



Full wwPDB EM Validation Report ⓘ

Mar 9, 2025 – 03:49 am GMT

PDB ID : 9GVJ
EMDB ID : EMD-51636
Title : MUC5AC mucin amino acids 28 to 1483
Authors : Haberman, M.; Kamyshinsky, R.; Fass, D.
Deposited on : 2024-09-24
Resolution : 2.91 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.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

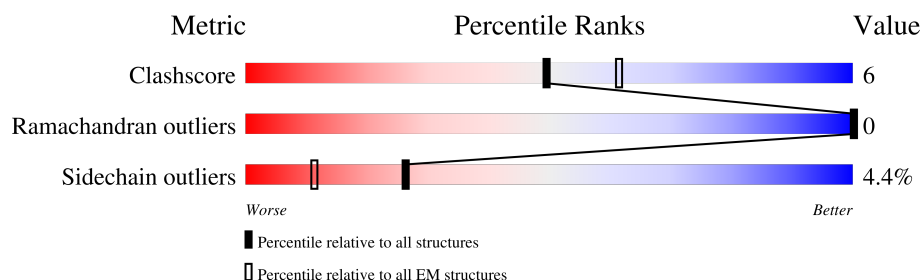
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.91 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1456	
1	B	1456	
1	C	1456	
1	D	1456	

2 Entry composition [i](#)

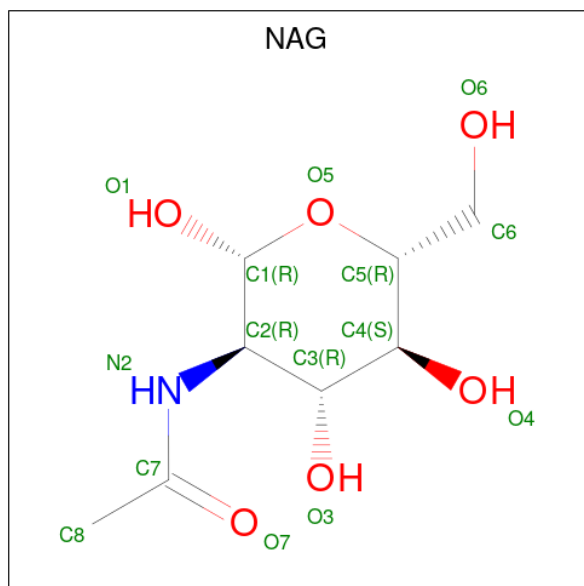
There are 5 unique types of molecules in this entry. The entry contains 17636 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Mucin-5AC.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	690	Total	C	N	O	S	4	0
			5230	3250	903	1008	69		
1	B	688	Total	C	N	O	S	4	0
			5219	3242	903	1005	69		
1	C	463	Total	C	N	O	S	3	0
			3453	2138	596	663	56		
1	D	463	Total	C	N	O	S	4	0
			3465	2144	602	663	56		

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Ca	0
			2	2	
3	B	2	Total	Ca	0
			2	2	
3	C	1	Total	Ca	0
			1	1	
3	D	1	Total	Ca	0
			1	1	

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Cu	0
			1	1	
4	B	1	Total	Cu	0
			1	1	

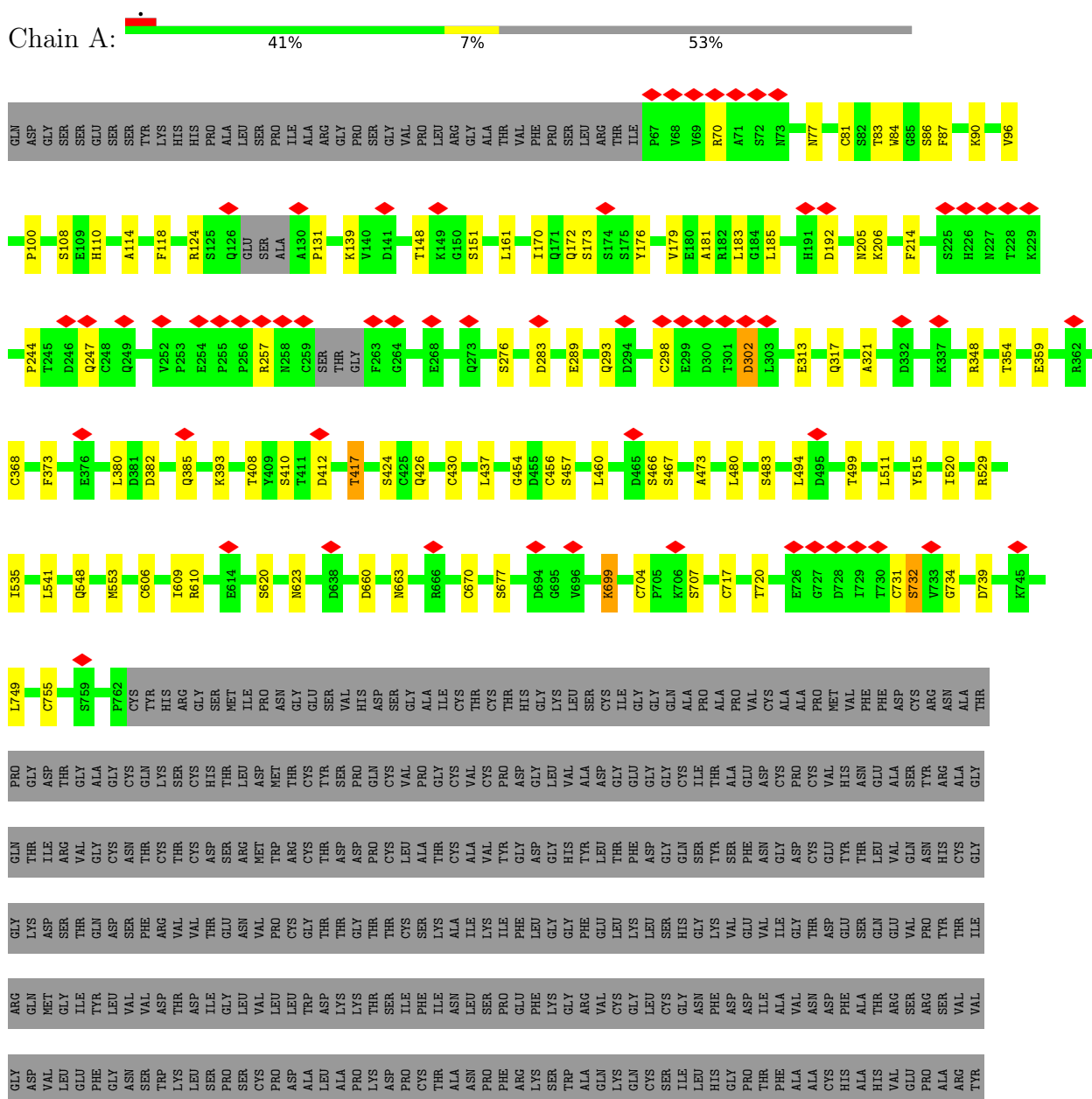
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	A	64	Total	O	0
			64	64	
5	B	39	Total	O	0
			39	39	
5	C	45	Total	O	0
			45	45	
5	D	29	Total	O	0
			29	29	

3 Residue-property plots

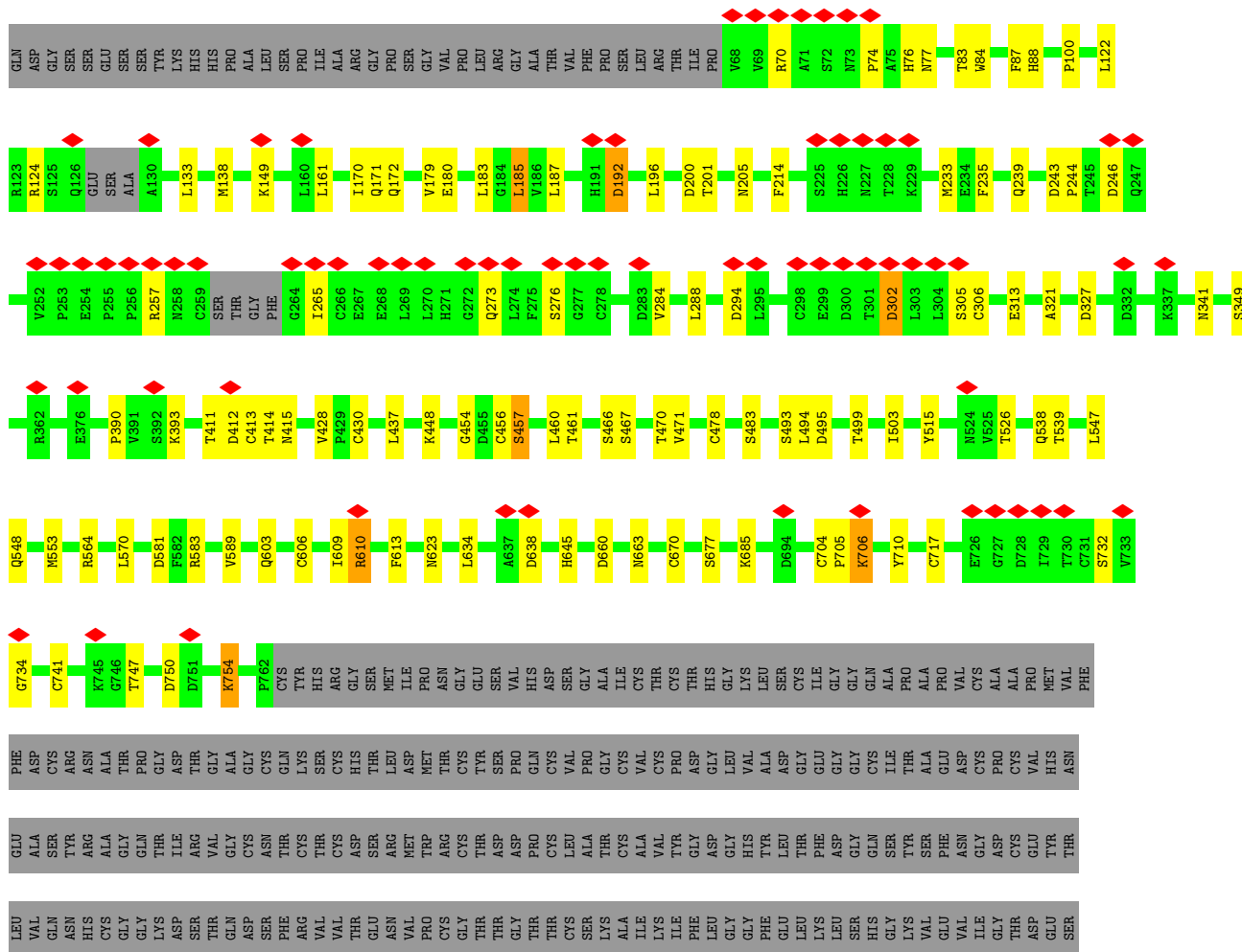
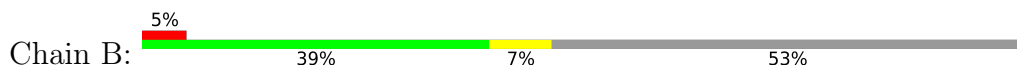
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Mucin-5AC



