



Full wwPDB EM Validation Report ⓘ

Aug 4, 2025 – 04:50 PM EDT

PDB ID : 9D0Y / pdb_00009d0y
EMDB ID : EMD-46466
Title : Map of endoH-treated hemagglutinin A/Sing/INFIMH/16
Authors : Torrents de la Pena, A.; Ward, A.B.; de Paiva Froes Rocha, R.
Deposited on : 2024-08-07
Resolution : 3.10 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.dev126
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) : 2.45.1

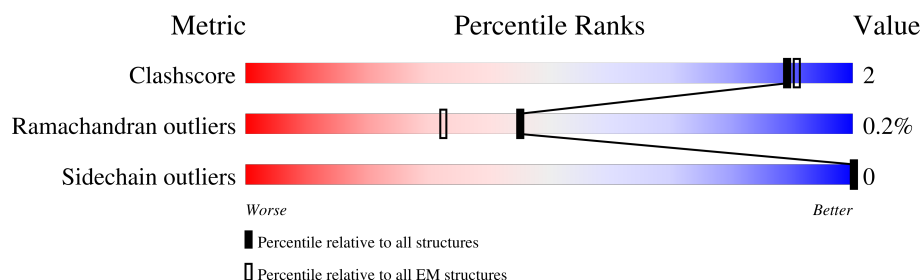
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	340	
1	B	340	
1	C	340	
2	D	486	
2	E	486	
2	F	486	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11781 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	313	Total	C	N	O	S	0	0
			2442	1534	433	463	12		
1	B	313	Total	C	N	O	S	0	0
			2442	1534	433	463	12		
1	C	313	Total	C	N	O	S	0	0
			2442	1534	433	463	12		

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP A0A2R4U332
A	-12	PRO	-	expression tag	UNP A0A2R4U332
A	-11	MET	-	expression tag	UNP A0A2R4U332
A	-10	GLY	-	expression tag	UNP A0A2R4U332
A	-9	SER	-	expression tag	UNP A0A2R4U332
A	-8	LEU	-	expression tag	UNP A0A2R4U332
A	-7	GLN	-	expression tag	UNP A0A2R4U332
A	-6	PRO	-	expression tag	UNP A0A2R4U332
A	-5	LEU	-	expression tag	UNP A0A2R4U332
A	-4	ALA	-	expression tag	UNP A0A2R4U332
A	-3	THR	-	expression tag	UNP A0A2R4U332
A	-2	LEU	-	expression tag	UNP A0A2R4U332
A	-1	TYR	-	expression tag	UNP A0A2R4U332
A	0	LEU	-	expression tag	UNP A0A2R4U332
A	1	LEU	-	expression tag	UNP A0A2R4U332
A	2	GLY	-	expression tag	UNP A0A2R4U332
A	3	MET	-	expression tag	UNP A0A2R4U332
A	4	LEU	-	expression tag	UNP A0A2R4U332
A	5	VAL	-	expression tag	UNP A0A2R4U332
A	6	ALA	-	expression tag	UNP A0A2R4U332
A	7	SER	-	expression tag	UNP A0A2R4U332
A	8	VAL	-	expression tag	UNP A0A2R4U332
A	9	LEU	-	expression tag	UNP A0A2R4U332
A	10	ALA	-	expression tag	UNP A0A2R4U332

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	MET	-	initiating methionine	UNP A0A2R4U332
B	-12	PRO	-	expression tag	UNP A0A2R4U332
B	-11	MET	-	expression tag	UNP A0A2R4U332
B	-10	GLY	-	expression tag	UNP A0A2R4U332
B	-9	SER	-	expression tag	UNP A0A2R4U332
B	-8	LEU	-	expression tag	UNP A0A2R4U332
B	-7	GLN	-	expression tag	UNP A0A2R4U332
B	-6	PRO	-	expression tag	UNP A0A2R4U332
B	-5	LEU	-	expression tag	UNP A0A2R4U332
B	-4	ALA	-	expression tag	UNP A0A2R4U332
B	-3	THR	-	expression tag	UNP A0A2R4U332
B	-2	LEU	-	expression tag	UNP A0A2R4U332
B	-1	TYR	-	expression tag	UNP A0A2R4U332
B	0	LEU	-	expression tag	UNP A0A2R4U332
B	1	LEU	-	expression tag	UNP A0A2R4U332
B	2	GLY	-	expression tag	UNP A0A2R4U332
B	3	MET	-	expression tag	UNP A0A2R4U332
B	4	LEU	-	expression tag	UNP A0A2R4U332
B	5	VAL	-	expression tag	UNP A0A2R4U332
B	6	ALA	-	expression tag	UNP A0A2R4U332
B	7	SER	-	expression tag	UNP A0A2R4U332
B	8	VAL	-	expression tag	UNP A0A2R4U332
B	9	LEU	-	expression tag	UNP A0A2R4U332
B	10	ALA	-	expression tag	UNP A0A2R4U332
C	-13	MET	-	initiating methionine	UNP A0A2R4U332
C	-12	PRO	-	expression tag	UNP A0A2R4U332
C	-11	MET	-	expression tag	UNP A0A2R4U332
C	-10	GLY	-	expression tag	UNP A0A2R4U332
C	-9	SER	-	expression tag	UNP A0A2R4U332
C	-8	LEU	-	expression tag	UNP A0A2R4U332
C	-7	GLN	-	expression tag	UNP A0A2R4U332
C	-6	PRO	-	expression tag	UNP A0A2R4U332
C	-5	LEU	-	expression tag	UNP A0A2R4U332
C	-4	ALA	-	expression tag	UNP A0A2R4U332
C	-3	THR	-	expression tag	UNP A0A2R4U332
C	-2	LEU	-	expression tag	UNP A0A2R4U332
C	-1	TYR	-	expression tag	UNP A0A2R4U332
C	0	LEU	-	expression tag	UNP A0A2R4U332
C	1	LEU	-	expression tag	UNP A0A2R4U332
C	2	GLY	-	expression tag	UNP A0A2R4U332
C	3	MET	-	expression tag	UNP A0A2R4U332
C	4	LEU	-	expression tag	UNP A0A2R4U332

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Chain	Residue	Modelled	Actual	Comment	Reference
C	5	VAL	-	expression tag	UNP A0A2R4U332
C	6	ALA	-	expression tag	UNP A0A2R4U332
C	7	SER	-	expression tag	UNP A0A2R4U332
C	8	VAL	-	expression tag	UNP A0A2R4U332
C	9	LEU	-	expression tag	UNP A0A2R4U332
C	10	ALA	-	expression tag	UNP A0A2R4U332

- Molecule 2 is a protein called Hemagglutinin HA2 chain, Green fluorescent protein fusion.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	164	Total	C	N	O	S	0	0
			1345	832	238	269	6		
2	E	164	Total	C	N	O	S	0	0
			1345	832	238	269	6		
2	F	164	Total	C	N	O	S	0	0
			1345	832	238	269	6		

