



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 11:39 AM UTC

PDB ID : 8I4G / pdb_00008i4g
EMDB ID : EMD-35172
Title : Omicron spike variant BQ.1.1 with n3130v-Fc
Authors : Hao, A.H.; Zhang, X.; Chen, Z.G.; Sun, L.
Deposited on : 2023-01-19
Resolution : 3.68 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

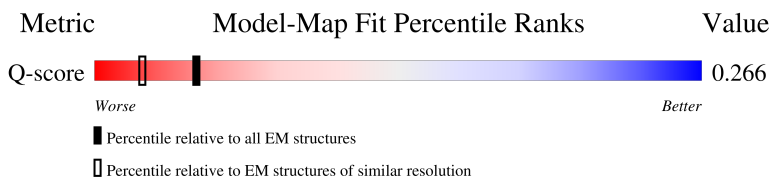
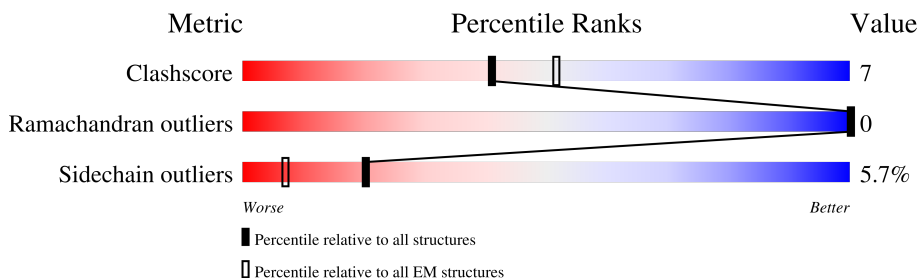
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.68 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	11376 (3.18 - 4.18)

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	C	383	
2	A	1294	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6057 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 n3130v-Fc.

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

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	649	Total	C	N	O	S	0	0
			5135	3293	854	967	21		

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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
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	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	148	ASP	GLY	variant	UNP P0DTC2
A	219	GLY	VAL	variant	UNP P0DTC2
A	345	ASP	GLY	variant	UNP P0DTC2
A	352	THR	ARG	variant	UNP P0DTC2
A	377	PHE	SER	variant	UNP P0DTC2
A	379	PRO	SER	variant	UNP P0DTC2
A	381	PHE	SER	variant	UNP P0DTC2
A	382	ALA	THR	variant	UNP P0DTC2
A	411	ASN	ASP	variant	UNP P0DTC2
A	414	SER	ARG	variant	UNP P0DTC2
A	423	ASN	LYS	variant	UNP P0DTC2
A	446	LYS	ASN	variant	UNP P0DTC2
A	450	THR	LYS	variant	UNP P0DTC2
A	458	ARG	LEU	variant	UNP P0DTC2
A	466	LYS	ASN	variant	UNP P0DTC2
A	483	ASN	SER	variant	UNP P0DTC2
A	484	LYS	THR	variant	UNP P0DTC2
A	490	ALA	GLU	variant	UNP P0DTC2
A	492	VAL	PHE	variant	UNP P0DTC2
A	504	ARG	GLN	variant	UNP P0DTC2
A	507	TYR	ASN	variant	UNP P0DTC2
A	511	HIS	TYR	variant	UNP P0DTC2
A	620	GLY	ASP	variant	UNP P0DTC2
A	661	TYR	HIS	variant	UNP P0DTC2
A	685	LYS	ASN	variant	UNP P0DTC2
A	687	HIS	PRO	conflict	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	688	GLY	ARG	engineered mutation	UNP P0DTC2
A	689	SER	ARG	engineered mutation	UNP P0DTC2
A	691	SER	ARG	engineered mutation	UNP P0DTC2
A	770	LYS	ASN	variant	UNP P0DTC2
A	802	TYR	ASP	variant	UNP P0DTC2
A	960	HIS	GLN	variant	UNP P0DTC2
A	975	LYS	ASN	variant	UNP P0DTC2
A	1215	GLY	-	expression tag	UNP P0DTC2
A	1216	SER	-	expression tag	UNP P0DTC2
A	1217	GLY	-	expression tag	UNP P0DTC2
A	1218	TYR	-	expression tag	UNP P0DTC2
A	1219	ILE	-	expression tag	UNP P0DTC2
A	1220	PRO	-	expression tag	UNP P0DTC2
A	1221	GLU	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	PRO	-	expression tag	UNP P0DTC2
A	1224	ARG	-	expression tag	UNP P0DTC2
A	1225	ASP	-	expression tag	UNP P0DTC2
A	1226	GLY	-	expression tag	UNP P0DTC2
A	1227	GLN	-	expression tag	UNP P0DTC2
A	1228	ALA	-	expression tag	UNP P0DTC2
A	1229	TYR	-	expression tag	UNP P0DTC2
A	1230	VAL	-	expression tag	UNP P0DTC2
A	1231	ARG	-	expression tag	UNP P0DTC2
A	1232	LYS	-	expression tag	UNP P0DTC2
A	1233	ASP	-	expression tag	UNP P0DTC2
A	1234	GLY	-	expression tag	UNP P0DTC2
A	1235	GLU	-	expression tag	UNP P0DTC2
A	1236	TRP	-	expression tag	UNP P0DTC2
A	1237	VAL	-	expression tag	UNP P0DTC2
A	1238	PHE	-	expression tag	UNP P0DTC2
A	1239	LEU	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	THR	-	expression tag	UNP P0DTC2
A	1242	PHE	-	expression tag	UNP P0DTC2
A	1243	LEU	-	expression tag	UNP P0DTC2
A	1244	SER	-	expression tag	UNP P0DTC2
A	1245	GLY	-	expression tag	UNP P0DTC2
A	1246	LEU	-	expression tag	UNP P0DTC2
A	1247	GLU	-	expression tag	UNP P0DTC2
A	1248	VAL	-	expression tag	UNP P0DTC2
A	1249	LEU	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1250	PHE	-	expression tag	UNP P0DTC2
A	1251	GLN	-	expression tag	UNP P0DTC2
A	1252	GLY	-	expression tag	UNP P0DTC2
A	1253	PRO	-	expression tag	UNP P0DTC2
A	1254	GLY	-	expression tag	UNP P0DTC2
A	1255	GLY	-	expression tag	UNP P0DTC2
A	1256	TRP	-	expression tag	UNP P0DTC2
A	1257	SER	-	expression tag	UNP P0DTC2
A	1258	HIS	-	expression tag	UNP P0DTC2
A	1259	PRO	-	expression tag	UNP P0DTC2
A	1260	GLN	-	expression tag	UNP P0DTC2
A	1261	PHE	-	expression tag	UNP P0DTC2
A	1262	GLU	-	expression tag	UNP P0DTC2
A	1263	LYS	-	expression tag	UNP P0DTC2
A	1264	GLY	-	expression tag	UNP P0DTC2
A	1265	GLY	-	expression tag	UNP P0DTC2
A	1266	GLY	-	expression tag	UNP P0DTC2
A	1267	SER	-	expression tag	UNP P0DTC2
A	1268	GLY	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	GLY	-	expression tag	UNP P0DTC2
A	1274	SER	-	expression tag	UNP P0DTC2
A	1275	ALA	-	expression tag	UNP P0DTC2
A	1276	TRP	-	expression tag	UNP P0DTC2
A	1277	SER	-	expression tag	UNP P0DTC2
A	1278	HIS	-	expression tag	UNP P0DTC2
A	1279	PRO	-	expression tag	UNP P0DTC2
A	1280	GLN	-	expression tag	UNP P0DTC2
A	1281	PHE	-	expression tag	UNP P0DTC2
A	1282	GLU	-	expression tag	UNP P0DTC2
A	1283	LYS	-	expression tag	UNP P0DTC2
A	1284	GLY	-	expression tag	UNP P0DTC2
A	1285	GLY	-	expression tag	UNP P0DTC2
A	1286	SER	-	expression tag	UNP P0DTC2
A	1287	HIS	-	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

Continued on next page...

