



Full wwPDB EM Validation Report ⓘ

Aug 8, 2024 – 12:12 PM JST

PDB ID : 8KEJ
EMDB ID : EMD-37160
Title : Monomer state of SARS-CoV-2 XBB Variant Spike protein trimer complexed with antibody PW5-5
Authors : Sun, L.; Mao, Q.; Wang, Y.
Deposited on : 2023-08-11
Resolution : 3.73 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:

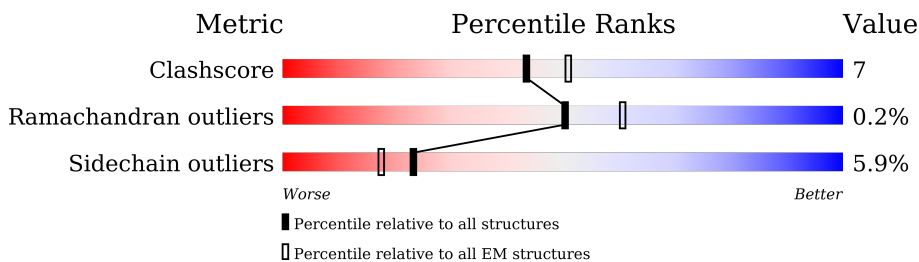
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

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 3.73 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	H	450	
2	L	216	
3	A	1295	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8377 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 PW5-5 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	H	218	1638	1038	268	324	8	0	0

- Molecule 2 is a protein called PW5-5 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	L	213	1653	1037	283	328	5	0	0

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	644	5086	3257	843	964	22	0	0

There are 159 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP P0DTC2
A	-5	PRO	-	insertion	UNP P0DTC2
A	-4	MET	-	insertion	UNP P0DTC2
A	-3	GLY	-	insertion	UNP P0DTC2
A	-2	SER	-	insertion	UNP P0DTC2
A	-1	LEU	-	insertion	UNP P0DTC2
A	0	GLN	-	insertion	UNP P0DTC2
A	1	PRO	-	insertion	UNP P0DTC2
A	2	LEU	-	insertion	UNP P0DTC2
A	3	ALA	-	insertion	UNP P0DTC2
A	4	THR	-	insertion	UNP P0DTC2
A	5	LEU	-	insertion	UNP P0DTC2
A	6	TYR	-	insertion	UNP P0DTC2
A	7	LEU	-	insertion	UNP P0DTC2
A	8	LEU	-	insertion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLY	-	insertion	UNP P0DTC2
A	10	MET	-	insertion	UNP P0DTC2
A	11	LEU	-	insertion	UNP P0DTC2
A	12	VAL	-	insertion	UNP P0DTC2
A	13	ALA	-	insertion	UNP P0DTC2
A	14	SER	-	insertion	UNP P0DTC2
A	15	VAL	-	insertion	UNP P0DTC2
A	16	LEU	-	insertion	UNP P0DTC2
A	17	ALA	-	insertion	UNP P0DTC2
A	18	GLN	-	insertion	UNP P0DTC2
A	19	CYS	-	insertion	UNP P0DTC2
A	20	VAL	-	insertion	UNP P0DTC2
A	21	ASN	-	insertion	UNP P0DTC2
A	22	LEU	-	insertion	UNP P0DTC2
A	23	ILE	-	insertion	UNP P0DTC2
A	24	THR	-	insertion	UNP P0DTC2
A	25	ARG	-	insertion	UNP P0DTC2
A	26	THR	-	insertion	UNP P0DTC2
A	27	GLN	-	insertion	UNP P0DTC2
A	28	SER	-	insertion	UNP P0DTC2
A	143	ASP	GLY	variant	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	146	GLN	HIS	variant	UNP P0DTC2
A	183	GLU	GLN	variant	UNP P0DTC2
A	213	GLU	VAL	variant	UNP P0DTC2
A	339	HIS	GLY	variant	UNP P0DTC2
A	346	THR	ARG	variant	UNP P0DTC2
A	368	ILE	LEU	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	445	PRO	VAL	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	460	LYS	ASN	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	486	SER	PHE	variant	UNP P0DTC2
A	490	SER	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	PHE	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	SER	-	expression tag	UNP P0DTC2
A	1239	GLY	-	expression tag	UNP P0DTC2
A	1240	LEU	-	expression tag	UNP P0DTC2
A	1241	GLU	-	expression tag	UNP P0DTC2
A	1242	VAL	-	expression tag	UNP P0DTC2
A	1243	LEU	-	expression tag	UNP P0DTC2
A	1244	PHE	-	expression tag	UNP P0DTC2
A	1245	GLN	-	expression tag	UNP P0DTC2
A	1246	GLY	-	expression tag	UNP P0DTC2
A	1247	PRO	-	expression tag	UNP P0DTC2
A	1248	GLY	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	TRP	-	expression tag	UNP P0DTC2
A	1251	SER	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	PRO	-	expression tag	UNP P0DTC2
A	1254	GLN	-	expression tag	UNP P0DTC2
A	1255	PHE	-	expression tag	UNP P0DTC2
A	1256	GLU	-	expression tag	UNP P0DTC2
A	1257	LYS	-	expression tag	UNP P0DTC2
A	1258	GLY	-	expression tag	UNP P0DTC2
A	1259	GLY	-	expression tag	UNP P0DTC2
A	1260	GLY	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	GLY	-	expression tag	UNP P0DTC2
A	1263	GLY	-	expression tag	UNP P0DTC2
A	1264	GLY	-	expression tag	UNP P0DTC2
A	1265	SER	-	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	ALA	-	expression tag	UNP P0DTC2
A	1270	TRP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	HIS	-	expression tag	UNP P0DTC2
A	1273	PRO	-	expression tag	UNP P0DTC2
A	1274	GLN	-	expression tag	UNP P0DTC2
A	1275	PHE	-	expression tag	UNP P0DTC2
A	1276	GLU	-	expression tag	UNP P0DTC2
A	1277	LYS	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	GLY	-	expression tag	UNP P0DTC2
A	1280	SER	-	expression tag	UNP P0DTC2
A	1281	HIS	-	expression tag	UNP P0DTC2
A	1282	HIS	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	HIS	-	expression tag	UNP P0DTC2
A	1285	HIS	-	expression tag	UNP P0DTC2
A	1286	HIS	-	expression tag	UNP P0DTC2
A	1287	HIS	-	expression tag	UNP P0DTC2
A	1288	HIS	-	expression tag	UNP P0DTC2

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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	166548	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)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.142	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.1	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	H	0.25	0/1679	0.42	0/2291
2	L	0.27	0/1691	0.45	0/2298
3	A	0.26	0/5218	0.42	0/7100
All	All	0.26	0/8588	0.43	0/11689

