



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:47 PM UTC

PDB ID : 3IY4 / pdb_00003iy4
EMDB ID : EMD-5109
Title : Variable domains of the computer generated model (WAM) of Fab 15 fitted into the cryoEM reconstruction of the virus-Fab 15 complex
Authors : Hafenstein, S.; Bowman, V.D.; Sun, T.; Nelson, C.D.; Palermo, L.M.; Chipman, P.R.; Battisti, A.J.; Parrish, C.R.; Rossmann, M.G.
Deposited on : 2009-04-09
Resolution : 11.70 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

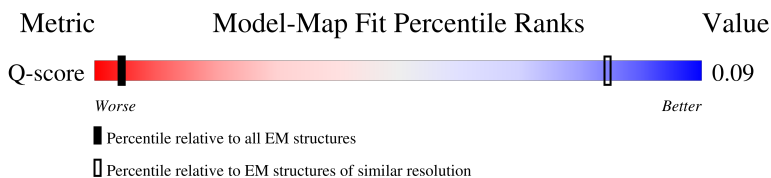
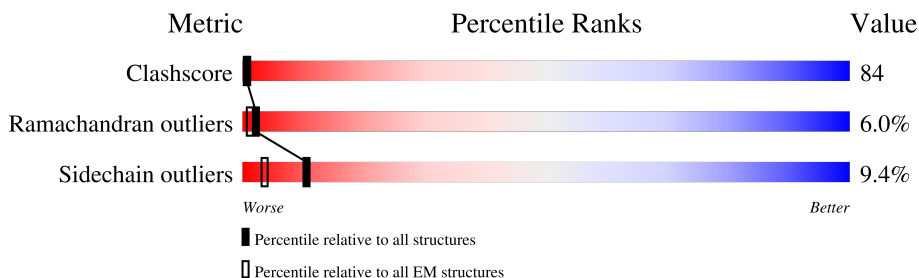
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 11.70 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	89 (11.30 - 12.20)

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	111	 39% 50% 8%
2	B	111	 36% 34% 20% 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1713 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 fragment of neutralizing antibody 15 (light chain).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	111	Total	C	N	O	S	0	0
			841	524	140	173	4		

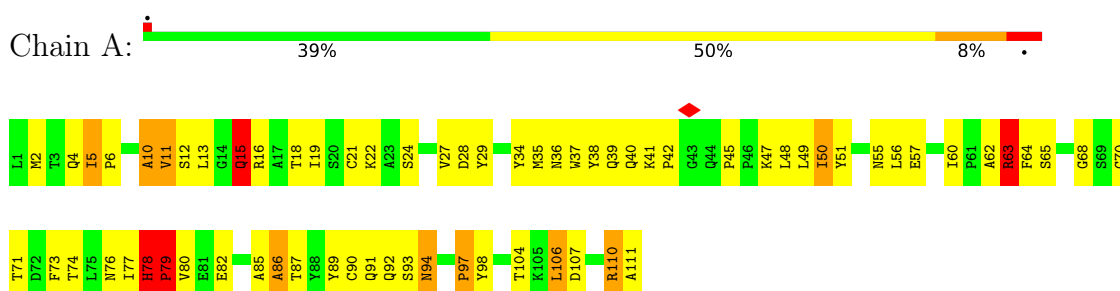
- Molecule 2 is a protein called fragment of neutralizing antibody 15 (heavy chain).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	111	Total	C	N	O	S	0	0
			872	560	143	164	5		

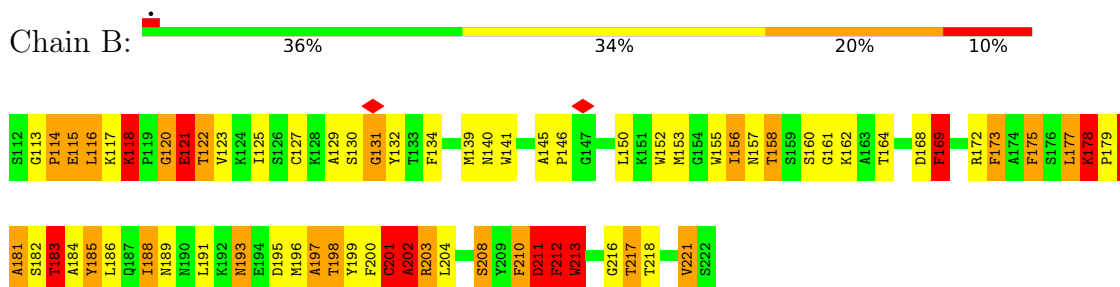
3 Residue-property plots

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

- Molecule 1: fragment of neutralizing antibody 15 (light chain)



- Molecule 2: fragment of neutralizing antibody 15 (heavy chain)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	4798	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	robem	Depositor
Microscope	FEI/PHILIPS CM300FEG/T	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	34.52	Depositor
Minimum defocus (nm)	0.9	Depositor
Maximum defocus (nm)	3.4	Depositor
Magnification	47190	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	6.132	Depositor
Minimum map value	-3.064	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1	Depositor
Map size ($\text{\AA}$)	528.07996, 528.07996, 528.07996	wwPDB
Map dimensions	184, 184, 184	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.8699996, 2.8699996, 2.8699996	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.06	3/860 (0.3%)	2.13	17/1166 (1.5%)
2	B	1.89	18/897 (2.0%)	2.76	54/1210 (4.5%)
All	All	1.54	21/1757 (1.2%)	2.47	71/2376 (3.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	4
2	B	1	10
All	All	2	14

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	213	TRP	NE1-CE2	-24.56	1.10	1.37
2	B	180	SER	CA-CB	16.02	1.79	1.53
2	B	180	SER	CB-OG	11.47	1.65	1.42
1	A	78	HIS	CG-ND1	-11.25	1.25	1.38
2	B	122	THR	CA-C	11.10	1.65	1.52
1	A	78	HIS	CG-CD2	10.76	1.47	1.35
2	B	122	THR	CA-CB	-10.57	1.35	1.53
2	B	122	THR	N-CA	10.22	1.58	1.45
2	B	121	GLU	C-N	9.38	1.46	1.33
2	B	201	CYS	C-N	-8.21	1.22	1.33
2	B	213	TRP	CD2-CE3	-8.20	1.27	1.40
2	B	180	SER	CA-C	-7.73	1.42	1.52
2	B	169	PHE	CE1-CZ	-6.66	1.18	1.38
2	B	188	ILE	CA-CB	6.46	1.62	1.54
2	B	180	SER	N-CA	6.44	1.54	1.46
2	B	188	ILE	CA-C	6.18	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	125	ILE	CA-CB	6.10	1.63	1.54
2	B	125	ILE	CA-C	6.09	1.60	1.52
2	B	202	ALA	C-N	5.68	1.41	1.33
1	A	79	PRO	N-CD	-5.39	1.40	1.47
2	B	169	PHE	CD2-CE2	-5.26	1.22	1.38

