Full wwPDB EM Validation Report

Jan 20, 2025 – 05:08 PM JST

PDB ID	:	8Z6R
EMDB ID	:	EMD-39802
Title	:	Structure of XBB.1.16 S trimer with 3 down-RBDs complex with antibody CYFN1006-1.
Authors	:	Wang, Y.J.; Sun, L.
Deposited on	:	2024-04-19
Resolution	:	2.87 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:

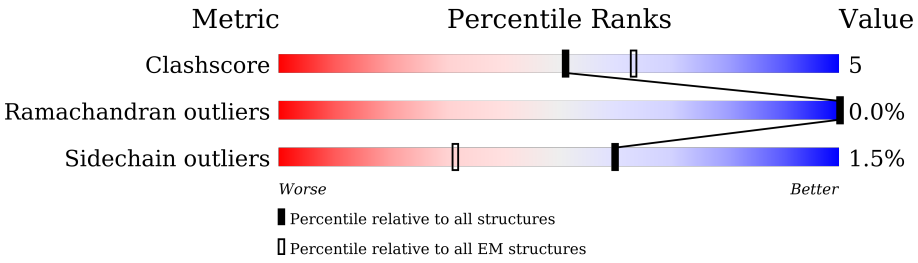
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.87 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	A	1299	67% 13% 19%
1	B	1299	67% 14% 19%
1	C	1299	68% 12% · 19%
2	D	215	6% 78% 11% 11%
2	F	215	6% 80% 9% 11%
2	H	215	7% 80% 9% 11%
3	E	451	7% 40% · 55%
3	G	451	· 37% 6% 56%

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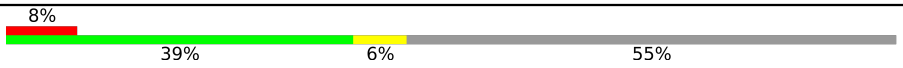
Mol	Chain	Length	Quality of chain
3	I	451	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 33554 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein,Fibritin,Spike glycoprotein,Fibritin,Spike glycoprotein,Fibritin,Expression Tag.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1051	Total	C	N	O	S	0	0
			8229	5274	1361	1554	40		
1	B	1050	Total	C	N	O	S	0	0
			8221	5270	1359	1552	40		
1	C	1051	Total	C	N	O	S	0	0
			8229	5274	1361	1554	40		

There are 243 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP P0DTC2
A	-5	PRO	-	expression tag	UNP P0DTC2
A	-4	MET	-	expression tag	UNP P0DTC2
A	-3	GLY	-	expression tag	UNP P0DTC2
A	-2	SER	-	expression tag	UNP P0DTC2
A	-1	LEU	-	expression tag	UNP P0DTC2
A	0	GLN	-	expression tag	UNP P0DTC2
A	1	PRO	-	expression tag	UNP P0DTC2
A	2	LEU	-	expression tag	UNP P0DTC2
A	3	ALA	-	expression tag	UNP P0DTC2
A	4	THR	-	expression tag	UNP P0DTC2
A	5	LEU	-	expression tag	UNP P0DTC2
A	6	TYR	-	expression tag	UNP P0DTC2
A	7	LEU	-	expression tag	UNP P0DTC2
A	8	LEU	-	expression tag	UNP P0DTC2
A	9	GLY	-	expression tag	UNP P0DTC2
A	10	MET	-	expression tag	UNP P0DTC2
A	11	LEU	-	expression tag	UNP P0DTC2
A	12	VAL	-	expression tag	UNP P0DTC2
A	13	ALA	-	expression tag	UNP P0DTC2
A	14	SER	-	expression tag	UNP P0DTC2
A	15	VAL	-	expression tag	UNP P0DTC2
A	16	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	17	ALA	-	expression tag	UNP P0DTC2
A	23	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	28	SER	ALA	variant	UNP P0DTC2
A	84	ALA	VAL	variant	UNP P0DTC2
A	143	ASP	GLY	variant	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	146	GLN	HIS	variant	UNP P0DTC2
A	180	VAL	GLU	conflict	UNP P0DTC2
A	183	GLU	GLN	variant	UNP P0DTC2
A	213	GLU	VAL	variant	UNP P0DTC2
A	252	VAL	GLY	variant	UNP P0DTC2
A	339	HIS	GLY	variant	UNP P0DTC2
A	346	THR	ARG	variant	UNP P0DTC2
A	368	ILE	LEU	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	445	PRO	VAL	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	460	LYS	ASN	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	ARG	THR	conflict	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	486	PRO	PHE	variant	UNP P0DTC2
A	490	SER	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	685	SER	-	insertion	UNP P0DTC2
A	686	SER	-	insertion	UNP P0DTC2
A	687	LYS	-	insertion	UNP P0DTC2
A	689	SER	-	insertion	UNP P0DTC2
A	768	LYS	ASN	variant	UNP P0DTC2
A	800	TYR	ASP	variant	UNP P0DTC2
A	821	PRO	PHE	conflict	UNP P0DTC2
A	896	PRO	ALA	conflict	UNP P0DTC2
A	903	PRO	ALA	conflict	UNP P0DTC2
A	946	PRO	ALA	conflict	UNP P0DTC2
A	958	HIS	GLN	variant	UNP P0DTC2
A	973	LYS	ASN	variant	UNP P0DTC2
A	990	PRO	LYS	variant	UNP P0DTC2
A	991	PRO	VAL	variant	UNP P0DTC2
A	1213	GLY	-	linker	UNP P0DTC2
A	1214	SER	-	linker	UNP P0DTC2
B	-6	MET	-	initiating methionine	UNP P0DTC2
B	-5	PRO	-	expression tag	UNP P0DTC2
B	-4	MET	-	expression tag	UNP P0DTC2
B	-3	GLY	-	expression tag	UNP P0DTC2
B	-2	SER	-	expression tag	UNP P0DTC2
B	-1	LEU	-	expression tag	UNP P0DTC2
B	0	GLN	-	expression tag	UNP P0DTC2
B	1	PRO	-	expression tag	UNP P0DTC2
B	2	LEU	-	expression tag	UNP P0DTC2
B	3	ALA	-	expression tag	UNP P0DTC2
B	4	THR	-	expression tag	UNP P0DTC2
B	5	LEU	-	expression tag	UNP P0DTC2
B	6	TYR	-	expression tag	UNP P0DTC2
B	7	LEU	-	expression tag	UNP P0DTC2
B	8	LEU	-	expression tag	UNP P0DTC2
B	9	GLY	-	expression tag	UNP P0DTC2
B	10	MET	-	expression tag	UNP P0DTC2
B	11	LEU	-	expression tag	UNP P0DTC2
B	12	VAL	-	expression tag	UNP P0DTC2
B	13	ALA	-	expression tag	UNP P0DTC2
B	14	SER	-	expression tag	UNP P0DTC2
B	15	VAL	-	expression tag	UNP P0DTC2
B	16	LEU	-	expression tag	UNP P0DTC2
B	17	ALA	-	expression tag	UNP P0DTC2
B	23	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	28	SER	ALA	variant	UNP P0DTC2
B	84	ALA	VAL	variant	UNP P0DTC2
B	143	ASP	GLY	variant	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	146	GLN	HIS	variant	UNP P0DTC2
B	180	VAL	GLU	conflict	UNP P0DTC2
B	183	GLU	GLN	variant	UNP P0DTC2
B	213	GLU	VAL	variant	UNP P0DTC2
B	252	VAL	GLY	variant	UNP P0DTC2
B	339	HIS	GLY	variant	UNP P0DTC2
B	346	THR	ARG	variant	UNP P0DTC2
B	368	ILE	LEU	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	445	PRO	VAL	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	460	LYS	ASN	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	ARG	THR	conflict	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	486	PRO	PHE	variant	UNP P0DTC2
B	490	SER	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	-	insertion	UNP P0DTC2
B	686	SER	-	insertion	UNP P0DTC2
B	687	LYS	-	insertion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	689	SER	-	insertion	UNP P0DTC2
B	768	LYS	ASN	variant	UNP P0DTC2
B	800	TYR	ASP	variant	UNP P0DTC2
B	821	PRO	PHE	conflict	UNP P0DTC2
B	896	PRO	ALA	conflict	UNP P0DTC2
B	903	PRO	ALA	conflict	UNP P0DTC2
B	946	PRO	ALA	conflict	UNP P0DTC2
B	958	HIS	GLN	variant	UNP P0DTC2
B	973	LYS	ASN	variant	UNP P0DTC2
B	990	PRO	LYS	variant	UNP P0DTC2
B	991	PRO	VAL	variant	UNP P0DTC2
B	1213	GLY	-	linker	UNP P0DTC2
B	1214	SER	-	linker	UNP P0DTC2
C	-6	MET	-	initiating methionine	UNP P0DTC2
C	-5	PRO	-	expression tag	UNP P0DTC2
C	-4	MET	-	expression tag	UNP P0DTC2
C	-3	GLY	-	expression tag	UNP P0DTC2
C	-2	SER	-	expression tag	UNP P0DTC2
C	-1	LEU	-	expression tag	UNP P0DTC2
C	0	GLN	-	expression tag	UNP P0DTC2
C	1	PRO	-	expression tag	UNP P0DTC2
C	2	LEU	-	expression tag	UNP P0DTC2
C	3	ALA	-	expression tag	UNP P0DTC2
C	4	THR	-	expression tag	UNP P0DTC2
C	5	LEU	-	expression tag	UNP P0DTC2
C	6	TYR	-	expression tag	UNP P0DTC2
C	7	LEU	-	expression tag	UNP P0DTC2
C	8	LEU	-	expression tag	UNP P0DTC2
C	9	GLY	-	expression tag	UNP P0DTC2
C	10	MET	-	expression tag	UNP P0DTC2
C	11	LEU	-	expression tag	UNP P0DTC2
C	12	VAL	-	expression tag	UNP P0DTC2
C	13	ALA	-	expression tag	UNP P0DTC2
C	14	SER	-	expression tag	UNP P0DTC2
C	15	VAL	-	expression tag	UNP P0DTC2
C	16	LEU	-	expression tag	UNP P0DTC2
C	17	ALA	-	expression tag	UNP P0DTC2
C	23	ILE	THR	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	28	SER	ALA	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	84	ALA	VAL	variant	UNP P0DTC2
C	143	ASP	GLY	variant	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	146	GLN	HIS	variant	UNP P0DTC2
C	180	VAL	GLU	conflict	UNP P0DTC2
C	183	GLU	GLN	variant	UNP P0DTC2
C	213	GLU	VAL	variant	UNP P0DTC2
C	252	VAL	GLY	variant	UNP P0DTC2
C	339	HIS	GLY	variant	UNP P0DTC2
C	346	THR	ARG	variant	UNP P0DTC2
C	368	ILE	LEU	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	445	PRO	VAL	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	460	LYS	ASN	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	ARG	THR	conflict	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	486	PRO	PHE	variant	UNP P0DTC2
C	490	SER	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	-	insertion	UNP P0DTC2
C	686	SER	-	insertion	UNP P0DTC2
C	687	LYS	-	insertion	UNP P0DTC2
C	689	SER	-	insertion	UNP P0DTC2
C	768	LYS	ASN	variant	UNP P0DTC2
C	800	TYR	ASP	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	821	PRO	PHE	conflict	UNP P0DTC2
C	896	PRO	ALA	conflict	UNP P0DTC2
C	903	PRO	ALA	conflict	UNP P0DTC2
C	946	PRO	ALA	conflict	UNP P0DTC2
C	958	HIS	GLN	variant	UNP P0DTC2
C	973	LYS	ASN	variant	UNP P0DTC2
C	990	PRO	LYS	variant	UNP P0DTC2
C	991	PRO	VAL	variant	UNP P0DTC2
C	1213	GLY	-	linker	UNP P0DTC2
C	1214	SER	-	linker	UNP P0DTC2

