



wwPDB EM Validation Summary Report ⓘ

Oct 13, 2024 – 03:41 pm BST

PDB ID : 8AQW
EMDB ID : EMD-15592
Title : BA.4/5 SARS-CoV-2 Spike bound to mouse ACE2 (local)
Authors : Lau, K.; Ni, D.; Beckert, B.; Nazarov, S.; Myasnikov, A.; Pojer, F.; Stahlberg, H.; Uchikawa, E.
Deposited on : 2022-08-13
Resolution : 3.30 Å(reported)

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

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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.dev113
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) : 2.39

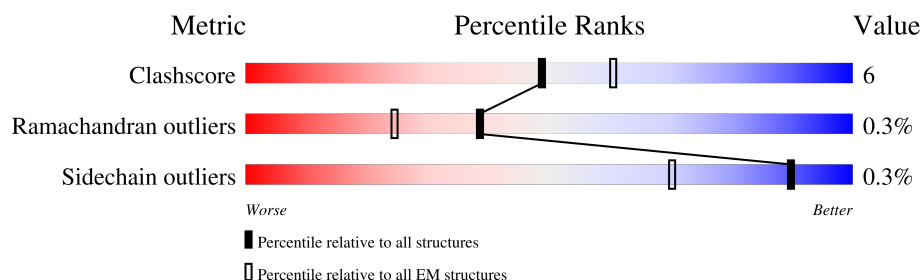
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	B	1283	
2	A	884	
3	C	2	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6457 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 Spike glycoprotein,Fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	193	Total	C	N	O	S	0	0
			1543	994	261	280	8		

There are 95 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	24	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	29	SER	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	452	ARG	LEU	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	486	VAL	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	682	GLY	ARG	variant	UNP P0DTC2
B	683	SER	ARG	variant	UNP P0DTC2
B	685	SER	ARG	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1209	GLY	-	linker	UNP P0DTC2
B	1210	SER	-	linker	UNP P0DTC2
B	1211	GLY	-	linker	UNP P0DTC2
B	1212	TYR	-	linker	UNP P0DTC2
B	1232	LEU	PHE	engineered mutation	UNP P10104
B	1238	GLY	-	expression tag	UNP P10104
B	1239	ARG	-	expression tag	UNP P10104
B	1240	SER	-	expression tag	UNP P10104
B	1241	LEU	-	expression tag	UNP P10104
B	1242	GLU	-	expression tag	UNP P10104
B	1243	VAL	-	expression tag	UNP P10104
B	1244	LEU	-	expression tag	UNP P10104
B	1245	PHE	-	expression tag	UNP P10104
B	1246	GLN	-	expression tag	UNP P10104
B	1247	GLY	-	expression tag	UNP P10104
B	1248	PRO	-	expression tag	UNP P10104
B	1249	GLY	-	expression tag	UNP P10104
B	1250	HIS	-	expression tag	UNP P10104
B	1251	HIS	-	expression tag	UNP P10104
B	1252	HIS	-	expression tag	UNP P10104
B	1253	HIS	-	expression tag	UNP P10104
B	1254	HIS	-	expression tag	UNP P10104
B	1255	HIS	-	expression tag	UNP P10104
B	1256	HIS	-	expression tag	UNP P10104
B	1257	HIS	-	expression tag	UNP P10104
B	1258	SER	-	expression tag	UNP P10104
B	1259	ALA	-	expression tag	UNP P10104
B	1260	TRP	-	expression tag	UNP P10104
B	1261	SER	-	expression tag	UNP P10104
B	1262	HIS	-	expression tag	UNP P10104
B	1263	PRO	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1264	GLN	-	expression tag	UNP P10104
B	1265	PHE	-	expression tag	UNP P10104
B	1266	GLU	-	expression tag	UNP P10104
B	1267	LYS	-	expression tag	UNP P10104
B	1268	GLY	-	expression tag	UNP P10104
B	1269	GLY	-	expression tag	UNP P10104
B	1270	GLY	-	expression tag	UNP P10104
B	1271	SER	-	expression tag	UNP P10104
B	1272	GLY	-	expression tag	UNP P10104
B	1273	GLY	-	expression tag	UNP P10104
B	1274	GLY	-	expression tag	UNP P10104
B	1275	GLY	-	expression tag	UNP P10104
B	1276	SER	-	expression tag	UNP P10104
B	1277	GLY	-	expression tag	UNP P10104
B	1278	GLY	-	expression tag	UNP P10104
B	1279	SER	-	expression tag	UNP P10104
B	1280	ALA	-	expression tag	UNP P10104
B	1281	TRP	-	expression tag	UNP P10104
B	1282	SER	-	expression tag	UNP P10104
B	1283	HIS	-	expression tag	UNP P10104
B	1284	PRO	-	expression tag	UNP P10104
B	1285	GLN	-	expression tag	UNP P10104
B	1286	PHE	-	expression tag	UNP P10104
B	1287	GLU	-	expression tag	UNP P10104
B	1288	LYS	-	expression tag	UNP P10104

- Molecule 2 is a protein called Processed angiotensin-converting enzyme 2,Ig gamma-2A chain C region, A allele.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	596	Total	C	N	O	S	1	0
			4872	3103	819	921	29		

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP Q8R0I0
A	-14	GLY	-	expression tag	UNP Q8R0I0
A	-13	THR	-	expression tag	UNP Q8R0I0
A	-12	LEU	-	expression tag	UNP Q8R0I0
A	-11	SER	-	expression tag	UNP Q8R0I0
A	-10	ALA	-	expression tag	UNP Q8R0I0

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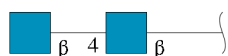
Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	PRO	-	expression tag	UNP Q8R0I0
A	-8	PRO	-	expression tag	UNP Q8R0I0
A	-7	CYS	-	expression tag	UNP Q8R0I0
A	-6	THR	-	expression tag	UNP Q8R0I0
A	-5	GLN	-	expression tag	UNP Q8R0I0
A	-4	ARG	-	expression tag	UNP Q8R0I0
A	-3	ILE	-	expression tag	UNP Q8R0I0
A	-2	LYS	-	expression tag	UNP Q8R0I0
A	-1	TRP	-	expression tag	UNP Q8R0I0
A	0	LYS	-	expression tag	UNP Q8R0I0
A	1	GLY	-	expression tag	UNP Q8R0I0
A	2	LEU	-	expression tag	UNP Q8R0I0
A	3	LEU	-	expression tag	UNP Q8R0I0
A	4	LEU	-	expression tag	UNP Q8R0I0
A	5	THR	-	expression tag	UNP Q8R0I0
A	6	ALA	-	expression tag	UNP Q8R0I0
A	7	SER	-	expression tag	UNP Q8R0I0
A	8	LEU	-	expression tag	UNP Q8R0I0
A	9	LEU	-	expression tag	UNP Q8R0I0
A	10	ASN	-	expression tag	UNP Q8R0I0
A	11	PHE	-	expression tag	UNP Q8R0I0
A	12	TRP	-	expression tag	UNP Q8R0I0
A	13	ASN	-	expression tag	UNP Q8R0I0
A	14	LEU	-	expression tag	UNP Q8R0I0
A	15	PRO	-	expression tag	UNP Q8R0I0
A	16	THR	-	expression tag	UNP Q8R0I0
A	17	THR	-	expression tag	UNP Q8R0I0
A	18	ALA	-	expression tag	UNP Q8R0I0
A	616	LEU	-	linker	UNP Q8R0I0
A	617	GLU	-	linker	UNP Q8R0I0
A	618	VAL	-	linker	UNP Q8R0I0
A	619	LEU	-	linker	UNP Q8R0I0
A	620	PHE	-	linker	UNP Q8R0I0
A	621	GLN	-	linker	UNP Q8R0I0
A	622	GLY	-	linker	UNP Q8R0I0
A	623	PRO	-	linker	UNP Q8R0I0
A	624	MET	-	linker	UNP Q8R0I0
A	625	ASP	-	linker	UNP Q8R0I0
A	859	HIS	-	expression tag	UNP P01863
A	860	HIS	-	expression tag	UNP P01863
A	861	HIS	-	expression tag	UNP P01863
A	862	HIS	-	expression tag	UNP P01863