There are 288 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	32	ARG	THR	conflict	UNP Q38SQ8
D	45	ILE	VAL	conflict	UNP Q38SQ8
D	57	GLY	GLU	conflict	UNP Q38SQ8
D	77	VAL	ILE	conflict	UNP Q38SQ8
D	123	LYS	ARG	conflict	UNP Q38SQ8
D	150	GLU	GLY	conflict	UNP Q38SQ8
D	155	GLU	GLY	conflict	UNP Q38SQ8
D	160	ASN	ASP	conflict	UNP Q38SQ8
D	175	ARG	-	linker	UNP Q38SQ8
D	176	MET	-	linker	UNP Q38SQ8
D	177	LYS	-	linker	UNP Q38SQ8
D	178	GLN	-	linker	UNP Q38SQ8
D	179	ILE	-	linker	UNP Q38SQ8
D	180	GLU	-	linker	UNP Q38SQ8
D	181	ASP	-	linker	UNP Q38SQ8
D	182	LYS	-	linker	UNP Q38SQ8
D	183	ILE	-	linker	UNP Q38SQ8
D	184	GLU	-	linker	UNP Q38SQ8
D	185	GLU	-	linker	UNP Q38SQ8
D	186	ILE	-	linker	UNP Q38SQ8
D	187	GLU	-	linker	UNP Q38SQ8
D	188	SER	-	linker	UNP Q38SQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	189	LYS	-	linker	UNP Q38SQ8
D	190	GLN	-	linker	UNP Q38SQ8
D	191	LYS	-	linker	UNP Q38SQ8
D	192	LYS	-	linker	UNP Q38SQ8
D	193	ILE	-	linker	UNP Q38SQ8
D	194	GLU	-	linker	UNP Q38SQ8
D	195	ASN	-	linker	UNP Q38SQ8
D	196	GLU	-	linker	UNP Q38SQ8
D	197	ILE	-	linker	UNP Q38SQ8
D	198	ALA	-	linker	UNP Q38SQ8
D	199	ARG	-	linker	UNP Q38SQ8
D	200	ILE	-	linker	UNP Q38SQ8
D	201	LYS	-	linker	UNP Q38SQ8
D	202	LYS	-	linker	UNP Q38SQ8
D	203	ILE	-	linker	UNP Q38SQ8
D	204	LYS	-	linker	UNP Q38SQ8
D	205	LEU	-	linker	UNP Q38SQ8
D	206	VAL	-	linker	UNP Q38SQ8
D	207	PRO	-	linker	UNP Q38SQ8
D	208	ARG	-	linker	UNP Q38SQ8
D	209	GLY	-	linker	UNP Q38SQ8
D	210	SER	-	linker	UNP Q38SQ8
D	211	VAL	-	linker	UNP Q38SQ8
D	212	ASP	-	linker	UNP Q38SQ8
D	213	GLU	-	linker	UNP Q38SQ8
D	214	ASN	-	linker	UNP Q38SQ8
D	215	LEU	-	linker	UNP Q38SQ8
D	216	TYR	-	linker	UNP Q38SQ8
D	217	PHE	-	linker	UNP Q38SQ8
D	218	GLN	-	linker	UNP Q38SQ8
D	219	ALA	-	linker	UNP Q38SQ8
D	249	ARG	SER	conflict	UNP P42212
D	258	ASN	TYR	conflict	UNP P42212
D	283	LEU	PHE	conflict	UNP P42212
D	284	THR	SER	conflict	UNP P42212
D	299	ARG	GLN	conflict	UNP P42212
D	318	SER	PHE	conflict	UNP P42212
D	324	THR	ASN	conflict	UNP P42212
D	364	PHE	TYR	conflict	UNP P42212
D	372	THR	MET	conflict	UNP P42212
D	382	ALA	VAL	conflict	UNP P42212
D	390	VAL	ILE	conflict	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
D	425	VAL	ALA	conflict	UNP P42212
D	453	SER	-	expression tag	UNP P42212
D	454	SER	-	expression tag	UNP P42212
D	455	ALA	-	expression tag	UNP P42212
D	456	TRP	-	expression tag	UNP P42212
D	457	SER	-	expression tag	UNP P42212
D	458	HIS	-	expression tag	UNP P42212
D	459	PRO	-	expression tag	UNP P42212
D	460	GLN	-	expression tag	UNP P42212
D	461	PHE	-	expression tag	UNP P42212
D	462	GLU	-	expression tag	UNP P42212
D	463	LYS	-	expression tag	UNP P42212
D	464	GLY	-	expression tag	UNP P42212
D	465	GLY	-	expression tag	UNP P42212
D	466	GLY	-	expression tag	UNP P42212
D	467	SER	-	expression tag	UNP P42212
D	468	GLY	-	expression tag	UNP P42212
D	469	GLY	-	expression tag	UNP P42212
D	470	GLY	-	expression tag	UNP P42212
D	471	SER	-	expression tag	UNP P42212
D	472	GLY	-	expression tag	UNP P42212
D	473	GLY	-	expression tag	UNP P42212
D	474	SER	-	expression tag	UNP P42212
D	475	ALA	-	expression tag	UNP P42212
D	476	TRP	-	expression tag	UNP P42212
D	477	SER	-	expression tag	UNP P42212
D	478	HIS	-	expression tag	UNP P42212
D	479	PRO	-	expression tag	UNP P42212
D	480	GLN	-	expression tag	UNP P42212
D	481	PHE	-	expression tag	UNP P42212
D	482	GLU	-	expression tag	UNP P42212
D	483	LYS	-	expression tag	UNP P42212
E	32	ARG	THR	conflict	UNP Q38SQ8
E	45	ILE	VAL	conflict	UNP Q38SQ8
E	57	GLY	GLU	conflict	UNP Q38SQ8
E	77	VAL	ILE	conflict	UNP Q38SQ8
E	123	LYS	ARG	conflict	UNP Q38SQ8
E	150	GLU	GLY	conflict	UNP Q38SQ8
E	155	GLU	GLY	conflict	UNP Q38SQ8
E	160	ASN	ASP	conflict	UNP Q38SQ8
E	175	ARG	-	linker	UNP Q38SQ8
E	176	MET	-	linker	UNP Q38SQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	177	LYS	-	linker	UNP Q38SQ8
E	178	GLN	-	linker	UNP Q38SQ8
E	179	ILE	-	linker	UNP Q38SQ8
E	180	GLU	-	linker	UNP Q38SQ8
E	181	ASP	-	linker	UNP Q38SQ8
E	182	LYS	-	linker	UNP Q38SQ8
E	183	ILE	-	linker	UNP Q38SQ8
E	184	GLU	-	linker	UNP Q38SQ8
E	185	GLU	-	linker	UNP Q38SQ8
E	186	ILE	-	linker	UNP Q38SQ8
E	187	GLU	-	linker	UNP Q38SQ8
E	188	SER	-	linker	UNP Q38SQ8
E	189	LYS	-	linker	UNP Q38SQ8
E	190	GLN	-	linker	UNP Q38SQ8
E	191	LYS	-	linker	UNP Q38SQ8
E	192	LYS	-	linker	UNP Q38SQ8
E	193	ILE	-	linker	UNP Q38SQ8
E	194	GLU	-	linker	UNP Q38SQ8
E	195	ASN	-	linker	UNP Q38SQ8
E	196	GLU	-	linker	UNP Q38SQ8
E	197	ILE	-	linker	UNP Q38SQ8
E	198	ALA	-	linker	UNP Q38SQ8
E	199	ARG	-	linker	UNP Q38SQ8
E	200	ILE	-	linker	UNP Q38SQ8
E	201	LYS	-	linker	UNP Q38SQ8
E	202	LYS	-	linker	UNP Q38SQ8
E	203	ILE	-	linker	UNP Q38SQ8
E	204	LYS	-	linker	UNP Q38SQ8
E	205	LEU	-	linker	UNP Q38SQ8
E	206	VAL	-	linker	UNP Q38SQ8
E	207	PRO	-	linker	UNP Q38SQ8
E	208	ARG	-	linker	UNP Q38SQ8
E	209	GLY	-	linker	UNP Q38SQ8
E	210	SER	-	linker	UNP Q38SQ8
E	211	VAL	-	linker	UNP Q38SQ8
E	212	ASP	-	linker	UNP Q38SQ8
E	213	GLU	-	linker	UNP Q38SQ8
E	214	ASN	-	linker	UNP Q38SQ8
E	215	LEU	-	linker	UNP Q38SQ8
E	216	TYR	-	linker	UNP Q38SQ8
E	217	PHE	-	linker	UNP Q38SQ8
E	218	GLN	-	linker	UNP Q38SQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	219	ALA	-	linker	UNP Q38SQ8
E	249	ARG	SER	conflict	UNP P42212
E	258	ASN	TYR	conflict	UNP P42212
E	283	LEU	PHE	conflict	UNP P42212
E	284	THR	SER	conflict	UNP P42212
E	299	ARG	GLN	conflict	UNP P42212
E	318	SER	PHE	conflict	UNP P42212
E	324	THR	ASN	conflict	UNP P42212
E	364	PHE	TYR	conflict	UNP P42212
E	372	THR	MET	conflict	UNP P42212
E	382	ALA	VAL	conflict	UNP P42212
E	390	VAL	ILE	conflict	UNP P42212
E	425	VAL	ALA	conflict	UNP P42212
E	453	SER	-	expression tag	UNP P42212
E	454	SER	-	expression tag	UNP P42212
E	455	ALA	-	expression tag	UNP P42212
E	456	TRP	-	expression tag	UNP P42212
E	457	SER	-	expression tag	UNP P42212
E	458	HIS	-	expression tag	UNP P42212
E	459	PRO	-	expression tag	UNP P42212
E	460	GLN	-	expression tag	UNP P42212
E	461	PHE	-	expression tag	UNP P42212
E	462	GLU	-	expression tag	UNP P42212
E	463	LYS	-	expression tag	UNP P42212
E	464	GLY	-	expression tag	UNP P42212
E	465	GLY	-	expression tag	UNP P42212
E	466	GLY	-	expression tag	UNP P42212
E	467	SER	-	expression tag	UNP P42212
E	468	GLY	-	expression tag	UNP P42212
E	469	GLY	-	expression tag	UNP P42212
E	470	GLY	-	expression tag	UNP P42212
E	471	SER	-	expression tag	UNP P42212
E	472	GLY	-	expression tag	UNP P42212
E	473	GLY	-	expression tag	UNP P42212
E	474	SER	-	expression tag	UNP P42212
E	475	ALA	-	expression tag	UNP P42212
E	476	TRP	-	expression tag	UNP P42212
E	477	SER	-	expression tag	UNP P42212
E	478	HIS	-	expression tag	UNP P42212
E	479	PRO	-	expression tag	UNP P42212
E	480	GLN	-	expression tag	UNP P42212
E	481	PHE	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
E	482	GLU	-	expression tag	UNP P42212
E	483	LYS	-	expression tag	UNP P42212
F	32	ARG	THR	conflict	UNP Q38SQ8
F	45	ILE	VAL	conflict	UNP Q38SQ8
F	57	GLY	GLU	conflict	UNP Q38SQ8
F	77	VAL	ILE	conflict	UNP Q38SQ8
F	123	LYS	ARG	conflict	UNP Q38SQ8
F	150	GLU	GLY	conflict	UNP Q38SQ8
F	155	GLU	GLY	conflict	UNP Q38SQ8
F	160	ASN	ASP	conflict	UNP Q38SQ8
F	175	ARG	-	linker	UNP Q38SQ8
F	176	MET	-	linker	UNP Q38SQ8
F	177	LYS	-	linker	UNP Q38SQ8
F	178	GLN	-	linker	UNP Q38SQ8
F	179	ILE	-	linker	UNP Q38SQ8
F	180	GLU	-	linker	UNP Q38SQ8
F	181	ASP	-	linker	UNP Q38SQ8
F	182	LYS	-	linker	UNP Q38SQ8
F	183	ILE	-	linker	UNP Q38SQ8
F	184	GLU	-	linker	UNP Q38SQ8
F	185	GLU	-	linker	UNP Q38SQ8
F	186	ILE	-	linker	UNP Q38SQ8
F	187	GLU	-	linker	UNP Q38SQ8
F	188	SER	-	linker	UNP Q38SQ8
F	189	LYS	-	linker	UNP Q38SQ8
F	190	GLN	-	linker	UNP Q38SQ8
F	191	LYS	-	linker	UNP Q38SQ8
F	192	LYS	-	linker	UNP Q38SQ8
F	193	ILE	-	linker	UNP Q38SQ8
F	194	GLU	-	linker	UNP Q38SQ8
F	195	ASN	-	linker	UNP Q38SQ8
F	196	GLU	-	linker	UNP Q38SQ8
F	197	ILE	-	linker	UNP Q38SQ8
F	198	ALA	-	linker	UNP Q38SQ8
F	199	ARG	-	linker	UNP Q38SQ8
F	200	ILE	-	linker	UNP Q38SQ8
F	201	LYS	-	linker	UNP Q38SQ8
F	202	LYS	-	linker	UNP Q38SQ8
F	203	ILE	-	linker	UNP Q38SQ8
F	204	LYS	-	linker	UNP Q38SQ8
F	205	LEU	-	linker	UNP Q38SQ8
F	206	VAL	-	linker	UNP Q38SQ8

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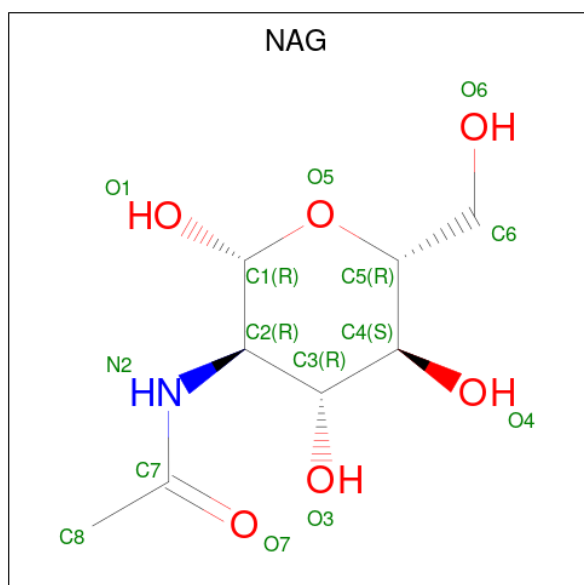
Chain	Residue	Modelled	Actual	Comment	Reference
F	207	PRO	-	linker	UNP Q38SQ8
F	208	ARG	-	linker	UNP Q38SQ8
F	209	GLY	-	linker	UNP Q38SQ8
F	210	SER	-	linker	UNP Q38SQ8
F	211	VAL	-	linker	UNP Q38SQ8
F	212	ASP	-	linker	UNP Q38SQ8
F	213	GLU	-	linker	UNP Q38SQ8
F	214	ASN	-	linker	UNP Q38SQ8
F	215	LEU	-	linker	UNP Q38SQ8
F	216	TYR	-	linker	UNP Q38SQ8
F	217	PHE	-	linker	UNP Q38SQ8
F	218	GLN	-	linker	UNP Q38SQ8
F	219	ALA	-	linker	UNP Q38SQ8
F	249	ARG	SER	conflict	UNP P42212
F	258	ASN	TYR	conflict	UNP P42212
F	283	LEU	PHE	conflict	UNP P42212
F	284	THR	SER	conflict	UNP P42212
F	299	ARG	GLN	conflict	UNP P42212
F	318	SER	PHE	conflict	UNP P42212
F	324	THR	ASN	conflict	UNP P42212
F	364	PHE	TYR	conflict	UNP P42212
F	372	THR	MET	conflict	UNP P42212
F	382	ALA	VAL	conflict	UNP P42212
F	390	VAL	ILE	conflict	UNP P42212
F	425	VAL	ALA	conflict	UNP P42212
F	453	SER	-	expression tag	UNP P42212
F	454	SER	-	expression tag	UNP P42212
F	455	ALA	-	expression tag	UNP P42212
F	456	TRP	-	expression tag	UNP P42212
F	457	SER	-	expression tag	UNP P42212
F	458	HIS	-	expression tag	UNP P42212
F	459	PRO	-	expression tag	UNP P42212
F	460	GLN	-	expression tag	UNP P42212
F	461	PHE	-	expression tag	UNP P42212
F	462	GLU	-	expression tag	UNP P42212
F	463	LYS	-	expression tag	UNP P42212
F	464	GLY	-	expression tag	UNP P42212
F	465	GLY	-	expression tag	UNP P42212
F	466	GLY	-	expression tag	UNP P42212
F	467	SER	-	expression tag	UNP P42212
F	468	GLY	-	expression tag	UNP P42212
F	469	GLY	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
F	470	GLY	-	expression tag	UNP P42212
F	471	SER	-	expression tag	UNP P42212
F	472	GLY	-	expression tag	UNP P42212
F	473	GLY	-	expression tag	UNP P42212
F	474	SER	-	expression tag	UNP P42212
F	475	ALA	-	expression tag	UNP P42212
F	476	TRP	-	expression tag	UNP P42212
F	477	SER	-	expression tag	UNP P42212
F	478	HIS	-	expression tag	UNP P42212
F	479	PRO	-	expression tag	UNP P42212
F	480	GLN	-	expression tag	UNP P42212
F	481	PHE	-	expression tag	UNP P42212
F	482	GLU	-	expression tag	UNP P42212
F	483	LYS	-	expression tag	UNP P42212

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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