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	H	1638	0	1601	23	0
2	L	1653	0	1611	23	0
3	A	5086	0	4906	76	0
All	All	8377	0	8118	116	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 (116) 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:L:149:GLN:HB2	2:L:197:GLU:HB3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:330:PRO:HB2	3:A:579:PRO:HB2	1.76	0.68
3:A:329:PHE:HB3	3:A:528:LYS:HB3	1.77	0.67
2:L:33:LEU:HB3	2:L:51:ALA:HB2	1.78	0.65
1:H:126:PRO:HB3	1:H:152:TYR:HB3	1.79	0.65
2:L:54:ARG:NH1	2:L:62:PHE:O	2.31	0.64
3:A:53:GLN:NE2	3:A:274:THR:OG1	2.31	0.63
1:H:107:ASN:HD22	2:L:91:ARG:HH11	1.46	0.63
3:A:87:PHE:H	3:A:237:ARG:HA	1.66	0.61
3:A:131:VAL:HG11	3:A:231:ILE:HG12	1.82	0.60
3:A:391:CYS:HA	3:A:525:CYS:HA	1.82	0.60
1:H:124:LYS:HZ1	1:H:151:ASP:HB3	1.65	0.60
3:A:361:CYS:SG	3:A:362:VAL:N	2.74	0.60
1:H:67:ARG:NH2	1:H:85:SER:O	2.34	0.60
3:A:191:GLU:HG2	3:A:223:LEU:HD21	1.85	0.59
3:A:100:ASN:HB3	3:A:103:ARG:HE	1.68	0.58
2:L:18:ARG:HH12	2:L:20:THR:HG23	1.68	0.58
3:A:109:THR:HG23	3:A:110:THR:HG23	1.85	0.57
3:A:292:ALA:HB1	3:A:320:VAL:HG13	1.85	0.57
1:H:40:ALA:HB3	1:H:43:GLN:HB2	1.87	0.57
3:A:555:SER:HB3	3:A:586:ASP:HB2	1.87	0.57
1:H:128:VAL:HG22	1:H:149:VAL:HG13	1.86	0.57
3:A:244:LEU:HG	3:A:246:ARG:HG2	1.88	0.56
3:A:656:VAL:HG12	3:A:658:ASN:H	1.71	0.55
3:A:358:ILE:HB	3:A:395:VAL:HG13	1.89	0.55
2:L:94:TRP:HB3	2:L:95:PRO:HD3	1.88	0.54
2:L:107:GLU:OE1	2:L:175:TYR:OH	2.25	0.54
2:L:118:PHE:HB2	2:L:137:LEU:HB3	1.88	0.54
3:A:291:CYS:H	3:A:297:SER:HB3	1.73	0.54
2:L:122:PRO:HD3	2:L:134:VAL:HG22	1.90	0.54
2:L:138:LEU:HB2	2:L:177:LEU:HB3	1.89	0.54
3:A:476:GLY:H	3:A:487:ASN:HD21	1.57	0.53
3:A:381:GLY:HA3	3:A:430:THR:HA	1.90	0.53
2:L:140:ASN:HA	2:L:174:THR:HB	1.91	0.52
3:A:336:CYS:N	3:A:361:CYS:SG	2.83	0.52
3:A:430:THR:OG1	3:A:515:PHE:O	2.28	0.52
3:A:295:PRO:HB3	3:A:610:VAL:HG13	1.91	0.51
1:H:150:LYS:NZ	1:H:151:ASP:OD1	2.43	0.51
3:A:187:LYS:HB2	3:A:210:ILE:HD11	1.92	0.50
3:A:194:PHE:HE1	3:A:203:ILE:HG23	1.77	0.50
3:A:613:GLN:HA	3:A:648:GLY:HA3	1.92	0.50
3:A:323:THR:HB	3:A:539:VAL:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:188:TYR:O	2:L:194:TYR:OH	2.30	0.50
3:A:271:GLN:OE1	3:A:273:ARG:NH2	2.45	0.49
2:L:14:SER:HB3	2:L:109:LYS:HE2	1.93	0.49
3:A:424:LYS:NZ	3:A:461:LEU:O	2.38	0.49
3:A:599:THR:HG22	3:A:601:GLY:H	1.76	0.49
3:A:120:ILE:HG23	3:A:129:ILE:HG12	1.95	0.49
2:L:34:ALA:N	2:L:89:GLN:O	2.46	0.49
3:A:457:ARG:NH2	3:A:459:SER:OG	2.46	0.48
3:A:310:LYS:HB3	3:A:664:ILE:HG12	1.94	0.48
3:A:357:ARG:HB2	3:A:394:ASN:HD21	1.79	0.48
3:A:661:GLU:O	3:A:695:TYR:OH	2.30	0.48
3:A:446:SER:O	3:A:498:ARG:NH1	2.47	0.47
1:H:102:PHE:HB2	3:A:464:PHE:HB2	1.96	0.47
3:A:435:ALA:HB2	3:A:510:VAL:HG13	1.96	0.47
3:A:474:GLN:HE21	3:A:478:LYS:H	1.60	0.47
1:H:100:LEU:HG	1:H:110:ASP:HB2	1.96	0.47
2:L:149:GLN:NE2	2:L:197:GLU:O	2.47	0.47
3:A:388:ASN:HB3	3:A:527:PRO:HD2	1.96	0.47
3:A:333:THR:OG1	3:A:334:ASN:N	2.47	0.46
3:A:204:TYR:HB3	3:A:223:LEU:HB3	1.98	0.46
3:A:97:GLU:O	3:A:188:ASN:ND2	2.44	0.46
3:A:276:LEU:HB3	3:A:289:VAL:HB	1.97	0.46
3:A:595:VAL:HG22	3:A:612:TYR:HD2	1.80	0.46
3:A:457:ARG:NH1	3:A:467:ASP:OD2	2.48	0.46
3:A:124:ALA:O	3:A:126:ASN:ND2	2.49	0.45
3:A:403:ARG:HH21	3:A:495:TYR:HE2	1.64	0.45
3:A:531:THR:HG22	3:A:532:ASN:H	1.81	0.45
2:L:142:TYR:CD2	2:L:143:PRO:HD2	2.52	0.45
1:H:97:ALA:HB1	1:H:109:PHE:HB3	1.98	0.45
1:H:174:PRO:HD3	2:L:166:THR:HG22	1.98	0.45
2:L:147:LYS:H	2:L:147:LYS:HG3	1.43	0.45
1:H:101:PHE:CE1	1:H:107:ASN:HB2	2.52	0.44
2:L:32:TYR:OH	3:A:428:ASP:OD1	2.28	0.44
3:A:541:PHE:CE2	3:A:587:ILE:HG21	2.53	0.44
3:A:144:VAL:HG23	3:A:245:HIS:HB2	1.98	0.44
3:A:294:ASP:HB2	3:A:297:SER:HB2	1.99	0.44
3:A:676:THR:HA	3:A:690:GLN:HG2	1.98	0.44
3:A:320:VAL:HG12	3:A:322:PRO:HG3	2.00	0.44
3:A:206:LYS:NZ	3:A:222:ALA:O	2.46	0.44
2:L:35:TRP:N	2:L:48:ILE:O	2.49	0.44
3:A:671:CYS:SG	3:A:697:MET:HB3	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:175:ALA:HA	1:H:185:LEU:HB3	2.00	0.43
1:H:153:PHE:HB3	1:H:154:PRO:HD3	1.99	0.43
1:H:39:GLN:NE2	1:H:43:GLN:O	2.50	0.43
3:A:328:ARG:HB3	3:A:530:SER:HA	1.99	0.43
1:H:48:MET:HG2	2:L:98:PHE:N	2.34	0.43
1:H:35:TYR:CZ	1:H:50:VAL:HB	2.54	0.43
1:H:175:ALA:HB1	1:H:183:TYR:HB3	2.00	0.43
3:A:78:LYS:HD2	3:A:246:ARG:HG3	2.01	0.42
3:A:341:VAL:HG11	3:A:397:ALA:HB1	2.00	0.42
3:A:118:LEU:HD13	3:A:131:VAL:HG22	2.01	0.42
3:A:119:LEU:HD11	3:A:130:LYS:HD2	2.01	0.42
3:A:124:ALA:O	3:A:125:THR:HG22	2.19	0.42
3:A:379:CYS:HA	3:A:432:CYS:HA	2.02	0.42
2:L:14:SER:HB3	2:L:109:LYS:HB3	2.00	0.42
1:H:155:GLU:N	1:H:156:PRO:HD3	2.34	0.42
3:A:328:ARG:HD2	3:A:529:LYS:O	2.20	0.42
3:A:549:THR:OG1	3:A:550:GLY:N	2.53	0.42
3:A:213:GLU:HG3	3:A:214:ARG:HG2	2.02	0.42
3:A:65:TRP:HE1	3:A:264:ALA:HB1	1.85	0.41
1:H:175:ALA:HB2	1:H:185:LEU:HD23	2.02	0.41
3:A:183:GLU:HG3	3:A:184:GLY:H	1.84	0.41
3:A:587:ILE:H	3:A:587:ILE:HG12	1.74	0.41
3:A:176:LEU:HD11	3:A:203:ILE:HG21	2.03	0.41
3:A:520:ALA:HB1	3:A:521:PRO:HD2	2.03	0.41
3:A:444:LYS:HE3	3:A:445:PRO:HD2	2.03	0.41
1:H:31:ASP:HB3	1:H:102:PHE:CD1	2.56	0.41
3:A:197:ILE:HG22	3:A:199:GLY:H	1.86	0.41
1:H:107:ASN:HA	2:L:91:ARG:HD2	2.02	0.41
3:A:66:PHE:HD1	3:A:66:PHE:HA	1.80	0.40
3:A:317:ASN:H	3:A:319:ARG:CZ	2.33	0.40
3:A:70:HIS:CE1	3:A:72:SER:HB2	2.57	0.40
3:A:119:LEU:HG	3:A:130:LYS:HB3	2.04	0.40
1:H:6:GLN:HG2	1:H:7:SER:H	1.86	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	H	216/450 (48%)	205 (95%)	11 (5%)	0	100	100
2	L	211/216 (98%)	195 (92%)	14 (7%)	2 (1%)	17	53
3	A	638/1295 (49%)	581 (91%)	57 (9%)	0	100	100
All	All	1065/1961 (54%)	981 (92%)	82 (8%)	2 (0%)	50	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	143	PRO
2	L	144	ARG

