



wwPDB EM Validation Summary Report ⓘ

Nov 2, 2024 – 08:34 pm GMT

PDB ID : 6S8D
EMDB ID : EMD-10118
Title : Structure of ZEBOV GP in complex with 1T0227 antibody
Authors : Diskin, R.; Cohen-Dvashi, H.
Deposited on : 2019-07-09
Resolution : 3.49 Å(reported)
Based on initial model : 5JQ3

This is a wwPDB EM Validation Summary 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.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

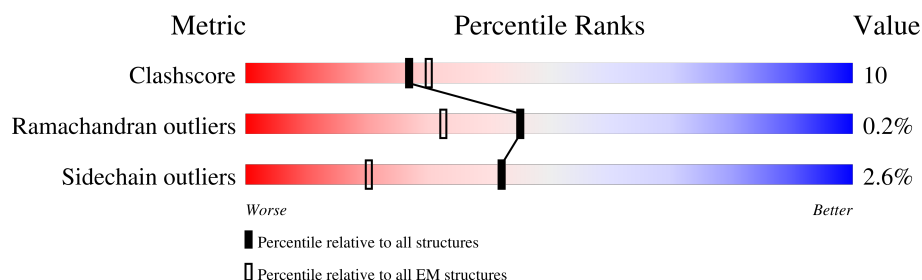
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.49 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	L	218	<div> <div>34%</div> <div>15%</div> <div>.</div> <div>50%</div> </div>
1	O	218	<div> <div>35%</div> <div>14%</div> <div>.</div> <div>50%</div> </div>
1	U	218	<div> <div>35%</div> <div>15%</div> <div>.</div> <div>50%</div> </div>
2	H	231	<div> <div>34%</div> <div>18%</div> <div></div> <div>47%</div> </div>
2	P	231	<div> <div>35%</div> <div>18%</div> <div></div> <div>47%</div> </div>
2	Y	231	<div> <div>33%</div> <div>19%</div> <div></div> <div>47%</div> </div>
3	A	323	<div> <div>49%</div> <div>8%</div> <div></div> <div>42%</div> </div>
3	C	323	<div> <div>49%</div> <div>8%</div> <div></div> <div>42%</div> </div>

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Mol	Chain	Length	Quality of chain
3	E	323	 49% 9% 42%
4	B	168	 57% 8% 35%
4	D	168	 57% 8% 35%
4	F	168	 57% 8% 35%
5	G	2	 100%
5	I	2	 100%
5	J	2	 100%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12267 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 Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	110	Total	C	N	O	S	0	0
			817	510	137	168	2		
1	O	110	Total	C	N	O	S	0	0
			817	510	137	168	2		
1	U	110	Total	C	N	O	S	0	0
			817	510	137	168	2		

- Molecule 2 is a protein called Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	122	Total	C	N	O	S	0	0
			949	603	165	177	4		
2	P	122	Total	C	N	O	S	0	0
			949	603	165	177	4		
2	Y	122	Total	C	N	O	S	0	0
			949	603	165	177	4		

- Molecule 3 is a protein called Envelope glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	186	Total	C	N	O	S	0	0
			1437	917	244	271	5		
3	C	186	Total	C	N	O	S	0	0
			1437	917	244	271	5		
3	E	186	Total	C	N	O	S	0	0
			1437	917	244	271	5		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	GLU	-	expression tag	UNP A0A0U3BWW0
A	29	THR	-	expression tag	UNP A0A0U3BWW0
A	30	GLY	-	expression tag	UNP A0A0U3BWW0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	31	ARG	-	expression tag	UNP A0A0U3BWW0
A	42	ALA	THR	conflict	UNP A0A0U3BWW0
A	310	VAL	ALA	conflict	UNP A0A0U3BWW0
A	313	THR	ASN	conflict	UNP A0A0U3BWW0
A	314	HIS	ARG	conflict	UNP A0A0U3BWW0
A	315	HIS	ALA	conflict	UNP A0A0U3BWW0
A	316	GLN	LYS	conflict	UNP A0A0U3BWW0
A	317	ASP	ASN	conflict	UNP A0A0U3BWW0
A	318	THR	ILE	conflict	UNP A0A0U3BWW0
A	319	GLY	SER	conflict	UNP A0A0U3BWW0
A	320	GLU	GLY	conflict	UNP A0A0U3BWW0
A	321	GLU	GLN	conflict	UNP A0A0U3BWW0
A	323	ALA	PRO	conflict	UNP A0A0U3BWW0
A	324	SER	ALA	conflict	UNP A0A0U3BWW0
A	325	SER	ARG	conflict	UNP A0A0U3BWW0
A	326	GLY	THR	conflict	UNP A0A0U3BWW0
A	327	LYS	SER	conflict	UNP A0A0U3BWW0
A	328	LEU	SER	conflict	UNP A0A0U3BWW0
A	329	GLY	ASP	conflict	UNP A0A0U3BWW0
A	330	LEU	PRO	conflict	UNP A0A0U3BWW0
A	331	ILE	GLY	conflict	UNP A0A0U3BWW0
A	335	ILE	-	expression tag	UNP A0A0U3BWW0
A	336	ALA	-	expression tag	UNP A0A0U3BWW0
A	337	GLY	-	expression tag	UNP A0A0U3BWW0
A	338	VAL	-	expression tag	UNP A0A0U3BWW0
A	339	ALA	-	expression tag	UNP A0A0U3BWW0
A	340	GLY	-	expression tag	UNP A0A0U3BWW0
A	341	LEU	-	expression tag	UNP A0A0U3BWW0
A	342	ILE	-	expression tag	UNP A0A0U3BWW0
A	343	THR	-	expression tag	UNP A0A0U3BWW0
A	344	GLY	-	expression tag	UNP A0A0U3BWW0
A	345	GLY	-	expression tag	UNP A0A0U3BWW0
A	346	ARG	-	expression tag	UNP A0A0U3BWW0
A	347	ARG	-	expression tag	UNP A0A0U3BWW0
A	348	THR	-	expression tag	UNP A0A0U3BWW0
A	349	ARG	-	expression tag	UNP A0A0U3BWW0
A	350	ARG	-	expression tag	UNP A0A0U3BWW0
C	28	GLU	-	expression tag	UNP A0A0U3BWW0
C	29	THR	-	expression tag	UNP A0A0U3BWW0
C	30	GLY	-	expression tag	UNP A0A0U3BWW0
C	31	ARG	-	expression tag	UNP A0A0U3BWW0
C	42	ALA	THR	conflict	UNP A0A0U3BWW0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	310	VAL	ALA	conflict	UNP A0A0U3BWW0
C	313	THR	ASN	conflict	UNP A0A0U3BWW0
C	314	HIS	ARG	conflict	UNP A0A0U3BWW0
C	315	HIS	ALA	conflict	UNP A0A0U3BWW0
C	316	GLN	LYS	conflict	UNP A0A0U3BWW0
C	317	ASP	ASN	conflict	UNP A0A0U3BWW0
C	318	THR	ILE	conflict	UNP A0A0U3BWW0
C	319	GLY	SER	conflict	UNP A0A0U3BWW0
C	320	GLU	GLY	conflict	UNP A0A0U3BWW0
C	321	GLU	GLN	conflict	UNP A0A0U3BWW0
C	323	ALA	PRO	conflict	UNP A0A0U3BWW0
C	324	SER	ALA	conflict	UNP A0A0U3BWW0
C	325	SER	ARG	conflict	UNP A0A0U3BWW0
C	326	GLY	THR	conflict	UNP A0A0U3BWW0
C	327	LYS	SER	conflict	UNP A0A0U3BWW0
C	328	LEU	SER	conflict	UNP A0A0U3BWW0
C	329	GLY	ASP	conflict	UNP A0A0U3BWW0
C	330	LEU	PRO	conflict	UNP A0A0U3BWW0
C	331	ILE	GLY	conflict	UNP A0A0U3BWW0
C	335	ILE	-	expression tag	UNP A0A0U3BWW0
C	336	ALA	-	expression tag	UNP A0A0U3BWW0
C	337	GLY	-	expression tag	UNP A0A0U3BWW0
C	338	VAL	-	expression tag	UNP A0A0U3BWW0
C	339	ALA	-	expression tag	UNP A0A0U3BWW0
C	340	GLY	-	expression tag	UNP A0A0U3BWW0
C	341	LEU	-	expression tag	UNP A0A0U3BWW0
C	342	ILE	-	expression tag	UNP A0A0U3BWW0
C	343	THR	-	expression tag	UNP A0A0U3BWW0
C	344	GLY	-	expression tag	UNP A0A0U3BWW0
C	345	GLY	-	expression tag	UNP A0A0U3BWW0
C	346	ARG	-	expression tag	UNP A0A0U3BWW0
C	347	ARG	-	expression tag	UNP A0A0U3BWW0
C	348	THR	-	expression tag	UNP A0A0U3BWW0
C	349	ARG	-	expression tag	UNP A0A0U3BWW0
C	350	ARG	-	expression tag	UNP A0A0U3BWW0
E	28	GLU	-	expression tag	UNP A0A0U3BWW0
E	29	THR	-	expression tag	UNP A0A0U3BWW0
E	30	GLY	-	expression tag	UNP A0A0U3BWW0
E	31	ARG	-	expression tag	UNP A0A0U3BWW0
E	42	ALA	THR	conflict	UNP A0A0U3BWW0
E	310	VAL	ALA	conflict	UNP A0A0U3BWW0
E	313	THR	ASN	conflict	UNP A0A0U3BWW0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	314	HIS	ARG	conflict	UNP A0A0U3BWW0
E	315	HIS	ALA	conflict	UNP A0A0U3BWW0
E	316	GLN	LYS	conflict	UNP A0A0U3BWW0
E	317	ASP	ASN	conflict	UNP A0A0U3BWW0
E	318	THR	ILE	conflict	UNP A0A0U3BWW0
E	319	GLY	SER	conflict	UNP A0A0U3BWW0
E	320	GLU	GLY	conflict	UNP A0A0U3BWW0
E	321	GLU	GLN	conflict	UNP A0A0U3BWW0
E	323	ALA	PRO	conflict	UNP A0A0U3BWW0
E	324	SER	ALA	conflict	UNP A0A0U3BWW0
E	325	SER	ARG	conflict	UNP A0A0U3BWW0
E	326	GLY	THR	conflict	UNP A0A0U3BWW0
E	327	LYS	SER	conflict	UNP A0A0U3BWW0
E	328	LEU	SER	conflict	UNP A0A0U3BWW0
E	329	GLY	ASP	conflict	UNP A0A0U3BWW0
E	330	LEU	PRO	conflict	UNP A0A0U3BWW0
E	331	ILE	GLY	conflict	UNP A0A0U3BWW0
E	335	ILE	-	expression tag	UNP A0A0U3BWW0
E	336	ALA	-	expression tag	UNP A0A0U3BWW0
E	337	GLY	-	expression tag	UNP A0A0U3BWW0
E	338	VAL	-	expression tag	UNP A0A0U3BWW0
E	339	ALA	-	expression tag	UNP A0A0U3BWW0
E	340	GLY	-	expression tag	UNP A0A0U3BWW0
E	341	LEU	-	expression tag	UNP A0A0U3BWW0
E	342	ILE	-	expression tag	UNP A0A0U3BWW0
E	343	THR	-	expression tag	UNP A0A0U3BWW0
E	344	GLY	-	expression tag	UNP A0A0U3BWW0
E	345	GLY	-	expression tag	UNP A0A0U3BWW0
E	346	ARG	-	expression tag	UNP A0A0U3BWW0
E	347	ARG	-	expression tag	UNP A0A0U3BWW0
E	348	THR	-	expression tag	UNP A0A0U3BWW0
E	349	ARG	-	expression tag	UNP A0A0U3BWW0
E	350	ARG	-	expression tag	UNP A0A0U3BWW0