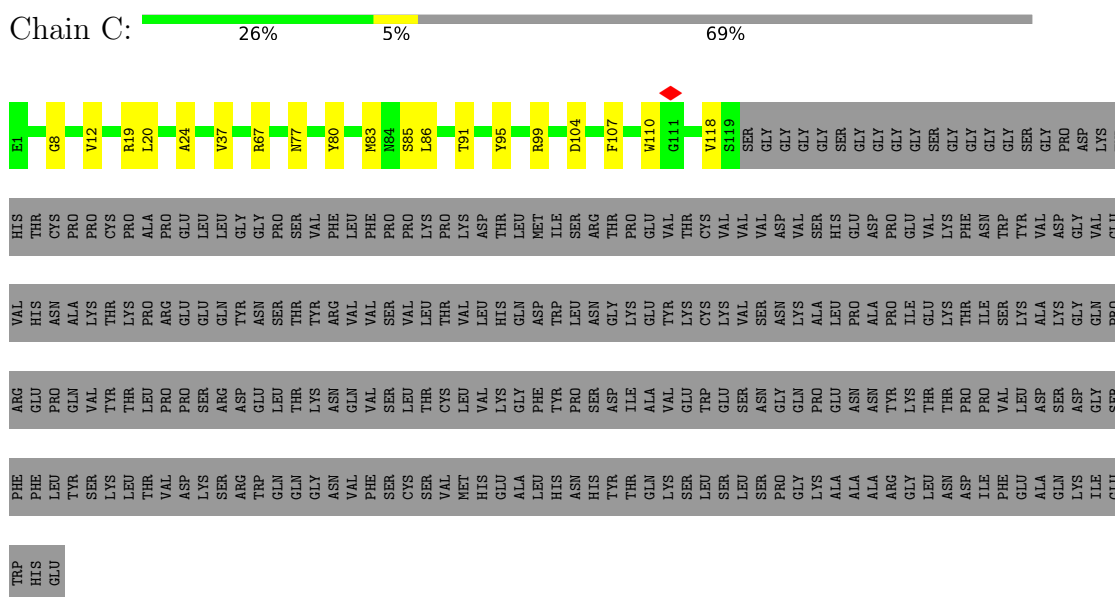
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1292	HIS	-	expression tag	UNP P0DTC2
A	1293	HIS	-	expression tag	UNP P0DTC2
A	1294	HIS	-	expression tag	UNP P0DTC2

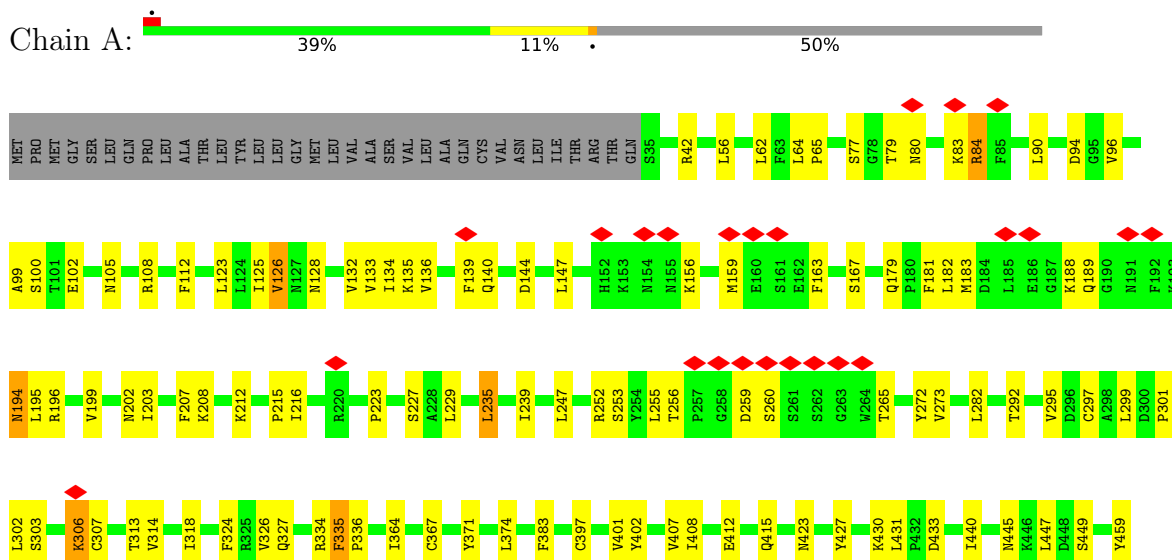
3 Residue-property plots

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: n3130v-Fc



• Molecule 2: Spike glycoprotein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	498235	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 ($e^-/\text{\AA}^2$)	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	2.207	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.029	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 [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	C	0.13	0/945	0.36	0/1283
2	A	0.15	0/5274	0.41	0/7185
All	All	0.15	0/6219	0.41	0/8468

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	C	922	0	866	10	0
2	A	5135	0	4948	72	0
All	All	6057	0	5814	82	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 7.