- Molecule 2 is a protein called CYFN1006-1 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	191	Total	C	N	O	S	0	0
			1419	889	234	289	7		
2	F	192	Total	C	N	O	S	0	0
			1429	895	237	290	7		
2	H	192	Total	C	N	O	S	0	0
			1429	895	237	290	7		

- Molecule 3 is a protein called CYFN1006-1 heavy chain.

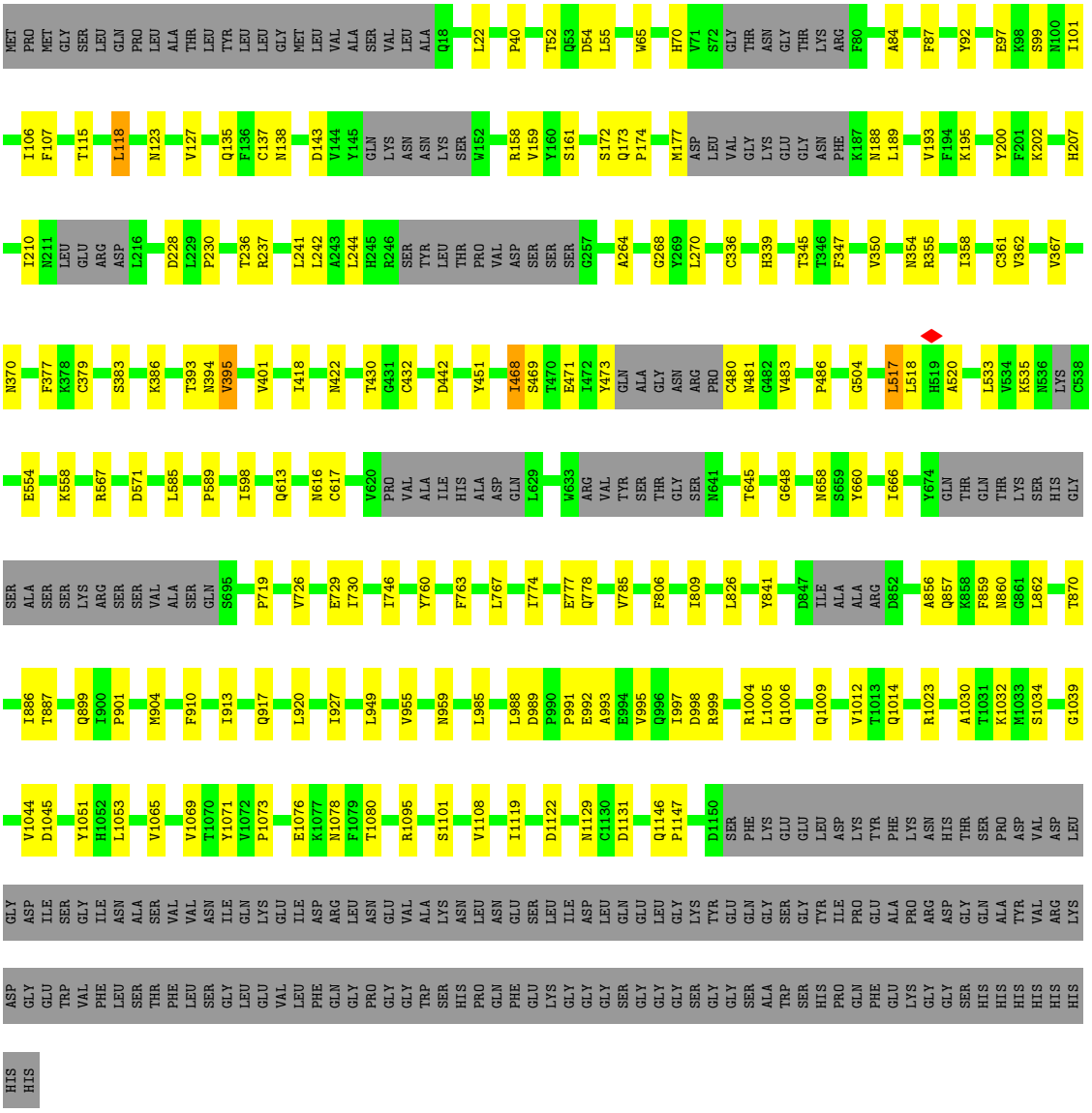
Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	202	Total	C	N	O	S	0	0
			1544	992	251	293	8		
3	G	198	Total	C	N	O	S	0	0
			1510	971	245	287	7		
3	I	202	Total	C	N	O	S	0	0
			1544	992	251	293	8		

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.