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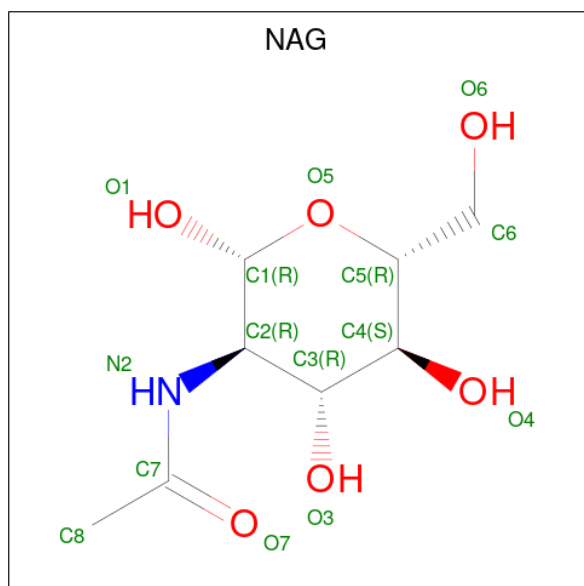
Chain	Residue	Modelled	Actual	Comment	Reference
A	863	HIS	-	expression tag	UNP P01863
A	864	HIS	-	expression tag	UNP P01863
A	865	HIS	-	expression tag	UNP P01863
A	866	HIS	-	expression tag	UNP P01863
A	867	HIS	-	expression tag	UNP P01863
A	868	HIS	-	expression tag	UNP P01863

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	2	Total	C	N	O	0	0
			28	16	2	10		

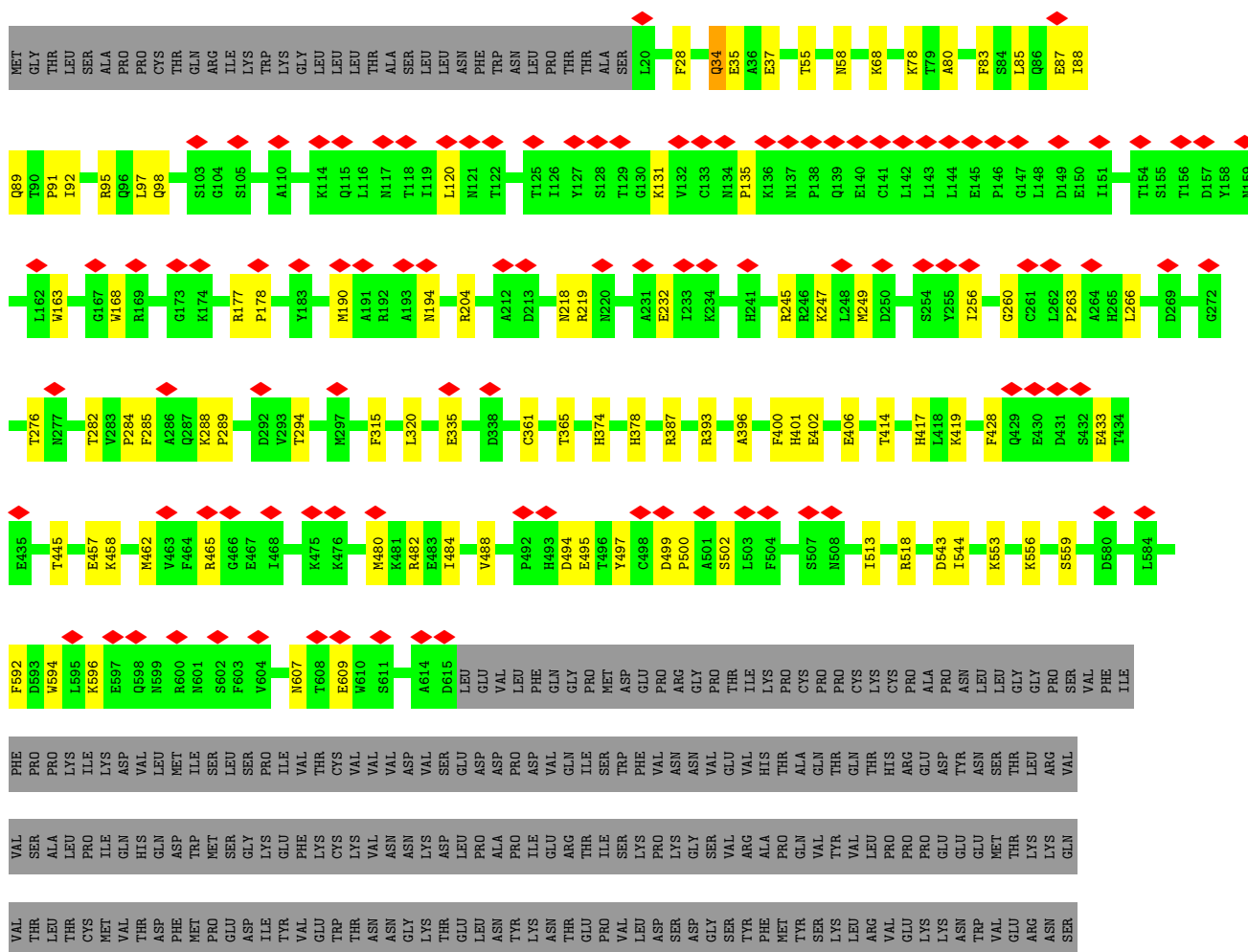
- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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

- Molecule 2: Processed angiotensin-converting enzyme 2,Ig gamma-2A chain C region, A allele



TYR
SER
CYS
SER
VAL
HIS
GLY
LEU
HIS
ASN
HIS
HIS
THR
LYS
SER
PHE
SER
ARG
THR
PRO
GLY
LYS
HIS
HIS
HIS
HIS
HIS
HIS
HIS
HIS

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

100%

NAG1
NAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103496	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.114	Depositor
Minimum map value	-0.745	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.172	Depositor
Map size (\AA)	365.184, 365.184, 365.184	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0144, 1.0144, 1.0144	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	B	0.26	0/1589	0.52	0/2163
2	A	0.24	0/5010	0.45	0/6801
All	All	0.25	0/6599	0.46	0/8964

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	B	1543	0	1466	16	0
2	A	4872	0	4639	55	0
3	C	28	0	25	0	0
4	B	14	0	13	0	0
All	All	6457	0	6143	71	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.

The worst 5 of 71 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:A:85:LEU:HD11	2:A:97:LEU:HD23	1.69	0.72
2:A:34[C]:GLN:OE1	2:A:35:GLU:N	2.23	0.70
2:A:458:LYS:O	2:A:462:MET:HG2	1.95	0.66
1:B:393:THR:HG22	1:B:394:ASN:H	1.61	0.66
2:A:419:LYS:NZ	2:A:428:PHE:O	2.29	0.65

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	B	191/1283 (15%)	174 (91%)	15 (8%)	2 (1%)	13	42
2	A	596/884 (67%)	560 (94%)	36 (6%)	0	100	100
All	All	787/2167 (36%)	734 (93%)	51 (6%)	2 (0%)	38	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	372	ALA
1	B	486	VAL

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	166/1107 (15%)	166 (100%)	0	100	100
2	A	522/788 (66%)	518 (99%)	4 (1%)	79	87
All	All	688/1895 (36%)	684 (99%)	4 (1%)	90	90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	34[A]	GLN
2	A	34[B]	GLN
2	A	34[C]	GLN
2	A	131	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	24	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 ⓘ

2 monosaccharides are modelled in this entry.