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	HIS	CE1-NE2-CD2	-37.64	71.36	109.00
2	B	180	SER	CB-CA-C	-31.97	57.08	110.79
2	B	180	SER	N-CA-CB	20.65	140.70	110.13
2	B	188	ILE	CA-CB-CG2	18.93	142.68	110.50
1	A	78	HIS	ND1-CE1-NE2	18.89	127.30	108.40
2	B	188	ILE	N-CA-CB	-16.50	92.55	110.53
2	B	188	ILE	CB-CA-C	16.06	132.03	111.15
1	A	78	HIS	CG-ND1-CE1	-15.77	82.50	109.30
2	B	125	ILE	CA-CB-CG2	15.76	137.28	110.50
1	A	79	PRO	CA-N-CD	-15.29	90.59	112.00
2	B	122	THR	CA-CB-OG1	-14.82	87.37	109.60
2	B	203	ARG	N-CA-C	-14.51	86.81	110.17
2	B	125	ILE	CB-CA-C	14.02	132.47	111.31
2	B	175	PHE	N-CA-CB	-13.75	89.39	110.29
1	A	79	PRO	N-CD-CG	13.45	123.37	103.20
2	B	169	PHE	CE1-CZ-CE2	12.84	143.12	120.00
2	B	169	PHE	CD1-CE1-CZ	-11.79	98.77	120.00
2	B	156	ILE	N-CA-CB	11.26	129.80	111.23
2	B	201	CYS	O-C-N	-11.01	107.94	122.59
2	B	158	THR	N-CA-CB	-10.82	91.45	110.39
2	B	156	ILE	CB-CA-C	-10.68	93.78	111.29
2	B	183	THR	CA-CB-CG2	-10.66	92.38	110.50
2	B	130	SER	O-C-N	9.89	134.55	123.48
1	A	63	ARG	CA-C-O	9.74	134.44	120.51
2	B	169	PHE	CZ-CE2-CD2	-9.09	103.64	120.00
2	B	180	SER	CA-CB-OG	9.05	129.20	111.10
2	B	122	THR	N-CA-C	8.88	124.07	109.95
2	B	156	ILE	CA-CB-CG2	8.80	125.47	110.50
1	A	63	ARG	CA-CB-CG	-8.59	96.92	114.10
2	B	193	ASN	OD1-CG-ND2	-8.57	114.03	122.60
1	A	79	PRO	CB-CG-CD	-8.43	79.13	106.10
2	B	202	ALA	N-CA-CB	7.95	123.93	110.49
2	B	221	VAL	O-C-N	-7.79	113.51	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	156	ILE	CA-CB-CG1	7.41	122.99	110.40
2	B	121	GLU	CA-C-O	-7.40	109.93	120.51
1	A	94	ASN	CB-CA-C	-7.30	98.53	110.79
2	B	178	LYS	CG-CD-CE	7.27	128.02	111.30
2	B	181	ALA	N-CA-C	-7.17	104.27	113.16
2	B	213	TRP	CD2-CE2-CZ2	7.08	129.48	122.40
2	B	118	LYS	CD-CE-NZ	6.94	134.11	111.90
1	A	78	HIS	C-N-CD	-6.70	97.52	125.00
2	B	213	TRP	CG-CD1-NE1	-6.54	101.70	110.20
2	B	180	SER	CA-C-O	-6.50	113.60	120.55
2	B	125	ILE	N-CA-CB	-6.39	97.83	111.37
2	B	121	GLU	CB-CA-C	6.20	122.76	110.42
2	B	201	CYS	CA-C-O	6.17	129.34	120.51
2	B	201	CYS	N-CA-C	-6.16	97.68	110.80
2	B	175	PHE	CB-CA-C	-6.08	98.27	109.46
2	B	212	PHE	N-CA-CB	-6.07	100.23	110.49
1	A	45	PRO	CB-CA-C	5.93	118.15	110.92
2	B	211	ASP	CB-CA-C	5.90	119.11	110.26
2	B	212	PHE	O-C-N	-5.73	114.97	122.59
2	B	125	ILE	N-CA-C	-5.66	100.20	108.97
2	B	156	ILE	O-C-N	5.59	129.55	122.57
2	B	213	TRP	CD1-NE1-CE2	5.56	118.91	108.90
2	B	160	SER	N-CA-C	-5.44	106.65	113.72
1	A	10	ALA	CB-CA-C	5.42	118.67	109.84
1	A	24	SER	N-CA-C	-5.40	106.20	112.89
2	B	131	GLY	N-CA-C	-5.39	100.42	113.18
2	B	169	PHE	CD1-CG-CD2	5.38	126.66	118.60
2	B	213	TRP	NE1-CE2-CD2	-5.36	100.43	107.40
2	B	188	ILE	CA-CB-CG1	-5.28	101.42	110.40
2	B	212	PHE	N-CA-C	5.22	121.92	110.80
2	B	178	LYS	CD-CE-NZ	5.16	128.41	111.90
2	B	118	LYS	CG-CD-CE	5.08	122.99	111.30
1	A	28	ASP	N-CA-C	5.08	117.00	108.73
1	A	97	PRO	CB-CA-C	-5.04	99.39	112.00
1	A	15	GLN	OE1-CD-NE2	-5.02	117.58	122.60
2	B	120	GLY	CA-C-N	-5.01	111.97	121.54
2	B	120	GLY	C-N-CA	-5.01	111.97	121.54
1	A	97	PRO	CA-CB-CG	5.00	113.51	104.00

All (2) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
1	A	63	ARG	CA
2	B	212	PHE	CA

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	62	ALA	Peptide
1	A	63	ARG	Mainchain
1	A	78	HIS	Mainchain,Sidechain
2	B	121	GLU	Peptide,Mainchain
2	B	131	GLY	Peptide
2	B	164	THR	Peptide
2	B	169	PHE	Sidechain
2	B	173	PHE	Sidechain
2	B	185	TYR	Sidechain
2	B	201	CYS	Mainchain
2	B	202	ALA	Peptide
2	B	210	PHE	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	841	0	801	95	0
2	B	872	0	837	194	0
All	All	1713	0	1638	280	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 84.

