



# wwPDB EM Validation Summary Report ⓘ

Feb 10, 2025 – 01:21 PM EST

PDB ID : 9DM0  
EMDB ID : EMD-46994  
Title : Cryo-EM structure of the SFV009 3G01 Fab in complex with A/California/04/2009  
Authors : Fernandez Quintero, M.L.; Ferguson, J.A.; Han, J.; Ward, A.B.  
Deposited on : 2024-09-11  
Resolution : 2.90 Å (reported)  
Based on initial models : ., 4m4y

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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 : 2022.3.0, CSD as543be (2022)  
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) : 2.40

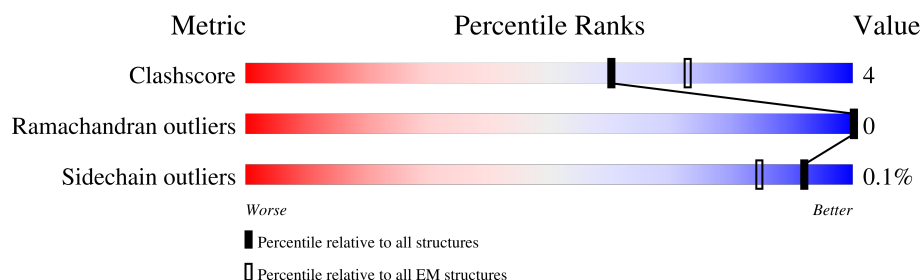
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 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  $\geq 3$ , 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	D	108	<div> <div>20%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
2	C	122	<div> <div>15%</div> <div>86%</div> <div>14%</div> </div>
3	A	324	<div> <div>.</div> <div>90%</div> <div>10%</div> </div>
3	E	324	<div> <div>.</div> <div>85%</div> <div>15%</div> </div>
3	F	324	<div> <div>.</div> <div>91%</div> <div>8%</div> </div>
4	B	231	<div> <div>.</div> <div>62%</div> <div>9%</div> <div>29%</div> </div>
4	G	231	<div> <div>.</div> <div>65%</div> <div>5%</div> <div>29%</div> </div>
4	I	231	<div> <div>.</div> <div>60%</div> <div>10%</div> <div>29%</div> </div>

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Mol	Chain	Length	Quality of chain
5	S	2	<div><div>50%</div><div><div></div><div></div></div><div>50%</div></div>
5	T	2	<div><div>50%</div><div><div></div><div></div></div><div>50%</div></div>
5	U	2	<div><div>50%</div><div><div></div><div></div></div><div>100%</div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13642 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 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	108	Total	C	N	O	S	0	0
			832	523	143	164	2		

- Molecule 2 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	122	Total	C	N	O	S	0	0
			951	597	171	179	4		

- Molecule 3 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	324	Total	C	N	O	S	0	0
			2529	1599	436	483	11		
3	E	324	Total	C	N	O	S	0	0
			2529	1599	436	483	11		
3	F	324	Total	C	N	O	S	0	0
			2529	1599	436	483	11		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	GLY	ALA	conflict	UNP R9RVT8
A	186	SER	PRO	conflict	UNP R9RVT8
A	200	THR	ALA	conflict	UNP R9RVT8
E	10	GLY	ALA	conflict	UNP R9RVT8
E	186	SER	PRO	conflict	UNP R9RVT8
E	200	THR	ALA	conflict	UNP R9RVT8
F	10	GLY	ALA	conflict	UNP R9RVT8
F	186	SER	PRO	conflict	UNP R9RVT8
F	200	THR	ALA	conflict	UNP R9RVT8

- Molecule 4 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	163	Total	C	N	O	S	0	0
			1326	830	226	264	6		
4	G	163	Total	C	N	O	S	0	0
			1326	830	226	264	6		
4	I	163	Total	C	N	O	S	0	0
			1326	830	226	264	6		

There are 204 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	ILE	-	expression tag	UNP A0A1D5AK66
B	-2	GLN	-	expression tag	UNP A0A1D5AK66
B	-1	SER	-	expression tag	UNP A0A1D5AK66
B	0	ARG	-	expression tag	UNP A0A1D5AK66
B	1	GLY	-	expression tag	UNP A0A1D5AK66
B	2	LEU	-	expression tag	UNP A0A1D5AK66
B	3	PHE	-	expression tag	UNP A0A1D5AK66
B	4	GLY	-	expression tag	UNP A0A1D5AK66
B	5	ALA	-	expression tag	UNP A0A1D5AK66
B	6	ILE	-	expression tag	UNP A0A1D5AK66
B	7	ALA	-	expression tag	UNP A0A1D5AK66
B	8	GLY	-	expression tag	UNP A0A1D5AK66
B	172	GLU	-	expression tag	UNP A0A1D5AK66
B	173	ILE	-	expression tag	UNP A0A1D5AK66
B	174	ASP	-	expression tag	UNP A0A1D5AK66
B	175	GLY	-	expression tag	UNP A0A1D5AK66
B	176	SER	-	expression tag	UNP A0A1D5AK66
B	177	GLY	-	expression tag	UNP A0A1D5AK66
B	178	TYR	-	expression tag	UNP A0A1D5AK66
B	179	ILE	-	expression tag	UNP A0A1D5AK66
B	180	PRO	-	expression tag	UNP A0A1D5AK66
B	181	GLU	-	expression tag	UNP A0A1D5AK66
B	182	ALA	-	expression tag	UNP A0A1D5AK66
B	183	PRO	-	expression tag	UNP A0A1D5AK66
B	184	ARG	-	expression tag	UNP A0A1D5AK66
B	185	ASP	-	expression tag	UNP A0A1D5AK66
B	186	GLY	-	expression tag	UNP A0A1D5AK66
B	187	GLN	-	expression tag	UNP A0A1D5AK66
B	188	ALA	-	expression tag	UNP A0A1D5AK66
B	189	TYR	-	expression tag	UNP A0A1D5AK66
B	190	VAL	-	expression tag	UNP A0A1D5AK66
B	191	ARG	-	expression tag	UNP A0A1D5AK66
B	192	LYS	-	expression tag	UNP A0A1D5AK66

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Chain	Residue	Modelled	Actual	Comment	Reference
B	193	ASP	-	expression tag	UNP A0A1D5AK66
B	194	GLY	-	expression tag	UNP A0A1D5AK66
B	195	GLU	-	expression tag	UNP A0A1D5AK66
B	196	TRP	-	expression tag	UNP A0A1D5AK66
B	197	VAL	-	expression tag	UNP A0A1D5AK66
B	198	LEU	-	expression tag	UNP A0A1D5AK66
B	199	LEU	-	expression tag	UNP A0A1D5AK66
B	200	SER	-	expression tag	UNP A0A1D5AK66
B	201	THR	-	expression tag	UNP A0A1D5AK66
B	202	PHE	-	expression tag	UNP A0A1D5AK66
B	203	LEU	-	expression tag	UNP A0A1D5AK66
B	204	GLY	-	expression tag	UNP A0A1D5AK66
B	205	SER	-	expression tag	UNP A0A1D5AK66
B	206	GLY	-	expression tag	UNP A0A1D5AK66
B	207	LEU	-	expression tag	UNP A0A1D5AK66
B	208	ASN	-	expression tag	UNP A0A1D5AK66
B	209	ASP	-	expression tag	UNP A0A1D5AK66
B	210	ILE	-	expression tag	UNP A0A1D5AK66
B	211	PHE	-	expression tag	UNP A0A1D5AK66
B	212	GLU	-	expression tag	UNP A0A1D5AK66
B	213	ALA	-	expression tag	UNP A0A1D5AK66
B	214	GLN	-	expression tag	UNP A0A1D5AK66
B	215	LYS	-	expression tag	UNP A0A1D5AK66
B	216	ILE	-	expression tag	UNP A0A1D5AK66
B	217	GLU	-	expression tag	UNP A0A1D5AK66
B	218	TRP	-	expression tag	UNP A0A1D5AK66
B	219	HIS	-	expression tag	UNP A0A1D5AK66
B	220	GLU	-	expression tag	UNP A0A1D5AK66
B	221	GLY	-	expression tag	UNP A0A1D5AK66
B	222	HIS	-	expression tag	UNP A0A1D5AK66
B	223	HIS	-	expression tag	UNP A0A1D5AK66
B	224	HIS	-	expression tag	UNP A0A1D5AK66
B	225	HIS	-	expression tag	UNP A0A1D5AK66
B	226	HIS	-	expression tag	UNP A0A1D5AK66
B	227	HIS	-	expression tag	UNP A0A1D5AK66
G	-3	ILE	-	expression tag	UNP A0A1D5AK66
G	-2	GLN	-	expression tag	UNP A0A1D5AK66
G	-1	SER	-	expression tag	UNP A0A1D5AK66
G	0	ARG	-	expression tag	UNP A0A1D5AK66
G	1	GLY	-	expression tag	UNP A0A1D5AK66
G	2	LEU	-	expression tag	UNP A0A1D5AK66
G	3	PHE	-	expression tag	UNP A0A1D5AK66

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Chain	Residue	Modelled	Actual	Comment	Reference
G	4	GLY	-	expression tag	UNP A0A1D5AK66
G	5	ALA	-	expression tag	UNP A0A1D5AK66
G	6	ILE	-	expression tag	UNP A0A1D5AK66
G	7	ALA	-	expression tag	UNP A0A1D5AK66
G	8	GLY	-	expression tag	UNP A0A1D5AK66
G	172	GLU	-	expression tag	UNP A0A1D5AK66
G	173	ILE	-	expression tag	UNP A0A1D5AK66
G	174	ASP	-	expression tag	UNP A0A1D5AK66
G	175	GLY	-	expression tag	UNP A0A1D5AK66
G	176	SER	-	expression tag	UNP A0A1D5AK66
G	177	GLY	-	expression tag	UNP A0A1D5AK66
G	178	TYR	-	expression tag	UNP A0A1D5AK66
G	179	ILE	-	expression tag	UNP A0A1D5AK66
G	180	PRO	-	expression tag	UNP A0A1D5AK66
G	181	GLU	-	expression tag	UNP A0A1D5AK66
G	182	ALA	-	expression tag	UNP A0A1D5AK66
G	183	PRO	-	expression tag	UNP A0A1D5AK66
G	184	ARG	-	expression tag	UNP A0A1D5AK66
G	185	ASP	-	expression tag	UNP A0A1D5AK66
G	186	GLY	-	expression tag	UNP A0A1D5AK66
G	187	GLN	-	expression tag	UNP A0A1D5AK66
G	188	ALA	-	expression tag	UNP A0A1D5AK66
G	189	TYR	-	expression tag	UNP A0A1D5AK66
G	190	VAL	-	expression tag	UNP A0A1D5AK66
G	191	ARG	-	expression tag	UNP A0A1D5AK66
G	192	LYS	-	expression tag	UNP A0A1D5AK66
G	193	ASP	-	expression tag	UNP A0A1D5AK66
G	194	GLY	-	expression tag	UNP A0A1D5AK66
G	195	GLU	-	expression tag	UNP A0A1D5AK66
G	196	TRP	-	expression tag	UNP A0A1D5AK66
G	197	VAL	-	expression tag	UNP A0A1D5AK66
G	198	LEU	-	expression tag	UNP A0A1D5AK66
G	199	LEU	-	expression tag	UNP A0A1D5AK66
G	200	SER	-	expression tag	UNP A0A1D5AK66
G	201	THR	-	expression tag	UNP A0A1D5AK66
G	202	PHE	-	expression tag	UNP A0A1D5AK66
G	203	LEU	-	expression tag	UNP A0A1D5AK66
G	204	GLY	-	expression tag	UNP A0A1D5AK66
G	205	SER	-	expression tag	UNP A0A1D5AK66
G	206	GLY	-	expression tag	UNP A0A1D5AK66
G	207	LEU	-	expression tag	UNP A0A1D5AK66
G	208	ASN	-	expression tag	UNP A0A1D5AK66

