



Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 10:04 PM UTC

PDB ID : 9LY5 / pdb_00009ly5
EMDB ID : EMD-63503
Title : antibody 20G5 Fab in complex with human B7-H3 (IgC)
Authors : Bin, L.; Shuaixiang, Z.; kaijie, H.
Deposited on : 2025-02-19
Resolution : 2.98 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

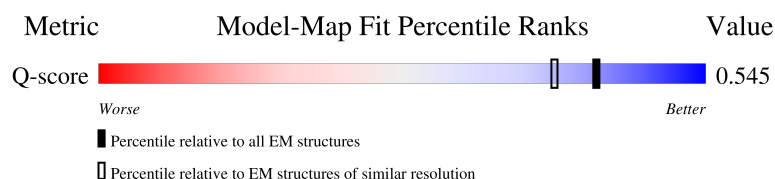
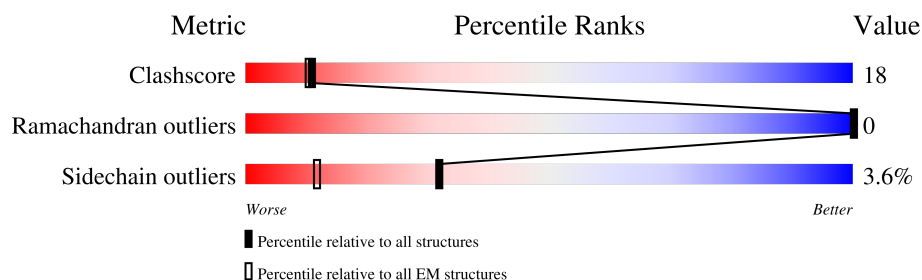
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 2.98 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13236 (2.48 - 3.48)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	223	
2	B	213	
3	C	448	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7833 atoms, of which 3200 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 antibody 20G5 Fab heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	218	Total	C	H	N	O	S	0	0
			3253	1034	1616	277	319	7		

- Molecule 2 is a protein called antibody 20G5 Fab light chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	213	Total	C	H	N	O	S	0	0
			3224	1028	1584	275	332	5		

- Molecule 3 is a protein called CD276 antigen.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	181	Total	C	N	O	S		0	0
			1356	845	234	270	7			

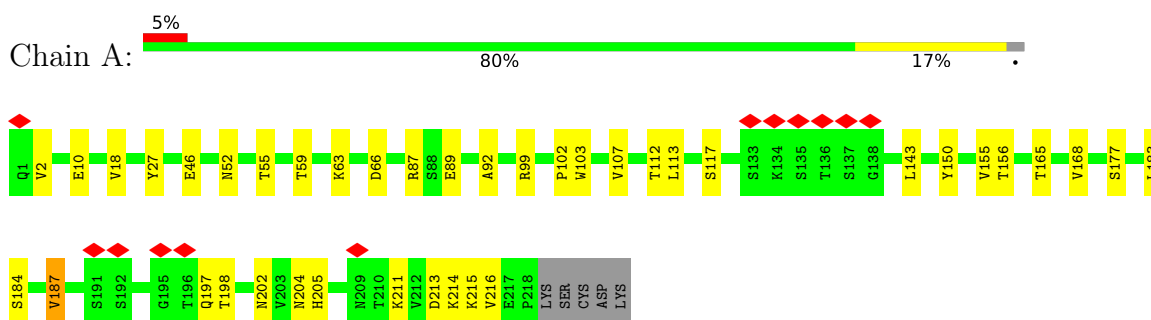
There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	462	GLY	-	expression tag	UNP Q5ZPR3
C	463	GLY	-	expression tag	UNP Q5ZPR3
C	464	GLY	-	expression tag	UNP Q5ZPR3
C	465	GLY	-	expression tag	UNP Q5ZPR3
C	466	SER	-	expression tag	UNP Q5ZPR3
C	467	HIS	-	expression tag	UNP Q5ZPR3
C	468	HIS	-	expression tag	UNP Q5ZPR3
C	469	HIS	-	expression tag	UNP Q5ZPR3
C	470	HIS	-	expression tag	UNP Q5ZPR3
C	471	HIS	-	expression tag	UNP Q5ZPR3
C	472	HIS	-	expression tag	UNP Q5ZPR3
C	473	HIS	-	expression tag	UNP Q5ZPR3
C	474	HIS	-	expression tag	UNP Q5ZPR3
C	475	HIS	-	expression tag	UNP Q5ZPR3
C	476	HIS	-	expression tag	UNP Q5ZPR3

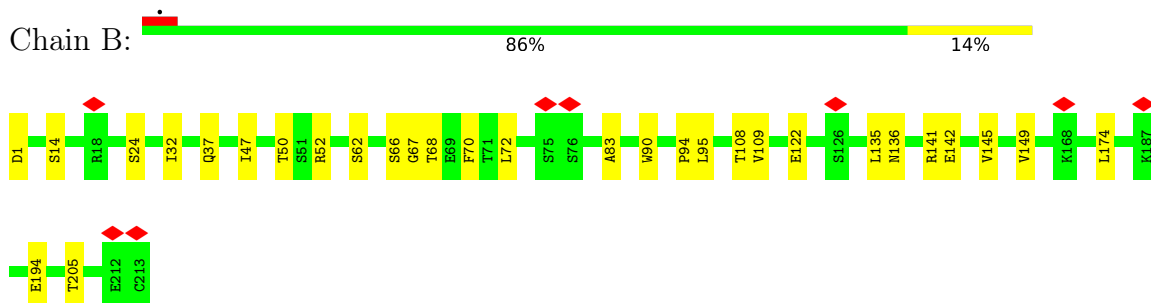
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

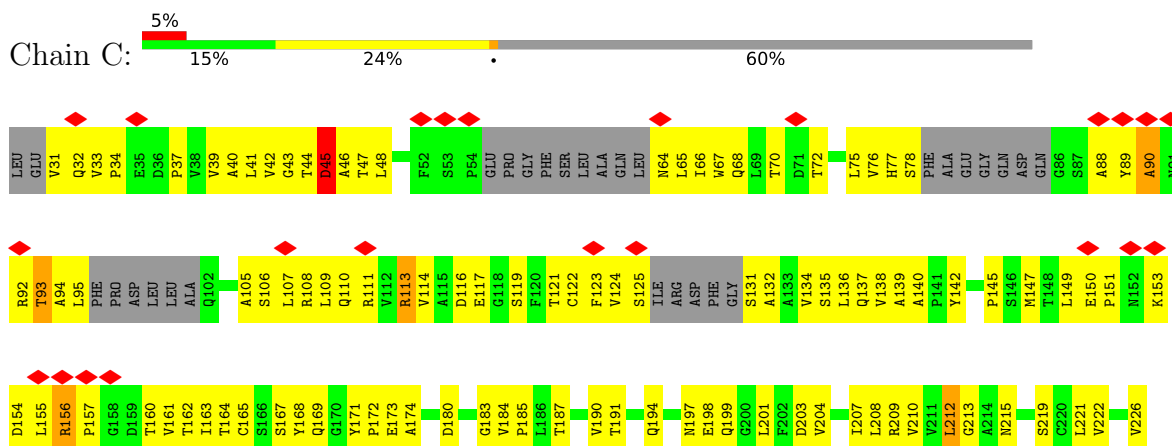
- Molecule 1: antibody 20G5 Fab heavy chain