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
3	NAG	C	1	3,2	14,14,15	0.20	0	17,19,21	0.51	0
3	NAG	C	2	3	14,14,15	0.33	0	17,19,21	0.37	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
3	NAG	C	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	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.

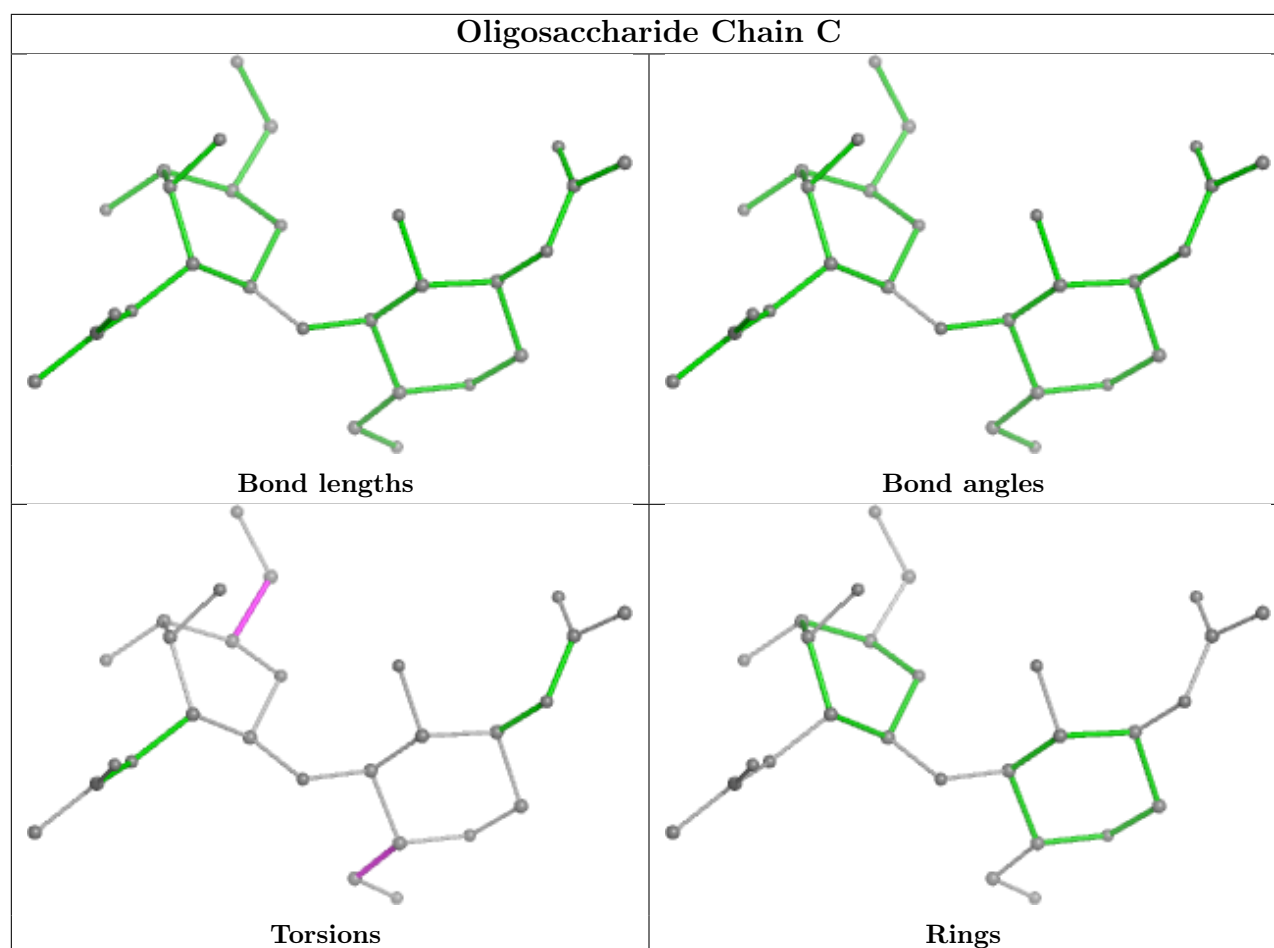
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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	$\# Z > 2$
4	NAG	B	1301	1	14,14,15	0.23	0	17,19,21	0.45	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
4	NAG	B	1301	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1301	NAG	O5-C5-C6-O6
4	B	1301	NAG	C4-C5-C6-O6
4	B	1301	NAG	C8-C7-N2-C2
4	B	1301	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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.

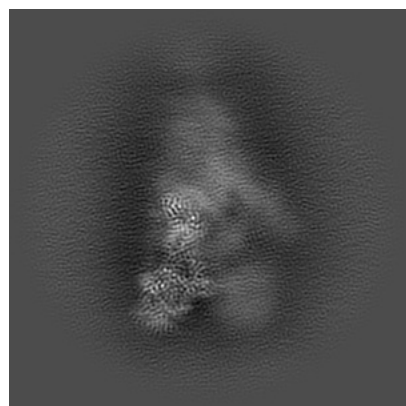
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15592. These allow visual inspection of the internal detail of the map and identification of artifacts.

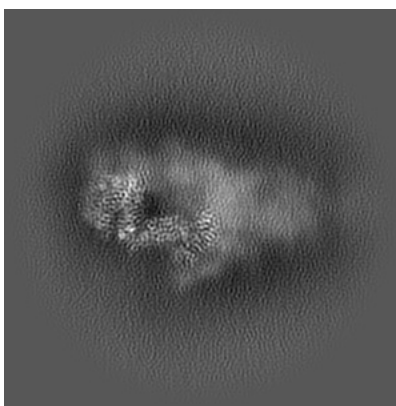
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

