



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:42 AM UTC

PDB ID : 8KDR / pdb_00008kdr
EMDB ID : EMD-37143
Title : The local refined map of SARS-CoV-2 XBB Variant Spike protein complexed with antibody PW5-535
Authors : Sun, L.; Mao, Q.; Wang, Y.
Deposited on : 2023-08-10
Resolution : 3.40 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

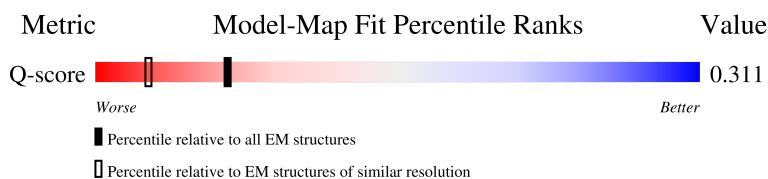
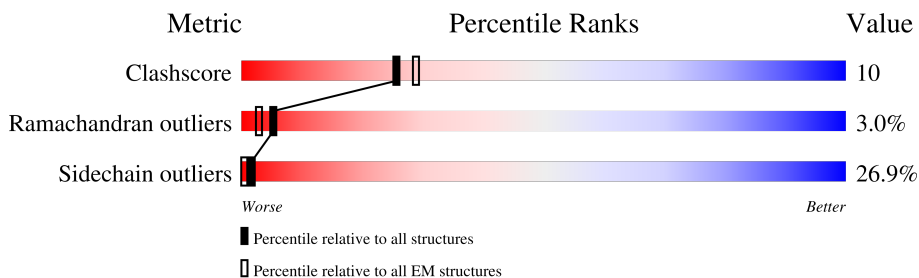
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	L	215	
2	H	450	
3	A	1295	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5454 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 PW5-535 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	212	Total	C	N	O	S	0	0
			1631	1024	277	326	4		

- Molecule 2 is a protein called PW5-535 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	218	Total	C	N	O	S	0	0
			1639	1033	278	321	7		

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	276	Total	C	N	O	S	0	0
			2184	1398	370	406	10		

There are 153 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLY	-	expression tag	UNP P0DTC2
A	10	MET	-	expression tag	UNP P0DTC2
A	11	LEU	-	expression tag	UNP P0DTC2
A	12	VAL	-	expression tag	UNP P0DTC2
A	13	ALA	-	expression tag	UNP P0DTC2
A	14	SER	-	expression tag	UNP P0DTC2
A	15	VAL	-	expression tag	UNP P0DTC2
A	16	LEU	-	expression tag	UNP P0DTC2
A	17	ALA	-	expression tag	UNP P0DTC2
A	23	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	28	SER	ALA	variant	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

Chain A: 14% 6% 79%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	298238	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	3.030	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	380.80002, 380.80002, 380.80002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.19, 1.19, 1.19	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	L	0.70	0/1670	1.04	7/2272 (0.3%)
2	H	0.81	0/1677	1.13	4/2282 (0.2%)
3	A	0.60	0/2244	0.92	6/3054 (0.2%)
All	All	0.70	0/5591	1.02	17/7608 (0.2%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	166	LEU	N-CA-C	-7.30	103.35	111.82
3	A	541	PHE	CA-CB-CG	6.57	120.37	113.80
1	L	53	THR	CB-CA-C	-5.90	101.68	111.41
3	A	565	PHE	CA-CB-CG	5.78	119.58	113.80
3	A	374	PHE	CA-CB-CG	5.71	119.51	113.80
2	H	101	SER	CA-C-O	-5.62	114.85	120.64
1	L	114	PRO	N-CA-C	5.58	123.97	112.47
1	L	59	PRO	N-CA-CB	-5.52	97.46	103.25
1	L	57	GLY	N-CA-C	-5.48	107.75	115.32
3	A	553	THR	CB-CA-C	-5.47	104.56	113.37
1	L	127	LYS	N-CA-C	-5.40	105.55	111.82
2	H	162	ASN	N-CA-CB	5.22	119.31	110.49
1	L	99	PHE	CA-C-N	5.21	127.97	121.83
1	L	99	PHE	C-N-CA	5.21	127.97	121.83
2	H	192	PRO	CB-CA-C	-5.16	103.45	111.40
3	A	562	PHE	CA-CB-CG	5.13	118.93	113.80
3	A	418	ILE	N-CA-C	-5.07	108.35	113.47

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	L	1631	0	1592	32	0
2	H	1639	0	1609	53	0
3	A	2184	0	2110	30	0
All	All	5454	0	5311	111	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 10.