CYS	THR	HIS	PRO	GLY	ARG	TRP	TYR
	THR	GLY	SER	THR	THR	HIS	GLU
PRO	PRO	ARG	SER	SER	GLY	HIS	ALA
PRO	PRO	VAL	TRP	TRP	VAL	VAL	CYS
CYS	CYS	CYS	PRO	ILE	SER	GLY	ASN
SER	SER	GLU	THR	SER	LYS	CYS	ASP
THR	THR	THR	THR	ALA	SER	VAL	ALA
	PRO	PRO	ALA	ARG	TYR	PRO	CYS
	ARG	ARG	GLY	CYS	ARG	CYS	ALA
	ALA	ALA	ILE	ILE	PRO	ASN	CYS
	GLU	GLU	LEU	GLU	SER	PRO	CYS
	ASP	ASP	PRO	ARG	ASP	ARG	GLY
	PRO	PRO	THR	ARG	LYS	CYS	CYS
	ALA	ALA	ALA	VAL	ASN	ASP	PHE
	LEU	LEU	VAL	THR	CYS	CYS	THR
	GLY	GLY	PRO	PRO	GLN	LEU	ALA
	ARG	ARG	GLY	VAL	ARG	GLU	GLN
	VAL	VAL	PRO	PRO	GLY	GLY	ALA
	GLN	GLN	CYS	THR	VAL	CYS	CYS
	CYS	CYS	LEU	THR	CYS	PRO	GLU
	SER	SER	TRP	PHE	THR	LYS	VAL
	PRO	PRO	SER	SER	TYR	CYS	GLY
	ASP	ASP	PRO	PHE	LYS	PRO	LEU
	VAL	VAL	TRP	SER	ALA	PRO	CYS
	GLY	GLY	MET	THR	GLU	GLU	VAL
	LEU	LEU	ASP	PRO	ALA	SER	ALA
	THR	THR	VAL	PRO	CYS	PRO	TRP
	CYS	CYS	SER	LEU	VAL	ILE	ARG
	ARG	ARG	ARG	VAL	CYS	PHE	THR
	ASN	ASN	PRO	VAL	ASP	ASP	PRO
	ARG	ARG	GLY	SER	TYR	GLY	SER
	GLU	GLU	ARG	SER	THR	LYS	CYS
	GLN	GLN	THR	HIS	GLN	MET	PRO
	SER	SER	ASP	THR	ARG	GLN	LEU
	GLY	GLY	SER	PRO	PHE	CYS	PHE
	LEU	LEU	GLY	SER	HIS	VAL	CYS
	THR	THR	ASP	THR	GLY	ALA	ASP
	ASN	ASN	PHE	THR	TYR	THR	TYR
	ASN	ASN	ASP	PRO	ASP	CYS	ASN
	TYR	TYR	THR	SER	VAL	PRO	ASN
	GLN	GLN	LEU	SER	ILE	THR	PRO
	ILE	ILE	GLU	SER	TYR	PRO	GLU
	ARG	ARG	ASN	HIS	HIS	PRO	GLY
	VAL	VAL	LEU	THR	THR	LEU	GLN
	GLN	GLN	ARG	GLY	THR	PRO	CYS
	CYS	CYS	ALA	PRO	THR	PRO	GLN

- Molecule 1: Mucin-5AC



THR	TYR	THR	SER	VAL	PRO	ASN	HIS	THR	GLN
THR	GLN	THR	SER	ILE	THR	PRO	VAL	ARG	GLN
THR	ILE	THR	SER	TYR	PRO	GLY	GLU	SER	VAL
THR	ASN	THR	HIS	HIS	PRO	GLN	ALA	SER	TYR
THR	ARG	THR	GLY	PRO	PRO	GLU	TYR	VAL	THR
THR	ALA	THR	PRO	ASP	ARG	GLY	TYR	VAL	ILE
THR	CYS	THR	PRO	GLY	ARG	GLU	TYR	ARG	ILE
THR	CYS	THR	SER	THR	CYS	HIS	GLY	GLY	ARG
THR	PRO	THR	THR	ILE	GLY	CYS	ASN	PHE	TYR
THR	CYS	THR	THR	SER	LYS	GLY	ASP	PHE	TYR
THR	SER	THR	THR	ALA	ARG	VAL	ALA	ASN	LEU
THR	VAL	THR	ALA	ARG	TYR	PRO	CYS	TRP	ASP
THR	ARG	THR	GLY	GLY	PRO	LEU	CYS	LYS	THR
THR	SER	THR	SER	ALA	GLY	ARG	ASP	LYS	THR
THR	GLU	THR	PRO	ASN	ALA	THR	SER	SER	ILE
THR	CYS	THR	ARG	GLY	VAL	CYS	GLY	PRO	GLY
THR	ARG	THR	THR	THR	VAL	ARG	GLY	SER	LEU
THR	ALA	THR	ARG	ILE	PRO	ASN	ASP	CYS	VAL
THR	ASP	THR	LEU	GLU	SER	PRO	CYS	PRO	LEU
THR	ALA	THR	THR	ARG	LYS	ARG	GLU	ASP	LEU
THR	PRO	THR	ALA	VAL	ASN	GLY	CYS	ALA	TRP
THR	GLY	THR	SER	TYR	CYS	ASP	PHE	LEU	ASN
THR	VAL	THR	ALA	THR	CYS	TYR	THR	ALA	LYS
THR	PRO	THR	SER	PRO	GLN	LEU	THR	PRO	LYS
THR	LEU	THR	LEU	CYS	SER	ARG	ALA	LYS	THR
THR	LEU	THR	LEU	SER	CYS	ARG	VAL	ASP	SER
THR	ARG	THR	LEU	PRO	VAL	GLY	ALA	PRO	ILE
THR	GLN	THR	GLY	VAL	GLU	GLY	TYR	THR	ILE
THR	VAL	THR	CYS	PRO	GLU	LEU	ALA	ALA	ASN
THR	GLN	THR	GLY	ARG	ARG	GLU	GLN	ASN	LEU
THR	VAL	THR	LYS	VAL	GLY	GLY	ALA	PRO	SER
THR	GLN	THR	CYS	THR	VAL	CYS	CYS	PHE	PRO
THR	GLY	THR	THR	THR	GLU	TYR	HIS	ARG	GLY
THR	THR	THR	TRP	PHE	THR	LYS	VAL	SER	PHE
THR	PRO	THR	SER	SER	TYR	CYS	GLY	TRP	GLY
THR	ASP	THR	PRO	PHE	LYS	PRO	LEU	ALA	ARG
THR	VAL	THR	TRP	PHE	ALA	PRO	CYS	GLN	VAL
THR	GLY	THR	MET	THR	GLU	GLU	VAL	LYS	VAL
THR	LEU	THR	ASP	PRO	ALA	ALA	SER	GLN	CYS
THR	THR	THR	VAL	PRO	CYS	PRO	TRP	CYS	LEU
THR	CYS	THR	SER	LEU	ILE	ILE	ARG	SER	CYS
THR	ARG	THR	ARG	VAL	PHE	PHE	THR	ILE	GLY
THR	ASN	THR	PRO	VAL	THR	ASP	PRO	LEU	CYS
THR	ARG	THR	GLY	SER	TYR	GLU	SER	HIS	PHE
THR	GLN	THR	GLY	THR	ASN	ASP	ILE	GLY	ASP
THR	ALA	THR	GLY	GLN	LYS	MET	CYS	PRO	ASP
THR	VAL	THR	THR	HIS	GLN	THR	PRO	THR	ILE
THR	SER	THR	ASP	THR	ARG	GLN	LEU	PHE	ALA
THR	GLY	THR	GLY	PRO	PHE	CYS	PHE	ALA	VAL
THR	LEU	THR	GLY	SER	HIS	VAL	CYS	ALA	ASN
THR	CYS	THR	ASP	ASN	PRO	ALA	ASP	CYS	ASN
THR	THR	THR	PHE	GLY	GLY	THR	TYR	HIS	PHE
THR	ASN	THR	ASN	PRO	ASN	CYS	TYR	ALA	ALA

- Molecule 1: Mucin-5AC

[illegible]



WORLDWIDE
PDB
PROTEIN DATA BANK

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	198256	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.313	Depositor
Minimum map value	-0.925	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.256	Depositor
Map size (\AA)	453.31, 453.31, 453.31	wwPDB
Map dimensions	550, 550, 550	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.8242, 0.8242, 0.8242	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CU, CA, NAG

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	0.25	0/5356	0.48	0/7280
1	B	0.25	0/5344	0.49	1/7264 (0.0%)
1	C	0.25	0/3548	0.50	1/4831 (0.0%)
1	D	0.25	0/3563	0.50	0/4850
All	All	0.25	0/17811	0.49	2/24225 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1195	ASP	CB-CG-OD1	5.76	123.48	118.30
1	B	638	ASP	CB-CG-OD2	5.07	122.86	118.30

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	5230	0	4954	50	0
1	B	5219	0	4947	59	0
1	C	3453	0	3179	41	0
1	D	3465	0	3199	44	0
2	A	42	0	39	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	42	0	39	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	64	0	0	0	0
5	B	39	0	0	0	0
5	C	45	0	0	0	0
5	D	29	0	0	0	0
All	All	17636	0	16357	186	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 6.