- Molecule 4 is a protein called Envelope glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	110	Total	C	N	O	S	0	0
			858	548	149	155	6		
4	D	110	Total	C	N	O	S	0	0
			858	548	149	155	6		
4	F	110	Total	C	N	O	S	0	0
			858	548	149	155	6		

There are 111 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	633	GLY	-	expression tag	UNP A0A0U3BWW0
B	634	SER	-	expression tag	UNP A0A0U3BWW0
B	635	GLY	-	expression tag	UNP A0A0U3BWW0
B	636	TYR	-	expression tag	UNP A0A0U3BWW0
B	637	ILE	-	expression tag	UNP A0A0U3BWW0
B	638	PRO	-	expression tag	UNP A0A0U3BWW0
B	639	GLU	-	expression tag	UNP A0A0U3BWW0
B	640	ALA	-	expression tag	UNP A0A0U3BWW0
B	641	PRO	-	expression tag	UNP A0A0U3BWW0
B	642	ARG	-	expression tag	UNP A0A0U3BWW0
B	643	ASP	-	expression tag	UNP A0A0U3BWW0
B	644	GLY	-	expression tag	UNP A0A0U3BWW0
B	645	GLN	-	expression tag	UNP A0A0U3BWW0
B	646	ALA	-	expression tag	UNP A0A0U3BWW0
B	647	TYR	-	expression tag	UNP A0A0U3BWW0
B	648	VAL	-	expression tag	UNP A0A0U3BWW0
B	649	ARG	-	expression tag	UNP A0A0U3BWW0
B	650	LYS	-	expression tag	UNP A0A0U3BWW0
B	651	ASP	-	expression tag	UNP A0A0U3BWW0
B	652	GLY	-	expression tag	UNP A0A0U3BWW0
B	653	GLU	-	expression tag	UNP A0A0U3BWW0
B	654	TRP	-	expression tag	UNP A0A0U3BWW0
B	655	VAL	-	expression tag	UNP A0A0U3BWW0
B	656	LEU	-	expression tag	UNP A0A0U3BWW0
B	657	LEU	-	expression tag	UNP A0A0U3BWW0
B	658	SER	-	expression tag	UNP A0A0U3BWW0
B	659	THR	-	expression tag	UNP A0A0U3BWW0
B	660	PHE	-	expression tag	UNP A0A0U3BWW0
B	661	LEU	-	expression tag	UNP A0A0U3BWW0
B	662	GLY	-	expression tag	UNP A0A0U3BWW0
B	663	THR	-	expression tag	UNP A0A0U3BWW0
B	664	HIS	-	expression tag	UNP A0A0U3BWW0
B	665	HIS	-	expression tag	UNP A0A0U3BWW0
B	666	HIS	-	expression tag	UNP A0A0U3BWW0
B	667	HIS	-	expression tag	UNP A0A0U3BWW0
B	668	HIS	-	expression tag	UNP A0A0U3BWW0
B	669	HIS	-	expression tag	UNP A0A0U3BWW0
D	633	GLY	-	expression tag	UNP A0A0U3BWW0
D	634	SER	-	expression tag	UNP A0A0U3BWW0
D	635	GLY	-	expression tag	UNP A0A0U3BWW0
D	636	TYR	-	expression tag	UNP A0A0U3BWW0
D	637	ILE	-	expression tag	UNP A0A0U3BWW0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	638	PRO	-	expression tag	UNP A0A0U3BWW0
D	639	GLU	-	expression tag	UNP A0A0U3BWW0
D	640	ALA	-	expression tag	UNP A0A0U3BWW0
D	641	PRO	-	expression tag	UNP A0A0U3BWW0
D	642	ARG	-	expression tag	UNP A0A0U3BWW0
D	643	ASP	-	expression tag	UNP A0A0U3BWW0
D	644	GLY	-	expression tag	UNP A0A0U3BWW0
D	645	GLN	-	expression tag	UNP A0A0U3BWW0
D	646	ALA	-	expression tag	UNP A0A0U3BWW0
D	647	TYR	-	expression tag	UNP A0A0U3BWW0
D	648	VAL	-	expression tag	UNP A0A0U3BWW0
D	649	ARG	-	expression tag	UNP A0A0U3BWW0
D	650	LYS	-	expression tag	UNP A0A0U3BWW0
D	651	ASP	-	expression tag	UNP A0A0U3BWW0
D	652	GLY	-	expression tag	UNP A0A0U3BWW0
D	653	GLU	-	expression tag	UNP A0A0U3BWW0
D	654	TRP	-	expression tag	UNP A0A0U3BWW0
D	655	VAL	-	expression tag	UNP A0A0U3BWW0
D	656	LEU	-	expression tag	UNP A0A0U3BWW0
D	657	LEU	-	expression tag	UNP A0A0U3BWW0
D	658	SER	-	expression tag	UNP A0A0U3BWW0
D	659	THR	-	expression tag	UNP A0A0U3BWW0
D	660	PHE	-	expression tag	UNP A0A0U3BWW0
D	661	LEU	-	expression tag	UNP A0A0U3BWW0
D	662	GLY	-	expression tag	UNP A0A0U3BWW0
D	663	THR	-	expression tag	UNP A0A0U3BWW0
D	664	HIS	-	expression tag	UNP A0A0U3BWW0
D	665	HIS	-	expression tag	UNP A0A0U3BWW0
D	666	HIS	-	expression tag	UNP A0A0U3BWW0
D	667	HIS	-	expression tag	UNP A0A0U3BWW0
D	668	HIS	-	expression tag	UNP A0A0U3BWW0
D	669	HIS	-	expression tag	UNP A0A0U3BWW0
F	633	GLY	-	expression tag	UNP A0A0U3BWW0
F	634	SER	-	expression tag	UNP A0A0U3BWW0
F	635	GLY	-	expression tag	UNP A0A0U3BWW0
F	636	TYR	-	expression tag	UNP A0A0U3BWW0
F	637	ILE	-	expression tag	UNP A0A0U3BWW0
F	638	PRO	-	expression tag	UNP A0A0U3BWW0
F	639	GLU	-	expression tag	UNP A0A0U3BWW0
F	640	ALA	-	expression tag	UNP A0A0U3BWW0
F	641	PRO	-	expression tag	UNP A0A0U3BWW0
F	642	ARG	-	expression tag	UNP A0A0U3BWW0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	643	ASP	-	expression tag	UNP A0A0U3BWW0
F	644	GLY	-	expression tag	UNP A0A0U3BWW0
F	645	GLN	-	expression tag	UNP A0A0U3BWW0
F	646	ALA	-	expression tag	UNP A0A0U3BWW0
F	647	TYR	-	expression tag	UNP A0A0U3BWW0
F	648	VAL	-	expression tag	UNP A0A0U3BWW0
F	649	ARG	-	expression tag	UNP A0A0U3BWW0
F	650	LYS	-	expression tag	UNP A0A0U3BWW0
F	651	ASP	-	expression tag	UNP A0A0U3BWW0
F	652	GLY	-	expression tag	UNP A0A0U3BWW0
F	653	GLU	-	expression tag	UNP A0A0U3BWW0
F	654	TRP	-	expression tag	UNP A0A0U3BWW0
F	655	VAL	-	expression tag	UNP A0A0U3BWW0
F	656	LEU	-	expression tag	UNP A0A0U3BWW0
F	657	LEU	-	expression tag	UNP A0A0U3BWW0
F	658	SER	-	expression tag	UNP A0A0U3BWW0
F	659	THR	-	expression tag	UNP A0A0U3BWW0
F	660	PHE	-	expression tag	UNP A0A0U3BWW0
F	661	LEU	-	expression tag	UNP A0A0U3BWW0
F	662	GLY	-	expression tag	UNP A0A0U3BWW0
F	663	THR	-	expression tag	UNP A0A0U3BWW0
F	664	HIS	-	expression tag	UNP A0A0U3BWW0
F	665	HIS	-	expression tag	UNP A0A0U3BWW0
F	666	HIS	-	expression tag	UNP A0A0U3BWW0
F	667	HIS	-	expression tag	UNP A0A0U3BWW0
F	668	HIS	-	expression tag	UNP A0A0U3BWW0
F	669	HIS	-	expression tag	UNP A0A0U3BWW0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

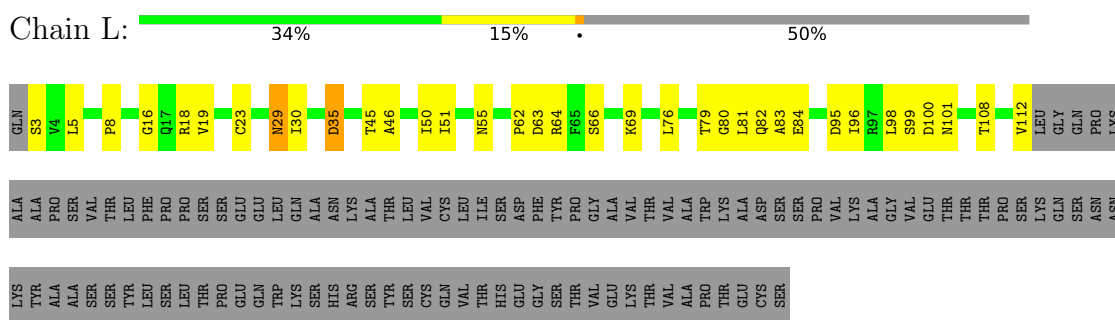


Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	2	Total	C	N	O	0	0
			28	16	2	10		
5	I	2	Total	C	N	O	0	0
			28	16	2	10		
5	J	2	Total	C	N	O	0	0
			28	16	2	10		