All (111) 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:H:164:GLY:H	2:H:166:LEU:HD23	1.37	0.89
1:L:121:PRO:HB3	1:L:132:SER:H	1.49	0.76
1:L:94:SER:HB3	3:A:384:PRO:HD3	1.68	0.74
2:H:34:ILE:HG12	2:H:78:VAL:HG21	1.70	0.73
2:H:151:ASP:HA	2:H:182:LEU:HB3	1.75	0.68
2:H:143:ALA:HB3	2:H:191:VAL:HG23	1.76	0.68
2:H:154:PRO:HB2	2:H:209:PRO:HG2	1.76	0.67
2:H:164:GLY:N	2:H:166:LEU:HD23	2.10	0.67
3:A:366:SER:O	3:A:370:ASN:ND2	2.29	0.65
3:A:330:PRO:HD3	3:A:544:ASN:HA	1.79	0.65
3:A:408:SER:O	3:A:414:GLN:NE2	2.31	0.63
2:H:20:LEU:HD22	2:H:116:THR:HG21	1.79	0.63
2:H:162:ASN:HB2	2:H:165:ALA:HB3	1.80	0.62
1:L:121:PRO:HD3	1:L:133:VAL:HG22	1.81	0.61
1:L:148:GLN:HB2	1:L:196:GLU:HB3	1.81	0.61
1:L:196:GLU:HA	1:L:207:THR:HG22	1.83	0.61
1:L:148:GLN:NE2	1:L:196:GLU:O	2.34	0.61
2:H:145:LEU:HD12	2:H:191:VAL:HG21	1.82	0.61
2:H:40:THR:HB	2:H:43:LYS:HB2	1.82	0.60
2:H:202:ILE:HA	2:H:217:LYS:HA	1.83	0.60
3:A:379:CYS:HB2	3:A:384:PRO:HG3	1.84	0.60
3:A:541:PHE:HE1	3:A:546:LEU:HD13	1.67	0.58
1:L:194:ALA:HB1	1:L:207:THR:HB	1.85	0.58
1:L:166:GLU:OE1	1:L:167:GLN:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:202:ILE:HG12	2:H:217:LYS:HB3	1.85	0.57
2:H:32:TYR:HE2	2:H:99:ASP:HB2	1.68	0.57
2:H:105:ILE:HG21	3:A:382:VAL:HG13	1.85	0.57
2:H:136:LYS:C	2:H:138:THR:H	2.13	0.57
2:H:98:GLY:HA2	2:H:109:MET:HA	1.86	0.56
2:H:161:TRP:HB2	2:H:170:VAL:HG22	1.87	0.56
2:H:153:PHE:HA	2:H:183:TYR:HD2	1.70	0.55
3:A:393:THR:HG21	3:A:518:LEU:HB2	1.88	0.55
2:H:29:PHE:HZ	2:H:78:VAL:HG13	1.72	0.55
2:H:162:ASN:CB	2:H:165:ALA:HB3	2.37	0.55
3:A:434:ILE:HB	3:A:511:VAL:HG13	1.89	0.55
2:H:161:TRP:CE2	2:H:203:CYS:HB3	2.42	0.54
2:H:189:VAL:HG13	2:H:191:VAL:HG22	1.89	0.54
1:L:125:GLN:HE22	1:L:132:SER:HB2	1.72	0.54
3:A:420:ASP:O	3:A:424:LYS:NZ	2.41	0.54
1:L:6:GLN:HA	1:L:22:THR:O	2.07	0.53
1:L:137:LEU:HB2	1:L:176:LEU:HB3	1.90	0.52
2:H:29:PHE:CZ	2:H:78:VAL:HG13	2.44	0.52
1:L:186:ASP:O	1:L:190:HIS:ND1	2.42	0.52
1:L:19:VAL:HG23	1:L:78:LEU:HD11	1.90	0.52
2:H:202:ILE:HA	2:H:217:LYS:HB3	1.92	0.51
2:H:164:GLY:H	2:H:166:LEU:CD2	2.16	0.51
3:A:395:VAL:HG12	3:A:524:VAL:HG21	1.94	0.50
3:A:452:LEU:HG	3:A:492:LEU:HB2	1.94	0.50
1:L:137:LEU:HD22	1:L:176:LEU:HD23	1.94	0.49
2:H:34:ILE:HD11	2:H:95:CYS:HB2	1.94	0.49
1:L:32:TYR:HB3	1:L:91:SER:HB3	1.93	0.49
1:L:94:SER:HB3	3:A:384:PRO:CD	2.40	0.49
2:H:44:GLY:O	2:H:45:LEU:C	2.56	0.49
3:A:401:VAL:HG22	3:A:509:ARG:HG2	1.94	0.48
1:L:94:SER:HB2	1:L:95:PRO:HD3	1.94	0.48
3:A:449:TYR:OH	3:A:498:ARG:NH2	2.45	0.48
3:A:556:ASN:HD22	3:A:556:ASN:HA	1.55	0.47
3:A:422:ASN:OD1	3:A:454:ARG:N	2.48	0.47
3:A:475:ALA:HB3	3:A:487:ASN:HD21	1.79	0.47
3:A:424:LYS:HZ2	3:A:424:LYS:HB2	1.80	0.47
1:L:136:LEU:HD21	2:H:188:VAL:HG21	1.95	0.46
2:H:4:LEU:HD11	2:H:27:PHE:HZ	1.80	0.46
1:L:104:LYS:HB2	1:L:104:LYS:HE2	1.48	0.46
3:A:398:ASP:HB2	3:A:512:VAL:HG23	1.97	0.46
1:L:108:LYS:HB3	1:L:108:LYS:HE3	1.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:353:TRP:HZ3	3:A:355:ARG:HD2	1.81	0.46
3:A:353:TRP:CZ3	3:A:355:ARG:HD2	2.51	0.46
3:A:537:LYS:HB2	3:A:537:LYS:HE2	1.51	0.45
3:A:391:CYS:HA	3:A:525:CYS:HA	1.98	0.45
2:H:82:MET:HG3	2:H:85:LEU:HD21	1.98	0.45
2:H:101:SER:O	2:H:102:PRO:C	2.60	0.45
2:H:136:LYS:HE3	2:H:136:LYS:HB2	1.61	0.45
1:L:134:VAL:HA	1:L:178:SER:O	2.17	0.45
3:A:560:LEU:O	3:A:562:PHE:N	2.50	0.44
1:L:39:ILE:HD11	1:L:42:LYS:HD2	1.99	0.44
2:H:18:LEU:HD23	2:H:18:LEU:H	1.83	0.44
2:H:108:TYR:O	2:H:109:MET:C	2.61	0.44
3:A:332:ILE:H	3:A:332:ILE:HG12	1.34	0.44
2:H:169:GLY:HA3	2:H:189:VAL:HG23	1.99	0.43
1:L:134:VAL:HG22	1:L:179:THR:HG22	2.00	0.43
2:H:213:LYS:HA	2:H:213:LYS:HD3	1.86	0.43
2:H:68:THR:HG23	2:H:81:GLN:HB3	2.00	0.43
1:L:152:ASP:HA	1:L:192:VAL:HB	2.00	0.43
2:H:53:THR:C	2:H:55:GLY:H	2.27	0.42
2:H:167:THR:O	2:H:168:SER:C	2.62	0.42
2:H:151:ASP:HB3	2:H:182:LEU:HD13	2.01	0.42
1:L:145:ALA:HB2	1:L:199:HIS:CD2	2.54	0.42
2:H:136:LYS:C	2:H:138:THR:N	2.78	0.42
2:H:215:ASP:HB2	2:H:216:LYS:H	1.41	0.42
2:H:92:MET:HB2	2:H:92:MET:HE2	1.63	0.42
2:H:185:LEU:HB2	2:H:186:SER:H	1.73	0.42
3:A:431:GLY:HA2	3:A:515:PHE:HD1	1.85	0.42
3:A:533:LEU:HD21	3:A:585:LEU:HD21	2.02	0.42
2:H:33:ASP:HA	2:H:71:ARG:HH12	1.85	0.42
2:H:66:ARG:HH12	2:H:86:ARG:H	1.68	0.42
2:H:97:ARG:HD3	2:H:97:ARG:HA	1.77	0.42
2:H:166:LEU:O	2:H:167:THR:C	2.63	0.42
1:L:90:GLN:HE21	1:L:90:GLN:HB2	1.65	0.41
1:L:104:LYS:H	1:L:104:LYS:HG3	1.51	0.41
2:H:35:HIS:HB2	2:H:96:VAL:HG12	2.01	0.41
1:L:143:ARG:HD3	1:L:164:VAL:HG11	2.02	0.41
2:H:105:ILE:H	2:H:105:ILE:HG12	1.79	0.41
2:H:162:ASN:ND2	2:H:202:ILE:HB	2.36	0.41
1:L:79:GLN:H	1:L:82:ASP:HB2	1.86	0.41
2:H:152:TYR:CE2	2:H:157:VAL:HG11	2.56	0.41
1:L:168:ASP:OD1	1:L:169:SER:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:33:LEU:HD11	1:L:88:CYS:HB3	2.02	0.41
3:A:541:PHE:CE1	3:A:546:LEU:HD13	2.51	0.41
1:L:89:GLN:HE21	1:L:89:GLN:HB3	1.65	0.40
3:A:379:CYS:HA	3:A:432:CYS:HA	2.03	0.40
2:H:178:GLN:O	2:H:179:SER:C	2.64	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	L	210/215 (98%)	179 (85%)	26 (12%)	5 (2%)	4	22
2	H	216/450 (48%)	148 (68%)	55 (26%)	13 (6%)	1	7
3	A	274/1295 (21%)	232 (85%)	39 (14%)	3 (1%)	11	38
All	All	700/1960 (36%)	559 (80%)	120 (17%)	21 (3%)	5	18