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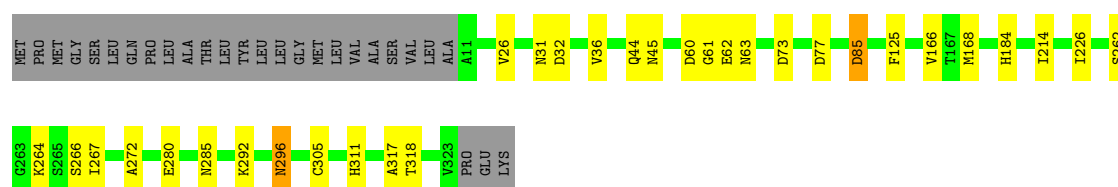
Mol	Chain	Residues	Atoms				AltConf
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	F	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots


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

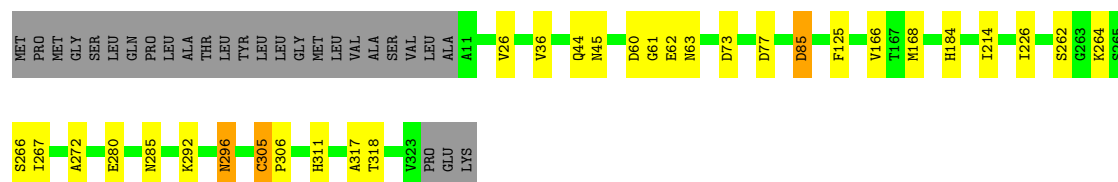
• Molecule 1: Hemagglutinin HA1 chain

Chain A: 



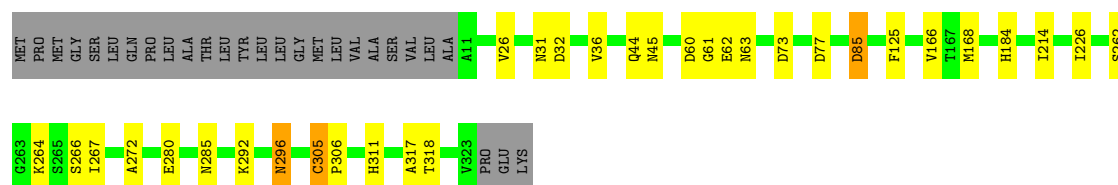
• Molecule 1: Hemagglutinin HA1 chain

Chain B: 



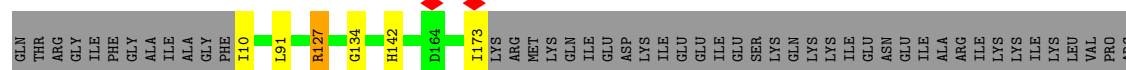
• Molecule 1: Hemagglutinin HA1 chain

Chain C: 



• Molecule 2: Hemagglutinin HA2 chain, Green fluorescent protein fusion

Chain D: 



[illegible]

- Molecule 2: Hemagglutinin HA2 chain, Green fluorescent protein fusion

Chain E:  33% 66%

[illegible]

- Molecule 2: Hemagglutinin HA2 chain, Green fluorescent protein fusion

Chain F:  33% 66%

[illegible]

WORLDWIDE
 **PDB**
PROTEIN DATA BANK

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	52046	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.583	Depositor
Minimum map value	-2.037	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	414.0, 414.0, 414.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.16	3/2498 (0.1%)	1.32	29/3394 (0.9%)
1	B	1.16	3/2498 (0.1%)	1.32	29/3394 (0.9%)
1	C	1.16	3/2498 (0.1%)	1.32	29/3394 (0.9%)
2	D	1.25	4/1367 (0.3%)	1.11	1/1836 (0.1%)
2	E	1.25	4/1367 (0.3%)	1.11	1/1836 (0.1%)
2	F	1.25	4/1367 (0.3%)	1.11	1/1836 (0.1%)
All	All	1.20	21/11595 (0.2%)	1.25	90/15690 (0.6%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	173	ILE	CB-CG1	7.16	1.67	1.53
2	D	173	ILE	CB-CG1	7.15	1.67	1.53
2	F	173	ILE	CB-CG1	7.14	1.67	1.53
1	C	267	ILE	CB-CG1	-6.22	1.41	1.53
1	A	267	ILE	CB-CG1	-6.21	1.41	1.53
1	B	267	ILE	CB-CG1	-6.21	1.41	1.53
2	E	10	ILE	CB-CG1	6.10	1.65	1.53
2	D	10	ILE	CB-CG1	6.10	1.65	1.53
2	F	10	ILE	CB-CG1	6.09	1.65	1.53
1	A	296	ASN	CB-CG	-5.63	1.38	1.52
1	B	296	ASN	CB-CG	-5.61	1.38	1.52
1	C	296	ASN	CB-CG	-5.61	1.38	1.52
2	F	91	LEU	CB-CG	-5.44	1.42	1.53
2	E	91	LEU	CB-CG	-5.43	1.42	1.53
2	D	91	LEU	CB-CG	-5.42	1.42	1.53
1	C	311	HIS	CB-CG	-5.33	1.42	1.50
2	E	127	ARG	NE-CZ	5.32	1.39	1.33
2	D	127	ARG	NE-CZ	5.30	1.38	1.33
1	A	311	HIS	CB-CG	-5.29	1.42	1.50
1	B	311	HIS	CB-CG	-5.27	1.42	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	127	ARG	NE-CZ	5.25	1.38	1.33

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	45	ASN	N-CA-C	-8.17	97.75	110.42
1	B	45	ASN	N-CA-C	-8.15	97.79	110.42
1	A	45	ASN	N-CA-C	-8.15	97.79	110.42
1	A	305	CYS	CA-C-N	7.63	127.64	119.78
1	A	305	CYS	C-N-CA	7.63	127.64	119.78
1	C	305	CYS	CA-C-N	7.62	127.63	119.78
1	C	305	CYS	C-N-CA	7.62	127.63	119.78
1	B	305	CYS	CA-C-N	7.60	127.61	119.78
1	B	305	CYS	C-N-CA	7.60	127.61	119.78
1	A	262	SER	N-CA-C	-7.41	100.54	110.55
1	B	262	SER	N-CA-C	-7.40	100.56	110.55
1	C	262	SER	N-CA-C	-7.38	100.59	110.55
1	A	280	GLU	N-CA-C	7.15	119.15	111.36
1	B	280	GLU	N-CA-C	7.15	119.15	111.36
1	C	280	GLU	N-CA-C	7.15	119.15	111.36
1	B	85	ASP	N-CA-C	-6.91	103.86	112.90
1	C	85	ASP	N-CA-C	-6.90	103.86	112.90
1	A	85	ASP	N-CA-C	-6.90	103.86	112.90
1	C	318	THR	N-CA-C	-6.80	104.67	114.12
1	A	318	THR	N-CA-C	-6.79	104.69	114.12
1	B	318	THR	N-CA-C	-6.78	104.70	114.12
1	C	168	MET	CA-C-N	6.77	126.69	119.85
1	C	168	MET	C-N-CA	6.77	126.69	119.85
1	B	168	MET	CA-C-N	6.77	126.69	119.85
1	B	168	MET	C-N-CA	6.77	126.69	119.85
1	A	168	MET	CA-C-N	6.74	126.66	119.85
1	A	168	MET	C-N-CA	6.74	126.66	119.85
1	A	184	HIS	CA-C-N	6.39	126.36	119.78
1	A	184	HIS	C-N-CA	6.39	126.36	119.78
1	C	184	HIS	CA-C-N	6.39	126.36	119.78
1	C	184	HIS	C-N-CA	6.39	126.36	119.78
1	B	184	HIS	CA-C-N	6.37	126.34	119.78
1	B	184	HIS	C-N-CA	6.37	126.34	119.78
1	A	272	ALA	CA-C-N	6.22	126.19	120.03
1	A	272	ALA	C-N-CA	6.22	126.19	120.03
1	B	272	ALA	CA-C-N	6.21	126.18	120.03
1	B	272	ALA	C-N-CA	6.21	126.18	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	272	ALA	CA-C-N	6.21	126.18	120.03
1	C	272	ALA	C-N-CA	6.21	126.18	120.03
2	E	142	HIS	CA-CB-CG	-5.98	107.82	113.80
2	F	142	HIS	CA-CB-CG	-5.96	107.84	113.80
2	D	142	HIS	CA-CB-CG	-5.95	107.85	113.80
1	A	292	LYS	CA-C-N	5.78	125.39	119.56
1	A	292	LYS	C-N-CA	5.78	125.39	119.56
1	C	292	LYS	CA-C-N	5.77	125.39	119.56
1	C	292	LYS	C-N-CA	5.77	125.39	119.56
1	B	292	LYS	CA-C-N	5.77	125.39	119.56
1	B	292	LYS	C-N-CA	5.77	125.39	119.56
1	A	73	ASP	CA-C-N	5.68	126.06	119.47
1	A	73	ASP	C-N-CA	5.68	126.06	119.47
1	B	73	ASP	CA-C-N	5.65	126.03	119.47
1	B	73	ASP	C-N-CA	5.65	126.03	119.47
1	C	73	ASP	CA-C-N	5.64	126.01	119.47
1	C	73	ASP	C-N-CA	5.64	126.01	119.47
1	C	267	ILE	CB-CA-C	-5.26	102.99	110.83
1	B	267	ILE	CB-CA-C	-5.25	103.00	110.83
1	A	267	ILE	CB-CA-C	-5.25	103.01	110.83
1	B	214	ILE	CA-C-N	5.25	125.16	119.76
1	B	214	ILE	C-N-CA	5.25	125.16	119.76
1	A	214	ILE	CA-C-N	5.24	125.16	119.76
1	A	214	ILE	C-N-CA	5.24	125.16	119.76
1	C	214	ILE	CA-C-N	5.23	125.15	119.76
1	C	214	ILE	C-N-CA	5.23	125.15	119.76
1	A	63	ASN	CA-C-N	-5.14	115.57	123.07
1	A	63	ASN	C-N-CA	-5.14	115.57	123.07
1	C	63	ASN	CA-C-N	-5.13	115.58	123.07
1	C	63	ASN	C-N-CA	-5.13	115.58	123.07
1	B	63	ASN	CA-C-N	-5.13	115.58	123.07
1	B	63	ASN	C-N-CA	-5.13	115.58	123.07
1	C	266	SER	N-CA-C	5.13	115.30	108.38
1	B	266	SER	N-CA-C	5.10	115.27	108.38
1	A	226	ILE	CA-C-N	5.09	125.54	120.04
1	A	226	ILE	C-N-CA	5.09	125.54	120.04
1	A	266	SER	N-CA-C	5.09	115.25	108.38
1	C	226	ILE	CA-C-N	5.09	125.53	120.04
1	C	226	ILE	C-N-CA	5.09	125.53	120.04
1	B	226	ILE	N-CA-C	5.07	113.51	107.73
1	B	262	SER	CA-C-N	-5.07	113.36	120.56
1	B	262	SER	C-N-CA	-5.07	113.36	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	226	ILE	CA-C-N	5.07	125.52	120.04
1	B	226	ILE	C-N-CA	5.07	125.52	120.04
1	C	262	SER	CA-C-N	-5.06	113.37	120.56
1	C	262	SER	C-N-CA	-5.06	113.37	120.56
1	A	262	SER	CA-C-N	-5.06	113.38	120.56
1	A	262	SER	C-N-CA	-5.06	113.38	120.56
1	C	226	ILE	N-CA-C	5.05	113.49	107.73
1	A	226	ILE	N-CA-C	5.04	113.48	107.73
1	C	44	GLN	O-C-N	5.02	129.31	122.48
1	B	44	GLN	O-C-N	5.02	129.30	122.48
1	A	44	GLN	O-C-N	5.01	129.30	122.48

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	A	2442	0	2400	12	0
1	B	2442	0	2400	12	0
1	C	2442	0	2400	13	0
2	D	1345	0	1271	2	0
2	E	1345	0	1271	2	0
2	F	1345	0	1271	2	0
3	A	126	0	117	0	0
3	B	126	0	117	0	0
3	C	126	0	117	0	0
3	D	14	0	13	0	0
3	E	14	0	13	0	0
3	F	14	0	13	0	0
All	All	11781	0	11403	40	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 2.