- Molecule 2: antibody 20G5 Fab light chain



- Molecule 3: CD276 antigen



HIS	ASN	PHE	LEU	L227
HIS	VAL	GLY	THR	Q228
HIS	THR	SER	ASP	Q230
HIS	THR	ALA	LYS	D230
HIS	GLN	VAL	GLN	H232
HIS	MET	SER	LEU	S233
HIS	ASN	LEU	VAL	S234
HIS	GLN	VAL	HIS	V235
HIS	GLN	ALA	PHE	T236
	GLY	ALA	THR	I237
	LEU	PRO	THR	T238
	PHE	TYR	GLY	PRO
	ASP	SER	GLY	GLN
	VAL	LYS	ARG	SER
	VAL	HIS	GLN	PRO
	SER	SER	GLY	THR
	VAL	MET	SER	GLY
	LEU	THR	ALA	ALA
	ARG	LEU	TYR	VAL
	VAL	GLU	ALA	GLU
	VAL	PRO	ASN	VAL
	LEU	ASN	ARG	GLN
	GLY	LYS	THR	VAL
	ALA	ASP	ALA	GLN
	ASN	LEU	LEU	PRO
	GLY	ARG	PHE	ASP
	THR	PRO	PRO	PRO
	THR	GLY	ASP	VAL
	SER	ASP	LEU	VAL
	CYS	THR	LEU	ALA
	LEU	VAL	ALA	LEU
	VAL	THR	GLN	VAL
	ARG	ILE	GLY	GLY
	ASN	THR	ASN	THR
	PRO	CYS	ALA	ASP
	VAL	SER	SER	ALA
	LEU	SER	LEU	THR
	GLN	TYR	ARG	LEU
	GLN	GLY	LEU	ARG
	ASP	GLY	GLN	CYS
	ALA	TYR	ARG	SER
	HIS	PRO	VAL	PHE
	GLY	GLU	VAL	SER
	SER	ALA	VAL	PRO
	VAL	GLU	ALA	GLU
	THR	VAL	ASP	PRO
	ILE	PHE	ASP	THR
	THR	TRP	GLY	GLY
	GLY	GLN	SER	PHE
	GLN	ASP	LEU	ALA
	PRO	GLY	THR	GLN
	MET	GLN	CYS	ASN
	THR	GLY	PHE	LEU
	GLY	VAL	VAL	ASN
	GLY	PRO	SER	LEU
	GLY	LEU	ILE	ILE
	GLY	THR	ARG	TRP
	SER	CYS	ASN	GLN

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	134476	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.252	Depositor
Minimum map value	-0.872	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.164	Depositor
Map size (\AA)	326.91998, 326.91998, 326.91998	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.743, 0.743, 0.743	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.24	0/1679	0.40	0/2292
2	B	0.31	0/1679	0.53	0/2280
3	C	0.36	0/1378	0.70	5/1879 (0.3%)
All	All	0.30	0/4736	0.55	5/6451 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	90	ALA	N-CA-C	6.61	120.65	112.58
3	C	235	VAL	N-CA-C	5.45	115.96	108.12
3	C	45	ASP	N-CA-C	-5.24	103.96	110.41
3	C	88	ALA	CB-CA-C	-5.12	104.67	111.88
3	C	93	THR	CB-CA-C	5.02	118.17	110.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1637	1616	1616	26	0
2	B	1640	1584	1584	21	0
3	C	1356	0	1318	130	0
All	All	4633	3200	4518	168	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 18.

