248:LEU:HB3	1.91	0.53
1:A:523:GLU:OE2	2:C:52:SER:OG	2.25	0.53
1:A:346:HIS:HE1	1:A:375:ILE:HA	1.74	0.53
1:A:400:THR:HG23	1:A:524:LEU:HD12	1.91	0.53
1:A:502:TYR:HD1	1:A:502:TYR:H	1.57	0.53
1:A:338:ASN:O	1:A:338:ASN:ND2	2.40	0.52
1:A:459:LEU:HD22	1:A:499:LEU:HB2	1.91	0.52
1:A:673:ILE:HD11	1:A:679:ALA:HB2	1.90	0.52
1:A:97:GLY:HA3	1:A:277:LEU:HD12	1.92	0.52
2:C:98:THR:O	2:C:108:SER:OG	2.24	0.52
1:A:444:ASN:ND2	1:A:513:GLN:OE1	2.40	0.52
1:A:360:TRP:HZ3	1:A:362:ARG:HB2	1.75	0.52
1:A:447:LYS:HD3	1:A:447:LYS:H	1.75	0.51
2:C:3:GLN:NE2	2:C:25:SER:OG	2.44	0.51
1:A:315:VAL:HG22	1:A:609:THR:HG23	1.93	0.51
1:A:107:ASN:HB3	1:A:110:ARG:HD3	1.92	0.50
1:A:583:VAL:HG13	1:A:594:ILE:HD11	1.92	0.50
2:C:99:ARG:NH1	2:C:104:ASP:O	2.45	0.50
1:A:213:LYS:HB2	1:A:230:LEU:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:ASN:ND2	1:A:598:SER:O	2.45	0.49
1:A:139:CYS:SG	1:A:140:GLU:N	2.85	0.49
1:A:142:GLN:HB2	1:A:169:SER:H	1.77	0.49
1:A:444:ASN:ND2	1:A:446:ASN:OD1	2.45	0.49
1:A:680:SER:HB3	1:A:700:ILE:HD11	1.94	0.49
1:A:113:ILE:HB	1:A:246:GLN:HB2	1.95	0.49
1:A:438:GLY:HA3	1:A:520:LEU:O	2.12	0.49
1:A:440:VAL:HG12	1:A:519:VAL:HG22	1.95	0.49
1:A:634:ASP:HA	1:A:641:ARG:HH22	1.78	0.48
1:A:437:THR:HG23	2:C:102:PHE:HB3	1.96	0.48
2:C:6:GLU:O	2:C:112:GLN:NE2	2.46	0.48
1:A:211:TYR:HB3	1:A:230:LEU:HB3	1.95	0.48
2:C:91:THR:HG23	2:C:117:THR:HA	1.94	0.48
1:A:663:VAL:HG12	1:A:665:ASN:H	1.79	0.48
1:A:481:GLN:NE2	1:A:488:ASN:OD1	2.46	0.48
1:A:633:ALA:HA	1:A:636:LEU:HD12	1.96	0.47
1:A:300:LEU:HG	1:A:301:ASP:H	1.80	0.47
1:A:410:ARG:HB3	1:A:502:TYR:HE2	1.80	0.47
1:A:362:ARG:HE	1:A:403:TYR:HB3	1.80	0.46
1:A:35:SER:OG	1:A:72:TRP:O	2.32	0.46
1:A:134:VAL:HG21	1:A:182:PHE:HB3	1.99	0.46
1:A:121:LYS:HG3	1:A:122:THR:H	1.81	0.45
1:A:565:LYS:HD3	1:A:566:PHE:HD2	1.81	0.45
1:A:116:THR:HG22	1:A:117:THR:HG23	1.97	0.45
1:A:330:THR:OG1	1:A:544:LYS:NZ	2.38	0.45
2:C:61:ALA:HB3	2:C:64:VAL:HG22	1.98	0.45
1:A:526:HIS:HE2	2:C:50:THR:HG1	1.63	0.45
1:A:50:VAL:HG12	1:A:51:PHE:H	1.82	0.44
1:A:343:CYS:HB3	1:A:345:PHE:HD2	1.82	0.44
1:A:649:VAL:HG12	1:A:658:ILE:HG12	1.97	0.44
2:C:20:LEU:HD12	2:C:81:LEU:HD23	1.99	0.44
1:A:213:LYS:HB2	1:A:230:LEU:HG	2.00	0.44
1:A:91:VAL:HG22	1:A:246:GLN:HE21	1.83	0.43
1:A:381:PHE:CG	1:A:441:ILE:HD11	2.53	0.43
1:A:434:ASP:OD1	1:A:434:ASP:N	2.52	0.43
1:A:109:ILE:HD11	1:A:270:ALA:HB1	2.00	0.43
2:C:69:THR:HG23	2:C:82:GLN:HB3	1.99	0.43
1:A:121:LYS:HD3	1:A:121:LYS:HA	1.77	0.43
1:A:333:ILE:HD11	1:A:541:VAL:HB	2.00	0.43
1:A:146:ASP:HB3	1:A:148:PHE:HD1	1.84	0.42
1:A:62:LEU:H	1:A:62:LEU:HD23	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ASN:ND2	1:A:146:ASP:OD1	2.53	0.42
1:A:681:TYR:CE2	1:A:697:GLN:HB3	2.55	0.42
2:C:51:ILE:HG13	2:C:70:ILE:HD12	2.01	0.42
1:A:73:PHE:HB3	1:A:88:ASP:HB3	2.02	0.41
2:C:72:ARG:HH22	2:C:77:ASN:HA	1.85	0.41
1:A:346:HIS:HA	1:A:349:PHE:HD2	1.85	0.41
1:A:334:VAL:O	1:A:550:PHE:HA	2.21	0.41
1:A:662:TYR:HA	1:A:701:ALA:HB3	2.01	0.41
1:A:399:PHE:HA	1:A:524:LEU:HD13	2.02	0.41
1:A:480:TYR:CZ	1:A:482:ALA:HB3	2.56	0.41
2:C:72:ARG:NH1	2:C:77:ASN:OD1	2.36	0.41
1:A:141:PHE:HB2	1:A:143:PHE:CE2	2.56	0.41
1:A:346:HIS:CE1	1:A:375:ILE:HA	2.56	0.40
2:C:90:ASP:HB2	2:C:118:VAL:HG21	2.03	0.40
2:C:34:MET:SD	2:C:98:THR:OG1	2.74	0.40
1:A:202:LYS:HG3	1:A:209:LYS:HB2	2.02	0.40
1:A:221:ARG:HG2	1:A:222:ASP:H	1.85	0.40
1:A:180:GLN:HE21	1:A:180:GLN:HB3	1.68	0.40
1:A:319:ILE:HB	1:A:605:ILE:HG12	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	607/1295 (47%)	564 (93%)	43 (7%)	0	100	100
2	C	117/258 (45%)	115 (98%)	2 (2%)	0	100	100
All	All	724/1553 (47%)	679 (94%)	45 (6%)	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	547/1116 (49%)	505 (92%)	42 (8%)	10 33
2	C	96/202 (48%)	93 (97%)	3 (3%)	35 56
All	All	643/1318 (49%)	598 (93%)	45 (7%)	15 35

