Full wwPDB EM Validation Report ⓘ

May 19, 2025 – 09:19 PM EDT

PDB ID	:	8U44 / pdb_00008u44
EMDB ID	:	EMD-41874
Title	:	CryoEM structure of A/Solomon Islands/3/2006 H1 HA in complex with 05.GC.w2.3C10-H1_SI06
Authors	:	Moore, N.; Han, J.; Ward, A.B.; Wilson, I.A.
Deposited on	:	2023-09-08
Resolution	:	3.41 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

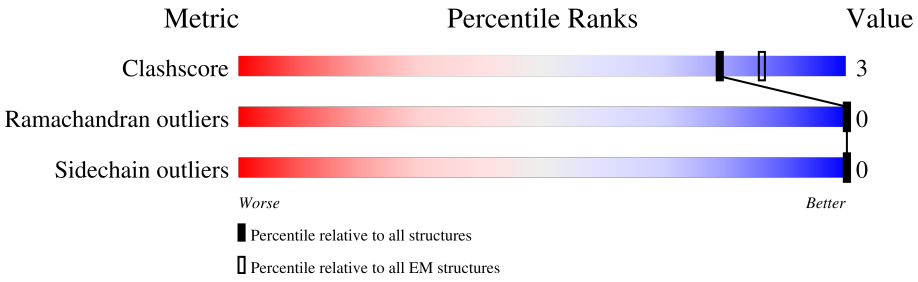
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.41 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 <=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	S	245	48% · 51%
1	U	245	49% · 51%
1	V	245	48% · 51%
2	T	235	43% · 54%
2	W	235	41% · 54%
2	X	235	41% · 54%
3	A	368	80% 8% 12%
3	G	368	80% 8% 12%

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Mol	Chain	Length	Quality of chain
3	H	368	
4	B	237	
4	I	237	
4	J	237	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17028 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 05.GC.w2.3C10-H1_SI06 Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	V	121	Total	C	N	O	S	0	0
			898	561	153	178	6		
1	S	121	Total	C	N	O	S	0	0
			898	561	153	178	6		
1	U	121	Total	C	N	O	S	0	0
			898	561	153	178	6		

- Molecule 2 is a protein called 05.GC.w2.3C10-H1_SI06 Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	X	107	Total	C	N	O	S	0	0
			815	510	138	164	3		
2	T	107	Total	C	N	O	S	0	0
			815	510	138	164	3		
2	W	107	Total	C	N	O	S	0	0
			815	510	138	164	3		

- Molecule 3 is a protein called Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	322	Total	C	N	O	S	0	0
			2527	1592	442	482	11		
3	G	322	Total	C	N	O	S	0	0
			2527	1592	442	482	11		
3	H	322	Total	C	N	O	S	0	0
			2527	1592	442	482	11		

There are 129 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-31	MET	-	initiating methionine	UNP A7Y8I1
A	-30	VAL	-	expression tag	UNP A7Y8I1
A	-29	LEU	-	expression tag	UNP A7Y8I1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-28	VAL	-	expression tag	UNP A7Y8I1
A	-27	ASN	-	expression tag	UNP A7Y8I1
A	-26	GLN	-	expression tag	UNP A7Y8I1
A	-25	SER	-	expression tag	UNP A7Y8I1
A	-24	HIS	-	expression tag	UNP A7Y8I1
A	-23	GLN	-	expression tag	UNP A7Y8I1
A	-22	GLY	-	expression tag	UNP A7Y8I1
A	-21	PHE	-	expression tag	UNP A7Y8I1
A	-20	ASN	-	expression tag	UNP A7Y8I1
A	-19	LYS	-	expression tag	UNP A7Y8I1
A	-18	GLU	-	expression tag	UNP A7Y8I1
A	-17	HIS	-	expression tag	UNP A7Y8I1
A	-16	THR	-	expression tag	UNP A7Y8I1
A	-15	SER	-	expression tag	UNP A7Y8I1
A	-14	LYS	-	expression tag	UNP A7Y8I1
A	-13	MET	-	expression tag	UNP A7Y8I1
A	-12	VAL	-	expression tag	UNP A7Y8I1
A	-11	SER	-	expression tag	UNP A7Y8I1
A	-10	ALA	-	expression tag	UNP A7Y8I1
A	-9	ILE	-	expression tag	UNP A7Y8I1
A	-8	VAL	-	expression tag	UNP A7Y8I1
A	-7	LEU	-	expression tag	UNP A7Y8I1
A	-6	TYR	-	expression tag	UNP A7Y8I1
A	-5	VAL	-	expression tag	UNP A7Y8I1
A	-4	LEU	-	expression tag	UNP A7Y8I1
A	-3	LEU	-	expression tag	UNP A7Y8I1
A	-2	ALA	-	expression tag	UNP A7Y8I1
A	-1	ALA	-	expression tag	UNP A7Y8I1
A	0	ALA	-	expression tag	UNP A7Y8I1
A	1	ALA	-	expression tag	UNP A7Y8I1
A	2	HIS	-	expression tag	UNP A7Y8I1
A	3	SER	-	expression tag	UNP A7Y8I1
A	4	ALA	-	expression tag	UNP A7Y8I1
A	5	PHE	-	expression tag	UNP A7Y8I1
A	6	ALA	-	expression tag	UNP A7Y8I1
A	7	ALA	-	expression tag	UNP A7Y8I1
A	8	ASP	-	expression tag	UNP A7Y8I1
A	9	PRO	-	expression tag	UNP A7Y8I1
A	10	GLY	-	expression tag	UNP A7Y8I1
A	53	ARG	LEU	conflict	UNP A7Y8I1
G	-31	MET	-	initiating methionine	UNP A7Y8I1
G	-30	VAL	-	expression tag	UNP A7Y8I1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-29	LEU	-	expression tag	UNP A7Y8I1
G	-28	VAL	-	expression tag	UNP A7Y8I1
G	-27	ASN	-	expression tag	UNP A7Y8I1
G	-26	GLN	-	expression tag	UNP A7Y8I1
G	-25	SER	-	expression tag	UNP A7Y8I1
G	-24	HIS	-	expression tag	UNP A7Y8I1
G	-23	GLN	-	expression tag	UNP A7Y8I1
G	-22	GLY	-	expression tag	UNP A7Y8I1
G	-21	PHE	-	expression tag	UNP A7Y8I1
G	-20	ASN	-	expression tag	UNP A7Y8I1
G	-19	LYS	-	expression tag	UNP A7Y8I1
G	-18	GLU	-	expression tag	UNP A7Y8I1
G	-17	HIS	-	expression tag	UNP A7Y8I1
G	-16	THR	-	expression tag	UNP A7Y8I1
G	-15	SER	-	expression tag	UNP A7Y8I1
G	-14	LYS	-	expression tag	UNP A7Y8I1
G	-13	MET	-	expression tag	UNP A7Y8I1
G	-12	VAL	-	expression tag	UNP A7Y8I1
G	-11	SER	-	expression tag	UNP A7Y8I1
G	-10	ALA	-	expression tag	UNP A7Y8I1
G	-9	ILE	-	expression tag	UNP A7Y8I1
G	-8	VAL	-	expression tag	UNP A7Y8I1
G	-7	LEU	-	expression tag	UNP A7Y8I1
G	-6	TYR	-	expression tag	UNP A7Y8I1
G	-5	VAL	-	expression tag	UNP A7Y8I1
G	-4	LEU	-	expression tag	UNP A7Y8I1
G	-3	LEU	-	expression tag	UNP A7Y8I1
G	-2	ALA	-	expression tag	UNP A7Y8I1
G	-1	ALA	-	expression tag	UNP A7Y8I1
G	0	ALA	-	expression tag	UNP A7Y8I1
G	1	ALA	-	expression tag	UNP A7Y8I1
G	2	HIS	-	expression tag	UNP A7Y8I1
G	3	SER	-	expression tag	UNP A7Y8I1
G	4	ALA	-	expression tag	UNP A7Y8I1
G	5	PHE	-	expression tag	UNP A7Y8I1
G	6	ALA	-	expression tag	UNP A7Y8I1
G	7	ALA	-	expression tag	UNP A7Y8I1
G	8	ASP	-	expression tag	UNP A7Y8I1
G	9	PRO	-	expression tag	UNP A7Y8I1
G	10	GLY	-	expression tag	UNP A7Y8I1
G	53	ARG	LEU	conflict	UNP A7Y8I1
H	-31	MET	-	initiating methionine	UNP A7Y8I1

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-30	VAL	-	expression tag	UNP A7Y8I1
H	-29	LEU	-	expression tag	UNP A7Y8I1
H	-28	VAL	-	expression tag	UNP A7Y8I1
H	-27	ASN	-	expression tag	UNP A7Y8I1
H	-26	GLN	-	expression tag	UNP A7Y8I1
H	-25	SER	-	expression tag	UNP A7Y8I1
H	-24	HIS	-	expression tag	UNP A7Y8I1
H	-23	GLN	-	expression tag	UNP A7Y8I1
H	-22	GLY	-	expression tag	UNP A7Y8I1
H	-21	PHE	-	expression tag	UNP A7Y8I1
H	-20	ASN	-	expression tag	UNP A7Y8I1
H	-19	LYS	-	expression tag	UNP A7Y8I1
H	-18	GLU	-	expression tag	UNP A7Y8I1
H	-17	HIS	-	expression tag	UNP A7Y8I1
H	-16	THR	-	expression tag	UNP A7Y8I1
H	-15	SER	-	expression tag	UNP A7Y8I1
H	-14	LYS	-	expression tag	UNP A7Y8I1
H	-13	MET	-	expression tag	UNP A7Y8I1
H	-12	VAL	-	expression tag	UNP A7Y8I1
H	-11	SER	-	expression tag	UNP A7Y8I1
H	-10	ALA	-	expression tag	UNP A7Y8I1
H	-9	ILE	-	expression tag	UNP A7Y8I1
H	-8	VAL	-	expression tag	UNP A7Y8I1
H	-7	LEU	-	expression tag	UNP A7Y8I1
H	-6	TYR	-	expression tag	UNP A7Y8I1
H	-5	VAL	-	expression tag	UNP A7Y8I1
H	-4	LEU	-	expression tag	UNP A7Y8I1
H	-3	LEU	-	expression tag	UNP A7Y8I1
H	-2	ALA	-	expression tag	UNP A7Y8I1
H	-1	ALA	-	expression tag	UNP A7Y8I1
H	0	ALA	-	expression tag	UNP A7Y8I1
H	1	ALA	-	expression tag	UNP A7Y8I1
H	2	HIS	-	expression tag	UNP A7Y8I1
H	3	SER	-	expression tag	UNP A7Y8I1
H	4	ALA	-	expression tag	UNP A7Y8I1
H	5	PHE	-	expression tag	UNP A7Y8I1
H	6	ALA	-	expression tag	UNP A7Y8I1
H	7	ALA	-	expression tag	UNP A7Y8I1
H	8	ASP	-	expression tag	UNP A7Y8I1
H	9	PRO	-	expression tag	UNP A7Y8I1
H	10	GLY	-	expression tag	UNP A7Y8I1
H	53	ARG	LEU	conflict	UNP A7Y8I1

- Molecule 4 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	173	Total	C	N	O	S	0	0
			1394	874	238	275	7		
4	I	173	Total	C	N	O	S	0	0
			1394	874	238	275	7		
4	J	173	Total	C	N	O	S	0	0
			1394	874	238	275	7		