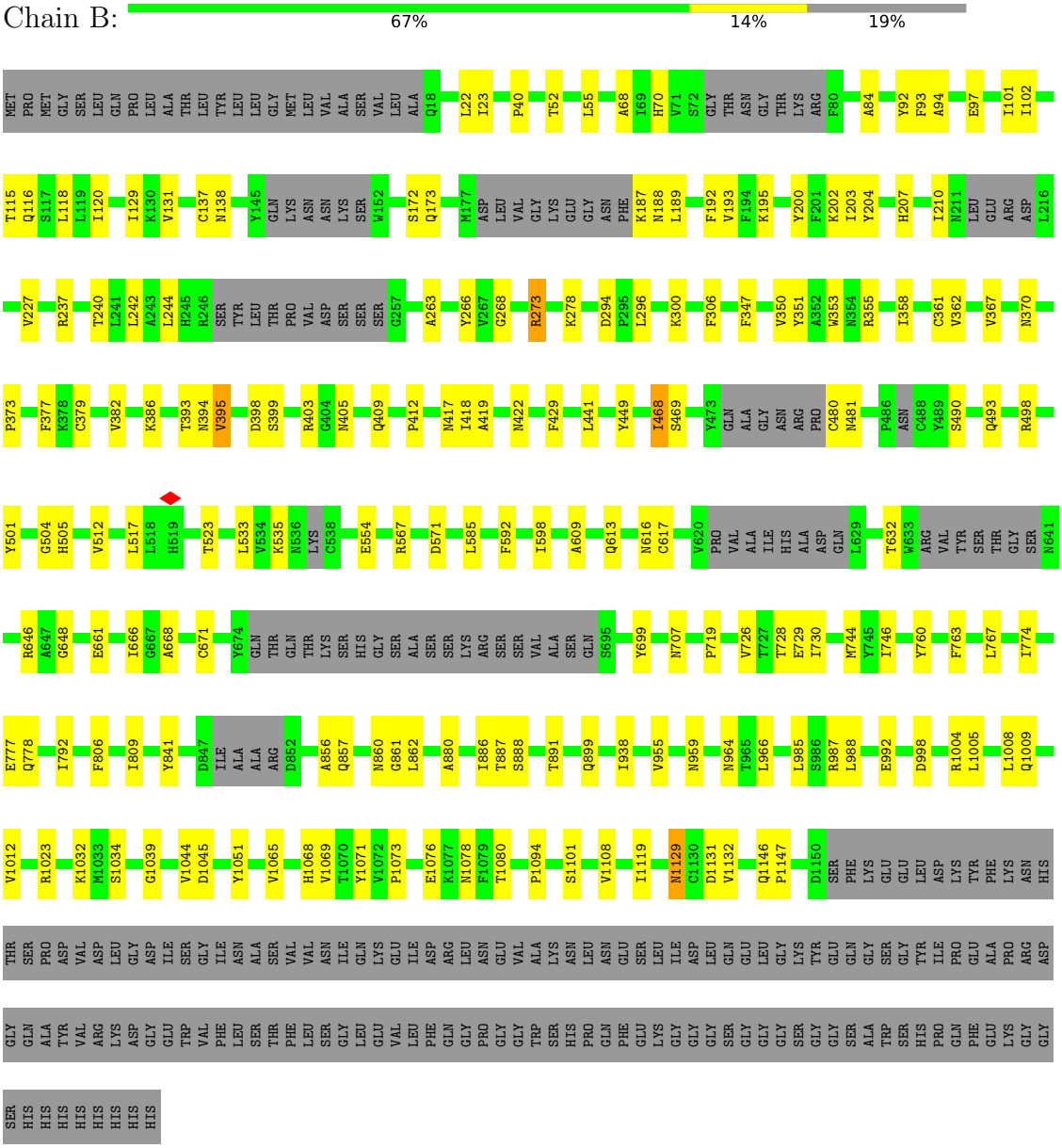
• Molecule 1: Spike glycoprotein,Fibritin,Spike glycoprotein,Fibritin,Spike glycoprotein,Fibritin, Expression Tag

Chain A:



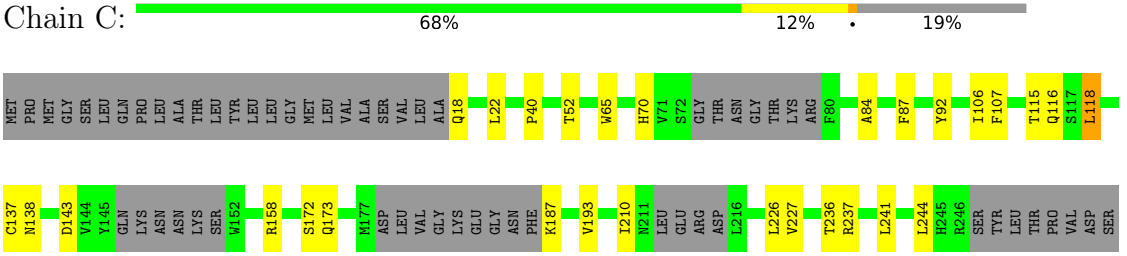
• Molecule 1: Spike glycoprotein,Fibritin,Spike glycoprotein,Fibritin,Spike glycoprotein,Fibritin, Expression Tag

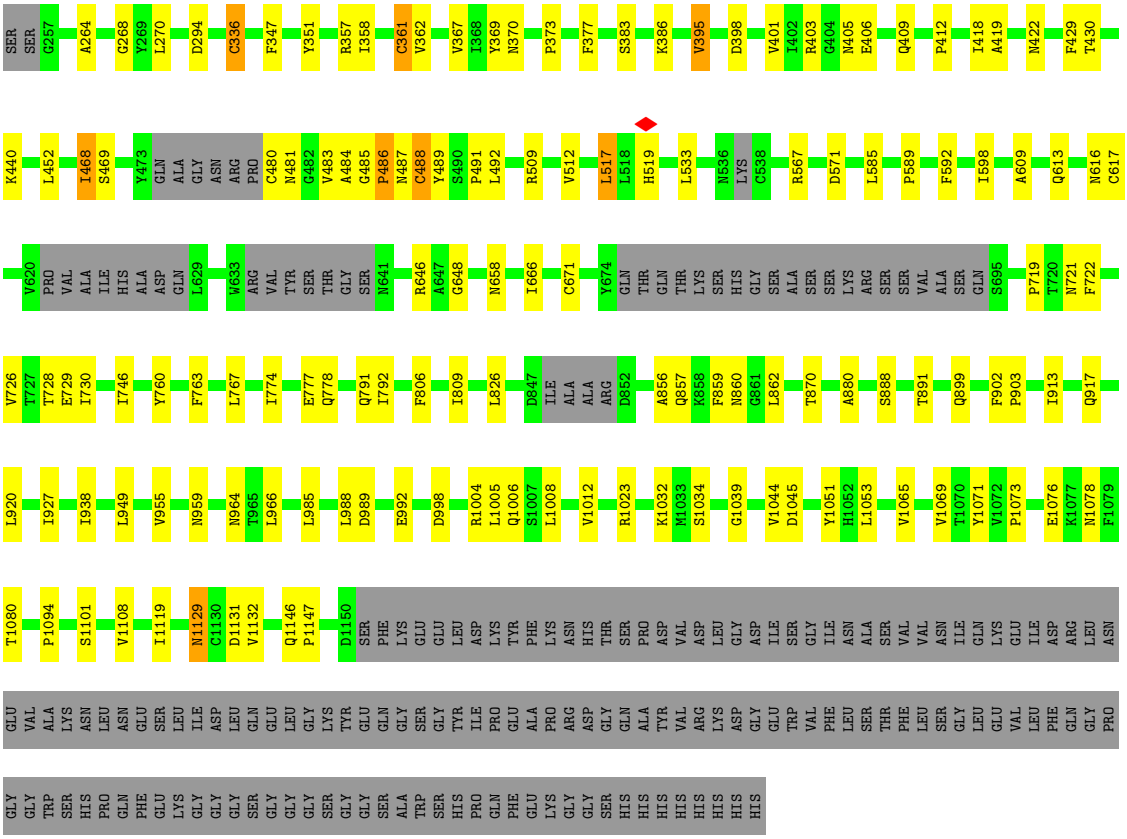
Chain B:



• Molecule 1: Spike glycoprotein,Fibritin,Spike glycoprotein,Fibritin,Spike glycoprotein,Fibritin, Expression Tag

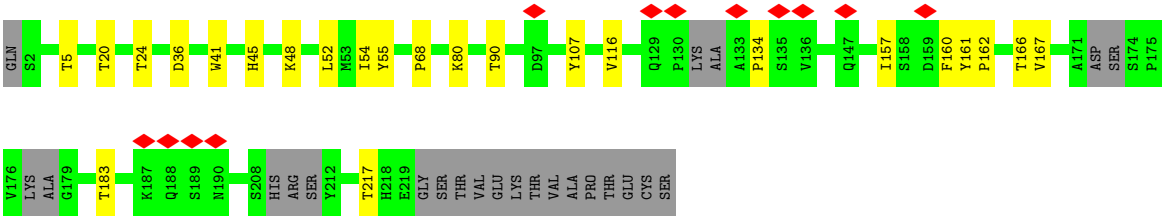
Chain C:





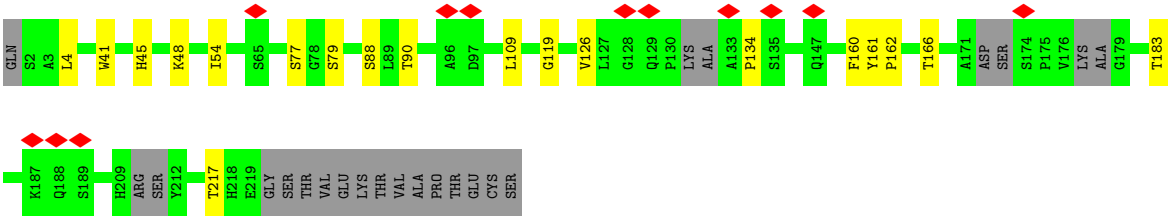
• Molecule 2: CYFN1006-1 light chain

Chain D:



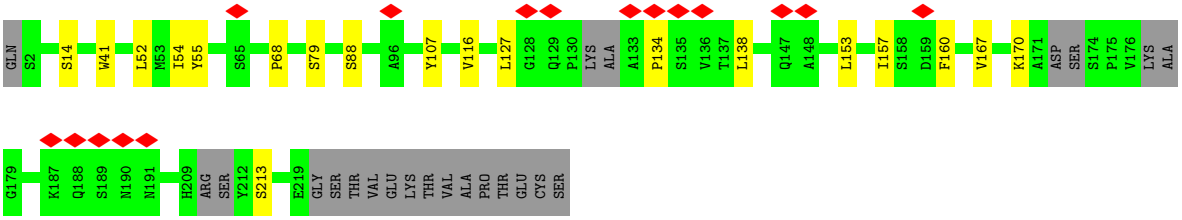
• Molecule 2: CYFN1006-1 light chain

Chain F:



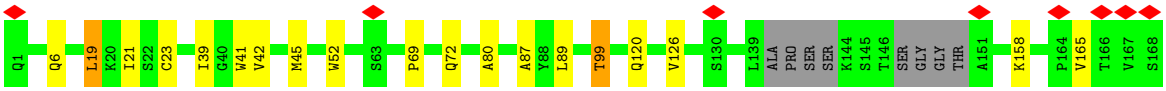
• Molecule 2: CYFN1006-1 light chain

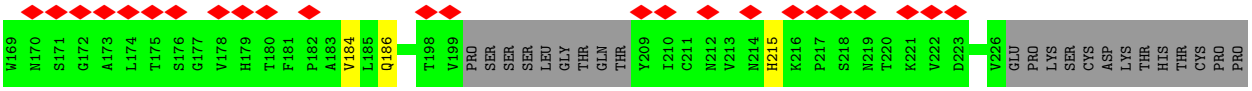
Chain H:

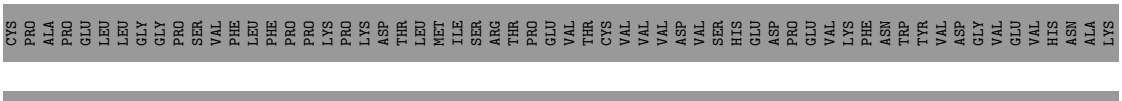


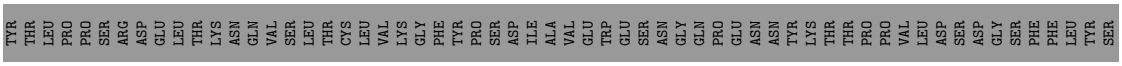
• Molecule 3: CYFN1006-1 heavy chain

Chain E:



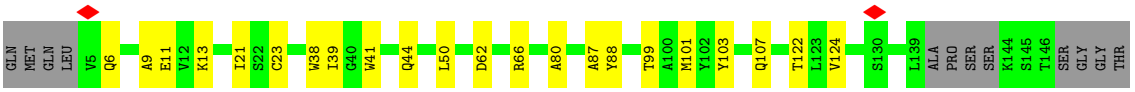


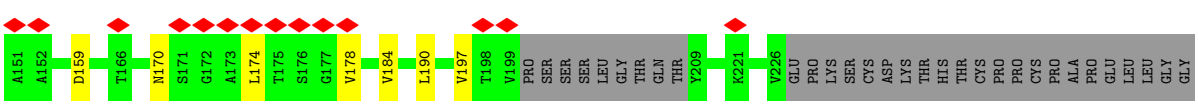


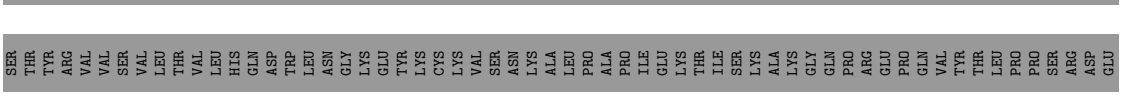


• Molecule 3: CYFN1006-1 heavy chain

Chain G:

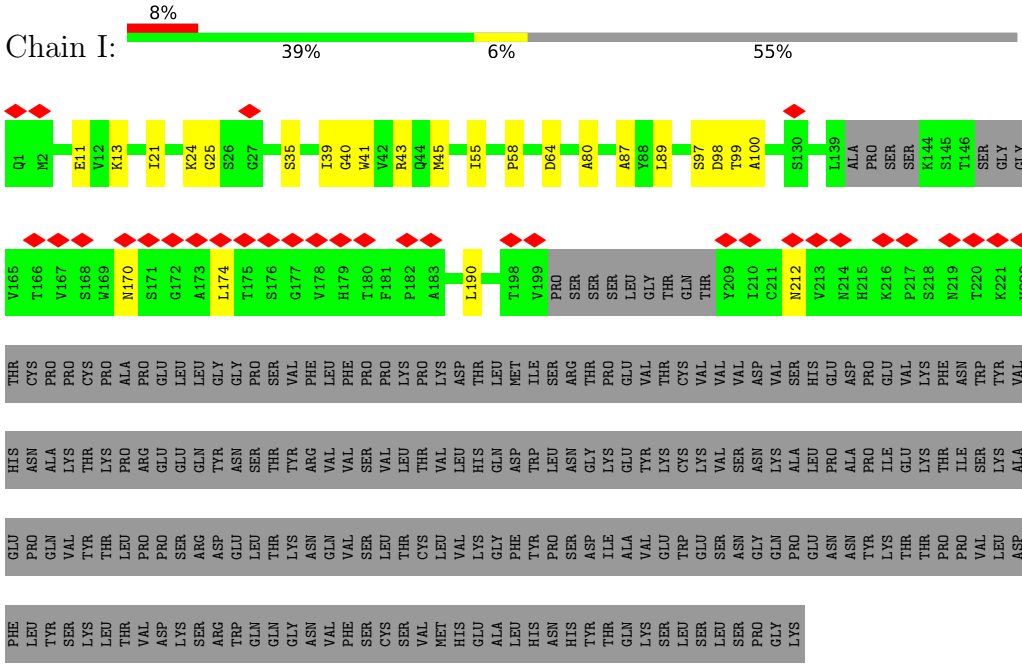






• Molecule 3: CYFN1006-1 heavy chain

Chain I:


8%
39%
6%
55%
Q1 M2 E11 V12 K13 I21 K24 G25 S26 G27 S35 I39 G40 W41 V42 R43 Q44 M45 I55 P58 D64 A80 A87 Y88 L89 S97 D98 T99 A100 S130 L139 ALA PRO SER SER K144 S145 T146 SER GLY GLY THR A151 D159 P164
V165 T166 V167 S168 W169 N170 S171 G172 A173 L174 T175 S176 G177 V178 H179 T180 F181 P182 A183 L190 T198 V199 PRO SER SER SER LEU GLY THR GLN THR Y209 I210 C211 N212 V213 N214 H215 K216 P217 S218 N219 T220 K221 V222 D223 K224 K225 V226 GLU PRO LYS SER CYS ASP LYS THR HIS
THR CYS PRO PRO CYS PRO ALA PRO GLU LEU LEU GLY GLY PRO SER VAL PHE LEU PHE PRO PRO LYS PRO LYS ASP THR LEU MET ILE SER ARG THR PRO GLU VAL THR CYS VAL VAL ASP VAL SER HIS GLU ASP PRO GLU VAL LYS PHE ASN TRP TYR VAL ASP GLY VAL GLU VAL
HIS ASN ALA LYS THR LYS PRO ARG GLU GLU GLN TYR ASN SER THR TYR ARG VAL VAL SER VAL LEU THR VAL LEU HIS GLN ASP TRP LEU ASN GLY LYS GLU TYR LYS CYS LYS VAL SER ASN LYS ALA LEU PRO ALA PRO ILE GLU LYS THR ILE SER LYS ALA LYS GLY GLN PRO ARG
GLU PRO GLN VAL TYR THR LEU PRO PRO SER ARG ASP GLU LEU THR LYS ASN GLN VAL SER LEU THR CYS LEU VAL LYS GLY PHE TYR PRO SER ASP ILE ALA VAL GLU TRP GLU SER ASN GLY GLN PRO GLU ASN ASN TYR LYS THR THR PRO PRO VAL LEU ASP SER ASP GLY SER PHE
PHE LEU TYR SER LYS LEU THR VAL ASP LYS SER ARG TRP GLN GLN GLY ASN VAL PHE SER CYS SER VAL MET HIS GLU ALA LEU HIS ASN HIS TYR THR GLN LYS SER LEU SER LEU SER PRO GLY LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	540576	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)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.040	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	298.24, 298.24, 298.24	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.932, 0.932, 0.932	Depositor

5 Model quality

5.1 Standard geometry

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	0.24	0/8424	0.41	0/11465
1	B	0.24	0/8415	0.41	0/11451
1	C	0.25	0/8424	0.41	0/11465
2	D	0.24	0/1449	0.42	0/1971
2	F	0.24	0/1460	0.42	0/1986
2	H	0.24	0/1460	0.43	0/1986
3	E	0.24	0/1584	0.43	0/2151
3	G	0.24	0/1550	0.42	0/2106
3	I	0.24	0/1584	0.43	0/2151
All	All	0.24	0/34350	0.42	0/46732

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	A	8229	0	8031	99	0
1	B	8221	0	8024	112	0
1	C	8229	0	8031	100	0
2	D	1419	0	1368	14	0
2	F	1429	0	1375	11	0
2	H	1429	0	1375	10	0
3	E	1544	0	1519	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1510	0	1480	16	0
3	I	1544	0	1519	15	0
All	All	33554	0	32722	348	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 5.