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	PHE
1	A	48	ASP
1	A	52	ARG
1	A	62	LEU
1	A	87	PHE
1	A	121	LYS
1	A	128	VAL
1	A	150	ASP
1	A	177	TYR
1	A	180	GLN
1	A	183	LEU
1	A	184	MET
1	A	234	VAL
1	A	235	ASP
1	A	236	LEU
1	A	273	TYR
1	A	307	LYS
1	A	336	PHE
1	A	338	ASN
1	A	368	CYS
1	A	384	PHE
1	A	421	GLN
1	A	447	LYS
1	A	459	LEU
1	A	485	LYS
1	A	499	LEU
1	A	502	TYR

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Mol	Chain	Res	Type
1	A	508	TYR
1	A	535	LYS
1	A	536	LYS
1	A	549	ASN
1	A	565	LYS
1	A	567	LEU
1	A	569	PHE
1	A	572	PHE
1	A	589	LEU
1	A	599	PHE
1	A	627	VAL
1	A	653	ARG
1	A	667	TYR
1	A	668	GLU
1	A	706	LEU
2	C	33	GLU
2	C	70	ILE
2	C	89	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	A	145	ASN
1	A	180	GLN
1	A	324	ASN
1	A	412	ASN
1	A	416	GLN
1	A	421	GLN
1	A	455	ASN
1	A	457	ASN
1	A	570	GLN
1	A	614	GLN
1	A	682	GLN
2	C	3	GLN
2	C	112	GLN

5.3.3 RNA

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 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.

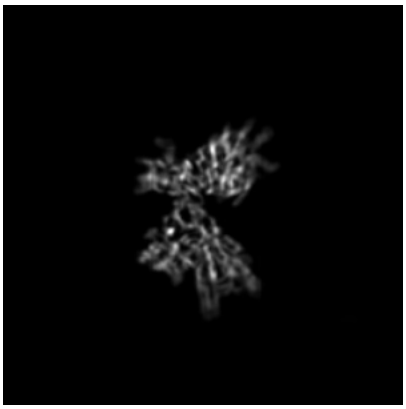
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35170. These allow visual inspection of the internal detail of the map and identification of artifacts.

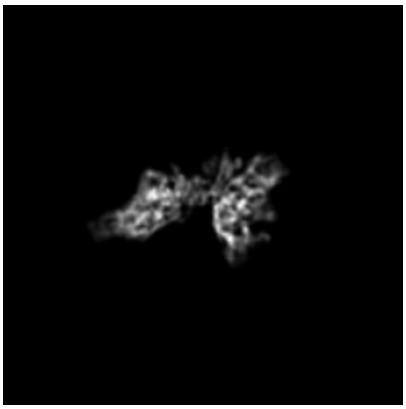
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