All (168) 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)
3:C:93:THR:HB	3:C:107:LEU:CD2	1.83	1.07
3:C:93:THR:HG22	3:C:109:LEU:HD13	1.36	1.07
3:C:93:THR:CB	3:C:107:LEU:HD23	1.85	1.04
1:A:204:ASN:OD1	1:A:211:LYS:NZ	2.11	0.84
3:C:150:GLU:HB3	3:C:151:PRO:HD3	1.62	0.81
3:C:173:GLU:HB3	3:C:194:GLN:NE2	1.95	0.81
2:B:194:GLU:OE2	2:B:205:THR:OG1	2.00	0.80
3:C:93:THR:HG22	3:C:109:LEU:CD1	2.12	0.80
1:A:87:ARG:NH2	1:A:89:GLU:OE1	2.15	0.79
3:C:173:GLU:HB3	3:C:194:GLN:HE22	1.48	0.79
2:B:141:ARG:NH1	2:B:141:ARG:O	2.18	0.76
1:A:59:THR:HG21	3:C:184:VAL:HG21	1.68	0.76
3:C:108:ARG:O	3:C:110:GLN:NE2	2.19	0.76
3:C:48:LEU:CD2	3:C:136:LEU:HD23	2.16	0.75
3:C:93:THR:HB	3:C:107:LEU:HD23	0.89	0.73
3:C:31:VAL:HG22	3:C:32:GLN:H	1.55	0.71
3:C:142:TYR:HB3	3:C:167:SER:OG	1.90	0.71
3:C:160:THR:HG22	3:C:209:ARG:HG3	1.73	0.70
3:C:92:ARG:NH1	3:C:113:ARG:HD2	2.06	0.70
1:A:197:GLN:OE1	1:A:198:THR:N	2.26	0.69
3:C:123:PHE:HA	3:C:131:SER:N	2.06	0.69
2:B:32:ILE:HD12	2:B:32:ILE:O	1.93	0.69
3:C:89:TYR:CE2	3:C:92:ARG:HD2	2.29	0.68
3:C:66:ILE:HG13	3:C:123:PHE:HB3	1.74	0.68
3:C:89:TYR:HE2	3:C:92:ARG:HD2	1.58	0.68
3:C:107:LEU:HB3	3:C:109:LEU:HD22	1.77	0.67
3:C:77:HIS:CE1	3:C:95:LEU:HD21	2.30	0.67
3:C:149:LEU:HD11	3:C:235:VAL:HG11	1.77	0.67
3:C:37:PRO:HA	3:C:135:SER:HB3	1.77	0.66
3:C:221:LEU:HD11	3:C:230:ASP:HB3	1.76	0.66
3:C:48:LEU:O	3:C:106:SER:HB2	1.94	0.66
3:C:31:VAL:HG22	3:C:32:GLN:N	2.10	0.65
3:C:77:HIS:ND1	3:C:95:LEU:HD21	2.14	0.62
2:B:52:ARG:NH2	3:C:228:GLN:HG3	2.14	0.62
3:C:48:LEU:HB3	3:C:134:VAL:HG11	1.81	0.62
3:C:136:LEU:CD1	3:C:138:VAL:HG23	2.29	0.62
1:A:10:GLU:OE1	1:A:18:VAL:HG23	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:TRP:O	3:C:185:PRO:HG3	2.00	0.61
3:C:194:GLN:OE1	3:C:204:VAL:HG22	2.00	0.61
2:B:47:ILE:HD12	2:B:72:LEU:HD13	1.82	0.61
3:C:89:TYR:CD2	3:C:89:TYR:O	2.54	0.60
3:C:145:PRO:HD3	3:C:231:ALA:HB1	1.81	0.60
2:B:90:TRP:NE1	3:C:183:GLY:O	2.28	0.59
3:C:139:ALA:HB2	3:C:226:VAL:HG11	1.82	0.59
2:B:90:TRP:CD1	3:C:185:PRO:HD3	2.38	0.59
3:C:198:GLU:N	3:C:198:GLU:OE2	2.35	0.59
3:C:114:VAL:CG2	3:C:201:LEU:HD23	2.33	0.59
3:C:68:GLN:OE1	3:C:75:LEU:HA	2.03	0.58
3:C:136:LEU:HD11	3:C:138:VAL:HG23	1.86	0.58
3:C:171:TYR:CD1	3:C:172:PRO:HA	2.38	0.58
3:C:70:THR:HB	3:C:119:SER:HB3	1.86	0.57
3:C:208:LEU:HG	3:C:210:VAL:HG13	1.85	0.57
3:C:75:LEU:HD21	3:C:78:SER:OG	2.05	0.55
1:A:214:LYS:NZ	2:B:122:GLU:OE2	2.22	0.55
3:C:44:THR:HG22	3:C:45:ASP:N	2.21	0.55
3:C:64:ASN:O	3:C:124:VAL:HA	2.07	0.55
3:C:114:VAL:HG21	3:C:201:LEU:HD23	1.89	0.55
1:A:52:ASN:ND2	1:A:55:THR:OG1	2.35	0.55
1:A:99:ARG:NH1	3:C:183:GLY:HA3	2.22	0.54
3:C:43:GLY:O	3:C:111:ARG:HA	2.07	0.54
3:C:153:LYS:HE2	3:C:155:LEU:HB2	1.88	0.54
3:C:92:ARG:O	3:C:110:GLN:HG2	2.07	0.54
3:C:212:LEU:CD2	3:C:237:ILE:HG21	2.37	0.54
3:C:66:ILE:CG1	3:C:123:PHE:HB3	2.38	0.53
3:C:43:GLY:C	3:C:111:ARG:HA	2.33	0.53
3:C:48:LEU:N	3:C:106:SER:OG	2.42	0.53
3:C:134:VAL:HG12	3:C:135:SER:H	1.73	0.53
3:C:89:TYR:O	3:C:90:ALA:HB3	2.09	0.53
3:C:33:VAL:HB	3:C:34:PRO:CD	2.39	0.53
1:A:52:ASN:HD22	1:A:55:THR:HG1	1.54	0.53
3:C:134:VAL:HG12	3:C:135:SER:N	2.24	0.52
3:C:212:LEU:HD23	3:C:237:ILE:HG21	1.90	0.52
3:C:142:TYR:OH	3:C:172:PRO:O	2.22	0.51
3:C:89:TYR:OH	3:C:116:ASP:OD1	2.22	0.51
3:C:161:VAL:HG22	3:C:212:LEU:HD13	1.93	0.51
3:C:68:GLN:O	3:C:121:THR:HG22	2.11	0.51
3:C:145:PRO:HB3	3:C:165:CYS:SG	2.51	0.50
3:C:197:ASN:OD1	3:C:199:GLN:N	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ASN:OD1	1:A:213:ASP:HB3	2.11	0.50
3:C:75:LEU:HD11	3:C:78:SER:OG	2.12	0.50
3:C:65:LEU:O	3:C:78:SER:HA	2.12	0.50
3:C:65:LEU:HD21	3:C:67:TRP:CD1	2.47	0.50
2:B:66:SER:O	2:B:67:GLY:C	2.54	0.49
3:C:64:ASN:HB3	3:C:125:SER:C	2.37	0.49
3:C:122:CYS:SG	3:C:122:CYS:O	2.70	0.49
3:C:162:THR:HG22	3:C:209:ARG:HE	1.77	0.49
1:A:2:VAL:HG12	1:A:107:VAL:HG11	1.92	0.49
3:C:65:LEU:O	3:C:65:LEU:HD23	2.12	0.49
3:C:150:GLU:CB	3:C:151:PRO:HD3	2.39	0.49
3:C:227:LEU:O	3:C:228:GLN:HB2	2.12	0.49
2:B:67:GLY:O	2:B:70:PHE:CZ	2.67	0.48
1:A:155:VAL:HG12	1:A:205:HIS:CD2	2.48	0.48
3:C:122:CYS:O	3:C:124:VAL:HG23	2.13	0.48
2:B:135:LEU:HD13	2:B:174:LEU:HD22	1.94	0.48
3:C:65:LEU:HD21	3:C:67:TRP:HD1	1.79	0.48
3:C:168:TYR:HD1	3:C:203:ASP:OD1	1.97	0.48
3:C:190:VAL:CG2	3:C:208:LEU:HD13	2.44	0.48
3:C:137:GLN:OE1	3:C:137:GLN:C	2.57	0.48
3:C:33:VAL:CG1	3:C:132:ALA:HB1	2.44	0.47
3:C:89:TYR:O	3:C:89:TYR:CG	2.68	0.47
3:C:41:LEU:HA	3:C:139:ALA:O	2.15	0.47
3:C:65:LEU:HD23	3:C:65:LEU:C	2.39	0.47
2:B:149:VAL:O	2:B:149:VAL:HG13	2.14	0.47
1:A:66:ASP:OD1	1:A:66:ASP:N	2.47	0.47
2:B:32:ILE:HD12	2:B:32:ILE:C	2.38	0.47
3:C:117:GLU:HG3	3:C:137:GLN:HA	1.96	0.47
3:C:157:PRO:HB3	3:C:213:GLY:HA2	1.95	0.47
1:A:59:THR:CG2	3:C:184:VAL:HG21	2.41	0.47
3:C:154:ASP:OD2	3:C:161:VAL:HG11	2.15	0.47
1:A:46:GLU:OE2	1:A:63:LYS:NZ	2.45	0.46
3:C:33:VAL:HG11	3:C:132:ALA:HB1	1.97	0.46
3:C:48:LEU:HB2	3:C:67:TRP:CH2	2.50	0.46
3:C:156:ARG:O	3:C:157:PRO:C	2.59	0.46
3:C:31:VAL:HG13	3:C:32:GLN:H	1.80	0.46
3:C:180:ASP:OD1	3:C:184:VAL:N	2.47	0.46
3:C:68:GLN:OE1	3:C:75:LEU:HD12	2.16	0.46
3:C:94:ALA:O	3:C:108:ARG:N	2.25	0.46
3:C:48:LEU:HD21	3:C:136:LEU:HD23	1.97	0.45
1:A:183:LEU:HD12	1:A:183:LEU:C	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:THR:O	2:B:50:THR:HG22	2.15	0.45
3:C:161:VAL:O	3:C:209:ARG:HA	2.16	0.45
3:C:66:ILE:CD1	3:C:123:PHE:HB3	2.47	0.45
1:A:143:LEU:HD12	1:A:216:VAL:HG11	1.98	0.45
2:B:108:THR:OG1	2:B:109:VAL:N	2.49	0.45
2:B:37:GLN:O	2:B:83:ALA:HB1	2.17	0.45
3:C:31:VAL:HG13	3:C:32:GLN:N	2.32	0.45
3:C:190:VAL:HG22	3:C:208:LEU:HD13	1.98	0.45
3:C:72:THR:O	3:C:72:THR:OG1	2.31	0.45
1:A:150:TYR:CE1	1:A:155:VAL:HG13	2.52	0.44
2:B:142:GLU:OE2	2:B:142:GLU:HA	2.17	0.44
3:C:149:LEU:CD1	3:C:235:VAL:HG11	2.44	0.44
3:C:219:SER:HB3	3:C:232:HIS:NE2	2.32	0.44
3:C:65:LEU:CD1	3:C:105:ALA:HB1	2.48	0.44
3:C:44:THR:CG2	3:C:45:ASP:N	2.81	0.43
3:C:174:ALA:HB1	3:C:222:VAL:CG1	2.48	0.43
3:C:48:LEU:HD12	3:C:67:TRP:CZ3	2.53	0.43
3:C:164:THR:HG23	3:C:207:ILE:HG13	2.00	0.43
3:C:76:VAL:CG1	3:C:93:THR:HG21	2.48	0.43
1:A:198:THR:HG23	1:A:215:LYS:NZ	2.34	0.43
1:A:2:VAL:HG22	1:A:27:TYR:HB3	2.01	0.43
1:A:183:LEU:HD12	1:A:184:SER:N	2.34	0.43
3:C:139:ALA:CB	3:C:226:VAL:HG11	2.46	0.43
2:B:145:VAL:O	2:B:145:VAL:HG13	2.19	0.43
3:C:149:LEU:HD23	3:C:154:ASP:OD2	2.18	0.43
3:C:169:GLN:HA	3:C:201:LEU:HB3	2.01	0.43
3:C:187:THR:HG22	3:C:187:THR:O	2.19	0.43
1:A:102:PRO:O	1:A:103:TRP:CD1	2.72	0.42
3:C:40:ALA:CB	3:C:46:ALA:HB2	2.49	0.42
1:A:2:VAL:HG11	1:A:107:VAL:HG21	2.01	0.42
3:C:136:LEU:HD11	3:C:138:VAL:CG2	2.50	0.42
3:C:66:ILE:HD11	3:C:123:PHE:CD2	2.54	0.42
3:C:40:ALA:HB1	3:C:46:ALA:HB2	2.01	0.42
3:C:42:VAL:HB	3:C:140:ALA:HB2	2.01	0.42
3:C:47:THR:HG23	3:C:47:THR:O	2.19	0.41
3:C:149:LEU:CD1	3:C:163:ILE:HD12	2.50	0.41
2:B:95:LEU:HD21	3:C:185:PRO:HD2	2.01	0.41
3:C:147:MET:HE3	3:C:147:MET:HB3	1.88	0.41
3:C:33:VAL:HB	3:C:34:PRO:HD2	2.02	0.41
3:C:39:VAL:HA	3:C:137:GLN:O	2.21	0.41
3:C:92:ARG:HH12	3:C:113:ARG:HD2	1.79	0.41

Continued on next page...