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	H	186/401 (46%)	178 (96%)	8 (4%)	29	58
2	L	186/188 (99%)	173 (93%)	13 (7%)	15	46
3	A	567/1118 (51%)	533 (94%)	34 (6%)	19	51
All	All	939/1707 (55%)	884 (94%)	55 (6%)	23	51

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	33	TYR

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Mol	Chain	Res	Type
1	H	48	MET
1	H	51	ILE
1	H	69	THR
1	H	91	THR
1	H	103	ILE
1	H	124	LYS
1	H	158	THR
2	L	3	VAL
2	L	10	THR
2	L	18	ARG
2	L	21	LEU
2	L	24	ARG
2	L	42	GLN
2	L	47	LEU
2	L	90	HIS
2	L	142	TYR
2	L	144	ARG
2	L	145	GLU
2	L	147	LYS
2	L	149	GLN
3	A	119	LEU
3	A	125	THR
3	A	136	PHE
3	A	173	GLN
3	A	208	THR
3	A	226	LEU
3	A	281	GLU
3	A	307	THR
3	A	318	PHE
3	A	319	ARG
3	A	320	VAL
3	A	321	GLN
3	A	323	THR
3	A	328	ARG
3	A	335	LEU
3	A	386	LYS
3	A	387	LEU
3	A	395	VAL
3	A	414	GLN
3	A	440	LYS
3	A	444	LYS
3	A	450	ASN

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Mol	Chain	Res	Type
3	A	457	ARG
3	A	460	LYS
3	A	495	TYR
3	A	517	LEU
3	A	524	VAL
3	A	531	THR
3	A	585	LEU
3	A	587	ILE
3	A	588	THR
3	A	592	PHE
3	A	596	SER
3	A	677	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	107	ASN
1	H	114	GLN
2	L	38	GLN
2	L	102	GLN
2	L	149	GLN
2	L	168	GLN
3	A	53	GLN
3	A	126	ASN
3	A	173	GLN
3	A	409	GLN
3	A	414	GLN
3	A	450	ASN
3	A	474	GLN
3	A	487	ASN
3	A	613	GLN
3	A	644	GLN
3	A	675	GLN
3	A	677	GLN
3	A	690	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

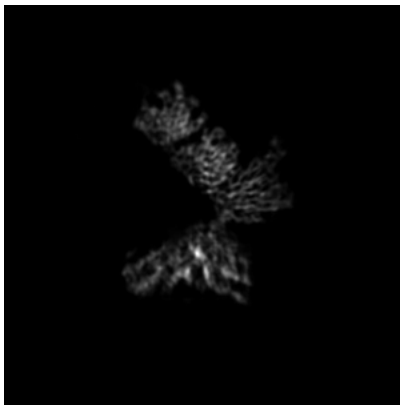
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37160. These allow visual inspection of the internal detail of the map and identification of artifacts.

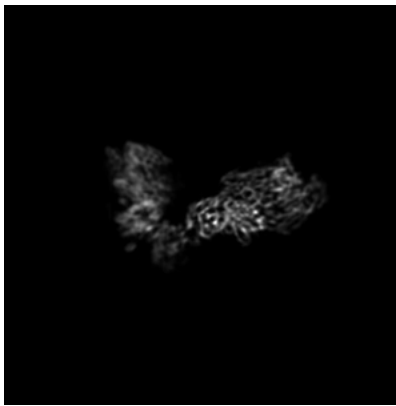
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