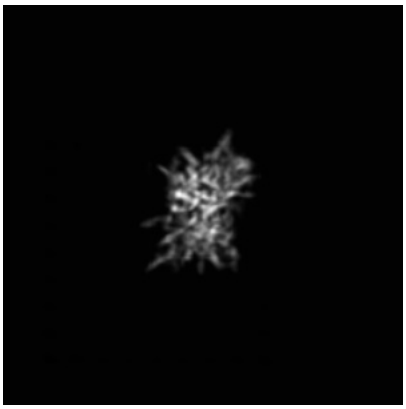
6.1.1 Primary map



X

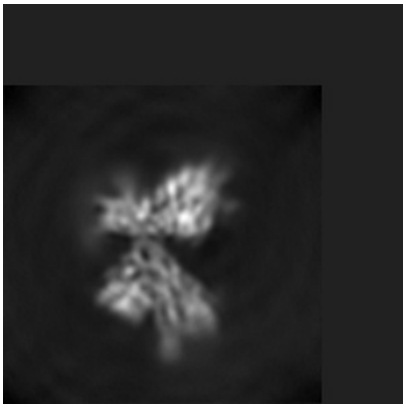


Y

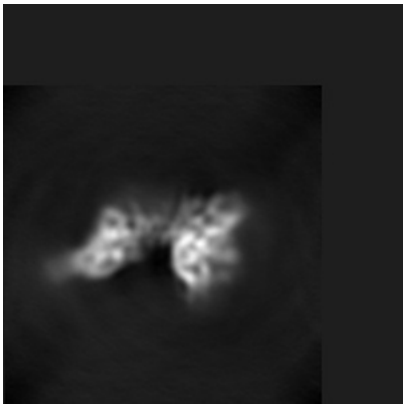


Z

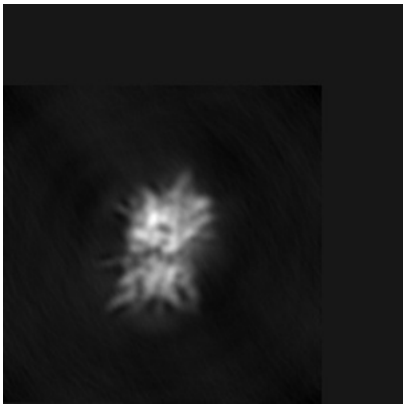
6.1.2 Raw map



X



Y



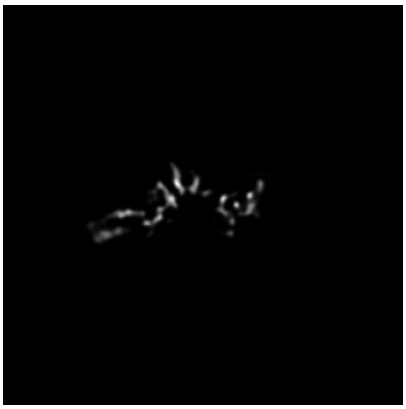
Z

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

6.2 Central slices (i)

6.2.1 Primary map

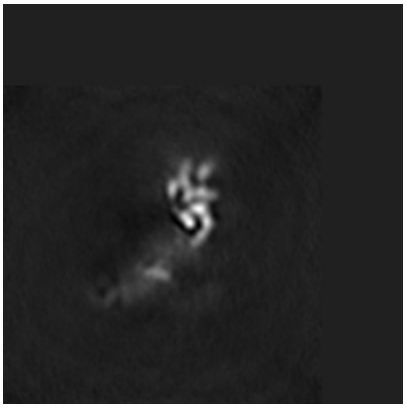
X Index: 128



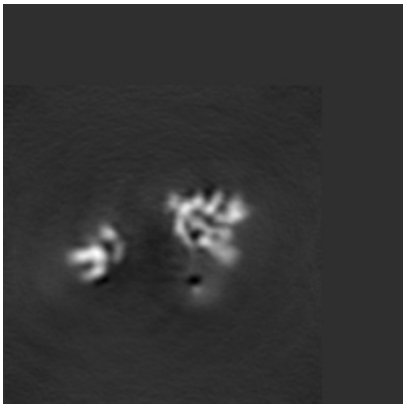
Y Index: 128

Z Index: 128

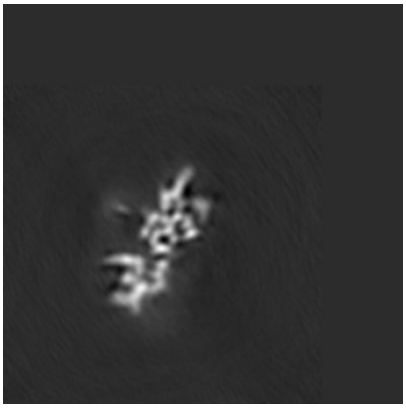
6.2.2 Raw map



X Index: 128



Y Index: 128



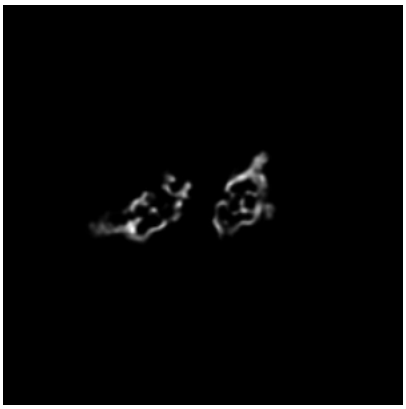
Z Index: 128

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

6.3 Largest variance slices (i)

6.3.1 Primary map

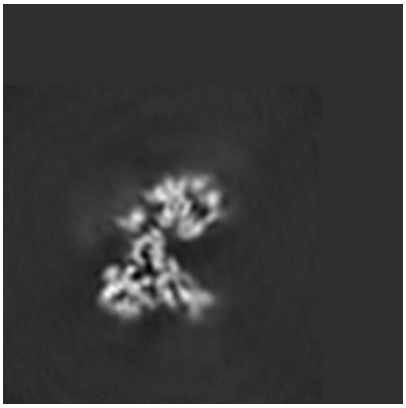