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Chain	Residue	Modelled	Actual	Comment	Reference
G	209	ASP	-	expression tag	UNP A0A1D5AK66
G	210	ILE	-	expression tag	UNP A0A1D5AK66
G	211	PHE	-	expression tag	UNP A0A1D5AK66
G	212	GLU	-	expression tag	UNP A0A1D5AK66
G	213	ALA	-	expression tag	UNP A0A1D5AK66
G	214	GLN	-	expression tag	UNP A0A1D5AK66
G	215	LYS	-	expression tag	UNP A0A1D5AK66
G	216	ILE	-	expression tag	UNP A0A1D5AK66
G	217	GLU	-	expression tag	UNP A0A1D5AK66
G	218	TRP	-	expression tag	UNP A0A1D5AK66
G	219	HIS	-	expression tag	UNP A0A1D5AK66
G	220	GLU	-	expression tag	UNP A0A1D5AK66
G	221	GLY	-	expression tag	UNP A0A1D5AK66
G	222	HIS	-	expression tag	UNP A0A1D5AK66
G	223	HIS	-	expression tag	UNP A0A1D5AK66
G	224	HIS	-	expression tag	UNP A0A1D5AK66
G	225	HIS	-	expression tag	UNP A0A1D5AK66
G	226	HIS	-	expression tag	UNP A0A1D5AK66
G	227	HIS	-	expression tag	UNP A0A1D5AK66
I	-3	ILE	-	expression tag	UNP A0A1D5AK66
I	-2	GLN	-	expression tag	UNP A0A1D5AK66
I	-1	SER	-	expression tag	UNP A0A1D5AK66
I	0	ARG	-	expression tag	UNP A0A1D5AK66
I	1	GLY	-	expression tag	UNP A0A1D5AK66
I	2	LEU	-	expression tag	UNP A0A1D5AK66
I	3	PHE	-	expression tag	UNP A0A1D5AK66
I	4	GLY	-	expression tag	UNP A0A1D5AK66
I	5	ALA	-	expression tag	UNP A0A1D5AK66
I	6	ILE	-	expression tag	UNP A0A1D5AK66
I	7	ALA	-	expression tag	UNP A0A1D5AK66
I	8	GLY	-	expression tag	UNP A0A1D5AK66
I	172	GLU	-	expression tag	UNP A0A1D5AK66
I	173	ILE	-	expression tag	UNP A0A1D5AK66
I	174	ASP	-	expression tag	UNP A0A1D5AK66
I	175	GLY	-	expression tag	UNP A0A1D5AK66
I	176	SER	-	expression tag	UNP A0A1D5AK66
I	177	GLY	-	expression tag	UNP A0A1D5AK66
I	178	TYR	-	expression tag	UNP A0A1D5AK66
I	179	ILE	-	expression tag	UNP A0A1D5AK66
I	180	PRO	-	expression tag	UNP A0A1D5AK66
I	181	GLU	-	expression tag	UNP A0A1D5AK66
I	182	ALA	-	expression tag	UNP A0A1D5AK66

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Chain	Residue	Modelled	Actual	Comment	Reference
I	183	PRO	-	expression tag	UNP A0A1D5AK66
I	184	ARG	-	expression tag	UNP A0A1D5AK66
I	185	ASP	-	expression tag	UNP A0A1D5AK66
I	186	GLY	-	expression tag	UNP A0A1D5AK66
I	187	GLN	-	expression tag	UNP A0A1D5AK66
I	188	ALA	-	expression tag	UNP A0A1D5AK66
I	189	TYR	-	expression tag	UNP A0A1D5AK66
I	190	VAL	-	expression tag	UNP A0A1D5AK66
I	191	ARG	-	expression tag	UNP A0A1D5AK66
I	192	LYS	-	expression tag	UNP A0A1D5AK66
I	193	ASP	-	expression tag	UNP A0A1D5AK66
I	194	GLY	-	expression tag	UNP A0A1D5AK66
I	195	GLU	-	expression tag	UNP A0A1D5AK66
I	196	TRP	-	expression tag	UNP A0A1D5AK66
I	197	VAL	-	expression tag	UNP A0A1D5AK66
I	198	LEU	-	expression tag	UNP A0A1D5AK66
I	199	LEU	-	expression tag	UNP A0A1D5AK66
I	200	SER	-	expression tag	UNP A0A1D5AK66
I	201	THR	-	expression tag	UNP A0A1D5AK66
I	202	PHE	-	expression tag	UNP A0A1D5AK66
I	203	LEU	-	expression tag	UNP A0A1D5AK66
I	204	GLY	-	expression tag	UNP A0A1D5AK66
I	205	SER	-	expression tag	UNP A0A1D5AK66
I	206	GLY	-	expression tag	UNP A0A1D5AK66
I	207	LEU	-	expression tag	UNP A0A1D5AK66
I	208	ASN	-	expression tag	UNP A0A1D5AK66
I	209	ASP	-	expression tag	UNP A0A1D5AK66
I	210	ILE	-	expression tag	UNP A0A1D5AK66
I	211	PHE	-	expression tag	UNP A0A1D5AK66
I	212	GLU	-	expression tag	UNP A0A1D5AK66
I	213	ALA	-	expression tag	UNP A0A1D5AK66
I	214	GLN	-	expression tag	UNP A0A1D5AK66
I	215	LYS	-	expression tag	UNP A0A1D5AK66
I	216	ILE	-	expression tag	UNP A0A1D5AK66
I	217	GLU	-	expression tag	UNP A0A1D5AK66
I	218	TRP	-	expression tag	UNP A0A1D5AK66
I	219	HIS	-	expression tag	UNP A0A1D5AK66
I	220	GLU	-	expression tag	UNP A0A1D5AK66
I	221	GLY	-	expression tag	UNP A0A1D5AK66
I	222	HIS	-	expression tag	UNP A0A1D5AK66
I	223	HIS	-	expression tag	UNP A0A1D5AK66
I	224	HIS	-	expression tag	UNP A0A1D5AK66

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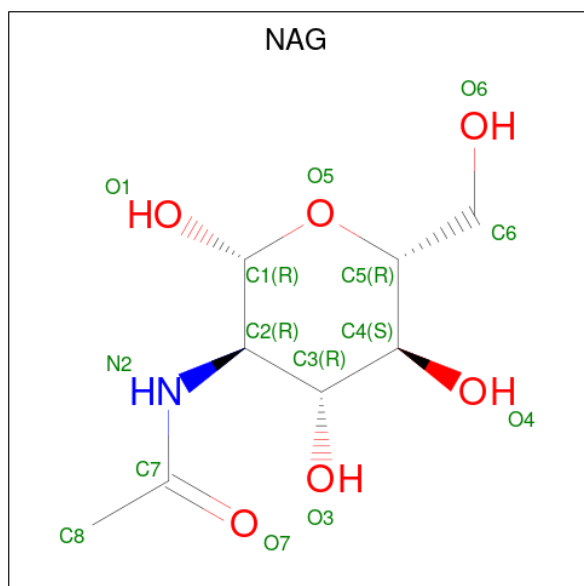
Chain	Residue	Modelled	Actual	Comment	Reference
I	225	HIS	-	expression tag	UNP A0A1D5AK66
I	226	HIS	-	expression tag	UNP A0A1D5AK66
I	227	HIS	-	expression tag	UNP A0A1D5AK66

- 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	S	2	Total	C	N	O	0	0
			28	16	2	10		
5	T	2	Total	C	N	O	0	0
			28	16	2	10		
5	U	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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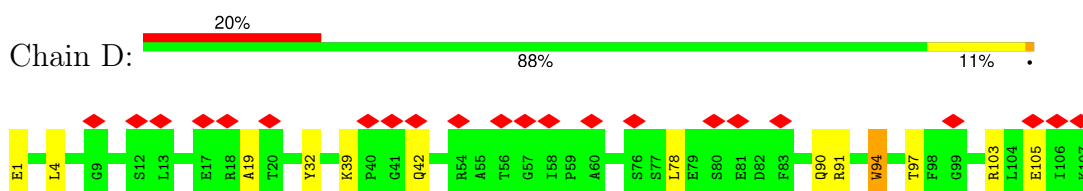
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Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total 14	C 8	N 1	O 5	0
6	A	1	Total 14	C 8	N 1	O 5	0
6	A	1	Total 14	C 8	N 1	O 5	0
6	B	1	Total 14	C 8	N 1	O 5	0
6	E	1	Total 14	C 8	N 1	O 5	0
6	E	1	Total 14	C 8	N 1	O 5	0
6	E	1	Total 14	C 8	N 1	O 5	0
6	E	1	Total 14	C 8	N 1	O 5	0
6	G	1	Total 14	C 8	N 1	O 5	0
6	F	1	Total 14	C 8	N 1	O 5	0
6	F	1	Total 14	C 8	N 1	O 5	0
6	F	1	Total 14	C 8	N 1	O 5	0
6	F	1	Total 14	C 8	N 1	O 5	0
6	I	1	Total 14	C 8	N 1	O 5	0

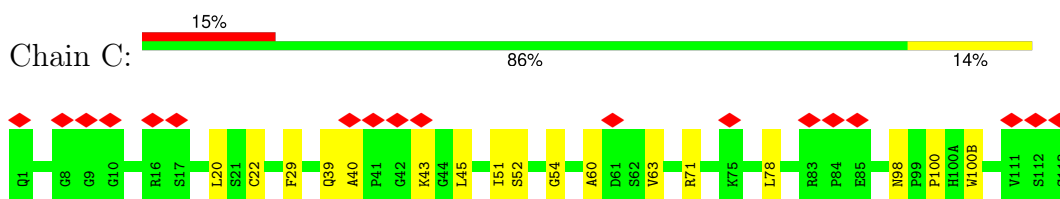
### 3 Residue-property plots [i](#)

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.