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	94	SER
2	H	102	PRO
1	L	55	HIS
1	L	59	PRO
2	H	153	PHE
2	H	169	GLY
2	H	170	VAL
2	H	200	THR
3	A	561	PRO
3	A	562	PHE
1	L	93	SER
2	H	109	MET

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Mol	Chain	Res	Type
2	H	156	PRO
2	H	167	THR
1	L	97	TRP
2	H	46	GLU
2	H	137	SER
2	H	41	THR
2	H	162	ASN
2	H	115	GLY
3	A	569	ILE

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	L	187/189 (99%)	146 (78%)	41 (22%)	1	3
2	H	183/398 (46%)	123 (67%)	60 (33%)	0	0
3	A	243/1118 (22%)	179 (74%)	64 (26%)	0	1
All	All	613/1705 (36%)	448 (73%)	165 (27%)	2	1

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	4	VAL
1	L	5	THR
1	L	8	PRO
1	L	11	LEU
1	L	14	SER
1	L	15	VAL
1	L	35	TRP
1	L	45	LYS
1	L	48	ILE
1	L	49	SER
1	L	53	THR
1	L	54	LEU
1	L	58	VAL

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Mol	Chain	Res	Type
1	L	61	ARG
1	L	63	SER
1	L	65	ARG
1	L	69	THR
1	L	70	ASP
1	L	72	THR
1	L	74	THR
1	L	81	GLU
1	L	85	THR
1	L	89	GLN
1	L	90	GLN
1	L	98	THR
1	L	104	LYS
1	L	106	GLU
1	L	107	ILE
1	L	108	LYS
1	L	110	THR
1	L	111	VAL
1	L	118	ILE
1	L	119	PHE
1	L	124	GLU
1	L	128	SER
1	L	132	SER
1	L	133	VAL
1	L	148	GLN
1	L	166	GLU
1	L	182	LEU
1	L	202	LEU
2	H	1	GLU
2	H	30	ARG
2	H	32	TYR
2	H	34	ILE
2	H	40	THR
2	H	41	THR
2	H	43	LYS
2	H	46	GLU
2	H	48	VAL
2	H	53	THR
2	H	56	ASP
2	H	57	THR
2	H	63	VAL
2	H	64	LYS

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Mol	Chain	Res	Type
2	H	68	THR
2	H	82	MET
2	H	90	THR
2	H	92	MET
2	H	97	ARG
2	H	101	SER
2	H	102	PRO
2	H	103	ASP
2	H	105	ILE
2	H	107	TYR
2	H	109	MET
2	H	111	VAL
2	H	114	THR
2	H	116	THR
2	H	117	ARG
2	H	119	ILE
2	H	120	VAL
2	H	124	LYS
2	H	127	SER
2	H	128	VAL
2	H	136	LYS
2	H	158	THR
2	H	159	VAL
2	H	163	SER
2	H	166	LEU
2	H	172	THR
2	H	176	VAL
2	H	177	LEU
2	H	178	GLN
2	H	185	LEU
2	H	192	PRO
2	H	195	SER
2	H	196	LEU
2	H	199	GLN
2	H	200	THR
2	H	202	ILE
2	H	205	VAL
2	H	208	LYS
2	H	211	ASN
2	H	212	THR
2	H	213	LYS
2	H	214	VAL

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Mol	Chain	Res	Type
2	H	215	ASP
2	H	216	LYS
2	H	217	LYS
2	H	218	VAL
3	A	323	THR
3	A	324	GLU
3	A	326	ILE
3	A	328	ARG
3	A	332	ILE
3	A	335	LEU
3	A	336	CYS
3	A	339	HIS
3	A	340	GLU
3	A	341	VAL
3	A	345	THR
3	A	346	THR
3	A	350	VAL
3	A	356	LYS
3	A	374	PHE
3	A	378	LYS
3	A	395	VAL
3	A	402	ILE
3	A	406	GLU
3	A	424	LYS
3	A	440	LYS
3	A	457	ARG
3	A	460	LYS
3	A	489	TYR
3	A	492	LEU
3	A	495	TYR
3	A	511	VAL
3	A	512	VAL
3	A	523	THR
3	A	524	VAL
3	A	528	LYS
3	A	529	LYS
3	A	531	THR
3	A	534	VAL
3	A	535	LYS
3	A	537	LYS
3	A	541	PHE
3	A	544	ASN

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Mol	Chain	Res	Type
3	A	546	LEU
3	A	547	THR
3	A	549	THR
3	A	551	VAL
3	A	553	THR
3	A	554	GLU
3	A	555	SER
3	A	556	ASN
3	A	558	LYS
3	A	563	GLN
3	A	565	PHE
3	A	567	ARG
3	A	568	ASP
3	A	569	ILE
3	A	572	THR
3	A	574	ASP
3	A	577	ARG
3	A	578	ASP
3	A	580	GLN
3	A	581	THR
3	A	582	LEU
3	A	583	GLU
3	A	585	LEU
3	A	587	ILE
3	A	588	THR
3	A	591	SER

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

Mol	Chain	Res	Type
1	L	3	GLN
1	L	90	GLN
1	L	101	GLN
1	L	125	GLN
1	L	148	GLN
2	H	35	HIS
2	H	81	GLN
2	H	83	ASN
2	H	207	HIS
3	A	370	ASN
3	A	409	GLN
3	A	414	GLN

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Mol	Chain	Res	Type
3	A	417	ASN
3	A	448	ASN
3	A	487	ASN
3	A	540	ASN
3	A	556	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no 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-37143. 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](#)