All (186) 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)
1:C:1147:HIS:HB3	1:C:1202:GLY:HA3	1.69	0.73
1:B:548:GLN:O	1:B:553:MET:HA	1.89	0.72
1:A:660:ASP:HB3	1:A:670:CYS:HB3	1.73	0.71
1:D:1147:HIS:HB3	1:D:1202:GLY:HA3	1.74	0.70
1:C:1191:ASN:ND2	1:C:1195:ASP:O	2.25	0.70
1:C:1162:PRO:HG2	1:D:1162:PRO:HG2	1.75	0.69
1:B:183:LEU:HD11	1:B:185:LEU:HD23	1.74	0.68
1:B:430:CYS:HB3	1:B:564:ARG:HH21	1.59	0.67
1:C:1087:ARG:NH2	1:C:1131:ASP:OD2	2.20	0.67
1:A:483:SER:O	1:A:663:ASN:ND2	2.29	0.66
1:B:88:HIS:NE2	1:B:294:ASP:OD1	2.29	0.66
1:A:83:THR:OG1	1:A:124:ARG:NH2	2.29	0.65
1:D:1223:GLN:N	1:D:1223:GLN:OE1	2.30	0.65
1:B:461:THR:HG22	1:B:471:VAL:HB	1.79	0.64
1:A:548:GLN:O	1:A:553:MET:HA	1.98	0.62
1:B:454:GLY:HA2	1:B:609:ILE:HG13	1.82	0.61
1:C:968:LEU:HD23	1:C:992:PRO:HG2	1.82	0.61
1:A:354:THR:HG22	1:A:380:LEU:HB3	1.81	0.61
1:B:161:LEU:HD12	1:B:172:GLN:HB2	1.83	0.61
1:A:620:SER:HB3	1:A:623:ASN:HB2	1.83	0.61
1:C:971:PHE:HD1	1:C:984:GLY:HA2	1.66	0.60
1:A:623:ASN:HA	1:B:244:PRO:HG3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ALA:HB3	1:A:185:LEU:HG	1.83	0.60
1:B:170:ILE:HG23	1:B:179:VAL:HG22	1.84	0.60
1:A:382:ASP:O	1:A:385:GLN:NE2	2.35	0.59
1:B:83:THR:OG1	1:B:124:ARG:NH2	2.35	0.59
1:B:171:GLN:NE2	1:B:180:GLU:OE2	2.35	0.59
1:B:660:ASP:HB3	1:B:670:CYS:HB3	1.84	0.59
1:A:70:ARG:NH1	1:A:70:ARG:HB3	2.18	0.59
1:B:610:ARG:NH1	1:B:610:ARG:HB3	2.17	0.59
1:D:1080:PRO:HB3	1:D:1125:ALA:HB2	1.84	0.59
1:D:1081:CYS:HB3	1:D:1088:LYS:HG3	1.85	0.59
1:C:883:ASN:ND2	1:C:895:THR:O	2.28	0.58
1:C:1218:ASP:O	1:C:1222:MET:N	2.36	0.58
1:B:413:CYS:HA	1:B:428:VAL:HG23	1.85	0.58
1:A:183:LEU:HD11	1:A:185:LEU:HD23	1.85	0.58
1:D:930:VAL:HG12	1:D:946:VAL:HB	1.85	0.58
1:B:412:ASP:OD2	1:B:685:LYS:NZ	2.36	0.58
1:D:1049:THR:HG22	1:D:1061:PHE:HA	1.85	0.58
1:A:313:GLU:OE2	1:A:317:GLN:NE2	2.34	0.58
1:D:926:GLU:OE2	1:D:965:LYS:NZ	2.28	0.57
1:D:973:LEU:HD21	1:D:995:ILE:HD11	1.87	0.56
1:C:1049:THR:HG22	1:C:1061:PHE:HA	1.87	0.56
1:D:889:SER:O	1:D:889:SER:OG	2.24	0.56
1:A:302:ASP:N	1:A:302:ASP:OD1	2.37	0.56
1:B:483:SER:O	1:B:663:ASN:ND2	2.38	0.55
1:A:720:THR:HG22	1:A:749:LEU:HB3	1.87	0.55
1:A:410:SER:HB2	2:A:1503:NAG:H82	1.87	0.55
1:C:900:LEU:HD22	1:C:1023:ASN:HB3	1.87	0.55
1:C:778:ASP:N	1:C:778:ASP:OD1	2.38	0.55
1:C:930:VAL:HG12	1:C:946:VAL:HB	1.89	0.54
1:B:77:ASN:HD21	1:B:321:ALA:HB2	1.73	0.54
1:A:244:PRO:HG3	1:B:623:ASN:HA	1.90	0.54
1:D:1147:HIS:CD2	1:D:1152:CYS:HA	2.44	0.53
1:B:732:SER:O	1:B:734:GLY:N	2.41	0.53
1:D:946:VAL:HG22	1:D:966:ILE:HG23	1.89	0.53
1:C:946:VAL:HG22	1:C:966:ILE:HG23	1.90	0.53
1:C:1080:PRO:HB3	1:C:1125:ALA:HB2	1.90	0.53
1:D:922[A]:ASN:HD22	1:D:1077:PRO:HG3	1.73	0.53
1:C:940:THR:HG23	1:C:941:GLN:HG2	1.90	0.52
1:B:390:PRO:HD2	1:B:393:LYS:HD3	1.90	0.52
1:B:243:ASP:HB2	1:B:246:ASP:HB2	1.92	0.52
1:D:971:PHE:HD2	1:D:984:GLY:HA3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:706:LYS:H	1:B:706:LYS:CD	2.23	0.52
1:B:494:LEU:HB2	1:B:499:THR:HB	1.92	0.51
1:A:170:ILE:HG23	1:A:179:VAL:HG22	1.92	0.51
1:B:122:LEU:HD12	1:B:133:LEU:HD21	1.94	0.50
1:A:289:GLU:O	1:A:293:GLN:HG3	2.11	0.50
1:C:1012:LEU:HD23	1:C:1020:ILE:HD11	1.93	0.50
1:D:1152:CYS:HB3	1:D:1180:PRO:HB2	1.93	0.49
1:C:849:LEU:HB3	1:C:857:CYS:HB3	1.94	0.49
1:A:454:GLY:HA2	1:A:609:ILE:HG13	1.94	0.49
1:A:707:SER:HB2	1:A:755:CYS:HB2	1.94	0.49
1:D:1191:ASN:ND2	1:D:1195:ASP:O	2.46	0.49
1:B:265:ILE:HD12	1:B:265:ILE:H	1.78	0.49
1:C:905:VAL:HB	1:C:1020:ILE:HG22	1.95	0.49
1:D:928:THR:HA	1:D:947:VAL:HG22	1.95	0.49
1:B:192:ASP:N	1:B:192:ASP:OD1	2.46	0.48
1:B:87:PHE:CG	1:B:100:PRO:HA	2.48	0.48
1:D:973:LEU:HD13	1:D:993:TYR:CZ	2.48	0.48
1:A:90:LYS:HG3	1:A:96:VAL:HG22	1.96	0.48
1:B:411:THR:OG1	1:B:414:THR:HG22	2.13	0.48
1:A:610:ARG:HB2	1:A:610:ARG:NH1	2.28	0.48
1:A:732:SER:O	1:A:734:GLY:N	2.45	0.48
1:B:610:ARG:HB3	1:B:610:ARG:HH11	1.78	0.48
1:C:934:CYS:O	1:C:1052:ARG:NH2	2.47	0.48
1:A:460:LEU:HD11	1:A:473:ALA:HB2	1.95	0.48
1:C:1079:ASP:HB3	1:C:1082:THR:HB	1.96	0.48
1:B:74:PRO:O	1:B:76:HIS:ND1	2.46	0.47
1:D:1147:HIS:HD2	1:D:1152:CYS:HA	1.77	0.47
1:A:466:SER:OG	1:A:467:SER:N	2.47	0.47
1:C:765:HIS:O	1:C:768:SER:OG	2.32	0.47
1:A:529:ARG:HG3	1:A:535:ILE:HG12	1.97	0.46
1:C:973:LEU:HD11	1:C:995:ILE:HD11	1.96	0.46
1:A:87:PHE:CZ	1:A:131:PRO:HB3	2.50	0.46
1:B:273:GLN:HA	1:B:276:SER:HB3	1.96	0.46
1:D:1148:GLU:OE2	1:D:1201[A]:ARG:NH2	2.48	0.46
1:A:456:CYS:HB2	1:A:606:CYS:HB3	1.80	0.46
1:B:302:ASP:OD1	1:B:302:ASP:N	2.49	0.46
1:B:583[A]:ARG:HB2	1:B:589:VAL:HG22	1.98	0.46
1:B:84:TRP:CD2	1:B:313:GLU:HG2	2.51	0.46
1:A:408:THR:HG22	1:A:417:THR:HB	1.98	0.45
1:B:634:LEU:O	1:B:645:HIS:NE2	2.48	0.45
1:D:1012:LEU:HD23	1:D:1020:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1131:ASP:OD1	1:D:1131:ASP:N	2.49	0.45
1:A:511:LEU:HD22	1:A:520:ILE:HG21	1.99	0.45
1:B:460:LEU:HD23	1:B:570:LEU:HD12	1.98	0.45
1:B:466:SER:OG	1:B:467:SER:N	2.47	0.45
1:C:1132:CYS:SG	1:D:1132:CYS:HB2	2.56	0.45
1:D:800:PRO:HB2	1:D:808:PHE:HE2	1.80	0.45
1:A:313:GLU:O	1:A:317:GLN:HG2	2.16	0.45
1:B:750:ASP:OD2	1:B:754:LYS:NZ	2.37	0.45
1:C:1084:ASN:HB3	1:C:1087:ARG:HD3	1.98	0.45
1:A:205:ASN:N	1:A:214:PHE:O	2.39	0.45
1:C:922[A]:ASN:HD22	1:C:1077:PRO:HG3	1.81	0.45
1:D:975:LEU:HD23	1:D:980:VAL:HG13	1.99	0.45
1:D:832:MET:SD	1:D:890:ARG:NH1	2.87	0.45
1:D:919:TYR:OH	1:D:1035:LEU:O	2.33	0.45
1:A:348:ARG:HB2	1:A:373:PHE:CE2	2.53	0.44
1:A:494:LEU:HB2	1:A:499:THR:HB	1.99	0.44
1:D:1024:LEU:HD11	1:D:1032:VAL:HG11	2.00	0.44
1:D:1149:VAL:HG23	1:D:1151:LEU:HD12	1.99	0.44
1:B:456:CYS:SG	1:B:457:SER:N	2.91	0.44
1:D:1188:THR:HG23	1:D:1191:ASN:H	1.81	0.44
1:B:704:CYS:HB2	1:B:705:PRO:HD2	2.00	0.44
1:A:161:LEU:HD12	1:A:172:GLN:HB2	1.99	0.44
1:A:359:GLU:OE2	1:A:359:GLU:HA	2.17	0.44
1:A:382:ASP:OD1	1:A:382:ASP:N	2.47	0.44
1:B:448:LYS:HD2	1:B:581:ASP:HB2	2.00	0.44
1:C:877:THR:HG23	1:C:884:THR:HG23	2.00	0.44
1:A:87:PHE:CG	1:A:100:PRO:HA	2.53	0.43
1:B:138:MET:SD	1:B:187:LEU:HD22	2.59	0.43
1:B:235:PHE:O	1:B:239:GLN:HG2	2.18	0.43
1:D:922[A]:ASN:ND2	1:D:1077:PRO:HG3	2.32	0.43
1:A:437:LEU:HD13	1:A:677:SER:HB2	2.01	0.43
1:D:991:VAL:HG13	1:D:993:TYR:HD2	1.83	0.43
1:C:1090:TRP:CE2	1:C:1094:GLN:HG3	2.54	0.43
1:D:1218:ASP:O	1:D:1222:MET:N	2.52	0.43
1:C:971:PHE:CD1	1:C:984:GLY:HA2	2.51	0.43
1:A:192:ASP:OD1	1:A:192:ASP:N	2.42	0.43
1:A:84:TRP:CD2	1:A:313:GLU:HG2	2.54	0.42
1:C:1185:CYS:CA	1:C:1196:CYS:HB3	2.43	0.42
1:A:456:CYS:SG	1:A:457:SER:N	2.92	0.42
1:D:1185:CYS:HB3	1:D:1196:CYS:N	2.34	0.42
1:B:205:ASN:N	1:B:214:PHE:O	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:CYS:HA	1:D:775:SER:O	2.18	0.42
1:A:110:HIS:HB2	1:A:118:PHE:CE1	2.55	0.42
1:B:706:LYS:H	1:B:706:LYS:HD3	1.84	0.42
1:C:945:ARG:HG2	1:C:947:VAL:HG23	2.01	0.42
1:A:77:ASN:ND2	1:A:321:ALA:HB2	2.34	0.42
1:B:470:THR:HB	1:B:493:SER:HB3	2.02	0.42
1:D:933:HIS:HB3	1:D:937:LYS:HA	2.01	0.42
1:B:583[B]:ARG:HB2	1:B:589:VAL:HG22	2.02	0.42
1:D:1185:CYS:HB3	1:D:1196:CYS:CA	2.40	0.42
1:B:710:TYR:HA	1:B:741:CYS:HA	2.02	0.42
1:C:922[A]:ASN:ND2	1:C:1077:PRO:HG3	2.35	0.42
1:D:971:PHE:HB3	1:D:993:TYR:HE2	1.84	0.42
1:B:341:ASN:OD1	1:B:341:ASN:N	2.52	0.41
1:C:928:THR:HA	1:C:947:VAL:HG22	2.02	0.41
1:A:148:THR:OG1	1:A:151:SER:HB3	2.20	0.41
1:C:1210:CYS:HA	1:C:1211:PRO:HD3	1.95	0.41
1:D:877:THR:HG23	1:D:884:THR:HG23	2.02	0.41
1:B:503:ILE:HG21	1:B:547:LEU:HD13	2.03	0.41
1:B:430:CYS:HB3	1:B:564:ARG:NH2	2.30	0.41
1:B:437:LEU:HD13	1:B:677:SER:HB2	2.02	0.41
1:C:800:PRO:HG2	1:C:808:PHE:CE2	2.56	0.41
1:C:973:LEU:HG	1:C:993:TYR:CE2	2.56	0.41
1:B:538:GLN:NE2	1:B:539:THR:O	2.53	0.41
1:A:118:PHE:HA	1:A:139:LYS:O	2.21	0.41
1:C:975:LEU:HD23	1:C:980:VAL:HG13	2.02	0.41
1:C:1215:PRO:HD2	1:C:1226:ALA:HA	2.01	0.41
1:A:114:ALA:HB3	1:D:1096:SER:HB2	2.03	0.41
1:A:699:LYS:HB3	1:A:699:LYS:HE3	1.76	0.41
1:B:456:CYS:HB2	1:B:606:CYS:HB3	1.81	0.41
1:A:480:LEU:HD13	1:C:782:ILE:HG21	2.03	0.41
1:B:415:ASN:OD1	2:B:1503:NAG:N2	2.53	0.41
1:B:603:GLN:HG2	1:D:822:GLY:O	2.21	0.41
1:A:289:GLU:OE1	1:A:293:GLN:NE2	2.54	0.40
1:C:783:CYS:HA	1:C:792:CYS:HA	2.03	0.40
1:B:84:TRP:CE2	1:B:313:GLU:HG2	2.56	0.40
1:C:1181:CYS:HA	1:C:1202:GLY:HA2	2.03	0.40
1:D:1126:CYS:SG	1:D:1131:ASP:HA	2.61	0.40
1:D:852:ASP:HB3	1:D:854:GLU:HG3	2.03	0.40
1:B:200:ASP:OD1	1:B:201:THR:N	2.55	0.40
1:C:1191:ASN:ND2	1:C:1195:ASP:OD1	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	688/1456 (47%)	671 (98%)	17 (2%)	0	100	100
1	B	686/1456 (47%)	665 (97%)	21 (3%)	0	100	100
1	C	462/1456 (32%)	446 (96%)	16 (4%)	0	100	100
1	D	463/1456 (32%)	443 (96%)	20 (4%)	0	100	100
All	All	2299/5824 (40%)	2225 (97%)	74 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	591/1233 (48%)	564 (95%)	27 (5%)	23	54
1	B	590/1233 (48%)	566 (96%)	24 (4%)	26	58
1	C	378/1233 (31%)	358 (95%)	20 (5%)	19	48
1	D	380/1233 (31%)	364 (96%)	16 (4%)	25	57
All	All	1939/4932 (39%)	1852 (96%)	87 (4%)	26	54