All (40) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:VAL:HG21	1:A:317:ALA:HB1	1.80	0.63
1:C:36:VAL:HG21	1:C:317:ALA:HB1	1.80	0.63
1:B:36:VAL:HG21	1:B:317:ALA:HB1	1.80	0.62
2:E:127:ARG:HH21	2:F:134:GLY:H	1.54	0.56
1:C:26:VAL:CG1	1:C:36:VAL:HG11	2.37	0.55
1:A:26:VAL:CG1	1:A:36:VAL:HG11	2.37	0.55
1:B:26:VAL:CG1	1:B:36:VAL:HG11	2.37	0.55
1:C:60:ASP:N	1:C:60:ASP:OD1	2.39	0.55
2:D:127:ARG:HH21	2:E:134:GLY:H	1.54	0.55
2:D:134:GLY:H	2:F:127:ARG:HH21	1.54	0.54
1:B:60:ASP:N	1:B:60:ASP:OD1	2.39	0.53
1:A:60:ASP:N	1:A:60:ASP:OD1	2.39	0.53
1:A:26:VAL:HG13	1:A:36:VAL:HG11	1.93	0.51
1:B:26:VAL:HG13	1:B:36:VAL:HG11	1.93	0.51
1:B:125:PHE:HD1	1:B:166:VAL:HG11	1.76	0.51
1:A:125:PHE:HD1	1:A:166:VAL:HG11	1.76	0.51
1:C:26:VAL:HG13	1:C:36:VAL:HG11	1.93	0.50
1:C:125:PHE:HD1	1:C:166:VAL:HG11	1.76	0.50
1:A:26:VAL:HG13	1:A:36:VAL:CG1	2.42	0.50
1:B:26:VAL:HG13	1:B:36:VAL:CG1	2.42	0.50
1:C:26:VAL:HG13	1:C:36:VAL:CG1	2.42	0.50
1:C:77:ASP:N	1:C:77:ASP:OD1	2.45	0.49
1:A:85:ASP:OD1	1:A:264:LYS:NZ	2.46	0.49
1:B:85:ASP:OD1	1:B:264:LYS:NZ	2.46	0.49
1:C:85:ASP:OD1	1:C:264:LYS:NZ	2.46	0.48
1:B:61:GLY:O	1:B:62:GLU:C	2.56	0.47
1:A:61:GLY:O	1:A:62:GLU:C	2.56	0.47
1:B:77:ASP:OD1	1:B:77:ASP:N	2.45	0.46
1:C:61:GLY:O	1:C:62:GLU:C	2.56	0.46
1:A:77:ASP:N	1:A:77:ASP:OD1	2.45	0.44
1:A:296:ASN:N	1:A:296:ASN:OD1	2.50	0.44
1:B:305:CYS:HA	1:B:306:PRO:HD3	1.88	0.43
1:C:36:VAL:HG21	1:C:317:ALA:CB	2.49	0.42
1:A:36:VAL:HG21	1:A:317:ALA:CB	2.49	0.41
1:C:305:CYS:HA	1:C:306:PRO:HD3	1.88	0.41
1:A:31:ASN:OD1	1:A:32:ASP:N	2.54	0.41
1:B:296:ASN:OD1	1:B:296:ASN:N	2.50	0.41
1:C:296:ASN:OD1	1:C:296:ASN:N	2.50	0.41
1:B:36:VAL:HG21	1:B:317:ALA:CB	2.49	0.40
1:C:31:ASN:OD1	1:C:32:ASP:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	311/340 (92%)	301 (97%)	9 (3%)	1 (0%)	37	68
1	B	311/340 (92%)	301 (97%)	9 (3%)	1 (0%)	37	68
1	C	311/340 (92%)	301 (97%)	9 (3%)	1 (0%)	37	68
2	D	162/486 (33%)	160 (99%)	2 (1%)	0	100	100
2	E	162/486 (33%)	160 (99%)	2 (1%)	0	100	100
2	F	162/486 (33%)	160 (99%)	2 (1%)	0	100	100
All	All	1419/2478 (57%)	1383 (98%)	33 (2%)	3 (0%)	45	74

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	285	ASN
1	B	285	ASN
1	C	285	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	276/298 (93%)	276 (100%)	0	100	100
1	B	276/298 (93%)	276 (100%)	0	100	100
1	C	276/298 (93%)	276 (100%)	0	100	100
2	D	144/418 (34%)	144 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	144/418 (34%)	144 (100%)	0	100	100
2	F	144/418 (34%)	144 (100%)	0	100	100
All	All	1260/2148 (59%)	1260 (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 (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	47	GLN
2	E	47	GLN
2	F	47	GLN

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](#)

30 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	$\# Z > 2$
3	NAG	C	408	1	14,14,15	0.64	0	17,19,21	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	403	1	14,14,15	0.38	0	17,19,21	1.48	4 (23%)
3	NAG	B	401	1	14,14,15	0.48	0	17,19,21	1.21	2 (11%)
3	NAG	C	404	1	14,14,15	0.58	0	17,19,21	1.17	3 (17%)
3	NAG	A	406	1	14,14,15	0.33	0	17,19,21	1.47	2 (11%)
3	NAG	C	407	1	14,14,15	0.48	0	17,19,21	0.90	0
3	NAG	C	405	1	14,14,15	0.28	0	17,19,21	1.06	1 (5%)
3	NAG	B	409	1	14,14,15	0.36	0	17,19,21	0.73	0
3	NAG	A	407	1	14,14,15	0.49	0	17,19,21	0.91	0
3	NAG	A	404	1	14,14,15	0.57	0	17,19,21	1.17	2 (11%)
3	NAG	C	402	1	14,14,15	0.62	0	17,19,21	1.56	4 (23%)
3	NAG	A	402	1	14,14,15	0.61	0	17,19,21	1.57	4 (23%)
3	NAG	B	408	1	14,14,15	0.63	0	17,19,21	0.63	0
3	NAG	A	405	1	14,14,15	0.29	0	17,19,21	1.06	1 (5%)
3	NAG	C	401	1	14,14,15	0.48	0	17,19,21	1.21	2 (11%)
3	NAG	A	403	1	14,14,15	0.38	0	17,19,21	1.48	4 (23%)
3	NAG	F	501	2	14,14,15	0.74	0	17,19,21	0.78	0
3	NAG	B	402	1	14,14,15	0.62	0	17,19,21	1.57	4 (23%)
3	NAG	A	401	1	14,14,15	0.48	0	17,19,21	1.21	2 (11%)
3	NAG	C	406	1	14,14,15	0.32	0	17,19,21	1.46	2 (11%)
3	NAG	B	404	1	14,14,15	0.58	0	17,19,21	1.17	2 (11%)
3	NAG	A	409	1	14,14,15	0.36	0	17,19,21	0.73	0
3	NAG	A	408	1	14,14,15	0.63	0	17,19,21	0.63	0
3	NAG	B	406	1	14,14,15	0.32	0	17,19,21	1.46	2 (11%)
3	NAG	C	409	1	14,14,15	0.36	0	17,19,21	0.73	0
3	NAG	B	405	1	14,14,15	0.28	0	17,19,21	1.06	1 (5%)
3	NAG	B	407	1	14,14,15	0.49	0	17,19,21	0.91	0
3	NAG	E	501	2	14,14,15	0.73	0	17,19,21	0.78	0
3	NAG	D	501	2	14,14,15	0.74	0	17,19,21	0.78	0
3	NAG	C	403	1	14,14,15	0.38	0	17,19,21	1.48	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	408	1	-	2/6/23/26	0/1/1/1
3	NAG	B	403	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	401	1	-	4/6/23/26	0/1/1/1
3	NAG	C	404	1	-	2/6/23/26	0/1/1/1
3	NAG	A	406	1	-	5/6/23/26	0/1/1/1
3	NAG	C	407	1	-	3/6/23/26	0/1/1/1
3	NAG	C	405	1	-	3/6/23/26	0/1/1/1
3	NAG	B	409	1	-	2/6/23/26	0/1/1/1
3	NAG	A	407	1	-	3/6/23/26	0/1/1/1
3	NAG	A	404	1	-	2/6/23/26	0/1/1/1
3	NAG	C	402	1	-	2/6/23/26	0/1/1/1
3	NAG	A	402	1	-	2/6/23/26	0/1/1/1
3	NAG	B	408	1	-	2/6/23/26	0/1/1/1
3	NAG	A	405	1	-	3/6/23/26	0/1/1/1
3	NAG	C	401	1	-	4/6/23/26	0/1/1/1
3	NAG	A	403	1	-	4/6/23/26	0/1/1/1
3	NAG	F	501	2	-	2/6/23/26	0/1/1/1
3	NAG	B	402	1	-	2/6/23/26	0/1/1/1
3	NAG	A	401	1	-	4/6/23/26	0/1/1/1
3	NAG	C	406	1	-	5/6/23/26	0/1/1/1
3	NAG	B	404	1	-	2/6/23/26	0/1/1/1
3	NAG	A	409	1	-	2/6/23/26	0/1/1/1
3	NAG	A	408	1	-	2/6/23/26	0/1/1/1
3	NAG	B	406	1	-	5/6/23/26	0/1/1/1
3	NAG	C	409	1	-	2/6/23/26	0/1/1/1
3	NAG	B	405	1	-	3/6/23/26	0/1/1/1
3	NAG	B	407	1	-	3/6/23/26	0/1/1/1
3	NAG	E	501	2	-	2/6/23/26	0/1/1/1
3	NAG	D	501	2	-	2/6/23/26	0/1/1/1
3	NAG	C	403	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	NAG	C2-N2-C7	-4.66	116.65	122.90
3	C	402	NAG	C2-N2-C7	-4.66	116.66	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	NAG	C2-N2-C7	-4.65	116.66	122.90
3	C	406	NAG	C2-N2-C7	4.10	128.40	122.90
3	B	406	NAG	C2-N2-C7	4.10	128.40	122.90
3	A	406	NAG	C2-N2-C7	4.09	128.39	122.90
3	A	403	NAG	C1-O5-C5	4.04	117.60	112.19
3	B	403	NAG	C1-O5-C5	4.03	117.59	112.19
3	C	403	NAG	C1-O5-C5	4.01	117.56	112.19
3	A	406	NAG	C1-O5-C5	3.16	116.42	112.19
3	C	406	NAG	C1-O5-C5	3.14	116.40	112.19
3	B	406	NAG	C1-O5-C5	3.13	116.39	112.19
3	C	401	NAG	C4-C3-C2	-3.10	106.48	111.02
3	A	401	NAG	C4-C3-C2	-3.09	106.48	111.02
3	B	401	NAG	C4-C3-C2	-3.08	106.50	111.02
3	C	404	NAG	C4-C3-C2	-2.93	106.73	111.02
3	B	404	NAG	C4-C3-C2	-2.91	106.75	111.02
3	A	404	NAG	C4-C3-C2	-2.91	106.76	111.02
3	B	401	NAG	C2-N2-C7	-2.78	119.17	122.90
3	C	401	NAG	C2-N2-C7	-2.78	119.17	122.90
3	A	401	NAG	C2-N2-C7	-2.77	119.18	122.90
3	B	405	NAG	C2-N2-C7	2.61	126.40	122.90
3	A	405	NAG	C2-N2-C7	2.61	126.40	122.90
3	C	405	NAG	C2-N2-C7	2.60	126.38	122.90
3	A	402	NAG	O5-C1-C2	-2.36	107.64	111.29
3	B	402	NAG	O5-C1-C2	-2.34	107.67	111.29
3	C	402	NAG	O5-C1-C2	-2.34	107.67	111.29
3	A	403	NAG	O5-C1-C2	2.24	114.76	111.29
3	C	403	NAG	O5-C1-C2	2.24	114.76	111.29
3	B	403	NAG	O5-C1-C2	2.24	114.76	111.29
3	B	403	NAG	C3-C4-C5	2.23	114.27	110.23
3	A	403	NAG	C3-C4-C5	2.23	114.27	110.23
3	C	403	NAG	C3-C4-C5	2.21	114.25	110.23
3	A	402	NAG	C1-O5-C5	2.20	115.14	112.19
3	C	402	NAG	C1-O5-C5	2.19	115.12	112.19
3	B	402	NAG	C1-O5-C5	2.18	115.11	112.19
3	A	404	NAG	O5-C1-C2	-2.09	108.06	111.29
3	C	404	NAG	O5-C1-C2	-2.07	108.09	111.29
3	B	404	NAG	O5-C1-C2	-2.07	108.09	111.29
3	B	402	NAG	C4-C3-C2	-2.03	108.04	111.02
3	C	402	NAG	C4-C3-C2	-2.03	108.04	111.02
3	A	402	NAG	C4-C3-C2	-2.03	108.04	111.02
3	B	403	NAG	C1-C2-N2	-2.03	107.24	110.43
3	A	403	NAG	C1-C2-N2	-2.02	107.24	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	403	NAG	C1-C2-N2	-2.02	107.24	110.43
3	C	404	NAG	O5-C5-C4	-2.00	105.96	110.83