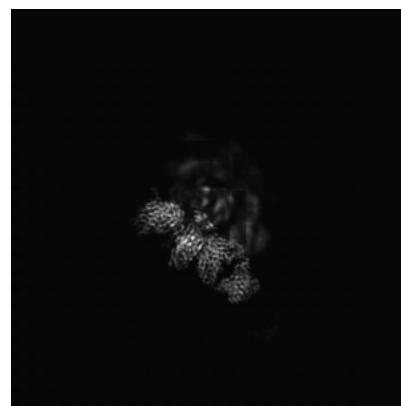
6.1.1 Primary map



X

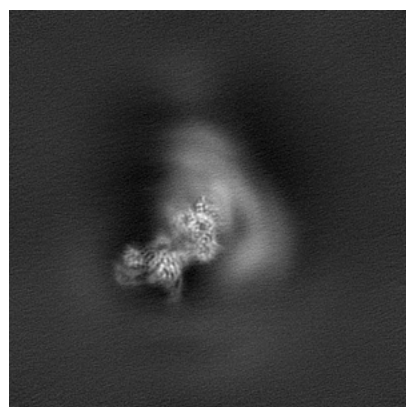


Y

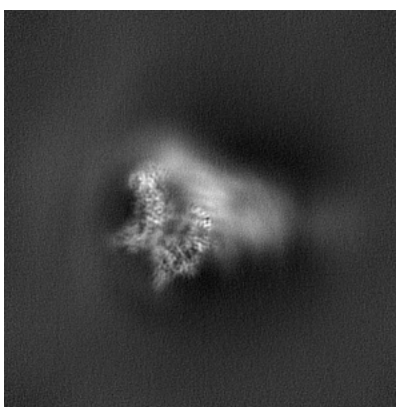


Z

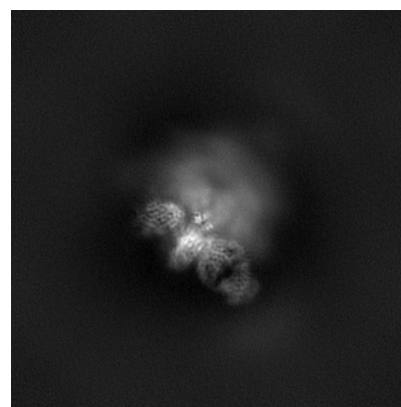
6.1.2 Raw map



X



Y

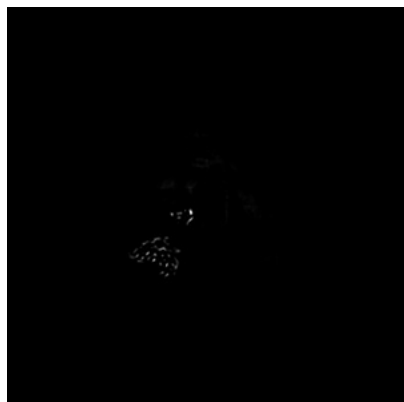


Z

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

6.2 Central slices [i](#)

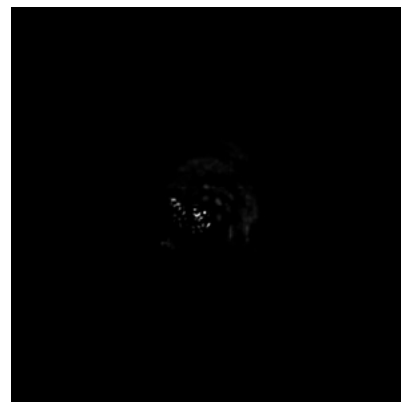
6.2.1 Primary map



X Index: 160

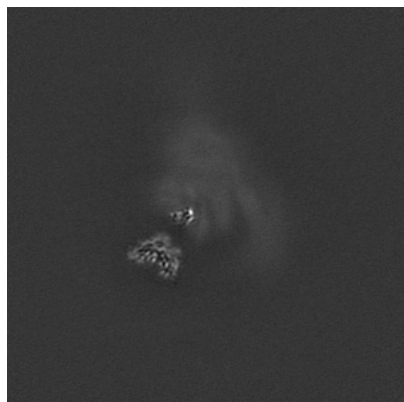


Y Index: 160



Z Index: 160

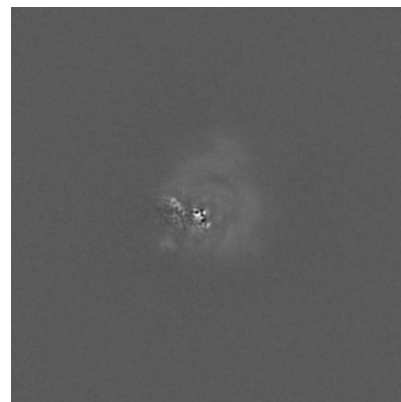
6.2.2 Raw map



X Index: 160



Y Index: 160

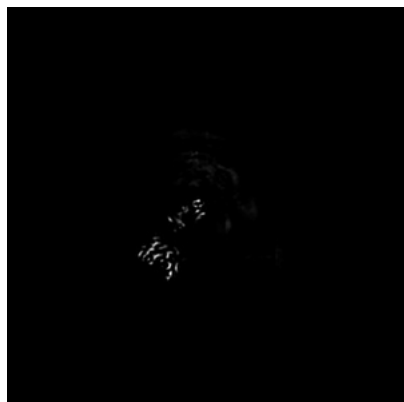


Z Index: 160

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

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 151

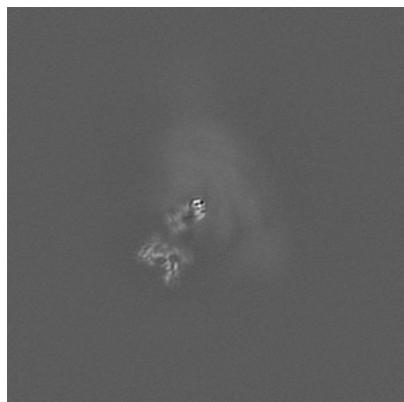