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	CYS
1	A	86	SER

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Mol	Chain	Res	Type
1	A	108	SER
1	A	173	SER
1	A	176	TYR
1	A	206	LYS
1	A	247	GLN
1	A	257	ARG
1	A	276	SER
1	A	283	ASP
1	A	298	CYS
1	A	302	ASP
1	A	368	CYS
1	A	393	LYS
1	A	412	ASP
1	A	417	THR
1	A	424	SER
1	A	426	GLN
1	A	430	CYS
1	A	515	TYR
1	A	541	LEU
1	A	699	LYS
1	A	704	CYS
1	A	717	CYS
1	A	731	CYS
1	A	732	SER
1	A	739	ASP
1	B	70	ARG
1	B	149	LYS
1	B	185	LEU
1	B	192	ASP
1	B	196	LEU
1	B	233	MET
1	B	257	ARG
1	B	284	VAL
1	B	288	LEU
1	B	302	ASP
1	B	305	SER
1	B	306	CYS
1	B	327	ASP
1	B	349	SER
1	B	457	SER
1	B	495	ASP
1	B	515	TYR

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Mol	Chain	Res	Type
1	B	526	THR
1	B	610	ARG
1	B	613	PHE
1	B	706	LYS
1	B	717	CYS
1	B	747	THR
1	B	754	LYS
1	C	769	MET
1	C	832	MET
1	C	838	GLN
1	C	861	GLU
1	C	876	GLN
1	C	883	ASN
1	C	888	ASP
1	C	900	LEU
1	C	943	SER
1	C	962	LYS
1	C	1005	ASP
1	C	1007	ASP
1	C	1015	ASP
1	C	1114[A]	ARG
1	C	1114[B]	ARG
1	C	1126	CYS
1	C	1157	THR
1	C	1164	PHE
1	C	1185	CYS
1	C	1222	MET
1	D	769	MET
1	D	809	PHE
1	D	871	SER
1	D	877	THR
1	D	888	ASP
1	D	889	SER
1	D	979	LYS
1	D	1005	ASP
1	D	1007	ASP
1	D	1016	LYS
1	D	1111	GLU
1	D	1114[A]	ARG
1	D	1114[B]	ARG
1	D	1164	PHE
1	D	1196	CYS

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Mol	Chain	Res	Type
1	D	1219	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	GLN
1	A	385	GLN
1	A	546	ASN
1	B	77	ASN
1	B	171	GLN
1	B	426	GLN
1	B	498	GLN
1	C	824	GLN
1	C	917	GLN
1	C	997	GLN
1	D	838	GLN
1	D	1147	HIS

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](#)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	B	1502	1	14,14,15	0.27	0	17,19,21	0.46	0
2	NAG	B	1501	1	14,14,15	0.23	0	17,19,21	0.42	0
2	NAG	A	1503	1	14,14,15	0.35	0	17,19,21	0.51	0
2	NAG	B	1503	1	14,14,15	0.33	0	17,19,21	0.53	0
2	NAG	A	1502	1	14,14,15	0.26	0	17,19,21	0.47	0
2	NAG	A	1501	1	14,14,15	0.22	0	17,19,21	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1502	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1501	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1503	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1503	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1502	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1501	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1501	NAG	C4-C5-C6-O6
2	B	1501	NAG	O5-C5-C6-O6
2	A	1501	NAG	C4-C5-C6-O6
2	B	1502	NAG	O5-C5-C6-O6
2	A	1501	NAG	O5-C5-C6-O6
2	A	1502	NAG	C4-C5-C6-O6
2	A	1502	NAG	O5-C5-C6-O6
2	B	1502	NAG	C4-C5-C6-O6
2	A	1503	NAG	C4-C5-C6-O6
2	A	1503	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1503	NAG	1	0
2	B	1503	NAG	1	0

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.

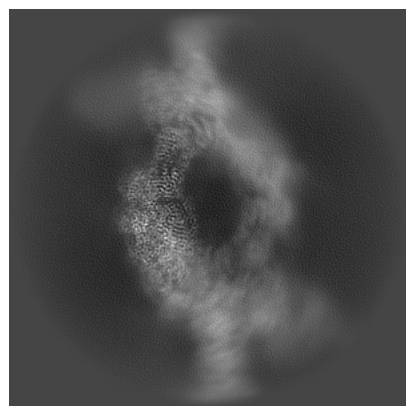
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51636. These allow visual inspection of the internal detail of the map and identification of artifacts.