All (280) 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:B:180:SER:CB	2:B:180:SER:OG	1.65	1.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:MET:HE3	2:B:173:PHE:CD2	1.67	1.28
2:B:118:LYS:HE3	2:B:121:GLU:CG	1.71	1.19
2:B:118:LYS:CE	2:B:121:GLU:HG3	1.77	1.14
2:B:153:MET:HE2	2:B:186:LEU:HD11	1.37	1.05
2:B:212:PHE:HA	2:B:213:TRP:HB3	1.35	1.05
1:A:78:HIS:CG	1:A:79:PRO:HD2	1.91	1.05
2:B:153:MET:HE3	2:B:173:PHE:CE2	1.92	1.05
2:B:118:LYS:HE3	2:B:121:GLU:HG3	1.03	1.02
2:B:183:THR:HG21	2:B:185:TYR:CZ	1.94	1.02
2:B:117:LYS:CD	2:B:191:LEU:HD12	1.88	1.02
2:B:153:MET:SD	2:B:186:LEU:HD21	2.00	1.01
2:B:153:MET:CE	2:B:186:LEU:HD21	1.92	1.00
2:B:117:LYS:HE2	2:B:121:GLU:CB	1.94	0.98
2:B:153:MET:HE1	2:B:188:ILE:HD11	1.47	0.96
1:A:97:PRO:HB3	2:B:152:TRP:CZ3	2.02	0.94
2:B:117:LYS:CG	2:B:121:GLU:HB2	1.97	0.94
2:B:183:THR:HG21	2:B:185:TYR:CE2	2.03	0.92
1:A:34:TYR:HB3	1:A:93:SER:HB3	1.49	0.91
1:A:57:GLU:O	1:A:60:ILE:HG22	1.72	0.90
1:A:78:HIS:CB	1:A:79:PRO:HD2	2.03	0.89
2:B:117:LYS:HD2	2:B:191:LEU:HD12	1.55	0.88
2:B:117:LYS:CD	2:B:121:GLU:HB2	2.04	0.86
2:B:117:LYS:HZ1	2:B:122:THR:HA	1.38	0.86
2:B:178:LYS:HD2	2:B:181:ALA:H	1.41	0.86
2:B:186:LEU:CG	2:B:188:ILE:HD11	2.05	0.84
2:B:186:LEU:CD2	2:B:188:ILE:HD11	2.07	0.84
1:A:27:VAL:HA	1:A:94:ASN:HB2	1.58	0.84
2:B:117:LYS:HE3	2:B:122:THR:O	1.78	0.83
2:B:123:VAL:HG12	2:B:188:ILE:HB	1.60	0.83
1:A:18:THR:HG23	1:A:74:THR:CG2	2.07	0.83
2:B:186:LEU:HG	2:B:188:ILE:HD11	1.60	0.83
2:B:118:LYS:HG2	2:B:121:GLU:CG	2.09	0.82
2:B:153:MET:HE2	2:B:186:LEU:CD1	2.09	0.82
2:B:117:LYS:HD3	2:B:191:LEU:HD12	1.58	0.82
2:B:156:ILE:HB	2:B:175:PHE:CE2	2.16	0.80
1:A:27:VAL:HG11	1:A:92:GLN:HB2	1.64	0.80
2:B:118:LYS:HE3	2:B:121:GLU:CD	2.07	0.80
2:B:196:MET:HG2	2:B:221:VAL:H	1.44	0.80
2:B:156:ILE:HB	2:B:175:PHE:CD2	2.18	0.79
1:A:40:GLN:O	1:A:86:ALA:HB1	1.81	0.79
1:A:5:ILE:HD12	1:A:6:PRO:HA	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:117:LYS:HG2	2:B:121:GLU:HB2	1.63	0.79
1:A:10:ALA:HA	1:A:107:ASP:OD1	1.82	0.79
1:A:78:HIS:CD2	1:A:79:PRO:HD2	2.18	0.78
1:A:15:GLN:HA	1:A:15:GLN:OE1	1.85	0.76
2:B:117:LYS:HE2	2:B:121:GLU:HB2	1.67	0.75
2:B:132:TYR:CE2	2:B:203:ARG:HD2	2.22	0.75
1:A:29:TYR:HB3	1:A:34:TYR:CE2	2.22	0.75
1:A:27:VAL:HA	1:A:94:ASN:CB	2.16	0.75
2:B:153:MET:HE1	2:B:186:LEU:HD21	1.70	0.74
2:B:153:MET:CE	2:B:186:LEU:CD2	2.66	0.74
2:B:114:PRO:O	2:B:115:GLU:HG2	1.87	0.74
2:B:118:LYS:HE2	2:B:118:LYS:H	1.53	0.74
2:B:202:ALA:HA	2:B:213:TRP:CD1	2.23	0.74
1:A:36:ASN:OD1	1:A:91:GLN:HB3	1.88	0.73
2:B:123:VAL:HG12	2:B:188:ILE:HG22	1.71	0.73
2:B:117:LYS:CE	2:B:121:GLU:HB2	2.18	0.72
1:A:34:TYR:HD2	1:A:94:ASN:HA	1.54	0.72
2:B:153:MET:HE1	2:B:188:ILE:CD1	2.19	0.72
2:B:158:THR:CA	2:B:177:LEU:HD21	2.21	0.71
1:A:29:TYR:HB2	1:A:94:ASN:ND2	2.04	0.71
2:B:123:VAL:CG1	2:B:188:ILE:HG22	2.22	0.70
2:B:178:LYS:HD2	2:B:181:ALA:N	2.06	0.70
2:B:178:LYS:C	2:B:178:LYS:HD3	2.16	0.69
2:B:193:ASN:O	2:B:196:MET:HG3	1.91	0.69
1:A:48:LEU:HB2	2:B:212:PHE:CE2	2.28	0.69
2:B:203:ARG:HB3	2:B:211:ASP:O	1.93	0.69
1:A:41:LYS:HA	1:A:86:ALA:CB	2.23	0.69
2:B:183:THR:HG22	2:B:183:THR:O	1.82	0.69
2:B:139:MET:SD	2:B:184:ALA:HB2	2.34	0.68
1:A:22:LYS:HA	1:A:71:THR:O	1.93	0.68
2:B:118:LYS:HG2	2:B:121:GLU:HG2	1.74	0.68
2:B:153:MET:CE	2:B:173:PHE:CD2	2.63	0.68
2:B:216:GLY:O	2:B:217:THR:HB	1.96	0.67
1:A:27:VAL:CA	1:A:94:ASN:HB2	2.24	0.66
2:B:117:LYS:HZ3	2:B:191:LEU:HD12	1.60	0.66
1:A:2:MET:HG2	1:A:90:CYS:SG	2.35	0.66
1:A:48:LEU:HB2	2:B:212:PHE:HE2	1.59	0.66
1:A:18:THR:HG23	1:A:74:THR:HG21	1.77	0.66
2:B:114:PRO:HD3	2:B:217:THR:OG1	1.96	0.65
1:A:89:TYR:CD1	2:B:150:LEU:HD12	2.31	0.65
2:B:117:LYS:HE2	2:B:121:GLU:HB3	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:VAL:HG21	1:A:35:MET:HE2	1.79	0.64
2:B:153:MET:HE1	2:B:186:LEU:CD2	2.26	0.64
2:B:186:LEU:HG	2:B:188:ILE:CD1	2.27	0.64
2:B:203:ARG:HE	2:B:211:ASP:CG	2.06	0.64
2:B:169:PHE:CD2	2:B:173:PHE:CE2	2.86	0.64
2:B:123:VAL:HG12	2:B:188:ILE:CG2	2.28	0.63
2:B:117:LYS:HE2	2:B:121:GLU:CA	2.27	0.63
2:B:117:LYS:HE2	2:B:121:GLU:C	2.23	0.63
2:B:178:LYS:HD3	2:B:180:SER:H	1.64	0.63
2:B:117:LYS:HE2	2:B:122:THR:N	2.14	0.62
2:B:117:LYS:HZ3	2:B:191:LEU:CD1	2.12	0.62
2:B:117:LYS:NZ	2:B:122:THR:HA	2.15	0.62
2:B:180:SER:CB	2:B:180:SER:HG	2.08	0.62
2:B:158:THR:O	2:B:177:LEU:HD11	2.00	0.61
2:B:117:LYS:NZ	2:B:191:LEU:HD12	2.14	0.61
1:A:41:LYS:HA	1:A:86:ALA:HB2	1.82	0.61
2:B:123:VAL:CG1	2:B:188:ILE:CG2	2.79	0.61
1:A:110:ARG:HG2	1:A:111:ALA:N	2.15	0.61
2:B:153:MET:HE2	2:B:186:LEU:CG	2.31	0.61
2:B:153:MET:CE	2:B:186:LEU:CG	2.79	0.61
1:A:76:ASN:HD22	1:A:77:ILE:N	1.99	0.60
2:B:198:THR:HG21	2:B:200:PHE:CZ	2.36	0.60
1:A:2:MET:HE1	1:A:35:MET:HE1	1.83	0.60
1:A:38:TYR:HE1	2:B:212:PHE:HZ	1.49	0.59
2:B:204:LEU:HA	2:B:210:PHE:HD1	1.67	0.59
1:A:29:TYR:HB3	1:A:34:TYR:HE2	1.66	0.59
1:A:18:THR:CG2	1:A:74:THR:CG2	2.81	0.59
2:B:186:LEU:HD23	2:B:188:ILE:HD11	1.85	0.59
1:A:49:LEU:HB3	1:A:60:ILE:HD12	1.84	0.58
1:A:49:LEU:CA	1:A:60:ILE:HD12	2.34	0.58
1:A:12:SER:O	1:A:15:GLN:HB2	2.03	0.58
2:B:114:PRO:HB2	2:B:218:THR:O	2.04	0.57
2:B:117:LYS:HZ3	2:B:191:LEU:CG	2.17	0.57
2:B:178:LYS:CD	2:B:181:ALA:H	2.15	0.57
1:A:5:ILE:HD12	1:A:6:PRO:CA	2.34	0.56
2:B:158:THR:HB	2:B:177:LEU:HD21	1.86	0.56
2:B:196:MET:CE	2:B:221:VAL:O	2.52	0.56
1:A:50:ILE:HD11	1:A:56:LEU:CD2	2.35	0.56
1:A:18:THR:HG23	1:A:74:THR:HG23	1.86	0.56
2:B:127:CYS:HG	2:B:201:CYS:HG	0.56	0.56
2:B:156:ILE:N	2:B:175:PHE:HE2	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:THR:HB	2:B:177:LEU:CD2	2.35	0.56
2:B:117:LYS:NZ	2:B:191:LEU:CD1	2.69	0.56
1:A:49:LEU:HB3	1:A:60:ILE:CD1	2.36	0.56
1:A:78:HIS:CD2	1:A:79:PRO:CG	2.88	0.56
2:B:118:LYS:O	2:B:121:GLU:HG2	2.06	0.56
1:A:27:VAL:HG11	1:A:92:GLN:CB	2.34	0.55
2:B:153:MET:CE	2:B:173:PHE:CE2	2.79	0.55
1:A:49:LEU:HA	1:A:60:ILE:HD12	1.89	0.55
1:A:42:PRO:HD3	1:A:86:ALA:HB2	1.87	0.55
1:A:50:ILE:CD1	1:A:56:LEU:HD23	2.37	0.55
2:B:156:ILE:HG13	2:B:162:LYS:C	2.32	0.54
1:A:16:ARG:HG3	1:A:76:ASN:HD21	1.73	0.54
1:A:15:GLN:OE1	1:A:15:GLN:CA	2.56	0.54
2:B:140:ASN:O	2:B:201:CYS:HA	2.07	0.54
2:B:158:THR:CB	2:B:177:LEU:HD21	2.38	0.53
1:A:49:LEU:CB	1:A:60:ILE:HD12	2.38	0.53
2:B:117:LYS:HZ1	2:B:122:THR:CA	2.16	0.53