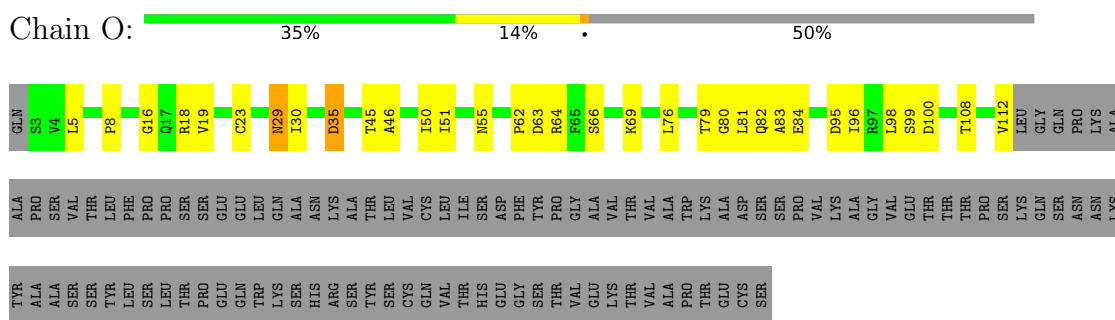
3 Residue-property plots [i](#)

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

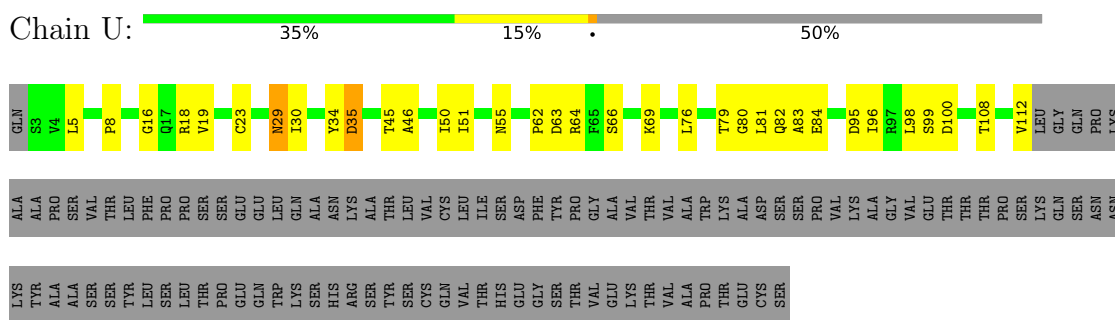
- Molecule 1: Light chain



- Molecule 1: Light chain



- Molecule 1: Light chain



- Molecule 2: Heavy chain

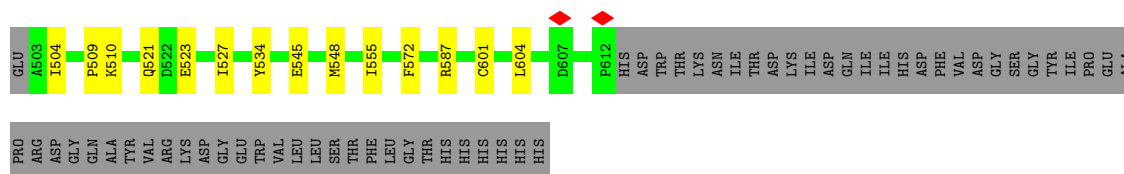
[illegible]

ALA	VAL	LEU	GLN	SER	GLY	LEU	LEU	TYR	SER	LEU	SER	PRO	SER	SER	LEU	GLY	THR	THR	GLN	THR	THR	TYR	ILE	CYS	ASN	VAL	ASN	HIS	LEU	PRO	SER	ASN	THR	LYS	THR	VAL	ASP	LYS	ARG	VAL	GLU	PRO	LYS	SER	CYS	ASP	LYS	THR	HIS							
L119	V120	T121	V122	S123	SER	GLY	SER	THR	LYS	GLY	PRO	PRO	SER	SER	LYS	GLY	THR	THR	GLY	GLY	THR	GLY	ALA	ALA	LEU	GLY	CYS	LEU	VAL	LYS	ASP	PRO	VAL	THR	THR	VAL	SER	TRP	ASN	SER	GLY	ALA	LEU	THR	SER	GLY	VAL	HIS	THR	PRO						
GLU	V2	K13	P14	G15		L18	R19		K33	K34	R35	V36	V37	R38	Q39		K43	G44		V48		L51	K52		T60	D61	V62	A63		K67	G68	R69		L72	S73	R74		O84	K85		L88	K89	G90	E91	D92	T93	A94	V95	Y96		T100	P103	Y110		G117	T119

[illegible][illegible]

- Molecule 4: Envelope glycoprotein

Chain F:  57% 8% 35%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	36227	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	4.693	Depositor
Minimum map value	-3.024	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.104	Depositor
Recommended contour level	0.23	Depositor
Map size (Å)	254.7, 254.7, 254.7	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.849, 0.849, 0.849	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: 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	L	0.35	0/836	0.53	0/1142
1	O	0.35	0/836	0.53	0/1142
1	U	0.36	0/836	0.53	0/1142
2	H	0.32	0/975	0.56	0/1326
2	P	0.32	0/975	0.57	0/1326
2	Y	0.32	0/975	0.57	0/1326
3	A	0.39	0/1473	0.54	0/2000
3	C	0.39	0/1473	0.54	0/2000
3	E	0.39	0/1473	0.54	0/2000
4	B	0.33	0/879	0.55	0/1198
4	D	0.33	0/879	0.55	0/1198
4	F	0.33	0/879	0.55	0/1198
All	All	0.35	0/12489	0.55	0/16998

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 [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	L	817	0	779	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	817	0	779	20	0
1	U	817	0	779	22	0
2	H	949	0	914	30	0
2	P	949	0	914	31	0
2	Y	949	0	914	32	0
3	A	1437	0	1377	20	0
3	C	1437	0	1377	20	0
3	E	1437	0	1377	21	0
4	B	858	0	837	8	0
4	D	858	0	837	8	0
4	F	858	0	837	8	0
5	G	28	0	25	0	0
5	I	28	0	25	0	0
5	J	28	0	25	0	0
All	All	12267	0	11796	233	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 233 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:P:85:MET:HB2	2:P:88:LEU:HD21	1.60	0.83
2:Y:85:MET:HB2	2:Y:88:LEU:HD21	1.60	0.82
2:H:85:MET:HB2	2:H:88:LEU:HD21	1.60	0.81
1:U:50:ILE:HG22	1:U:51:ILE:HG12	1.73	0.70
1:O:50:ILE:HG22	1:O:51:ILE:HG12	1.74	0.70

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	108/218 (50%)	101 (94%)	6 (6%)	1 (1%)	14	49
1	O	108/218 (50%)	101 (94%)	6 (6%)	1 (1%)	14	49
1	U	108/218 (50%)	101 (94%)	6 (6%)	1 (1%)	14	49
2	H	120/231 (52%)	112 (93%)	8 (7%)	0	100	100
2	P	120/231 (52%)	112 (93%)	8 (7%)	0	100	100
2	Y	120/231 (52%)	112 (93%)	8 (7%)	0	100	100
3	A	182/323 (56%)	177 (97%)	5 (3%)	0	100	100
3	C	182/323 (56%)	177 (97%)	5 (3%)	0	100	100
3	E	182/323 (56%)	177 (97%)	5 (3%)	0	100	100
4	B	108/168 (64%)	105 (97%)	3 (3%)	0	100	100
4	D	108/168 (64%)	105 (97%)	3 (3%)	0	100	100
4	F	108/168 (64%)	105 (97%)	3 (3%)	0	100	100
All	All	1554/2820 (55%)	1485 (96%)	66 (4%)	3 (0%)	45	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	63	ASP
1	O	63	ASP
1	U	63	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	90/183 (49%)	87 (97%)	3 (3%)	33	61
1	O	90/183 (49%)	87 (97%)	3 (3%)	33	61
1	U	90/183 (49%)	87 (97%)	3 (3%)	33	61
2	H	99/194 (51%)	98 (99%)	1 (1%)	73	84
2	P	99/194 (51%)	98 (99%)	1 (1%)	73	84
2	Y	99/194 (51%)	98 (99%)	1 (1%)	73	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	151/273 (55%)	147 (97%)	4 (3%)	41	66
3	C	151/273 (55%)	147 (97%)	4 (3%)	41	66
3	E	151/273 (55%)	147 (97%)	4 (3%)	41	66
4	B	89/140 (64%)	86 (97%)	3 (3%)	32	60
4	D	89/140 (64%)	86 (97%)	3 (3%)	32	60
4	F	89/140 (64%)	86 (97%)	3 (3%)	32	60
All	All	1287/2370 (54%)	1254 (97%)	33 (3%)	42	66

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	135	CYS
3	E	229	GLU
2	Y	85	MET
4	D	601	CYS
4	D	527	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	U	56	ASN
3	C	61	ASN
3	E	61	ASN
3	E	39	HIS
3	C	40	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 ⓘ

6 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	$\# Z > 2$
5	NAG	G	1	5,4	14,14,15	0.32	0	17,19,21	0.41	0
5	NAG	G	2	5	14,14,15	0.22	0	17,19,21	0.50	0
5	NAG	I	1	5,4	14,14,15	0.31	0	17,19,21	0.41	0
5	NAG	I	2	5	14,14,15	0.21	0	17,19,21	0.50	0
5	NAG	J	1	5,4	14,14,15	0.32	0	17,19,21	0.41	0
5	NAG	J	2	5	14,14,15	0.22	0	17,19,21	0.51	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
5	NAG	G	1	5,4	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	NAG	I	1	5,4	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
5	NAG	J	1	5,4	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	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.