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	NAG	C8-C7-N2-C2
3	A	402	NAG	O7-C7-N2-C2
3	A	403	NAG	C8-C7-N2-C2
3	A	403	NAG	O7-C7-N2-C2
3	A	405	NAG	C8-C7-N2-C2
3	A	405	NAG	O7-C7-N2-C2
3	A	406	NAG	C8-C7-N2-C2
3	A	406	NAG	O7-C7-N2-C2
3	A	407	NAG	C8-C7-N2-C2
3	A	407	NAG	O7-C7-N2-C2
3	B	402	NAG	C8-C7-N2-C2
3	B	402	NAG	O7-C7-N2-C2
3	B	403	NAG	C8-C7-N2-C2
3	B	403	NAG	O7-C7-N2-C2
3	B	405	NAG	C8-C7-N2-C2
3	B	405	NAG	O7-C7-N2-C2
3	B	406	NAG	C8-C7-N2-C2
3	B	406	NAG	O7-C7-N2-C2
3	B	407	NAG	C8-C7-N2-C2
3	B	407	NAG	O7-C7-N2-C2
3	C	402	NAG	C8-C7-N2-C2
3	C	402	NAG	O7-C7-N2-C2
3	C	403	NAG	C8-C7-N2-C2
3	C	403	NAG	O7-C7-N2-C2
3	C	405	NAG	C8-C7-N2-C2
3	C	405	NAG	O7-C7-N2-C2
3	C	406	NAG	C8-C7-N2-C2
3	C	406	NAG	O7-C7-N2-C2
3	C	407	NAG	C8-C7-N2-C2
3	C	407	NAG	O7-C7-N2-C2
3	A	404	NAG	O5-C5-C6-O6
3	B	404	NAG	O5-C5-C6-O6
3	C	404	NAG	O5-C5-C6-O6
3	A	403	NAG	C4-C5-C6-O6
3	B	403	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	C	403	NAG	C4-C5-C6-O6
3	A	409	NAG	C8-C7-N2-C2
3	A	409	NAG	O7-C7-N2-C2
3	D	501	NAG	C8-C7-N2-C2
3	D	501	NAG	O7-C7-N2-C2
3	B	409	NAG	C8-C7-N2-C2
3	B	409	NAG	O7-C7-N2-C2
3	E	501	NAG	C8-C7-N2-C2
3	E	501	NAG	O7-C7-N2-C2
3	C	409	NAG	O7-C7-N2-C2
3	F	501	NAG	C8-C7-N2-C2
3	F	501	NAG	O7-C7-N2-C2
3	A	403	NAG	O5-C5-C6-O6
3	B	403	NAG	O5-C5-C6-O6
3	C	403	NAG	O5-C5-C6-O6
3	A	404	NAG	C4-C5-C6-O6
3	B	404	NAG	C4-C5-C6-O6
3	C	404	NAG	C4-C5-C6-O6
3	A	406	NAG	C4-C5-C6-O6
3	B	406	NAG	C4-C5-C6-O6
3	C	406	NAG	C4-C5-C6-O6
3	C	409	NAG	C8-C7-N2-C2
3	A	406	NAG	O5-C5-C6-O6
3	B	406	NAG	O5-C5-C6-O6
3	C	406	NAG	O5-C5-C6-O6
3	A	401	NAG	C8-C7-N2-C2
3	B	401	NAG	C8-C7-N2-C2
3	C	401	NAG	C8-C7-N2-C2
3	A	401	NAG	O7-C7-N2-C2
3	B	401	NAG	O7-C7-N2-C2
3	C	401	NAG	O7-C7-N2-C2
3	A	401	NAG	C4-C5-C6-O6
3	B	401	NAG	C4-C5-C6-O6
3	C	401	NAG	C4-C5-C6-O6
3	A	407	NAG	O5-C5-C6-O6
3	B	407	NAG	O5-C5-C6-O6
3	C	407	NAG	O5-C5-C6-O6
3	A	401	NAG	O5-C5-C6-O6
3	B	401	NAG	O5-C5-C6-O6
3	C	401	NAG	O5-C5-C6-O6
3	A	405	NAG	C3-C2-N2-C7
3	A	406	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	B	405	NAG	C3-C2-N2-C7
3	B	406	NAG	C3-C2-N2-C7
3	C	405	NAG	C3-C2-N2-C7
3	C	406	NAG	C3-C2-N2-C7
3	A	408	NAG	C4-C5-C6-O6
3	B	408	NAG	C4-C5-C6-O6
3	C	408	NAG	C4-C5-C6-O6
3	A	408	NAG	O5-C5-C6-O6
3	C	408	NAG	O5-C5-C6-O6
3	B	408	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.

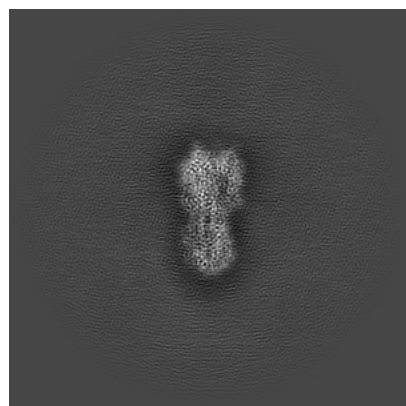
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46466. These allow visual inspection of the internal detail of the map and identification of artifacts.

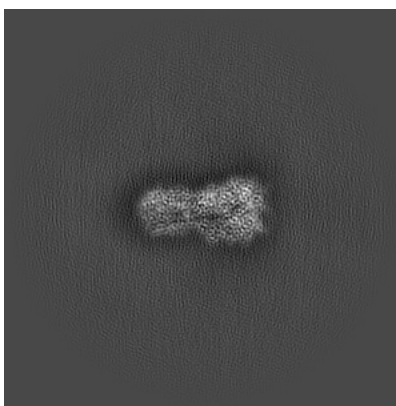
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

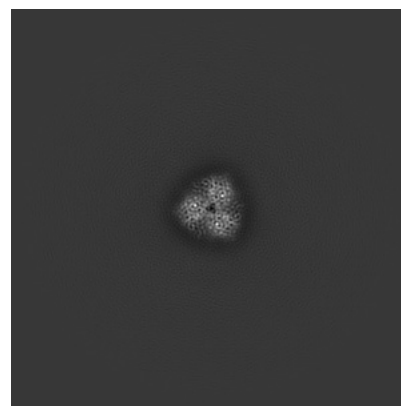
6.1.1 Primary map



X

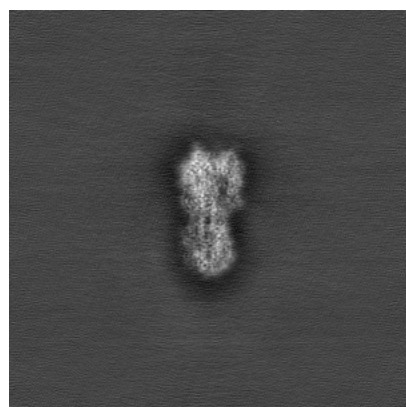


Y

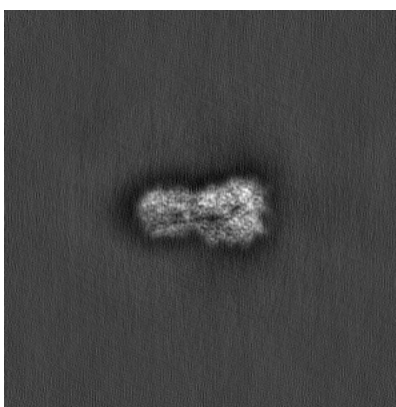


Z

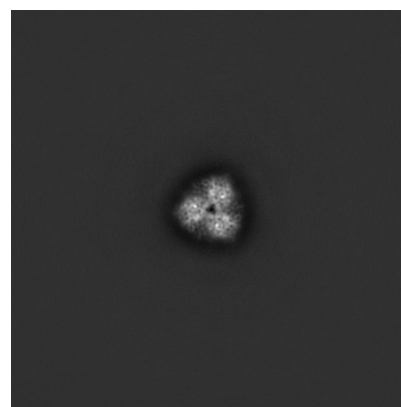
6.1.2 Raw map



X



Y

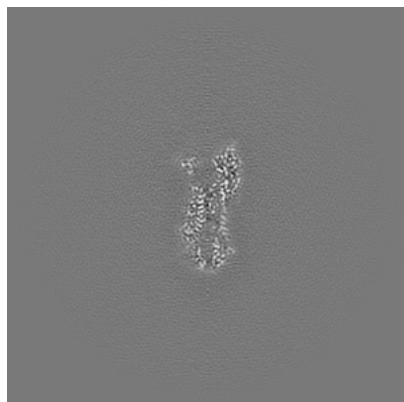


Z

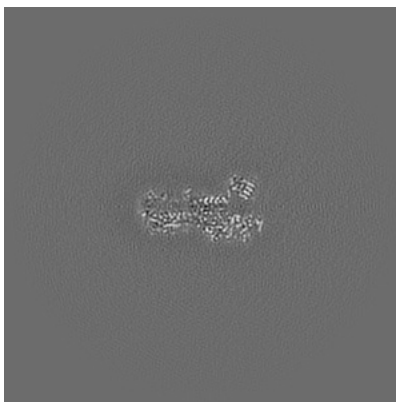
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

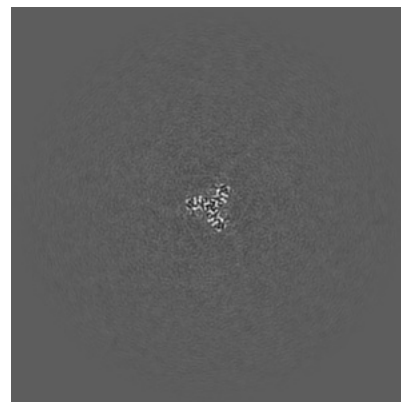
6.2.1 Primary map



X Index: 180

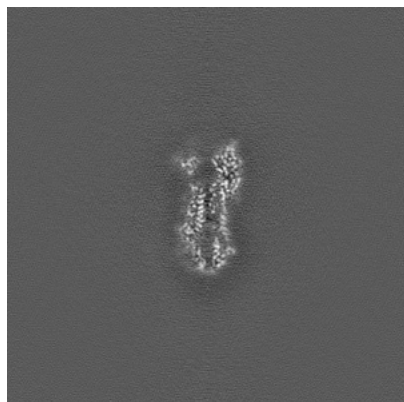


Y Index: 180

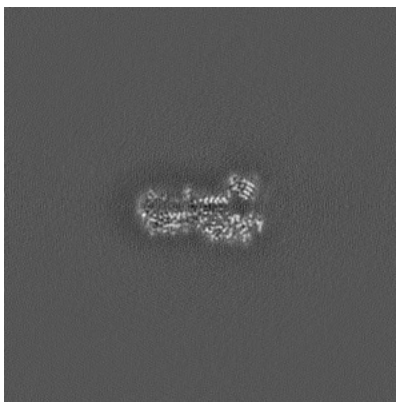


Z Index: 180

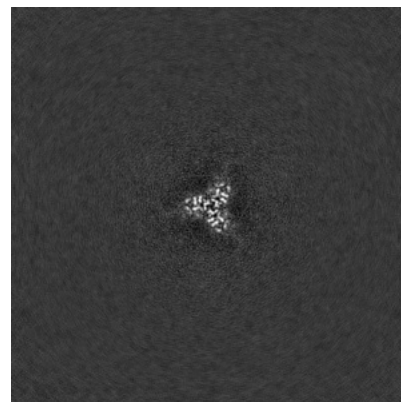
6.2.2 Raw map



X Index: 180



Y Index: 180

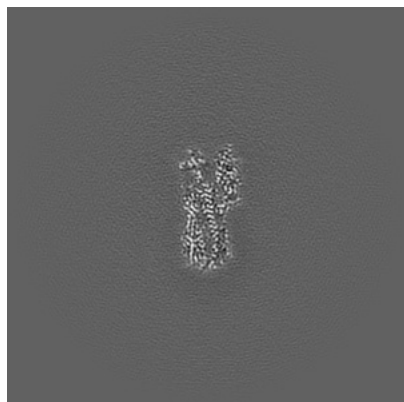


Z Index: 180

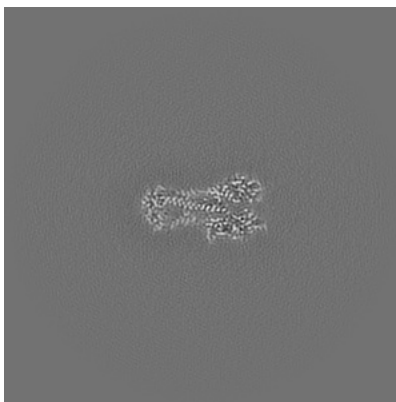
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