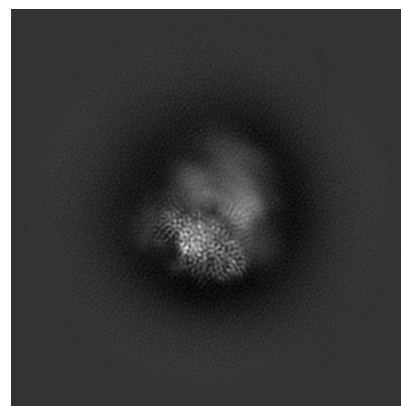
6.1.1 Primary map



X

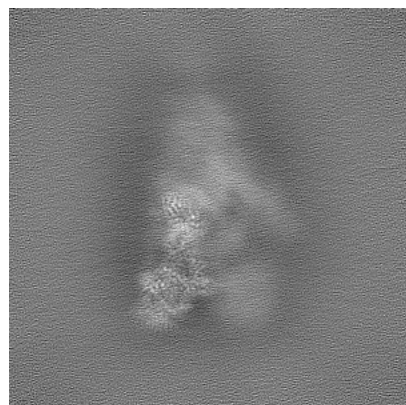


Y

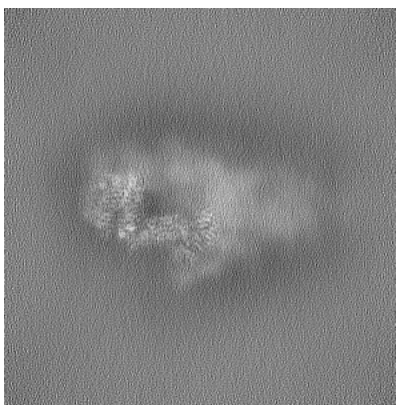


Z

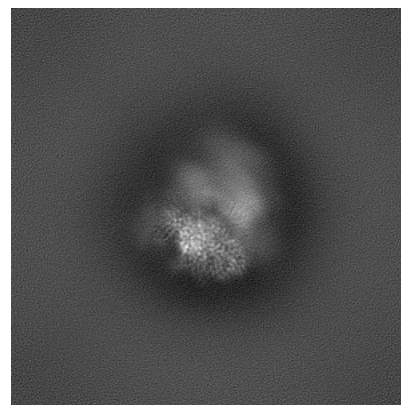
6.1.2 Raw map



X



Y

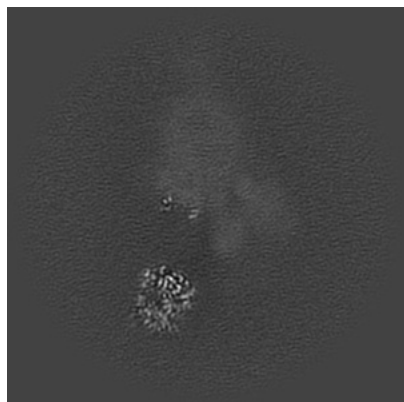


Z

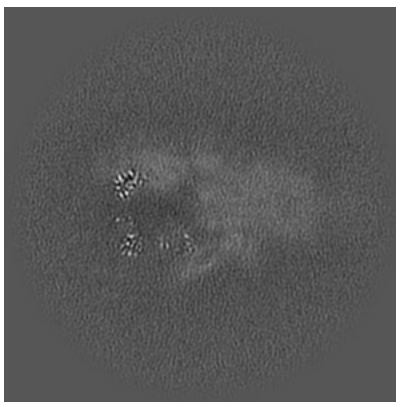
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

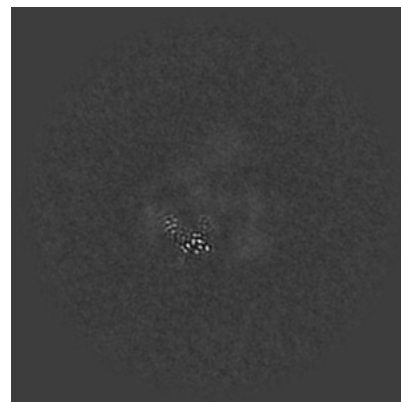
6.2.1 Primary map



X Index: 180

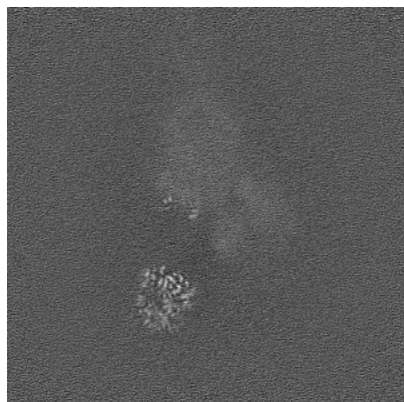


Y Index: 180

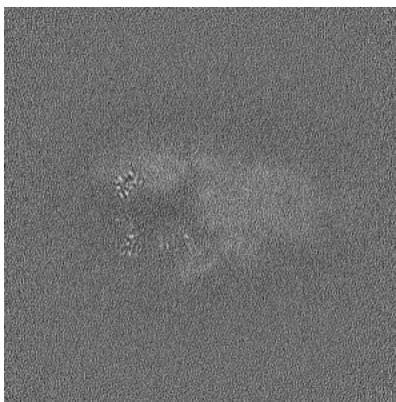


Z Index: 180

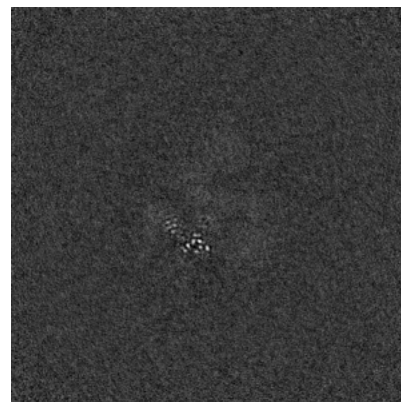
6.2.2 Raw map



X Index: 180



Y Index: 180

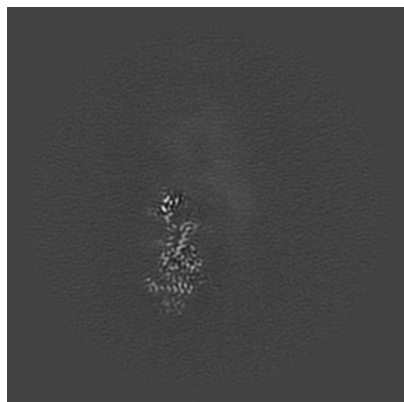


Z Index: 180

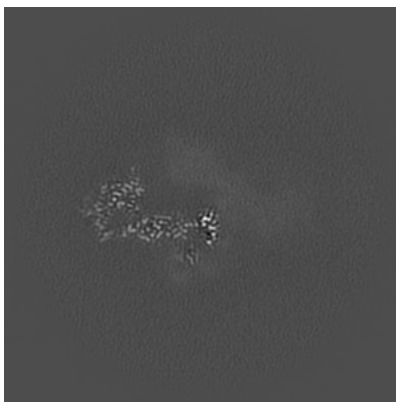
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