All (82) 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:A:105:ASN:HB3	2:A:108:ARG:HD3	1.72	0.71
2:A:212:LYS:HB2	2:A:229:LEU:HA	1.71	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:ARG:HD2	1:C:80:TYR:HB3	1.73	0.69
2:A:42:ARG:NH1	2:A:227:SER:OG	2.26	0.68
2:A:195:LEU:HB2	2:A:216:ILE:HD11	1.75	0.67
2:A:486:CYS:HB3	2:A:489:VAL:HG22	1.79	0.64
2:A:314:VAL:HG12	2:A:608:THR:HG23	1.78	0.64
2:A:62:LEU:HD13	2:A:94:ASP:HB3	1.79	0.63
2:A:326:VAL:HG21	2:A:596:CYS:HB3	1.81	0.62
2:A:99:ALA:HB3	2:A:272:TYR:HB2	1.81	0.62
2:A:626:VAL:HG13	2:A:627:PRO:HD3	1.82	0.62
2:A:402:TYR:HB2	2:A:520:SER:HB2	1.83	0.60
1:C:8:GLY:HA3	1:C:20:LEU:HA	1.85	0.59
2:A:99:ALA:HB1	2:A:195:LEU:HD11	1.85	0.58
2:A:336:PRO:O	2:A:586:GLN:NE2	2.36	0.58
2:A:301:PRO:HG3	2:A:616:VAL:HG22	1.85	0.58
2:A:463:ARG:NH2	2:A:473:ASP:OD2	2.36	0.58
2:A:364:ILE:HB	2:A:401:VAL:HG23	1.86	0.57
2:A:194:ASN:HA	2:A:215:PRO:HA	1.87	0.57
1:C:99:ARG:HB3	1:C:107:PHE:HA	1.87	0.57
2:A:64:LEU:HD12	2:A:65:PRO:HD2	1.87	0.57
2:A:216:ILE:HG12	2:A:223:PRO:HG3	1.86	0.56
1:C:67:ARG:NH2	1:C:85:SER:O	2.32	0.56
1:C:91:THR:HG22	1:C:118:VAL:H	1.71	0.56
2:A:501:TYR:H	2:A:501:TYR:HD1	1.54	0.55
2:A:105:ASN:HA	2:A:183:MET:HE3	1.90	0.54
2:A:430:LYS:HE3	2:A:431:LEU:H	1.73	0.54
1:C:24:ALA:O	1:C:77:ASN:ND2	2.41	0.54
2:A:80:ASN:HA	2:A:84:ARG:HG2	1.90	0.53
2:A:144:ASP:N	2:A:144:ASP:OD1	2.41	0.53
2:A:480:GLN:NE2	2:A:493:ASN:O	2.41	0.53
2:A:112:PHE:HB2	2:A:123:LEU:HB3	1.92	0.53
2:A:96:VAL:HG13	2:A:273:VAL:HG13	1.92	0.52
2:A:548:ASN:ND2	2:A:553:THR:OG1	2.43	0.52
2:A:427:TYR:HA	2:A:467:LEU:HD23	1.93	0.51
2:A:128:ASN:ND2	2:A:159:MET:SD	2.84	0.50
2:A:80:ASN:OD1	2:A:84:ARG:NH2	2.43	0.50
2:A:480:GLN:NE2	2:A:494:CYS:SG	2.83	0.50
2:A:302:LEU:HD21	2:A:608:THR:HG22	1.92	0.50
2:A:77:SER:OG	2:A:260:SER:O	2.30	0.49
2:A:462:PHE:HD2	2:A:497:PRO:HA	1.78	0.48
2:A:125:ILE:HG12	2:A:134:ILE:HG23	1.96	0.48
2:A:202:ASN:HB3	2:A:207:PHE:HD1	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:90:LEU:HD22	2:A:273:VAL:HG11	1.96	0.47
2:A:235:LEU:HD23	2:A:235:LEU:H	1.80	0.47
2:A:507:TYR:HB3	2:A:511:HIS:HB2	1.96	0.47
2:A:100:SER:OG	2:A:196:ARG:NH1	2.48	0.47
2:A:371:TYR:HA	2:A:374:LEU:HD13	1.96	0.47
2:A:299:LEU:HA	2:A:636:THR:HG21	1.97	0.46
2:A:123:LEU:HD13	2:A:136:VAL:HG22	1.98	0.46
2:A:334:ARG:HD2	2:A:586:GLN:HG3	1.99	0.46
2:A:297:CYS:H	2:A:303:SER:HB3	1.82	0.45
2:A:147:LEU:HB2	2:A:247:LEU:HD11	1.98	0.45
2:A:203:ILE:HD11	2:A:208:LYS:HD2	1.97	0.45
2:A:79:THR:HB	2:A:83:LYS:HB2	1.98	0.44
2:A:415:GLN:HE22	2:A:423:ASN:H	1.65	0.44
2:A:433:ASP:OD1	2:A:433:ASP:N	2.50	0.44
2:A:80:ASN:HD21	2:A:253:SER:HB2	1.83	0.44
2:A:324:PHE:O	2:A:327:GLN:NE2	2.51	0.44
2:A:630:ILE:H	2:A:630:ILE:HG13	1.69	0.44
2:A:445:ASN:O	2:A:449:SER:OG	2.35	0.44
1:C:83:MET:HB3	1:C:86:LEU:HD21	1.99	0.44
2:A:188:LYS:HG2	2:A:189:GLN:H	1.83	0.44
2:A:42:ARG:NH2	2:A:223:PRO:HB2	2.32	0.43
2:A:199:VAL:HG23	2:A:229:LEU:HD22	2.00	0.43
1:C:37:VAL:O	1:C:95:TYR:N	2.42	0.43
2:A:383:PHE:HD1	2:A:440:ILE:HD13	1.83	0.42
2:A:126:VAL:HG23	2:A:133:VAL:HB	2.00	0.42
2:A:252:ARG:HD3	2:A:265:THR:HG22	2.00	0.42
2:A:179:GLN:HE21	2:A:179:GLN:HB3	1.67	0.42
2:A:256:THR:OG1	2:A:259:ASP:OD1	2.28	0.42
2:A:140:GLN:HB2	2:A:167:SER:HB3	2.02	0.41
2:A:408:ILE:HD12	2:A:412:GLU:HG3	2.01	0.41
2:A:459:TYR:HE1	2:A:501:TYR:HB3	1.85	0.41
1:C:99:ARG:NH1	1:C:104:ASP:O	2.43	0.41
2:A:335:PHE:HE1	2:A:397:CYS:HB2	1.84	0.41
2:A:604:ILE:HB	2:A:615:ALA:HB3	2.01	0.41
1:C:83:MET:HB3	1:C:86:LEU:HD11	2.03	0.40
2:A:135:LYS:HD2	2:A:139:PHE:HZ	1.86	0.40
2:A:56:LEU:HB3	2:A:282:LEU:HD11	2.03	0.40
2:A:295:VAL:HG21	2:A:306:LYS:HG2	2.04	0.40
2:A:472:ARG:HG2	2:A:474:ILE:HG23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	C	117/383 (30%)	108 (92%)	9 (8%)	0	100	100
2	A	647/1294 (50%)	587 (91%)	60 (9%)	0	100	100
All	All	764/1677 (46%)	695 (91%)	69 (9%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	96/325 (30%)	94 (98%)	2 (2%)	47	63
2	A	569/1112 (51%)	533 (94%)	36 (6%)	16	43
All	All	665/1437 (46%)	627 (94%)	38 (6%)	20	45

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	12	VAL
1	C	110	TRP
2	A	84	ARG
2	A	102	GLU
2	A	126	VAL
2	A	132	VAL
2	A	156	LYS
2	A	163	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	181	PHE
2	A	182	LEU
2	A	194	ASN
2	A	235	LEU
2	A	239	ILE
2	A	255	LEU
2	A	292	THR
2	A	306	LYS
2	A	307	CYS
2	A	313	THR
2	A	318	ILE
2	A	335	PHE
2	A	367	CYS
2	A	407	VAL
2	A	447	LEU
2	A	464	LYS
2	A	484	LYS
2	A	495	TYR
2	A	501	TYR
2	A	516	VAL
2	A	524	LEU
2	A	530	VAL
2	A	566	LEU
2	A	605	THR
2	A	614	VAL
2	A	626	VAL
2	A	633	ASP
2	A	642	TYR
2	A	652	ARG
2	A	667	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	39	GLN
1	C	77	ASN
2	A	121	GLN
2	A	131	ASN
2	A	154	ASN
2	A	179	GLN
2	A	202	ASN
2	A	340	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	349	ASN
2	A	411	ASN
2	A	415	GLN
2	A	420	GLN
2	A	548	ASN
2	A	613	GLN
2	A	681	GLN
2	A	683	GLN

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 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-35172. These allow visual inspection of the internal detail of the map and identification of artifacts.