There are 189 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	expression tag	UNP A7Y8I1
B	176	GLY	-	expression tag	UNP A7Y8I1
B	177	GLY	-	expression tag	UNP A7Y8I1
B	178	GLY	-	expression tag	UNP A7Y8I1
B	179	GLY	-	expression tag	UNP A7Y8I1
B	180	LEU	-	expression tag	UNP A7Y8I1
B	181	ASN	-	expression tag	UNP A7Y8I1
B	182	ASP	-	expression tag	UNP A7Y8I1
B	183	ILE	-	expression tag	UNP A7Y8I1
B	184	PHE	-	expression tag	UNP A7Y8I1
B	185	GLU	-	expression tag	UNP A7Y8I1
B	186	ALA	-	expression tag	UNP A7Y8I1
B	187	GLN	-	expression tag	UNP A7Y8I1
B	188	LYS	-	expression tag	UNP A7Y8I1
B	189	ILE	-	expression tag	UNP A7Y8I1
B	190	GLU	-	expression tag	UNP A7Y8I1
B	191	TRP	-	expression tag	UNP A7Y8I1
B	192	HIS	-	expression tag	UNP A7Y8I1
B	193	GLU	-	expression tag	UNP A7Y8I1
B	194	ARG	-	expression tag	UNP A7Y8I1
B	195	LEU	-	expression tag	UNP A7Y8I1
B	196	VAL	-	expression tag	UNP A7Y8I1
B	197	PRO	-	expression tag	UNP A7Y8I1
B	198	ARG	-	expression tag	UNP A7Y8I1
B	199	GLY	-	expression tag	UNP A7Y8I1
B	200	SER	-	expression tag	UNP A7Y8I1
B	201	PRO	-	expression tag	UNP A7Y8I1
B	202	GLY	-	expression tag	UNP A7Y8I1
B	203	SER	-	expression tag	UNP A7Y8I1
B	204	GLY	-	expression tag	UNP A7Y8I1
B	205	TYR	-	expression tag	UNP A7Y8I1
B	206	ILE	-	expression tag	UNP A7Y8I1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	207	PRO	-	expression tag	UNP A7Y8I1
B	208	GLU	-	expression tag	UNP A7Y8I1
B	209	ALA	-	expression tag	UNP A7Y8I1
B	210	PRO	-	expression tag	UNP A7Y8I1
B	211	ARG	-	expression tag	UNP A7Y8I1
B	212	ASP	-	expression tag	UNP A7Y8I1
B	213	GLY	-	expression tag	UNP A7Y8I1
B	214	GLN	-	expression tag	UNP A7Y8I1
B	215	ALA	-	expression tag	UNP A7Y8I1
B	216	TYR	-	expression tag	UNP A7Y8I1
B	217	VAL	-	expression tag	UNP A7Y8I1
B	218	ARG	-	expression tag	UNP A7Y8I1
B	219	LYS	-	expression tag	UNP A7Y8I1
B	220	ASP	-	expression tag	UNP A7Y8I1
B	221	GLY	-	expression tag	UNP A7Y8I1
B	222	GLU	-	expression tag	UNP A7Y8I1
B	223	TRP	-	expression tag	UNP A7Y8I1
B	224	VAL	-	expression tag	UNP A7Y8I1
B	225	LEU	-	expression tag	UNP A7Y8I1
B	226	LEU	-	expression tag	UNP A7Y8I1
B	227	SER	-	expression tag	UNP A7Y8I1
B	228	THR	-	expression tag	UNP A7Y8I1
B	229	PHE	-	expression tag	UNP A7Y8I1
B	230	LEU	-	expression tag	UNP A7Y8I1
B	231	GLY	-	expression tag	UNP A7Y8I1
B	232	HIS	-	expression tag	UNP A7Y8I1
B	233	HIS	-	expression tag	UNP A7Y8I1
B	234	HIS	-	expression tag	UNP A7Y8I1
B	235	HIS	-	expression tag	UNP A7Y8I1
B	236	HIS	-	expression tag	UNP A7Y8I1
B	237	HIS	-	expression tag	UNP A7Y8I1
I	175	SER	-	expression tag	UNP A7Y8I1
I	176	GLY	-	expression tag	UNP A7Y8I1
I	177	GLY	-	expression tag	UNP A7Y8I1
I	178	GLY	-	expression tag	UNP A7Y8I1
I	179	GLY	-	expression tag	UNP A7Y8I1
I	180	LEU	-	expression tag	UNP A7Y8I1
I	181	ASN	-	expression tag	UNP A7Y8I1
I	182	ASP	-	expression tag	UNP A7Y8I1
I	183	ILE	-	expression tag	UNP A7Y8I1
I	184	PHE	-	expression tag	UNP A7Y8I1
I	185	GLU	-	expression tag	UNP A7Y8I1

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Chain	Residue	Modelled	Actual	Comment	Reference
I	186	ALA	-	expression tag	UNP A7Y8I1
I	187	GLN	-	expression tag	UNP A7Y8I1
I	188	LYS	-	expression tag	UNP A7Y8I1
I	189	ILE	-	expression tag	UNP A7Y8I1
I	190	GLU	-	expression tag	UNP A7Y8I1
I	191	TRP	-	expression tag	UNP A7Y8I1
I	192	HIS	-	expression tag	UNP A7Y8I1
I	193	GLU	-	expression tag	UNP A7Y8I1
I	194	ARG	-	expression tag	UNP A7Y8I1
I	195	LEU	-	expression tag	UNP A7Y8I1
I	196	VAL	-	expression tag	UNP A7Y8I1
I	197	PRO	-	expression tag	UNP A7Y8I1
I	198	ARG	-	expression tag	UNP A7Y8I1
I	199	GLY	-	expression tag	UNP A7Y8I1
I	200	SER	-	expression tag	UNP A7Y8I1
I	201	PRO	-	expression tag	UNP A7Y8I1
I	202	GLY	-	expression tag	UNP A7Y8I1
I	203	SER	-	expression tag	UNP A7Y8I1
I	204	GLY	-	expression tag	UNP A7Y8I1
I	205	TYR	-	expression tag	UNP A7Y8I1
I	206	ILE	-	expression tag	UNP A7Y8I1
I	207	PRO	-	expression tag	UNP A7Y8I1
I	208	GLU	-	expression tag	UNP A7Y8I1
I	209	ALA	-	expression tag	UNP A7Y8I1
I	210	PRO	-	expression tag	UNP A7Y8I1
I	211	ARG	-	expression tag	UNP A7Y8I1
I	212	ASP	-	expression tag	UNP A7Y8I1
I	213	GLY	-	expression tag	UNP A7Y8I1
I	214	GLN	-	expression tag	UNP A7Y8I1
I	215	ALA	-	expression tag	UNP A7Y8I1
I	216	TYR	-	expression tag	UNP A7Y8I1
I	217	VAL	-	expression tag	UNP A7Y8I1
I	218	ARG	-	expression tag	UNP A7Y8I1
I	219	LYS	-	expression tag	UNP A7Y8I1
I	220	ASP	-	expression tag	UNP A7Y8I1
I	221	GLY	-	expression tag	UNP A7Y8I1
I	222	GLU	-	expression tag	UNP A7Y8I1
I	223	TRP	-	expression tag	UNP A7Y8I1
I	224	VAL	-	expression tag	UNP A7Y8I1
I	225	LEU	-	expression tag	UNP A7Y8I1
I	226	LEU	-	expression tag	UNP A7Y8I1
I	227	SER	-	expression tag	UNP A7Y8I1

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Chain	Residue	Modelled	Actual	Comment	Reference
I	228	THR	-	expression tag	UNP A7Y8I1
I	229	PHE	-	expression tag	UNP A7Y8I1
I	230	LEU	-	expression tag	UNP A7Y8I1
I	231	GLY	-	expression tag	UNP A7Y8I1
I	232	HIS	-	expression tag	UNP A7Y8I1
I	233	HIS	-	expression tag	UNP A7Y8I1
I	234	HIS	-	expression tag	UNP A7Y8I1
I	235	HIS	-	expression tag	UNP A7Y8I1
I	236	HIS	-	expression tag	UNP A7Y8I1
I	237	HIS	-	expression tag	UNP A7Y8I1
J	175	SER	-	expression tag	UNP A7Y8I1
J	176	GLY	-	expression tag	UNP A7Y8I1
J	177	GLY	-	expression tag	UNP A7Y8I1
J	178	GLY	-	expression tag	UNP A7Y8I1
J	179	GLY	-	expression tag	UNP A7Y8I1
J	180	LEU	-	expression tag	UNP A7Y8I1
J	181	ASN	-	expression tag	UNP A7Y8I1
J	182	ASP	-	expression tag	UNP A7Y8I1
J	183	ILE	-	expression tag	UNP A7Y8I1
J	184	PHE	-	expression tag	UNP A7Y8I1
J	185	GLU	-	expression tag	UNP A7Y8I1
J	186	ALA	-	expression tag	UNP A7Y8I1
J	187	GLN	-	expression tag	UNP A7Y8I1
J	188	LYS	-	expression tag	UNP A7Y8I1
J	189	ILE	-	expression tag	UNP A7Y8I1
J	190	GLU	-	expression tag	UNP A7Y8I1
J	191	TRP	-	expression tag	UNP A7Y8I1
J	192	HIS	-	expression tag	UNP A7Y8I1
J	193	GLU	-	expression tag	UNP A7Y8I1
J	194	ARG	-	expression tag	UNP A7Y8I1
J	195	LEU	-	expression tag	UNP A7Y8I1
J	196	VAL	-	expression tag	UNP A7Y8I1
J	197	PRO	-	expression tag	UNP A7Y8I1
J	198	ARG	-	expression tag	UNP A7Y8I1
J	199	GLY	-	expression tag	UNP A7Y8I1
J	200	SER	-	expression tag	UNP A7Y8I1
J	201	PRO	-	expression tag	UNP A7Y8I1
J	202	GLY	-	expression tag	UNP A7Y8I1
J	203	SER	-	expression tag	UNP A7Y8I1
J	204	GLY	-	expression tag	UNP A7Y8I1
J	205	TYR	-	expression tag	UNP A7Y8I1
J	206	ILE	-	expression tag	UNP A7Y8I1