Y Index: 155

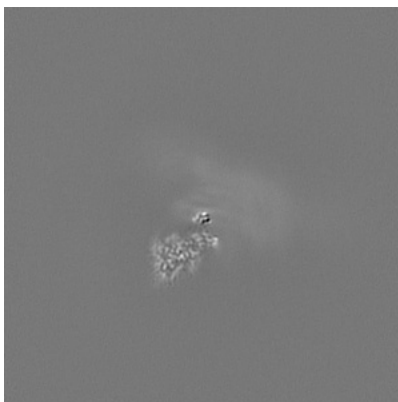


Z Index: 123

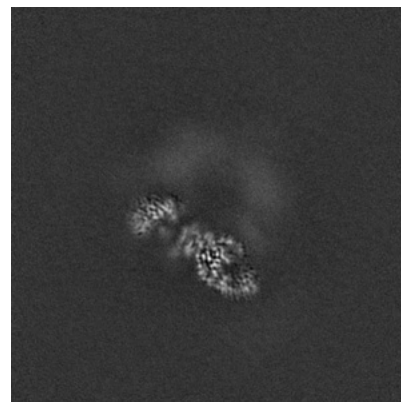
6.3.2 Raw map



X Index: 150



Y Index: 155

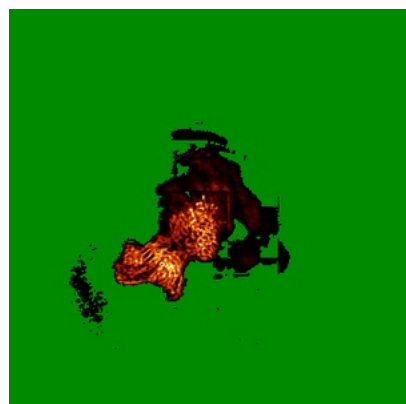


Z Index: 123

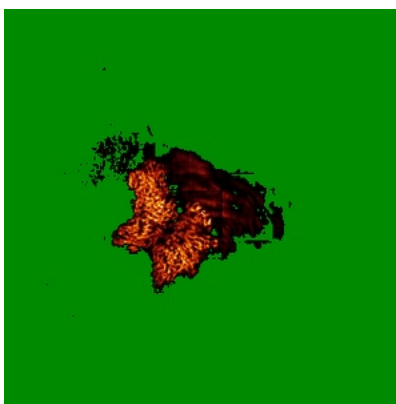
The images above show the largest variance slices of the map in three orthogonal directions.

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

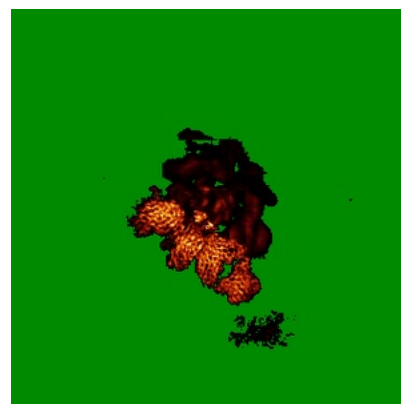
6.4.1 Primary map



X

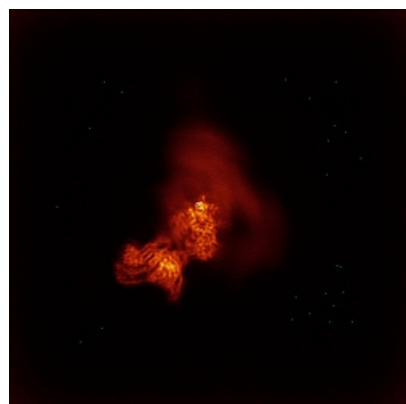


Y

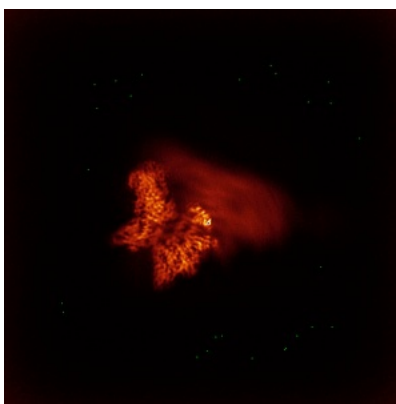


Z

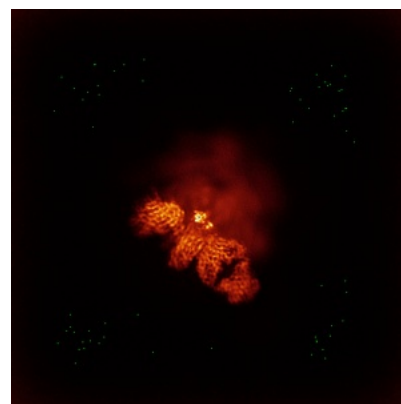
6.4.2 Raw map



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

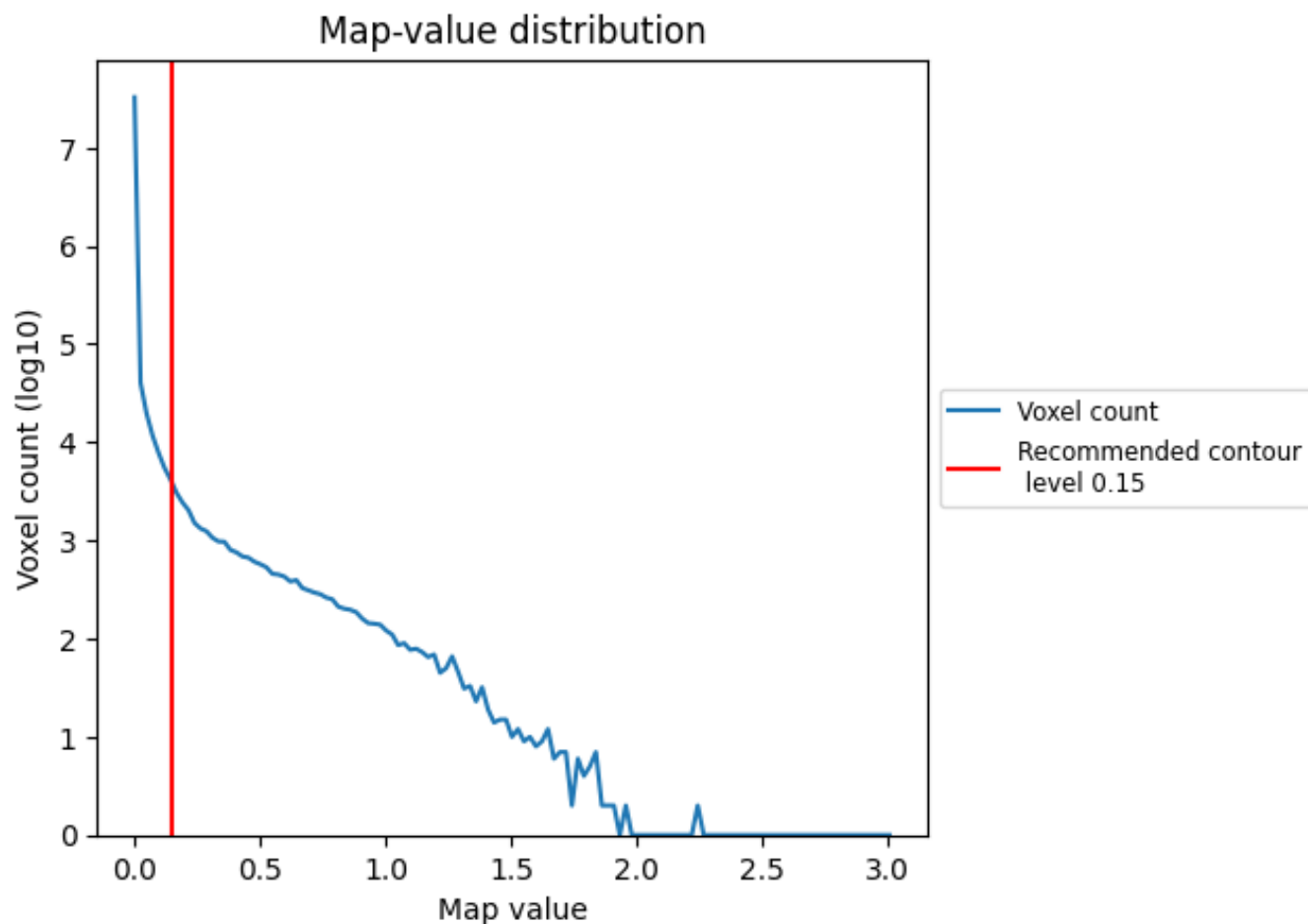
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