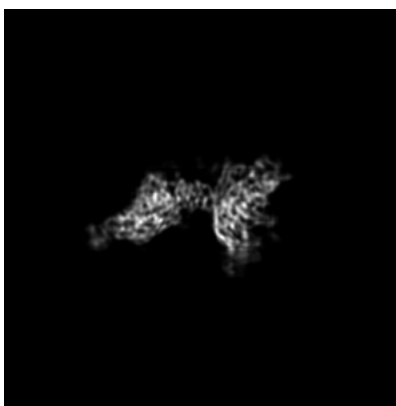
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

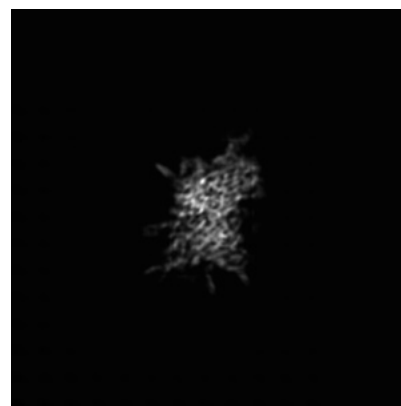
6.1.1 Primary map



X

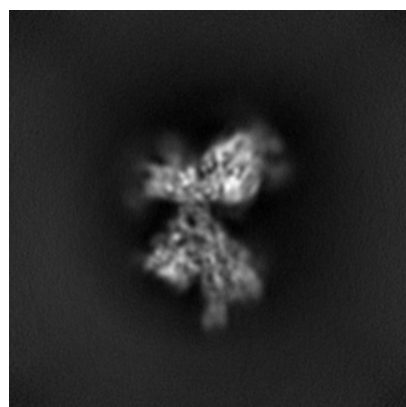


Y

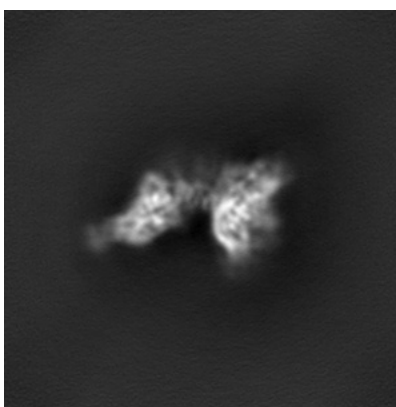


Z

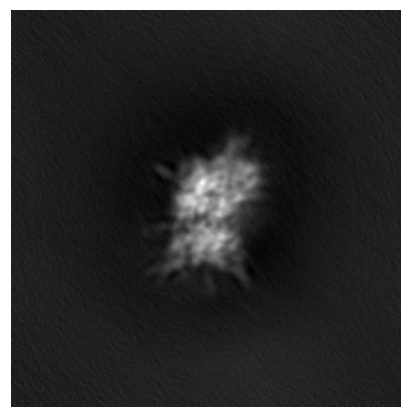
6.1.2 Raw map



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: 128

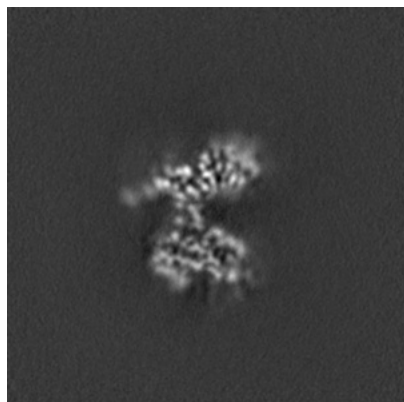


Y Index: 128

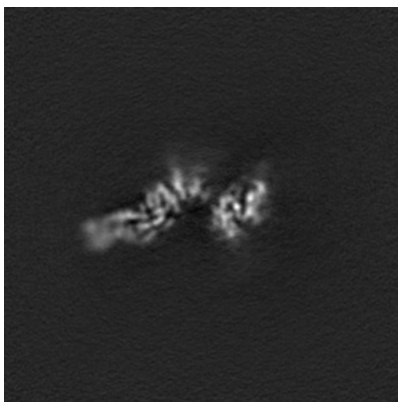


Z Index: 128

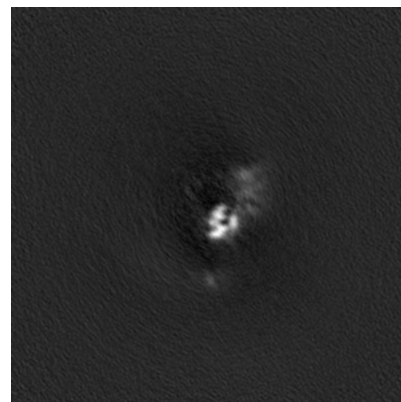
6.2.2 Raw map



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](#)