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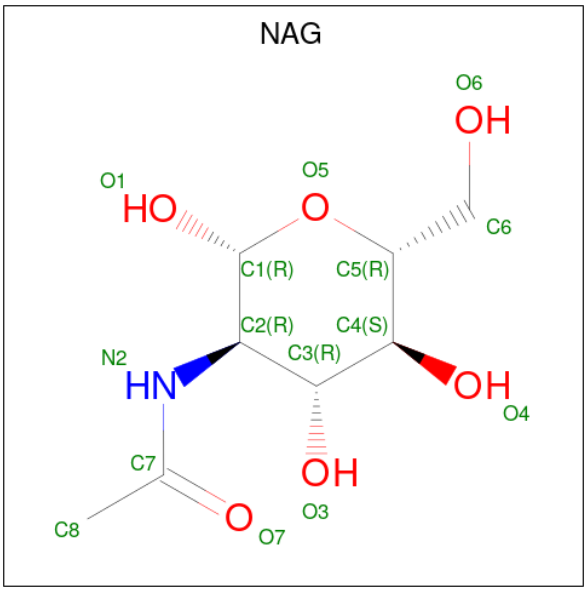
Chain	Residue	Modelled	Actual	Comment	Reference
J	207	PRO	-	expression tag	UNP A7Y8I1
J	208	GLU	-	expression tag	UNP A7Y8I1
J	209	ALA	-	expression tag	UNP A7Y8I1
J	210	PRO	-	expression tag	UNP A7Y8I1
J	211	ARG	-	expression tag	UNP A7Y8I1
J	212	ASP	-	expression tag	UNP A7Y8I1
J	213	GLY	-	expression tag	UNP A7Y8I1
J	214	GLN	-	expression tag	UNP A7Y8I1
J	215	ALA	-	expression tag	UNP A7Y8I1
J	216	TYR	-	expression tag	UNP A7Y8I1
J	217	VAL	-	expression tag	UNP A7Y8I1
J	218	ARG	-	expression tag	UNP A7Y8I1
J	219	LYS	-	expression tag	UNP A7Y8I1
J	220	ASP	-	expression tag	UNP A7Y8I1
J	221	GLY	-	expression tag	UNP A7Y8I1
J	222	GLU	-	expression tag	UNP A7Y8I1
J	223	TRP	-	expression tag	UNP A7Y8I1
J	224	VAL	-	expression tag	UNP A7Y8I1
J	225	LEU	-	expression tag	UNP A7Y8I1
J	226	LEU	-	expression tag	UNP A7Y8I1
J	227	SER	-	expression tag	UNP A7Y8I1
J	228	THR	-	expression tag	UNP A7Y8I1
J	229	PHE	-	expression tag	UNP A7Y8I1
J	230	LEU	-	expression tag	UNP A7Y8I1
J	231	GLY	-	expression tag	UNP A7Y8I1
J	232	HIS	-	expression tag	UNP A7Y8I1
J	233	HIS	-	expression tag	UNP A7Y8I1
J	234	HIS	-	expression tag	UNP A7Y8I1
J	235	HIS	-	expression tag	UNP A7Y8I1
J	236	HIS	-	expression tag	UNP A7Y8I1
J	237	HIS	-	expression tag	UNP A7Y8I1

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



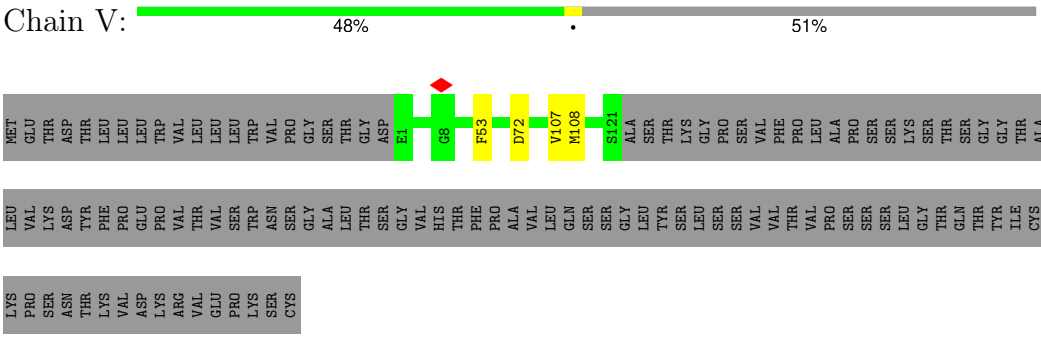
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	
5	H	1	Total	C	N	O	0
			14	8	1	5	
5	H	1	Total	C	N	O	0
			14	8	1	5	
5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

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.

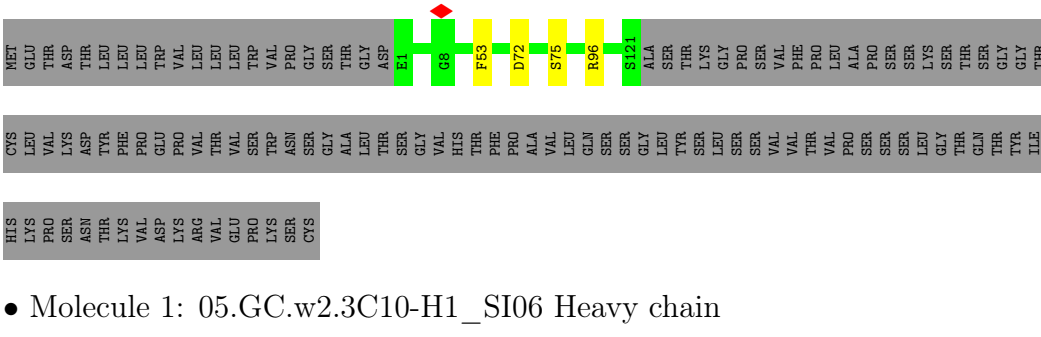
• Molecule 1: 05.GC.w2.3C10-H1_SI06 Heavy chain

Chain V:



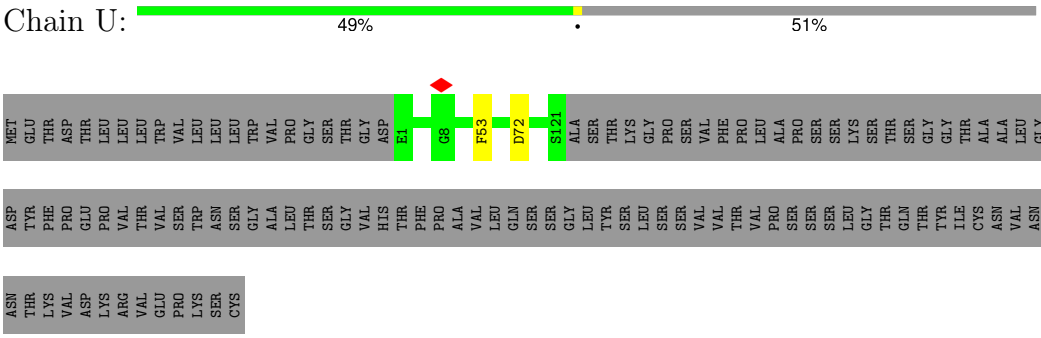
• Molecule 1: 05.GC.w2.3C10-H1_SI06 Heavy chain

Chain S:



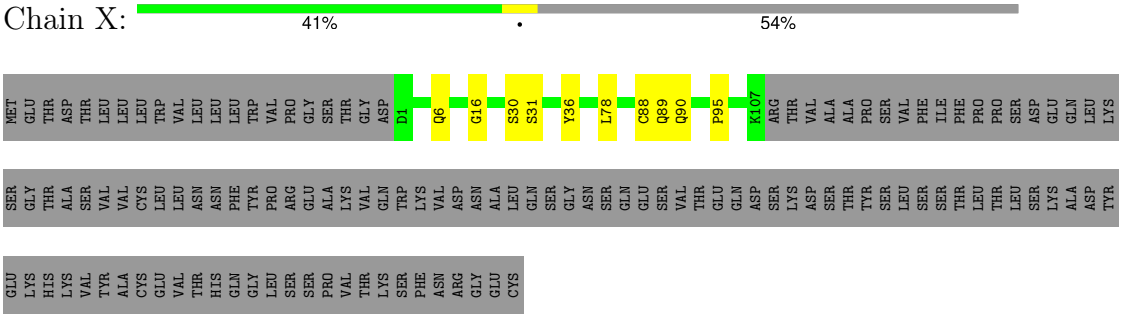
• Molecule 1: 05.GC.w2.3C10-H1_SI06 Heavy chain

Chain U:



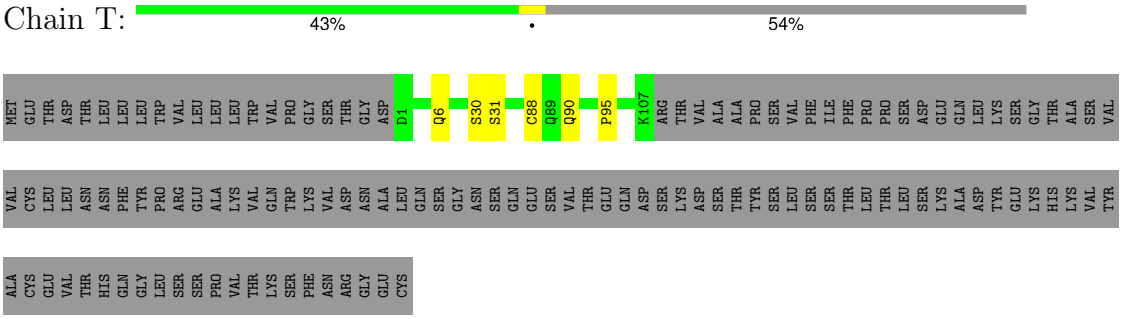
• Molecule 2: 05.GC.w2.3C10-H1_SI06 Light chain

Chain X:



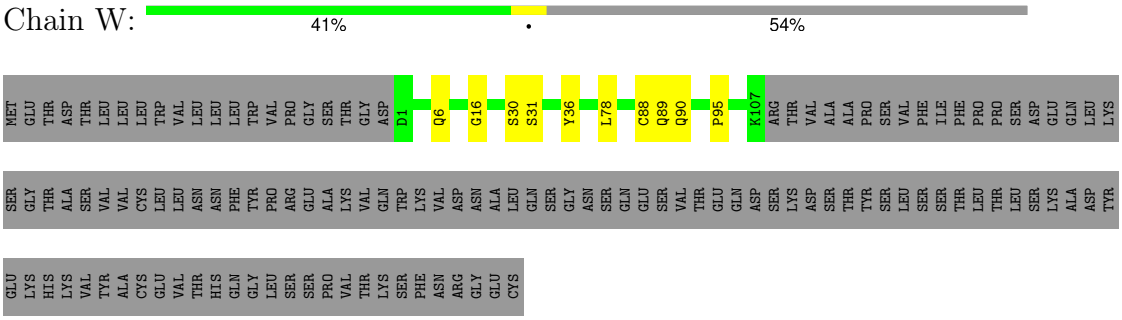
• Molecule 2: 05.GC.w2.3C10-H1_SI06 Light chain

Chain T:



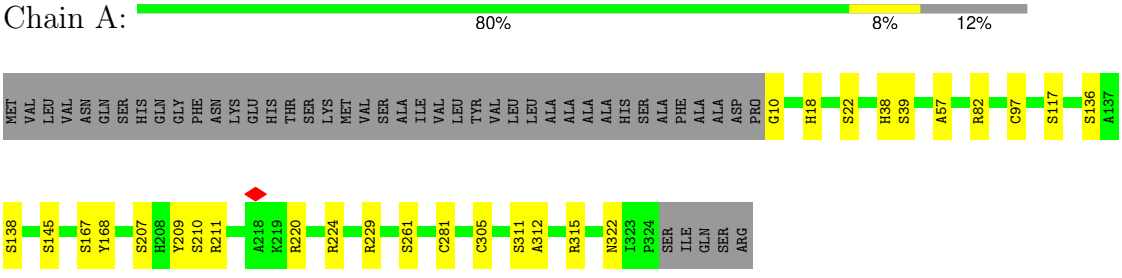
• Molecule 2: 05.GC.w2.3C10-H1_SI06 Light chain

Chain W:



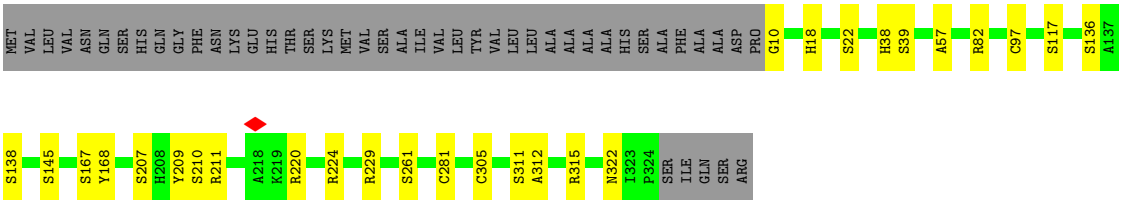
• Molecule 3: Hemagglutinin HA1 chain

Chain A:

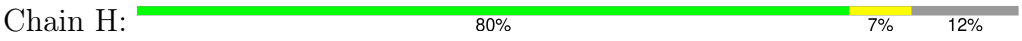


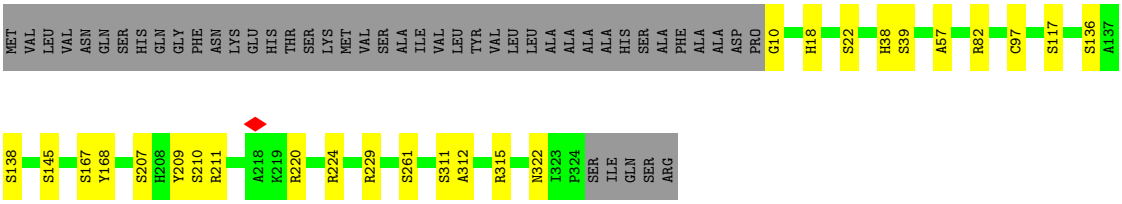
• Molecule 3: Hemagglutinin HA1 chain

Chain G:

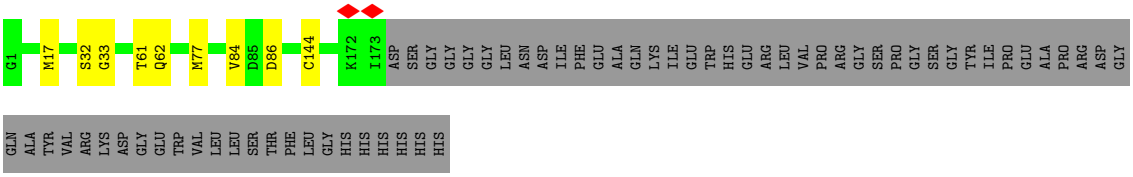


• Molecule 3: Hemagglutinin HA1 chain

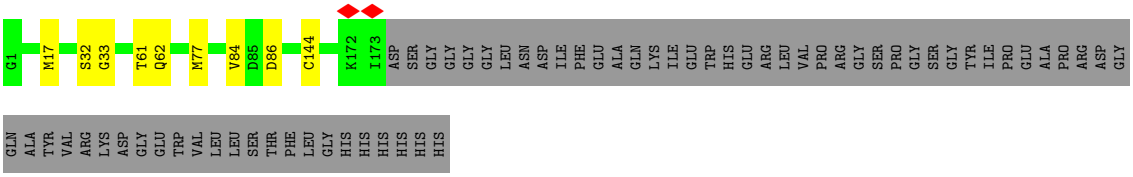




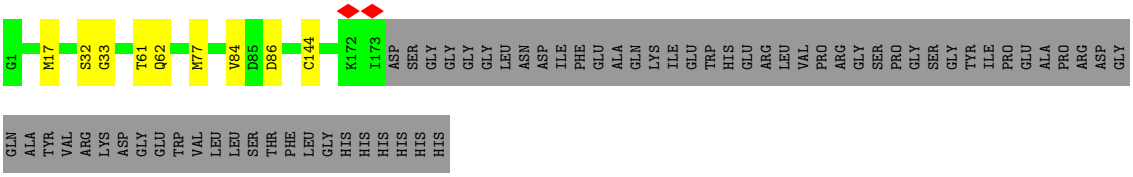
• Molecule 4: Hemagglutinin HA2 chain



• Molecule 4: Hemagglutinin HA2 chain



• Molecule 4: Hemagglutinin HA2 chain



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	53000	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.988	Depositor
Minimum map value	-0.343	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	300.96, 300.96, 300.96	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	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	S	0.27	0/915	0.58	0/1240
1	U	0.27	0/915	0.58	0/1240
1	V	0.27	0/915	0.58	0/1240
2	T	0.24	0/833	0.53	0/1129
2	W	0.24	0/833	0.53	0/1129
2	X	0.24	0/833	0.53	0/1129
3	A	0.24	0/2593	0.52	0/3527
3	G	0.24	0/2593	0.52	0/3527
3	H	0.24	0/2593	0.52	0/3527
4	B	0.27	0/1421	0.57	0/1909
4	I	0.27	0/1421	0.57	0/1909
4	J	0.27	0/1421	0.57	0/1909
All	All	0.25	0/17286	0.54	0/23415

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	S	898	0	877	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	898	0	877	2	0
1	V	898	0	877	3	0
2	T	815	0	795	3	0
2	W	815	0	795	5	0
2	X	815	0	795	5	0
3	A	2527	0	2438	22	0
3	G	2527	0	2438	22	0
3	H	2527	0	2438	21	0
4	B	1394	0	1327	10	0
4	I	1394	0	1327	10	0
4	J	1394	0	1327	10	0
5	A	42	0	39	0	0
5	G	42	0	39	0	0
5	H	42	0	39	0	0
All	All	17028	0	16428	86	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 3.

All (86) 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:77:MET:HE1	4:I:77:MET:SD	2.10	0.92
4:I:77:MET:HE1	4:J:77:MET:SD	2.10	0.92
4:B:77:MET:SD	4:J:77:MET:HE1	2.10	0.91
4:I:86:ASP:OD2	4:J:62:GLN:HG3	1.78	0.84
4:B:62:GLN:HG3	4:J:86:ASP:OD2	1.78	0.83
4:B:86:ASP:OD2	4:I:62:GLN:HG3	1.78	0.83
2:W:90:GLN:NE2	2:W:95:PRO:O	2.17	0.78
2:X:90:GLN:NE2	2:X:95:PRO:O	2.17	0.77
2:T:90:GLN:NE2	2:T:95:PRO:O	2.17	0.76
2:T:6:GLN:NE2	2:T:88:CYS:SG	2.62	0.72
2:W:6:GLN:NE2	2:W:88:CYS:SG	2.62	0.72
2:X:6:GLN:NE2	2:X:88:CYS:SG	2.62	0.72
3:H:22:SER:O	3:H:322:ASN:ND2	2.23	0.72
3:A:22:SER:O	3:A:322:ASN:ND2	2.23	0.71
3:G:22:SER:O	3:G:322:ASN:ND2	2.23	0.71
3:H:57:ALA:O	3:H:82:ARG:NH2	2.25	0.69
3:A:57:ALA:O	3:A:82:ARG:NH2	2.25	0.69
3:G:57:ALA:O	3:G:82:ARG:NH2	2.25	0.69
3:A:207:SER:HA	3:H:229:ARG:NH2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:229:ARG:NH2	3:G:207:SER:HA	2.22	0.54
3:G:229:ARG:NH2	3:H:207:SER:HA	2.22	0.54
3:G:10:GLY:N	4:I:144:CYS:O	2.41	0.53
3:A:10:GLY:N	4:B:144:CYS:O	2.41	0.53
3:H:10:GLY:N	4:J:144:CYS:O	2.41	0.53
3:G:209:TYR:OH	3:G:211:ARG:NH2	2.44	0.50
4:J:32:SER:OG	4:J:33:GLY:N	2.44	0.50
3:A:209:TYR:OH	3:A:211:ARG:NH2	2.44	0.50
4:I:32:SER:OG	4:I:33:GLY:N	2.44	0.50
4:B:32:SER:OG	4:B:33:GLY:N	2.44	0.49
3:H:209:TYR:OH	3:H:211:ARG:NH2	2.44	0.49
3:A:229:ARG:HH21	3:G:207:SER:HA	1.77	0.49
2:W:30:SER:OG	2:W:31:SER:N	2.45	0.49
3:G:229:ARG:HH21	3:H:207:SER:HA	1.77	0.49
3:A:207:SER:HA	3:H:229:ARG:HH21	1.77	0.48
3:G:167:SER:OG	3:G:168:TYR:N	2.46	0.48
3:H:167:SER:OG	3:H:168:TYR:N	2.46	0.48
3:A:210:SER:OG	3:H:220:ARG:CZ	2.62	0.48
3:G:220:ARG:CZ	3:H:210:SER:OG	2.62	0.48
3:A:18:HIS:ND1	4:B:17:MET:O	2.46	0.48
3:A:220:ARG:CZ	3:G:210:SER:OG	2.62	0.48
2:T:30:SER:OG	2:T:31:SER:N	2.45	0.47
3:H:39:SER:OG	3:H:315:ARG:NE	2.47	0.47
4:B:61:THR:O	4:B:62:GLN:NE2	2.46	0.47
3:G:39:SER:OG	3:G:315:ARG:NE	2.47	0.47
3:A:39:SER:OG	3:A:315:ARG:NE	2.47	0.47
4:J:61:THR:O	4:J:62:GLN:NE2	2.46	0.47
4:B:84:VAL:HG11	4:J:84:VAL:HG22	1.97	0.47
3:G:18:HIS:ND1	4:I:17:MET:O	2.46	0.47
1:V:53:PHE:O	3:A:38:HIS:ND1	2.49	0.46
1:S:53:PHE:O	3:G:38:HIS:ND1	2.49	0.46
1:S:72:ASP:N	1:S:72:ASP:OD1	2.49	0.46
3:A:167:SER:OG	3:A:168:TYR:N	2.46	0.46
4:B:84:VAL:HG22	4:I:84:VAL:HG11	1.97	0.46
1:U:72:ASP:OD1	1:U:72:ASP:N	2.49	0.46
4:I:84:VAL:HG22	4:J:84:VAL:HG11	1.97	0.46
3:H:18:HIS:ND1	4:J:17:MET:O	2.46	0.46
1:V:72:ASP:OD1	1:V:72:ASP:N	2.48	0.46
1:U:53:PHE:O	3:H:38:HIS:ND1	2.49	0.46
3:G:281:CYS:HB2	3:G:305:CYS:HB2	1.82	0.45
3:H:97:CYS:O	3:H:138:SER:OG	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:61:THR:O	4:I:62:GLN:NE2	2.46	0.45
3:A:311:SER:OG	3:A:312:ALA:N	2.50	0.45
3:A:97:CYS:O	3:A:138:SER:OG	2.34	0.45
2:X:30:SER:OG	2:X:31:SER:N	2.45	0.45
3:A:220:ARG:NE	3:G:210:SER:OG	2.50	0.45
3:H:311:SER:OG	3:H:312:ALA:N	2.50	0.45
3:G:311:SER:OG	3:G:312:ALA:N	2.50	0.44
3:H:117:SER:N	3:H:261:SER:OG	2.47	0.44
3:A:210:SER:OG	3:H:220:ARG:NE	2.50	0.44
3:G:220:ARG:NE	3:H:210:SER:OG	2.50	0.44
3:G:117:SER:N	3:G:261:SER:OG	2.47	0.44
3:G:97:CYS:O	3:G:138:SER:OG	2.34	0.43
2:X:36:TYR:OH	2:X:89:GLN:OE1	2.32	0.43
3:A:117:SER:N	3:A:261:SER:OG	2.47	0.43
3:G:138:SER:OG	3:G:224:ARG:NH1	2.52	0.42
3:H:138:SER:OG	3:H:224:ARG:NH1	2.52	0.42
2:W:36:TYR:OH	2:W:89:GLN:OE1	2.32	0.42
3:A:138:SER:OG	3:A:224:ARG:NH1	2.52	0.42
3:H:136:SER:N	3:H:145:SER:OG	2.53	0.41
3:G:136:SER:N	3:G:145:SER:OG	2.53	0.41
2:X:16:GLY:N	2:X:78:LEU:O	2.54	0.41
3:A:281:CYS:HB2	3:A:305:CYS:HB2	1.82	0.41
2:W:16:GLY:N	2:W:78:LEU:O	2.54	0.41
3:A:136:SER:N	3:A:145:SER:OG	2.53	0.40
1:V:107:VAL:HG12	1:V:108:MET:H	1.87	0.40
1:S:75:SER:O	1:S:96:ARG:NH2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	119/245 (49%)	112 (94%)	7 (6%)	0	100	100
1	U	119/245 (49%)	112 (94%)	7 (6%)	0	100	100
1	V	119/245 (49%)	112 (94%)	7 (6%)	0	100	100
2	T	105/235 (45%)	101 (96%)	4 (4%)	0	100	100
2	W	105/235 (45%)	101 (96%)	4 (4%)	0	100	100
2	X	105/235 (45%)	101 (96%)	4 (4%)	0	100	100
3	A	320/368 (87%)	306 (96%)	14 (4%)	0	100	100
3	G	320/368 (87%)	306 (96%)	14 (4%)	0	100	100
3	H	320/368 (87%)	306 (96%)	14 (4%)	0	100	100
4	B	171/237 (72%)	156 (91%)	15 (9%)	0	100	100
4	I	171/237 (72%)	155 (91%)	16 (9%)	0	100	100
4	J	171/237 (72%)	155 (91%)	16 (9%)	0	100	100
All	All	2145/3255 (66%)	2023 (94%)	122 (6%)	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	S	95/203 (47%)	95 (100%)	0	100	100
1	U	95/203 (47%)	95 (100%)	0	100	100
1	V	95/203 (47%)	95 (100%)	0	100	100
2	T	93/208 (45%)	93 (100%)	0	100	100
2	W	93/208 (45%)	93 (100%)	0	100	100
2	X	93/208 (45%)	93 (100%)	0	100	100
3	A	281/318 (88%)	281 (100%)	0	100	100
3	G	281/318 (88%)	281 (100%)	0	100	100
3	H	281/318 (88%)	281 (100%)	0	100	100