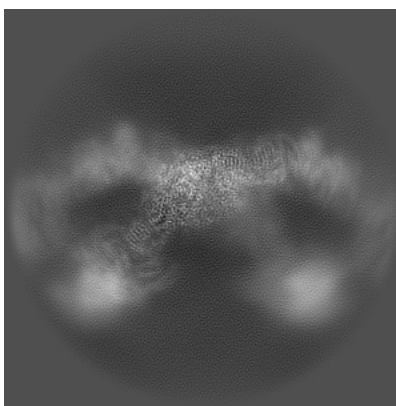
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

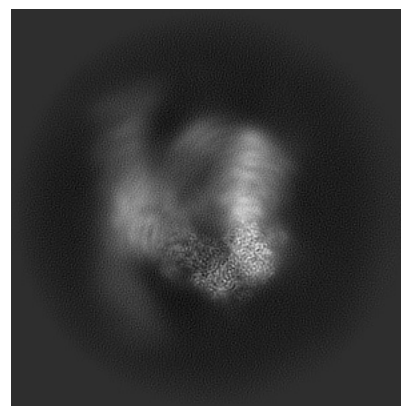
6.1.1 Primary map



X

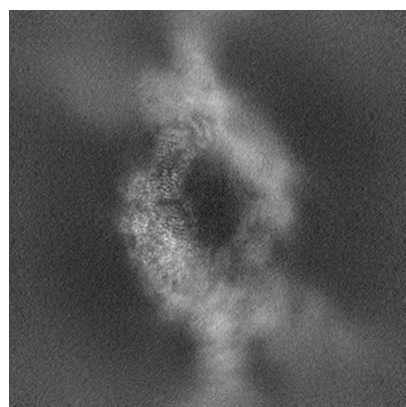


Y

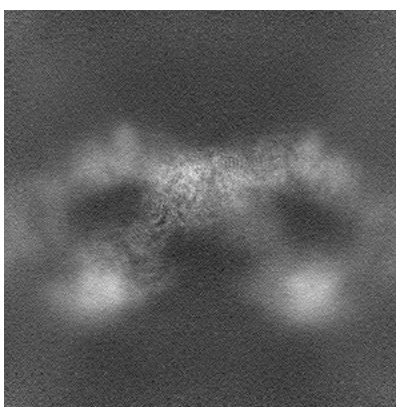


Z

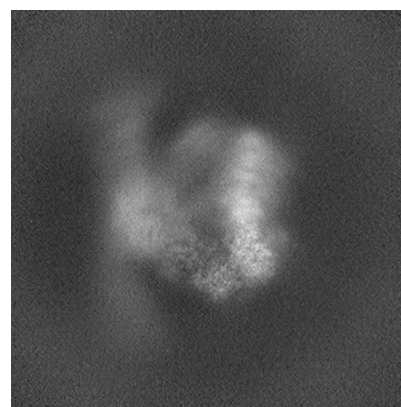
6.1.2 Raw map



X



Y

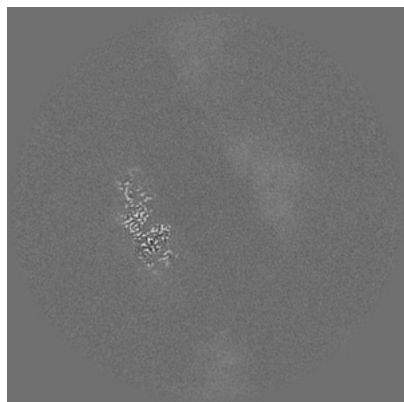


Z

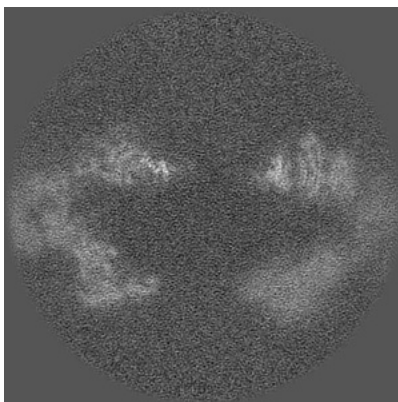
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

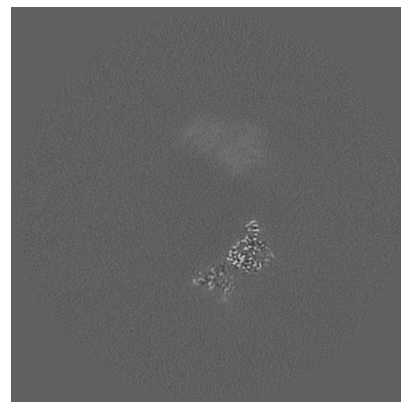
6.2.1 Primary map



X Index: 275

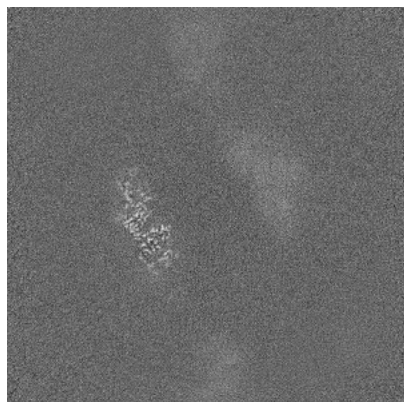


Y Index: 275

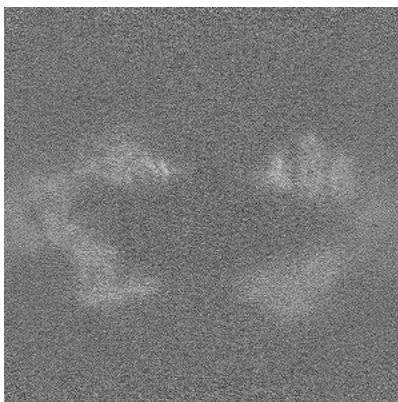


Z Index: 275

6.2.2 Raw map



X Index: 275



Y Index: 275

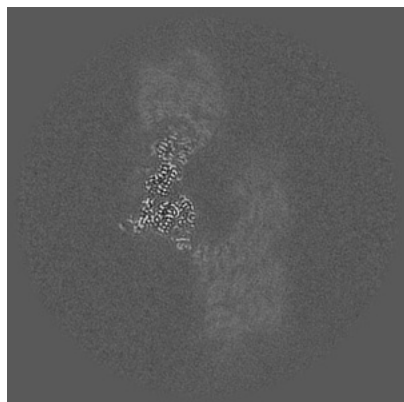


Z Index: 275

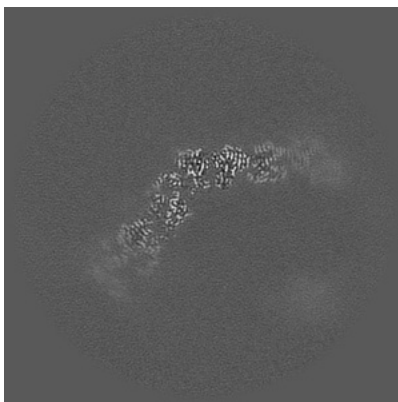
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

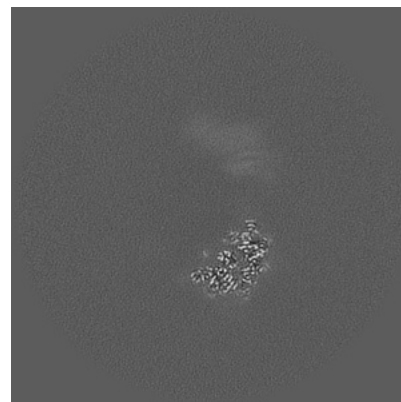
6.3.1 Primary map



X Index: 333

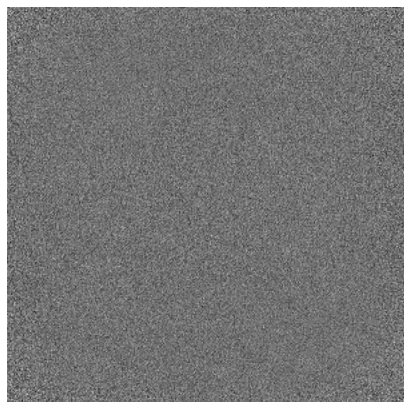


Y Index: 214

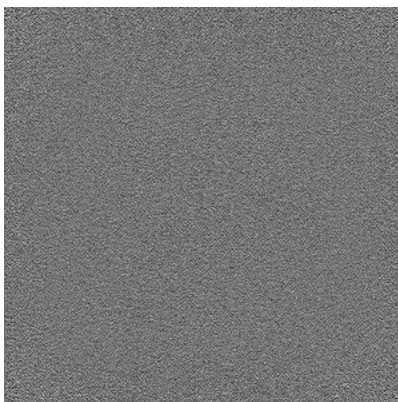


Z Index: 258

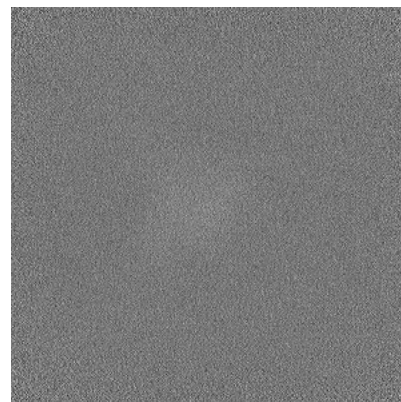
6.3.2 Raw map



X Index: 0



Y Index: 0

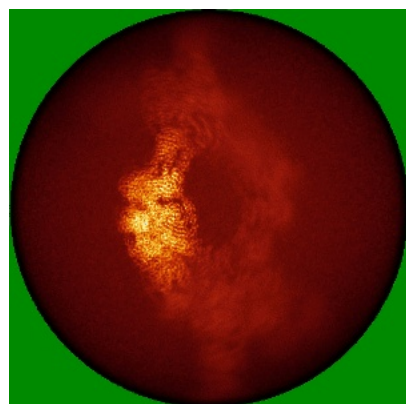


Z Index: 0

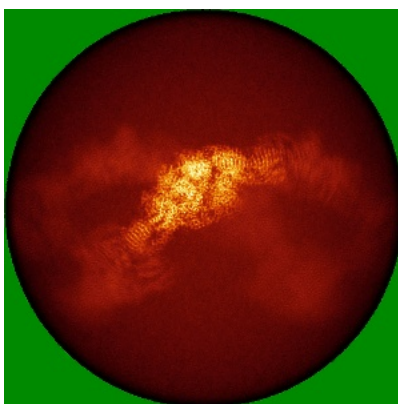
The images above show the largest variance slices of the map in three orthogonal directions.