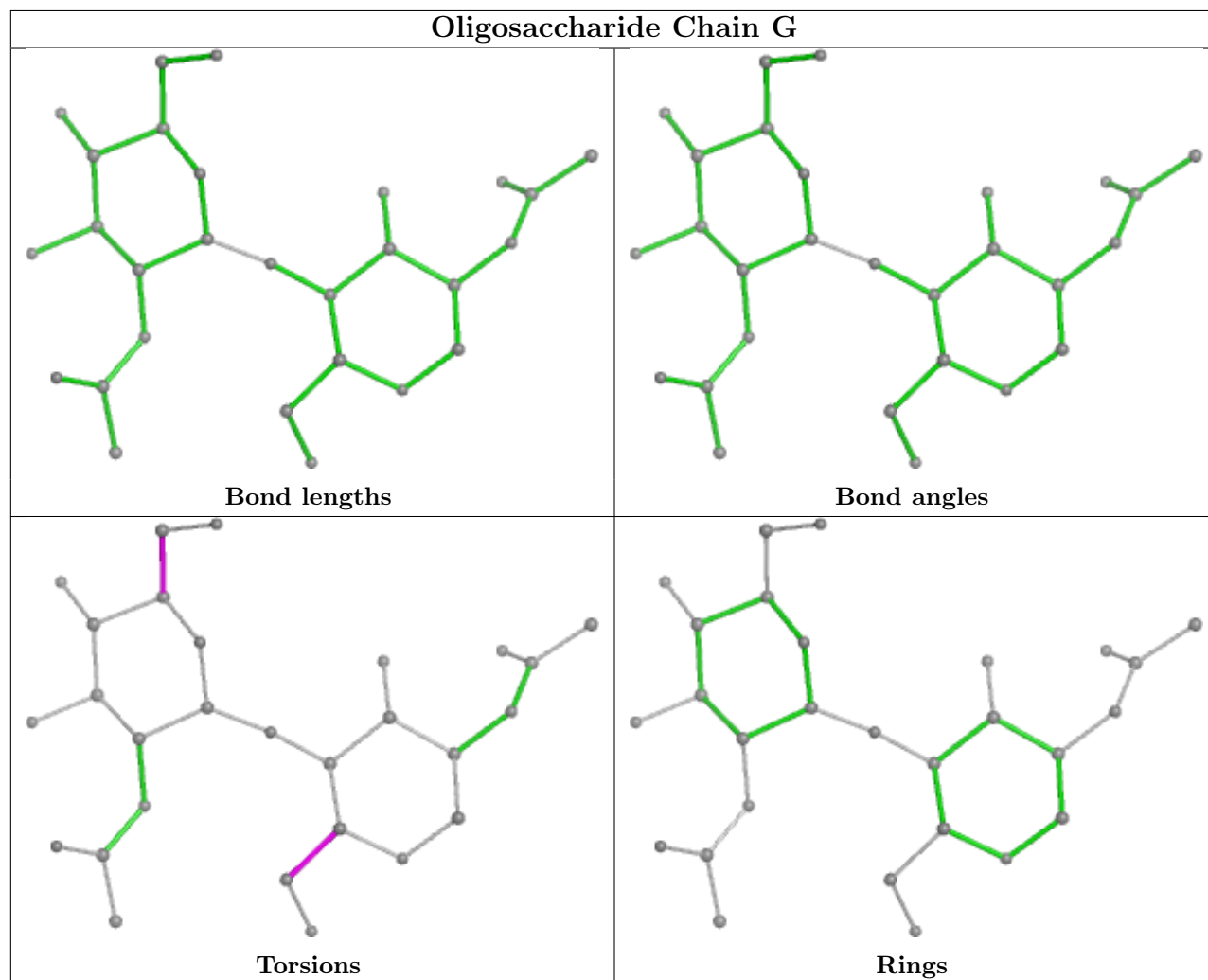
5 of 12 torsion outliers are listed below:

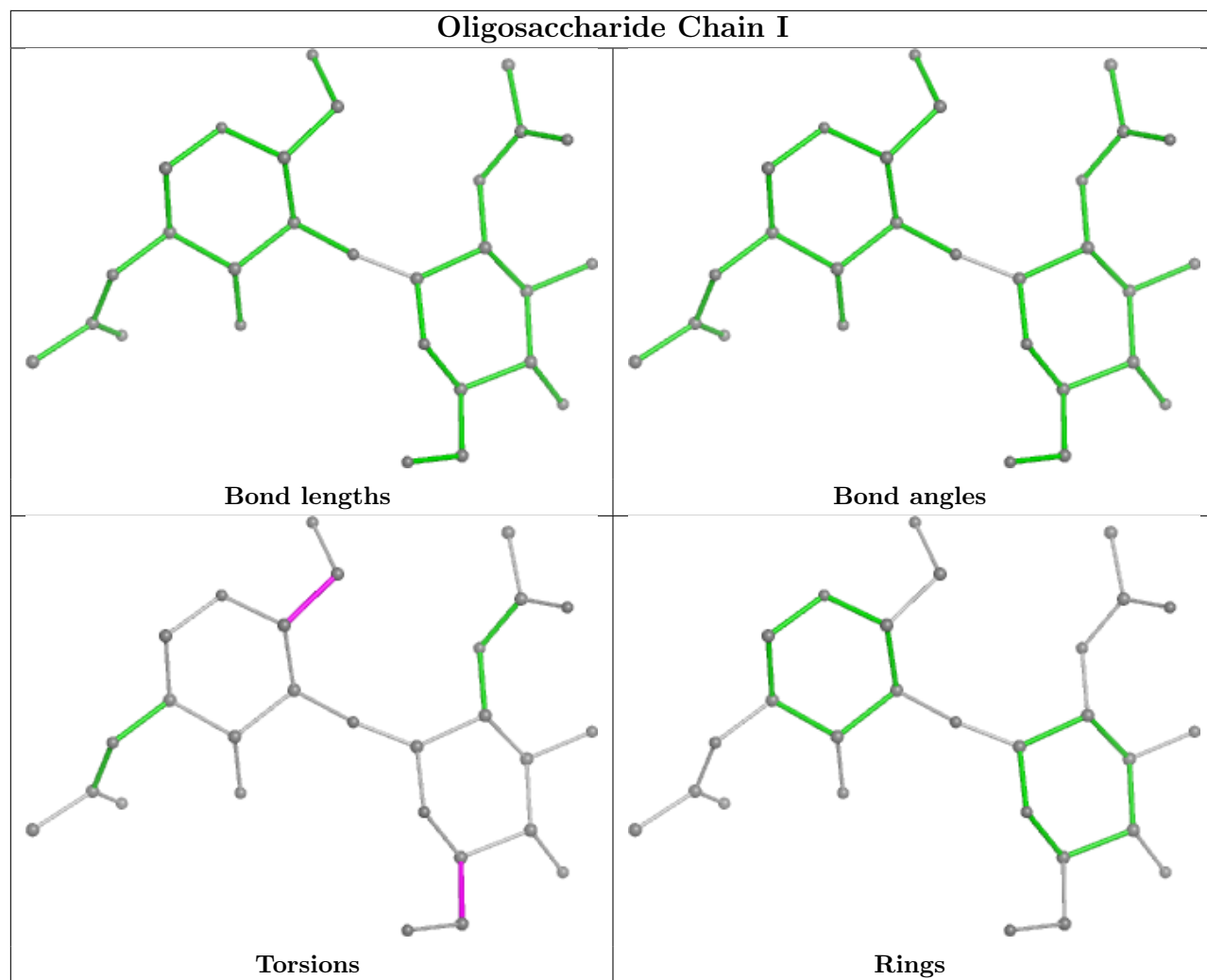
Mol	Chain	Res	Type	Atoms
5	G	1	NAG	O5-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6

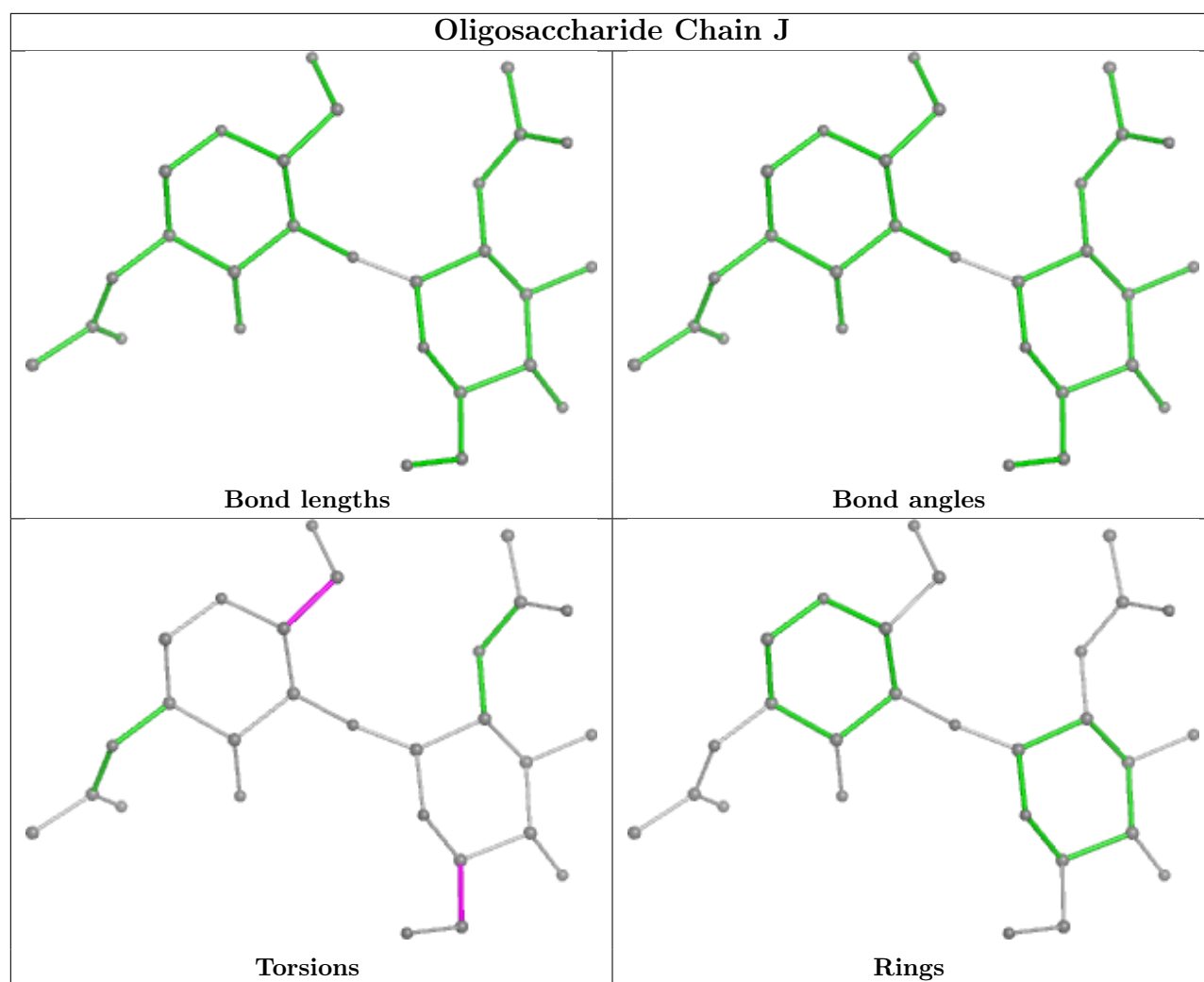
There are no ring outliers.

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](#)

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.