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	B	149/200 (74%)	149 (100%)	0	100	100
4	I	149/200 (74%)	149 (100%)	0	100	100
4	J	149/200 (74%)	149 (100%)	0	100	100
All	All	1854/2787 (66%)	1854 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	V	37	GLN
2	X	6	GLN
2	X	100	GLN
3	A	101	HIS
3	A	183	HIS
4	B	114	ASN
1	S	37	GLN
2	T	6	GLN
2	T	100	GLN
3	G	47	HIS
3	G	101	HIS
4	I	114	ASN
1	U	37	GLN
2	W	100	GLN
3	H	47	HIS
3	H	101	HIS
4	J	114	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

9 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	$\#\|Z\| > 2$
5	NAG	H	503	3	14,14,15	0.22	0	17,19,21	0.40	0
5	NAG	A	503	3	14,14,15	0.23	0	17,19,21	0.40	0
5	NAG	G	502	3	14,14,15	0.27	0	17,19,21	0.44	0
5	NAG	A	502	3	14,14,15	0.27	0	17,19,21	0.43	0
5	NAG	A	501	3	14,14,15	0.22	0	17,19,21	0.43	0
5	NAG	G	501	3	14,14,15	0.22	0	17,19,21	0.43	0
5	NAG	H	502	3	14,14,15	0.27	0	17,19,21	0.44	0
5	NAG	H	501	3	14,14,15	0.22	0	17,19,21	0.43	0
5	NAG	G	503	3	14,14,15	0.23	0	17,19,21	0.40	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	H	503	3	-	3/6/23/26	0/1/1/1
5	NAG	A	503	3	-	3/6/23/26	0/1/1/1
5	NAG	G	502	3	-	1/6/23/26	0/1/1/1
5	NAG	A	502	3	-	1/6/23/26	0/1/1/1
5	NAG	A	501	3	-	2/6/23/26	0/1/1/1
5	NAG	G	501	3	-	2/6/23/26	0/1/1/1
5	NAG	H	502	3	-	1/6/23/26	0/1/1/1
5	NAG	H	501	3	-	2/6/23/26	0/1/1/1
5	NAG	G	503	3	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	NAG	O5-C5-C6-O6
5	G	501	NAG	O5-C5-C6-O6
5	H	501	NAG	O5-C5-C6-O6
5	A	501	NAG	C4-C5-C6-O6
5	G	501	NAG	C4-C5-C6-O6
5	H	501	NAG	C4-C5-C6-O6
5	A	503	NAG	O5-C5-C6-O6
5	G	503	NAG	O5-C5-C6-O6
5	H	503	NAG	O5-C5-C6-O6
5	A	503	NAG	C4-C5-C6-O6
5	G	503	NAG	C4-C5-C6-O6
5	H	503	NAG	C4-C5-C6-O6
5	A	503	NAG	C1-C2-N2-C7
5	G	503	NAG	C1-C2-N2-C7
5	H	503	NAG	C1-C2-N2-C7
5	G	502	NAG	O5-C5-C6-O6
5	A	502	NAG	O5-C5-C6-O6
5	H	502	NAG	O5-C5-C6-O6

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.

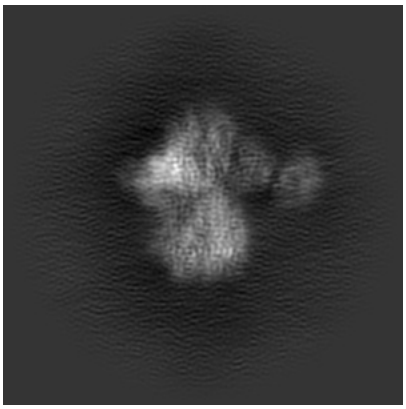
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41874. These allow visual inspection of the internal detail of the map and identification of artifacts.

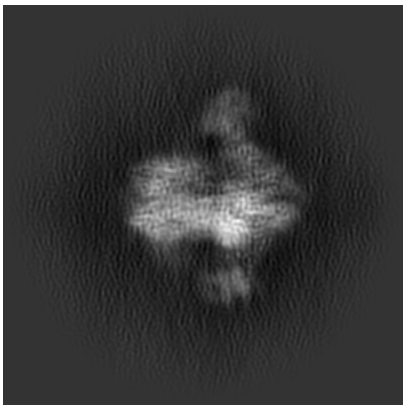
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

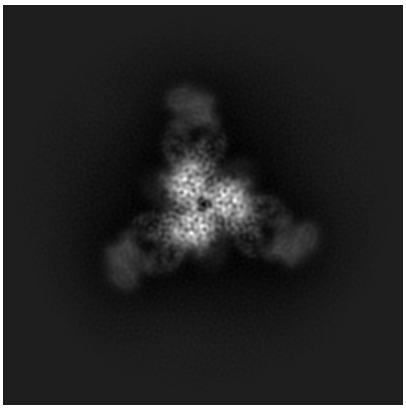
6.1.1 Primary map



X

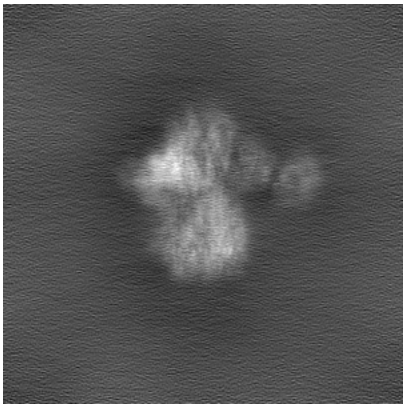


Y

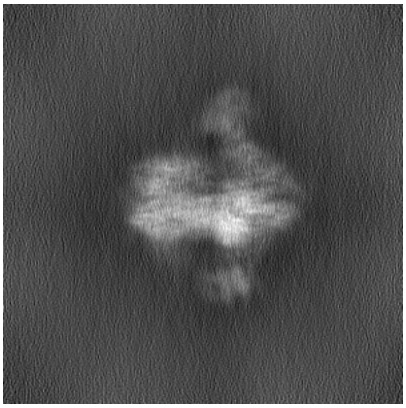


Z

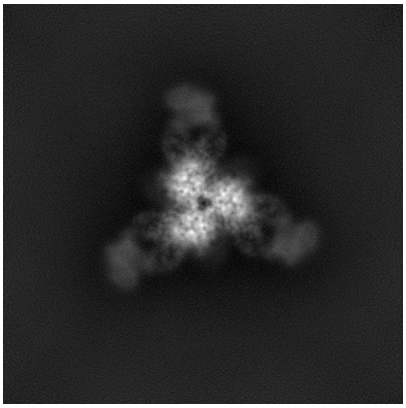
6.1.2 Raw map



X



Y

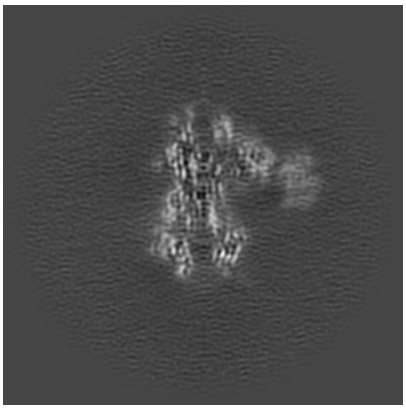


Z

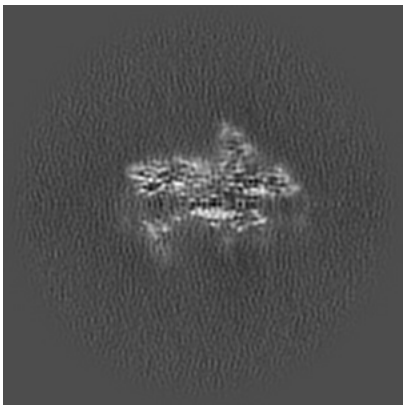
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

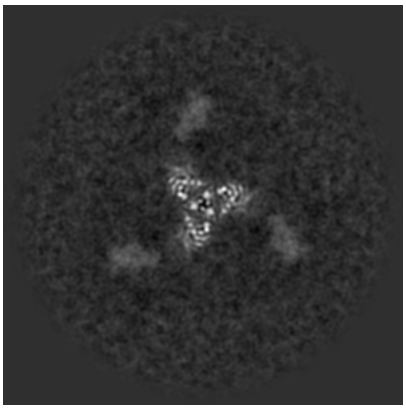
6.2.1 Primary map



X Index: 144

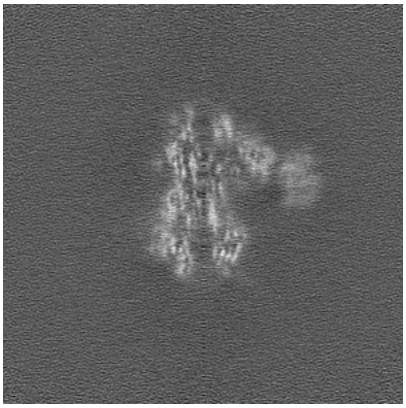


Y Index: 144

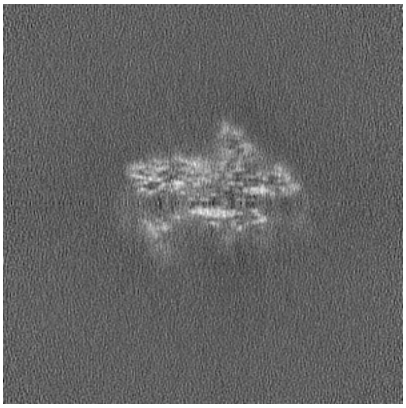


Z Index: 144

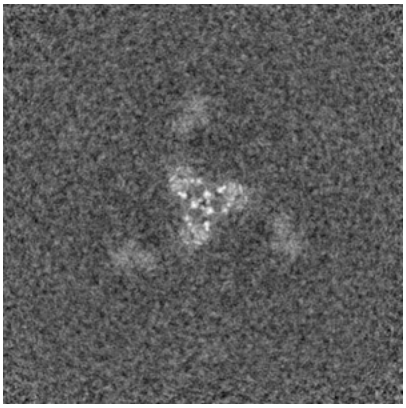
6.2.2 Raw map



X Index: 144



Y Index: 144

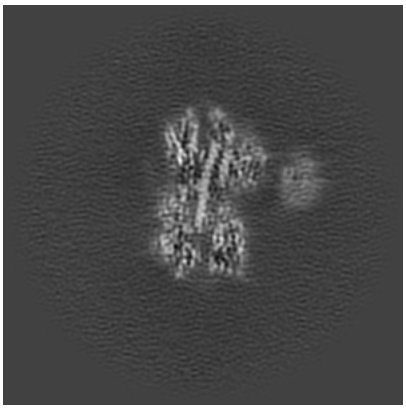


Z Index: 144

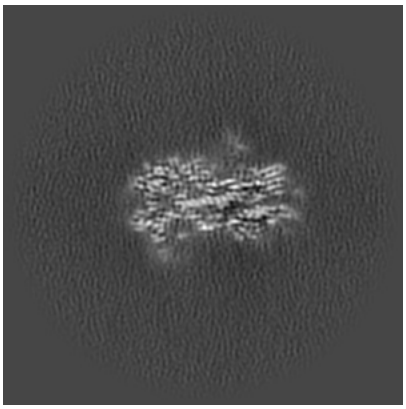
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