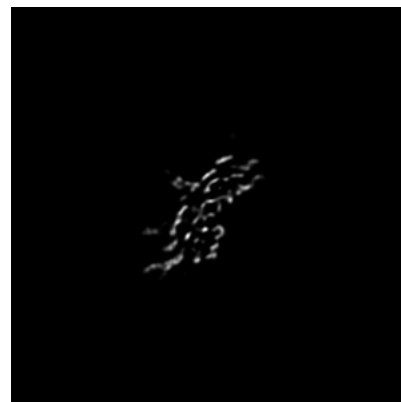
6.3.1 Primary map



X Index: 134

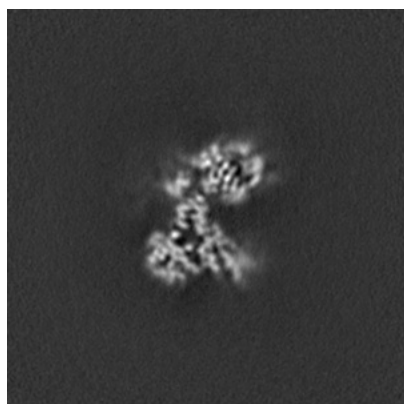


Y Index: 135

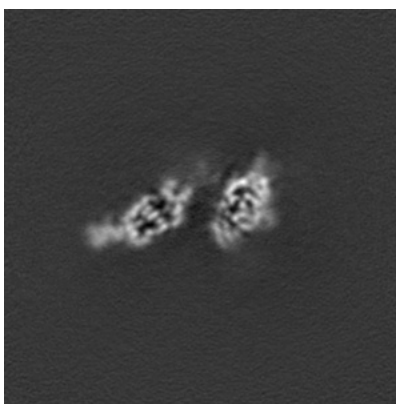


Z Index: 144

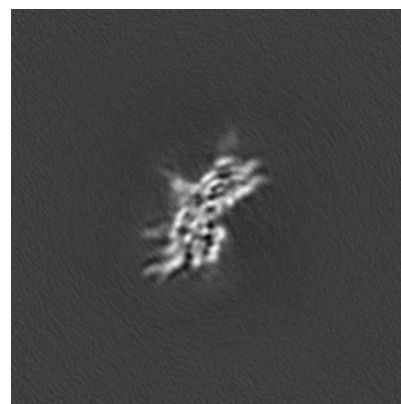
6.3.2 Raw map



X Index: 133



Y Index: 134

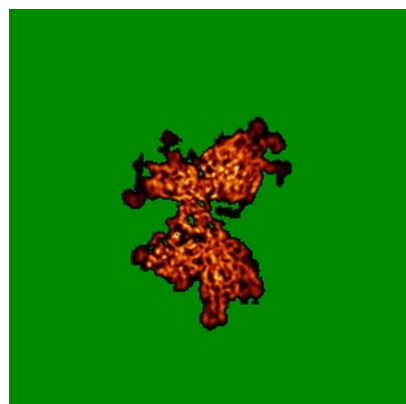


Z Index: 144

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

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

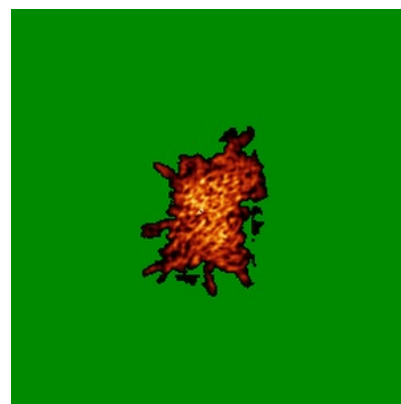
6.4.1 Primary map



X

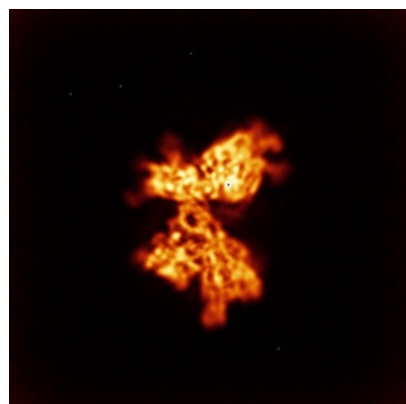


Y

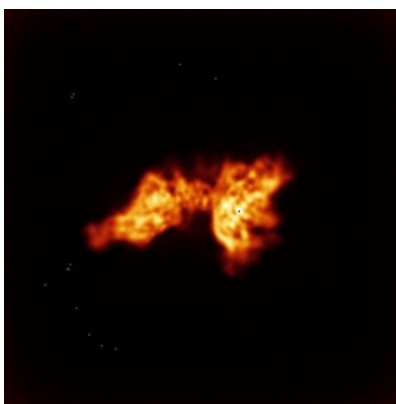


Z

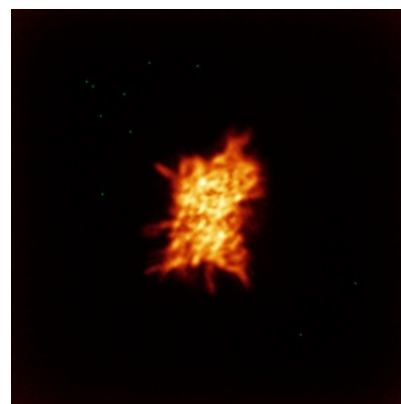
6.4.2 Raw map



X



Y

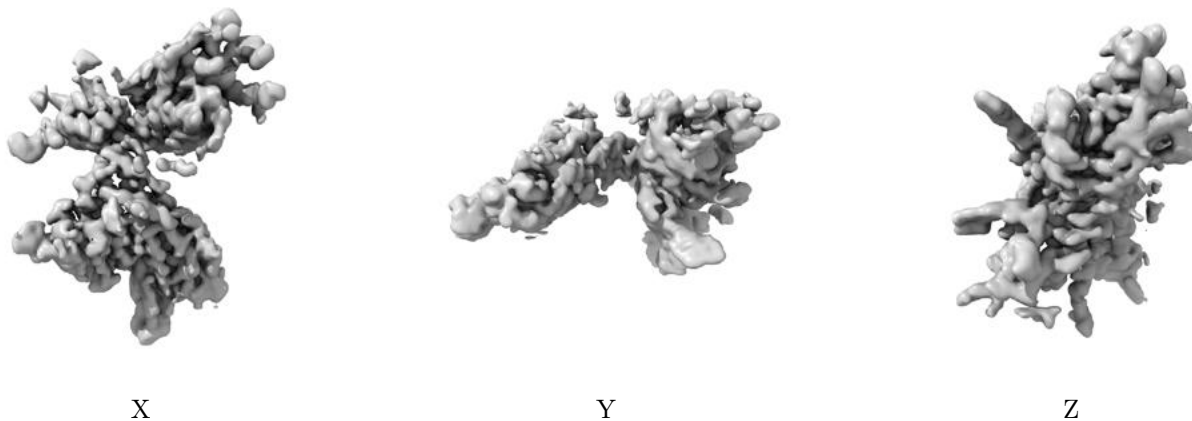


Z

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.

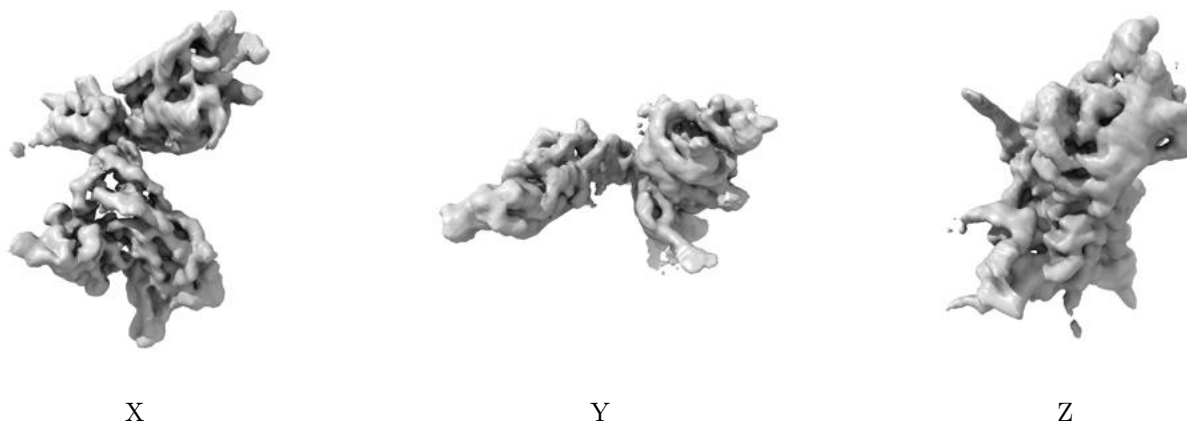
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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.