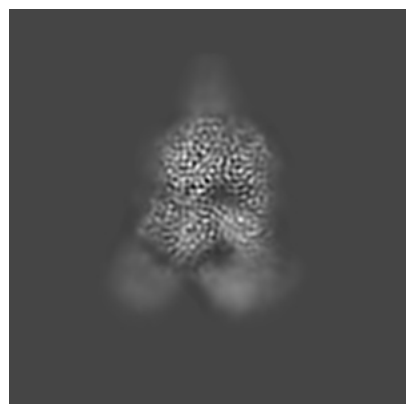
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10118. These allow visual inspection of the internal detail of the map and identification of artifacts.

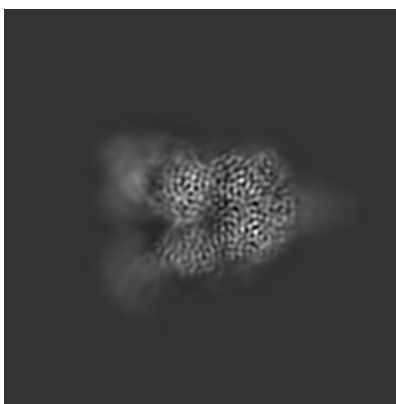
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

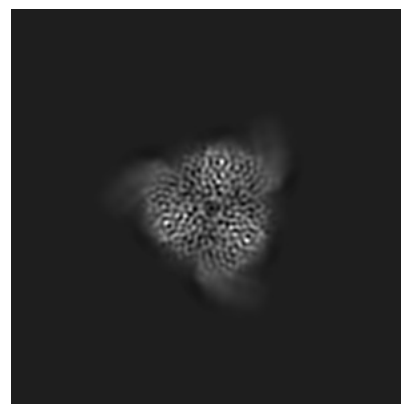
6.1.1 Primary map



X

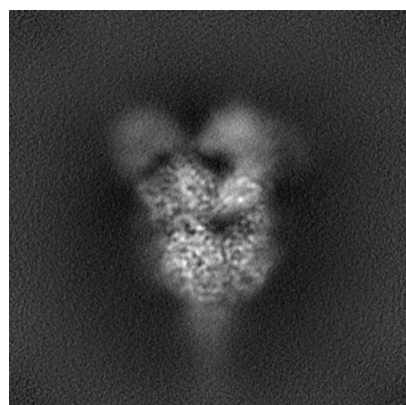


Y

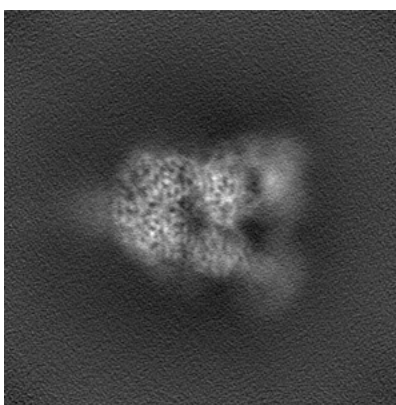


Z

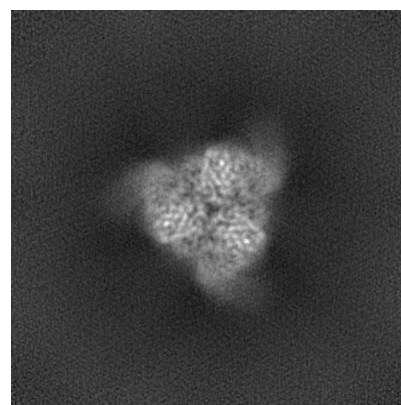
6.1.2 Raw map



X



Y

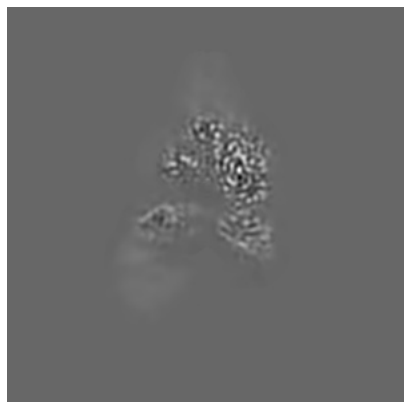


Z

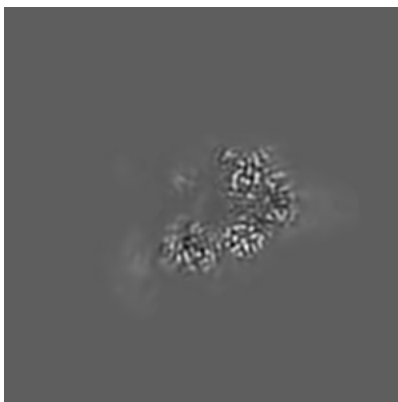
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

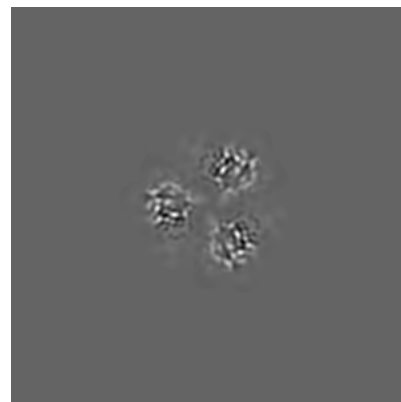
6.2.1 Primary map



X Index: 150



Y Index: 150

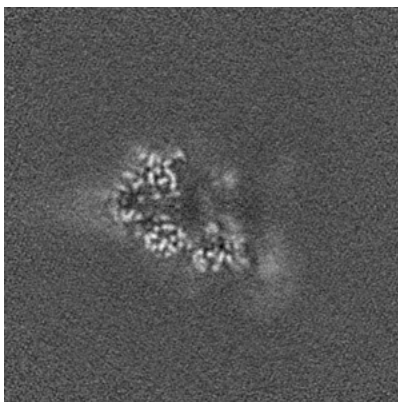


Z Index: 150

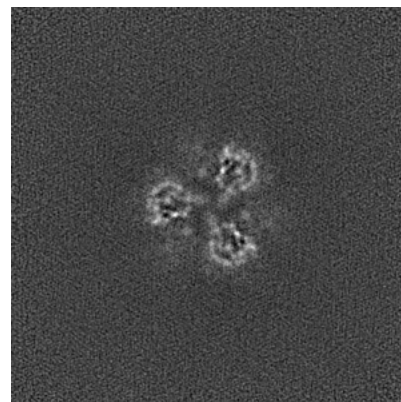
6.2.2 Raw map



X Index: 150



Y Index: 150



Z Index: 150

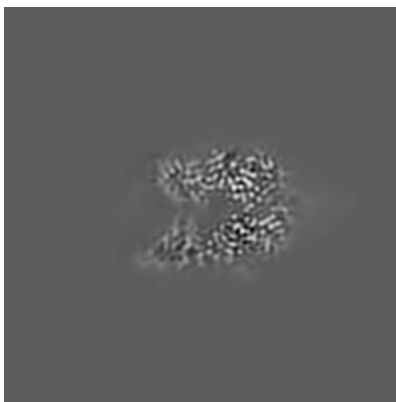
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

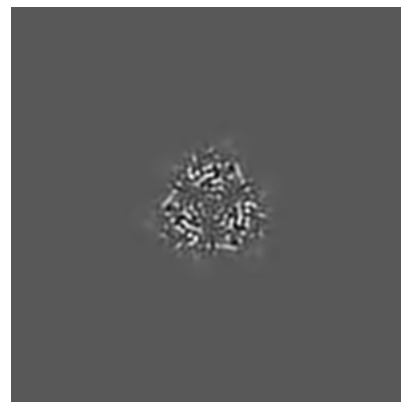
6.3.1 Primary map



X Index: 165

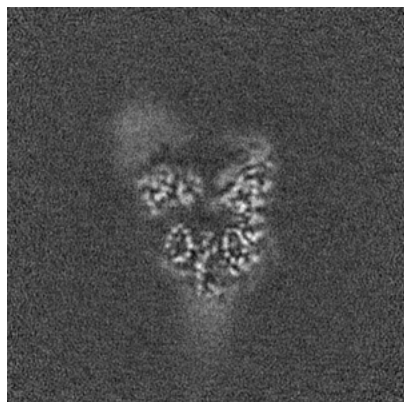


Y Index: 136

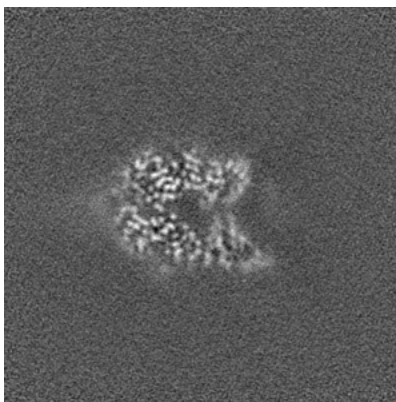


Z Index: 178

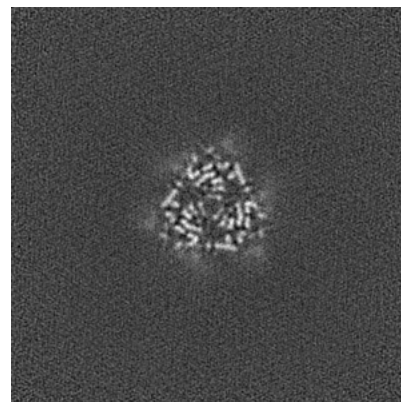
6.3.2 Raw map



X Index: 158



Y Index: 136

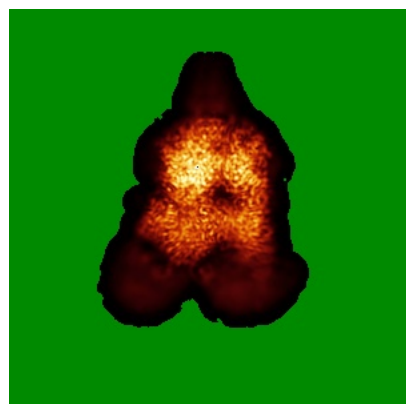


Z Index: 121

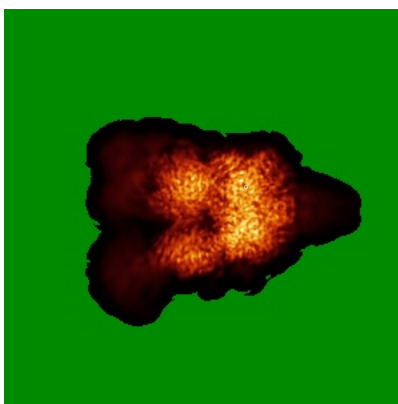
The images above show the largest variance slices of the map in three orthogonal directions.