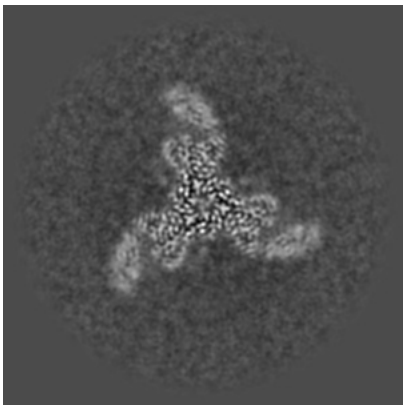
6.3.1 Primary map



X Index: 138

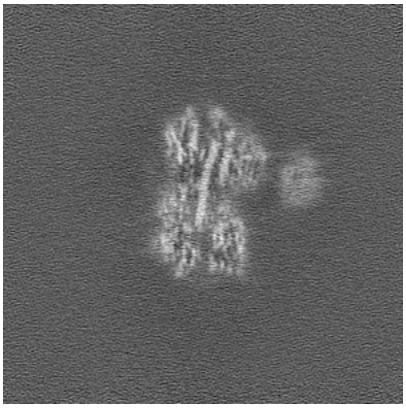


Y Index: 151

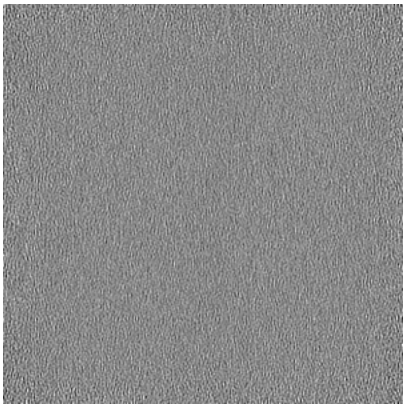


Z Index: 168

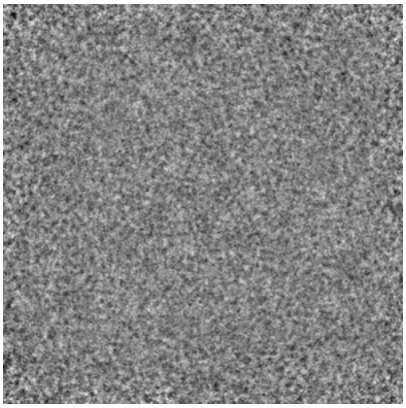
6.3.2 Raw map



X Index: 138



Y Index: 0

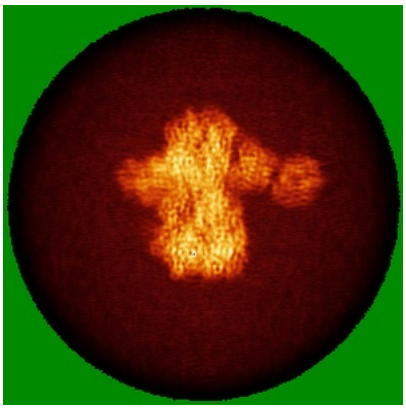


Z Index: 0

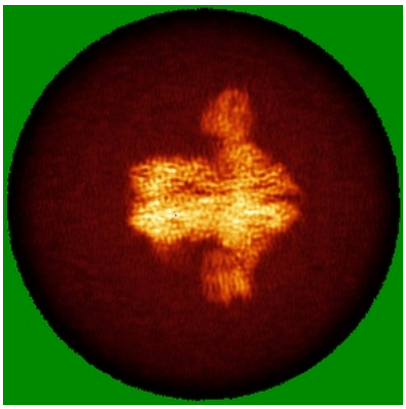
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

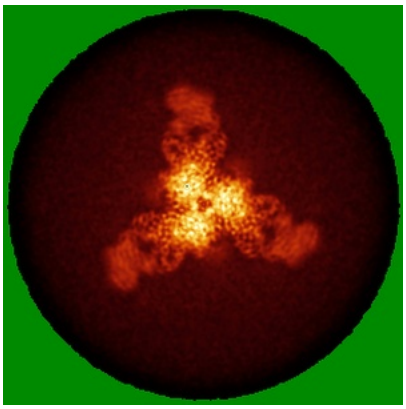
6.4.1 Primary map



X

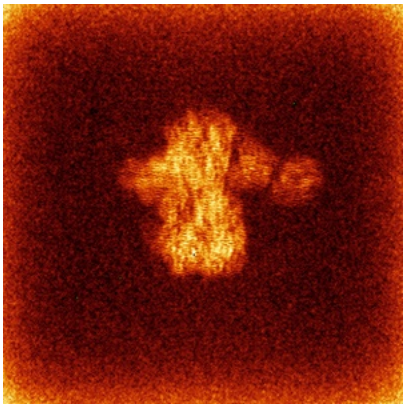


Y

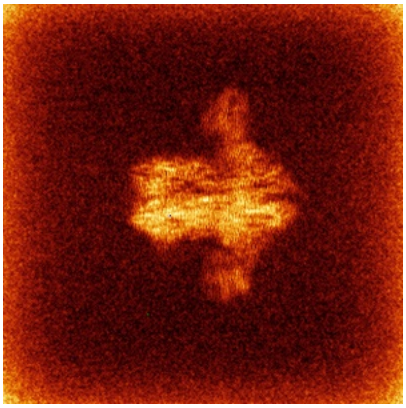


Z

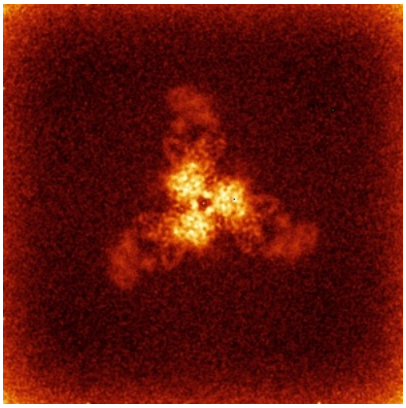
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X

Y

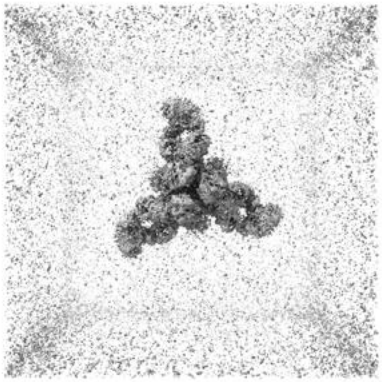
Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. 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

X

Y



Z

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.

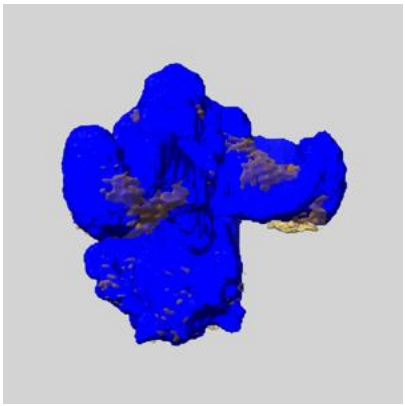
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

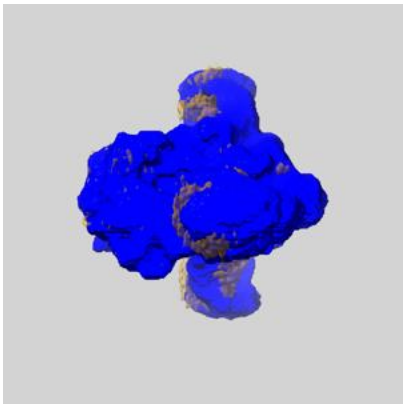
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

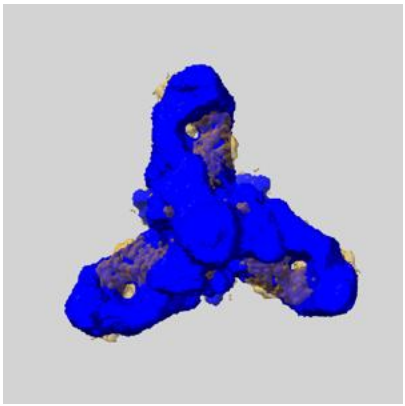
6.6.1 emd_41874_msk_1.map (i)