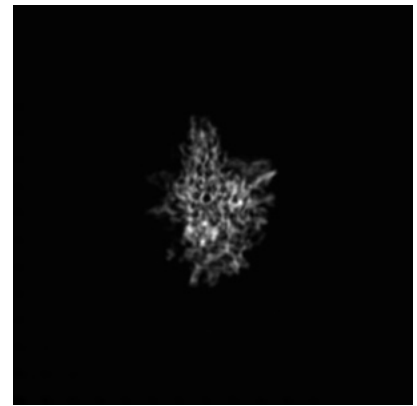
6.1.1 Primary map



X

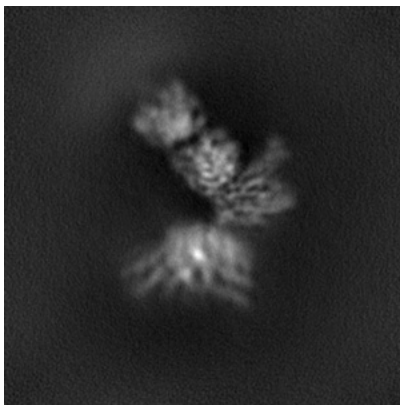


Y

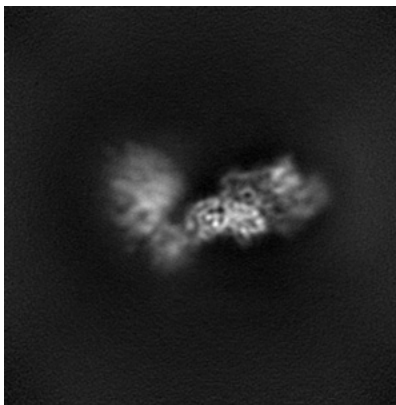


Z

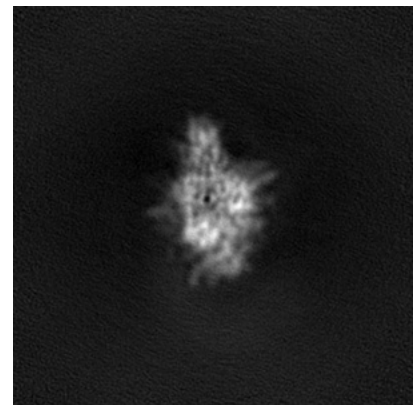
6.1.2 Raw map



X



Y

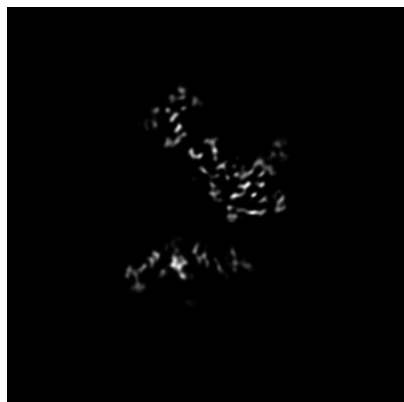


Z

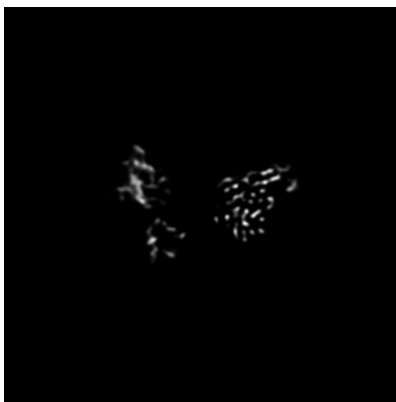
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

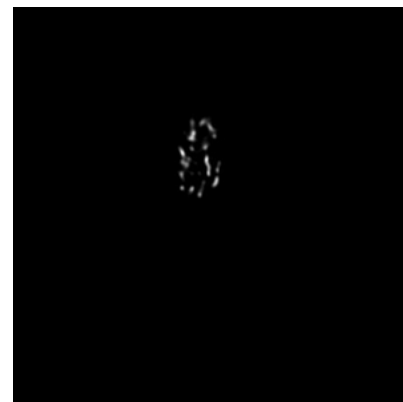
6.2.1 Primary map



X Index: 128

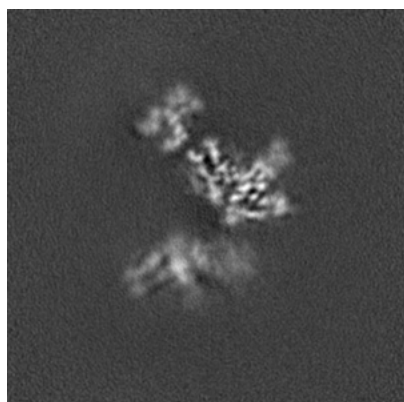


Y Index: 128

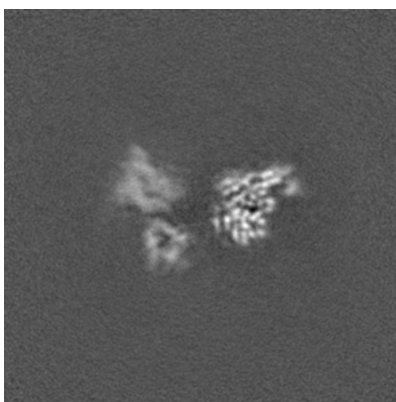


Z Index: 128

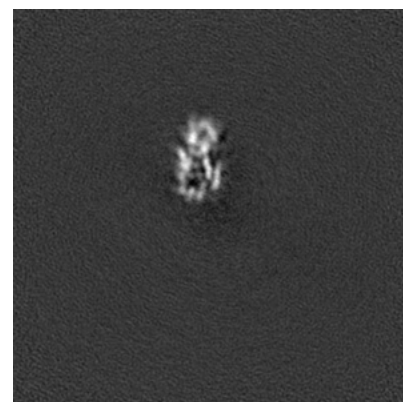
6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

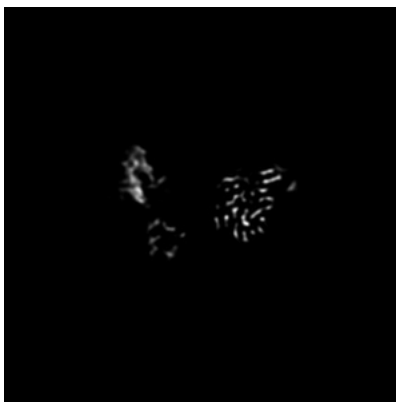
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 121

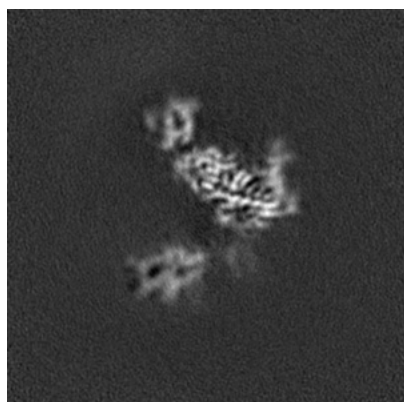


Y Index: 129

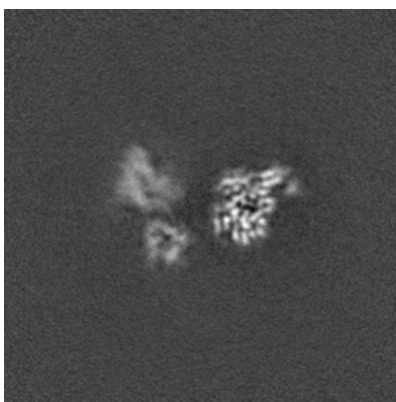


Z Index: 84

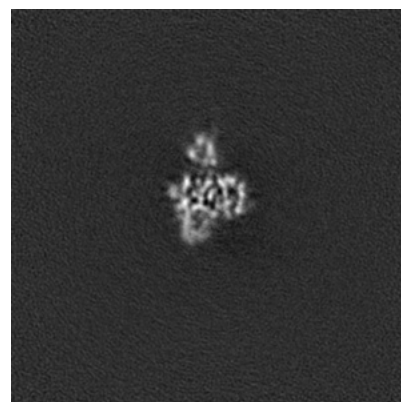
6.3.2 Raw map



X Index: 121



Y Index: 129



Z Index: 153

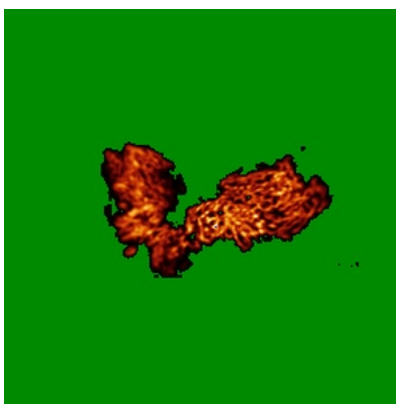
The images above show the largest variance slices of the map in three orthogonal directions.