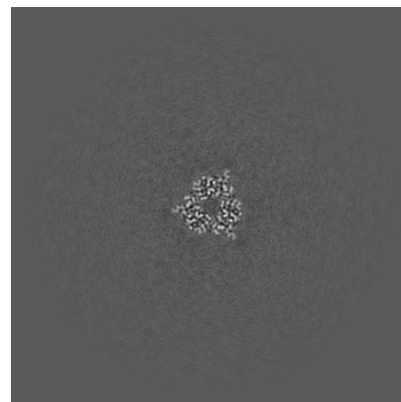
6.3.1 Primary map



X Index: 185

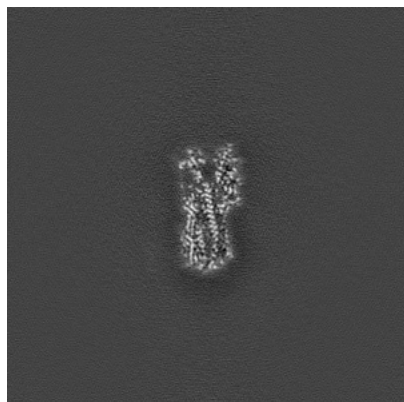


Y Index: 173

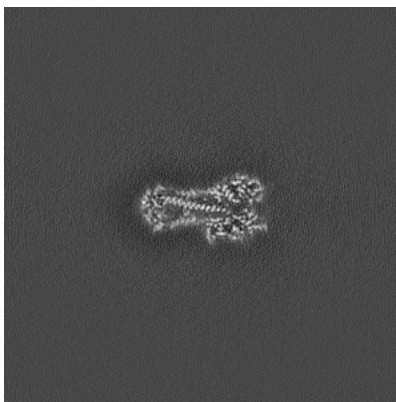


Z Index: 215

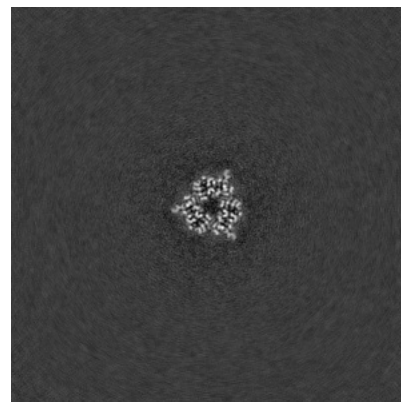
6.3.2 Raw map



X Index: 185



Y Index: 173

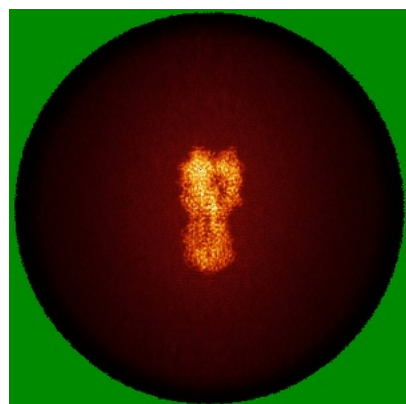


Z Index: 215

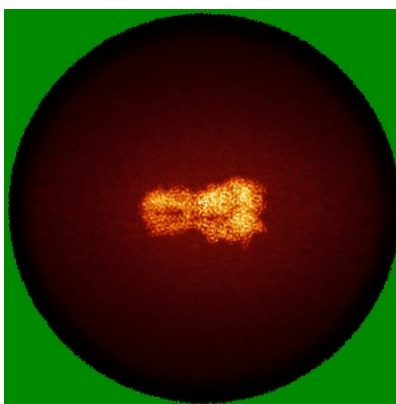
The images above show the largest variance slices of the map in three orthogonal directions.

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

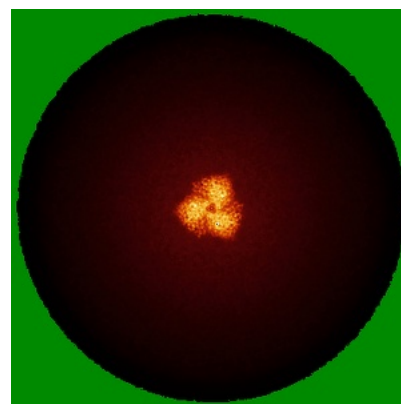
6.4.1 Primary map



X



Y

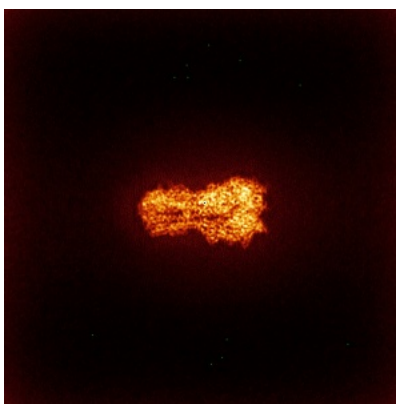


Z

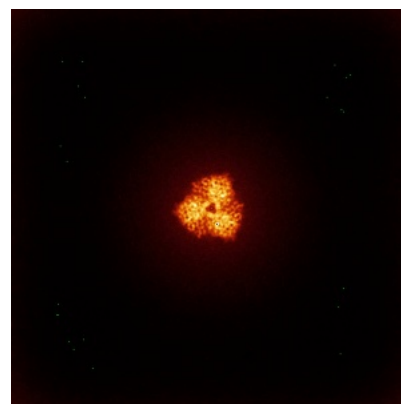
6.4.2 Raw map



X



Y

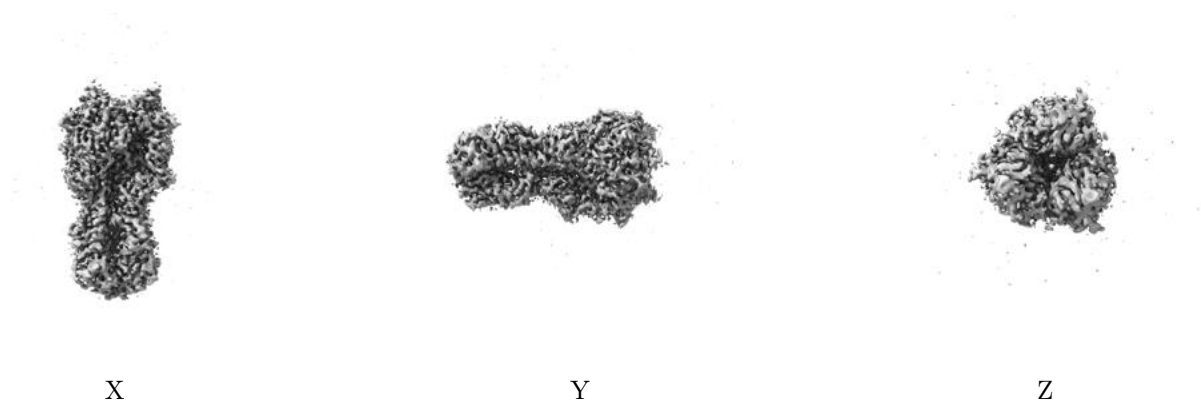


Z

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.

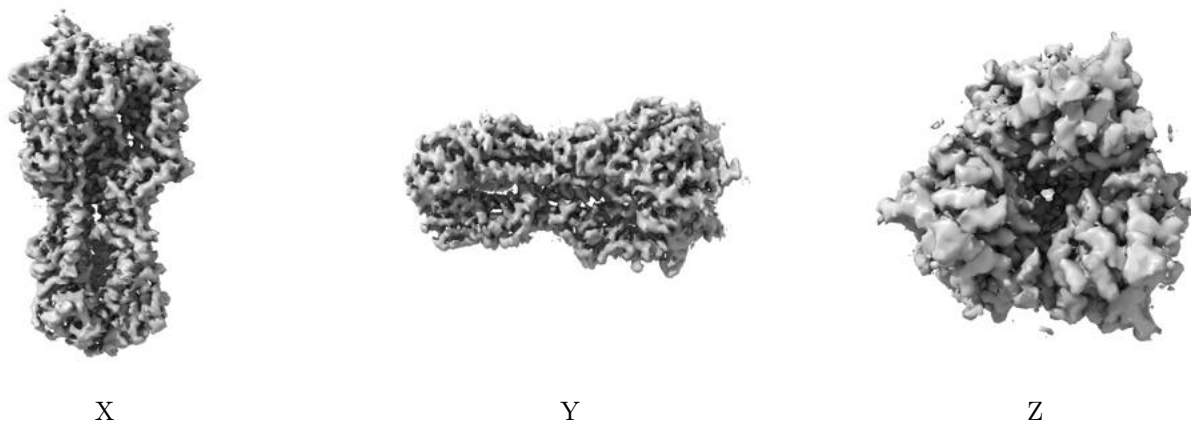
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. 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.

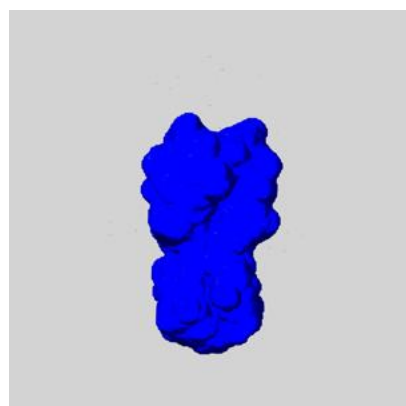
6.6 Mask visualisation [i](#)

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

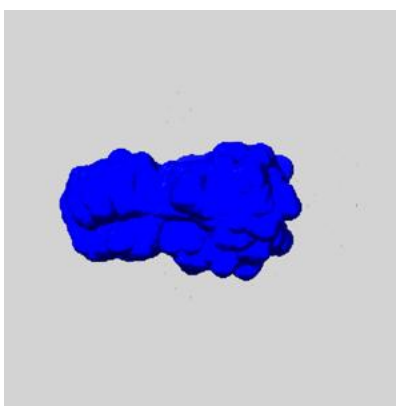
A mask typically either:

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

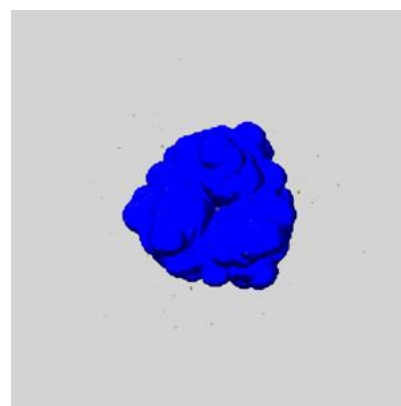
6.6.1 emd_46466_msk_1.map [i](#)