2:B:118:LYS:CE	2:B:118:LYS:H	2.20	0.53
2:B:188:ILE:HG23	2:B:191:LEU:HD21	1.90	0.53
2:B:196:MET:O	2:B:197:ALA:HB2	2.09	0.53
1:A:50:ILE:HD11	1:A:56:LEU:HD23	1.90	0.53
1:A:93:SER:HA	1:A:98:TYR:HD1	1.74	0.52
1:A:27:VAL:HG21	1:A:35:MET:CE	2.40	0.52
1:A:41:LYS:HZ2	1:A:47:LYS:NZ	2.07	0.52
2:B:129:ALA:HA	2:B:213:TRP:CZ3	2.44	0.52
2:B:145:ALA:HB1	2:B:146:PRO:HD2	1.92	0.52
1:A:27:VAL:CB	1:A:94:ASN:HB2	2.40	0.52
2:B:113:GLY:N	2:B:114:PRO:CD	2.73	0.51
2:B:204:LEU:HA	2:B:210:PHE:HA	1.92	0.51
2:B:183:THR:HG23	2:B:184:ALA:N	2.20	0.51
2:B:114:PRO:C	2:B:115:GLU:HG2	2.35	0.51
2:B:114:PRO:HG3	2:B:217:THR:OG1	2.10	0.51
1:A:56:LEU:HD21	1:A:64:PHE:O	2.09	0.51
2:B:183:THR:HG21	2:B:185:TYR:OH	2.07	0.51
2:B:118:LYS:HG2	2:B:121:GLU:HG3	1.90	0.51
1:A:11:VAL:HG12	1:A:106:LEU:HD11	1.93	0.51
2:B:188:ILE:CG2	2:B:191:LEU:HD21	2.41	0.51
2:B:178:LYS:CD	2:B:180:SER:H	2.24	0.50
2:B:158:THR:O	2:B:177:LEU:HD21	2.11	0.50
2:B:186:LEU:CG	2:B:188:ILE:CD1	2.85	0.50
2:B:114:PRO:CD	2:B:217:THR:OG1	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:PRO:CG	2:B:217:THR:OG1	2.59	0.50
2:B:158:THR:CA	2:B:177:LEU:CD2	2.90	0.50
1:A:41:LYS:HZ2	1:A:47:LYS:HZ2	1.60	0.50
1:A:93:SER:HA	1:A:98:TYR:CD1	2.46	0.50
2:B:169:PHE:CD2	2:B:173:PHE:CD2	3.00	0.50
2:B:177:LEU:CD1	2:B:177:LEU:C	2.85	0.50
1:A:106:LEU:HD12	1:A:107:ASP:N	2.26	0.50
2:B:158:THR:C	2:B:177:LEU:HD21	2.37	0.50
2:B:118:LYS:CD	2:B:121:GLU:HG3	2.39	0.49
2:B:217:THR:HG23	2:B:217:THR:O	2.11	0.49
1:A:18:THR:CG2	1:A:74:THR:HG23	2.42	0.49
1:A:63:ARG:HD3	1:A:79:PRO:O	2.12	0.49
2:B:127:CYS:HG	2:B:201:CYS:CB	2.21	0.49
1:A:18:THR:CG2	1:A:74:THR:HG21	2.42	0.49
2:B:122:THR:HG22	2:B:189:ASN:HA	1.95	0.49
1:A:34:TYR:HB3	1:A:93:SER:CB	2.33	0.48
1:A:34:TYR:O	1:A:92:GLN:HA	2.13	0.48
1:A:89:TYR:CE1	2:B:150:LEU:HD12	2.48	0.48
2:B:129:ALA:HB2	2:B:213:TRP:CH2	2.49	0.48
2:B:196:MET:HE2	2:B:221:VAL:O	2.11	0.48
2:B:114:PRO:O	2:B:115:GLU:CG	2.59	0.48
2:B:117:LYS:HZ1	2:B:121:GLU:C	2.21	0.48
2:B:127:CYS:SG	2:B:201:CYS:CB	3.01	0.48
2:B:158:THR:HA	2:B:177:LEU:HD21	1.96	0.48
2:B:218:THR:O	2:B:218:THR:HG23	2.14	0.48
1:A:37:TRP:CZ3	1:A:90:CYS:HB3	2.48	0.48
2:B:129:ALA:HA	2:B:213:TRP:HZ3	1.79	0.48
2:B:158:THR:HA	2:B:177:LEU:CD2	2.44	0.47
1:A:110:ARG:HG2	1:A:111:ALA:H	1.79	0.47
2:B:118:LYS:H	2:B:118:LYS:CD	2.27	0.47
2:B:156:ILE:CB	2:B:175:PHE:CE2	2.94	0.47
2:B:158:THR:CB	2:B:177:LEU:CD2	2.92	0.47
1:A:2:MET:CE	1:A:35:MET:HE1	2.44	0.47
2:B:203:ARG:N	2:B:213:TRP:CD1	2.82	0.47
1:A:85:ALA:O	1:A:86:ALA:HB2	2.14	0.47
2:B:178:LYS:HD3	2:B:180:SER:N	2.29	0.47
2:B:134:PHE:CD2	2:B:182:SER:HA	2.50	0.47
2:B:196:MET:HE3	2:B:221:VAL:O	2.13	0.47
1:A:27:VAL:HA	1:A:94:ASN:CG	2.39	0.46
2:B:117:LYS:HD2	2:B:191:LEU:CD1	2.35	0.46
2:B:198:THR:CG2	2:B:200:PHE:CZ	2.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:ALA:CA	2:B:213:TRP:HE1	2.27	0.46
1:A:15:GLN:O	1:A:80:VAL:HG23	2.16	0.46
1:A:41:LYS:NZ	1:A:47:LYS:NZ	2.64	0.46
2:B:117:LYS:CE	2:B:122:THR:N	2.78	0.46
2:B:129:ALA:HB1	2:B:132:TYR:HE1	1.80	0.46
1:A:78:HIS:CD2	1:A:79:PRO:CD	2.93	0.46
2:B:198:THR:CG2	2:B:200:PHE:CE2	2.98	0.46
2:B:117:LYS:CE	2:B:122:THR:O	2.57	0.46
1:A:51:TYR:O	1:A:55:ASN:HB2	2.16	0.46
1:A:63:ARG:O	1:A:77:ILE:HA	2.15	0.46
1:A:85:ALA:O	1:A:86:ALA:CB	2.64	0.46
1:A:93:SER:OG	2:B:208:SER:HA	2.16	0.46
2:B:134:PHE:CG	2:B:182:SER:HA	2.51	0.46
1:A:2:MET:HE1	1:A:35:MET:CE	2.45	0.46
2:B:198:THR:HG22	2:B:200:PHE:CE2	2.50	0.46
2:B:168:ASP:OD2	2:B:169:PHE:CE1	2.69	0.45
1:A:39:GLN:HB2	1:A:49:LEU:HD11	1.98	0.45
2:B:117:LYS:CE	2:B:121:GLU:C	2.88	0.45
2:B:127:CYS:HB2	2:B:141:TRP:CH2	2.51	0.45
2:B:153:MET:HE1	2:B:186:LEU:CG	2.47	0.45
2:B:115:GLU:HB3	2:B:116:LEU:H	1.61	0.45
2:B:193:ASN:OD1	2:B:196:MET:CE	2.65	0.45
2:B:132:TYR:CZ	2:B:203:ARG:HD2	2.51	0.45
2:B:156:ILE:HG22	2:B:175:PHE:CZ	2.52	0.44
1:A:68:GLY:HA3	1:A:73:PHE:HA	1.98	0.44
1:A:97:PRO:HB3	2:B:152:TRP:CE3	2.51	0.44
2:B:134:PHE:CE1	2:B:139:MET:SD	3.10	0.44
2:B:199:TYR:O	2:B:217:THR:HG22	2.17	0.44
2:B:123:VAL:CG1	2:B:188:ILE:HB	2.38	0.44
2:B:153:MET:SD	2:B:199:TYR:HE2	2.40	0.44
2:B:202:ALA:HA	2:B:213:TRP:NE1	2.32	0.44
1:A:106:LEU:HD12	1:A:106:LEU:C	2.43	0.44
2:B:134:PHE:HD2	2:B:179:PRO:HA	1.83	0.44
2:B:117:LYS:CE	2:B:121:GLU:CB	2.75	0.44
2:B:123:VAL:HG11	2:B:188:ILE:HG22	1.98	0.44
2:B:193:ASN:OD1	2:B:196:MET:HE3	2.18	0.43
2:B:120:GLY:O	2:B:121:GLU:C	2.59	0.43
2:B:156:ILE:HG22	2:B:175:PHE:CE2	2.53	0.43
1:A:78:HIS:HB2	1:A:79:PRO:HD2	1.94	0.43
2:B:156:ILE:HD11	2:B:161:GLY:C	2.43	0.43
2:B:203:ARG:O	2:B:210:PHE:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:VAL:HG22	1:A:15:GLN:CB	2.48	0.43
2:B:117:LYS:HZ3	2:B:191:LEU:HG	1.84	0.43
2:B:139:MET:CE	2:B:184:ALA:HB2	2.50	0.42
2:B:139:MET:HE1	2:B:184:ALA:HB2	1.99	0.42
1:A:35:MET:HE2	1:A:35:MET:HB2	1.79	0.42
2:B:118:LYS:CG	2:B:121:GLU:HG3	2.50	0.42
2:B:155:TRP:C	2:B:175:PHE:HE2	2.27	0.42
2:B:172:ARG:NH2	2:B:195:ASP:OD2	2.52	0.42
2:B:168:ASP:CG	2:B:169:PHE:CZ	2.97	0.42
2:B:118:LYS:CG	2:B:121:GLU:CG	2.91	0.42
2:B:117:LYS:NZ	2:B:121:GLU:C	2.78	0.42
2:B:183:THR:HG21	2:B:185:TYR:CE1	2.51	0.42
2:B:129:ALA:HB1	2:B:132:TYR:CE1	2.55	0.42
2:B:168:ASP:OD2	2:B:169:PHE:CZ	2.73	0.42
2:B:177:LEU:HD13	2:B:179:PRO:HD3	2.01	0.42
2:B:114:PRO:O	2:B:115:GLU:CB	2.68	0.42
1:A:27:VAL:HB	1:A:94:ASN:HB2	2.02	0.41
2:B:139:MET:HB2	2:B:139:MET:HE3	1.74	0.41
1:A:63:ARG:HB2	1:A:78:HIS:NE2	2.35	0.41
1:A:63:ARG:CB	1:A:78:HIS:NE2	2.83	0.41
1:A:13:LEU:HD21	1:A:82:GLU:OE1	2.20	0.41
2:B:114:PRO:HD3	2:B:217:THR:HG1	1.85	0.41
1:A:4:GLN:HG3	1:A:21:CYS:SG	2.60	0.41
1:A:19:ILE:HG12	1:A:104:THR:HG21	2.02	0.41
2:B:139:MET:SD	2:B:184:ALA:CB	3.05	0.41
1:A:40:GLN:HB3	1:A:87:THR:HG23	2.02	0.41
1:A:41:LYS:NZ	1:A:47:LYS:HZ2	2.19	0.41
1:A:38:TYR:CE1	2:B:212:PHE:HZ	2.36	0.40
1:A:50:ILE:HD11	1:A:56:LEU:HD21	2.02	0.40
2:B:168:ASP:OD2	2:B:169:PHE:HZ	2.04	0.40
2:B:212:PHE:CD1	2:B:212:PHE:C	3.00	0.40
2:B:113:GLY:N	2:B:114:PRO:HD2	2.35	0.40
2:B:156:ILE:HG12	2:B:157:ASN:O	2.21	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	109/111 (98%)	102 (94%)	3 (3%)	4 (4%)	2	20
2	B	109/111 (98%)	94 (86%)	6 (6%)	9 (8%)	0	9
All	All	218/222 (98%)	196 (90%)	9 (4%)	13 (6%)	2	13