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

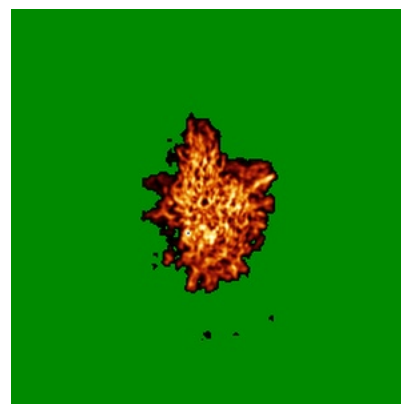
6.4.1 Primary map



X

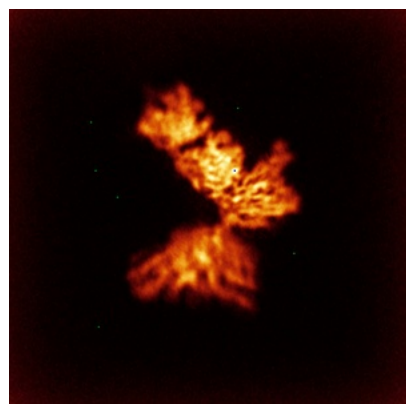


Y

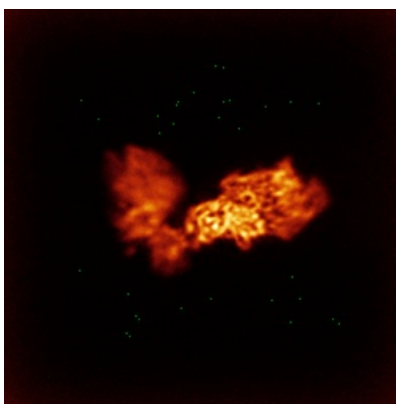


Z

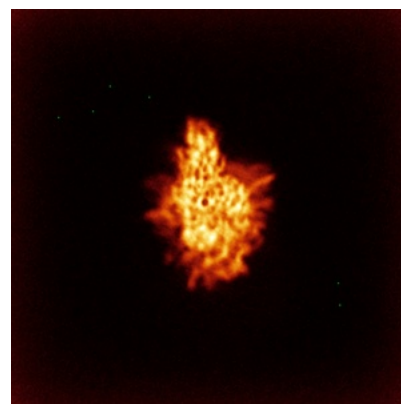
6.4.2 Raw map



X



Y

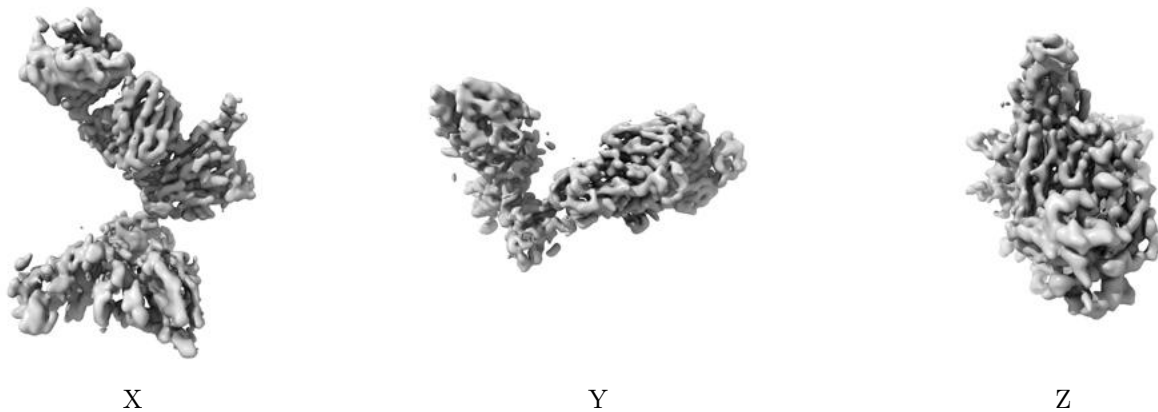


Z

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.

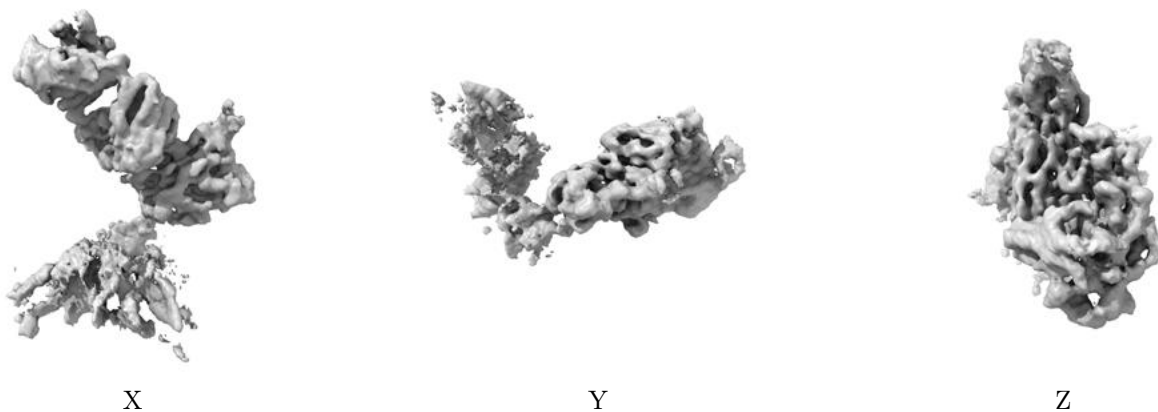
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

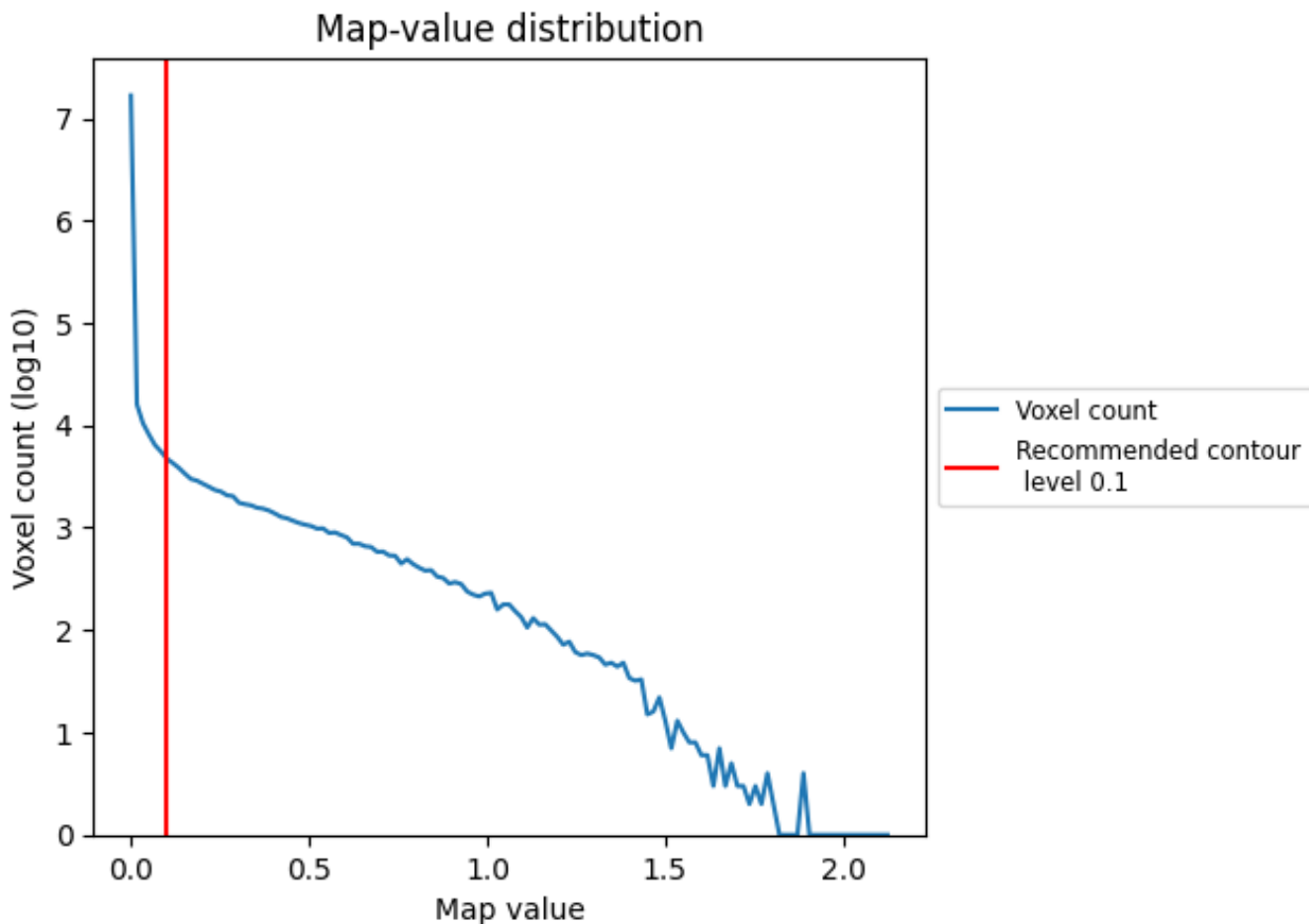
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