All (348) 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:C:767:LEU:HG	1:C:1012:VAL:HG21	1.73	0.71
1:A:367:VAL:O	1:A:370:ASN:ND2	2.25	0.69
1:C:106:ILE:HG13	1:C:241:LEU:HD21	1.75	0.69
1:A:767:LEU:HG	1:A:1012:VAL:HG21	1.75	0.68
1:B:767:LEU:HG	1:B:1012:VAL:HG21	1.76	0.67
1:C:1051:TYR:HB2	1:C:1071:TYR:HB3	1.78	0.66
2:H:107:TYR:HB3	2:H:116:VAL:HG12	1.78	0.65
1:B:1129:ASN:ND2	1:B:1131:ASP:OD1	2.30	0.65
1:C:1129:ASN:ND2	1:C:1131:ASP:OD1	2.29	0.65
2:D:134:PRO:HB3	2:D:160:PHE:HB3	1.80	0.64
1:C:1108:VAL:HG23	1:C:1119:ILE:HG12	1.79	0.64
1:B:1051:TYR:HB2	1:B:1071:TYR:HB3	1.81	0.63
1:A:106:ILE:HG13	1:A:241:LEU:HD21	1.81	0.63
3:I:159:ASP:HA	3:I:190:LEU:HD13	1.81	0.63
1:A:143:ASP:OD2	1:A:158:ARG:NH2	2.31	0.63
3:I:35:SER:HA	3:I:58:PRO:HB2	1.81	0.62
1:A:729:GLU:OE2	1:A:1032:LYS:NZ	2.27	0.62
1:A:1129:ASN:ND2	1:A:1131:ASP:OD1	2.33	0.62
1:A:1051:TYR:HB2	1:A:1071:TYR:HB3	1.81	0.62
2:H:134:PRO:HB3	2:H:160:PHE:HB3	1.80	0.62
1:B:730:ILE:HG13	1:B:1065:VAL:HG22	1.81	0.62
3:E:42:VAL:HG12	3:E:52:TRP:HA	1.82	0.61
1:B:68:ALA:HB3	1:B:263:ALA:HB3	1.82	0.61
1:C:143:ASP:OD2	1:C:158:ARG:NH2	2.34	0.61
1:A:123:ASN:H	1:A:127:VAL:HG12	1.64	0.61
1:C:856:ALA:O	1:C:860:ASN:ND2	2.32	0.61
1:A:856:ALA:O	1:A:860:ASN:ND2	2.33	0.61
1:C:567:ARG:NH2	1:C:571:ASP:OD1	2.34	0.60
1:B:195:LYS:HB2	1:B:202:LYS:HB2	1.83	0.60
1:C:777:GLU:OE2	1:C:1023:ARG:NE	2.34	0.60
1:C:1080:THR:HB	1:C:1101:SER:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ILE:HG21	1:B:240:THR:HB	1.84	0.60
3:I:170:ASN:HD22	3:I:174:LEU:HD23	1.66	0.59
2:F:45:HIS:HB2	2:F:48:LYS:HB2	1.83	0.59
1:B:188:ASN:HD21	1:B:207:HIS:HB2	1.68	0.59
1:B:806:PHE:HD1	1:B:809:ILE:HD11	1.67	0.59
1:A:746:ILE:O	1:A:1004:ARG:NH2	2.34	0.59
3:G:6:GLN:NE2	3:G:122:THR:OG1	2.36	0.59
1:B:412:PRO:HG3	1:B:429:PHE:HB3	1.83	0.59
1:C:729:GLU:OE2	1:C:1032:LYS:NZ	2.28	0.59
1:B:746:ILE:O	1:B:1004:ARG:NH2	2.36	0.58
1:A:730:ILE:HG13	1:A:1065:VAL:HG22	1.85	0.58
2:F:134:PRO:HB3	2:F:160:PHE:HB3	1.85	0.58
3:G:159:ASP:HA	3:G:190:LEU:HD13	1.86	0.58
3:I:43:ARG:NH1	3:I:97:SER:O	2.37	0.58
1:C:726:VAL:HG22	1:C:1069:VAL:HG22	1.86	0.58
1:C:746:ILE:O	1:C:1004:ARG:NH2	2.36	0.58
1:B:535:LYS:NZ	1:B:554:GLU:OE2	2.34	0.58
1:B:567:ARG:NH2	1:B:571:ASP:O	2.37	0.58
1:B:1080:THR:HB	1:B:1101:SER:HB3	1.86	0.58
1:B:856:ALA:O	1:B:860:ASN:ND2	2.37	0.58
1:C:358:ILE:HB	1:C:395:VAL:HG13	1.86	0.57
1:C:730:ILE:HG13	1:C:1065:VAL:HG22	1.86	0.57
3:E:158:LYS:NZ	3:E:186:GLN:OE1	2.38	0.57
1:C:137:CYS:SG	1:C:138:ASN:N	2.77	0.57
1:A:195:LYS:HB2	1:A:202:LYS:HB2	1.87	0.57
1:A:1108:VAL:HG23	1:A:1119:ILE:HG12	1.86	0.57
1:B:101:ILE:HG22	1:B:102:ILE:H	1.70	0.57
2:D:45:HIS:HB2	2:D:48:LYS:HB2	1.87	0.57
1:B:398:ASP:HB2	1:B:512:VAL:HB	1.86	0.57
1:C:955:VAL:O	1:C:959:ASN:ND2	2.36	0.57
1:A:726:VAL:HG22	1:A:1069:VAL:HG22	1.86	0.57
1:A:985:LEU:O	1:C:386:LYS:NZ	2.35	0.57
1:A:386:LYS:NZ	1:B:985:LEU:O	2.34	0.56
3:E:99:THR:HB	3:E:126:VAL:H	1.70	0.56
2:D:20:THR:HG22	2:D:90:THR:HG22	1.87	0.56
1:A:806:PHE:HD1	1:A:809:ILE:HD11	1.69	0.56
1:A:1078:ASN:OD1	1:B:899:GLN:NE2	2.39	0.56
1:A:137:CYS:SG	1:A:138:ASN:N	2.79	0.56
1:A:760:TYR:OH	1:A:998:ASP:OD1	2.24	0.56
1:B:40:PRO:HG3	1:B:52:THR:HG21	1.89	0.55
1:A:955:VAL:O	1:A:959:ASN:ND2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:726:VAL:HG22	1:B:1069:VAL:HG22	1.88	0.55
1:A:859:PHE:HA	1:C:592:PHE:HZ	1.72	0.55
3:G:11:GLU:OE1	3:G:13:LYS:NZ	2.38	0.55
1:B:1078:ASN:OD1	1:C:899:GLN:NE2	2.39	0.55
1:B:137:CYS:SG	1:B:138:ASN:N	2.80	0.54
1:A:899:GLN:NE2	1:C:1078:ASN:OD1	2.40	0.54
1:A:1039:GLY:HA3	1:C:1044:VAL:HG21	1.88	0.54
3:I:64:ASP:OD2	1:C:440:LYS:NZ	2.40	0.54
1:B:888:SER:OG	1:B:891:THR:OG1	2.26	0.54
1:B:777:GLU:OE2	1:B:1023:ARG:NE	2.41	0.54
3:E:6:GLN:H	3:E:120:GLN:HE22	1.56	0.54
3:E:80:ALA:HA	3:E:87:ALA:HA	1.89	0.54
1:B:1044:VAL:HG21	1:C:1039:GLY:HA3	1.90	0.54
1:A:358:ILE:HB	1:A:395:VAL:HG13	1.89	0.54
2:D:166:THR:HB	2:D:217:THR:HB	1.90	0.54
1:C:888:SER:OG	1:C:891:THR:OG1	2.24	0.53
3:E:69:PRO:HA	3:E:72:GLN:HE21	1.74	0.53
2:F:77:SER:HG	2:F:90:THR:HG1	1.55	0.53
2:D:157:ILE:HD12	2:D:167:VAL:HG22	1.90	0.53
3:E:23:CYS:HB2	3:E:41:TRP:HZ2	1.73	0.53
1:A:1006:GLN:NE2	1:B:1009:GLN:OE1	2.37	0.53
1:B:93:PHE:HB3	1:B:192:PHE:HB2	1.91	0.53
1:B:273:ARG:HH12	1:B:632:THR:HG21	1.74	0.53
1:B:405:ASN:ND2	1:C:369:TYR:O	2.40	0.52
1:B:955:VAL:O	1:B:959:ASN:ND2	2.36	0.52
1:A:777:GLU:OE2	1:A:1023:ARG:NE	2.32	0.52
1:A:841:TYR:OH	1:C:589:PRO:O	2.28	0.52