X



Y

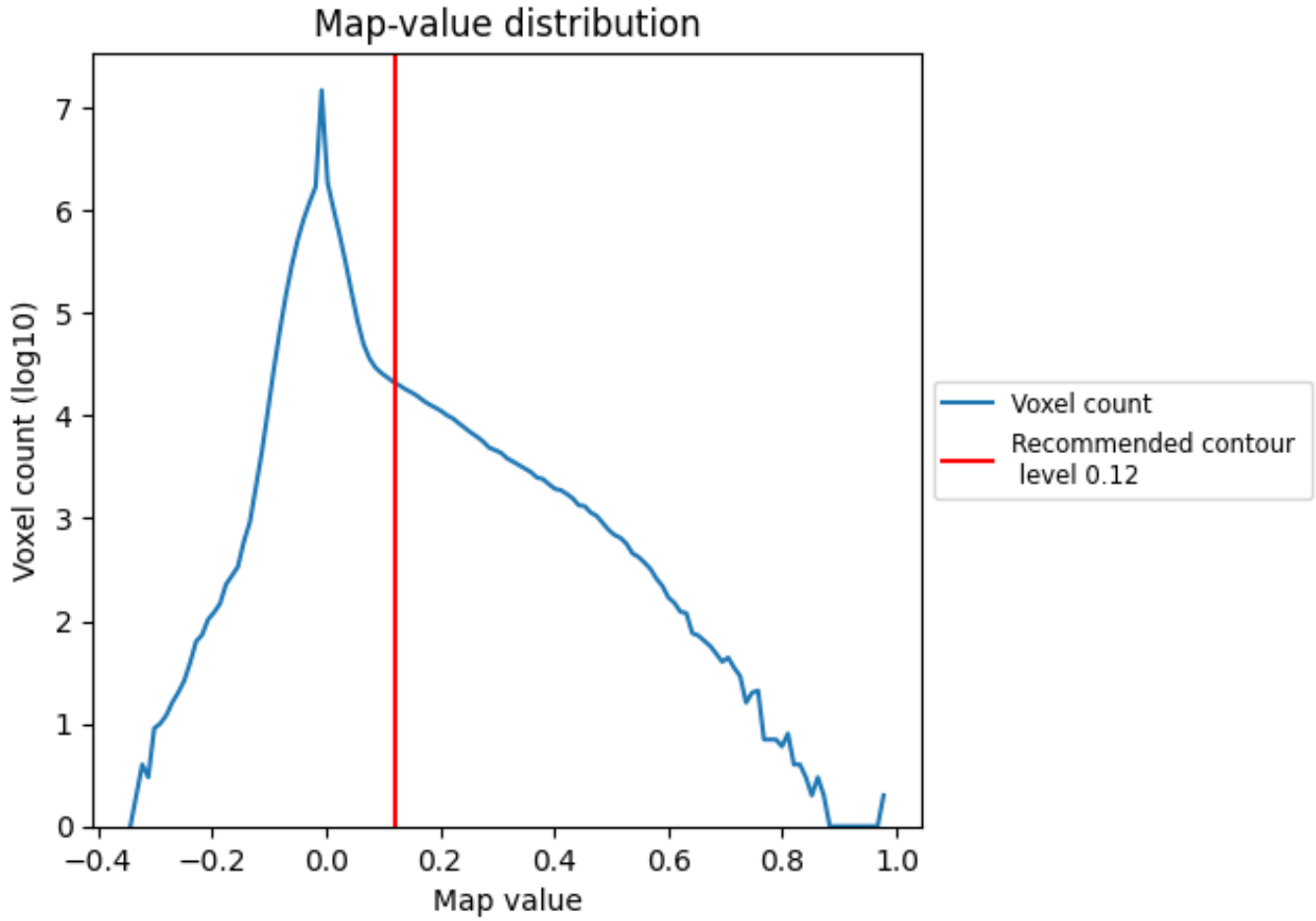


Z

7 Map analysis

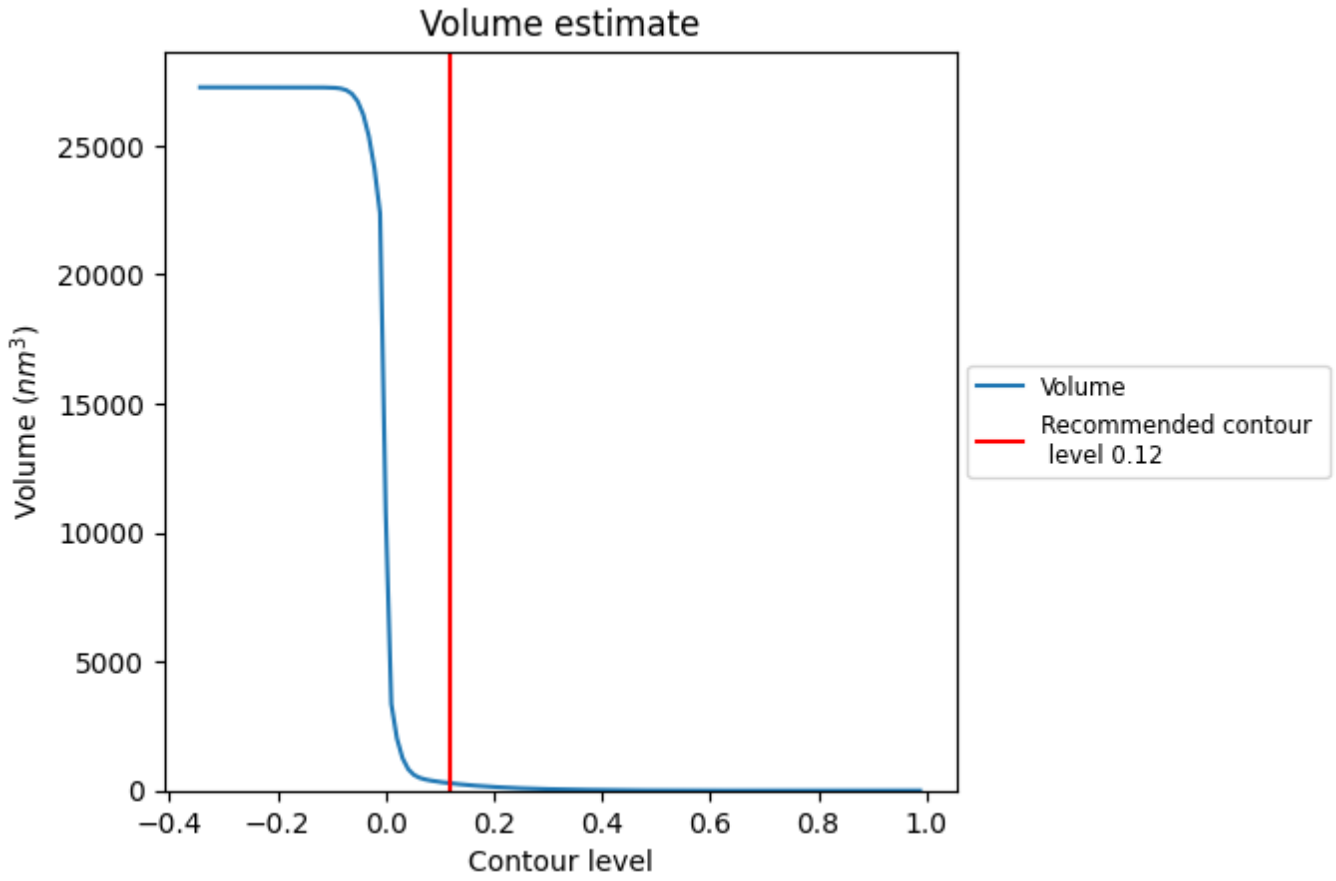
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

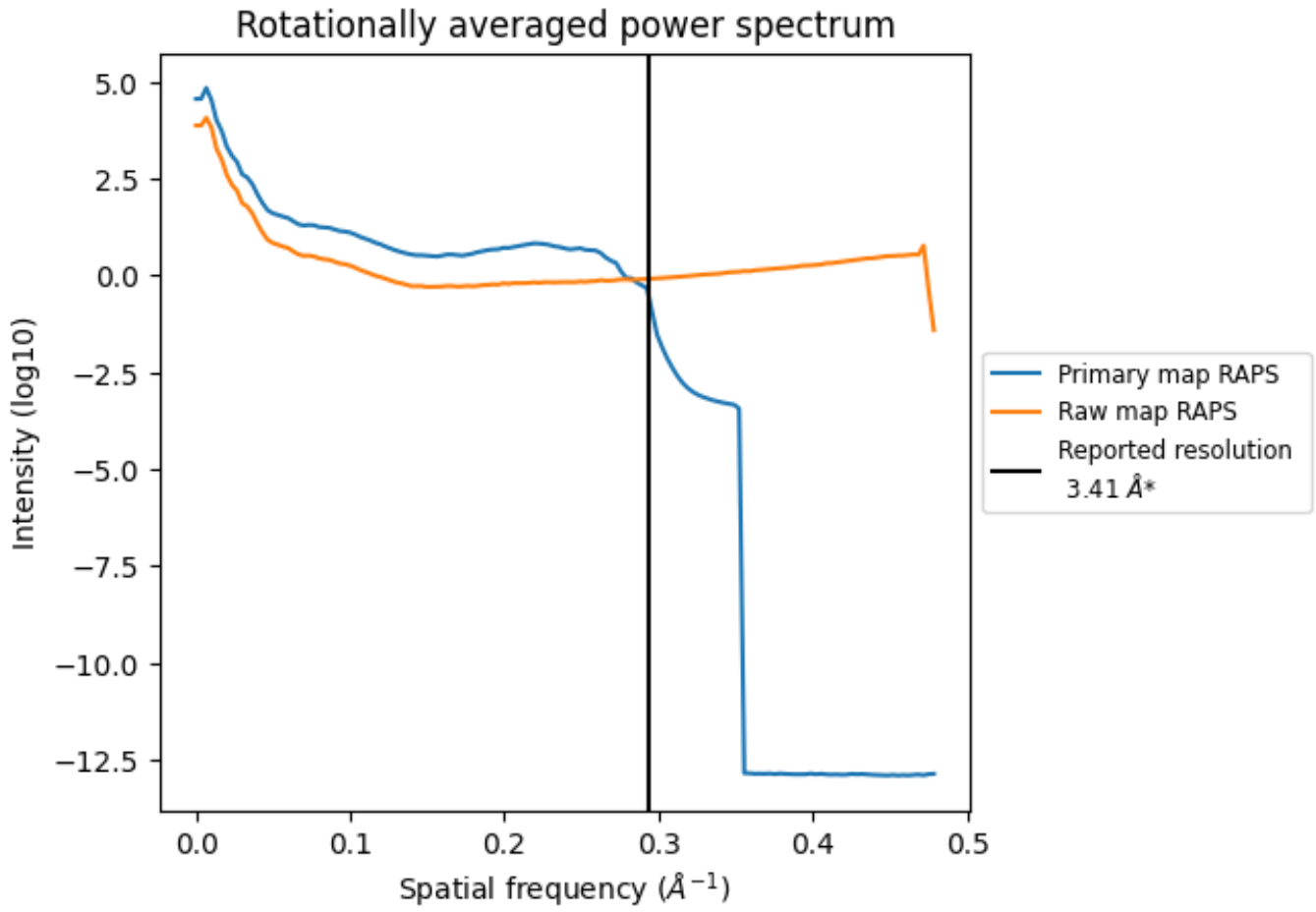
7.2 Volume estimate



The volume at the recommended contour level is 282 nm^3; this corresponds to an approximate mass of 255 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 (i)