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

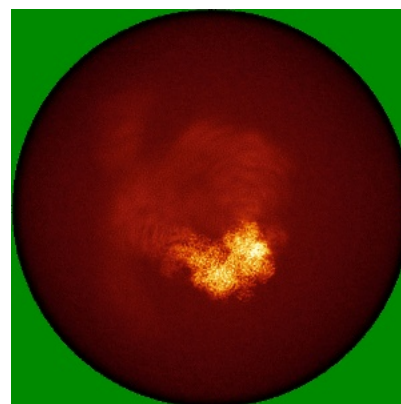
6.4.1 Primary map



X

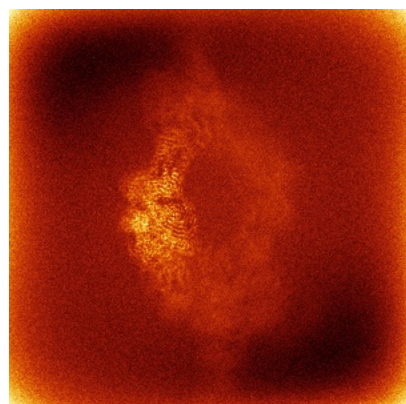


Y

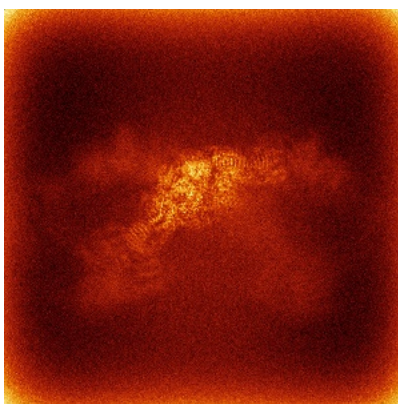


Z

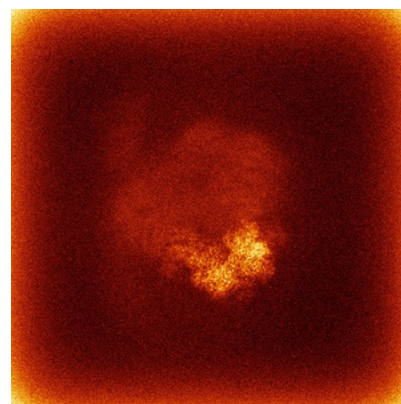
6.4.2 Raw map



X



Y

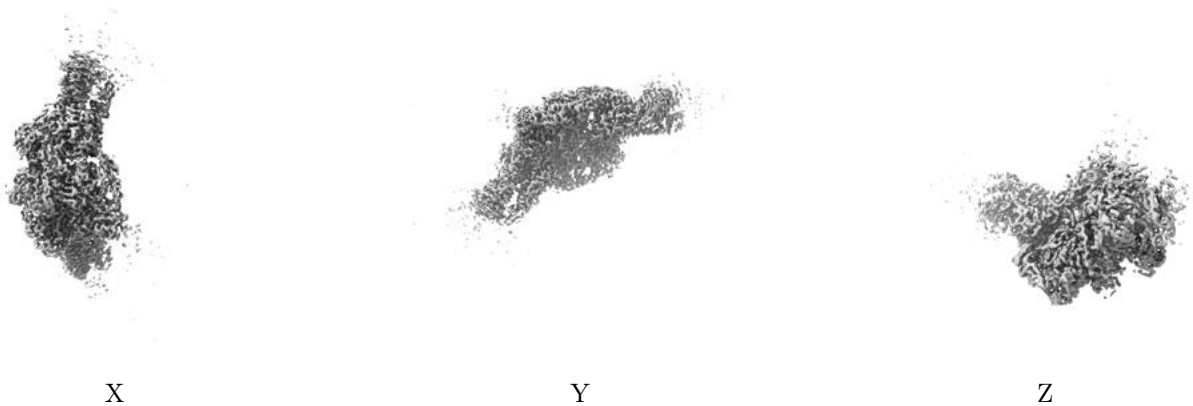


Z

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.

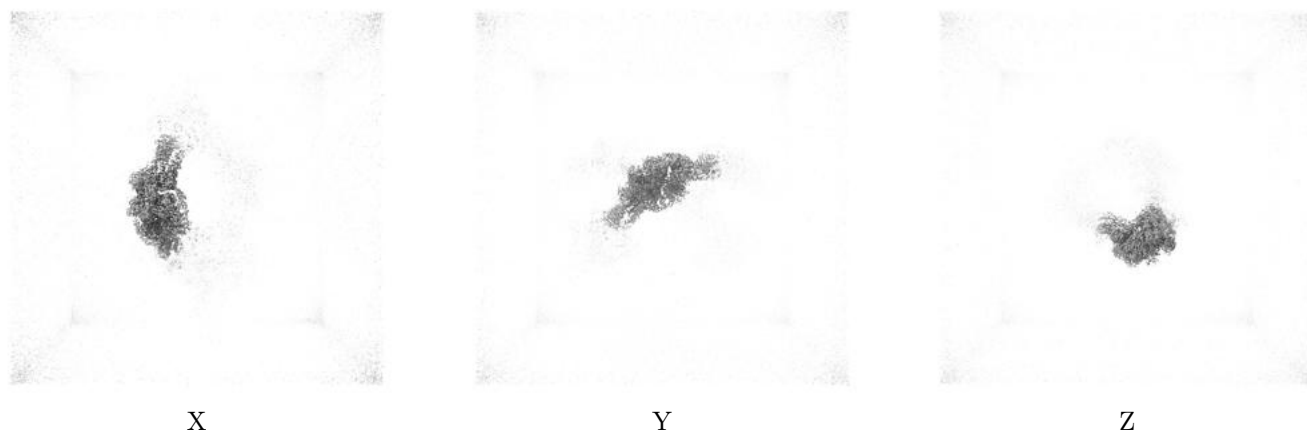
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.256. 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.

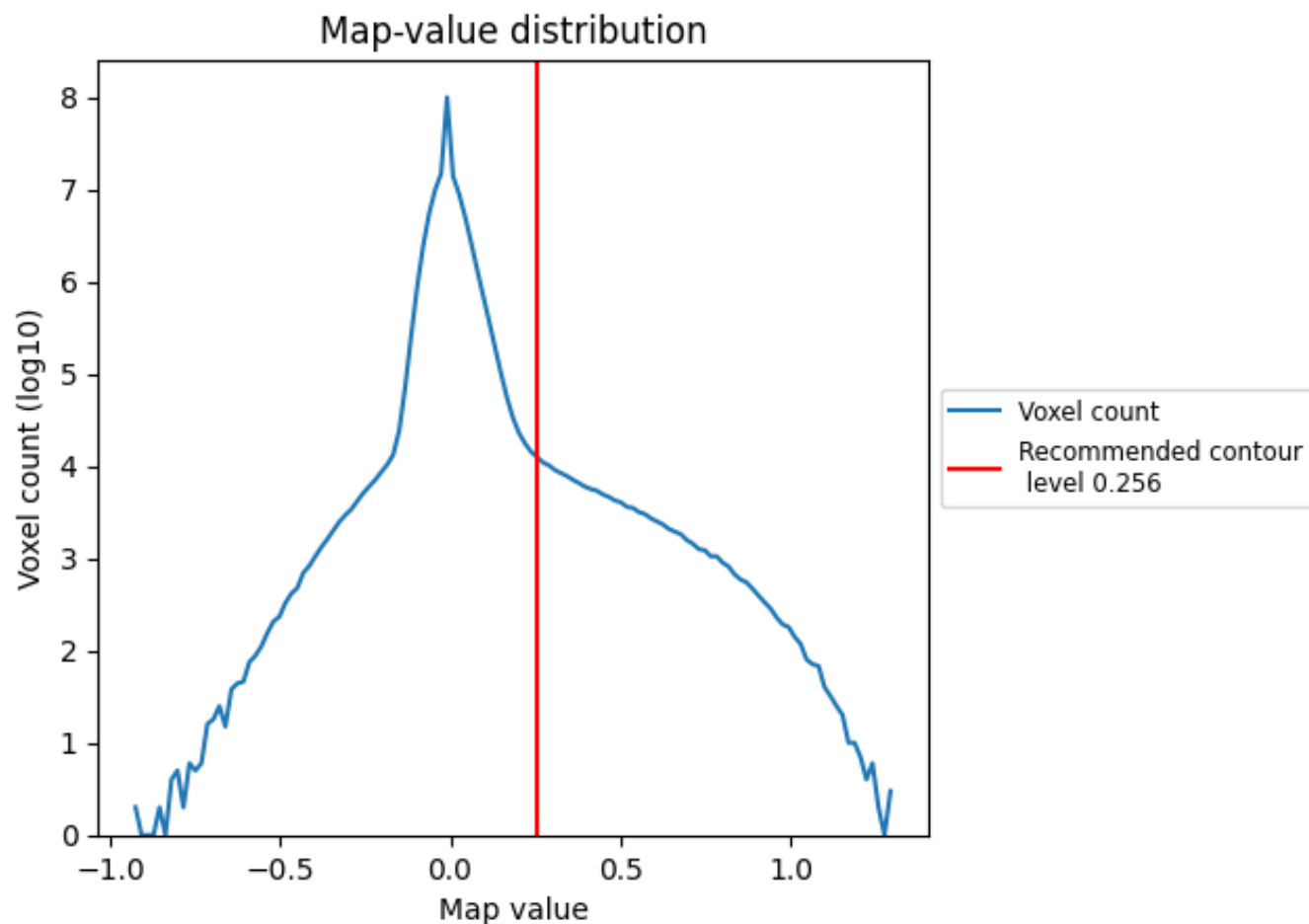
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