1:A:1095:ARG:NH1	1:A:1122:ASP:O	2.43	0.52
1:B:367:VAL:O	1:B:370:ASN:ND2	2.43	0.52
1:A:230:PRO:HD2	1:C:357:ARG:HH11	1.74	0.52
1:B:490:SER:O	1:B:493:GLN:NE2	2.43	0.52
2:F:41:TRP:HB2	2:F:54:ILE:HB	1.90	0.52
2:H:52:LEU:HD11	2:H:55:TYR:HB3	1.92	0.52
1:B:386:LYS:NZ	1:C:985:LEU:O	2.37	0.52
1:B:729:GLU:OE2	1:B:1032:LYS:NZ	2.29	0.52
1:B:102:ILE:HG12	1:B:242:LEU:HA	1.91	0.51
1:B:707:ASN:ND2	1:C:791:GLN:OE1	2.41	0.51
1:B:1108:VAL:HG23	1:B:1119:ILE:HG12	1.91	0.51
1:C:367:VAL:O	1:C:370:ASN:ND2	2.43	0.51
1:A:774:ILE:O	1:A:778:GLN:HG2	2.11	0.51
1:B:94:ALA:HB3	1:B:266:TYR:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ILE:HB	1:B:395:VAL:HG13	1.93	0.51
1:C:988:LEU:HB3	1:C:992:GLU:HG3	1.93	0.51
1:A:188:ASN:HD21	1:A:207:HIS:HB2	1.75	0.51
1:B:760:TYR:OH	1:B:998:ASP:OD1	2.23	0.51
3:G:170:ASN:HD22	3:G:174:LEU:HD23	1.75	0.51
1:B:92:TYR:N	1:B:268:GLY:O	2.42	0.50
1:A:189:LEU:HB2	1:A:210:ILE:HD13	1.92	0.50
1:B:1094:PRO:O	1:C:917:GLN:NE2	2.44	0.50
1:A:468:ILE:HD12	1:B:116:GLN:HG2	1.94	0.50
3:G:6:GLN:HG2	3:G:23:CYS:HA	1.93	0.50
1:C:187:LYS:HE3	1:C:210:ILE:HG13	1.93	0.50
1:C:491:PRO:HG2	1:C:492:LEU:HG	1.92	0.50
1:C:719:PRO:HG3	1:C:1073:PRO:HB3	1.93	0.50
1:B:203:ILE:HD12	1:B:227:VAL:HB	1.92	0.50
1:C:92:TYR:N	1:C:268:GLY:O	2.42	0.50
1:A:989:ASP:HB2	1:A:991:PRO:HD2	1.92	0.50
1:B:449:TYR:OH	1:B:498:ARG:NH1	2.44	0.50
1:C:172:SER:OG	1:C:173:GLN:OE1	2.30	0.50
1:B:55:LEU:HD23	1:B:195:LYS:HG2	1.93	0.49
1:A:469:SER:HB3	1:B:115:THR:HG22	1.94	0.49
1:A:658:ASN:ND2	1:A:660:TYR:OH	2.46	0.49
2:D:41:TRP:HB2	2:D:54:ILE:HB	1.93	0.49
1:A:1009:GLN:OE1	1:C:1006:GLN:NE2	2.39	0.49
1:A:1044:VAL:HG21	1:B:1039:GLY:HA3	1.94	0.49
1:B:774:ILE:O	1:B:778:GLN:HG2	2.13	0.49
1:A:535:LYS:NZ	1:A:554:GLU:OE2	2.40	0.49
1:C:412:PRO:HG3	1:C:429:PHE:HB3	1.93	0.49
1:B:172:SER:OG	1:B:173:GLN:OE1	2.30	0.49
1:B:598:ILE:HB	1:B:609:ALA:HB3	1.94	0.49
1:B:616:ASN:OD1	1:B:617:CYS:N	2.45	0.49
2:D:5:THR:OG1	2:D:24:THR:OG1	2.29	0.49
1:B:22:LEU:HB3	1:B:70:HIS:CE1	2.48	0.49
2:H:41:TRP:HB2	2:H:54:ILE:HB	1.95	0.49
1:B:379:CYS:HB3	1:B:382:VAL:HG23	1.93	0.49
1:A:1080:THR:HB	1:A:1101:SER:HB3	1.95	0.48
1:B:418:ILE:HA	1:B:422:ASN:HD22	1.77	0.48
1:C:294:ASP:OD1	1:C:294:ASP:N	2.45	0.48
1:C:774:ILE:O	1:C:778:GLN:HG2	2.13	0.48
1:A:115:THR:HG22	1:C:469:SER:HB3	1.94	0.48
3:G:44:GLN:HB2	3:G:50:LEU:HD23	1.95	0.48
1:A:172:SER:HG	1:A:173:GLN:H	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:616:ASN:OD1	1:A:617:CYS:N	2.46	0.48
1:A:886:ILE:HG13	1:A:887:THR:HG23	1.95	0.48
1:A:1034:SER:HB3	1:C:1045:ASP:HB2	1.95	0.48
2:D:183:THR:HG23	3:E:184:VAL:HG13	1.94	0.48
3:I:80:ALA:HA	3:I:87:ALA:HA	1.94	0.48
1:C:484:ALA:HA	1:C:488:CYS:HB2	1.96	0.48
1:C:18:GLN:HB2	1:C:158:ARG:HE	1.77	0.48
1:C:857:GLN:NE2	1:C:964:ASN:OD1	2.46	0.48
1:A:97:GLU:OE2	1:A:99:SER:OG	2.32	0.48
1:C:616:ASN:OD1	1:C:617:CYS:N	2.46	0.48
1:A:719:PRO:HA	1:A:1076:GLU:HA	1.96	0.48
1:C:519:HIS:HE1	1:C:567:ARG:HH11	1.61	0.48
2:H:14:SER:HA	2:H:127:LEU:H	1.79	0.47
1:A:920:LEU:HD12	1:A:927:ILE:HD12	1.96	0.47
2:H:79:SER:OG	2:H:88:SER:OG	2.32	0.47
1:B:393:THR:HG22	1:B:394:ASN:HD22	1.79	0.47
1:A:857:GLN:HB3	1:A:862:LEU:HB2	1.97	0.47
1:C:143:ASP:OD1	1:C:143:ASP:N	2.48	0.47
1:C:409:GLN:HB3	1:C:419:ALA:HB2	1.97	0.47
1:C:920:LEU:HD12	1:C:927:ILE:HD12	1.96	0.47
1:A:430:THR:HG21	1:A:517:LEU:HD11	1.96	0.47
1:A:645:THR:OG1	1:A:648:GLY:O	2.27	0.47
1:C:398:ASP:HB2	1:C:512:VAL:HB	1.96	0.47
3:I:11:GLU:OE1	3:I:13:LYS:NZ	2.48	0.47
1:C:418:ILE:HA	1:C:422:ASN:HD22	1.80	0.47
1:C:760:TYR:OH	1:C:998:ASP:OD1	2.25	0.47
3:G:178:VAL:HG22	3:G:197:VAL:HG23	1.97	0.47
1:B:728:THR:HG23	1:B:938:ILE:HD12	1.97	0.47
3:I:212:ASN:ND2	3:I:223:ASP:OD1	2.46	0.46
2:F:183:THR:HG23	3:G:184:VAL:HG13	1.97	0.46
3:I:40:GLY:HA3	3:I:55:ILE:HG22	1.96	0.46
1:A:442:ASP:HB3	1:A:451:TYR:HE2	1.79	0.46
1:B:403:ARG:NE	1:B:405:ASN:OD1	2.47	0.46
1:B:646:ARG:NH1	1:B:668:ALA:O	2.49	0.46
1:B:729:GLU:OE1	1:B:1068:HIS:NE2	2.48	0.46
1:B:719:PRO:HA	1:B:1076:GLU:HA	1.96	0.46
2:D:36:ASP:O	2:D:80:LYS:NZ	2.49	0.46
1:A:719:PRO:HG3	1:A:1073:PRO:HB3	1.96	0.46
1:B:1045:ASP:HB2	1:C:1034:SER:HB3	1.98	0.46
1:C:806:PHE:HD1	1:C:809:ILE:HD11	1.79	0.46
1:A:40:PRO:HG3	1:A:52:THR:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:ALA:O	1:B:263:ALA:N	2.48	0.46
1:B:886:ILE:HG13	1:B:887:THR:HG23	1.97	0.46
1:C:65:TRP:HE1	1:C:264:ALA:HB1	1.81	0.46
1:C:719:PRO:HA	1:C:1076:GLU:HA	1.98	0.46
1:A:174:PRO:HB2	1:A:177:MET:HB3	1.98	0.46
1:C:193:VAL:HG13	1:C:270:LEU:HD11	1.97	0.46