X Index: 135



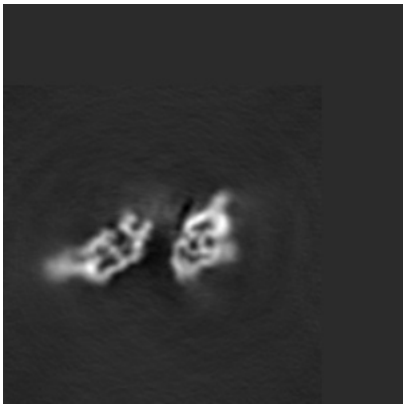
Y Index: 134

Z Index: 145

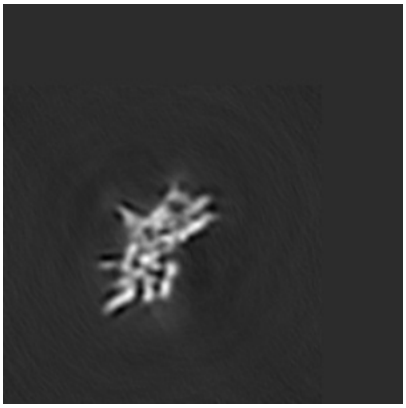
6.3.2 Raw map



X Index: 108



Y Index: 108

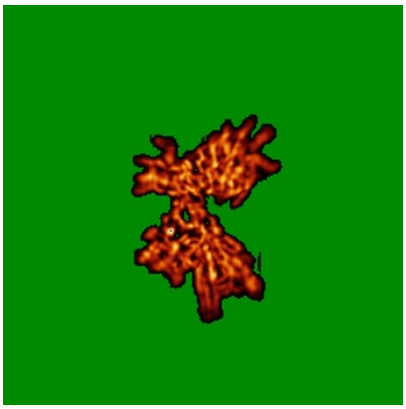


Z Index: 119

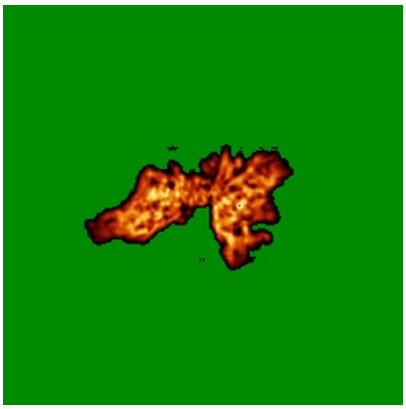
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



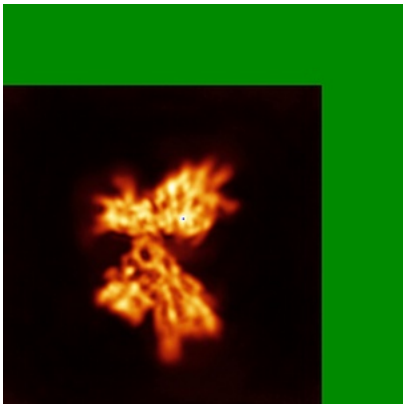
X



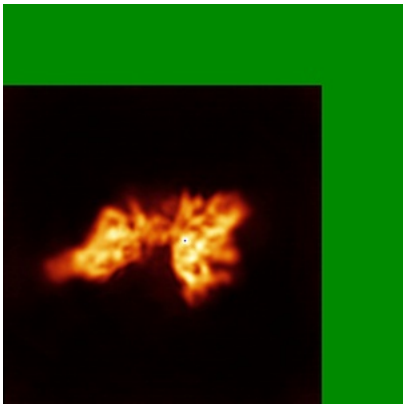
Y

Z

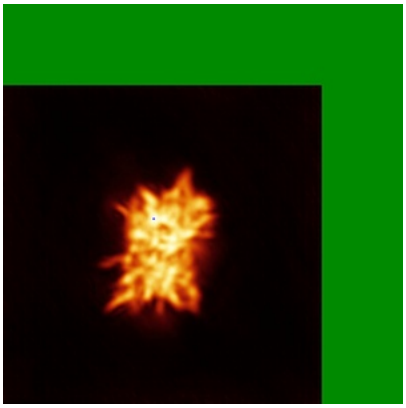
6.4.2 Raw map



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.

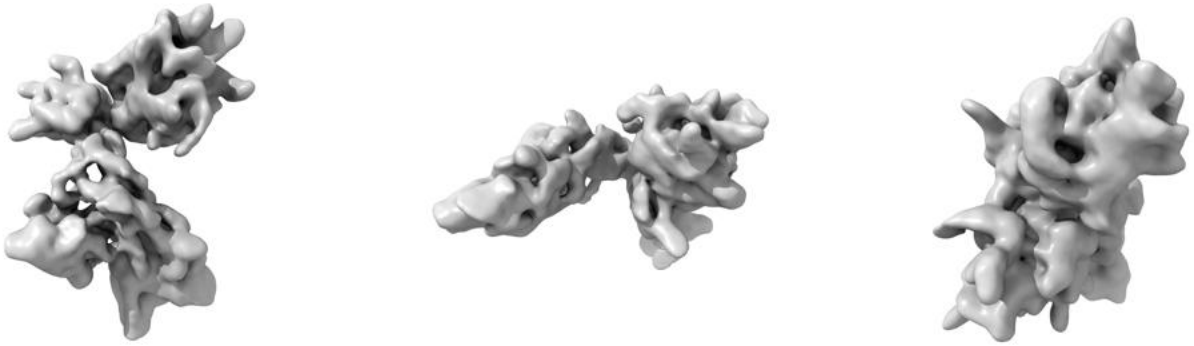
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.028. 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



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.