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:VAL:HG22	1:A:187:VAL:HG12	2.02	0.41
3:C:48:LEU:HD22	3:C:136:LEU:HD23	2.02	0.40
3:C:161:VAL:HG22	3:C:212:LEU:CD1	2.51	0.40
1:A:92:ALA:O	1:A:113:LEU:HD12	2.21	0.40
1:A:103:TRP:CD1	1:A:103:TRP:O	2.74	0.40
2:B:62:SER:O	2:B:72:LEU:HD12	2.21	0.40
3:C:76:VAL:HG13	3:C:93:THR:HG21	2.02	0.40
3:C:107:LEU:CB	3:C:109:LEU:HD22	2.48	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	216/223 (97%)	211 (98%)	5 (2%)	0	100	100
2	B	211/213 (99%)	206 (98%)	5 (2%)	0	100	100
3	C	171/448 (38%)	143 (84%)	28 (16%)	0	100	100
All	All	598/884 (68%)	560 (94%)	38 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	185/190 (97%)	179 (97%)	6 (3%)	34	65
2	B	187/187 (100%)	181 (97%)	6 (3%)	34	65
3	C	153/375 (41%)	146 (95%)	7 (5%)	24	57
All	All	525/752 (70%)	506 (96%)	19 (4%)	32	63

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	THR
1	A	117	SER
1	A	156	THR
1	A	165	THR
1	A	177	SER
1	A	187	VAL
2	B	1	ASP
2	B	14	SER
2	B	24	SER
2	B	68	THR
2	B	94	PRO
2	B	136	ASN
3	C	45	ASP
3	C	113	ARG
3	C	156	ARG
3	C	191	THR
3	C	212	LEU
3	C	215	ASN
3	C	234	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	HIS
1	A	176	GLN
2	B	78	GLN
2	B	137	ASN
3	C	77	HIS
3	C	215	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.

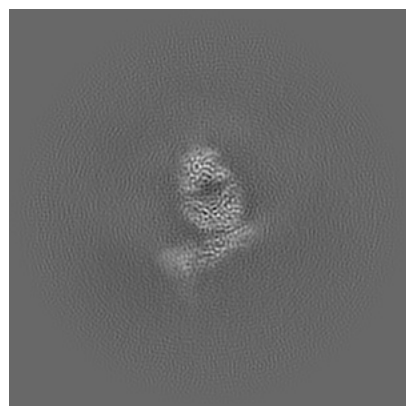
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63503. These allow visual inspection of the internal detail of the map and identification of artifacts.

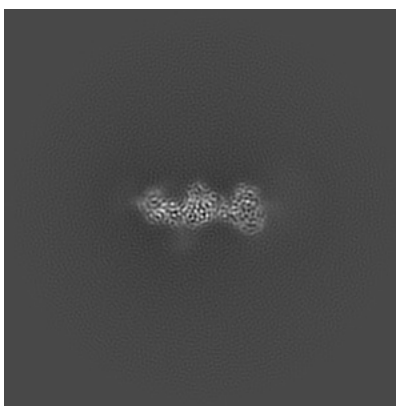
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

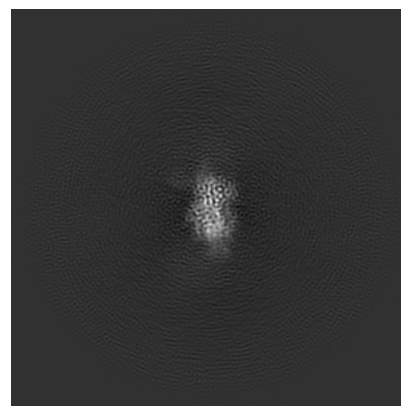
6.1.1 Primary map



X

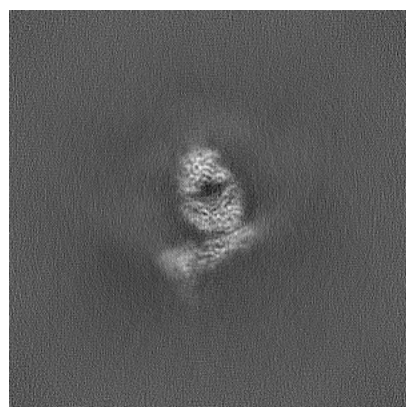


Y

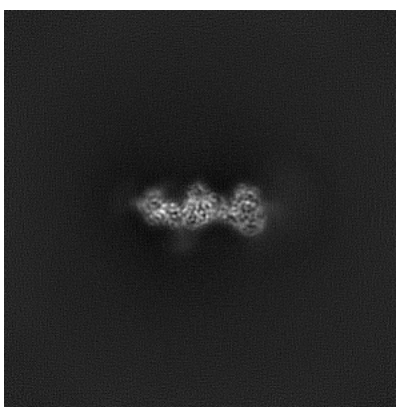


Z

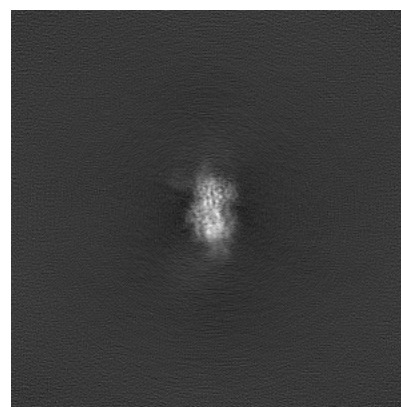
6.1.2 Raw map



X



Y

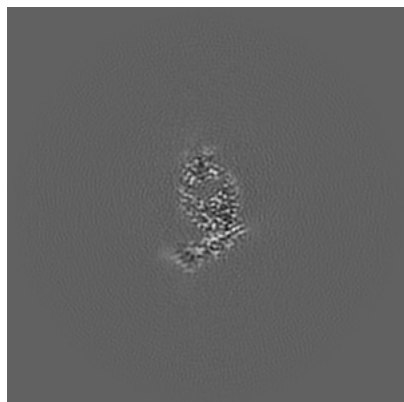


Z

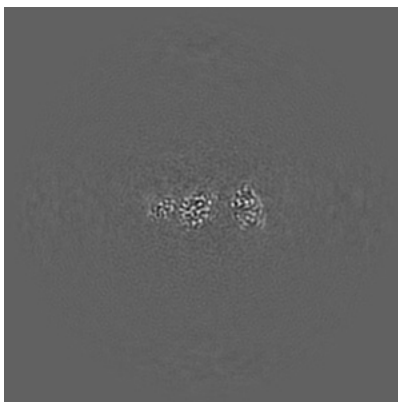
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

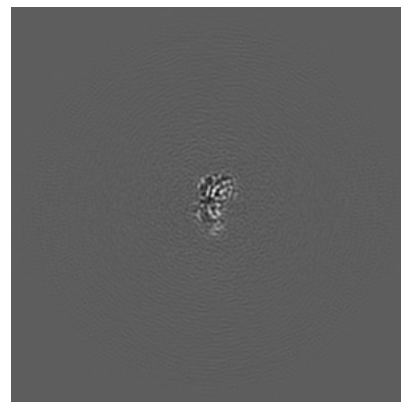
6.2.1 Primary map



X Index: 220

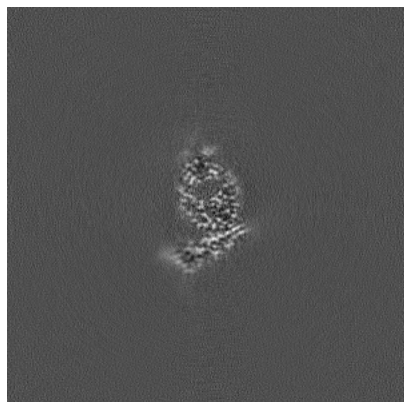


Y Index: 220

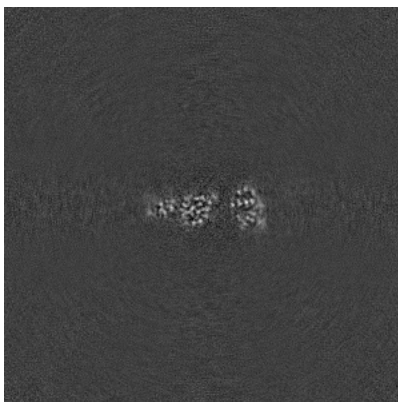


Z Index: 220

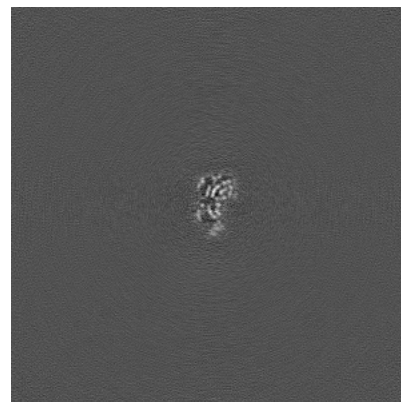
6.2.2 Raw map



X Index: 220



Y Index: 220

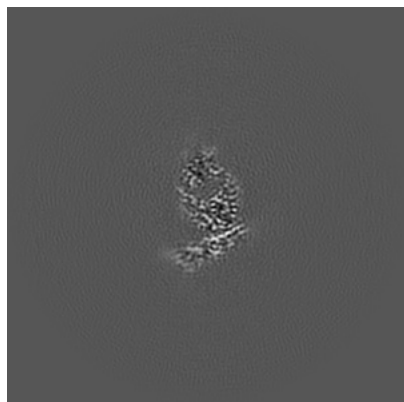


Z Index: 220

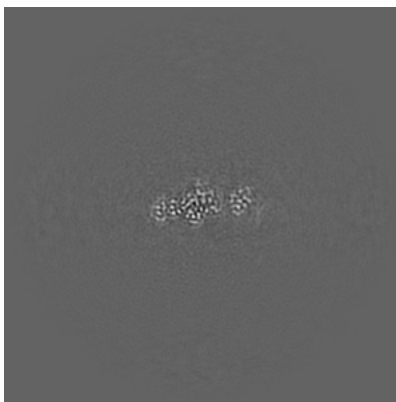
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