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	ARG
1	A	79	PRO
1	A	86	ALA
2	B	115	GLU
2	B	121	GLU
2	B	213	TRP
2	B	217	THR
2	B	208	SER
2	B	212	PHE
1	A	70	GLY
2	B	202	ALA
2	B	197	ALA
2	B	114	PRO

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	90/90 (100%)	82 (91%)	8 (9%)	9	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	90/90 (100%)	81 (90%)	9 (10%)	7 24
All	All	180/180 (100%)	163 (91%)	17 (9%)	10 26

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	11	VAL
1	A	15	GLN
1	A	50	ILE
1	A	63	ARG
1	A	65	SER
1	A	106	LEU
1	A	110	ARG
2	B	116	LEU
2	B	118	LYS
2	B	177	LEU
2	B	178	LYS
2	B	180	SER
2	B	183	THR
2	B	198	THR
2	B	201	CYS
2	B	211	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	94	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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.

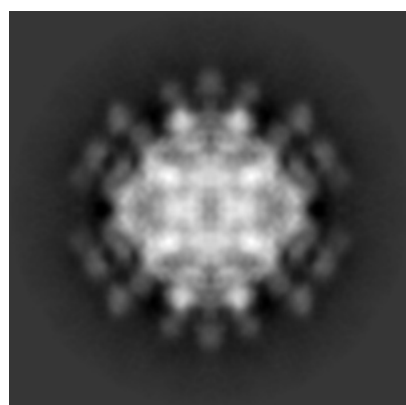
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5109. These allow visual inspection of the internal detail of the map and identification of artifacts.

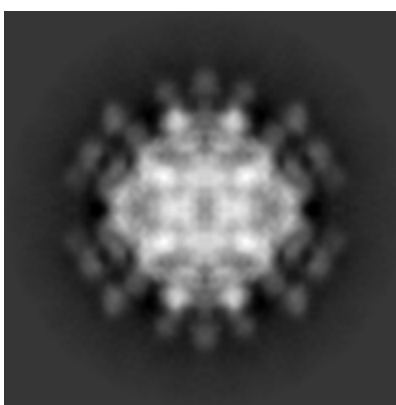
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

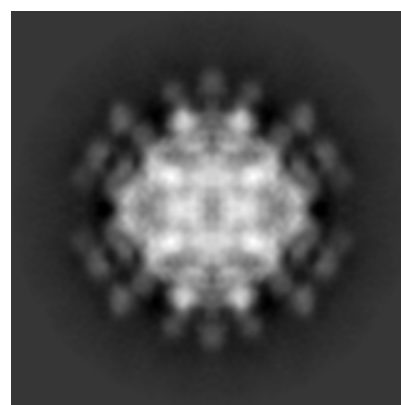
6.1.1 Primary map



X



Y

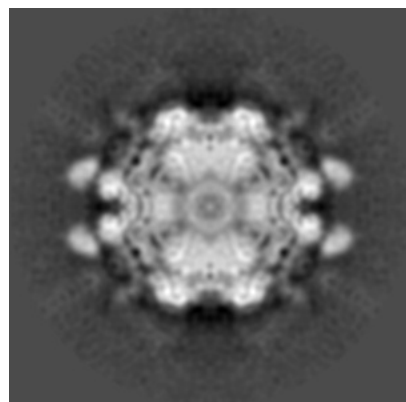


Z

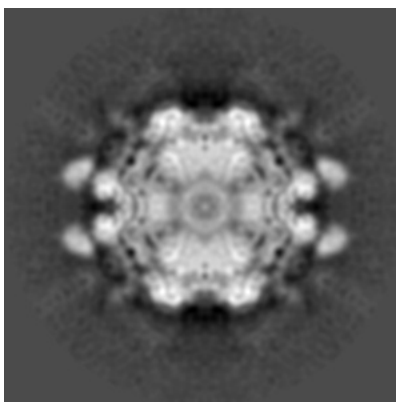
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

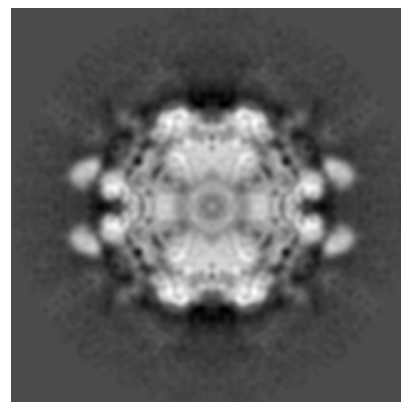
6.2.1 Primary map



X Index: 92



Y Index: 92

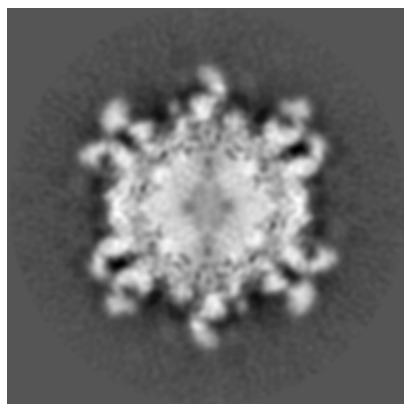


Z Index: 92

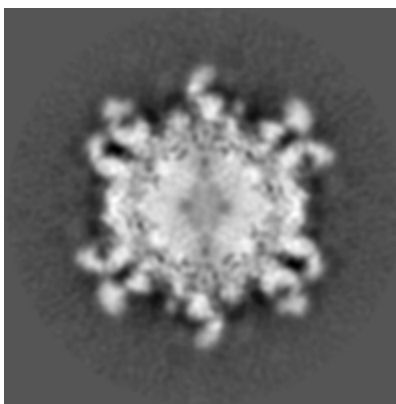
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