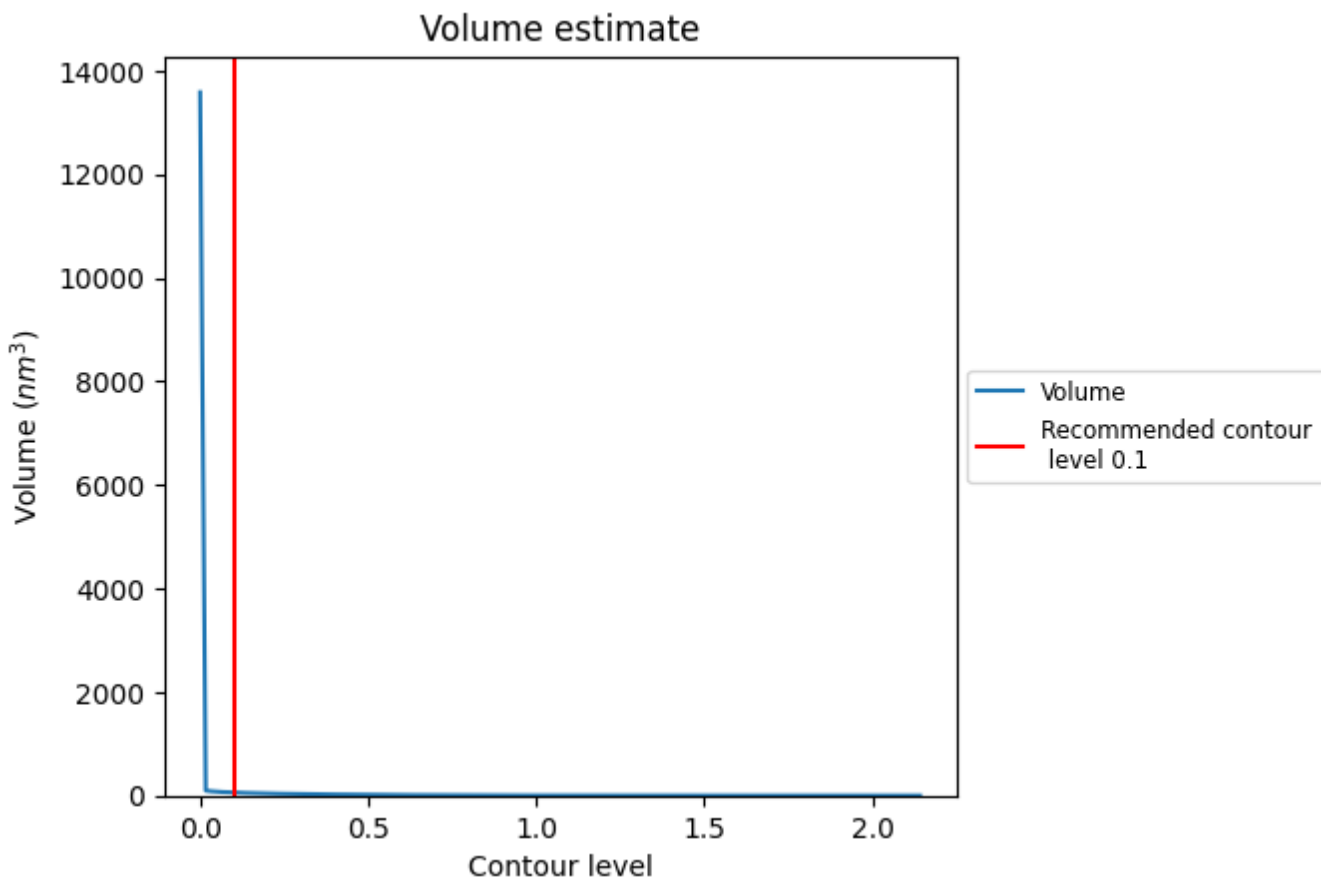
This section contains the results of statistical analysis of the map.

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.

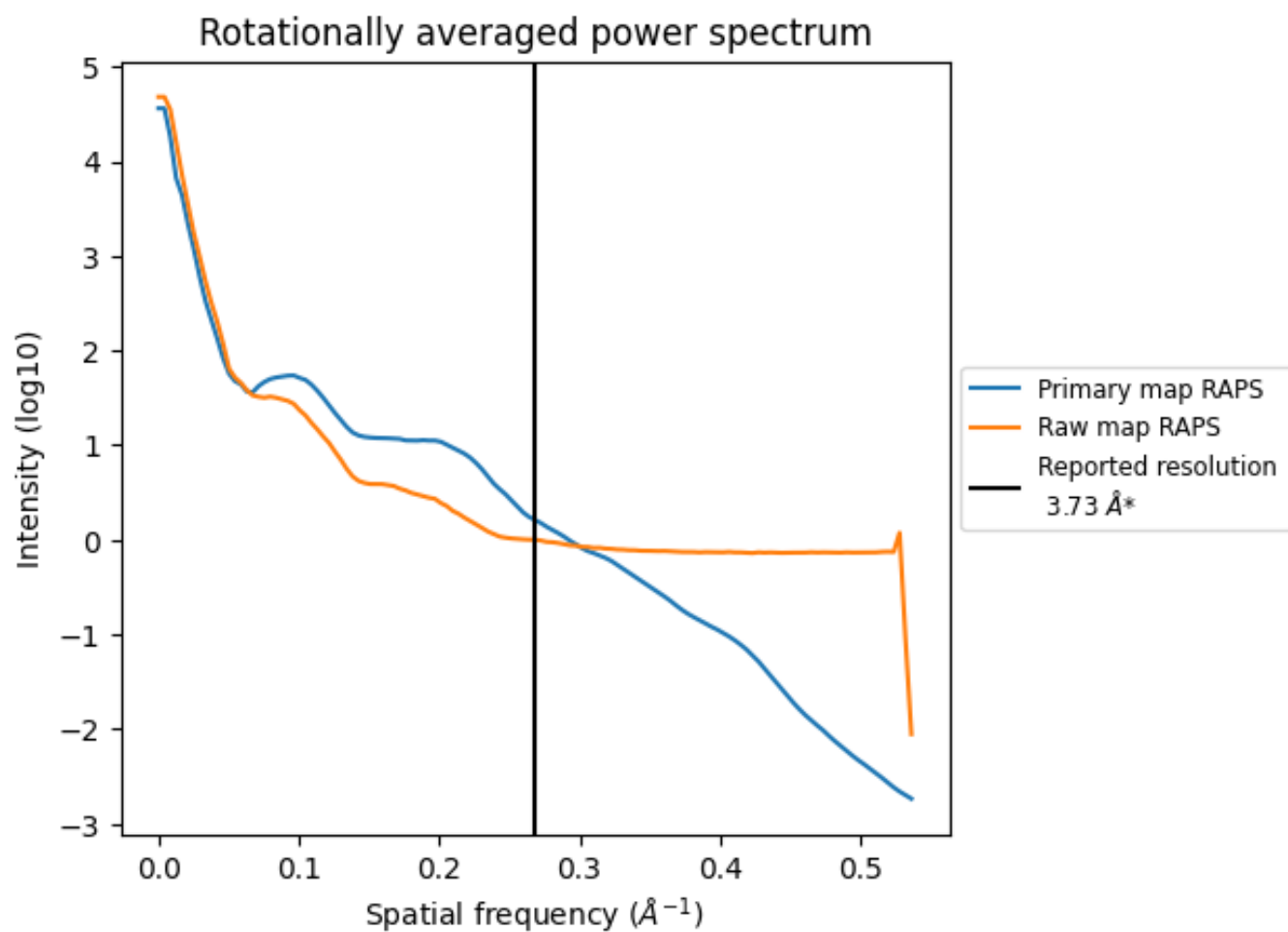
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 58 nm³; this corresponds to an approximate mass of 52 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](#)