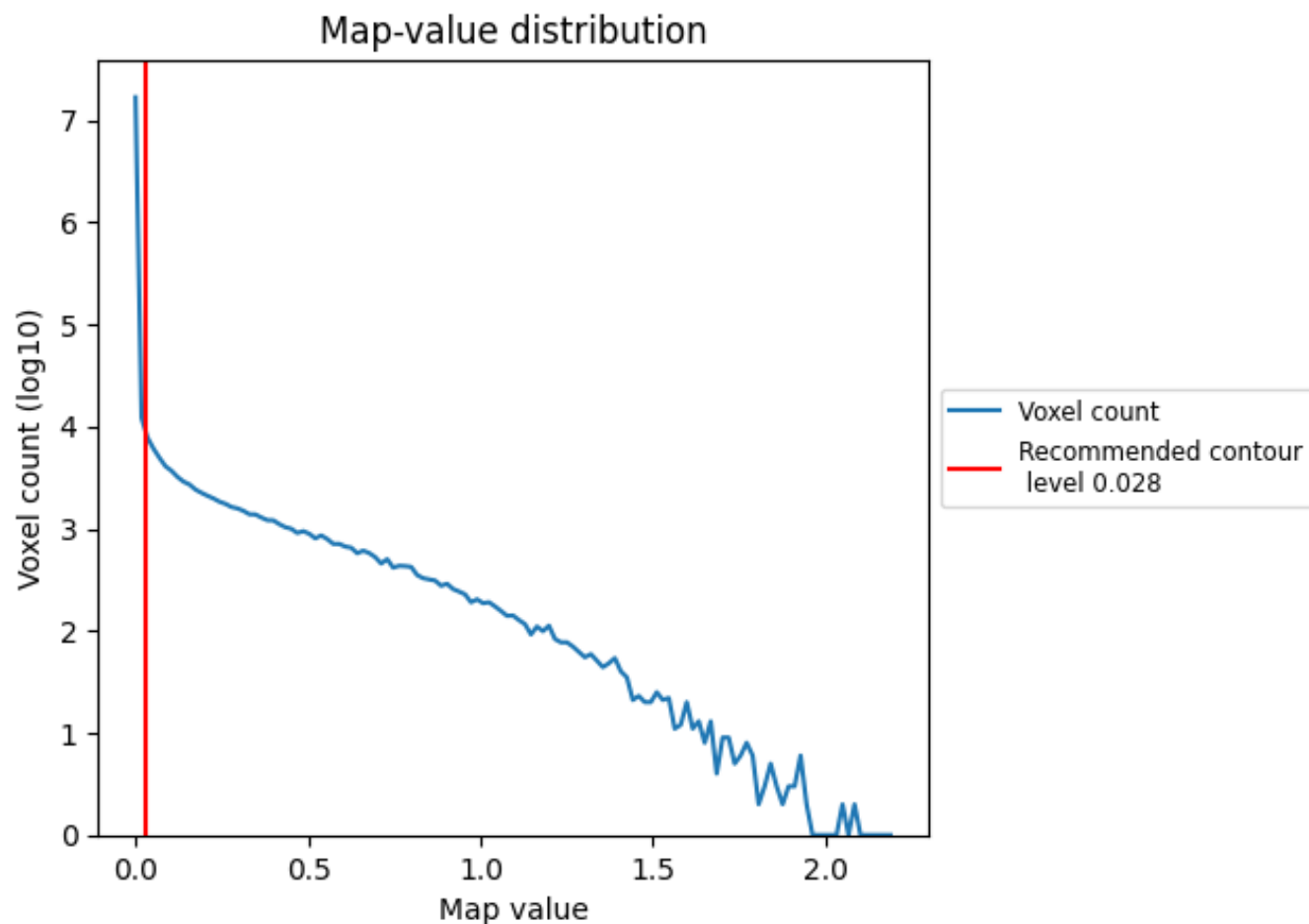
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

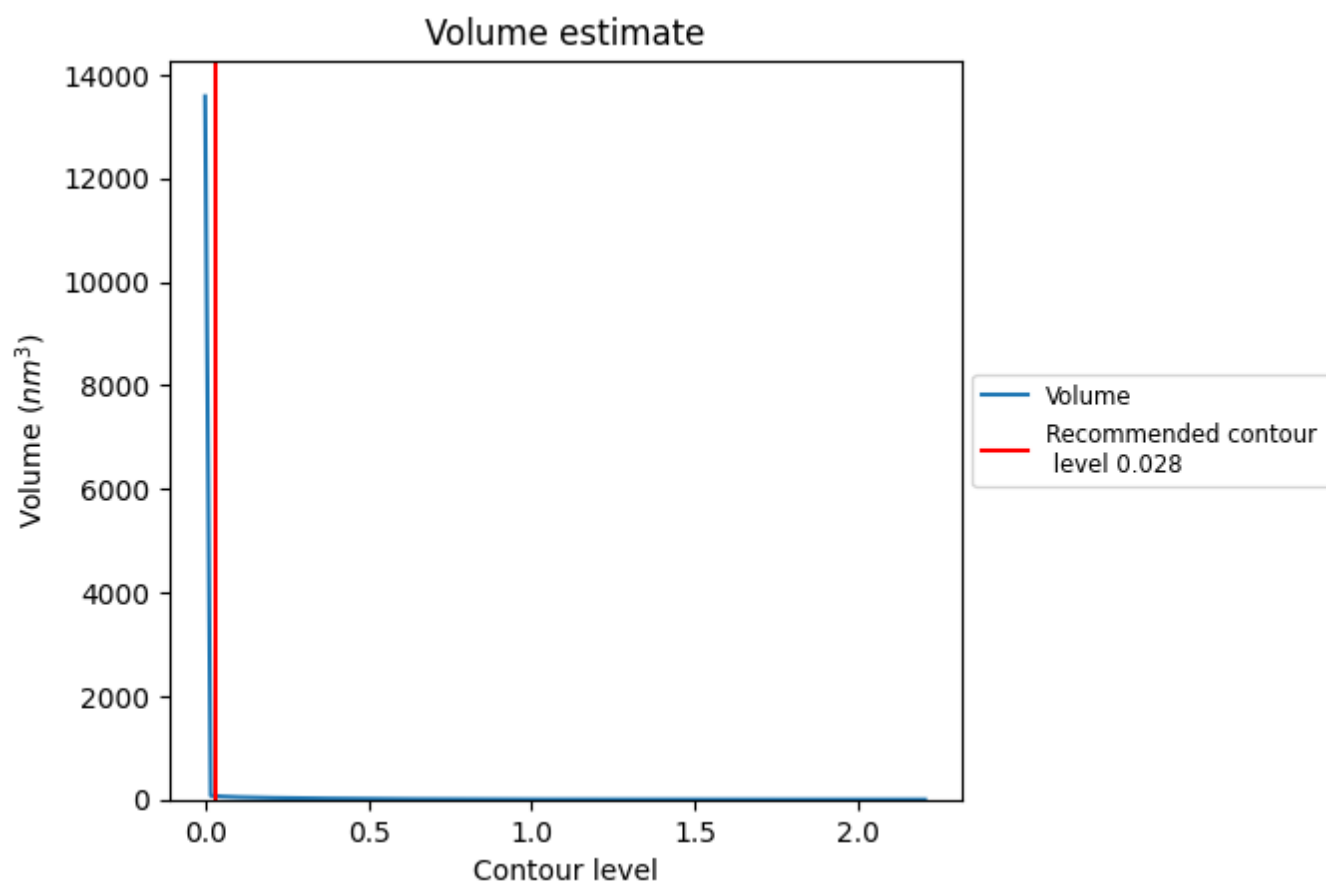
This section contains the results of statistical analysis of the map.