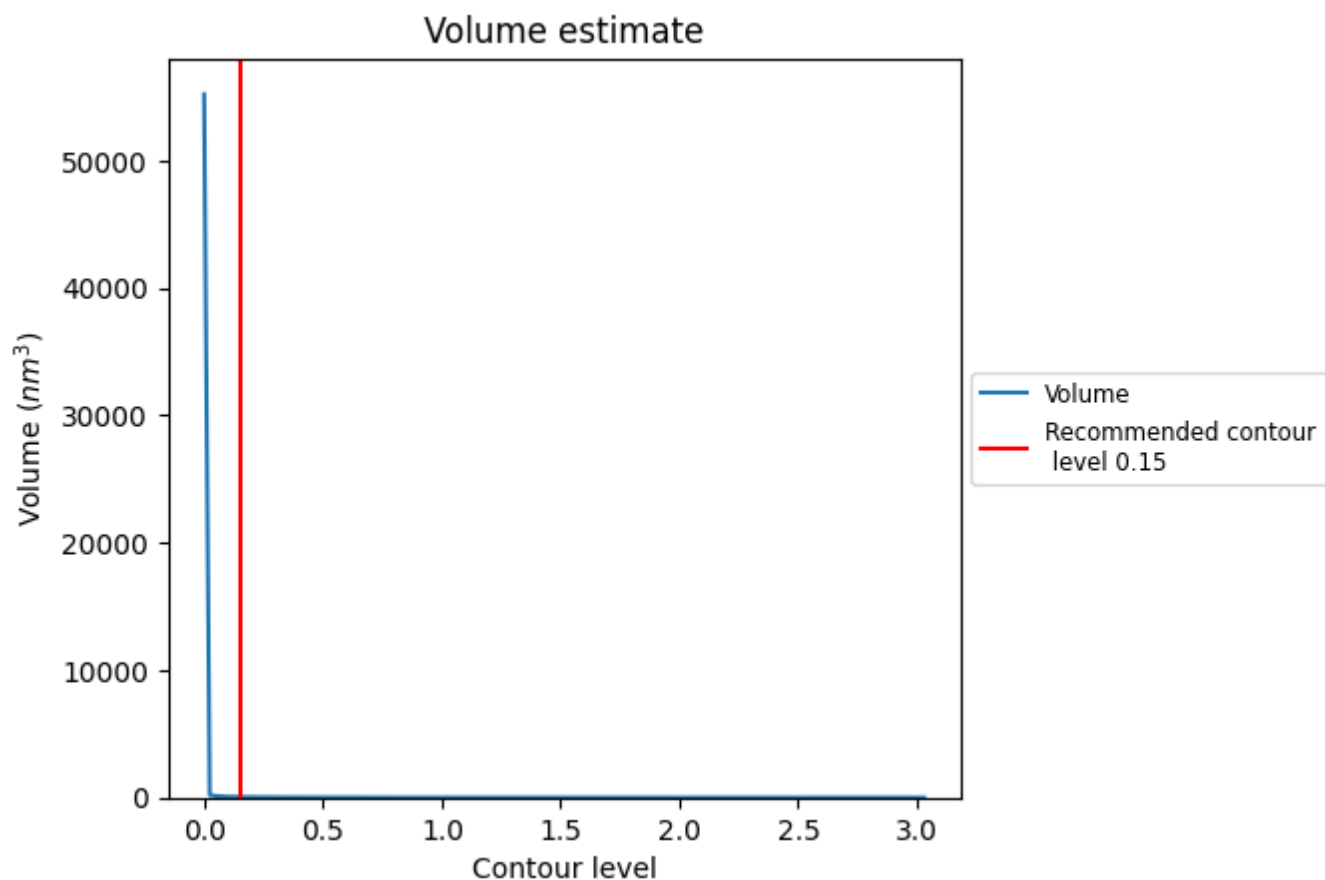
This section contains the results of statistical analysis of the map.

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.

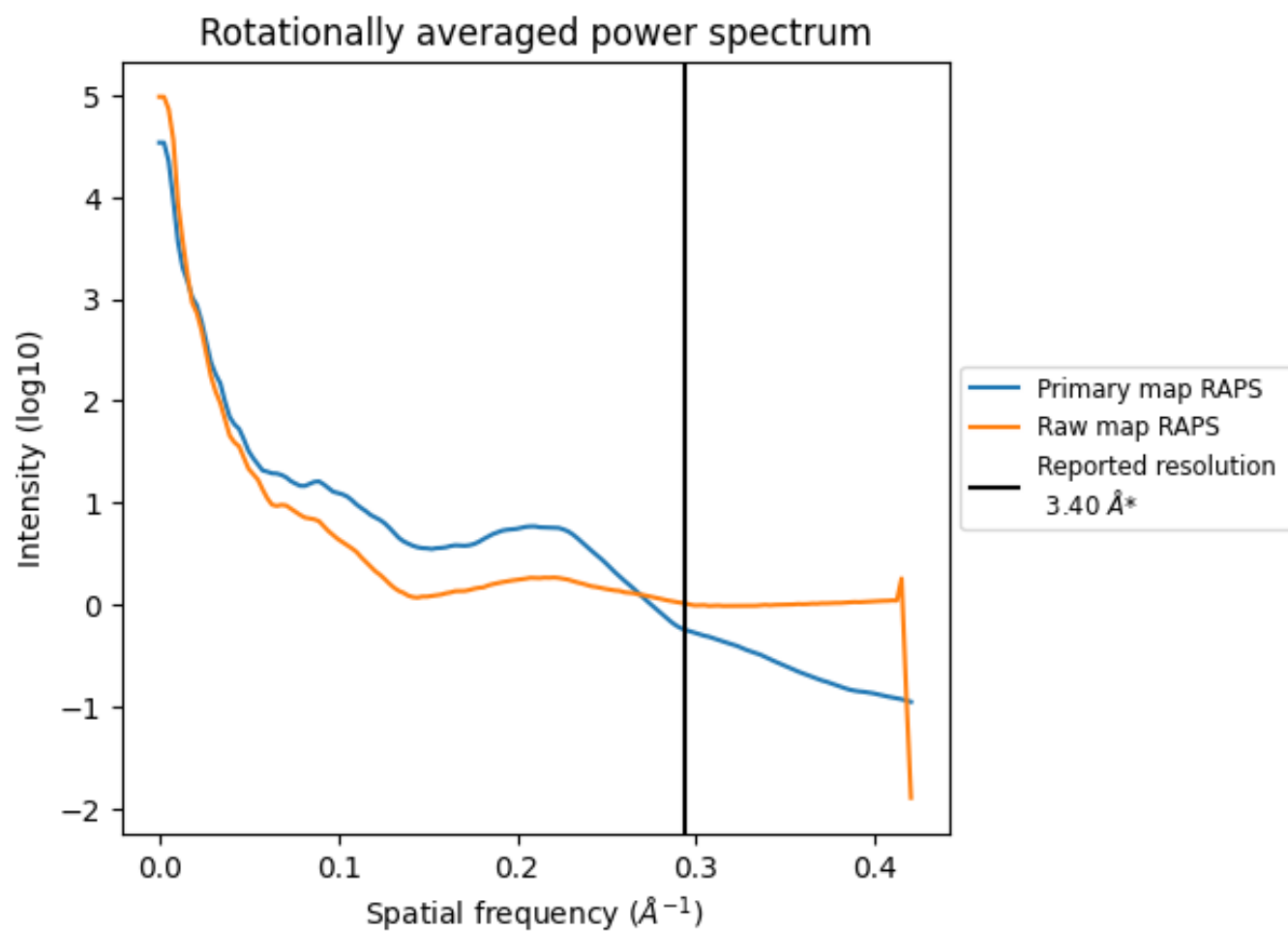
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 48 nm^3 ; this corresponds to an approximate mass of 43 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](#)