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

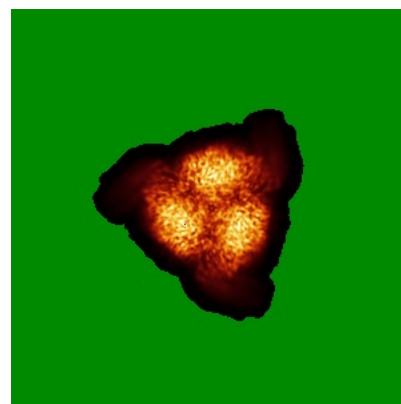
6.4.1 Primary map



X

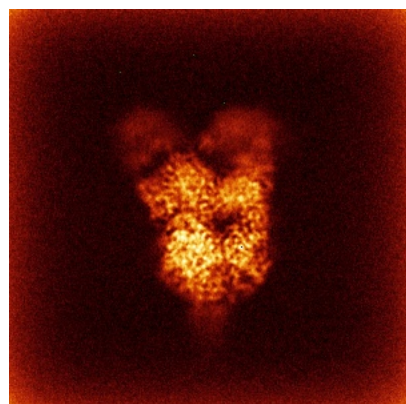


Y

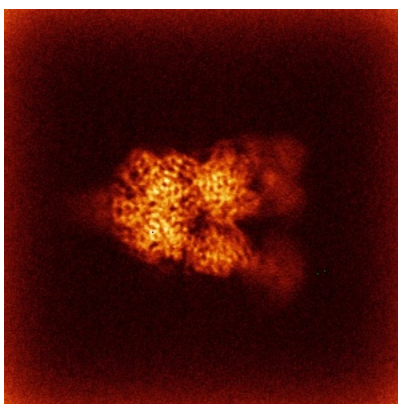


Z

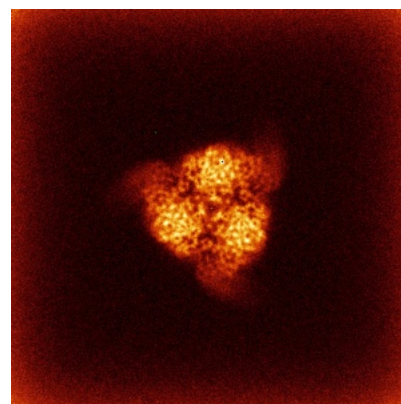
6.4.2 Raw map



X



Y

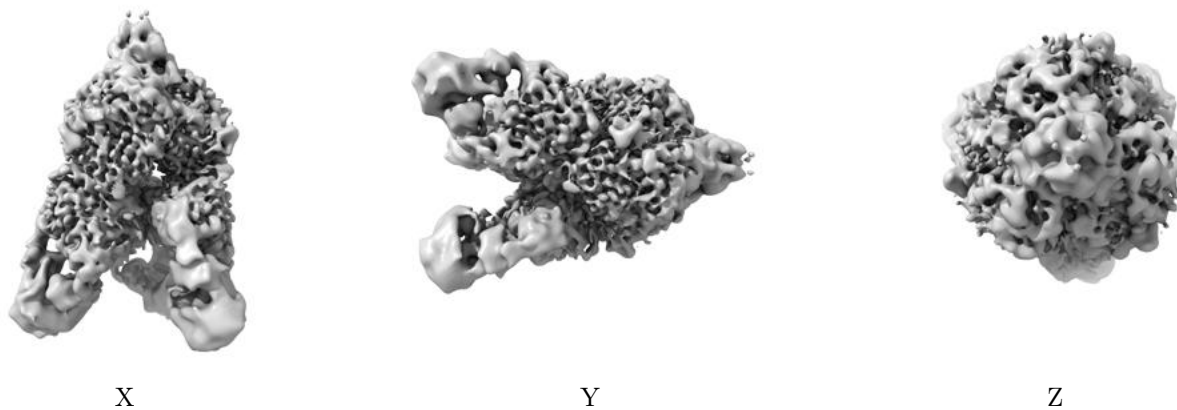


Z

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.

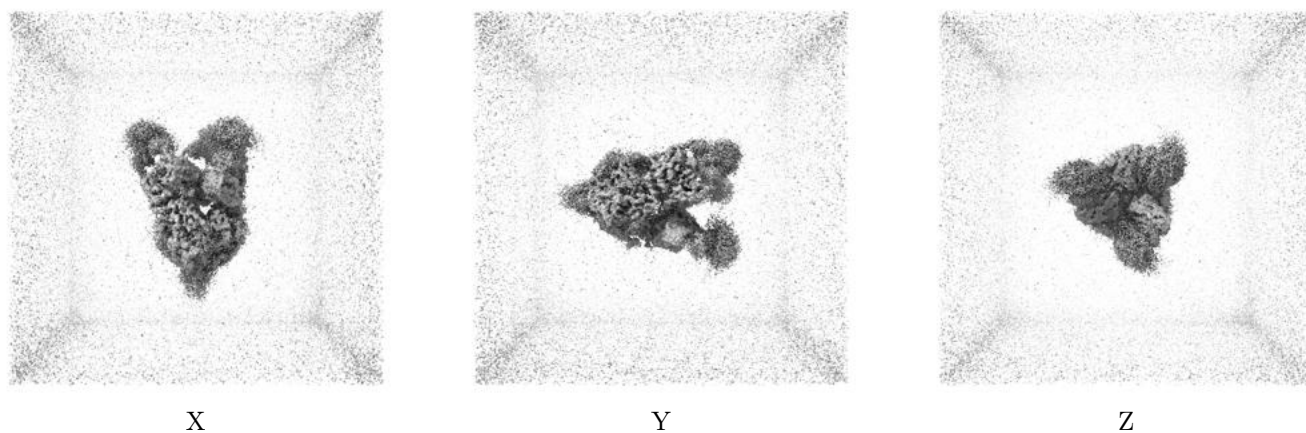
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.23. 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.

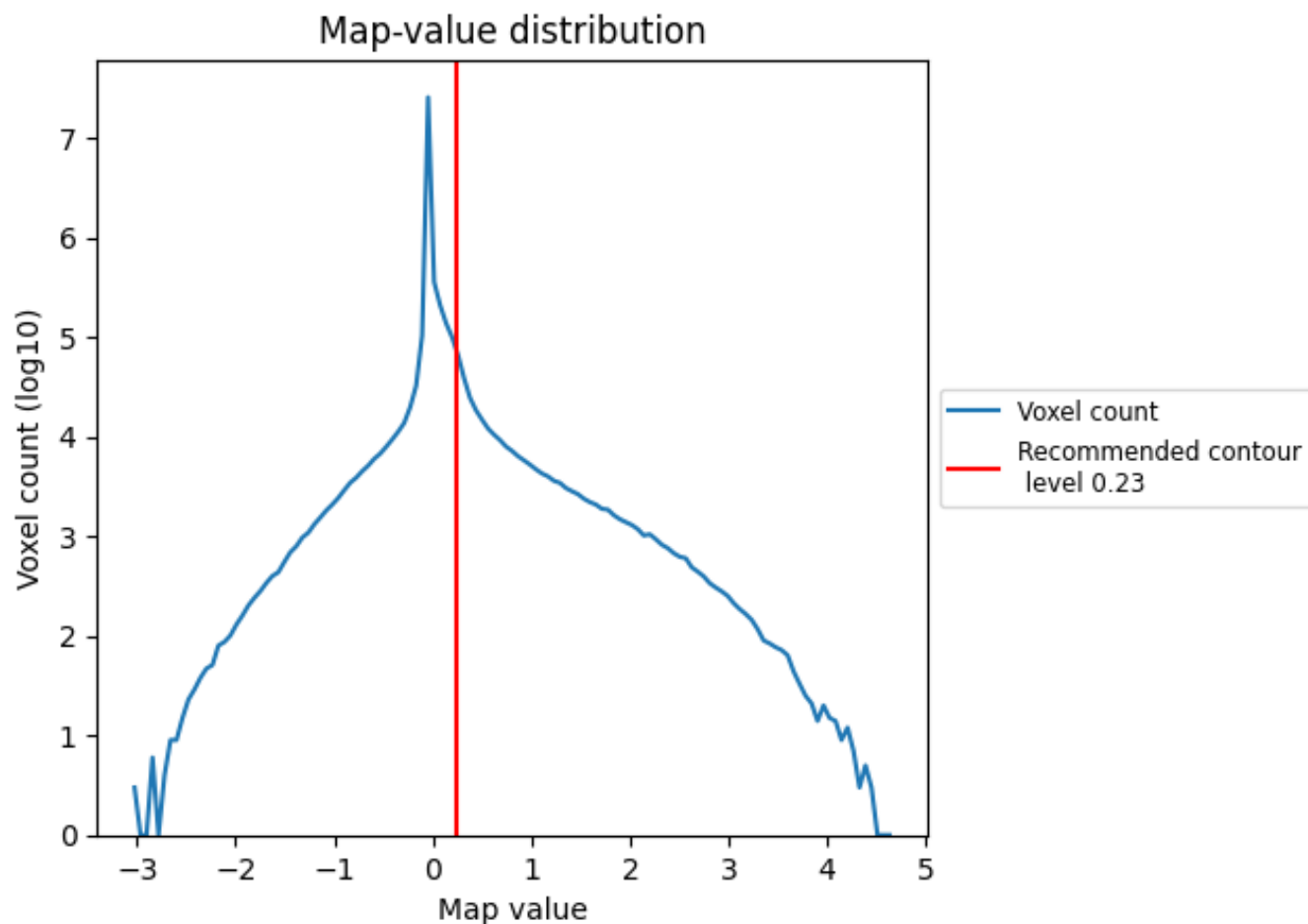
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