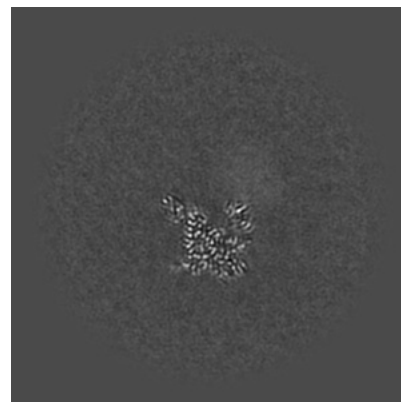
6.3.1 Primary map



X Index: 157

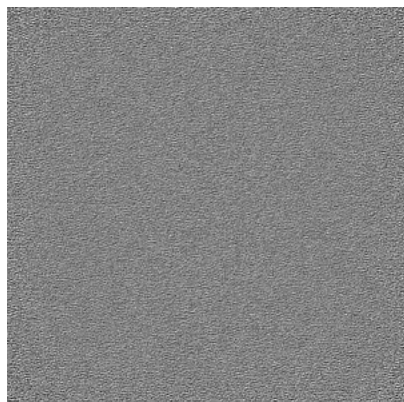


Y Index: 149

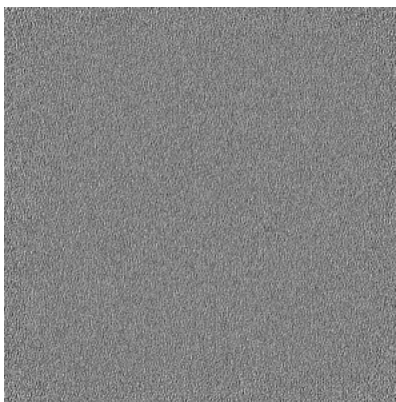


Z Index: 114

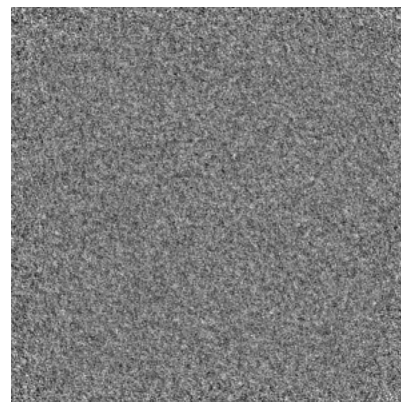
6.3.2 Raw map



X Index: 0



Y Index: 0

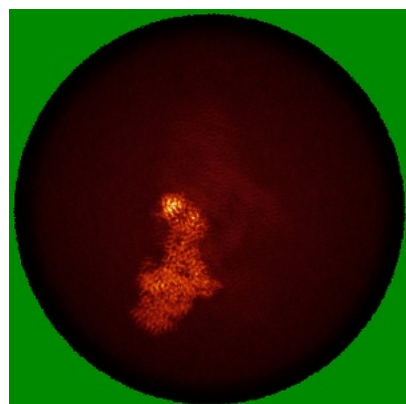


Z Index: 359

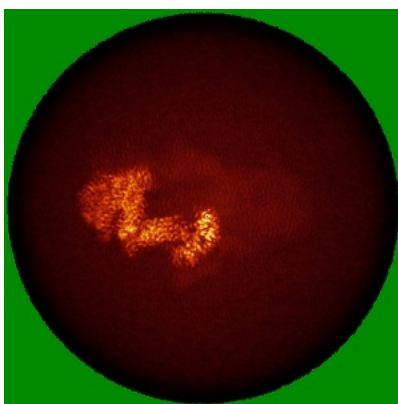
The images above show the largest variance slices of the map in three orthogonal directions.

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

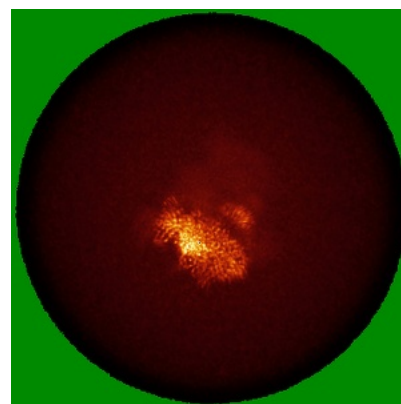
6.4.1 Primary map



X

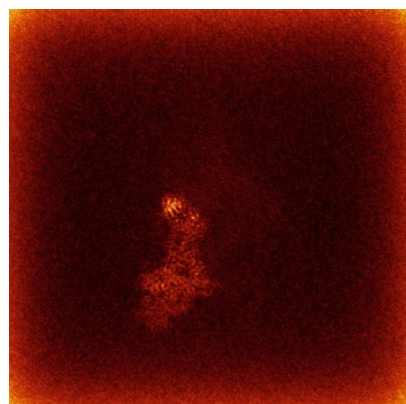


Y

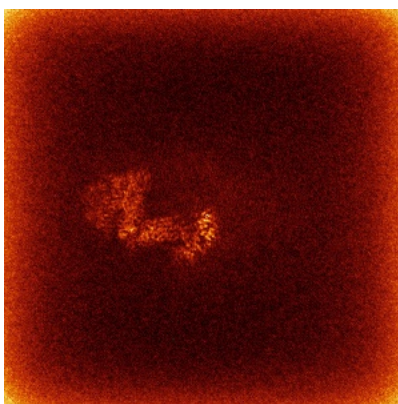


Z

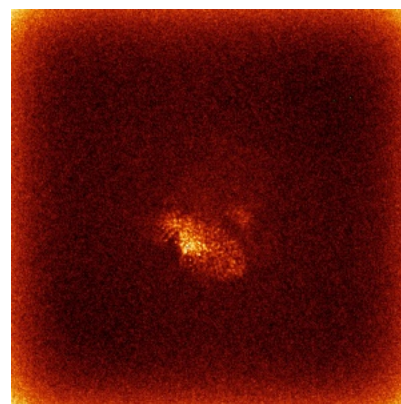
6.4.2 Raw map



X



Y

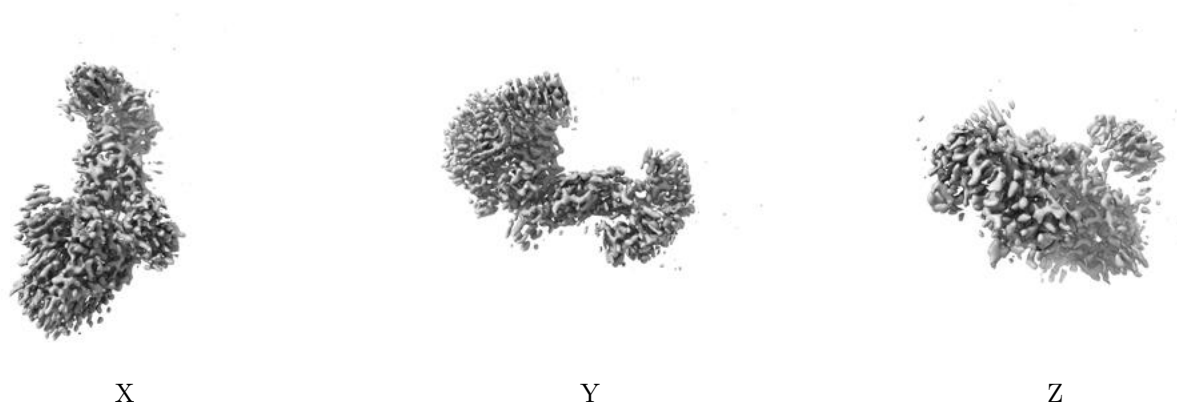


Z

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.

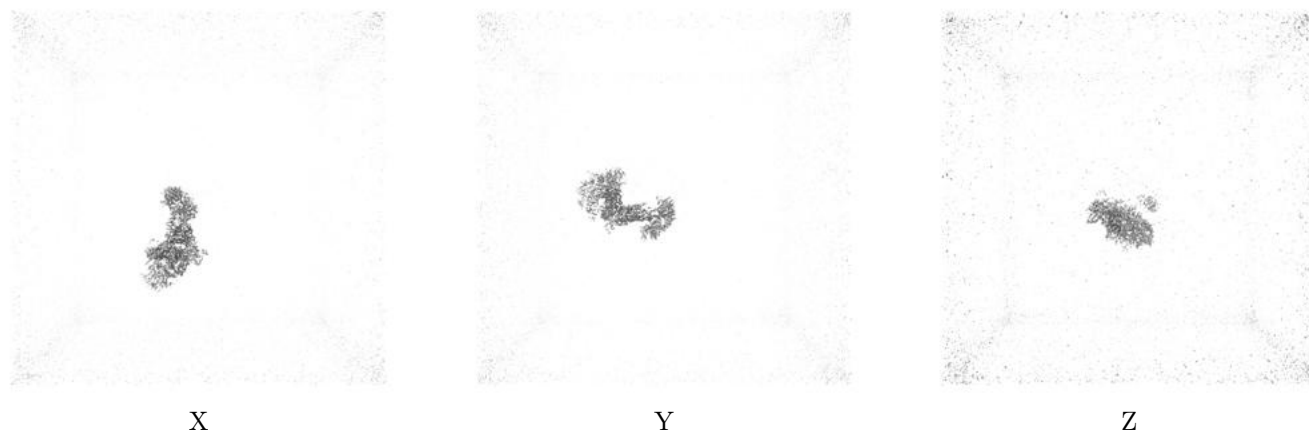
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.172. 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.