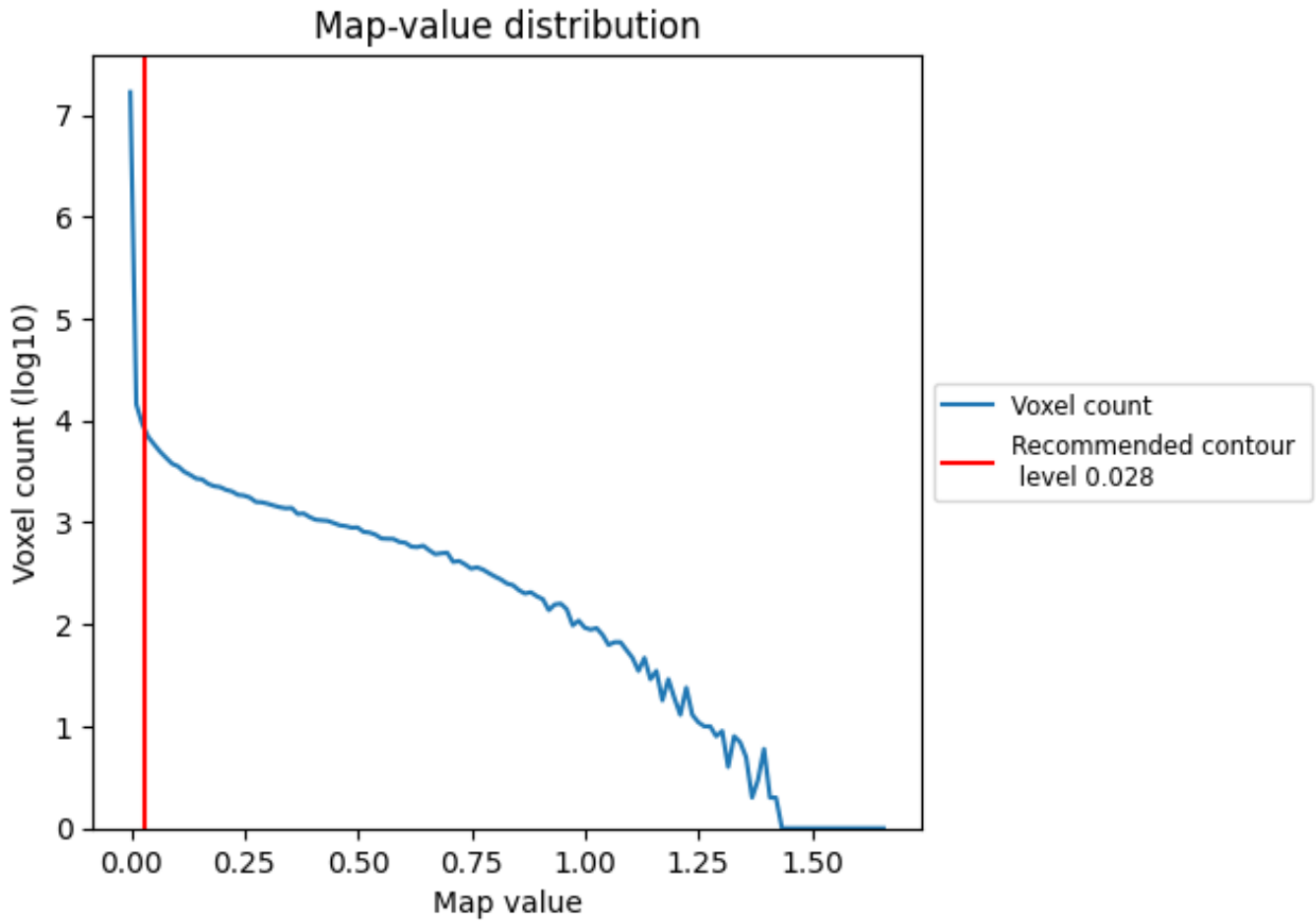
6.6 Mask visualisation (i)

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

7 Map analysis

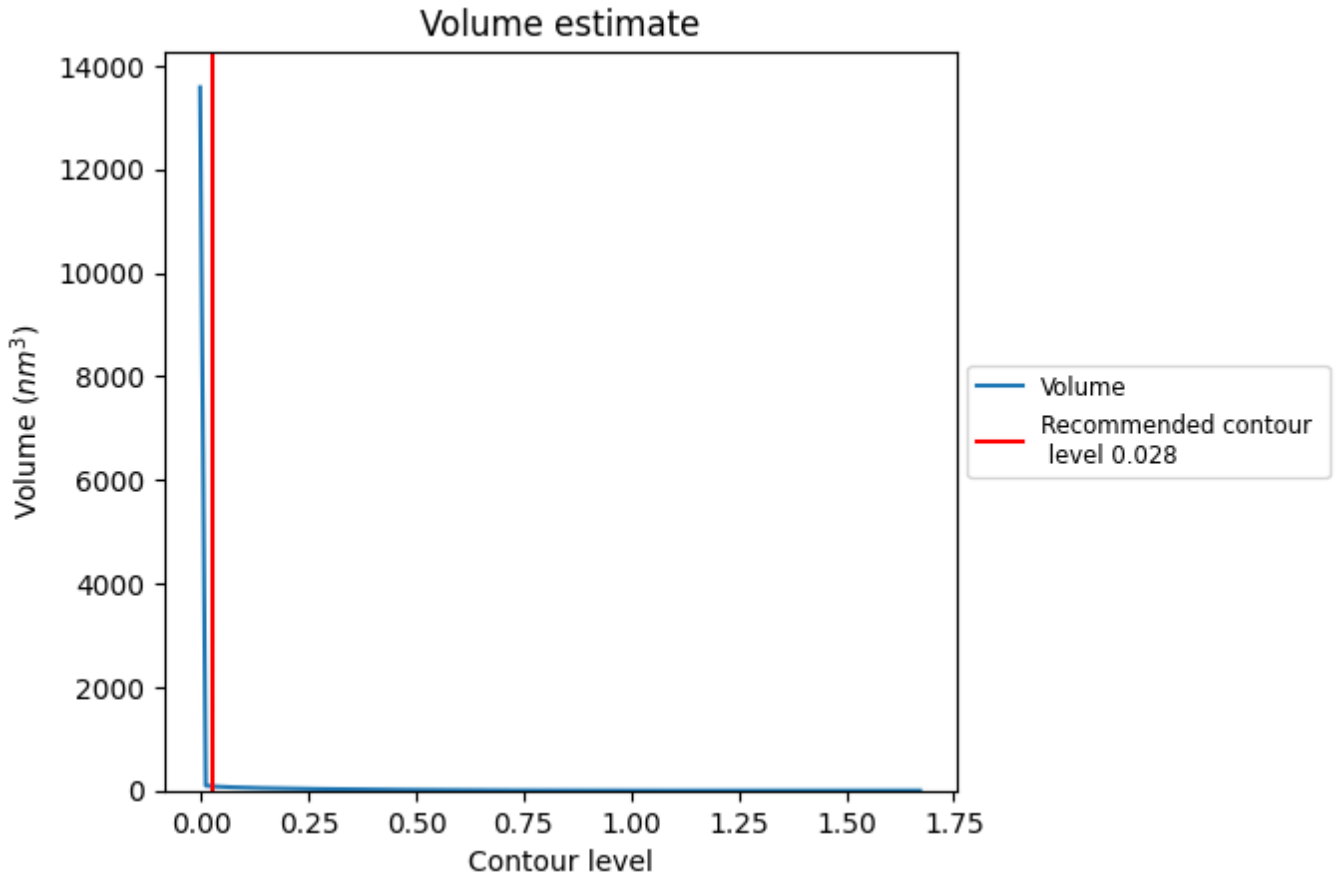
This section contains the results of statistical analysis of the map.