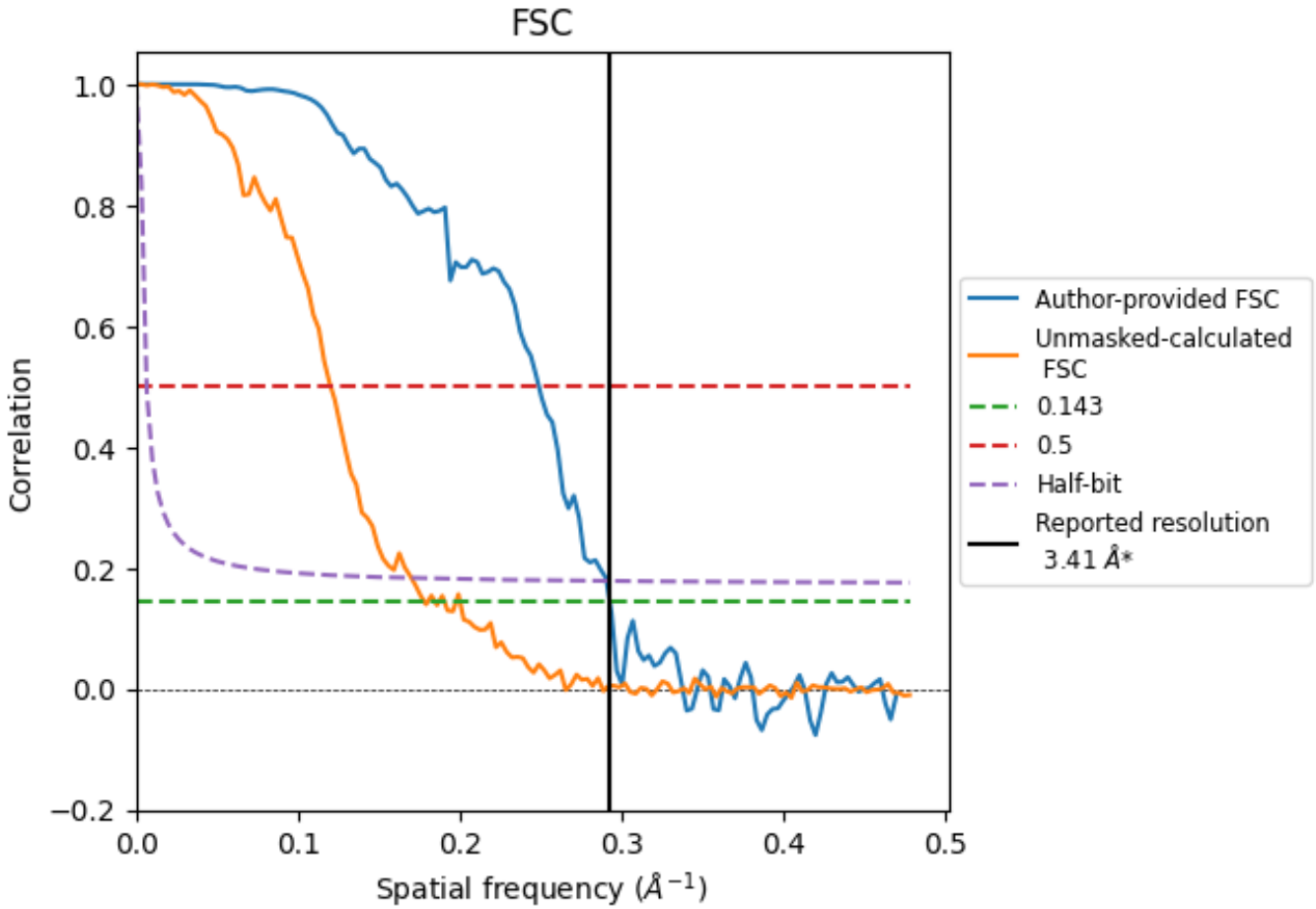


*Reported resolution corresponds to spatial frequency of 0.293 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.293 Å^{-1}

8.2 Resolution estimates (i)

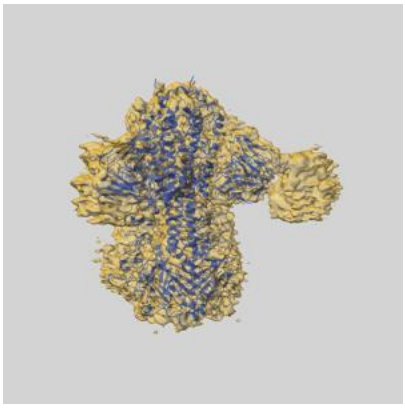
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.41	-	-
Author-provided FSC curve	3.41	4.01	3.44
Unmasked-calculated*	5.60	8.31	5.87

*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 5.60 differs from the reported value 3.41 by more than 10 %

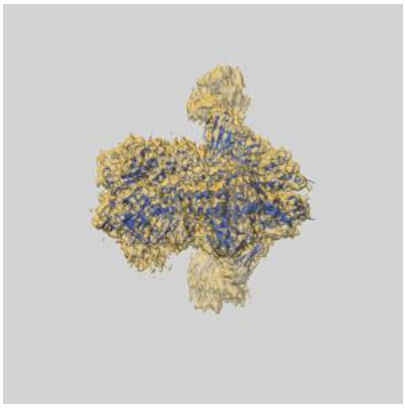
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41874 and PDB model 8U44. Per-residue inclusion information can be found in section 3 on page 14.

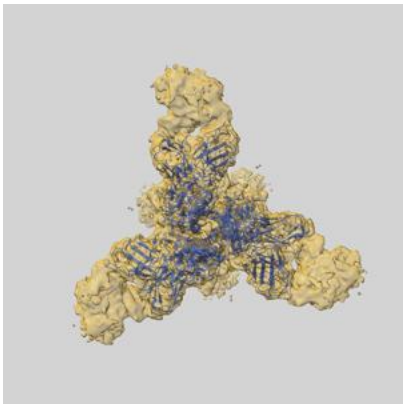
9.1 Map-model overlay



X



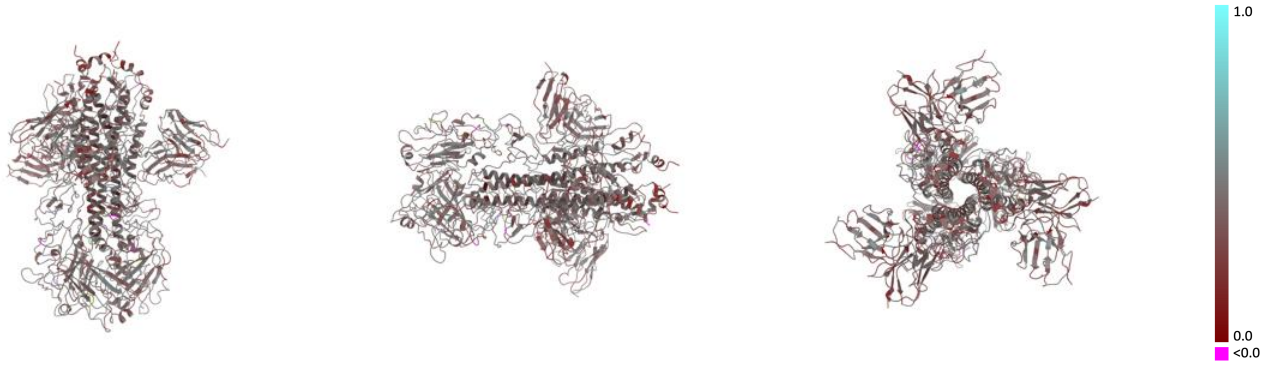
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 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.

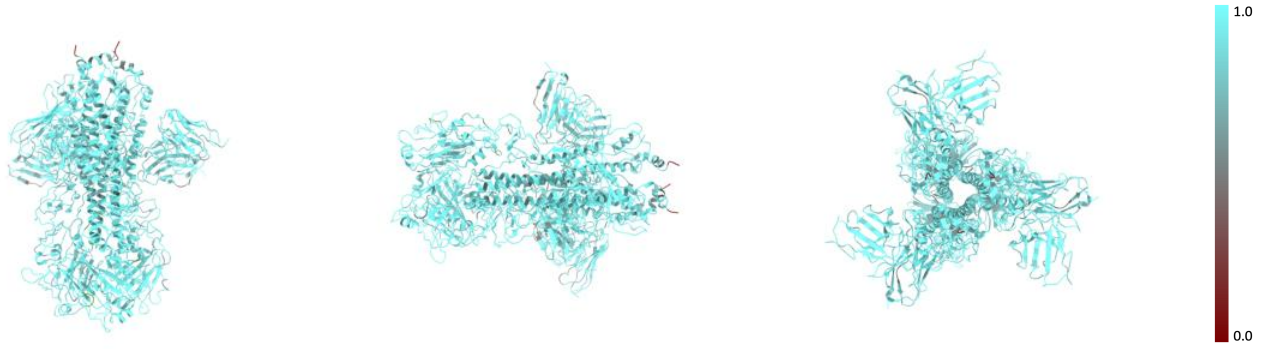
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

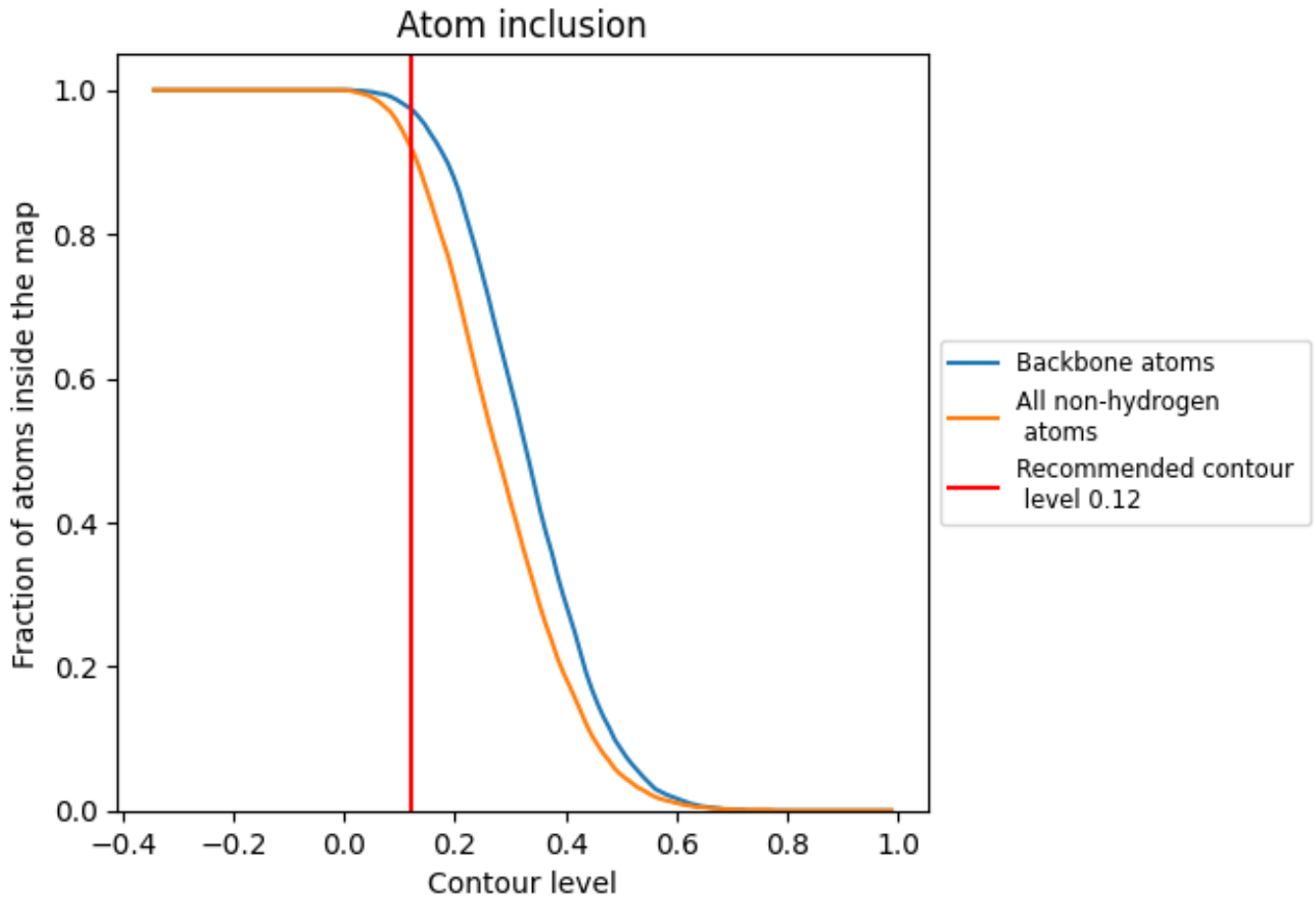
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.12).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 92% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9210	0.3870
A	0.9460	0.4020
B	0.9090	0.3840
G	0.9470	0.4010
H	0.9470	0.4030
I	0.9100	0.3820
J	0.9080	0.3850
S	0.8850	0.3620
T	0.9010	0.3760
U	0.8870	0.3620
V	0.8860	0.3600
W	0.9000	0.3760
X	0.9010	0.3760