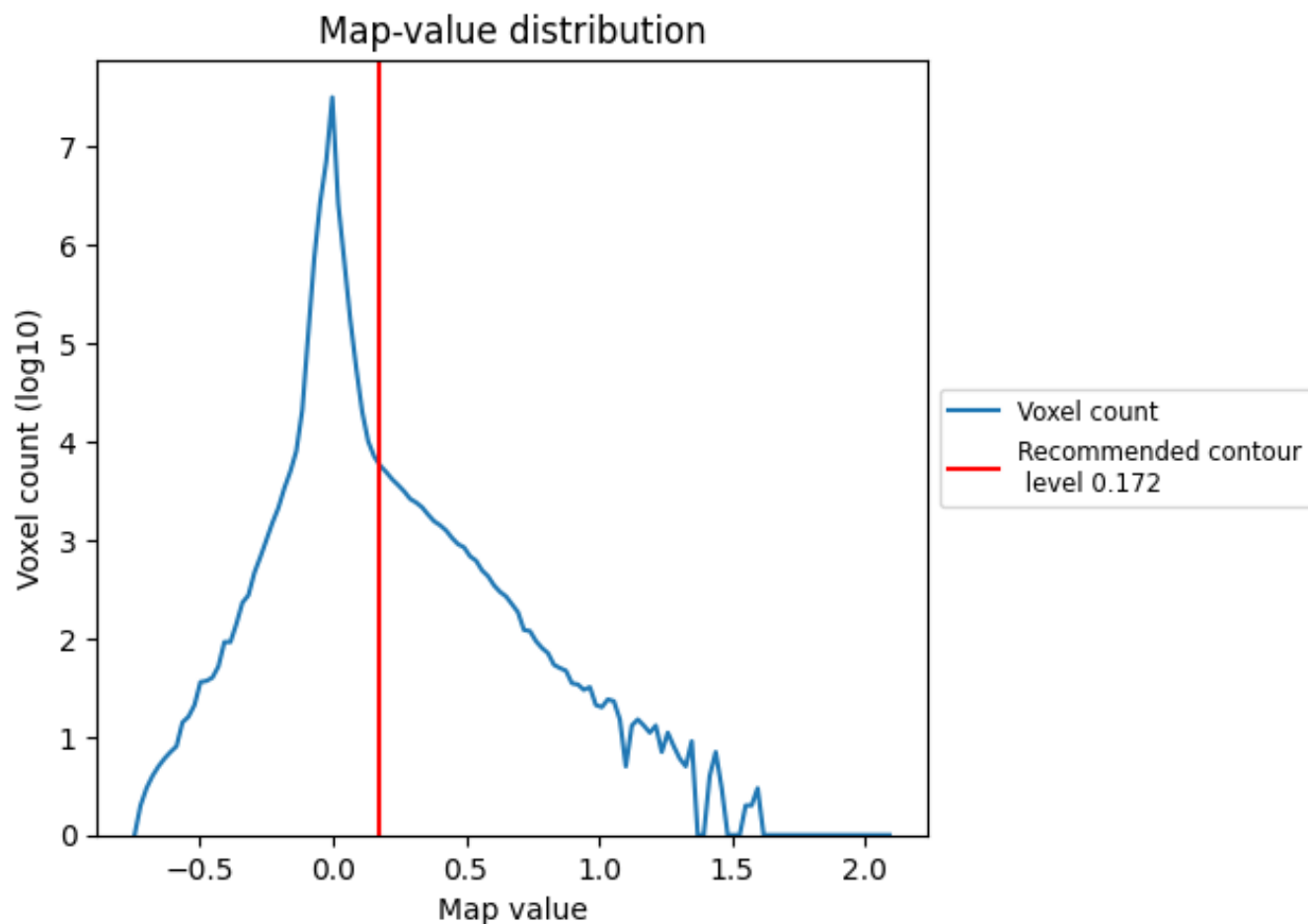
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

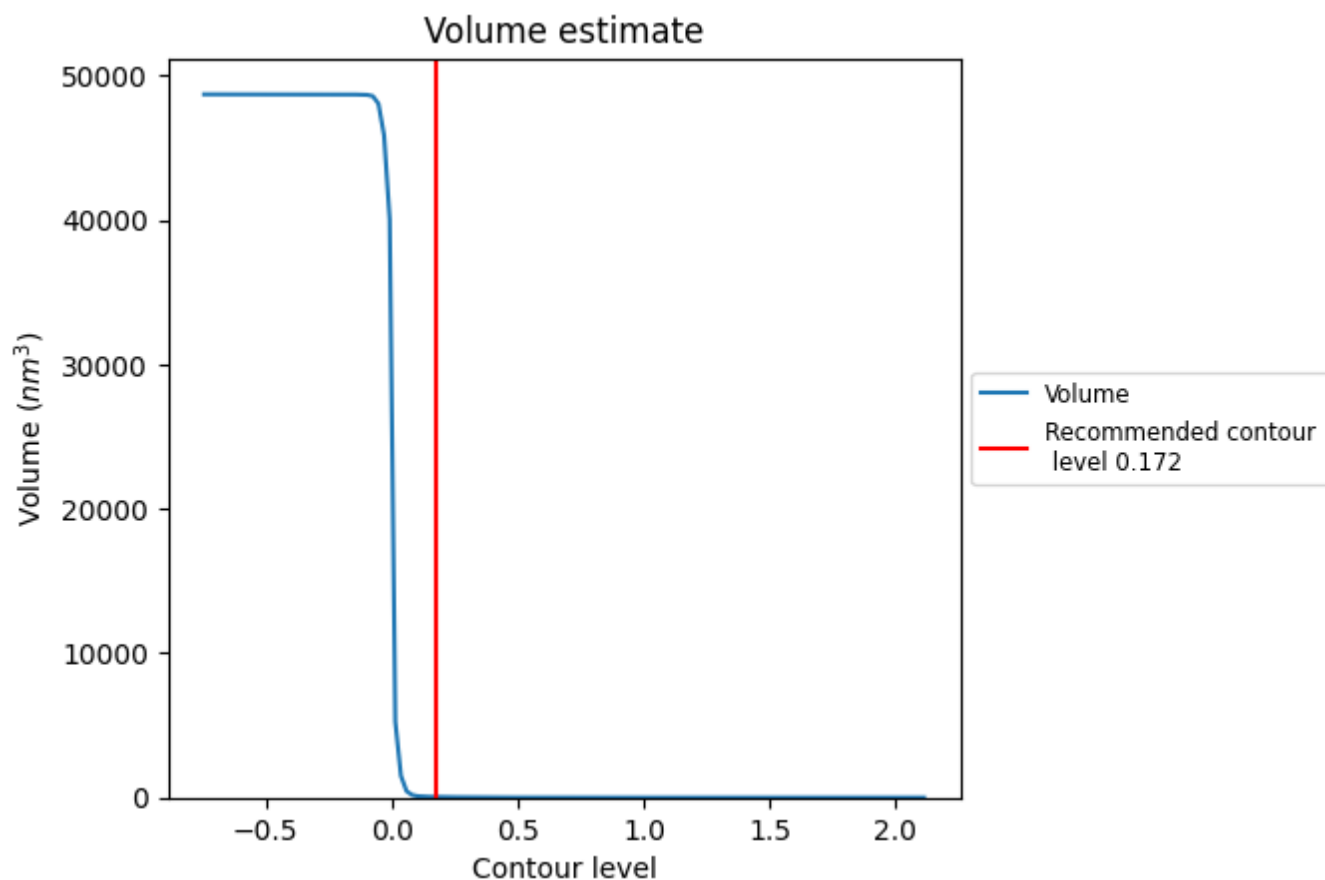
This section contains the results of statistical analysis of the map.

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.