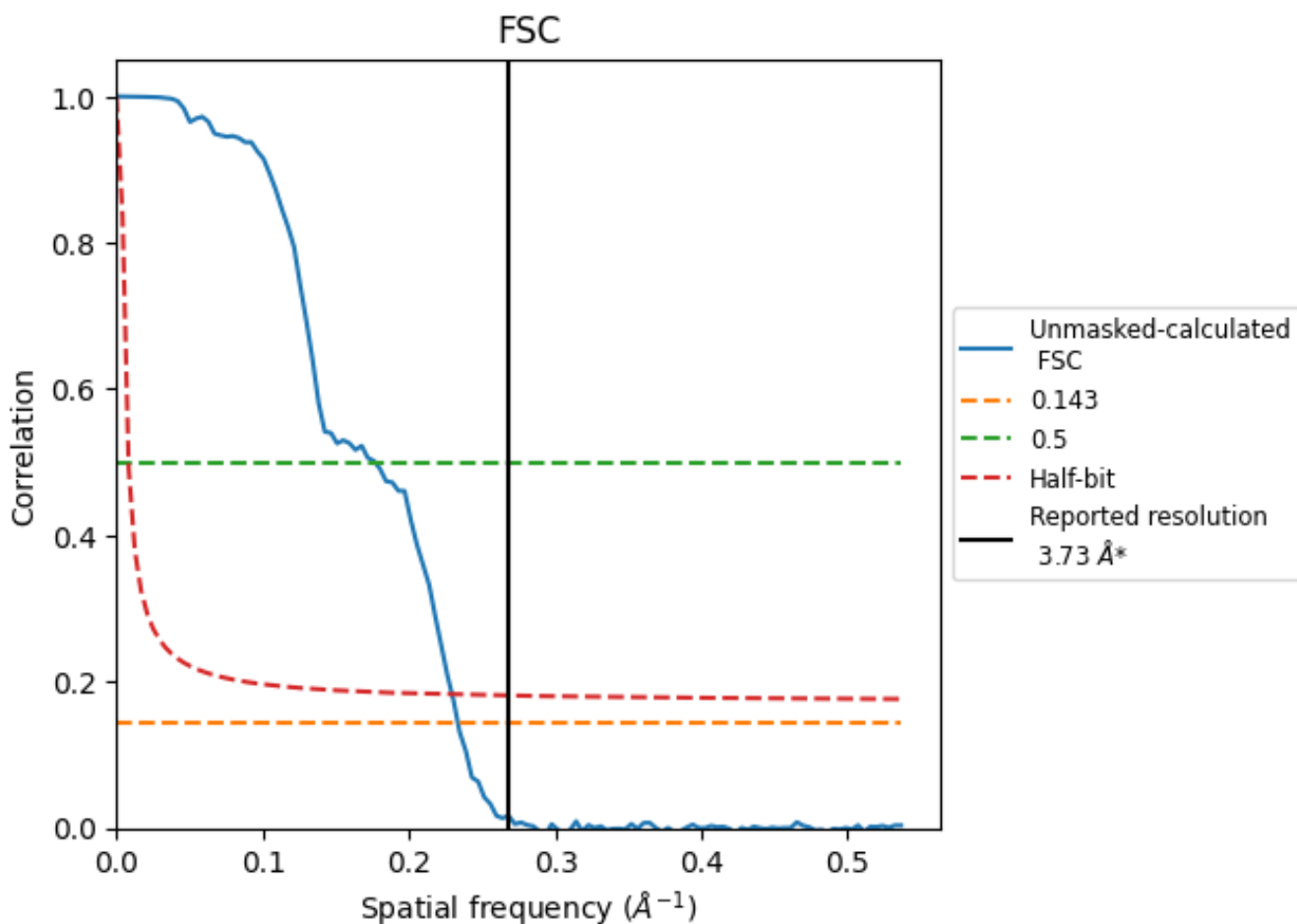


*Reported resolution corresponds to spatial frequency of 0.268 Å⁻¹

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 0.268 Å⁻¹

8.2 Resolution estimates [i](#)

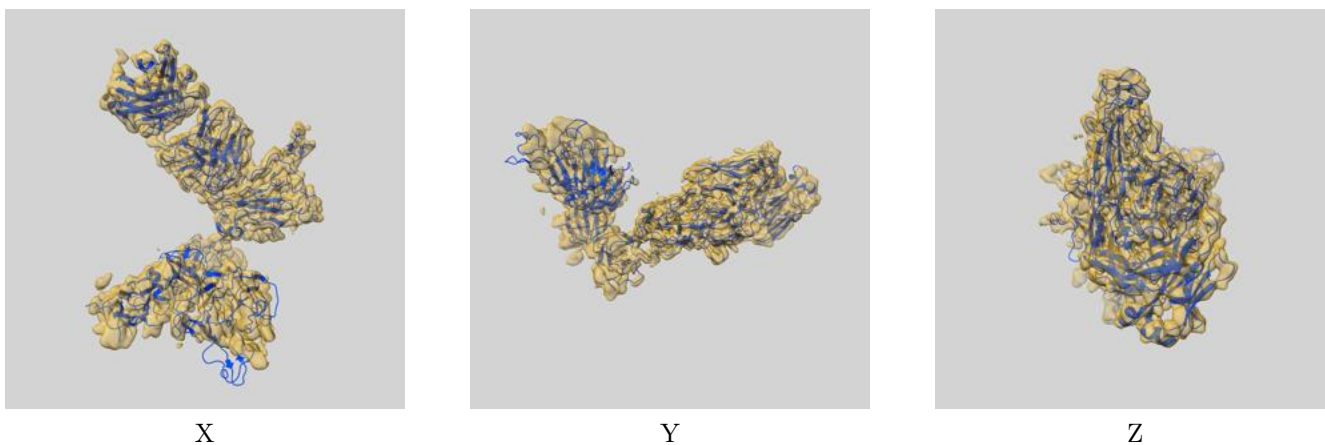
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.73	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.28	5.66	4.36

*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 4.28 differs from the reported value 3.73 by more than 10 %