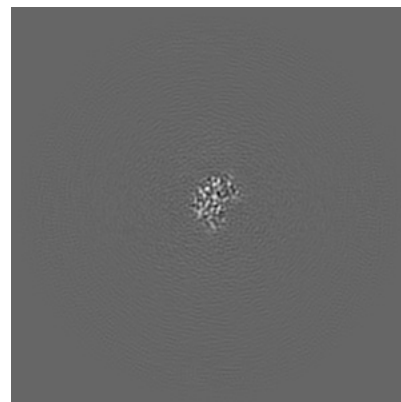
6.3.1 Primary map



X Index: 219

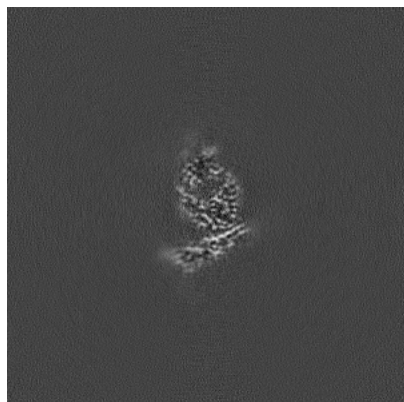


Y Index: 229

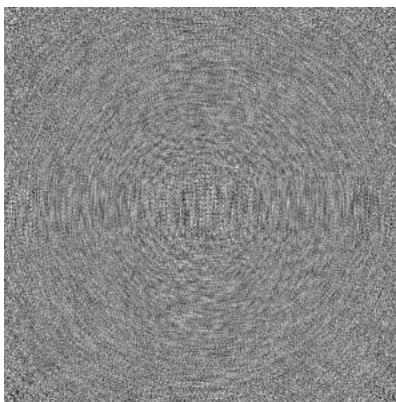


Z Index: 212

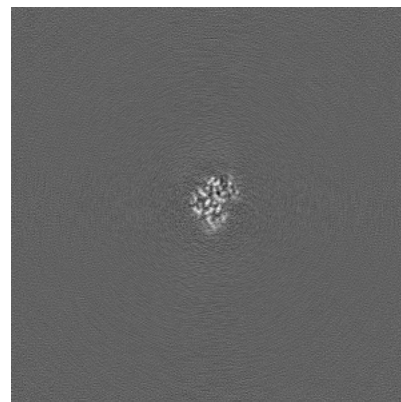
6.3.2 Raw map



X Index: 219



Y Index: 0

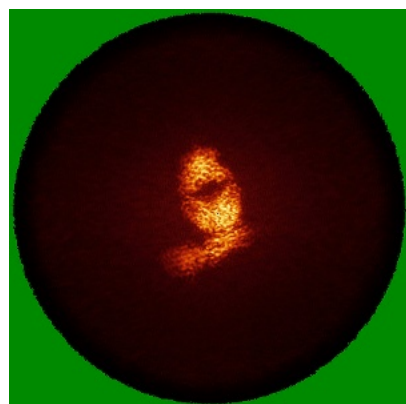


Z Index: 211

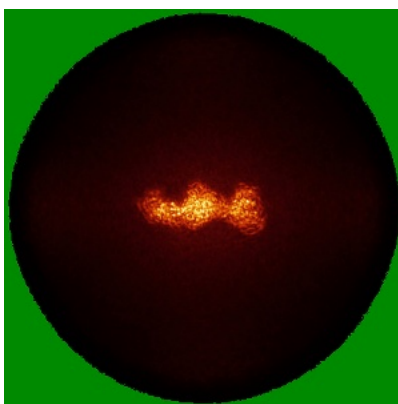
The images above show the largest variance slices of the map in three orthogonal directions.

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

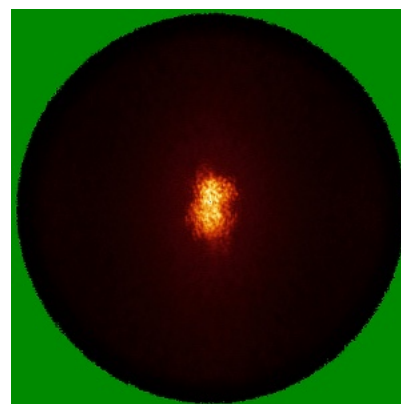
6.4.1 Primary map



X

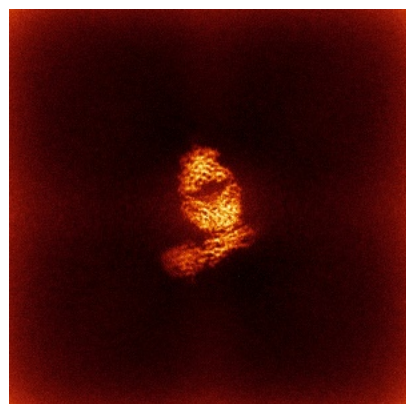


Y

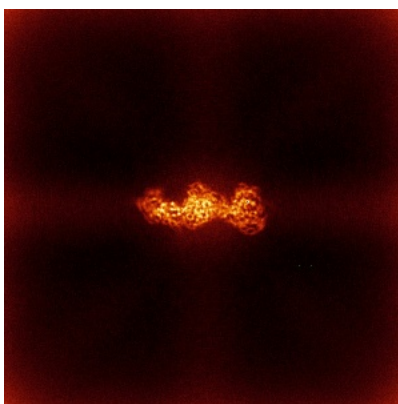


Z

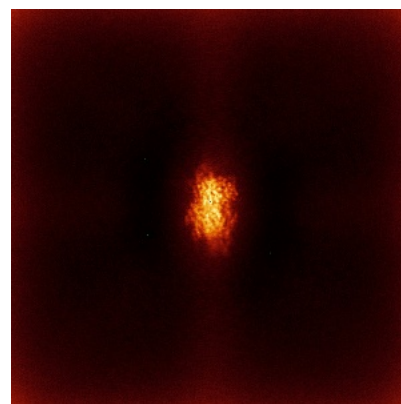
6.4.2 Raw map



X



Y

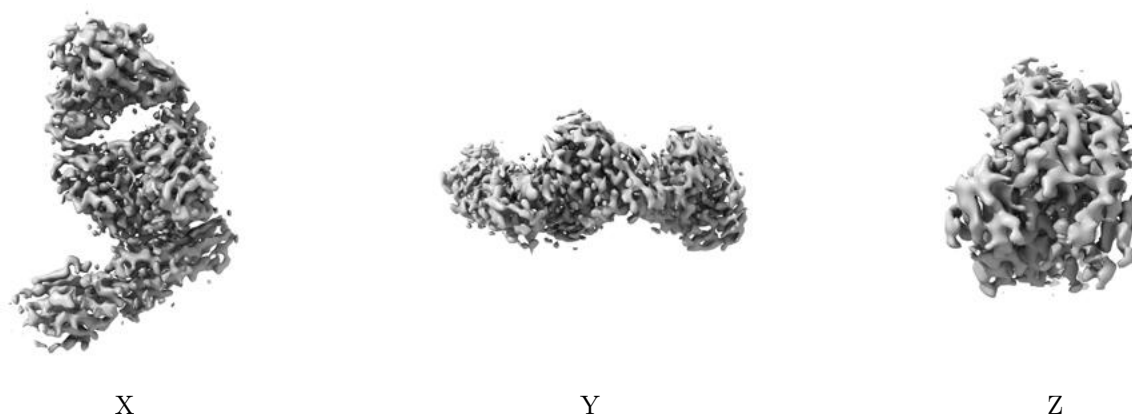


Z

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.