X



Y

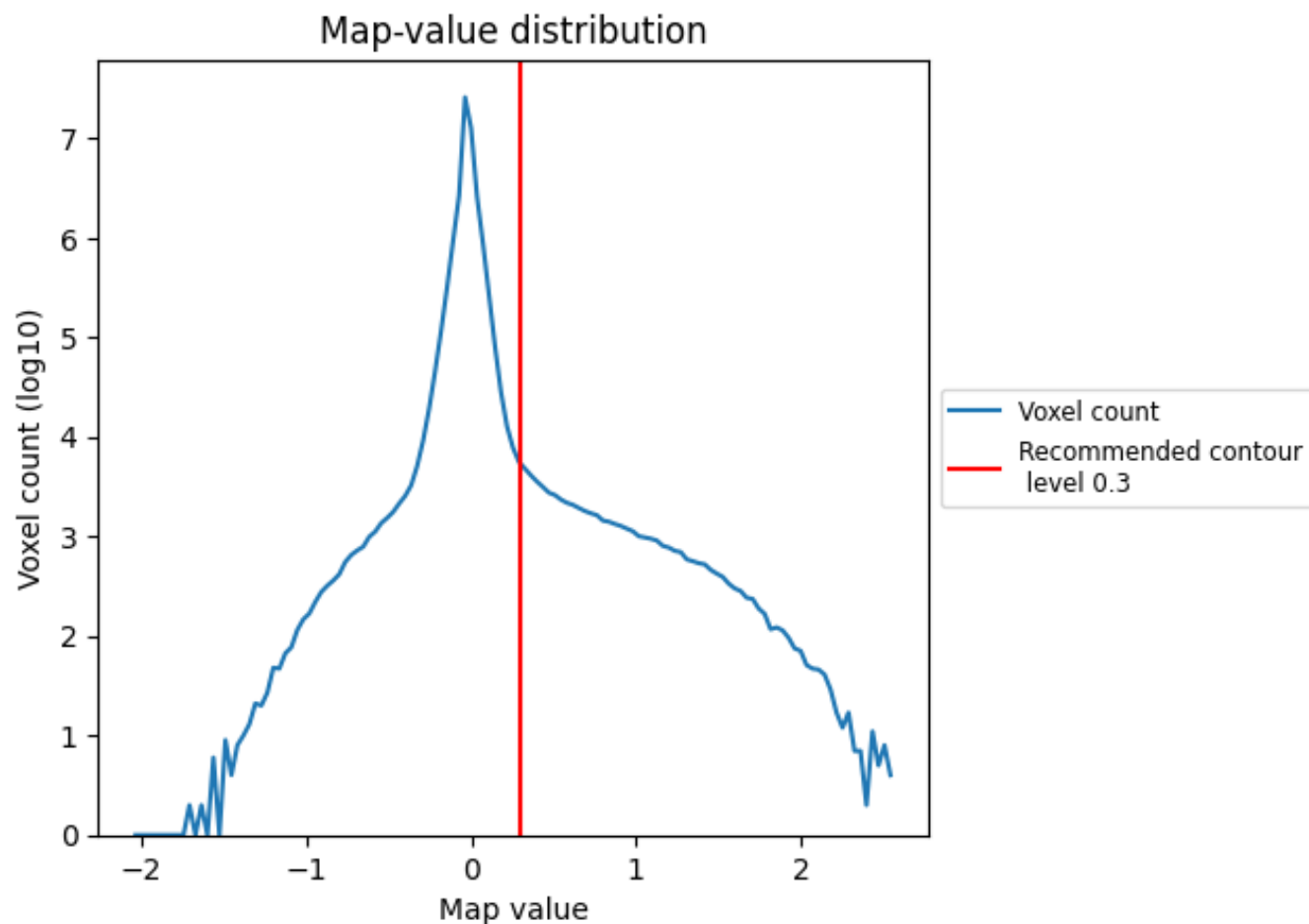


Z

7 Map analysis [i](#)

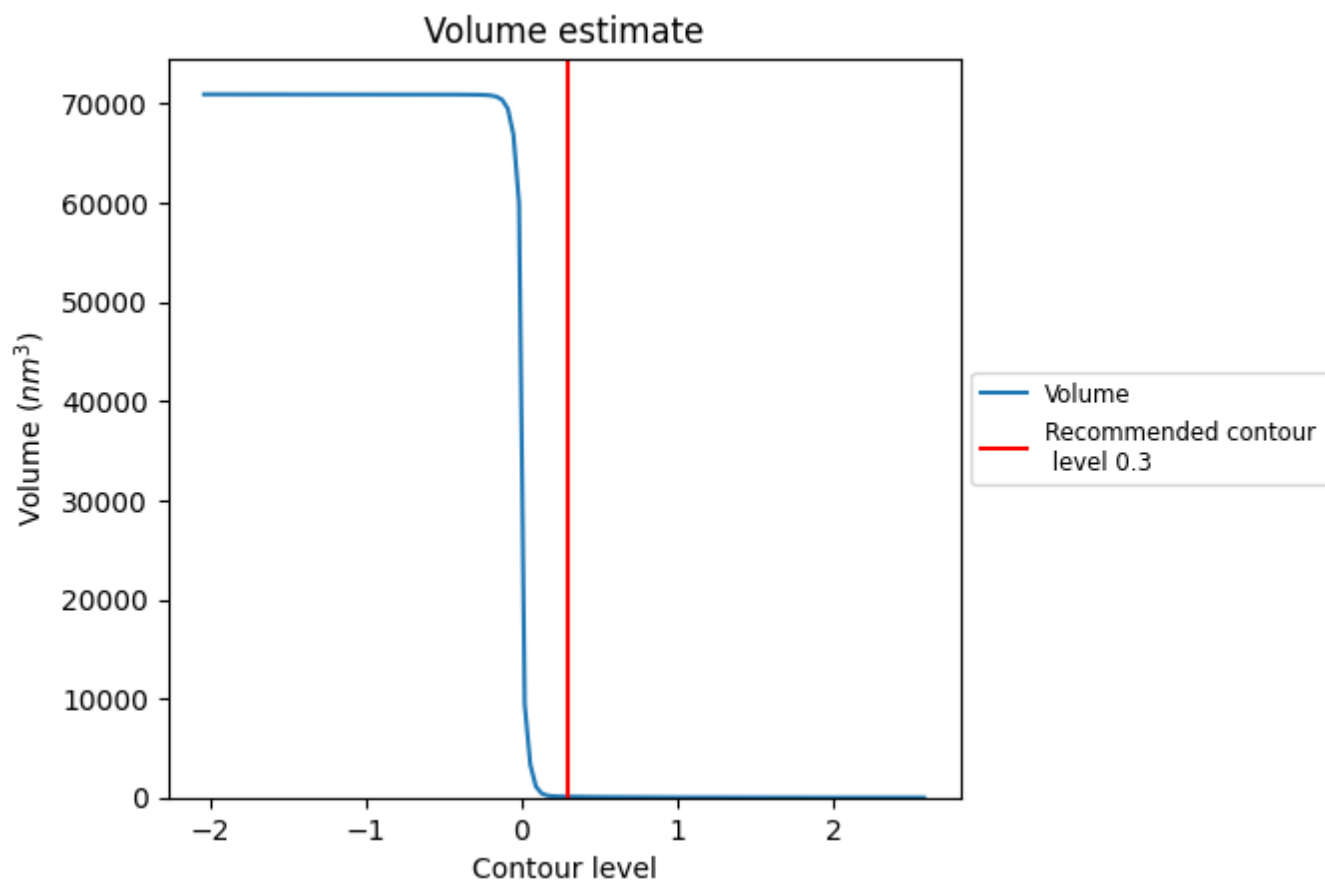
This section contains the results of statistical analysis of the map.

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.

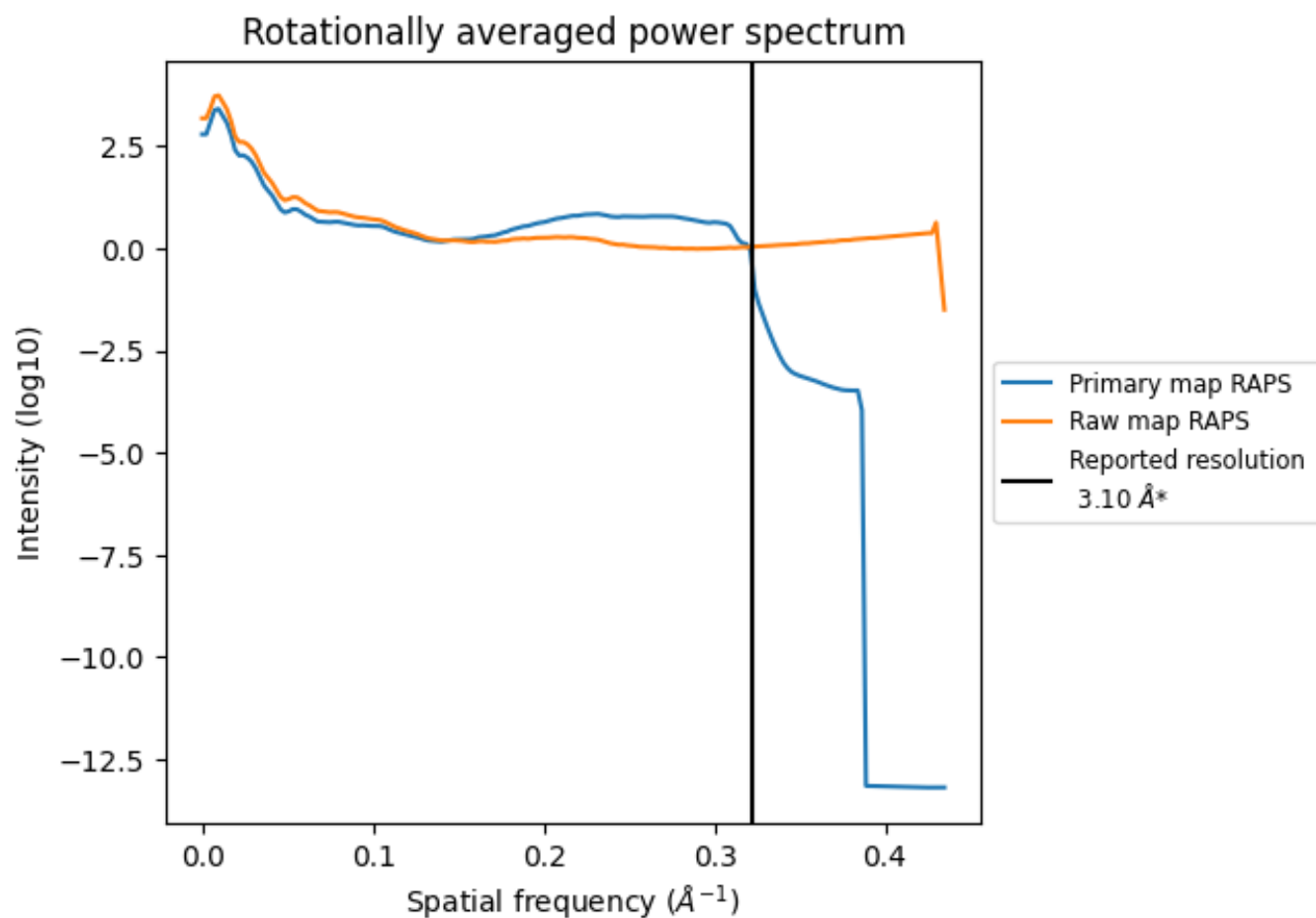
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 91 nm³; 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 ⓘ