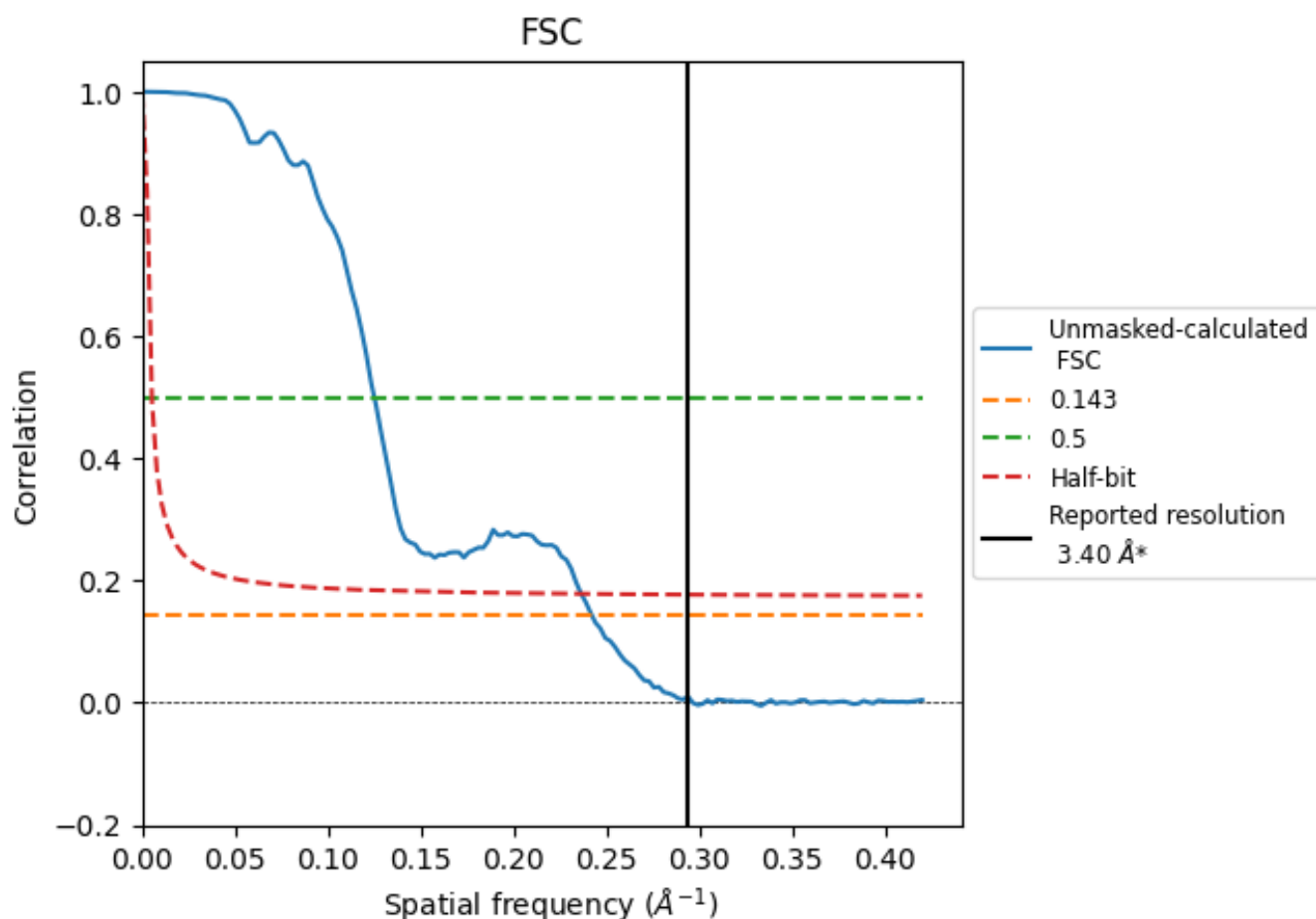


*Reported resolution corresponds to spatial frequency of $0.294 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

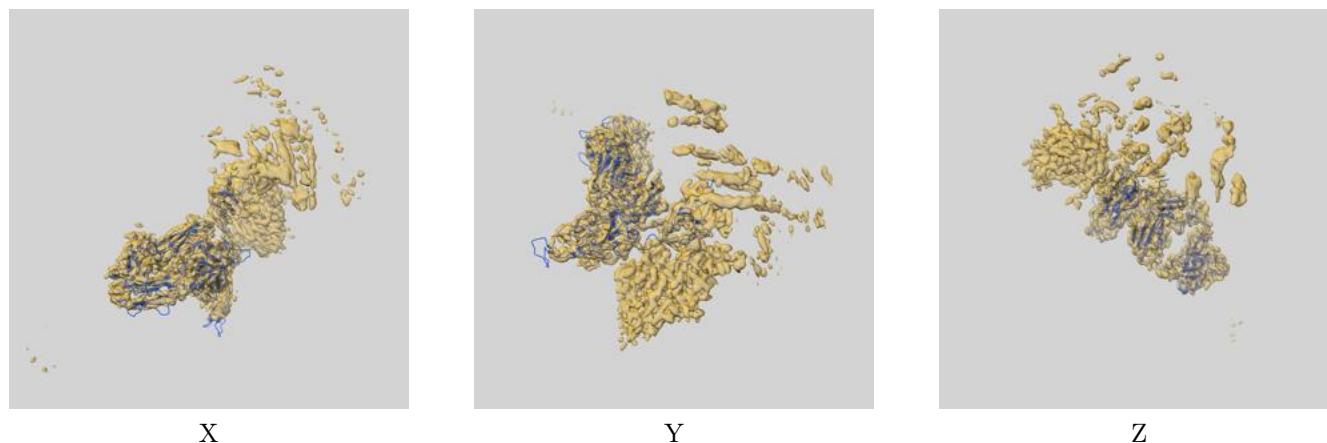
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.13	8.00	4.23