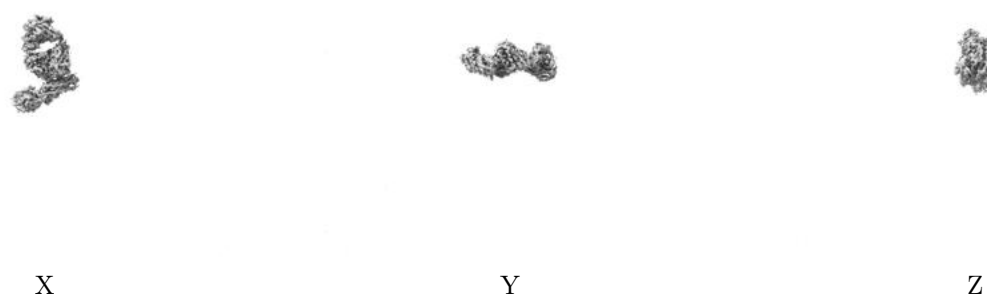
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.164. 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.

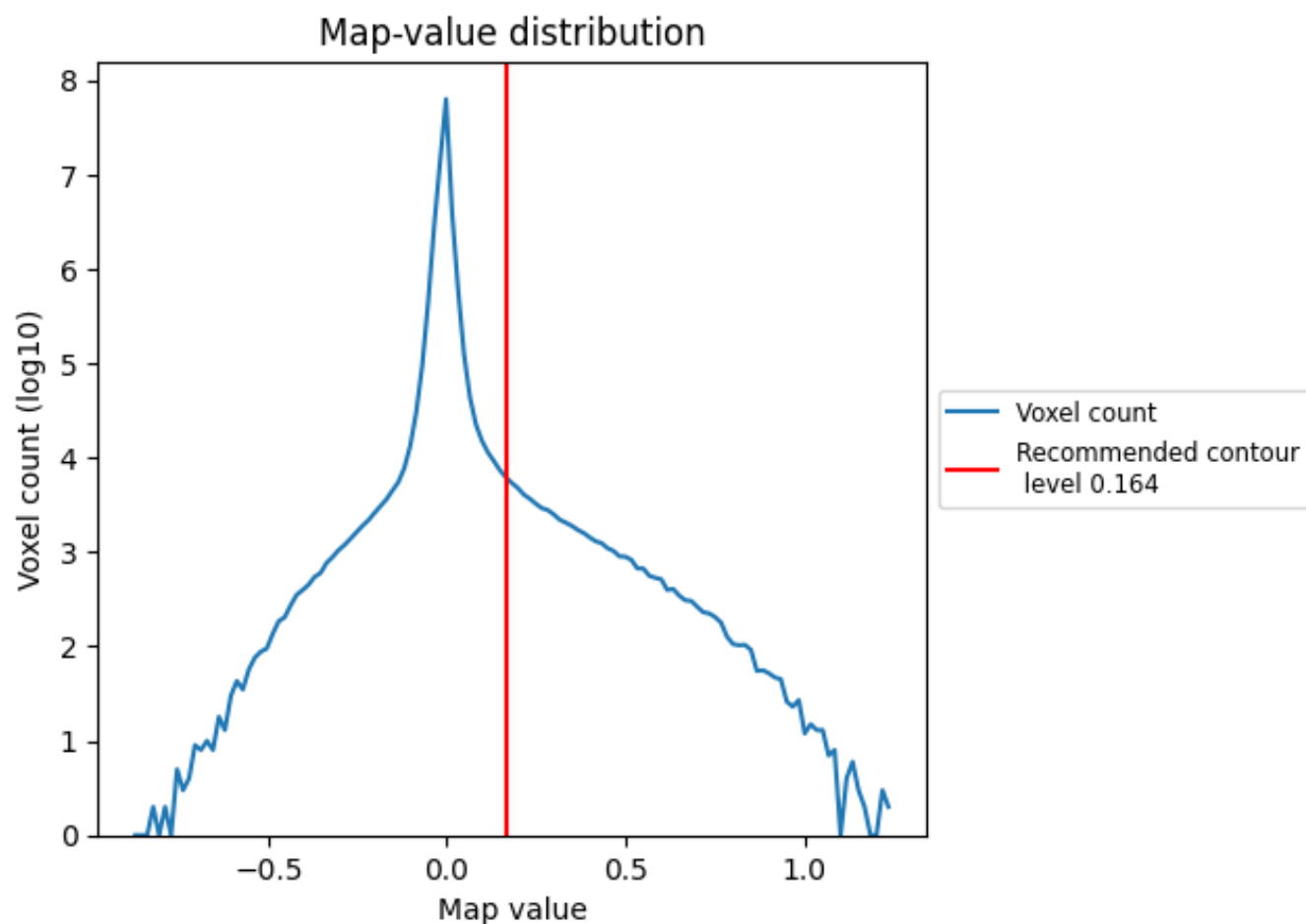
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

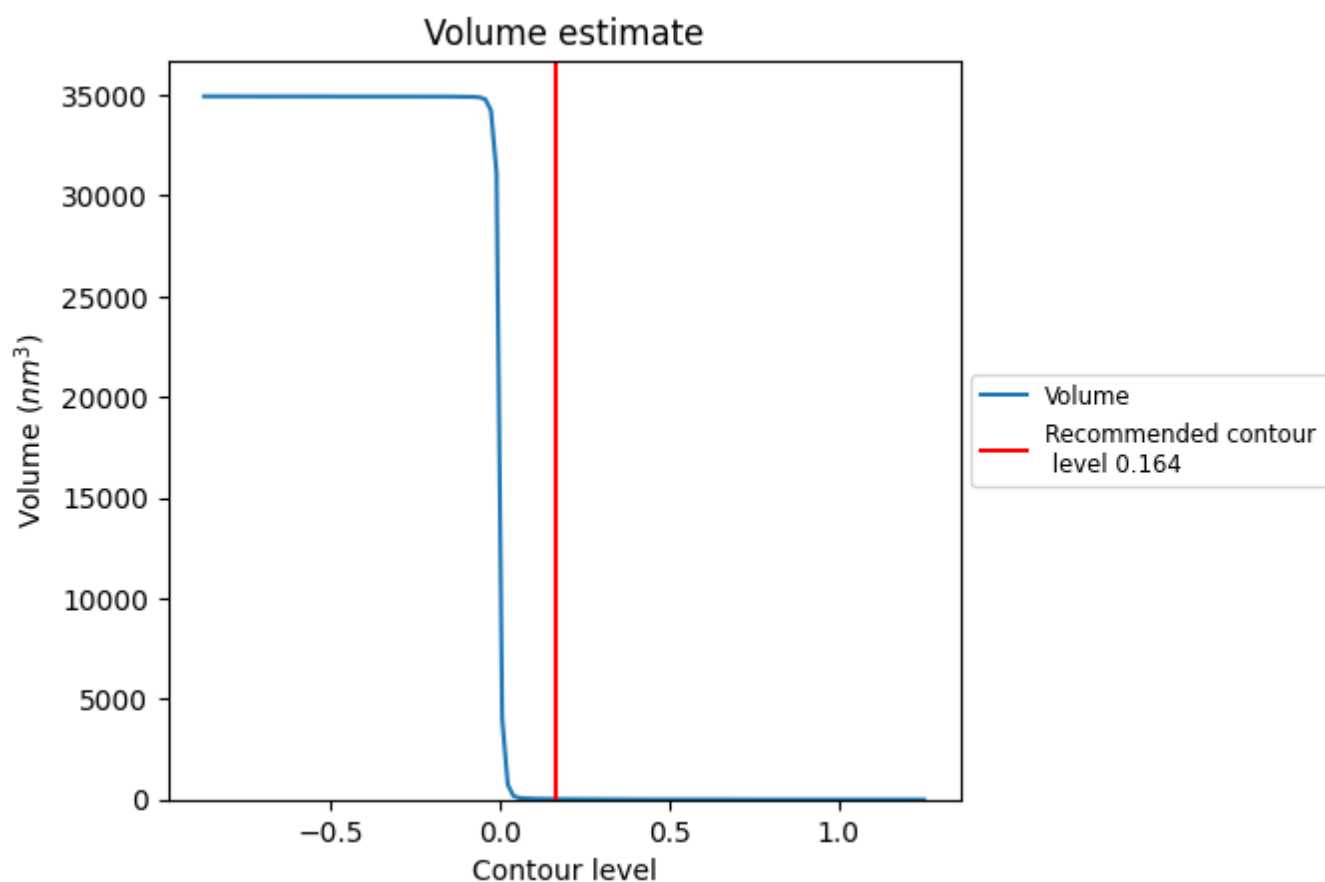
This section contains the results of statistical analysis of the map.