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.

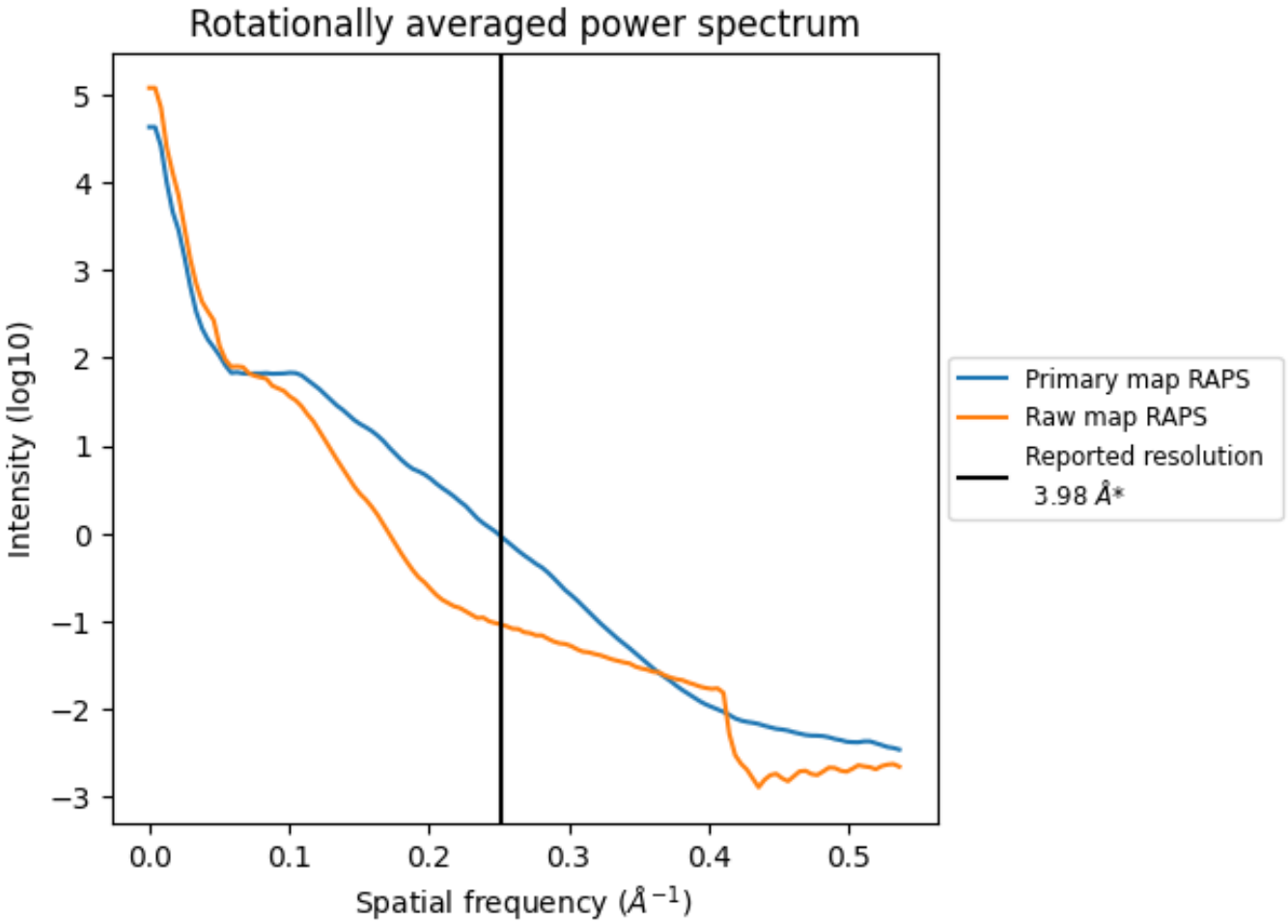
7.2 Volume estimate



The volume at the recommended contour level is 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)