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.

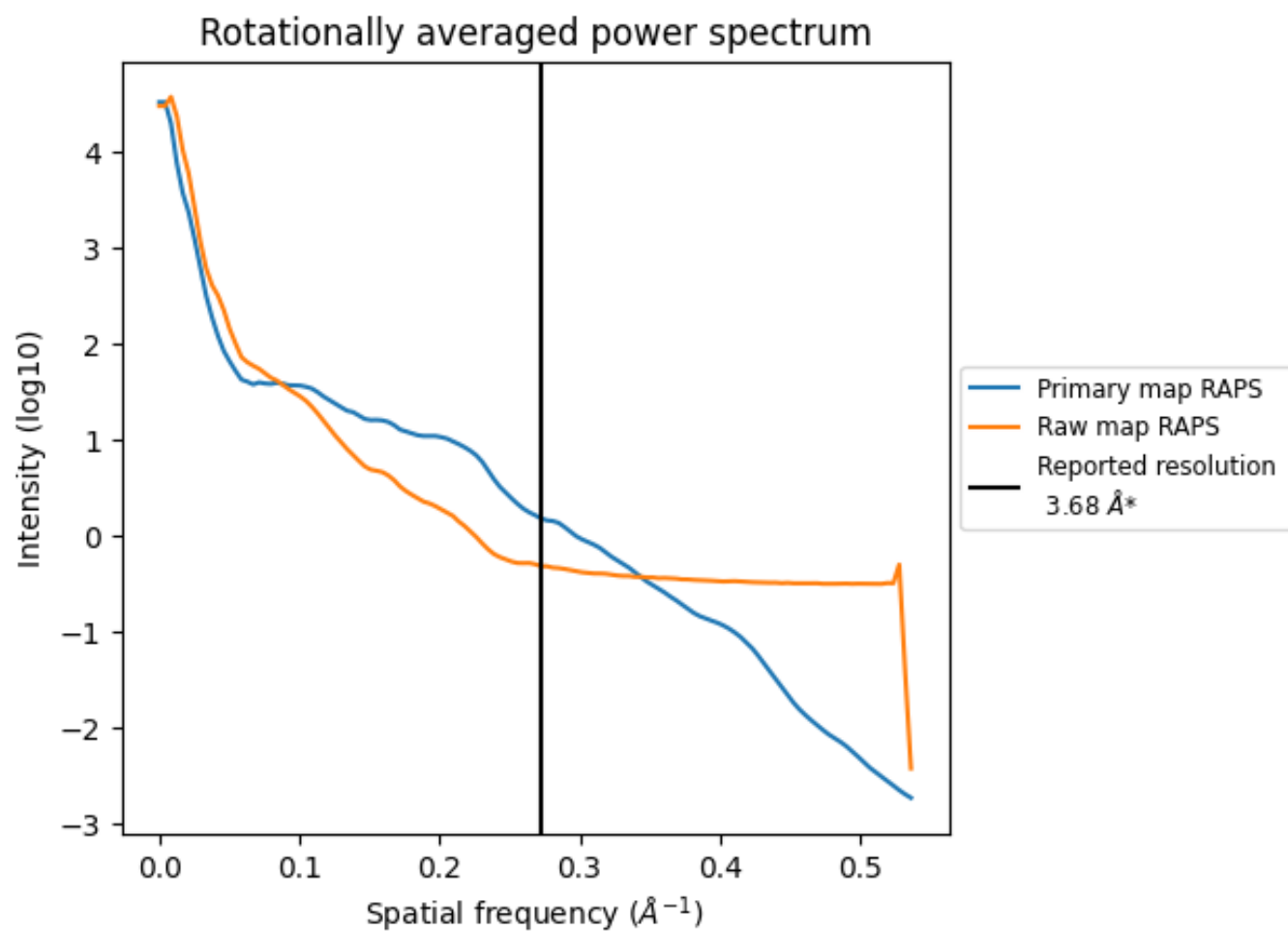
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 68 nm³; this corresponds to an approximate mass of 61 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 ⓘ