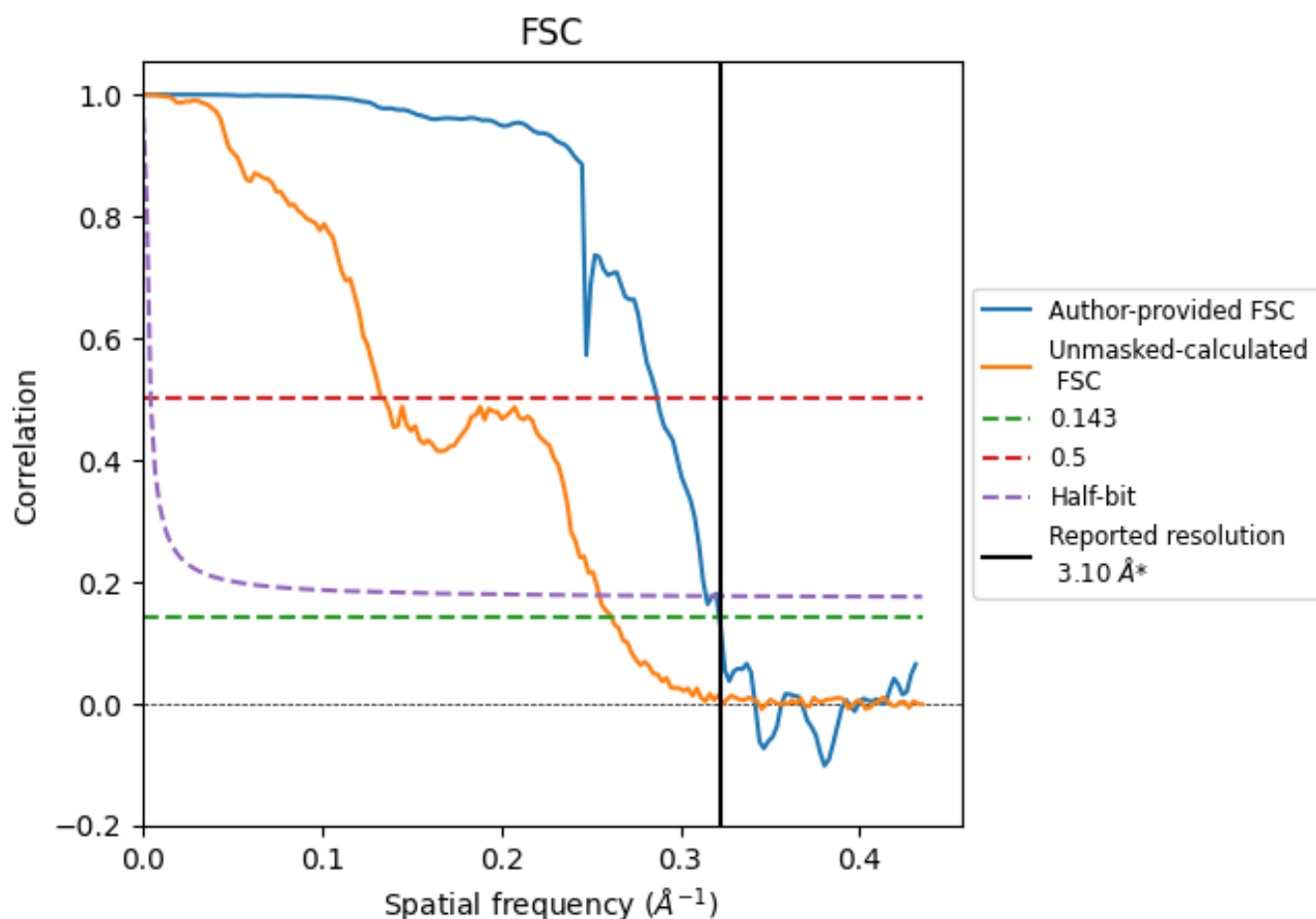


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 \AA^{-1}

8.2 Resolution estimates [i](#)

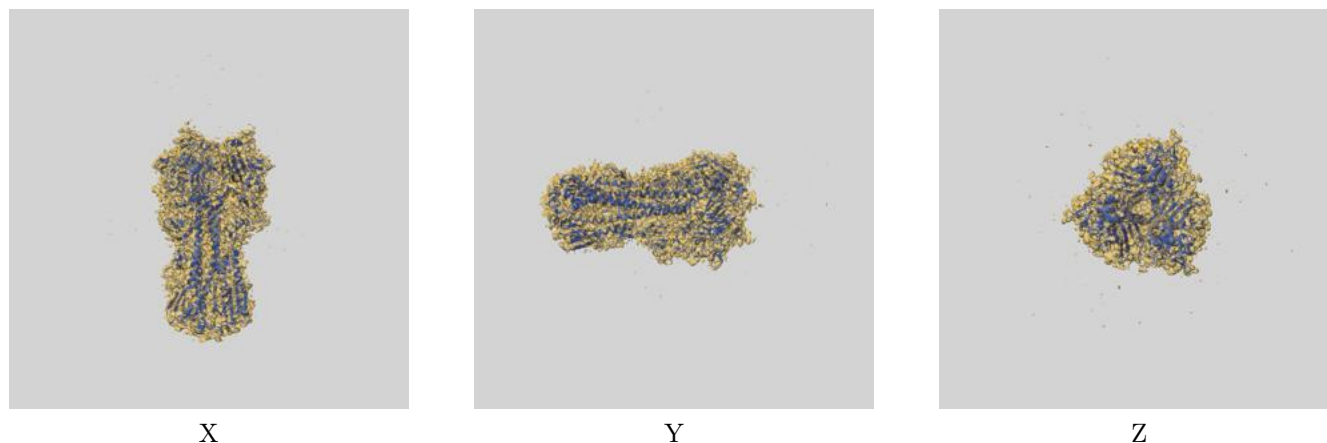
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.11	3.48	3.18
Unmasked-calculated*	3.83	7.43	3.92

*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 3.83 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

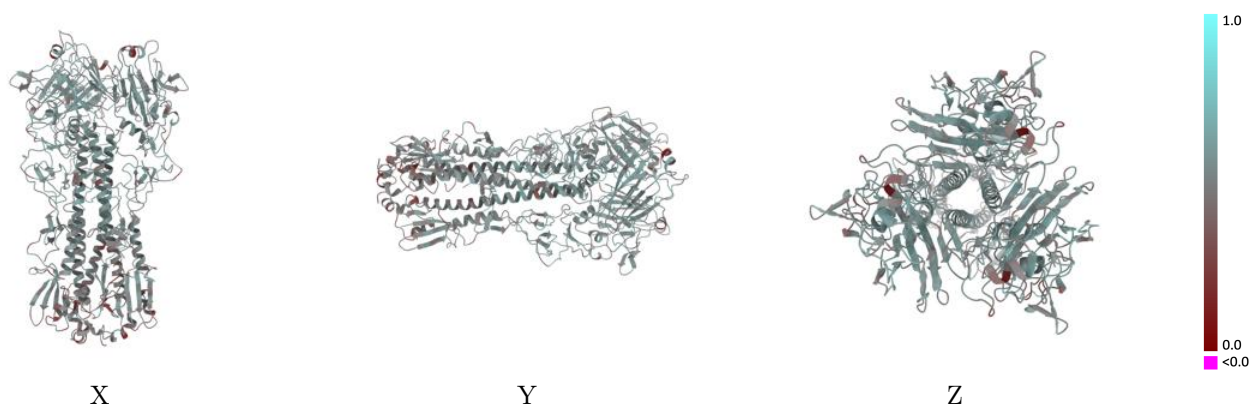
This section contains information regarding the fit between EMDB map EMD-46466 and PDB model 9D0Y. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



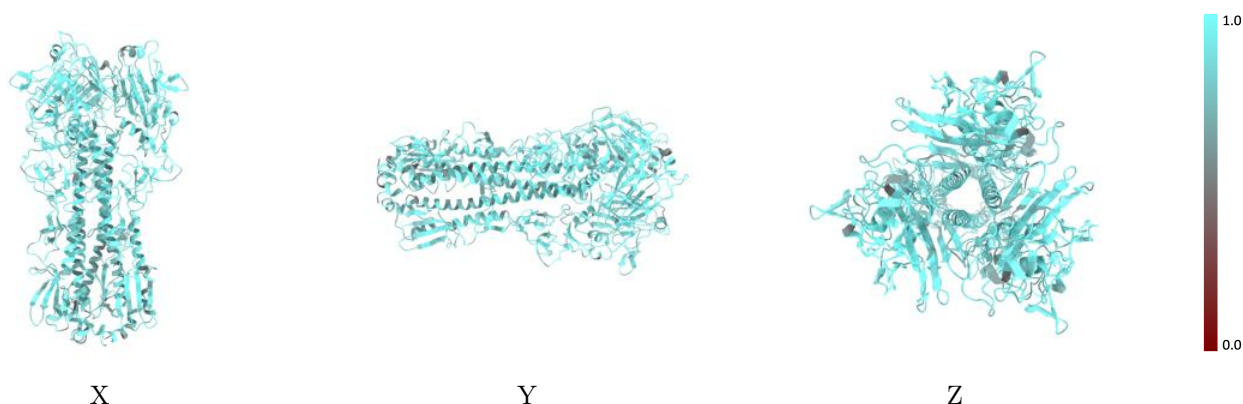
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



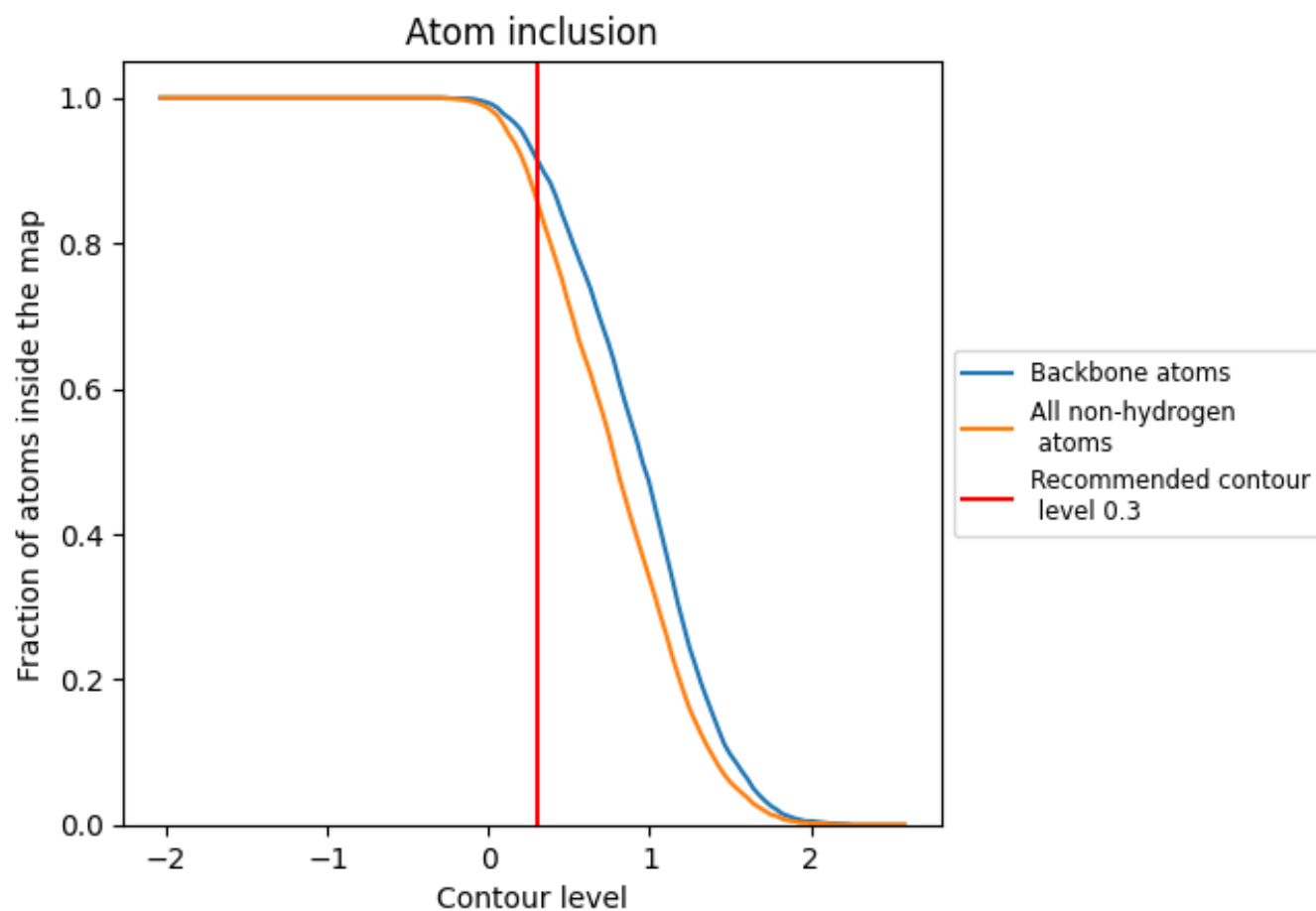
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 86% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8590	<div><div></div></div> 0.5080
A	<div><div></div></div> 0.8790	<div><div></div></div> 0.5250
B	<div><div></div></div> 0.8760	<div><div></div></div> 0.5230
C	<div><div></div></div> 0.8770	<div><div></div></div> 0.5230
D	<div><div></div></div> 0.8220	<div><div></div></div> 0.4790
E	<div><div></div></div> 0.8260	<div><div></div></div> 0.4760
F	<div><div></div></div> 0.8220	<div><div></div></div> 0.4750

1.0

0.0

<0.0