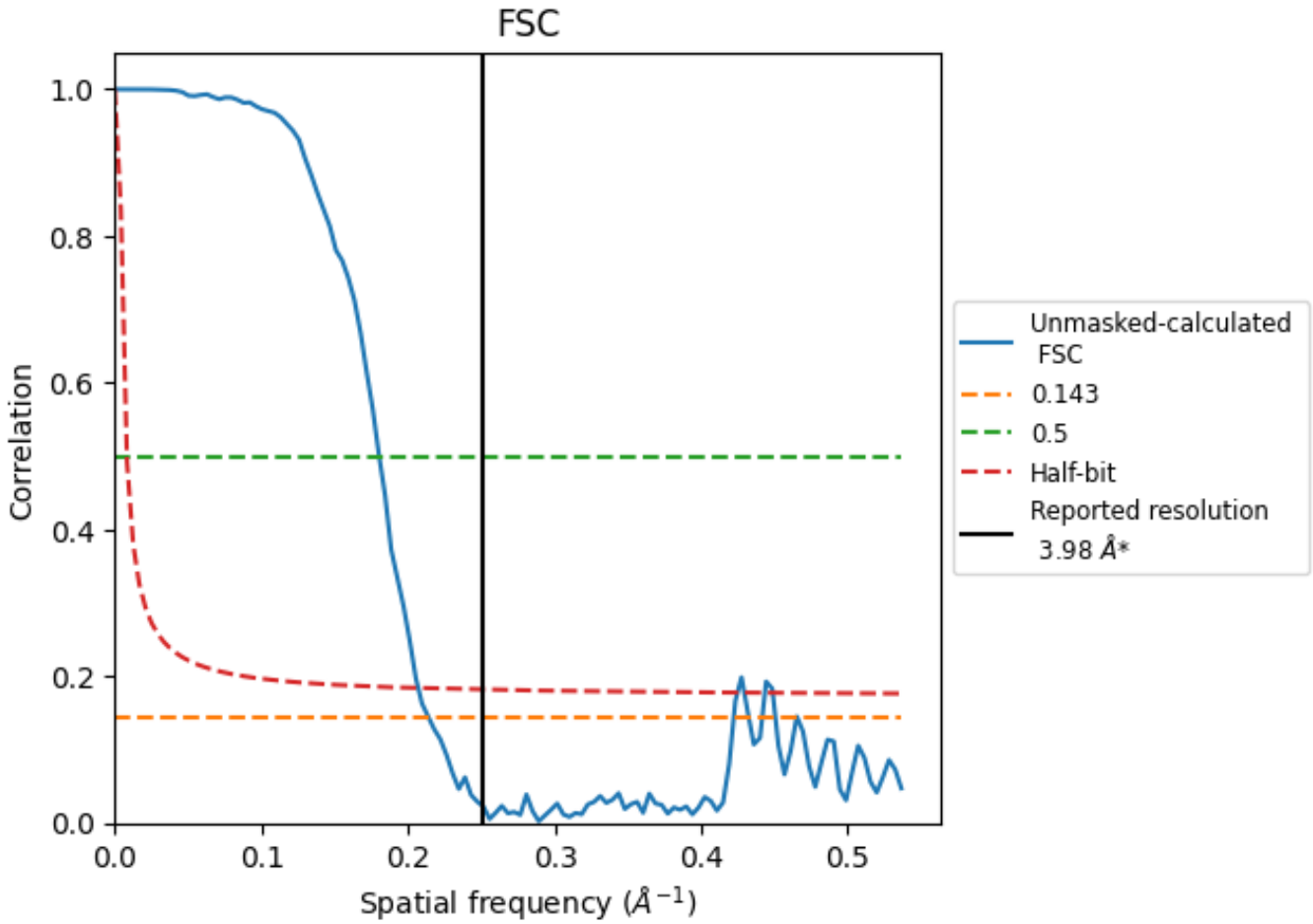


*Reported resolution corresponds to spatial frequency of 0.251 Å^{-1}

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 0.251 Å^{-1}

8.2 Resolution estimates (i)

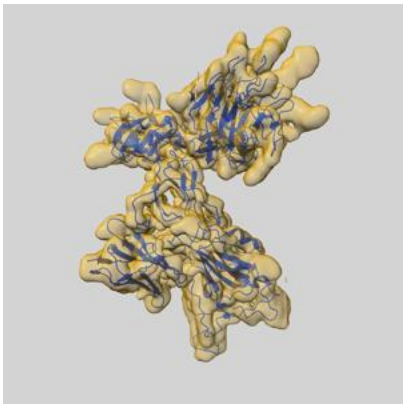
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.98	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.67	5.55	4.83

*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 4.67 differs from the reported value 3.98 by more than 10 %

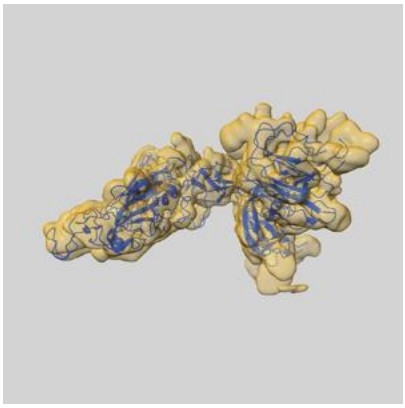
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35170 and PDB model 8I4E. Per-residue inclusion information can be found in section 3 on page 8.

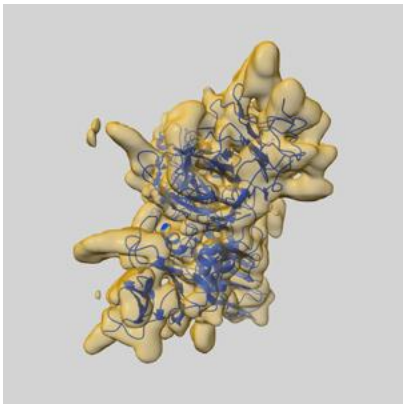
9.1 Map-model overlay



X



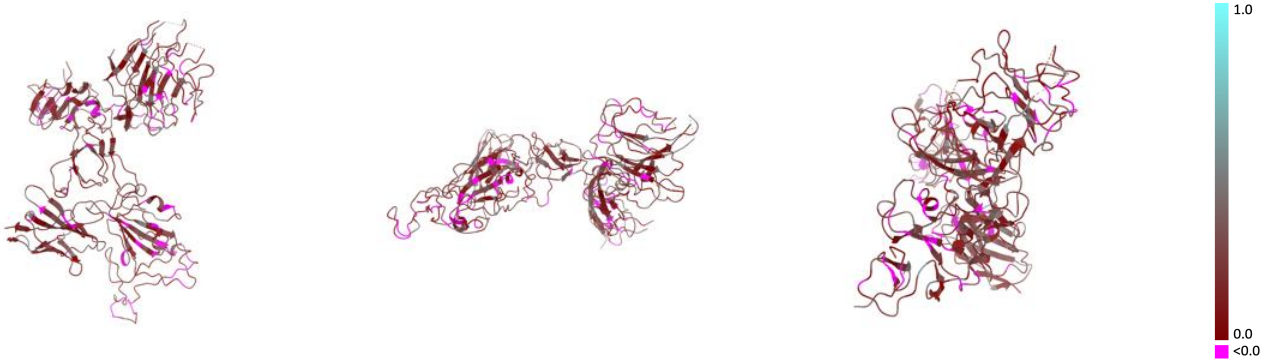
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.028 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.