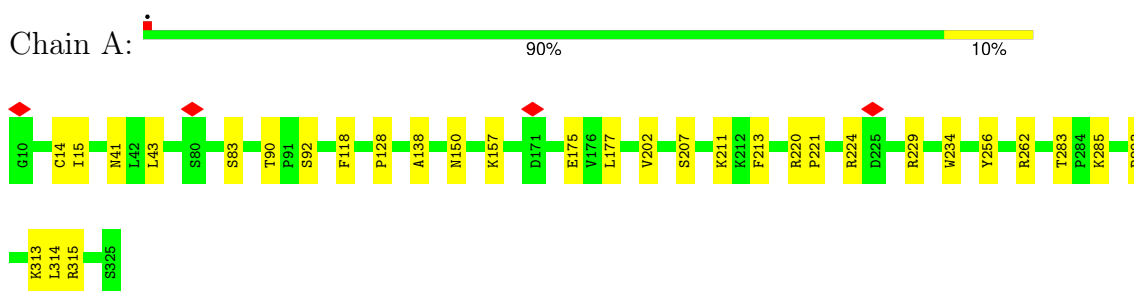
- Molecule 1: Fab light chain



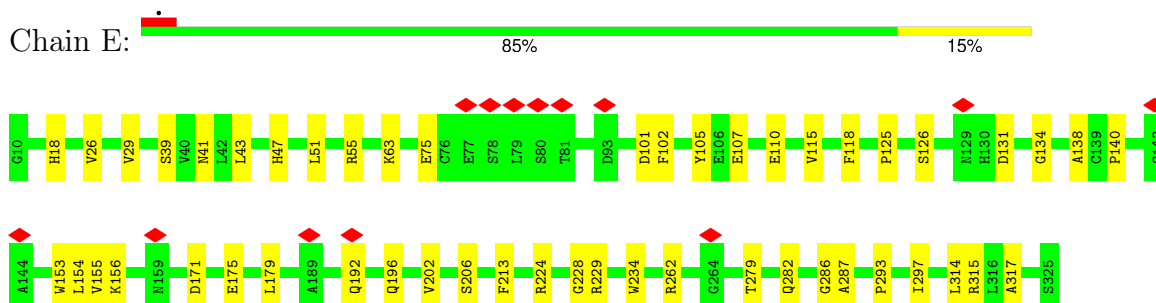
- Molecule 2: Fab heavy chain



- Molecule 3: Hemagglutinin



- Molecule 3: Hemagglutinin







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



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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	90138	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	44.94	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	190000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.703	Depositor
Minimum map value	-0.456	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.101	Depositor
Map size ( $\text{\AA}$ )	367.616, 367.616, 367.616	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.718, 0.718, 0.718	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	D	0.27	0/852	0.58	0/1156
2	C	0.27	0/976	0.62	1/1325 (0.1%)
3	A	0.27	0/2593	0.53	0/3524
3	E	0.28	0/2593	0.56	1/3524 (0.0%)
3	F	0.28	0/2593	0.53	0/3524
4	B	0.31	0/1353	0.56	1/1823 (0.1%)
4	G	0.27	0/1353	0.52	0/1823
4	I	0.27	0/1353	0.55	1/1823 (0.1%)
All	All	0.28	0/13666	0.55	4/18522 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
3	F	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	101	ASP	CB-CG-OD1	7.83	125.34	118.30
4	B	102	LEU	CA-CB-CG	5.75	128.53	115.30
2	C	20	LEU	CA-CB-CG	5.21	127.30	115.30
4	I	102	LEU	CA-CB-CG	5.16	127.16	115.30

There are no chirality outliers.



All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	94	TRP	Peptide
3	F	277	CYS	Peptide

## 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	D	832	0	812	7	0
2	C	951	0	912	10	0
3	A	2529	0	2474	24	0
3	E	2529	0	2474	31	0
3	F	2529	0	2474	19	0
4	B	1326	0	1243	17	0
4	G	1326	0	1244	11	0
4	I	1326	0	1244	16	0
5	S	28	0	25	0	0
5	T	28	0	25	1	0
5	U	28	0	25	0	0
6	A	56	0	52	0	0
6	B	14	0	13	0	0
6	E	56	0	52	0	0
6	F	56	0	52	1	0
6	G	14	0	13	1	0
6	I	14	0	13	0	0
All	All	13642	0	13147	116	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 4.

The worst 5 of 116 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)
4:B:141:TYR:O	4:B:169:ASN:ND2	2.18	0.77
3:E:43:LEU:HB2	3:E:314:LEU:HB2	1.79	0.65
4:G:150:GLU:HB2	6:G:201:NAG:H82	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:71:ASN:ND2	4:B:74:GLU:OE1	2.34	0.60
4:I:133:ILE:HD13	4:I:139:GLU:HB2	1.85	0.59

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	D	106/108 (98%)	96 (91%)	10 (9%)	0	100	100
2	C	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
3	A	322/324 (99%)	319 (99%)	3 (1%)	0	100	100
3	E	322/324 (99%)	312 (97%)	10 (3%)	0	100	100
3	F	322/324 (99%)	316 (98%)	6 (2%)	0	100	100
4	B	161/231 (70%)	157 (98%)	4 (2%)	0	100	100
4	G	161/231 (70%)	159 (99%)	2 (1%)	0	100	100
4	I	161/231 (70%)	159 (99%)	2 (1%)	0	100	100
All	All	1675/1895 (88%)	1632 (97%)	43 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	91/91 (100%)	91 (100%)	0	100	100
2	C	101/101 (100%)	101 (100%)	0	100	100
3	A	284/284 (100%)	284 (100%)	0	100	100
3	E	284/284 (100%)	283 (100%)	1 (0%)	89	97
3	F	284/284 (100%)	284 (100%)	0	100	100
4	B	143/197 (73%)	143 (100%)	0	100	100
4	G	143/197 (73%)	143 (100%)	0	100	100
4	I	143/197 (73%)	143 (100%)	0	100	100
All	All	1473/1635 (90%)	1472 (100%)	1 (0%)	92	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	55	ARG

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

Mol	Chain	Res	Type
3	F	38	HIS

### 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	S	1	5,3	14,14,15	0.28	0	17,19,21	0.63	1 (5%)
5	NAG	S	2	5	14,14,15	0.35	0	17,19,21	0.49	0
5	NAG	T	1	5,3	14,14,15	0.28	0	17,19,21	0.62	0
5	NAG	T	2	5	14,14,15	0.32	0	17,19,21	0.50	0
5	NAG	U	1	5,3	14,14,15	0.30	0	17,19,21	0.56	0
5	NAG	U	2	5	14,14,15	0.30	0	17,19,21	0.52	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	S	1	5,3	-	2/6/23/26	0/1/1/1
5	NAG	S	2	5	-	0/6/23/26	0/1/1/1
5	NAG	T	1	5,3	-	2/6/23/26	0/1/1/1
5	NAG	T	2	5	-	2/6/23/26	0/1/1/1
5	NAG	U	1	5,3	-	0/6/23/26	0/1/1/1
5	NAG	U	2	5	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	1	NAG	C1-O5-C5	2.18	115.11	112.19

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

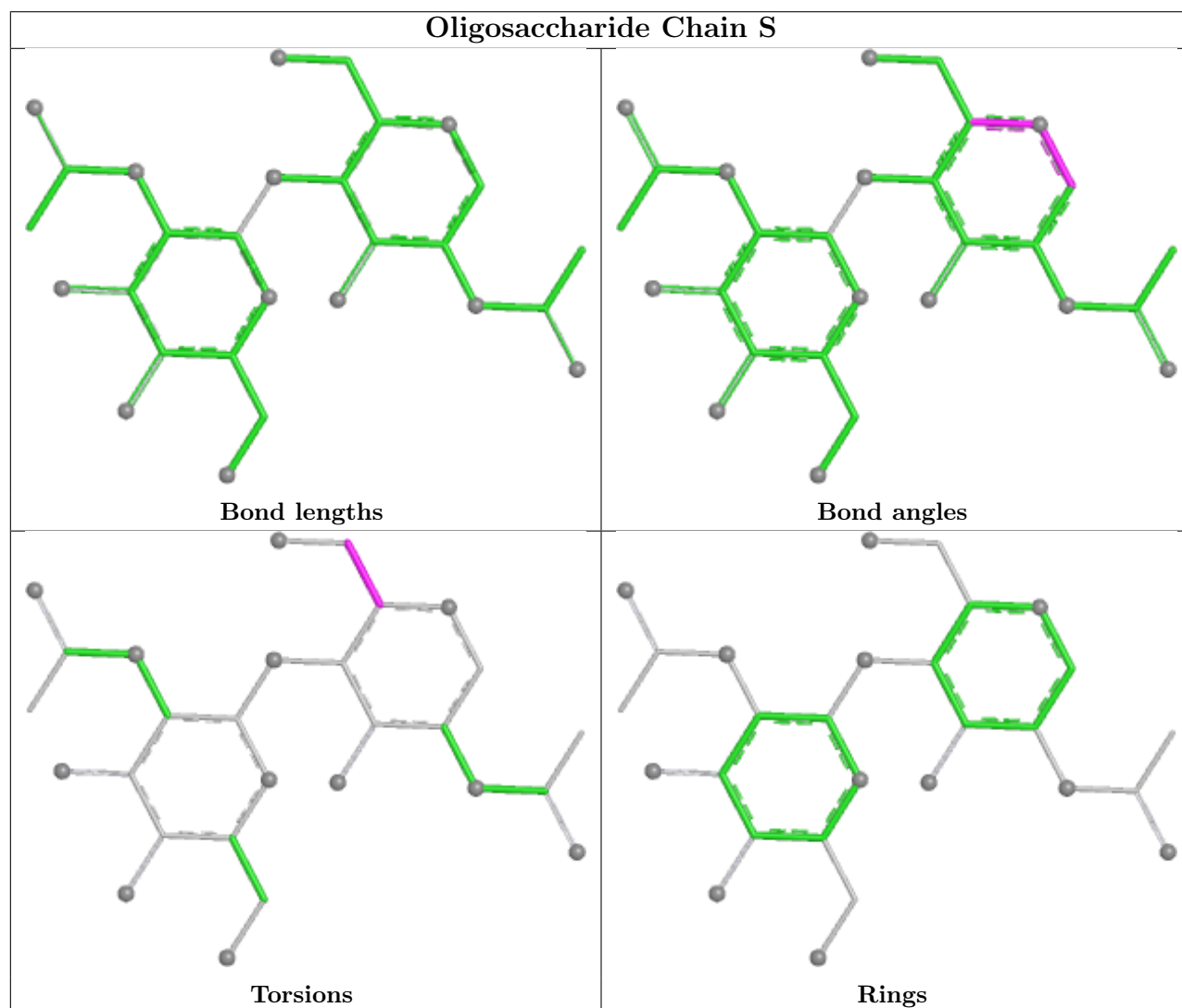
Mol	Chain	Res	Type	Atoms
5	S	1	NAG	O5-C5-C6-O6
5	T	1	NAG	O5-C5-C6-O6
5	T	1	NAG	C4-C5-C6-O6
5	S	1	NAG	C4-C5-C6-O6
5	U	2	NAG	O5-C5-C6-O6