*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 4.13 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

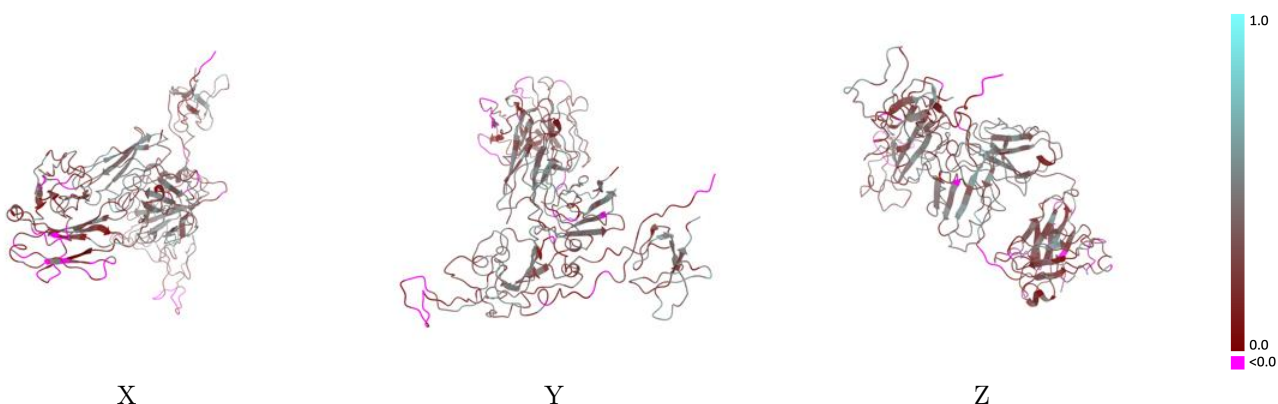
This section contains information regarding the fit between EMDB map EMD-37143 and PDB model 8KDR. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.15 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](#)

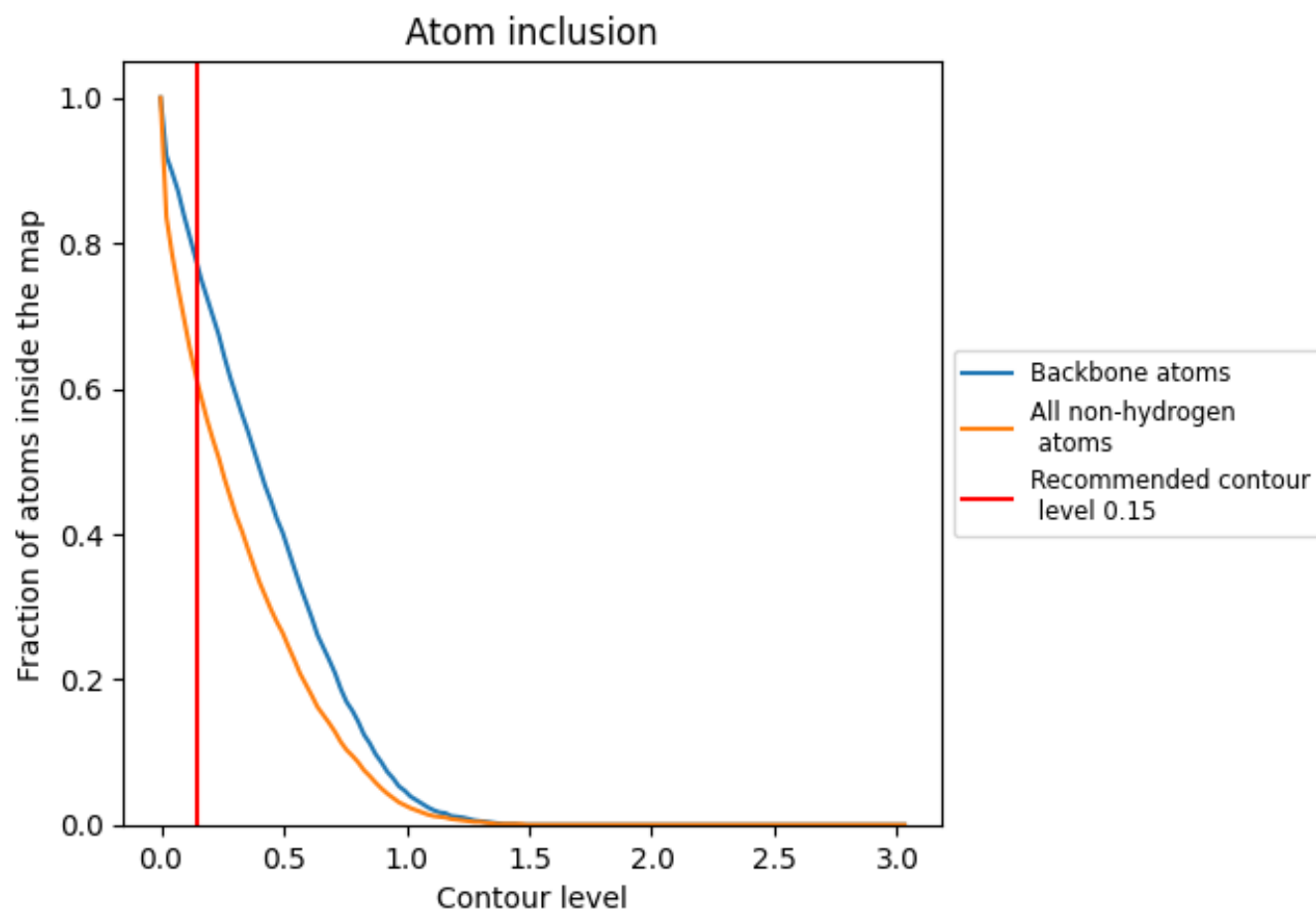


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 77% of all backbone atoms, 61% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6060	0.3110
A	0.5790	0.3070
H	0.6450	0.3300
L	0.6040	0.2980