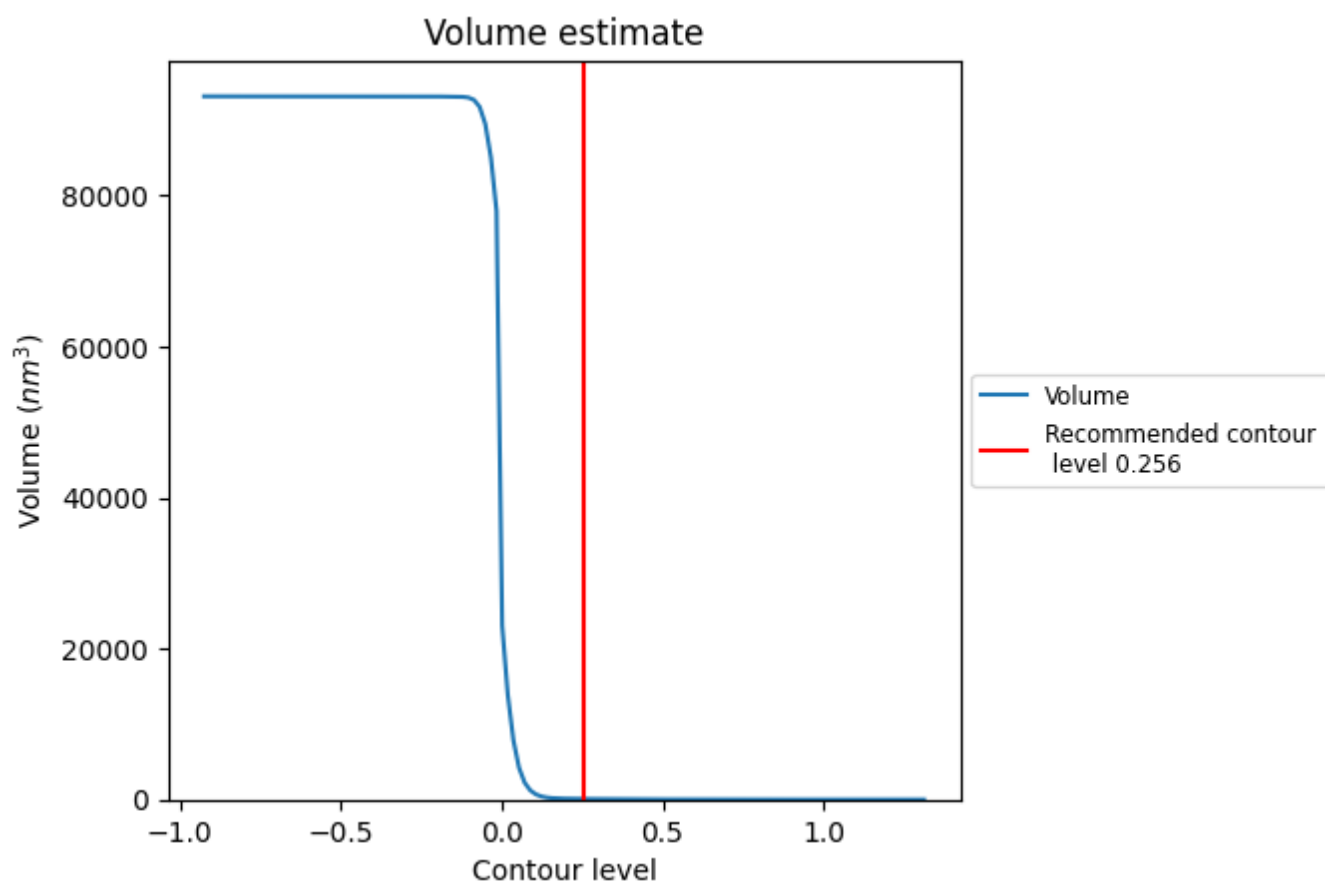
This section contains the results of statistical analysis of the map.

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.

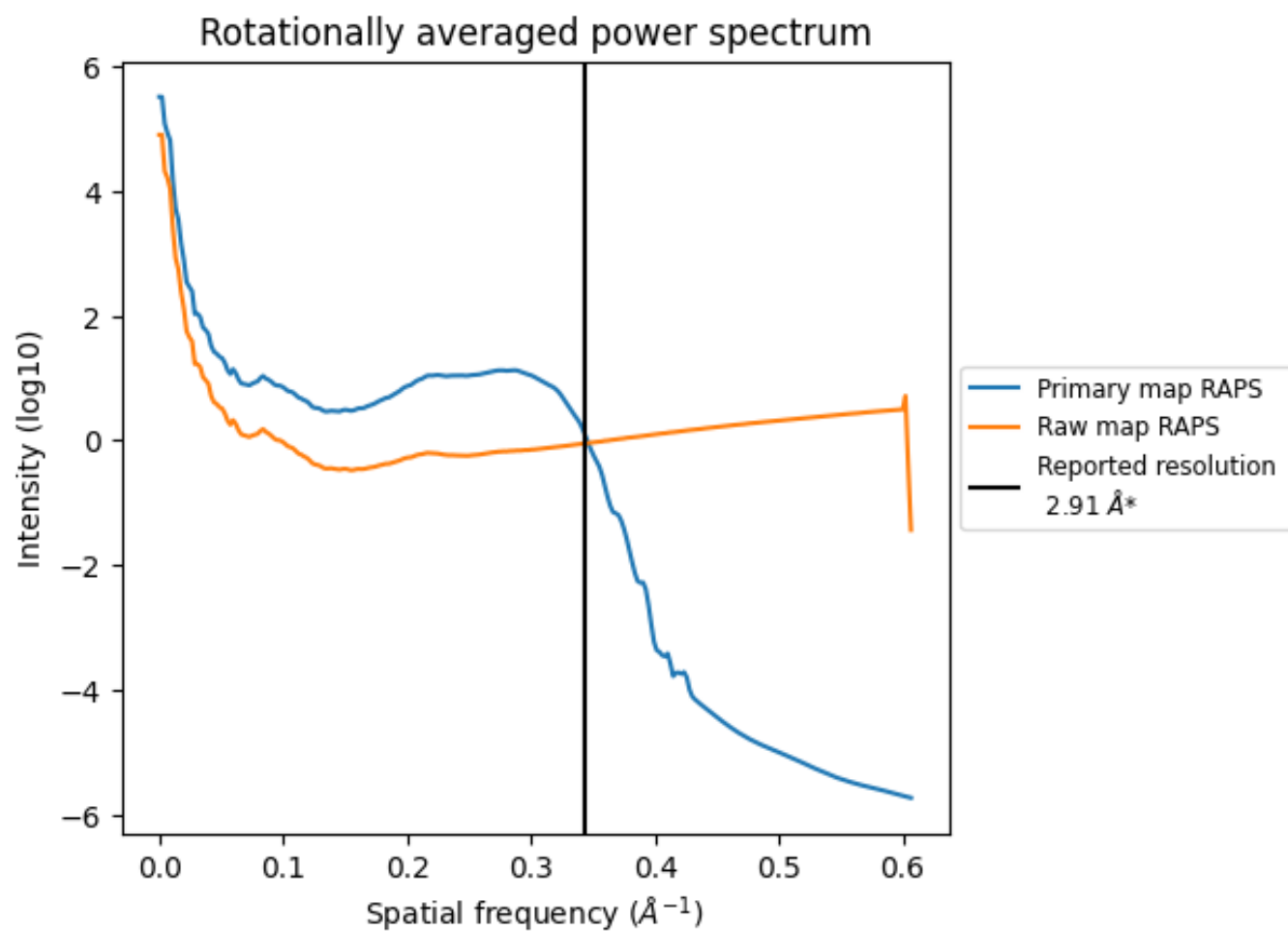
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 83 nm³; this corresponds to an approximate mass of 75 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 ⓘ