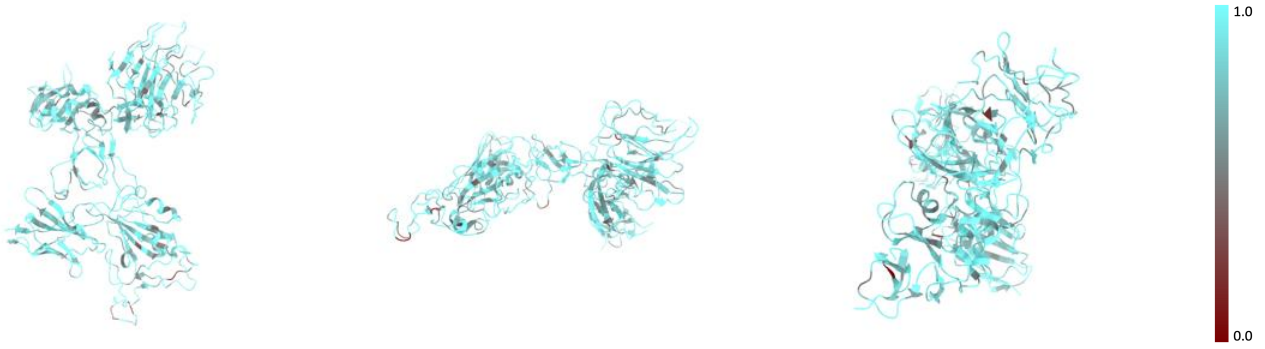
9.2 Q-score mapped to coordinate model



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.

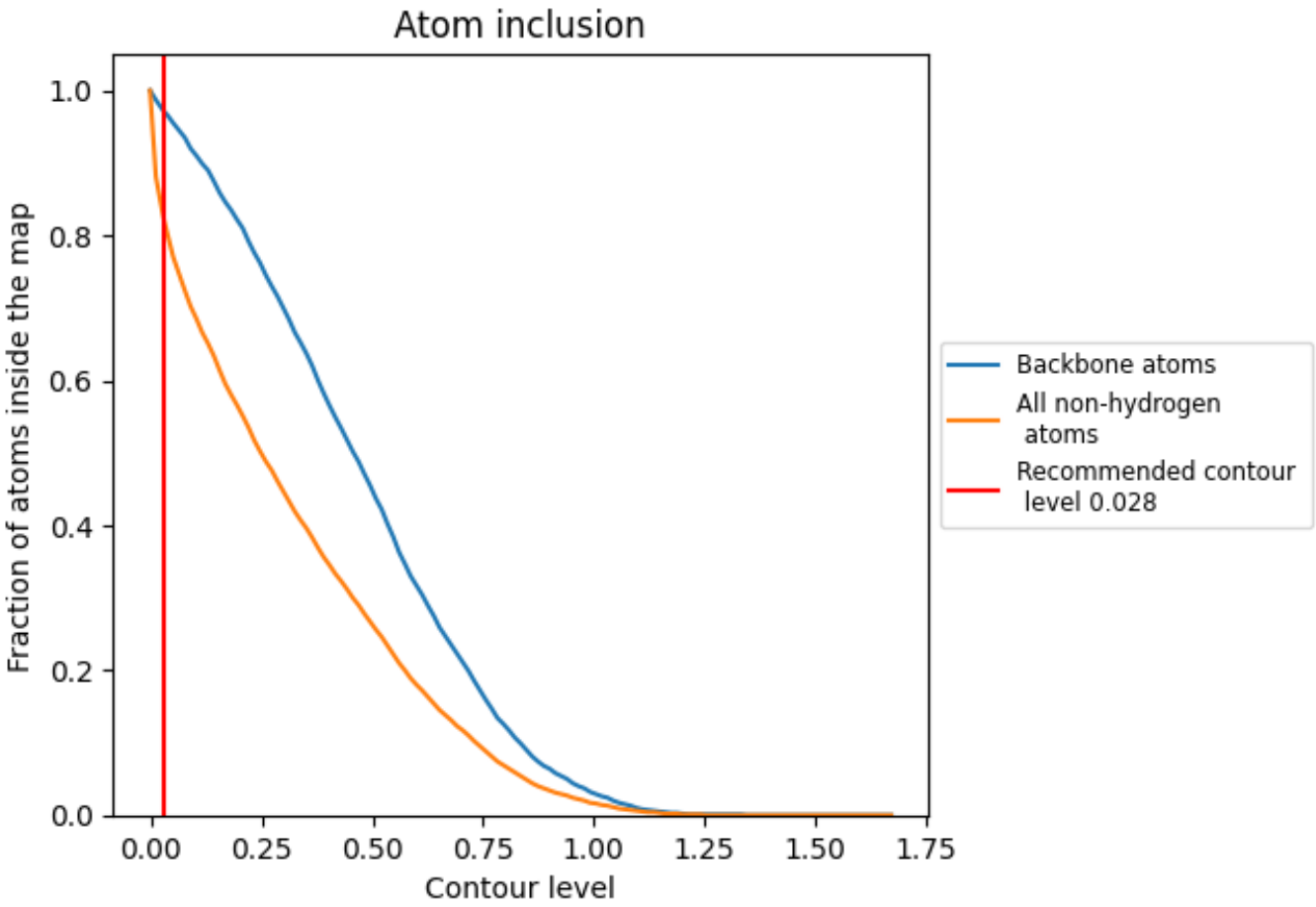
9.3 Atom inclusion mapped to coordinate model



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 (0.028).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 82% 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 (0.028) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8250	0.1810
A	0.8190	0.1780
C	0.8580	0.1990