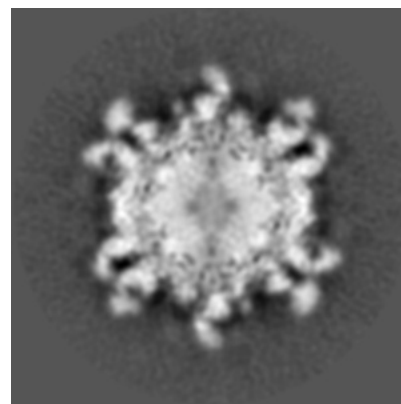
6.3.1 Primary map



X Index: 80



Y Index: 104

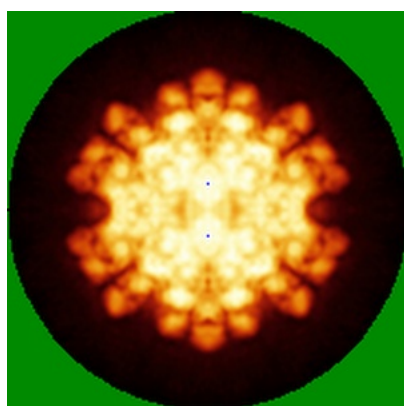


Z Index: 80

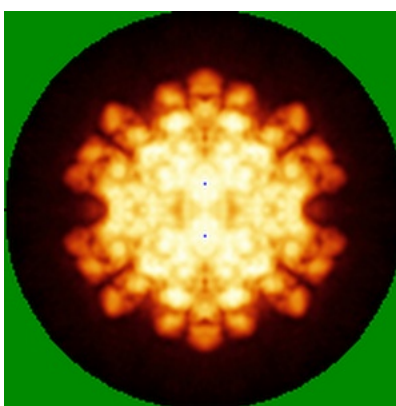
The images above show the largest variance slices of the map in three orthogonal directions.

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

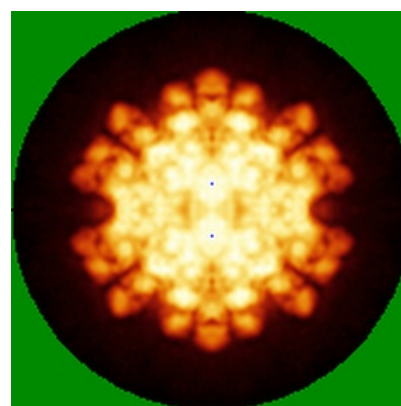
6.4.1 Primary map



X



Y

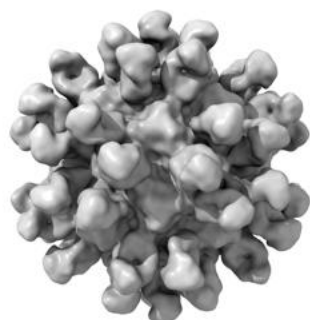


Z

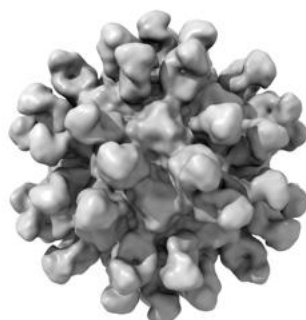
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

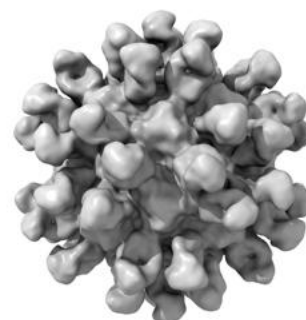
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

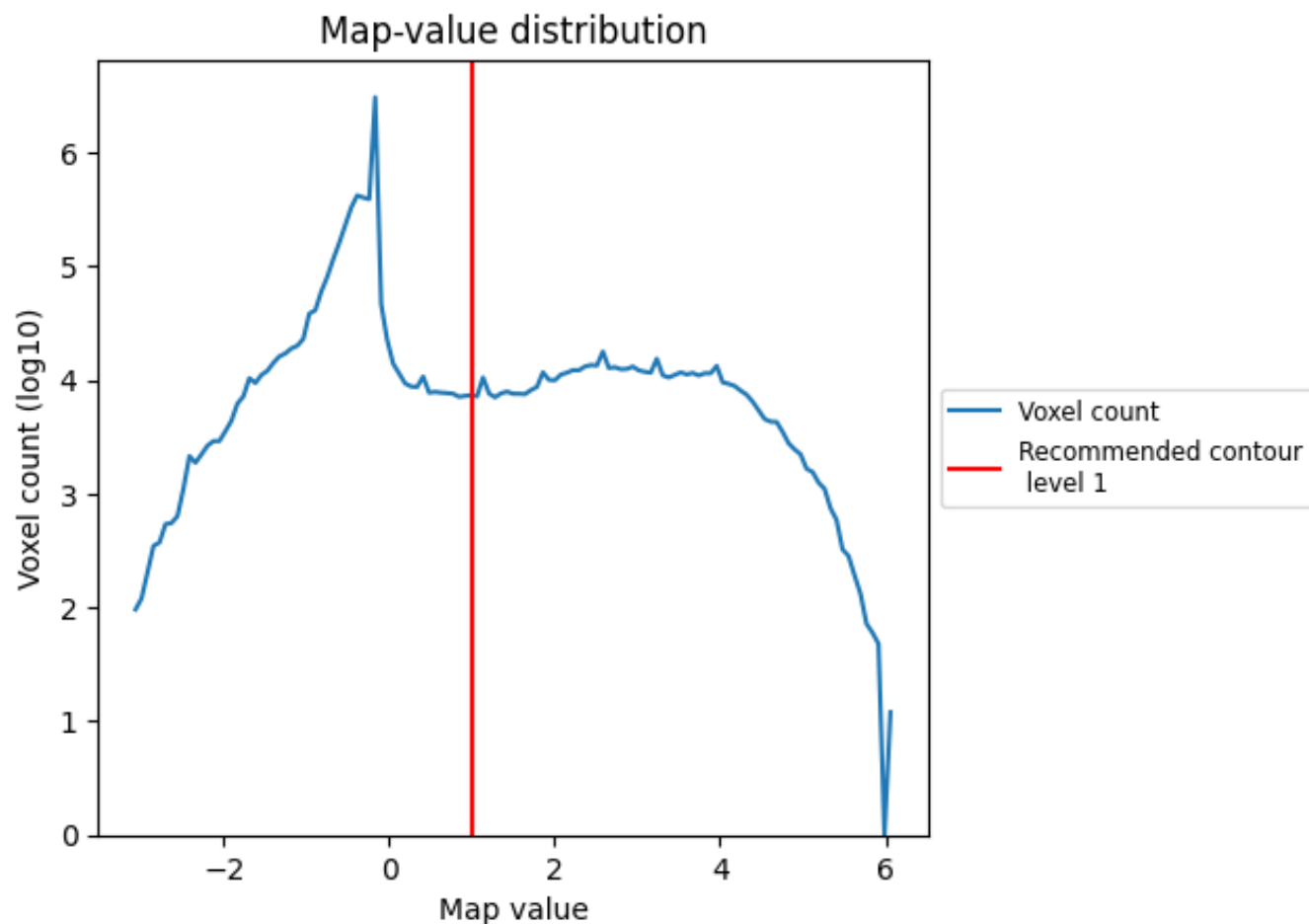
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