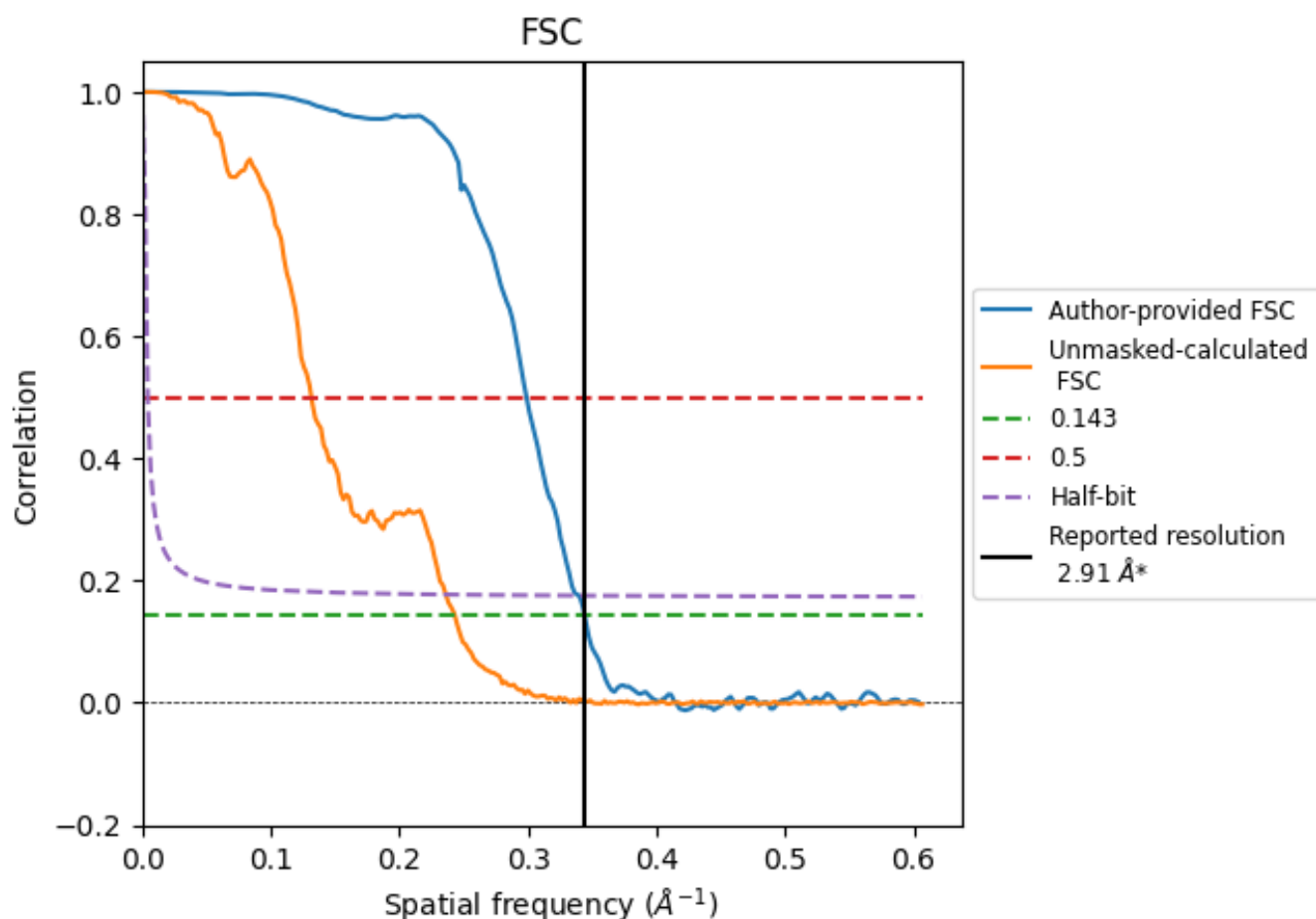


*Reported resolution corresponds to spatial frequency of 0.344 \AA^{-1}

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 0.344 \AA^{-1}

8.2 Resolution estimates [i](#)

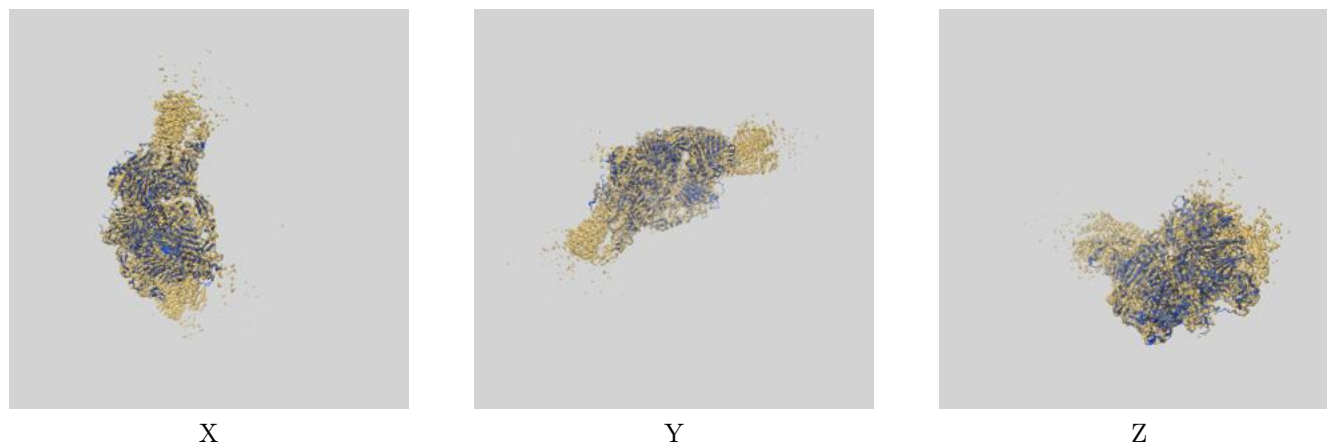
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.91	-	-
Author-provided FSC curve	2.91	3.34	2.95
Unmasked-calculated*	4.12	7.60	4.23

*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 4.12 differs from the reported value 2.91 by more than 10 %

9 Map-model fit [i](#)

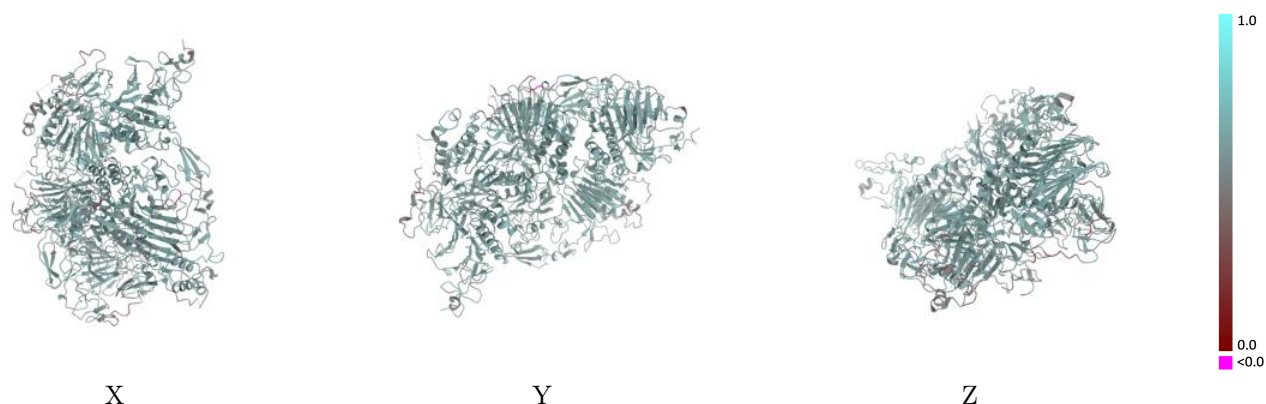
This section contains information regarding the fit between EMDB map EMD-51636 and PDB model 9GVJ. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



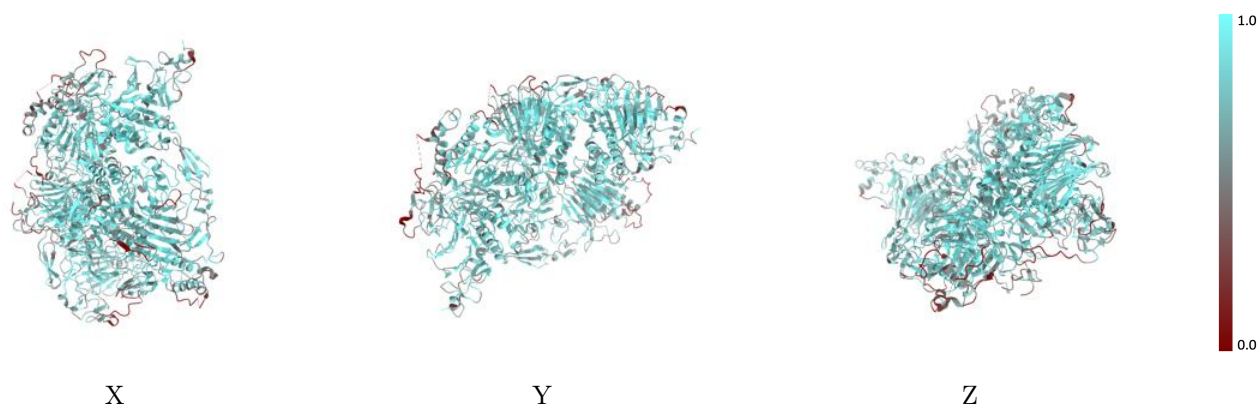
The images above show the 3D surface view of the map at the recommended contour level 0.256 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



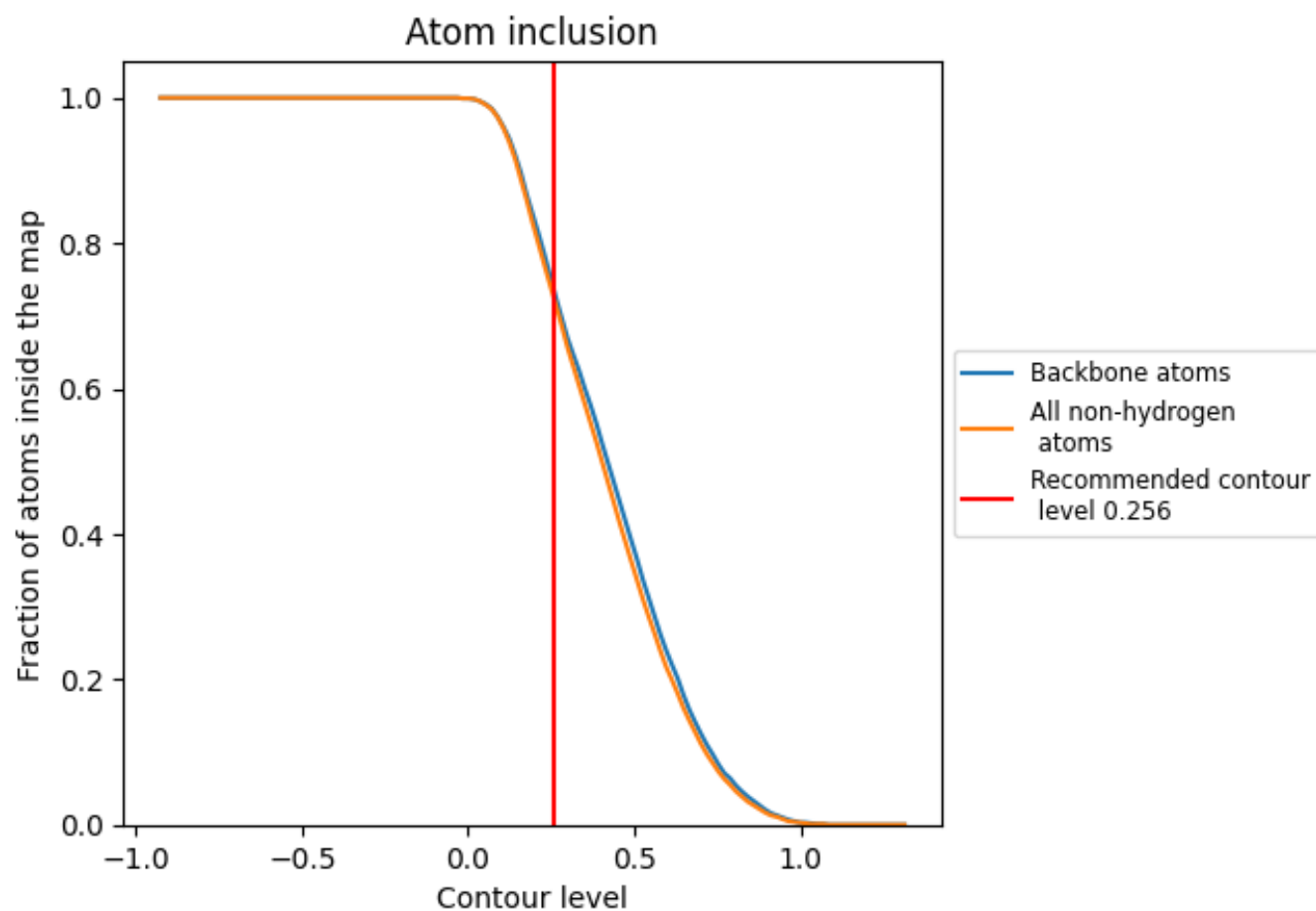
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.256).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 73% 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 (0.256) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7270	<div></div> 0.5810
A	<div></div> 0.7400	<div></div> 0.5890
B	<div></div> 0.7220	<div></div> 0.5810
C	<div></div> 0.7310	<div></div> 0.5750
D	<div></div> 0.7270	<div></div> 0.5720