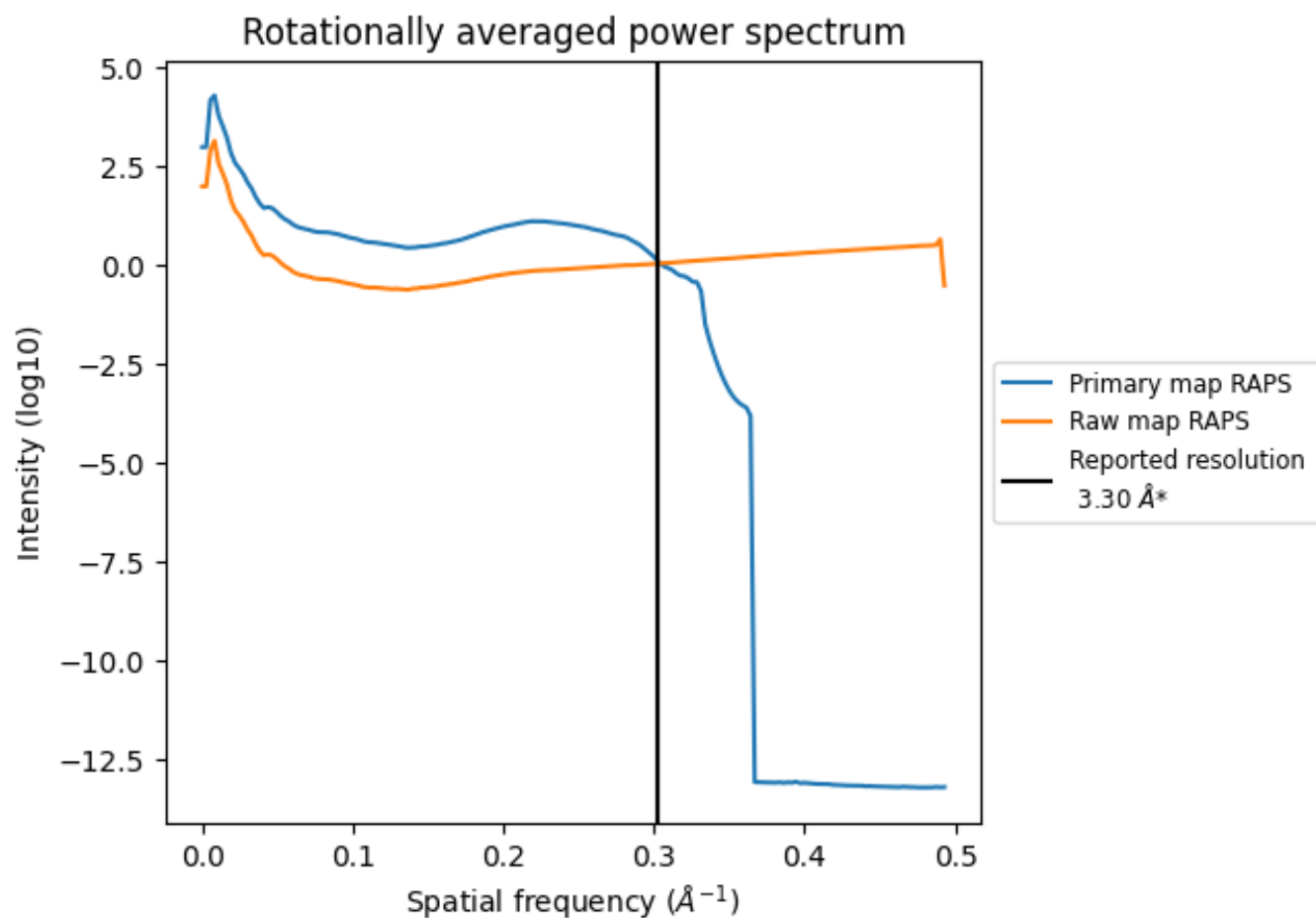
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 46 nm^3 ; this corresponds to an approximate mass of 41 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 ⓘ

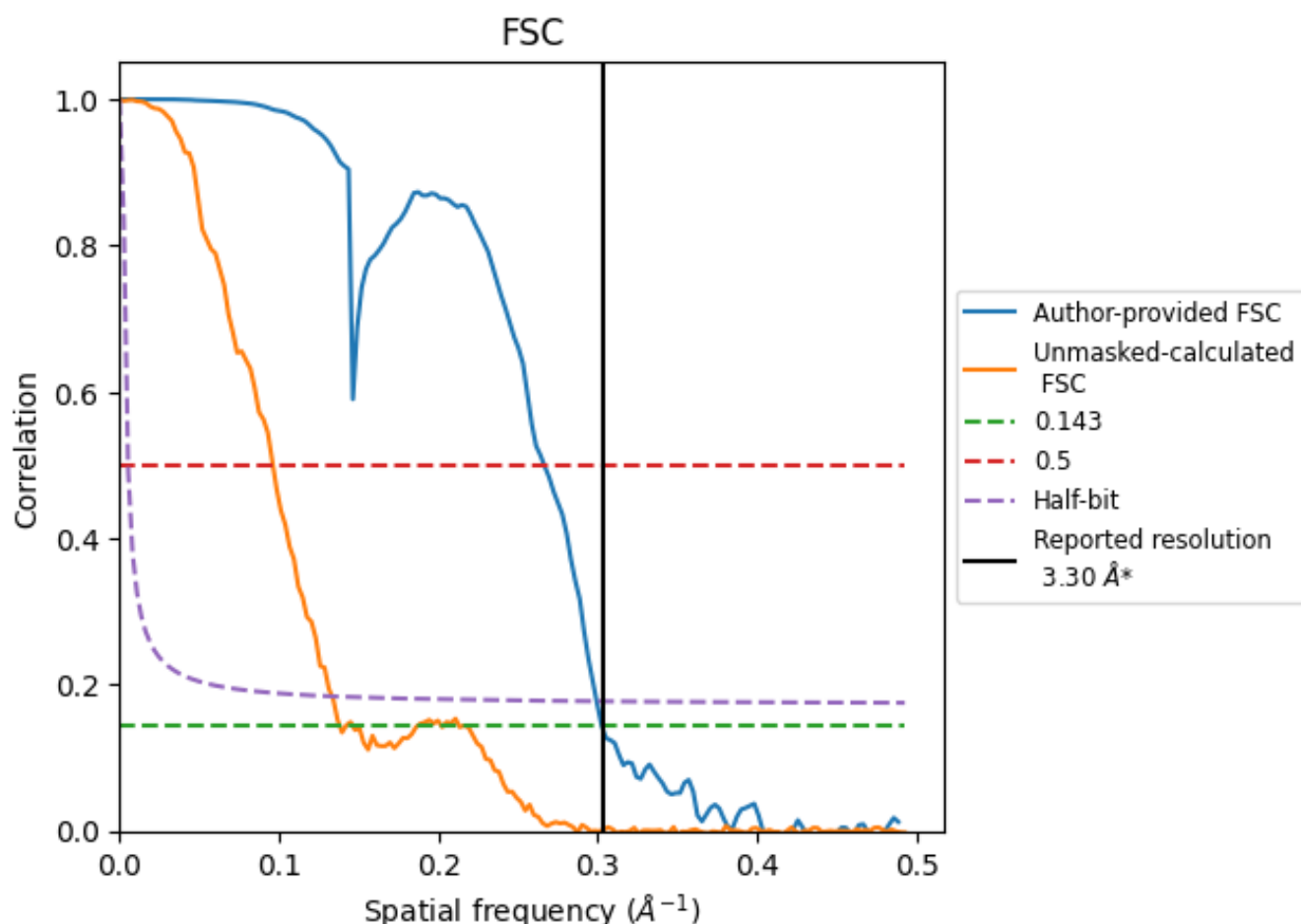


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

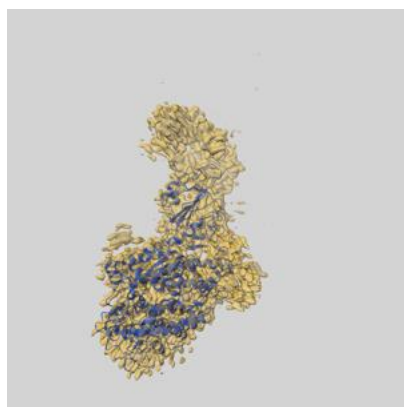
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.30	3.75	3.34
Unmasked-calculated*	7.23	10.38	7.50