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.

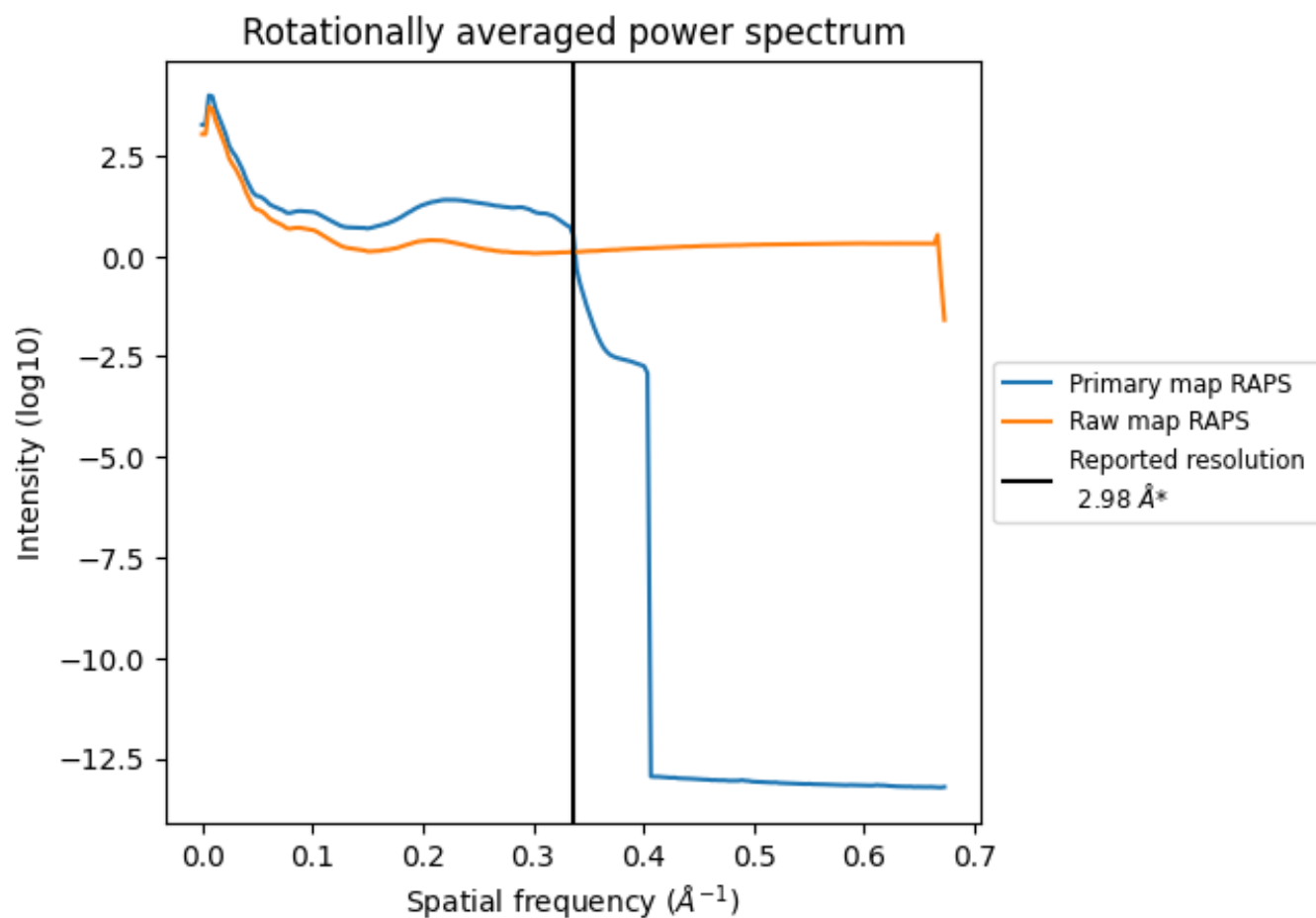
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 25 nm³; this corresponds to an approximate mass of 23 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 ⓘ

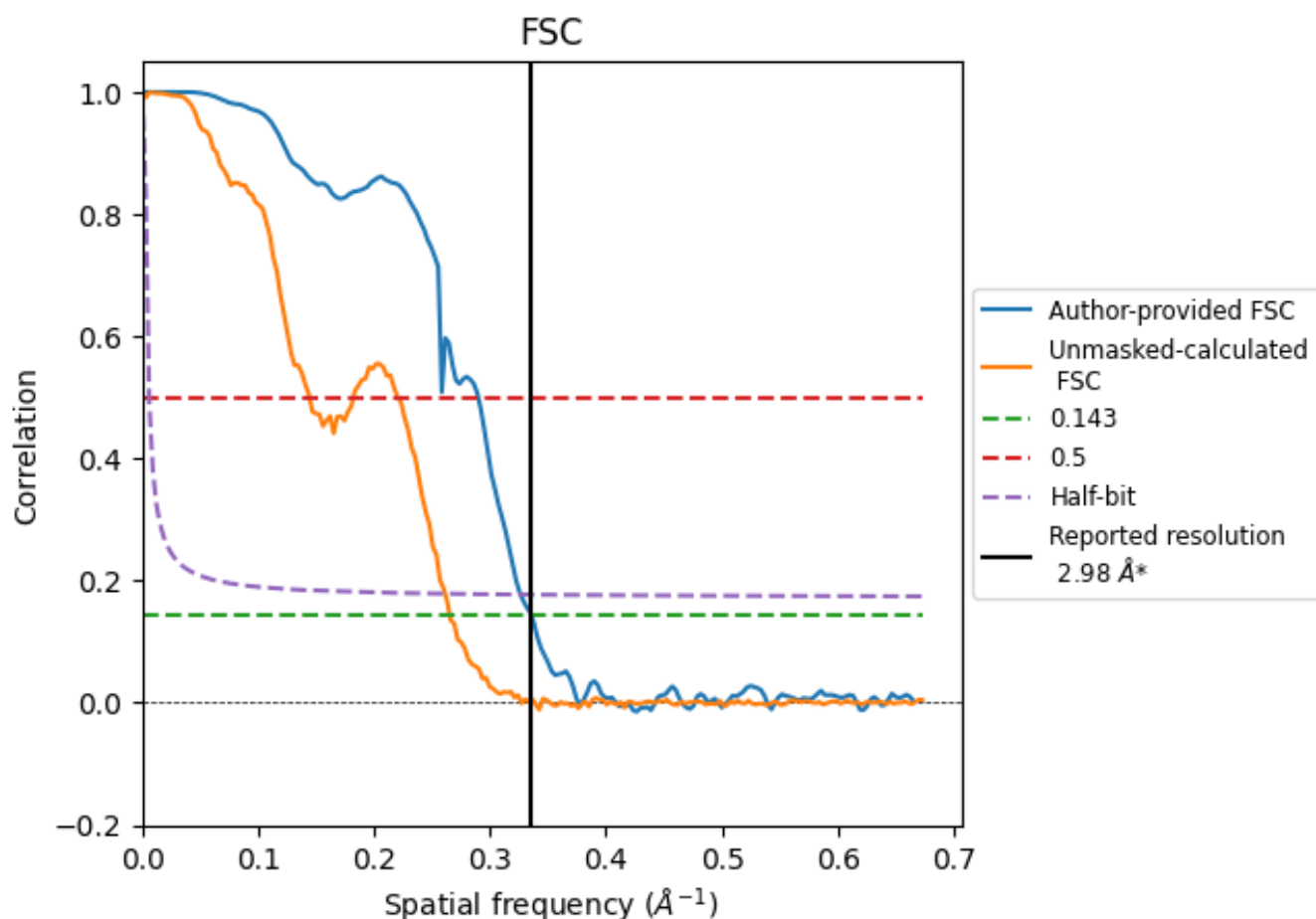


*Reported resolution corresponds to spatial frequency of 0.336 \AA^{-1}

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 0.336 Å⁻¹

8.2 Resolution estimates [i](#)

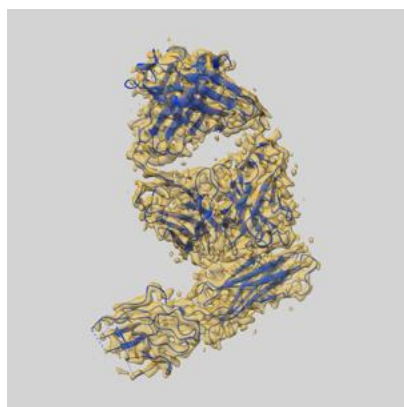
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.98	-	-
Author-provided FSC curve	2.98	3.45	3.06
Unmasked-calculated*	3.77	6.93	3.83