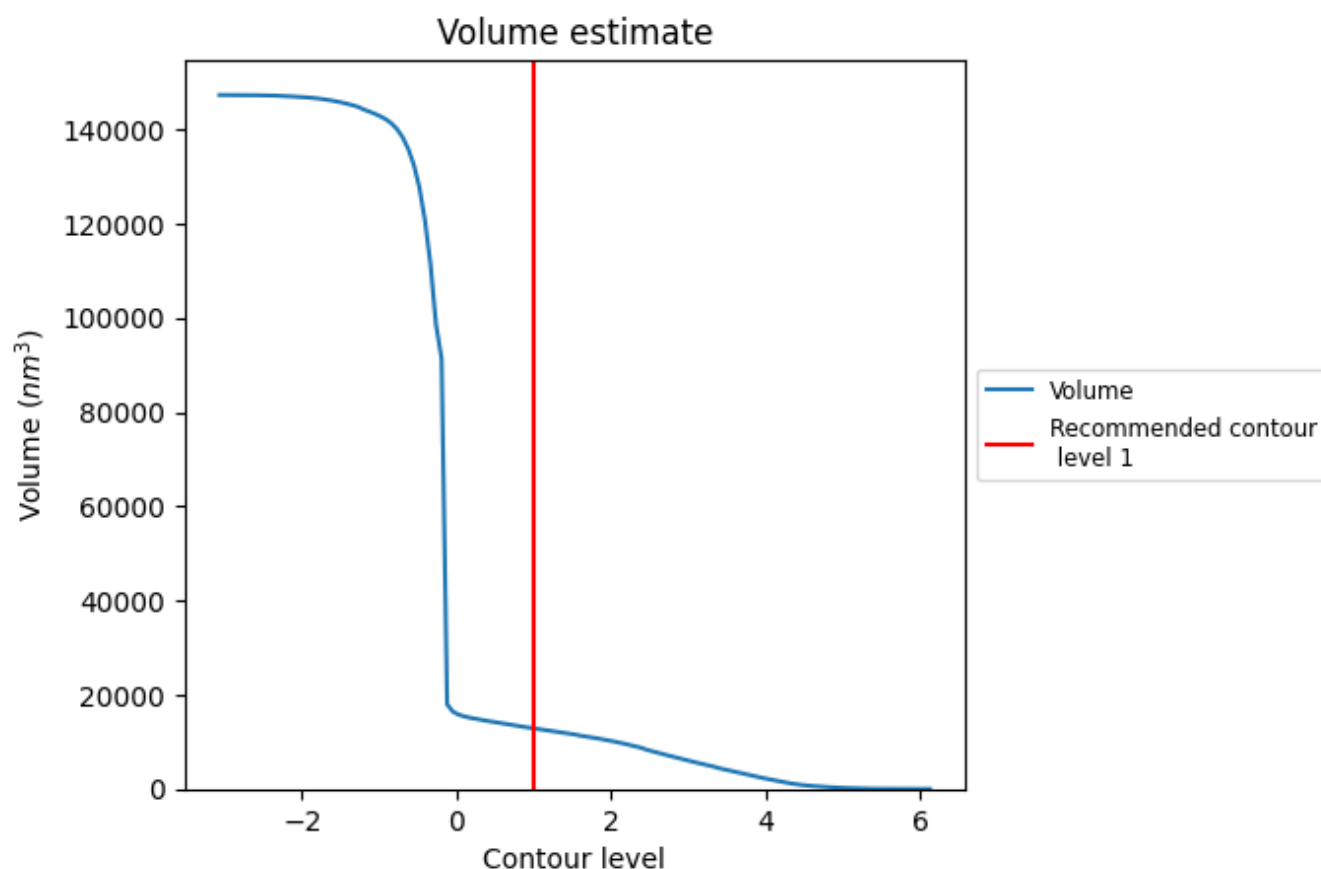
This section contains the results of statistical analysis of the map.

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.

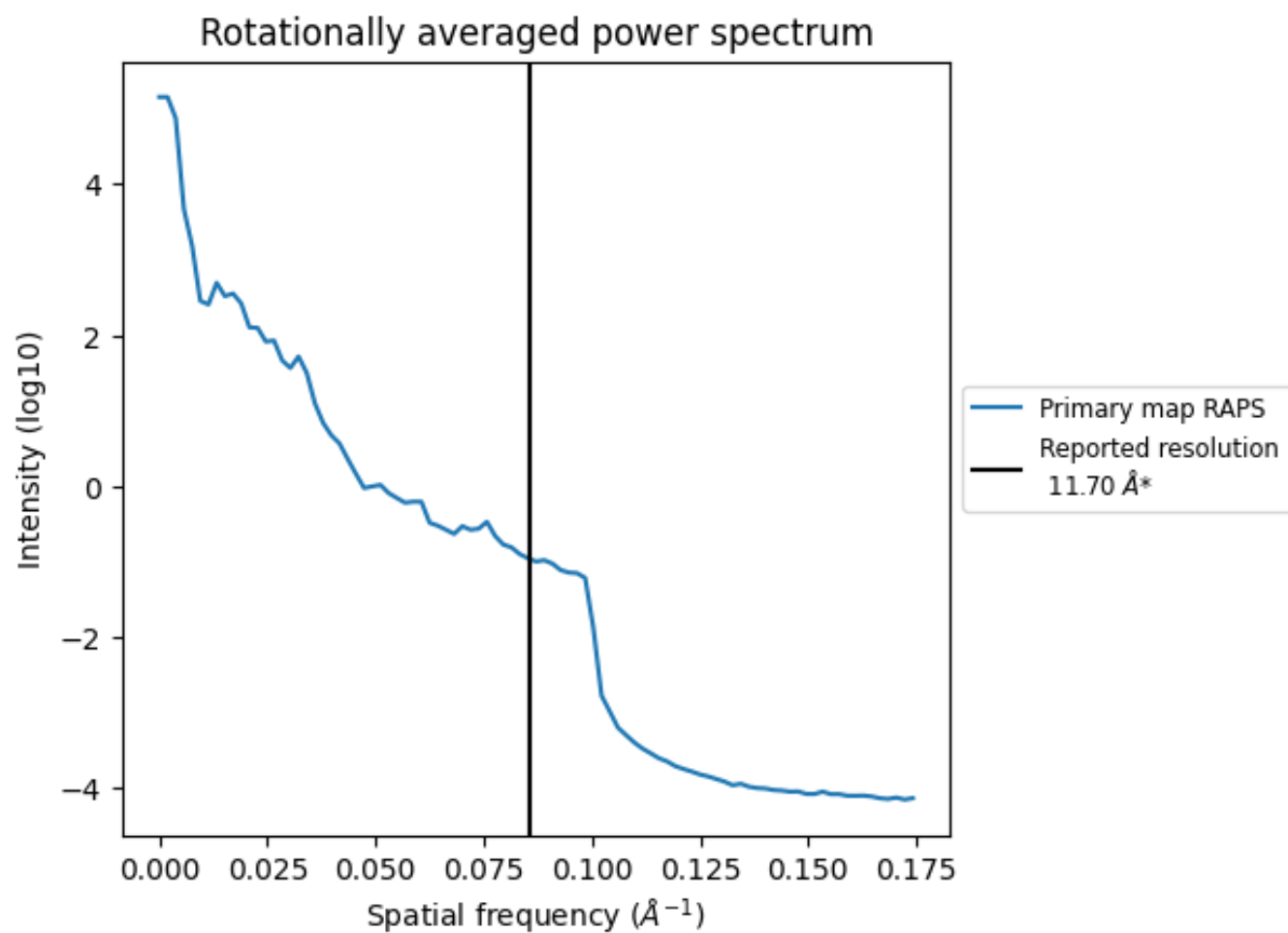
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 12874 nm^3 ; this corresponds to an approximate mass of 11630 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 0.085 Å⁻¹

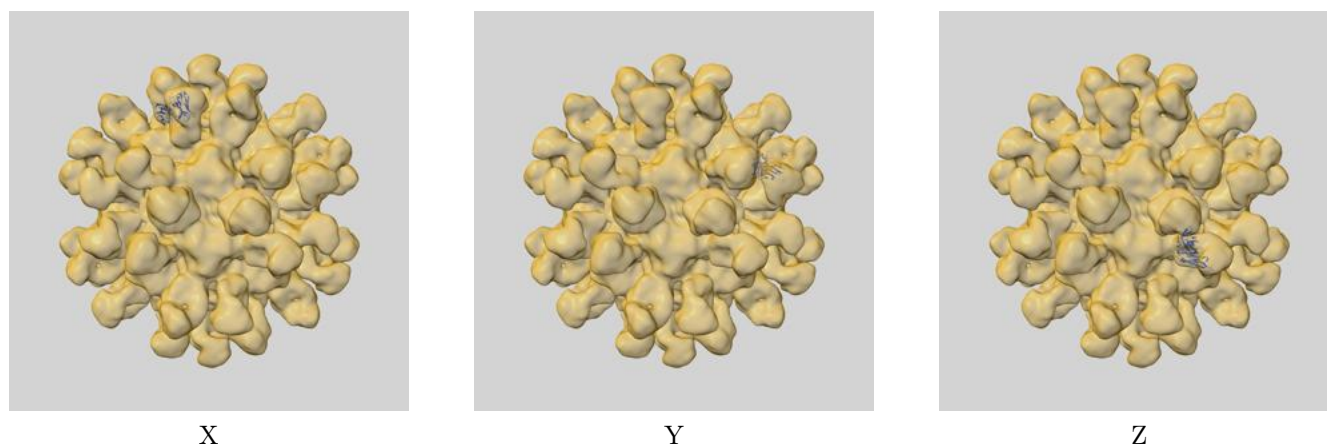
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