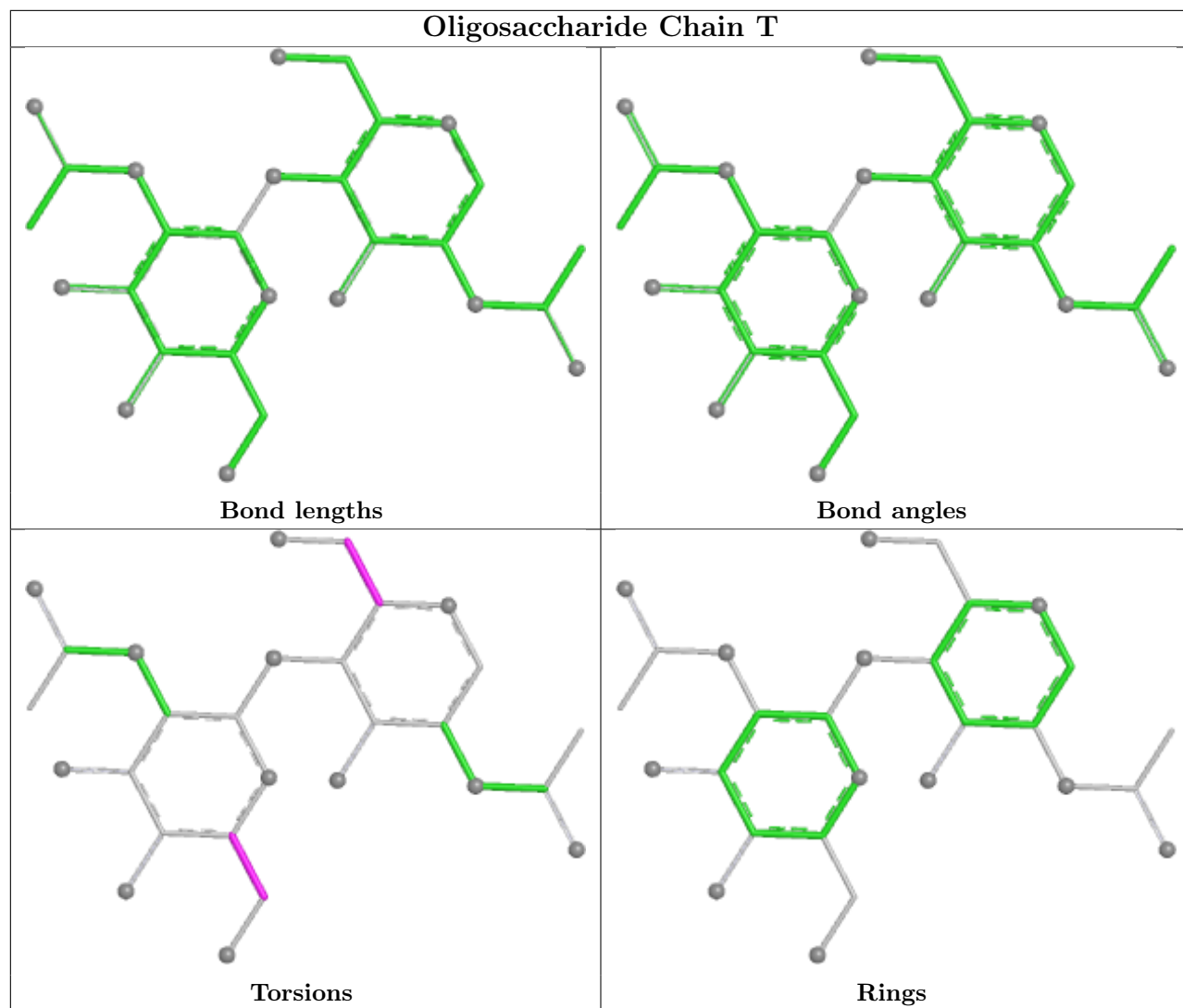
There are no ring outliers.

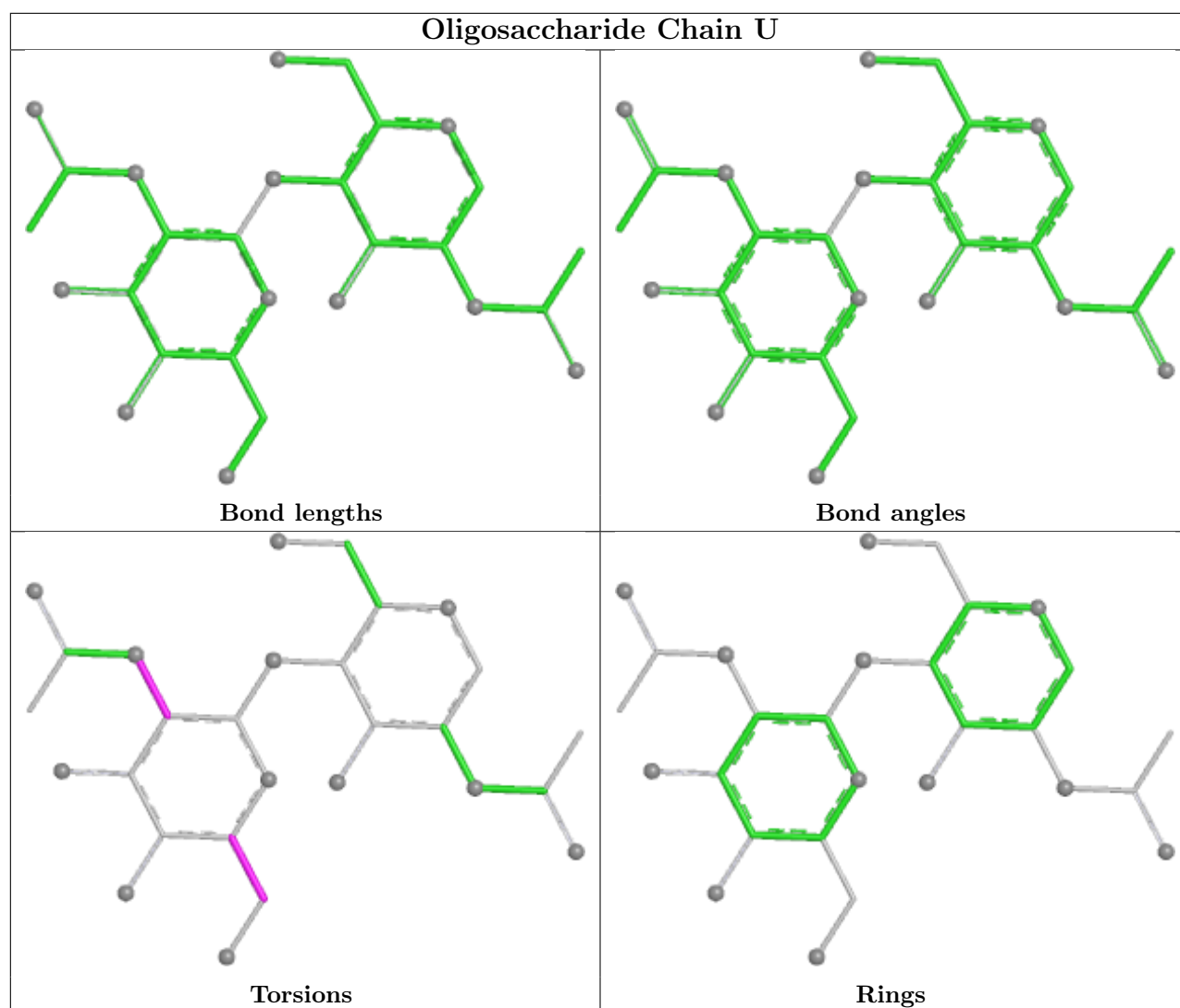
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	T	1	NAG	1	0

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](#)

15 ligands 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	$\# Z  > 2$
6	NAG	A	403	3	14,14,15	0.37	0	17,19,21	0.51	0
6	NAG	B	201	4	14,14,15	0.54	0	17,19,21	0.43	0
6	NAG	A	404	3	14,14,15	0.35	0	17,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	A	402	3	14,14,15	0.91	1 (7%)	17,19,21	0.98	1 (5%)
6	NAG	E	403	3	14,14,15	0.42	0	17,19,21	0.59	1 (5%)
6	NAG	G	201	4	14,14,15	0.93	1 (7%)	17,19,21	0.74	1 (5%)
6	NAG	I	201	4	14,14,15	0.60	0	17,19,21	0.72	1 (5%)
6	NAG	F	402	3	14,14,15	0.35	0	17,19,21	0.50	0
6	NAG	E	404	3	14,14,15	0.37	0	17,19,21	0.52	0
6	NAG	F	401	3	14,14,15	0.39	0	17,19,21	0.48	0
6	NAG	F	403	3	14,14,15	0.41	0	17,19,21	0.54	0
6	NAG	E	401	3	14,14,15	0.35	0	17,19,21	0.49	0
6	NAG	A	401	3	14,14,15	0.42	0	17,19,21	0.53	0
6	NAG	F	404	3	14,14,15	0.39	0	17,19,21	0.54	0
6	NAG	E	402	3	14,14,15	0.42	0	17,19,21	0.62	1 (5%)

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
6	NAG	A	403	3	-	1/6/23/26	0/1/1/1
6	NAG	B	201	4	-	0/6/23/26	0/1/1/1
6	NAG	A	404	3	-	2/6/23/26	0/1/1/1
6	NAG	A	402	3	-	0/6/23/26	0/1/1/1
6	NAG	E	403	3	-	2/6/23/26	0/1/1/1
6	NAG	G	201	4	-	2/6/23/26	0/1/1/1
6	NAG	I	201	4	-	0/6/23/26	0/1/1/1
6	NAG	F	402	3	-	2/6/23/26	0/1/1/1
6	NAG	E	404	3	-	2/6/23/26	0/1/1/1
6	NAG	F	401	3	-	2/6/23/26	0/1/1/1
6	NAG	F	403	3	-	2/6/23/26	0/1/1/1
6	NAG	E	401	3	-	0/6/23/26	0/1/1/1
6	NAG	A	401	3	-	0/6/23/26	0/1/1/1
6	NAG	F	404	3	-	1/6/23/26	0/1/1/1
6	NAG	E	402	3	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	402	NAG	C1-C2	2.85	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	201	NAG	C1-C2	2.63	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	402	NAG	C1-O5-C5	3.63	117.05	112.19
6	I	201	NAG	C1-O5-C5	2.58	115.65	112.19
6	G	201	NAG	C1-O5-C5	2.30	115.27	112.19
6	E	402	NAG	C1-O5-C5	2.15	115.07	112.19
6	E	403	NAG	C1-O5-C5	2.04	114.92	112.19

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	404	NAG	O5-C5-C6-O6
6	G	201	NAG	O5-C5-C6-O6
6	G	201	NAG	C4-C5-C6-O6
6	F	401	NAG	C4-C5-C6-O6
6	F	403	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
6	G	201	NAG	1	0
6	F	402	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.