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.77 differs from the reported value 2.98 by more than 10 %

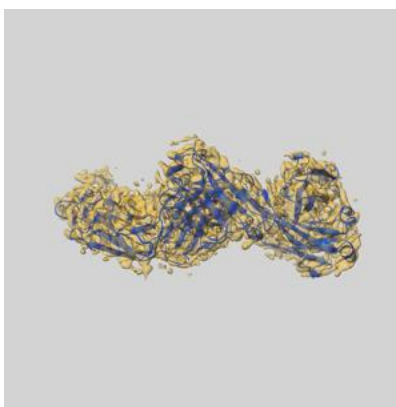
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-63503 and PDB model 9LY5. Per-residue inclusion information can be found in section [3](#) on page [4](#).

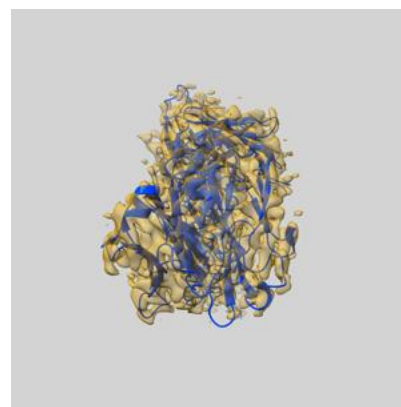
9.1 Map-model overlay [i](#)



X



Y



Z

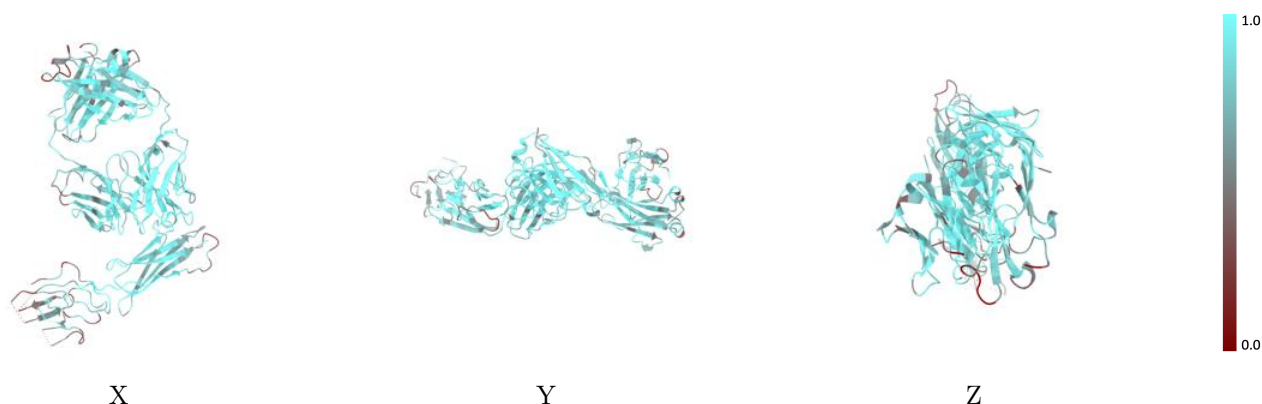
The images above show the 3D surface view of the map at the recommended contour level 0.164 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



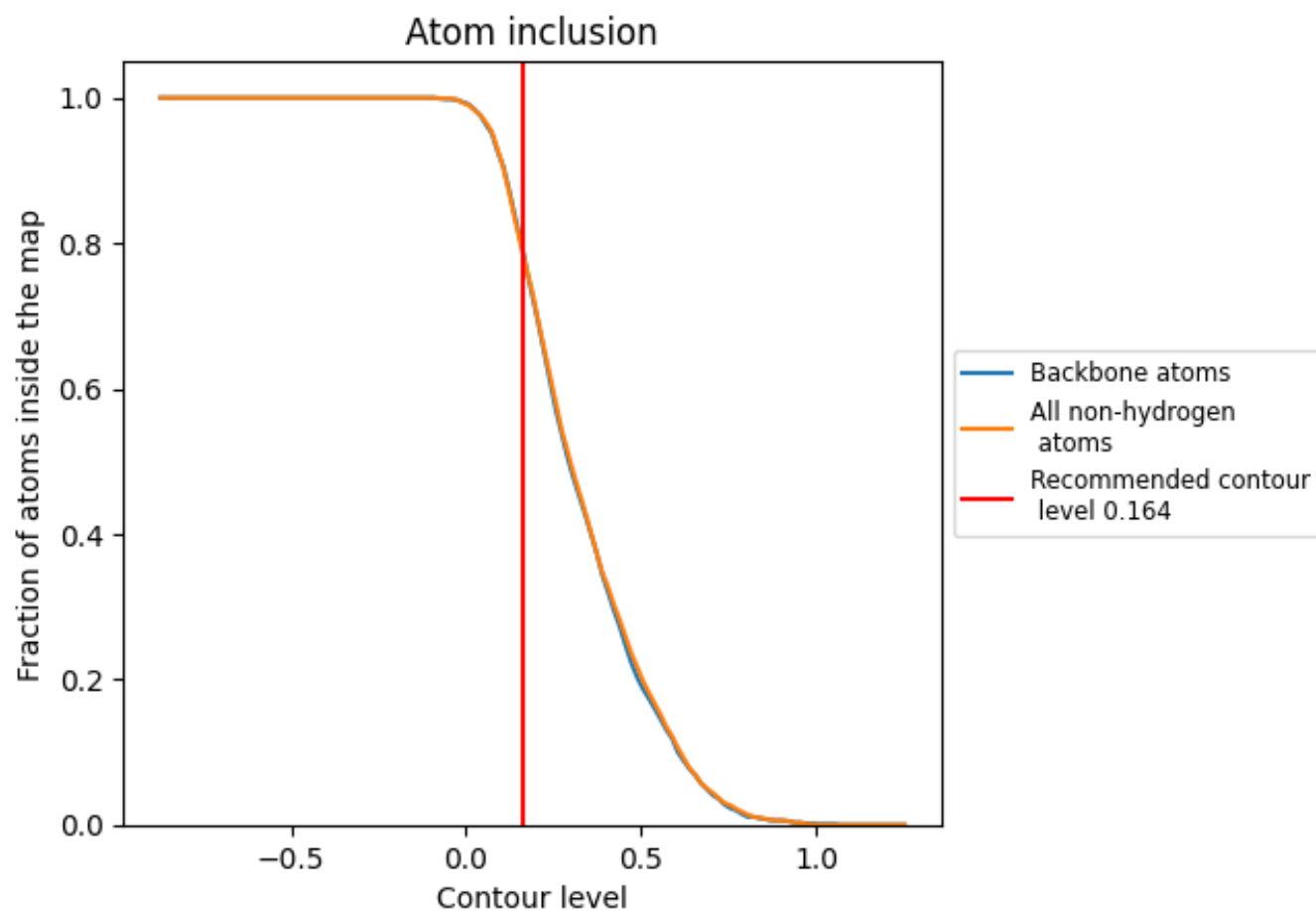
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.164).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 78% 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 (0.164) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7830	<div></div> 0.5450
A	<div></div> 0.8280	<div></div> 0.5590
B	<div></div> 0.8160	<div></div> 0.5590
C	<div></div> 0.7110	<div></div> 0.5120