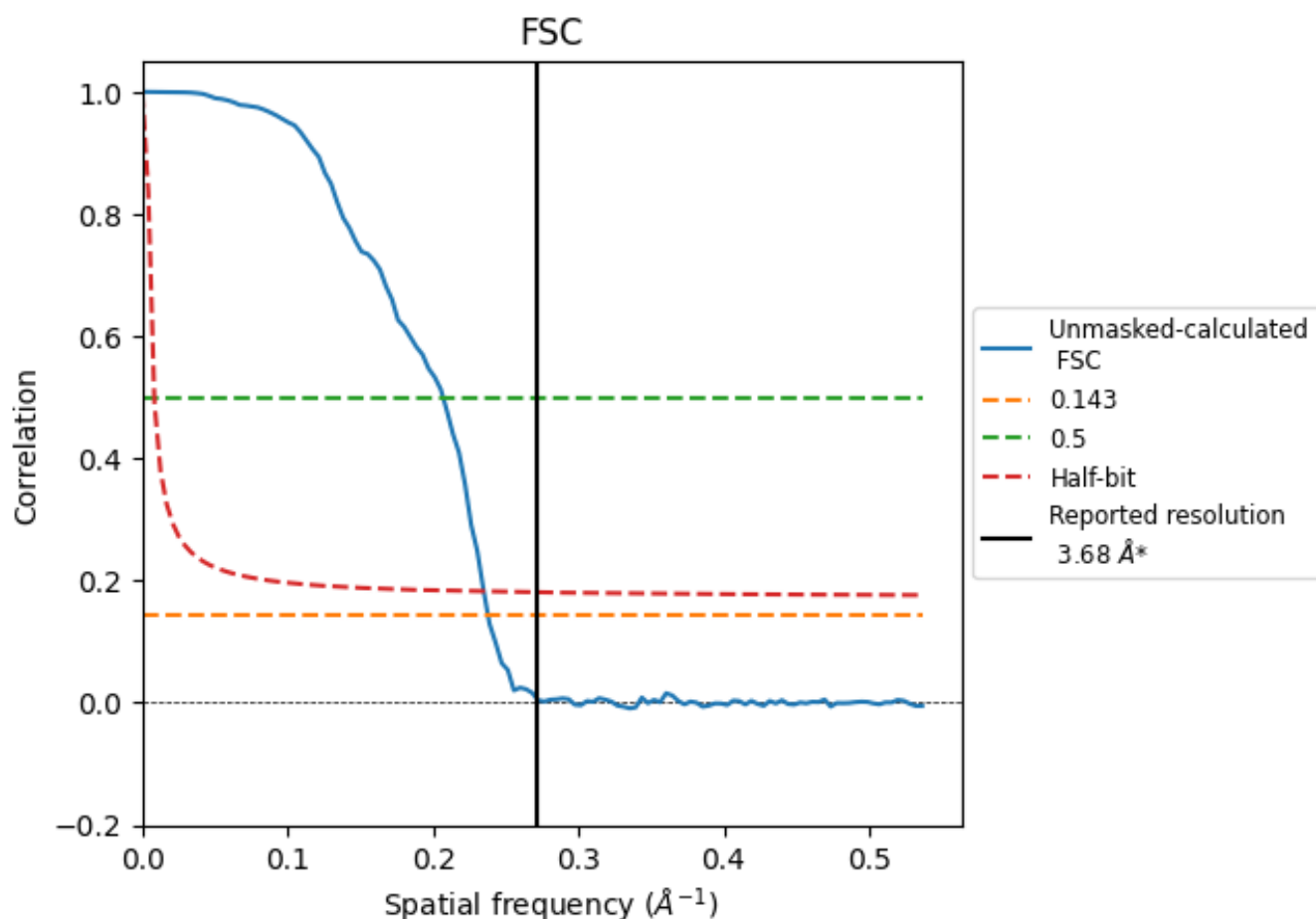


*Reported resolution corresponds to spatial frequency of 0.272 Å⁻¹

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 0.272 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.68	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.20	4.83	4.26

*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 4.20 differs from the reported value 3.68 by more than 10 %

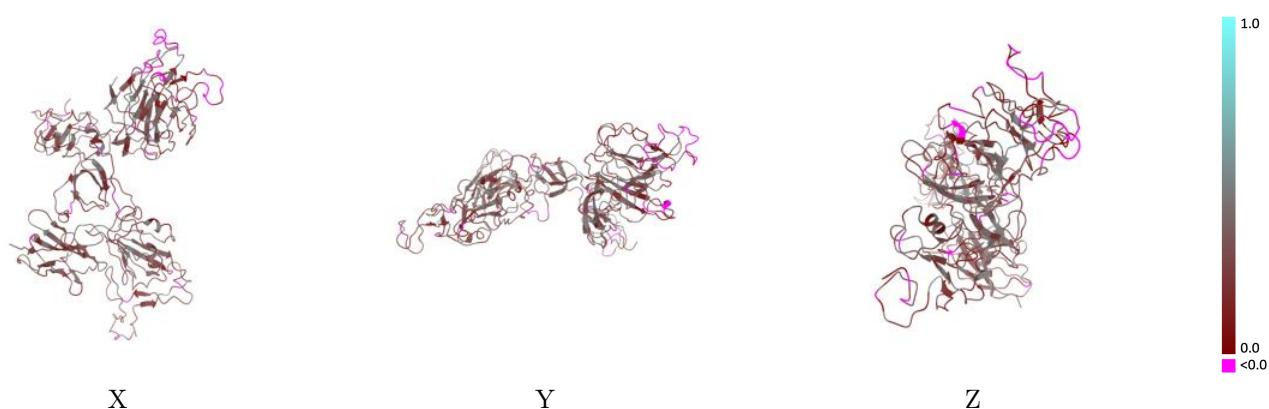
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-35172 and PDB model 8I4G. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

This section was not generated.

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

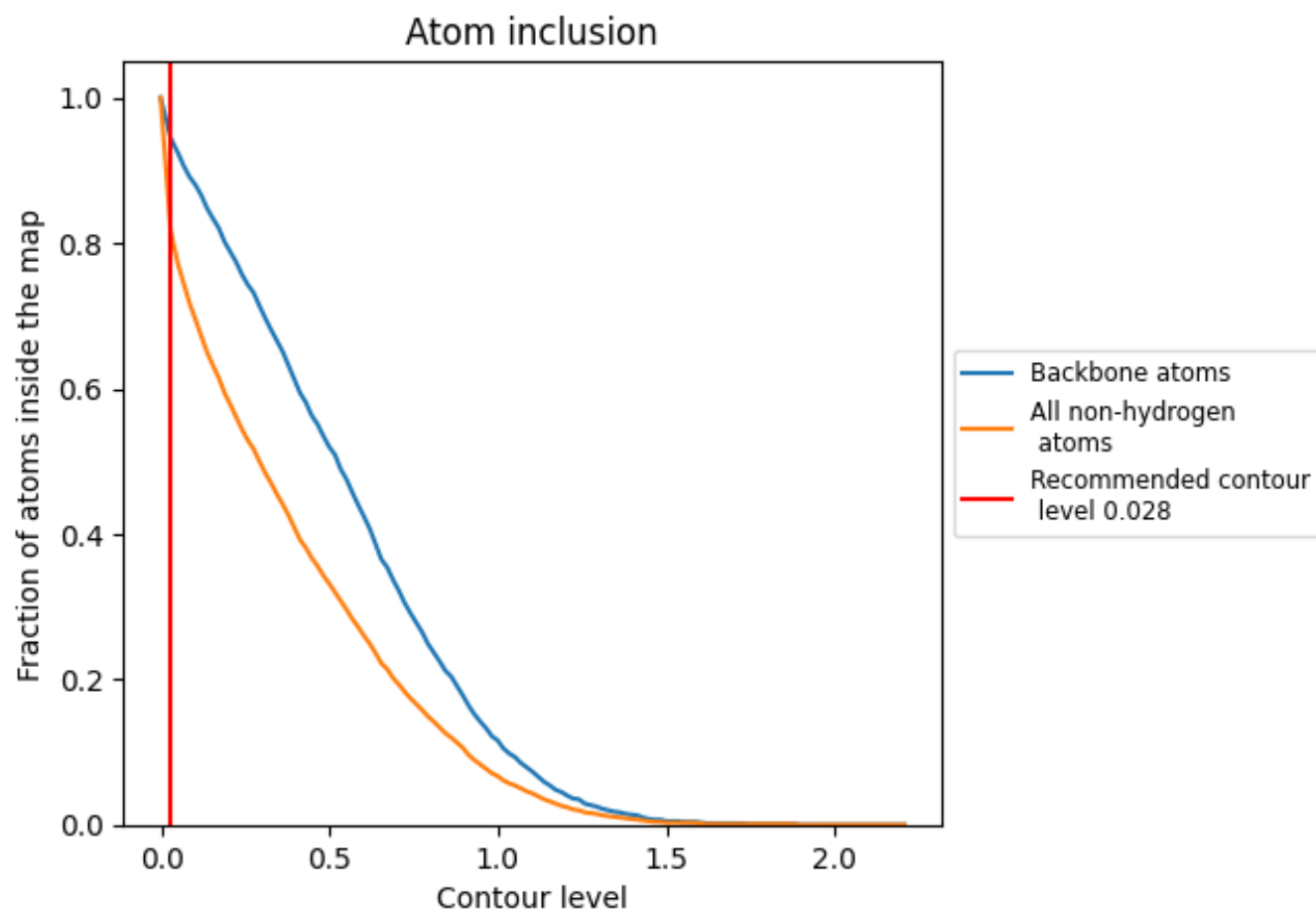


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 94% 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	0.8180	0.2660
A	0.8120	0.2600
C	0.8550	0.2990