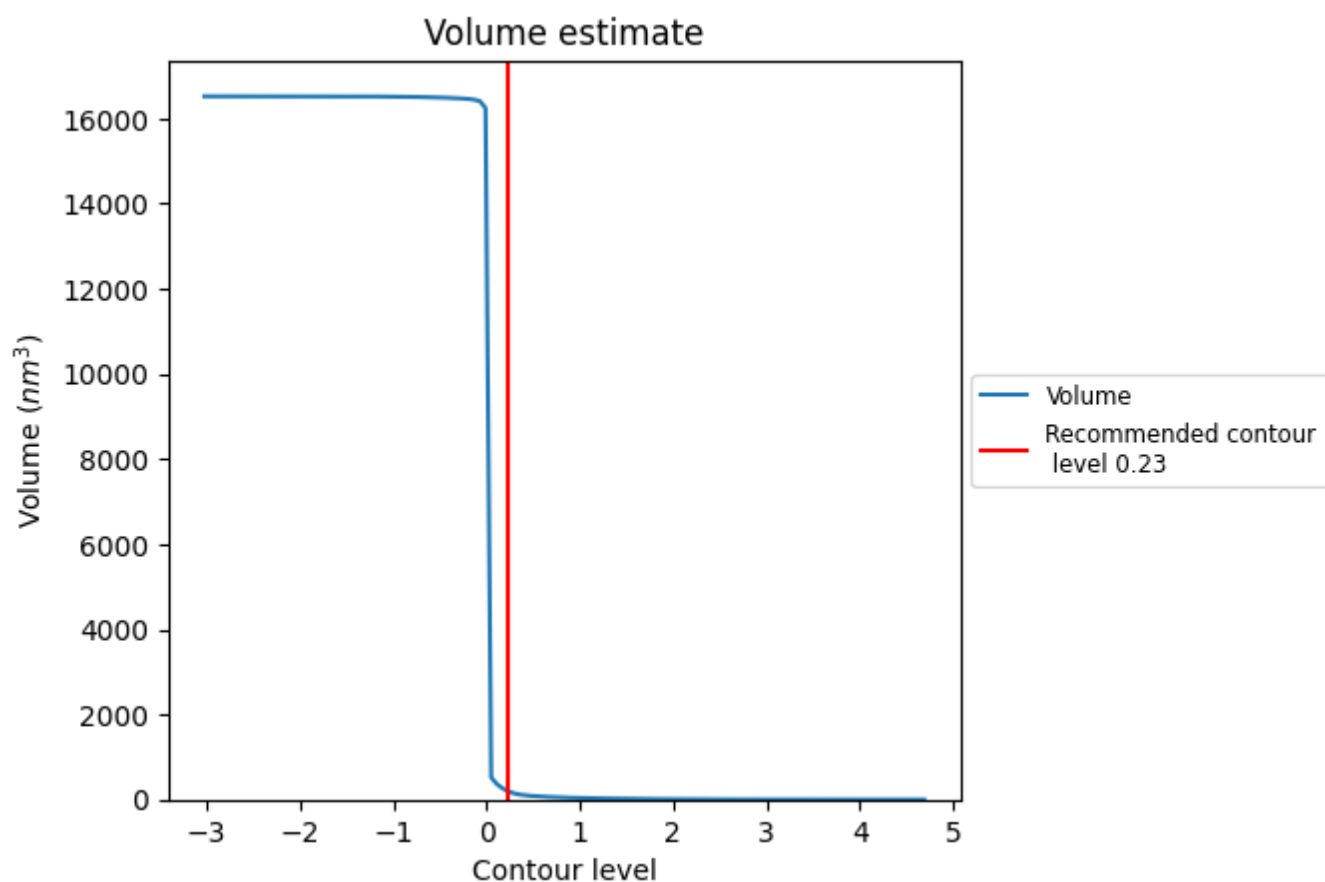
This section contains the results of statistical analysis of the map.

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.

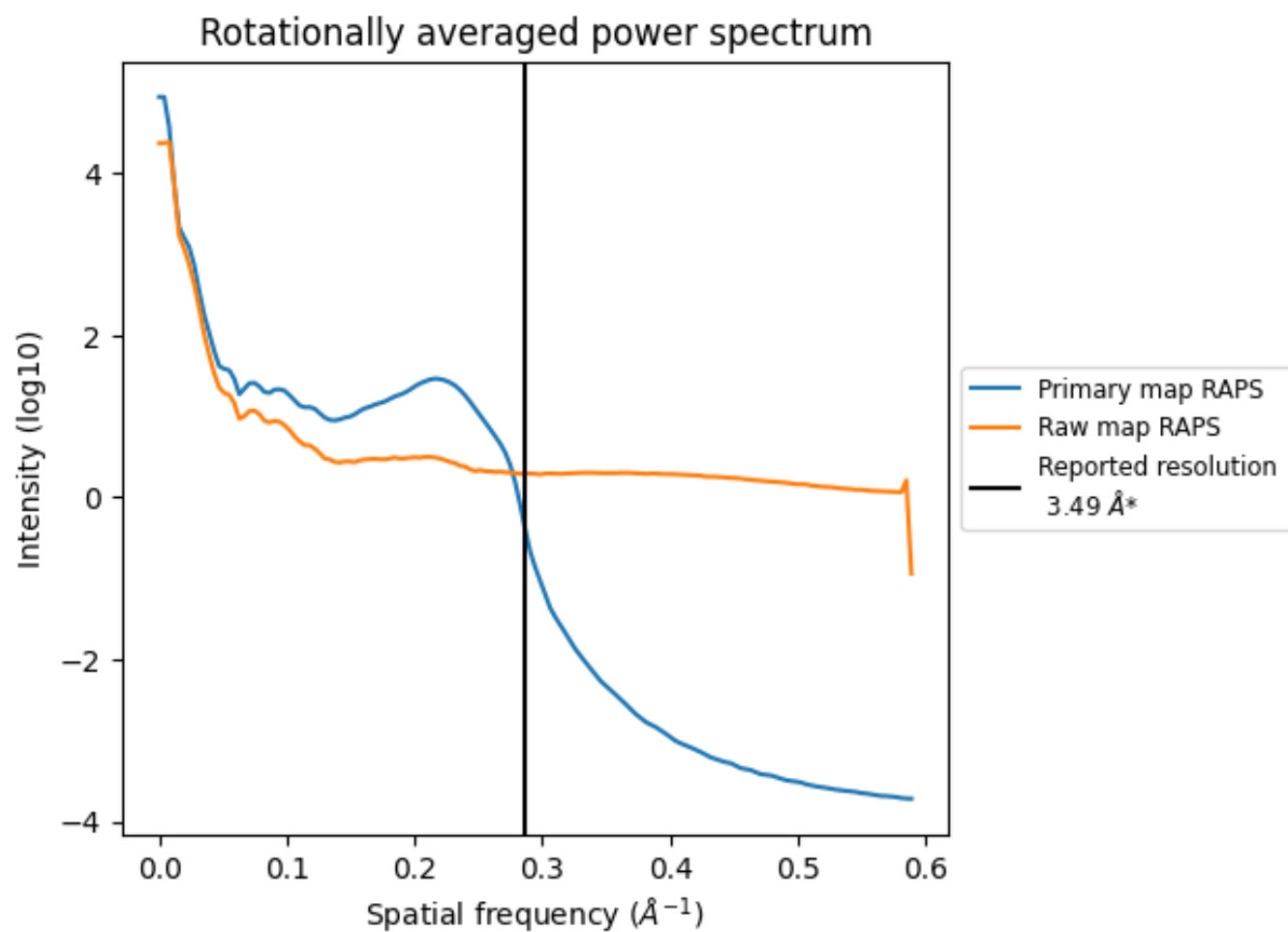
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 198 nm^3 ; this corresponds to an approximate mass of 179 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 ⓘ

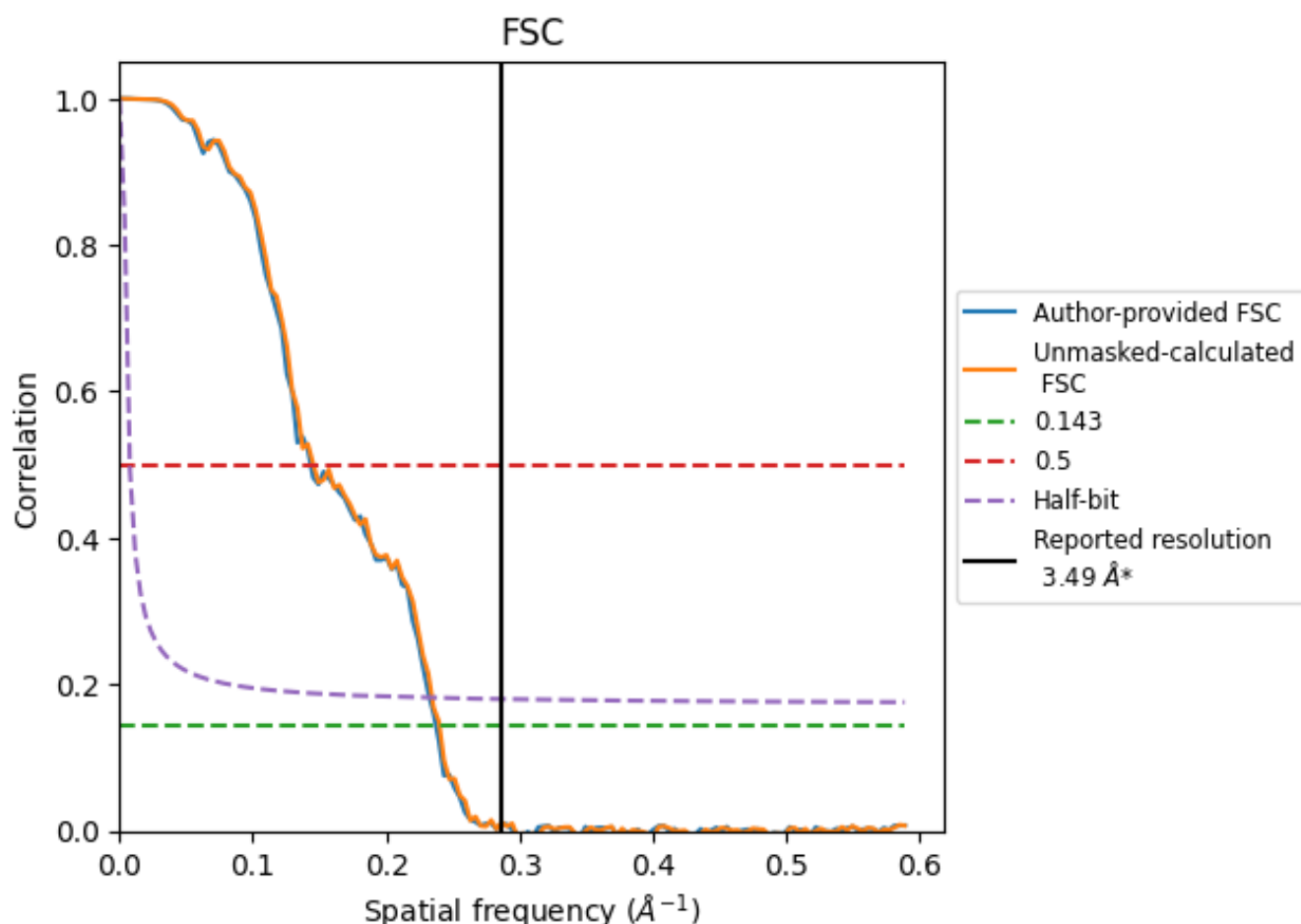


*Reported resolution corresponds to spatial frequency of 0.287 Å⁻¹

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 0.287 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.49	-	-
Author-provided FSC curve	4.21	6.97	4.30
Unmasked-calculated*	4.17	6.88	4.27

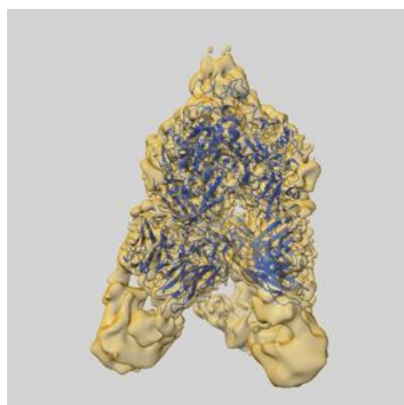
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.21 differs from the reported value 3.49 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.17 differs from the reported value 3.49 by more than 10 %

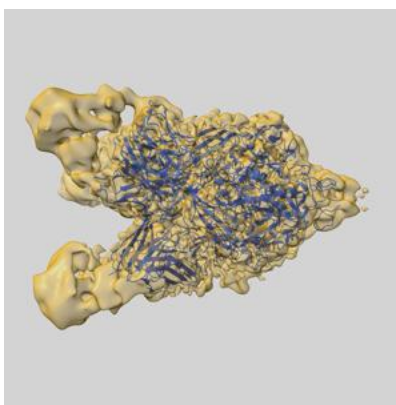
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10118 and PDB model 6S8D. Per-residue inclusion information can be found in section [3](#) on page [11](#).