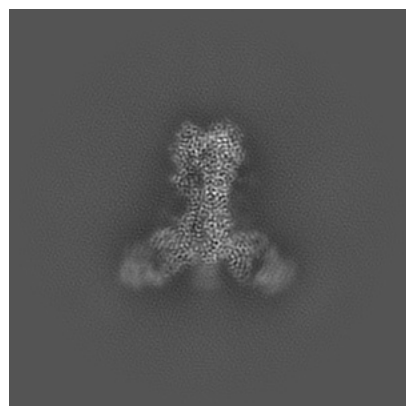
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46994. These allow visual inspection of the internal detail of the map and identification of artifacts.

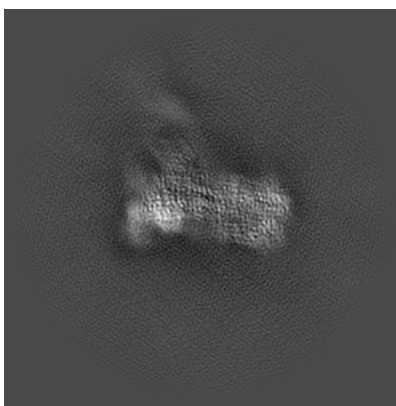
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

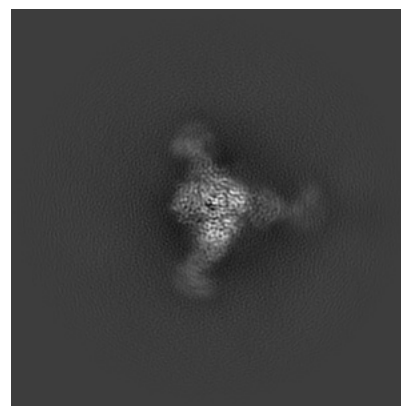
#### 6.1.1 Primary map



X

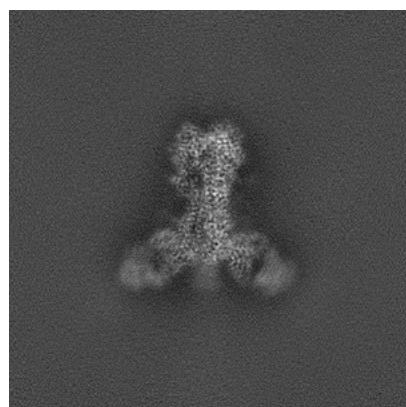


Y

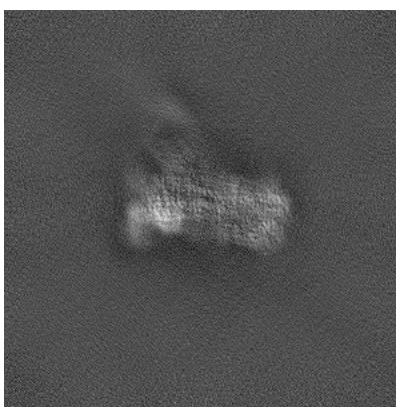


Z

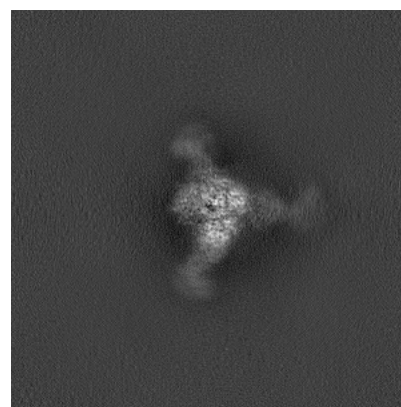
#### 6.1.2 Raw map



X



Y

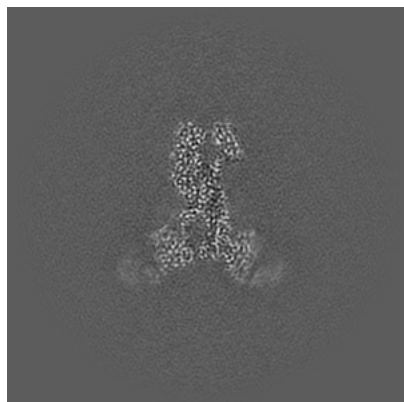


Z

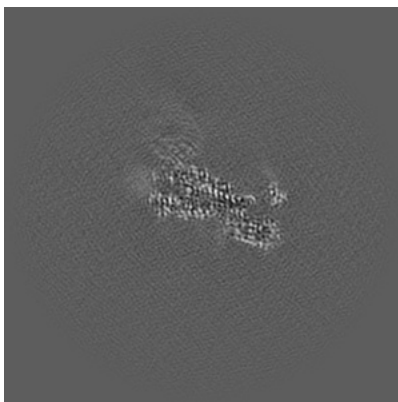
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

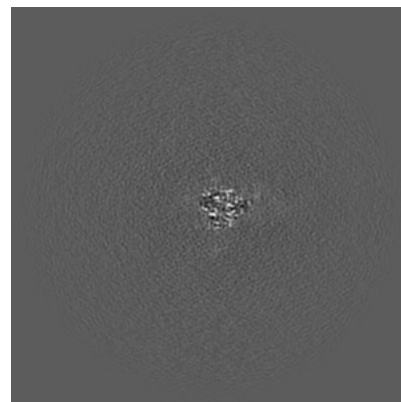
### 6.2.1 Primary map



X Index: 256

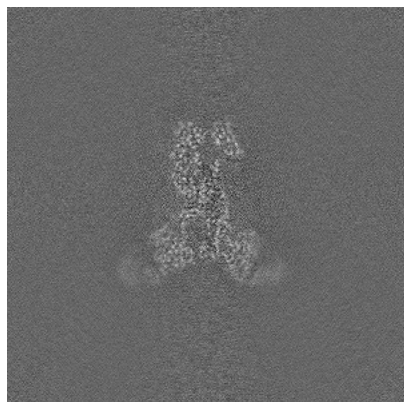


Y Index: 256

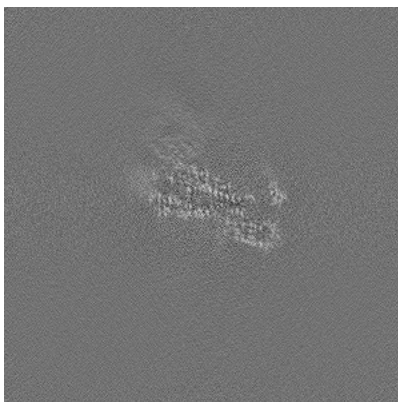


Z Index: 256

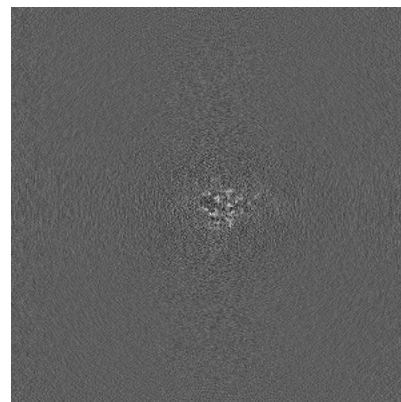
### 6.2.2 Raw map



X Index: 256



Y Index: 256

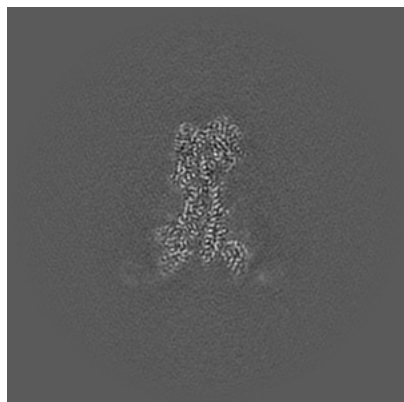


Z Index: 256

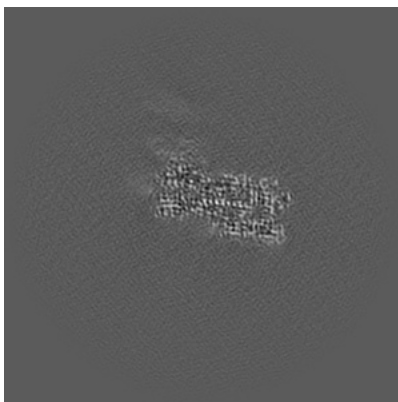
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