*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 7.23 differs from the reported value 3.3 by more than 10 %

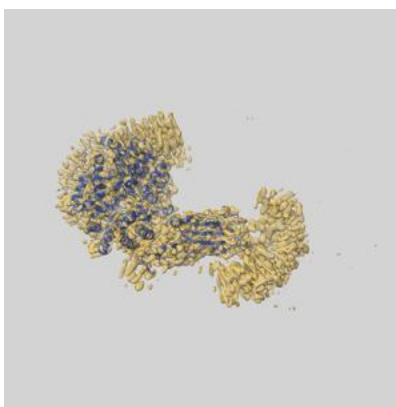
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15592 and PDB model 8AQW. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

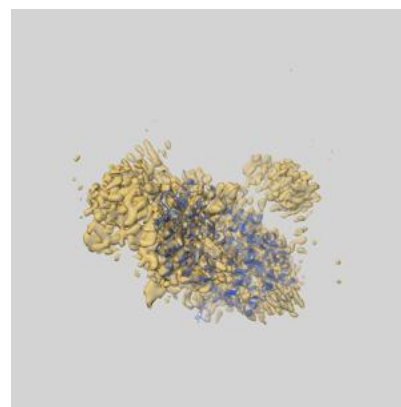
9.1 Map-model overlay [i](#)



X



Y



Z

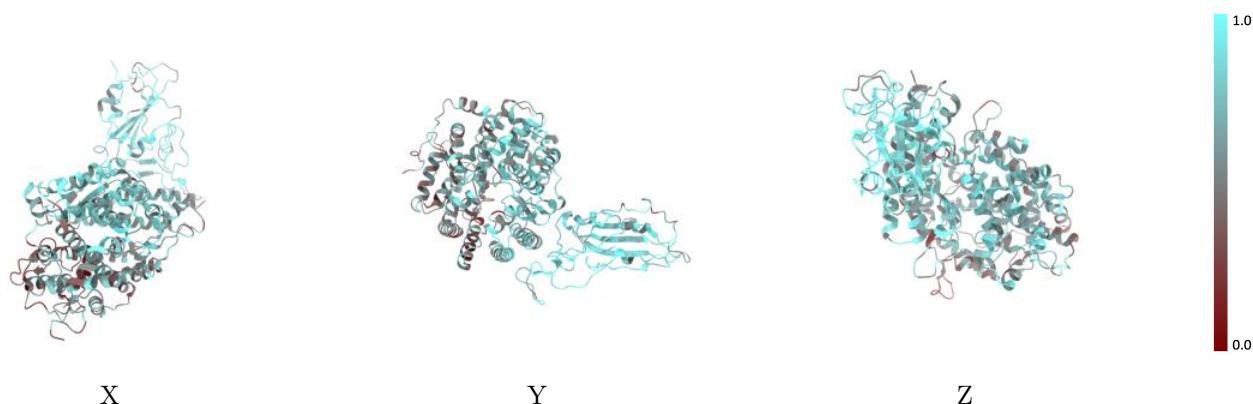
The images above show the 3D surface view of the map at the recommended contour level 0.172 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



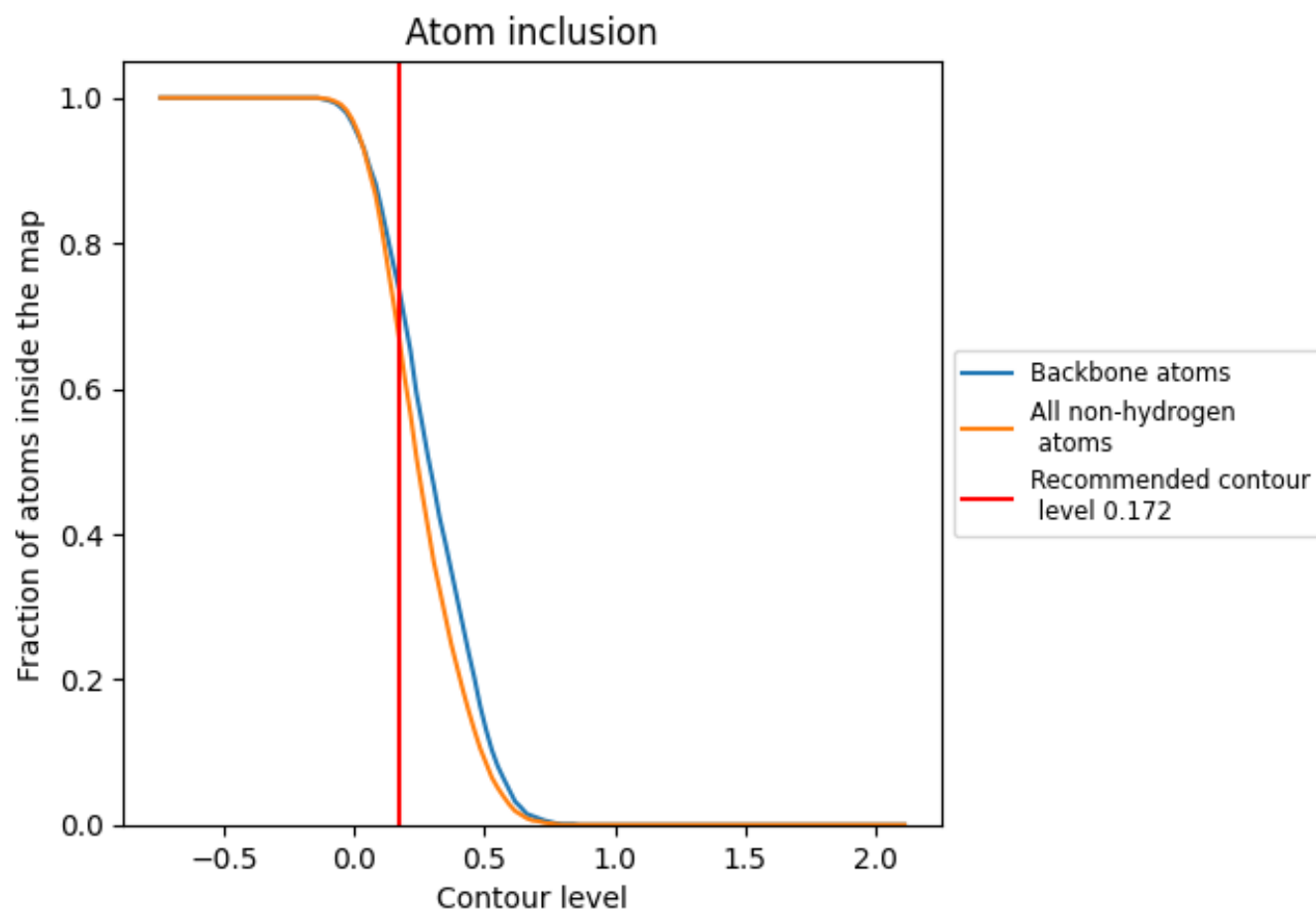
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.172).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 67% 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 (0.172) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6690	<div></div> 0.4520
A	<div></div> 0.6290	<div></div> 0.4350
B	<div></div> 0.7990	<div></div> 0.5080
C	<div></div> 0.5000	<div></div> 0.3640