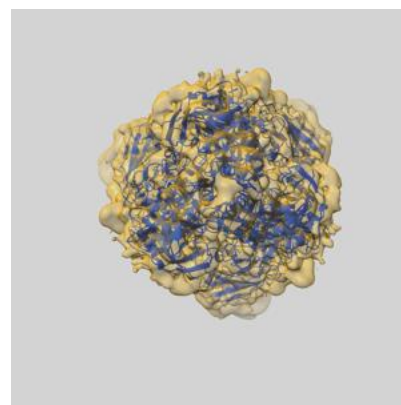
9.1 Map-model overlay [i](#)



X



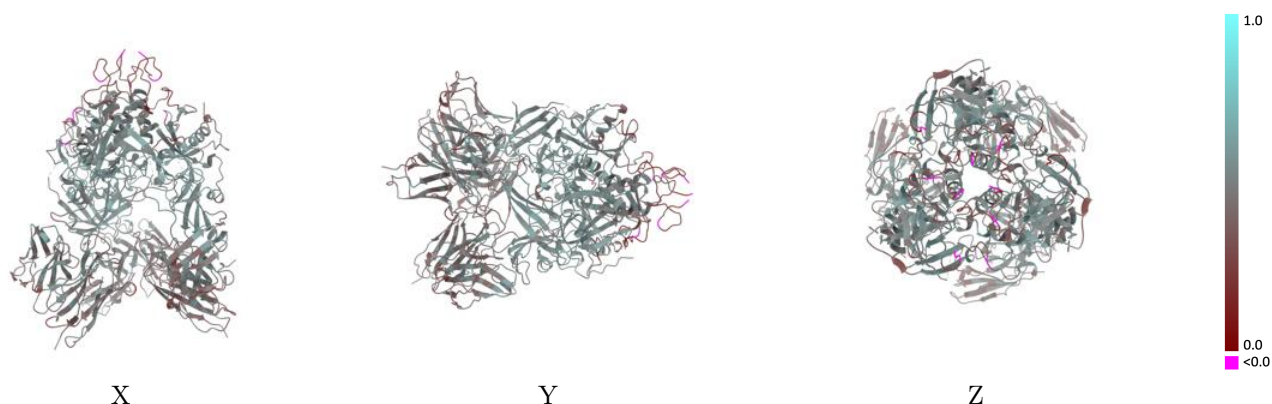
Y



Z

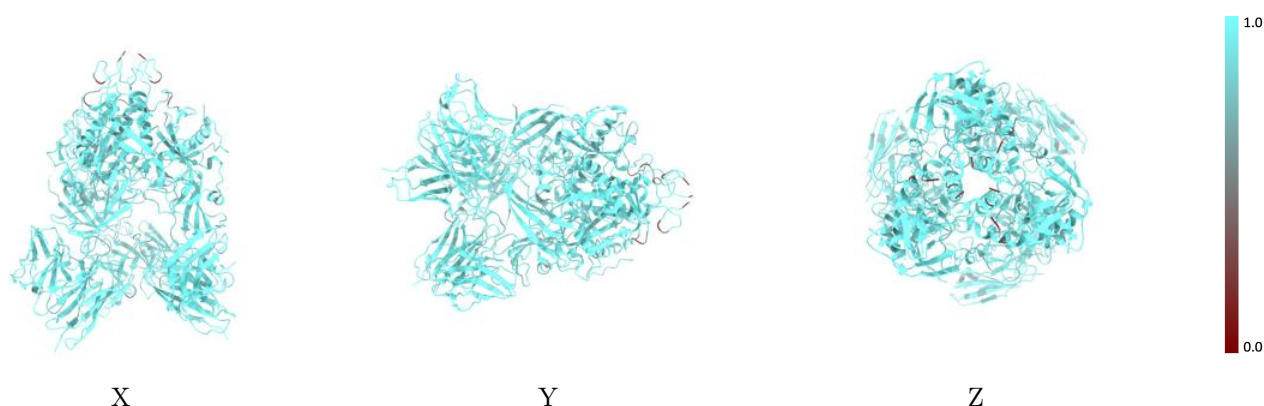
The images above show the 3D surface view of the map at the recommended contour level 0.23 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



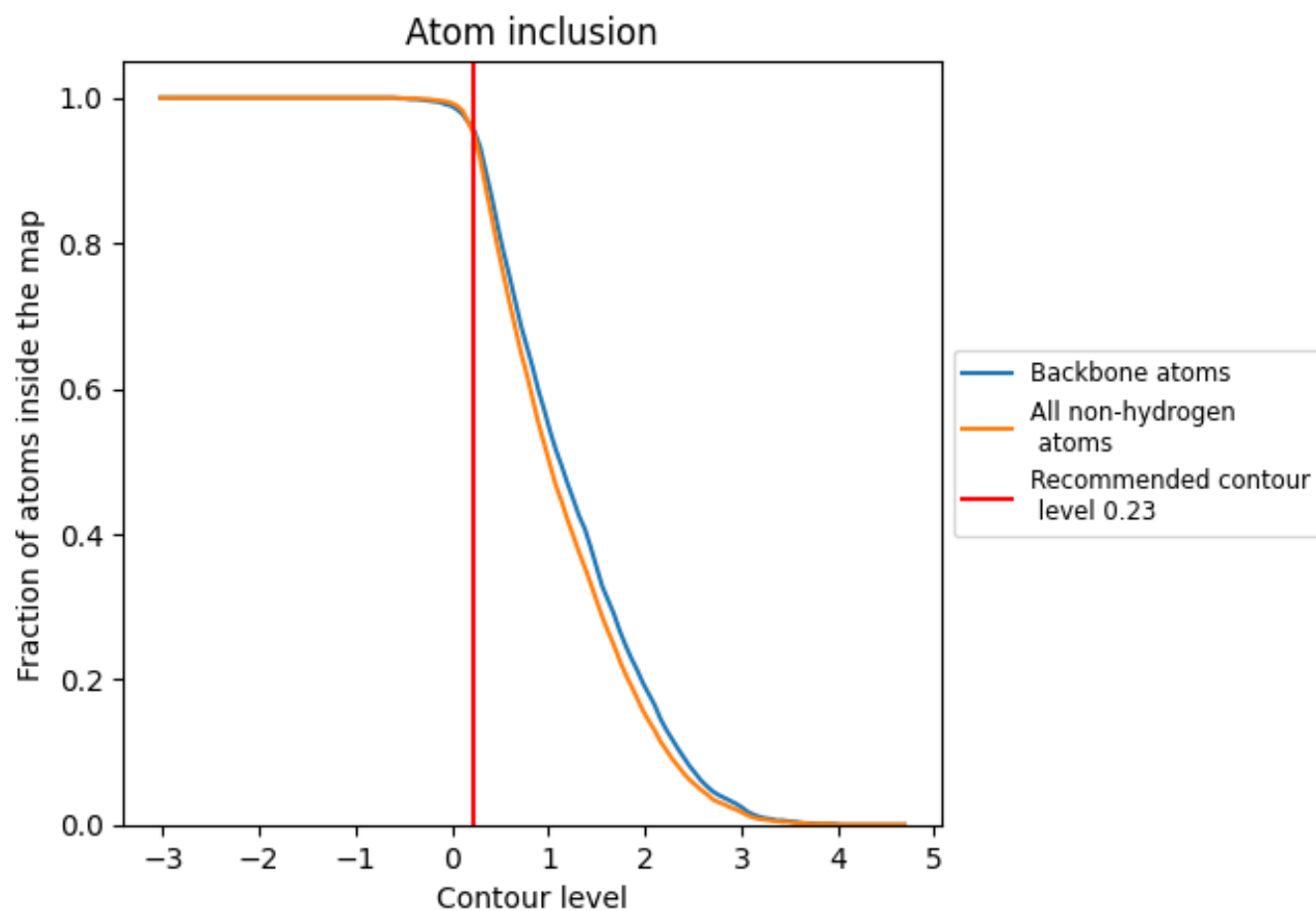
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.23).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.23) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9500	<div><div></div></div> 0.4760
A	<div><div></div></div> 0.9390	<div><div></div></div> 0.5080
B	<div><div></div></div> 0.9450	<div><div></div></div> 0.4700
C	<div><div></div></div> 0.9380	<div><div></div></div> 0.5070
D	<div><div></div></div> 0.9480	<div><div></div></div> 0.4690
E	<div><div></div></div> 0.9370	<div><div></div></div> 0.5060
F	<div><div></div></div> 0.9510	<div><div></div></div> 0.4710
G	<div><div></div></div> 0.9640	<div><div></div></div> 0.4790
H	<div><div></div></div> 0.9530	<div><div></div></div> 0.4550
I	<div><div></div></div> 0.9640	<div><div></div></div> 0.4670
J	<div><div></div></div> 0.9640	<div><div></div></div> 0.4900
L	<div><div></div></div> 0.9650	<div><div></div></div> 0.4520
O	<div><div></div></div> 0.9650	<div><div></div></div> 0.4490
P	<div><div></div></div> 0.9520	<div><div></div></div> 0.4590
U	<div><div></div></div> 0.9640	<div><div></div></div> 0.4480
Y	<div><div></div></div> 0.9600	<div><div></div></div> 0.4600

1.0

0.0

<0.0