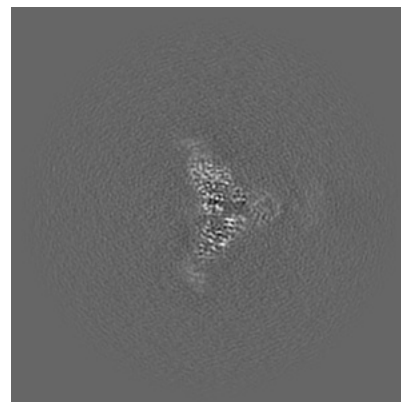
### 6.3.1 Primary map



X Index: 264

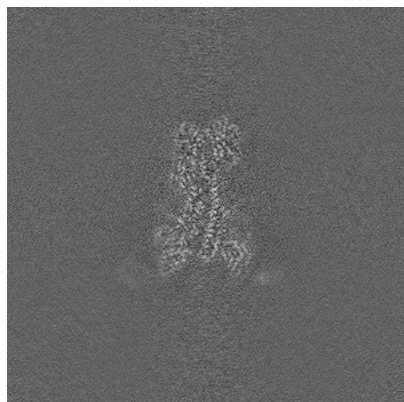


Y Index: 268

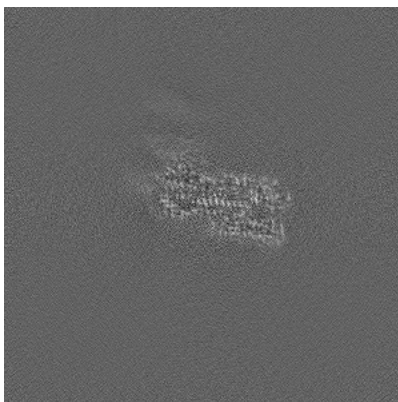


Z Index: 205

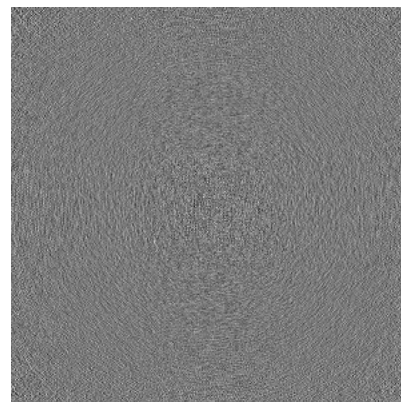
### 6.3.2 Raw map



X Index: 263



Y Index: 267



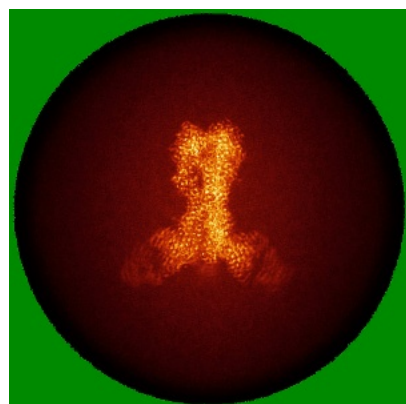
Z Index: 511

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

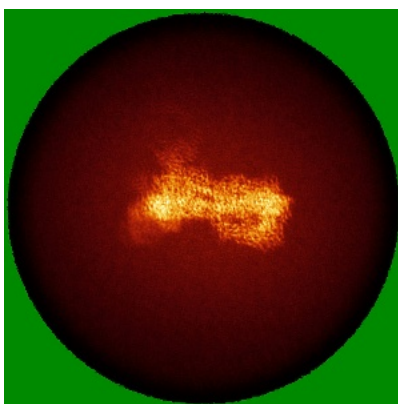


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

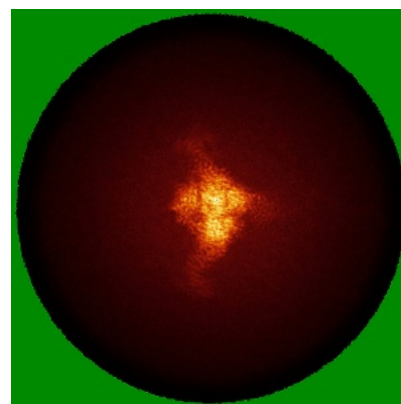
### 6.4.1 Primary map



X

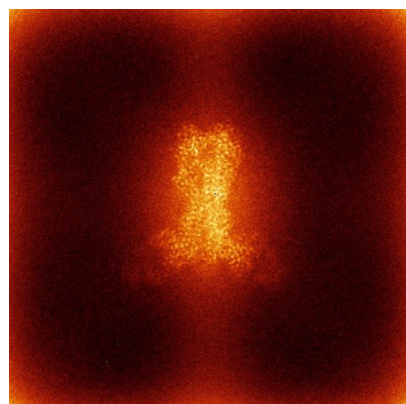


Y

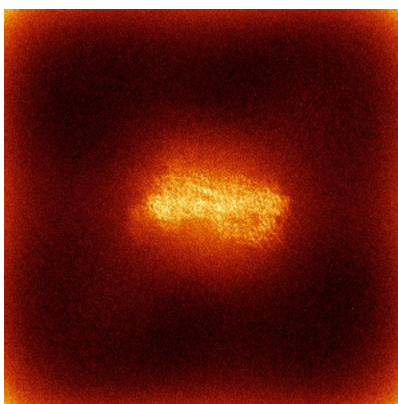


Z

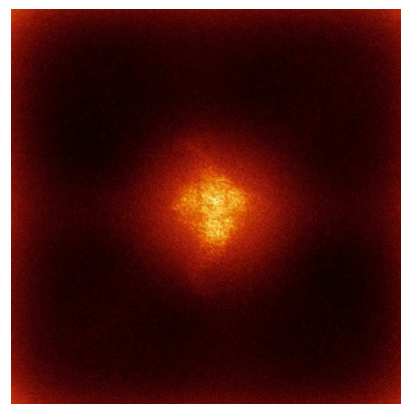
### 6.4.2 Raw map



X



Y

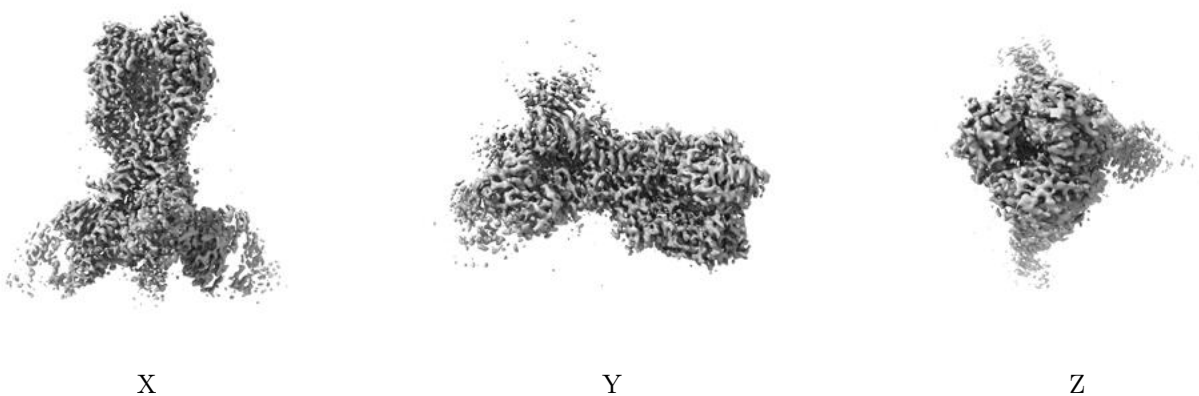


Z

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.

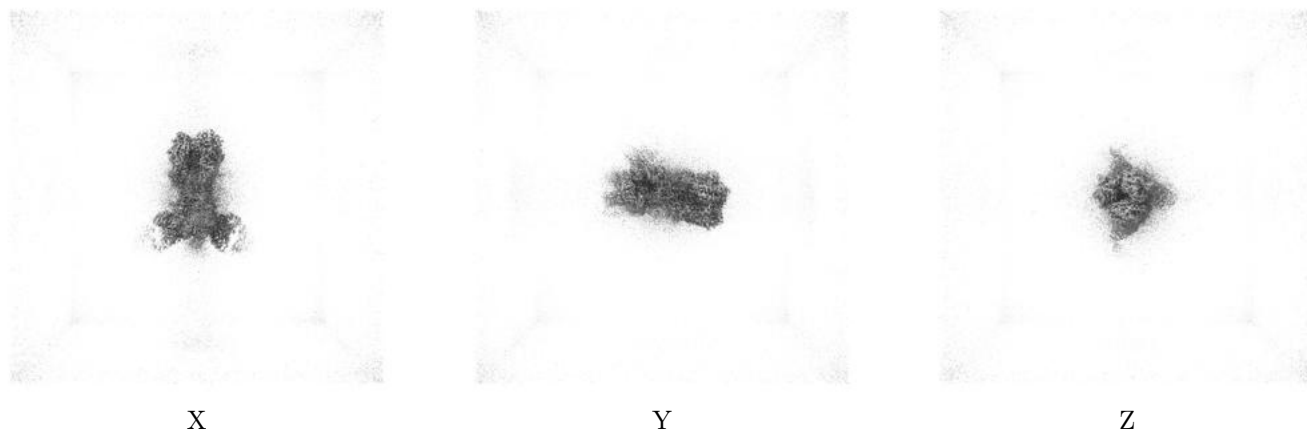
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.101. 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.

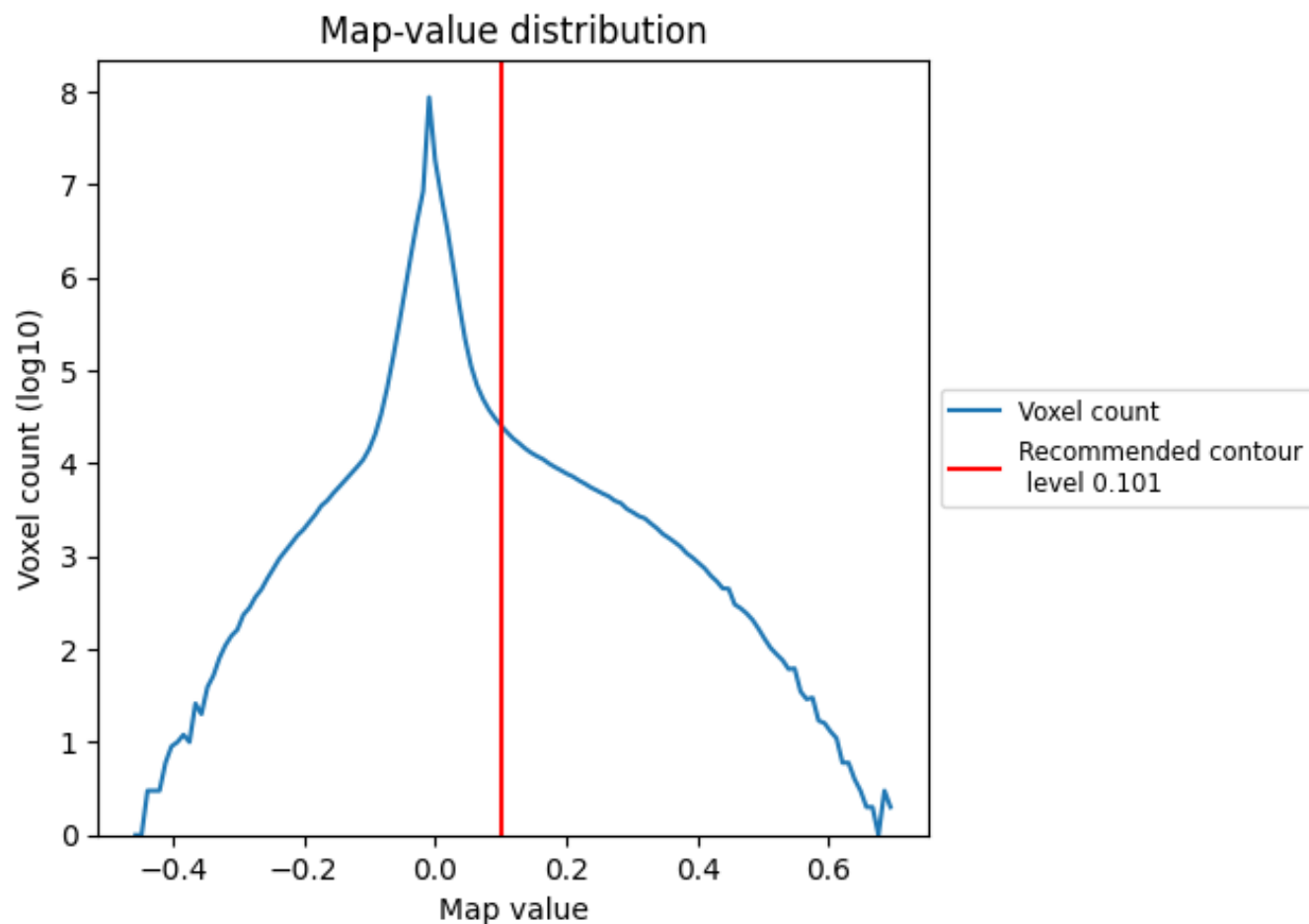
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