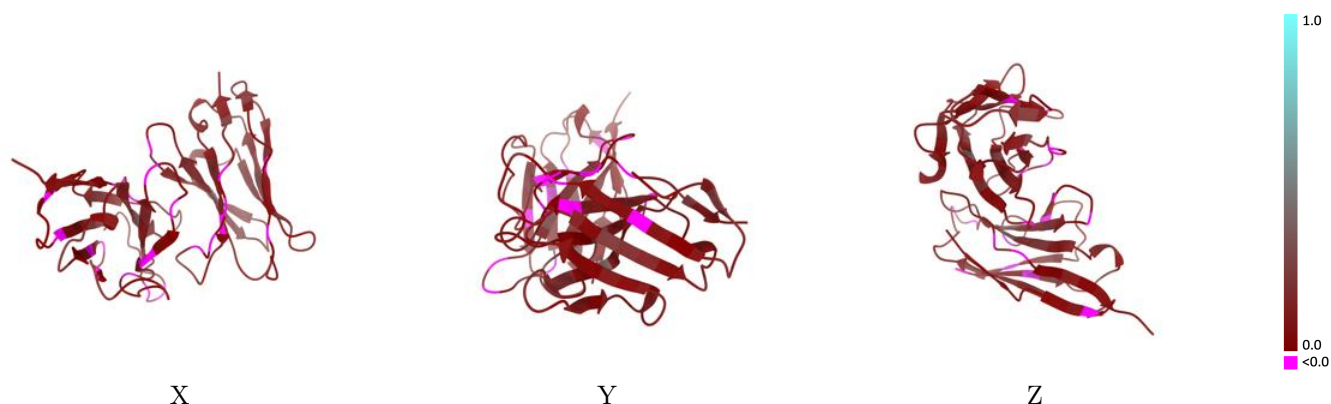
This section contains information regarding the fit between EMDB map EMD-5109 and PDB model 3IY4. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)



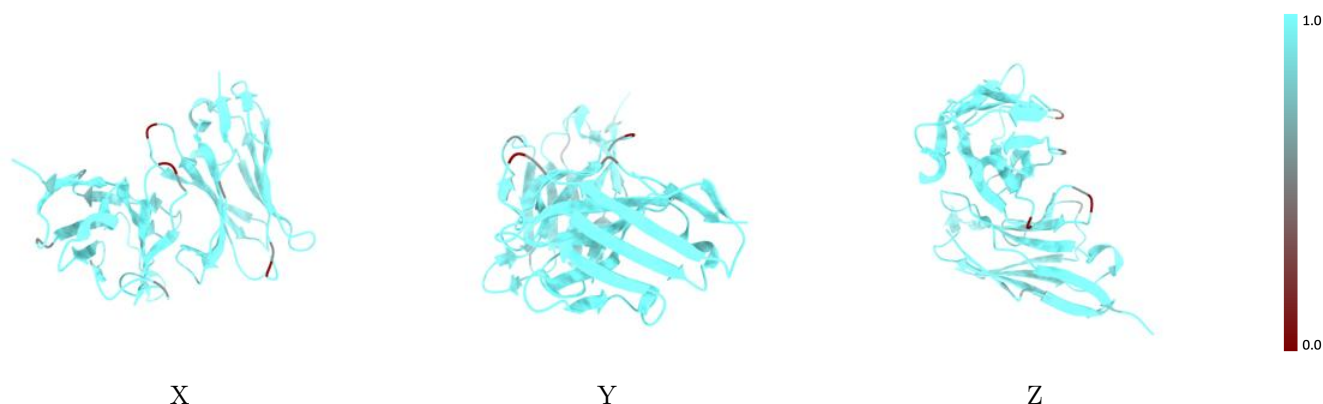
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



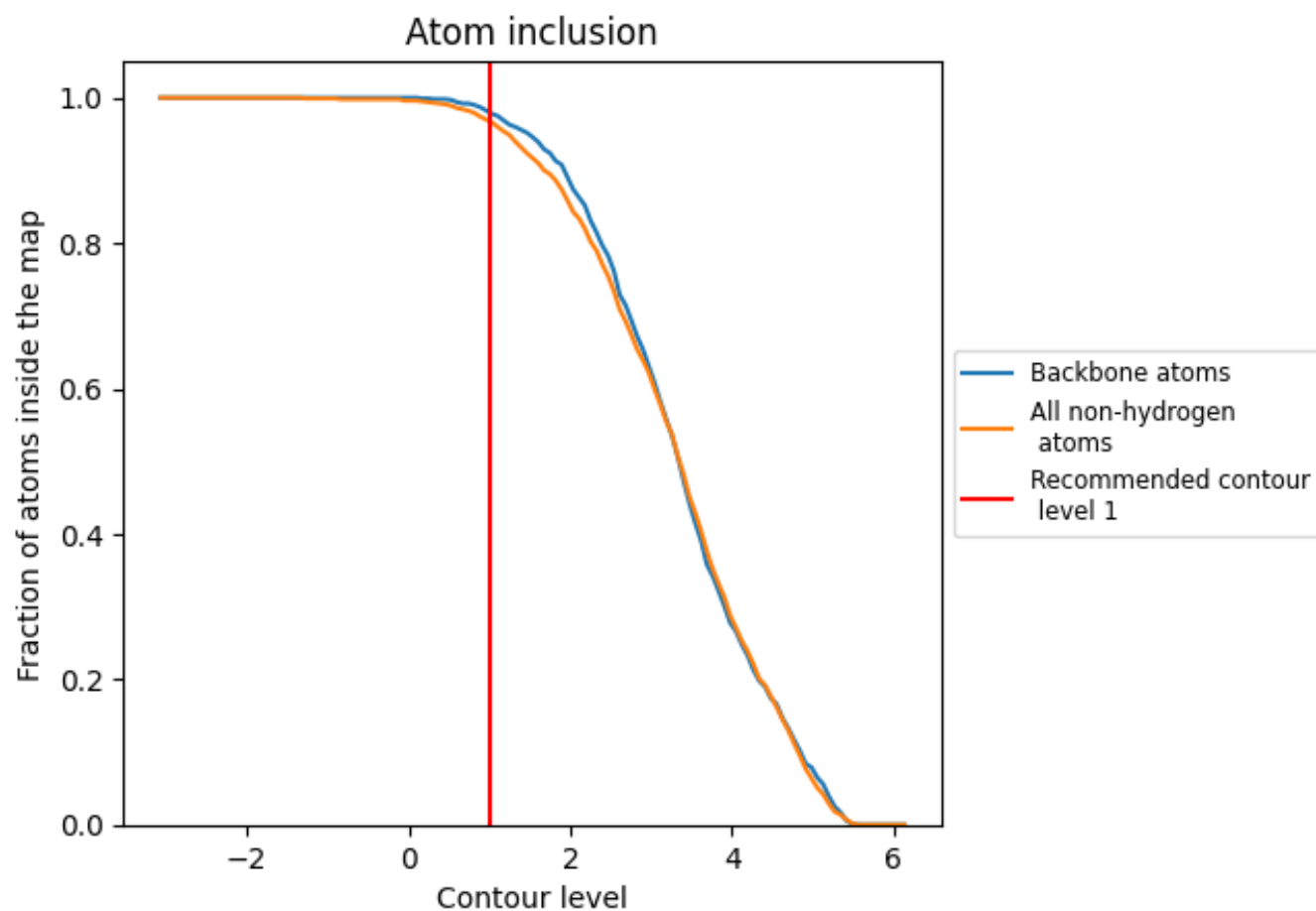
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9680	0.0900
A	0.9630	0.0850
B	0.9740	0.0940