9 Map-model fit [i](#)

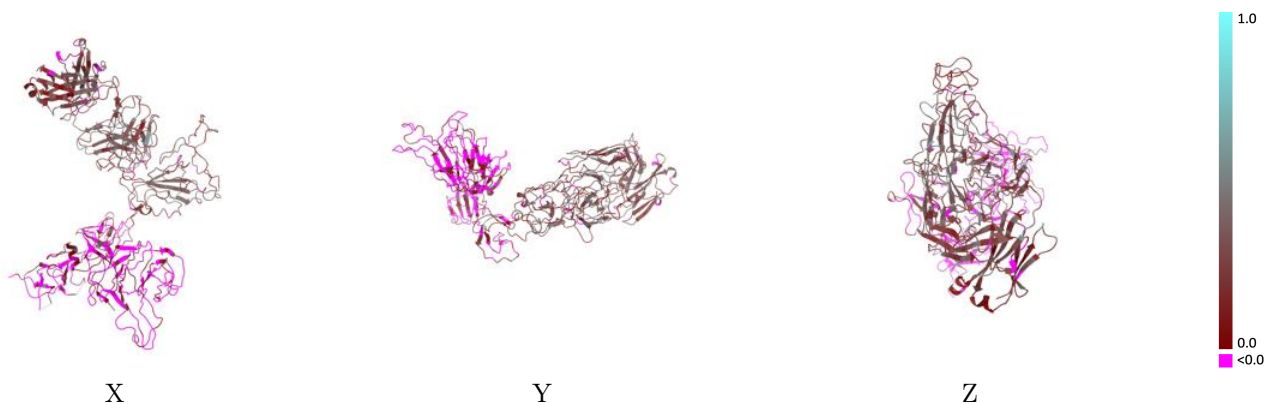
This section contains information regarding the fit between EMDB map EMD-37160 and PDB model 8KEJ. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



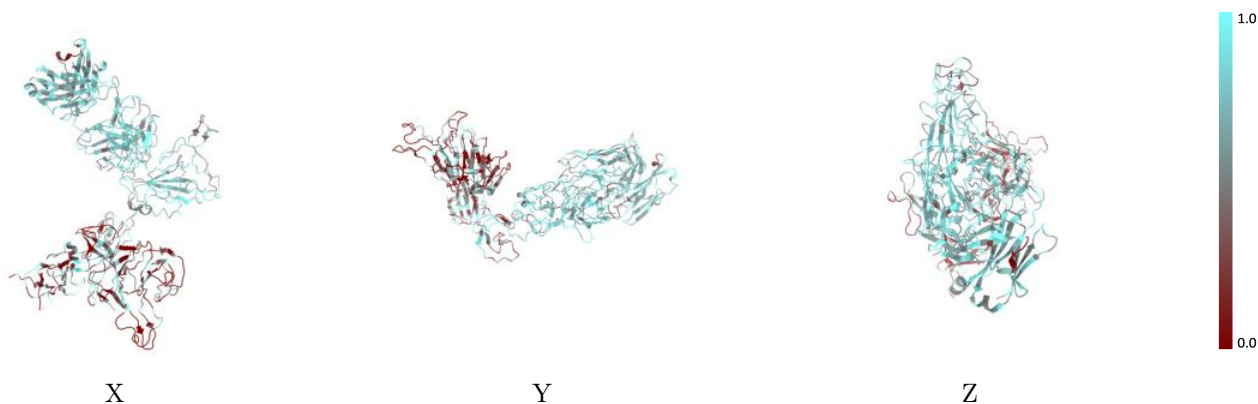
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



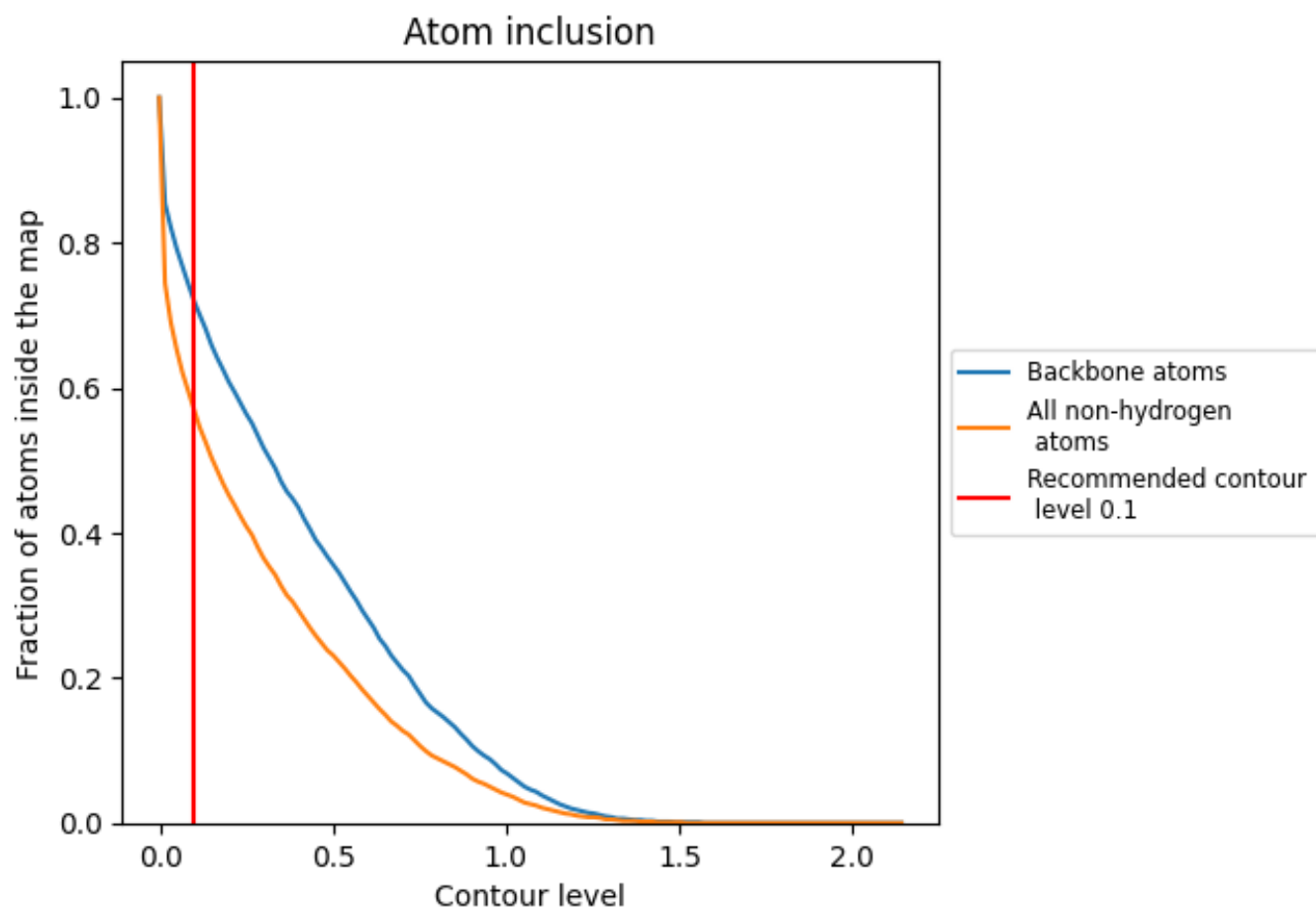
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).









9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5680	 0.1660
A	 0.4790	 0.0880
H	 0.7110	 0.2990
L	 0.7000	 0.2740