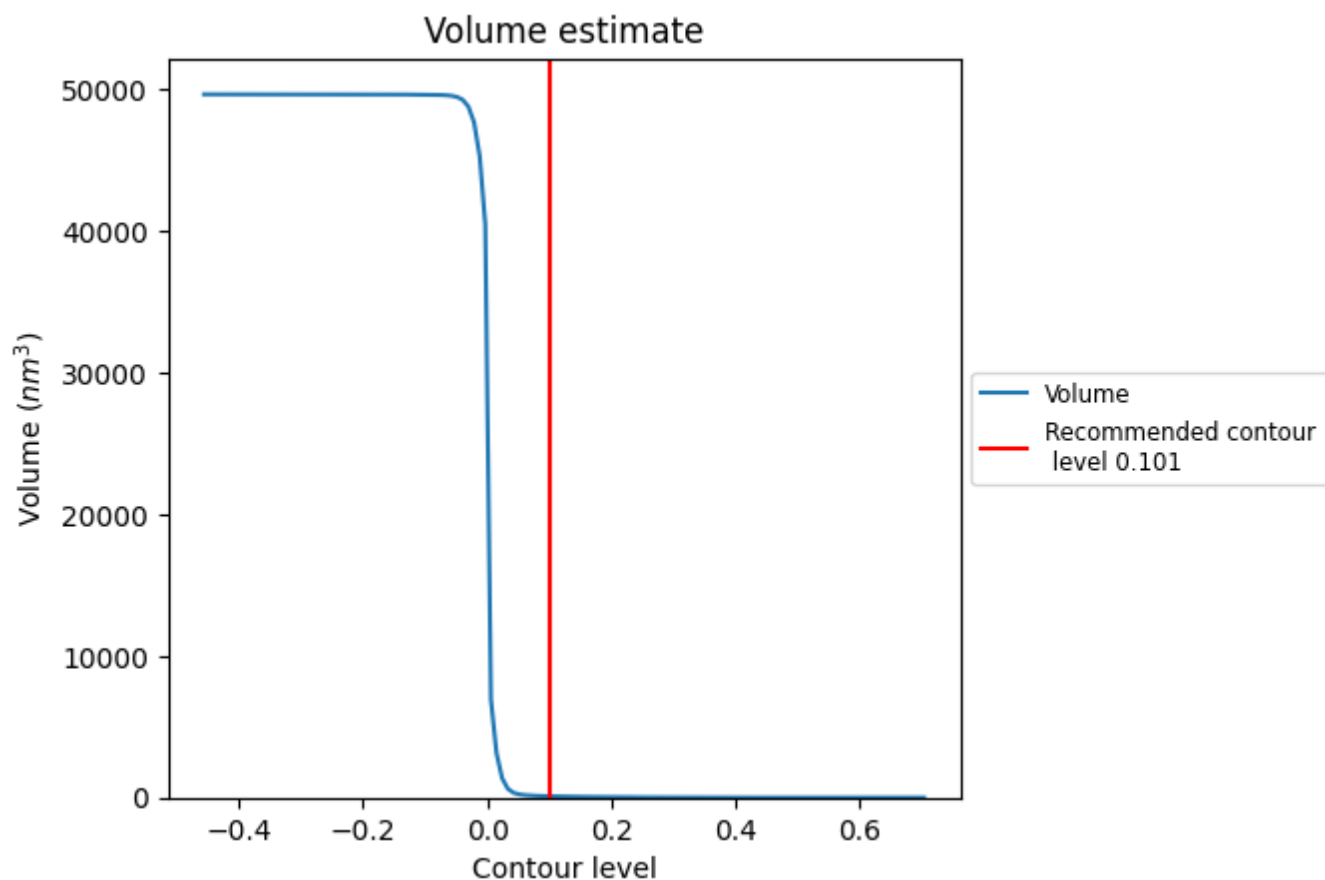
This section contains the results of statistical analysis of the map.

### 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](#)

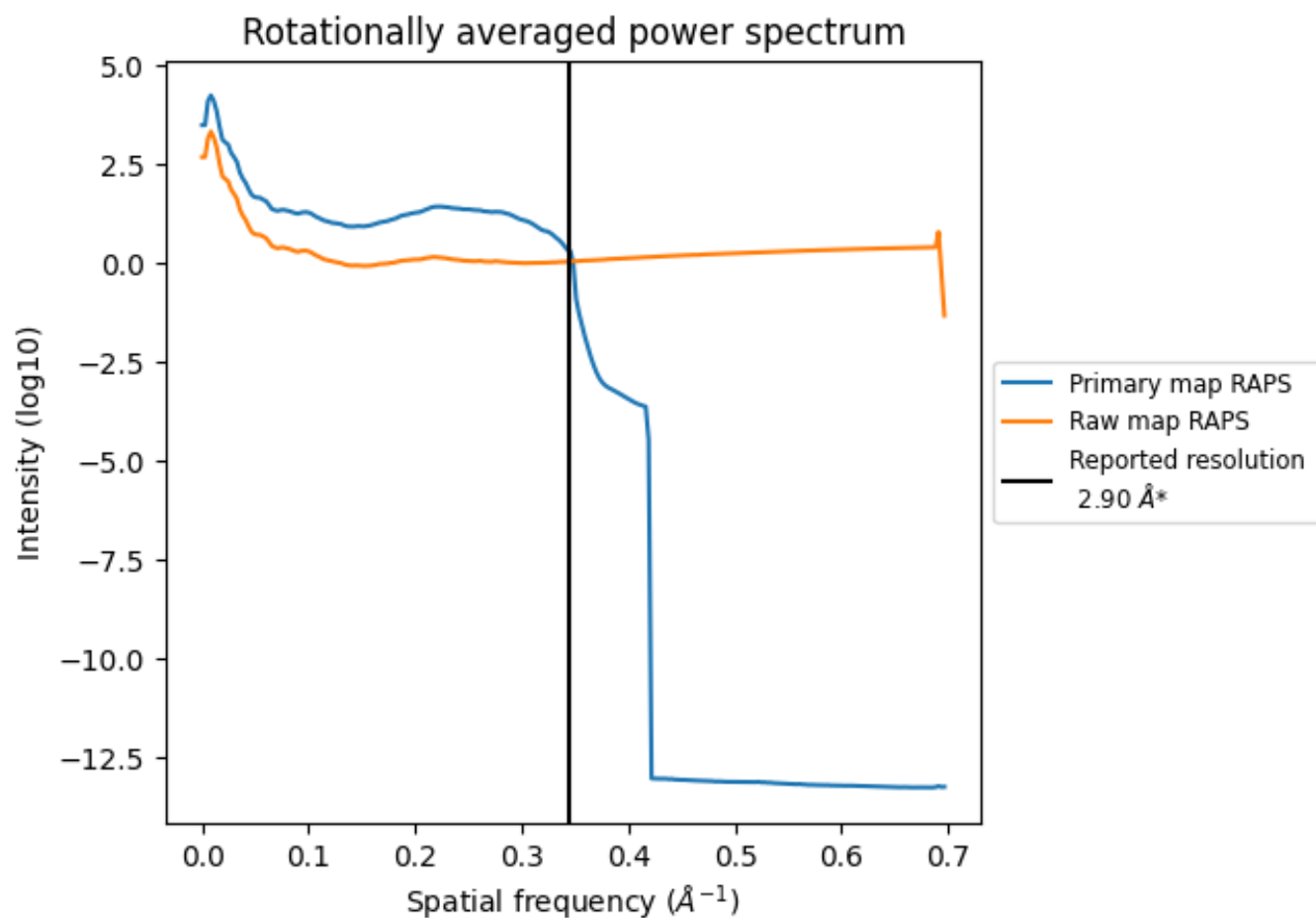


The volume at the recommended contour level is 90 nm<sup>3</sup>; this corresponds to an approximate mass of 82 kDa.

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 ⓘ

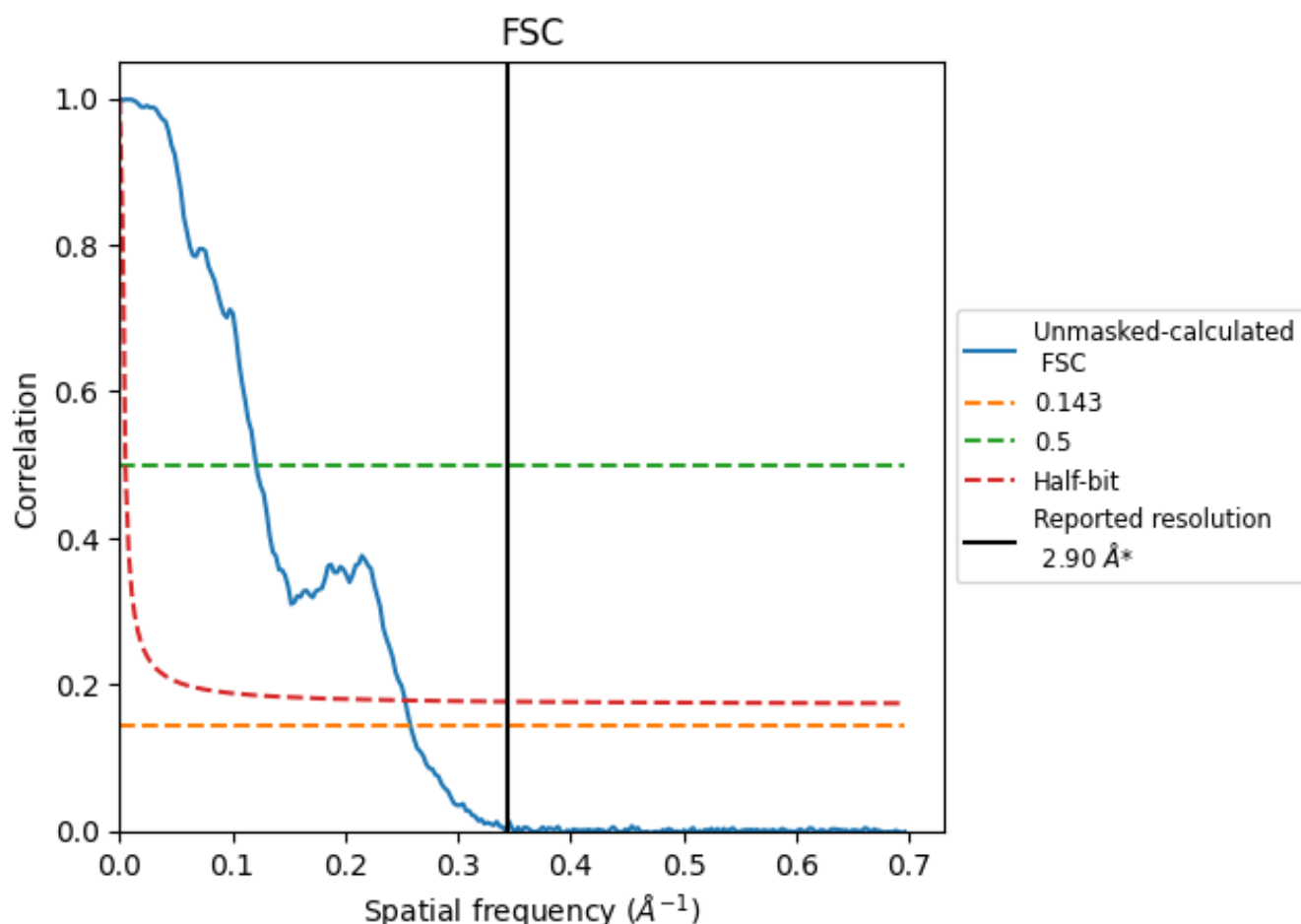


\*Reported resolution corresponds to spatial frequency of 0.345  $\text{\AA}^{-1}$

## 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 0.345 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

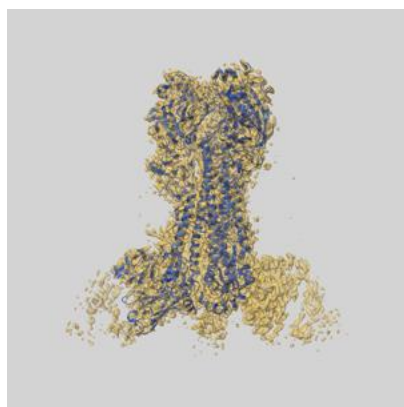
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.87	8.25	3.95

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.87 differs from the reported value 2.9 by more than 10 %

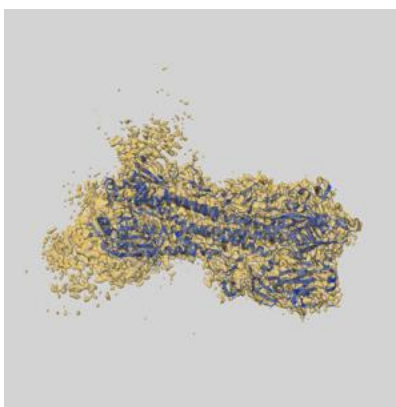
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-46994 and PDB model 9DM0. Per-residue inclusion information can be found in section 3 on page 12.

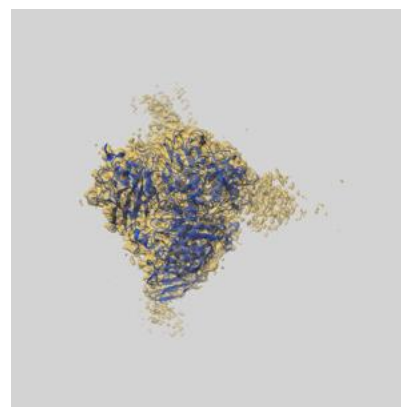
### 9.1 Map-model overlay [i](#)



X



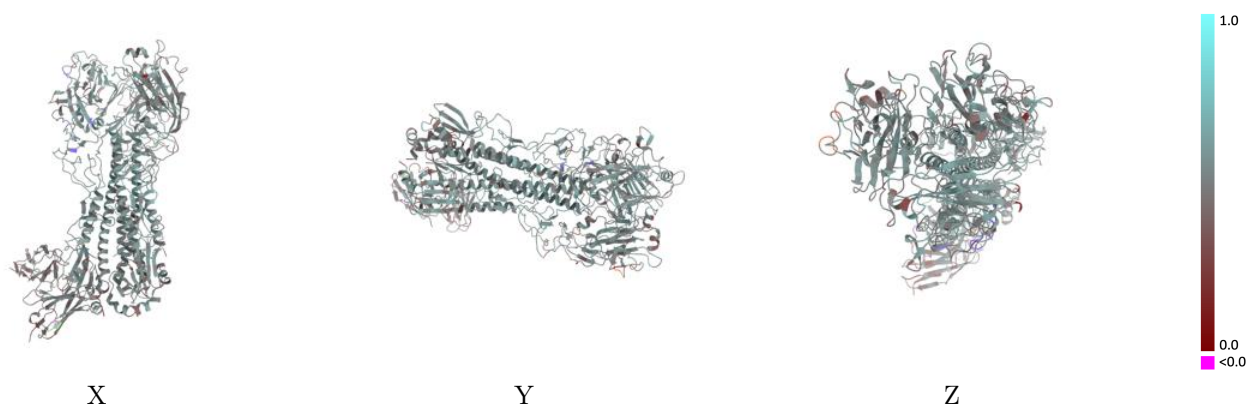
Y



Z

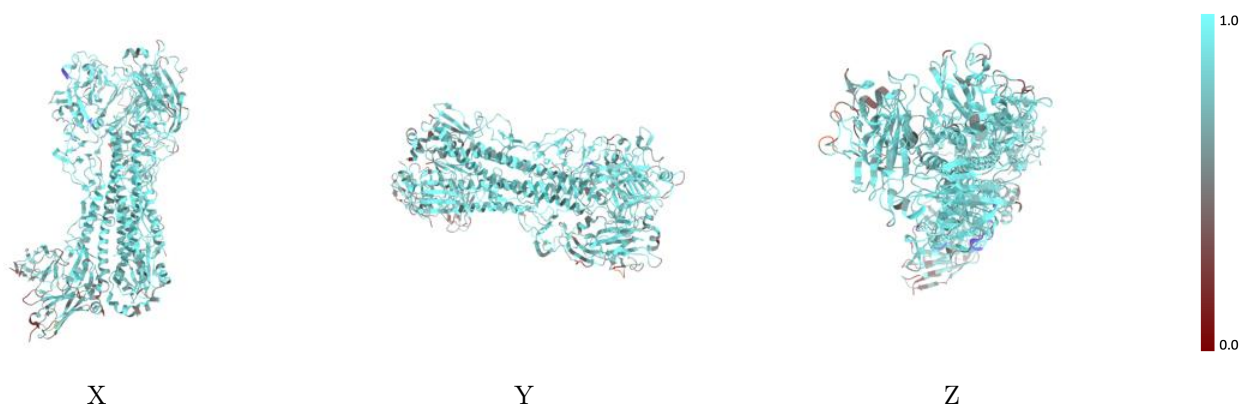
The images above show the 3D surface view of the map at the recommended contour level 0.101 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



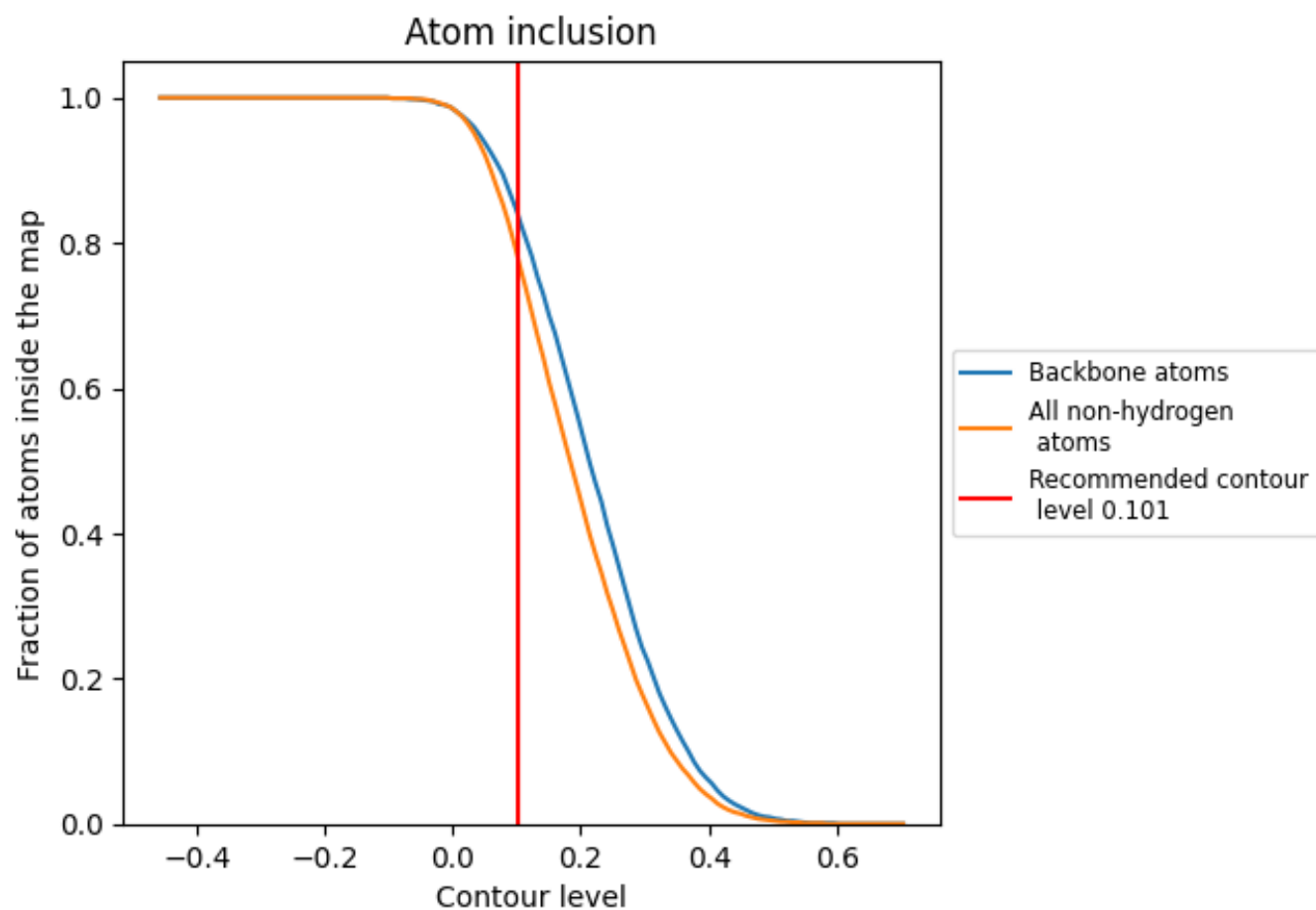
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.101).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.101) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7830	<div></div> 0.5110
A	<div></div> 0.8340	<div></div> 0.5320
B	<div></div> 0.7910	<div></div> 0.5180
C	<div></div> 0.6800	<div></div> 0.4640
D	<div></div> 0.6330	<div></div> 0.4170
E	<div></div> 0.7810	<div></div> 0.5140
F	<div></div> 0.7990	<div></div> 0.5190
G	<div></div> 0.8230	<div></div> 0.5290
I	<div></div> 0.7980	<div></div> 0.5190
S	<div></div> 0.5710	<div></div> 0.4460
T	<div></div> 0.3570	<div></div> 0.4360
U	<div></div> 0.5000	<div></div> 0.4390

1.0

0.0

<0.0