2:F:79:SER:OG	2:F:88:SER:OG	2.34	0.46
1:A:87:PHE:N	1:A:236:THR:O	2.43	0.46
1:B:504:GLY:HA3	1:C:373:PRO:HD3	1.99	0.46
1:A:913:ILE:HD13	1:A:1053:LEU:HD21	1.97	0.45
1:B:857:GLN:NE2	1:B:964:ASN:OD1	2.49	0.45
3:G:38:TRP:HB2	3:G:107:GLN:HB2	1.98	0.45
1:A:901:PRO:HB2	1:A:904:MET:HG3	1.98	0.45
3:G:62:ASP:OD1	3:G:62:ASP:N	2.48	0.45
1:A:22:LEU:HB3	1:A:70:HIS:CE1	2.50	0.45
1:B:347:PHE:CD2	1:B:399:SER:HB3	2.51	0.45
1:C:84:ALA:HB3	1:C:237:ARG:HE	1.80	0.45
1:C:403:ARG:NE	1:C:405:ASN:OD1	2.48	0.45
1:A:54:ASP:OD1	1:A:55:LEU:N	2.45	0.45
1:A:92:TYR:N	1:A:268:GLY:O	2.44	0.45
3:I:24:LYS:NZ	3:I:25:GLY:O	2.41	0.45
1:C:351:TYR:HE1	1:C:452:LEU:HB2	1.81	0.45
1:C:533:LEU:HD21	1:C:585:LEU:HD11	1.98	0.45
1:C:728:THR:HG23	1:C:938:ILE:HD12	1.99	0.45
1:C:1129:ASN:HD21	1:C:1132:VAL:HG23	1.82	0.45
1:A:193:VAL:HG13	1:A:270:LEU:HD11	1.98	0.45
2:F:109:LEU:HD23	2:F:109:LEU:H	1.82	0.45
1:B:294:ASP:N	1:B:294:ASP:OD1	2.49	0.45
1:B:1129:ASN:HD21	1:B:1132:VAL:HG23	1.80	0.45
1:A:383:SER:HB2	1:B:988:LEU:HA	1.97	0.45
3:G:66:ARG:HH12	1:B:441:LEU:HD11	1.82	0.45
3:I:21:ILE:HG22	3:I:89:LEU:HB2	1.98	0.45
1:A:533:LEU:HD21	1:A:585:LEU:HD11	1.99	0.44
1:C:966:LEU:HD11	1:C:1008:LEU:HD23	1.98	0.44
3:G:21:ILE:HD12	3:G:21:ILE:HA	1.91	0.44
1:B:966:LEU:HD11	1:B:1008:LEU:HD23	1.99	0.44
1:A:354:ASN:OD1	1:A:355:ARG:N	2.51	0.44
3:G:41:TRP:HE1	3:G:87:ALA:HB1	1.82	0.44
1:B:353:TRP:HZ3	1:B:355:ARG:HE	1.66	0.44
1:B:469:SER:HB3	1:C:115:THR:HG22	1.98	0.44
2:H:55:TYR:CD1	2:H:68:PRO:HG3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:988:LEU:HB3	1:B:992:GLU:HG3	1.98	0.44
1:A:84:ALA:HB3	1:A:237:ARG:HE	1.83	0.44
1:A:1146:GLN:HB2	1:A:1147:PRO:HD3	1.99	0.44
1:B:1146:GLN:HB2	1:B:1147:PRO:HD3	2.00	0.44
1:A:1045:ASP:HB2	1:B:1034:SER:HB3	1.99	0.44
1:B:468:ILE:HD12	1:C:116:GLN:HG2	2.00	0.44
1:B:613:GLN:HA	1:B:648:GLY:HA3	2.00	0.44
1:C:826:LEU:HD22	1:C:949:LEU:HD21	2.00	0.44
2:D:52:LEU:HD11	2:D:55:TYR:HB3	2.00	0.44
1:C:107:PHE:HB2	1:C:118:LEU:HB3	2.00	0.44
1:A:345:THR:OG1	2:D:107:TYR:O	2.32	0.43
2:F:166:THR:HB	2:F:217:THR:HB	1.99	0.43
1:C:403:ARG:HE	1:C:406:GLU:HG3	1.83	0.43
1:B:23:ILE:HG13	1:B:242:LEU:HG	1.99	0.43
1:A:143:ASP:OD1	1:A:143:ASP:N	2.45	0.43
1:C:347:PHE:HB2	1:C:401:VAL:HG23	2.01	0.43
1:A:347:PHE:HB2	1:A:401:VAL:HG23	2.00	0.43
2:F:161:TYR:HB3	2:F:162:PRO:HD3	2.01	0.43
1:B:857:GLN:HB3	1:B:862:LEU:HB2	2.01	0.43
1:C:913:ILE:HD13	1:C:1053:LEU:HD21	1.99	0.43
1:A:826:LEU:HD22	1:A:949:LEU:HD21	1.99	0.43
3:I:43:ARG:HH22	3:I:98:ASP:HA	1.83	0.43
1:B:120:ILE:HG12	1:B:129:ILE:HG23	1.99	0.43
1:B:187:LYS:HE3	1:B:210:ILE:HG13	2.01	0.43
1:A:107:PHE:HB2	1:A:118:LEU:HB3	1.99	0.43
1:C:40:PRO:HG3	1:C:52:THR:HG21	2.00	0.43
1:A:589:PRO:O	1:B:841:TYR:OH	2.33	0.43
2:F:4:LEU:HB2	2:F:119:GLY:HA2	2.00	0.43
1:B:592:PHE:HZ	1:C:859:PHE:HA	1.84	0.43
1:C:468:ILE:HD13	1:C:468:ILE:H	1.84	0.43
1:C:485:GLY:HA3	1:C:486:PRO:HD3	1.85	0.43
1:C:598:ILE:HB	1:C:609:ALA:HB3	2.01	0.43
1:C:857:GLN:HB3	1:C:862:LEU:HB2	2.00	0.43
1:B:84:ALA:HB3	1:B:237:ARG:HE	1.83	0.43
1:B:351:TYR:HD2	1:B:468:ILE:HA	1.84	0.43
1:B:189:LEU:HB2	1:B:210:ILE:HD13	2.01	0.43
1:A:383:SER:N	1:B:987:ARG:O	2.50	0.42
1:B:792:ILE:HG23	1:B:880:ALA:HB2	2.00	0.42
1:C:763:PHE:CD2	1:C:1005:LEU:HD21	2.54	0.42
1:C:989:ASP:OD1	1:C:989:ASP:N	2.48	0.42
1:A:101:ILE:HG22	1:A:242:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:ILE:HG12	1:A:666:ILE:HD12	2.00	0.42
3:G:80:ALA:HA	3:G:88:TYR:H	1.84	0.42
1:B:97:GLU:HB3	1:B:101:ILE:HD12	2.01	0.42
1:B:501:TYR:HB3	1:B:505:HIS:HB2	2.01	0.42
1:A:785:VAL:HG22	1:A:1030:ALA:HB2	2.01	0.42
3:E:165:VAL:HG22	3:E:215:HIS:HD2	1.85	0.42
3:I:41:TRP:CD1	3:I:89:LEU:HD21	2.54	0.42
1:B:409:GLN:HB3	1:B:419:ALA:HB2	2.01	0.42
1:A:995:VAL:O	1:A:999:ARG:NH2	2.53	0.42
1:C:351:TYR:HD2	1:C:468:ILE:HA	1.84	0.42
1:C:721:ASN:OD1	1:C:722:PHE:N	2.46	0.42
1:C:1146:GLN:HB2	1:C:1147:PRO:HD3	2.01	0.42
1:A:350:VAL:HG12	1:A:422:ASN:HB3	2.01	0.42
1:B:666:ILE:HG12	1:B:671:CYS:HA	2.01	0.42
1:B:719:PRO:HG3	1:B:1073:PRO:HB3	2.00	0.42
3:E:19:LEU:HD13	3:E:21:ILE:HD13	2.02	0.42
1:A:993:ALA:O	1:A:997:ILE:HG12	2.20	0.42
2:D:55:TYR:CD1	2:D:68:PRO:HG3	2.55	0.42
3:G:101:MET:HG2	3:G:103:TYR:CZ	2.55	0.42
2:H:157:ILE:HD12	2:H:167:VAL:HG22	2.02	0.42
1:B:661:GLU:O	1:B:699:TYR:OH	2.32	0.42
1:B:278:LYS:HB2	1:B:306:PHE:CZ	2.55	0.41
1:B:296:LEU:HG	1:B:300:LYS:HE3	2.02	0.41
1:C:336:CYS:HA	1:C:361:CYS:HB2	2.02	0.41
1:C:401:VAL:HG22	1:C:509:ARG:HG2	2.02	0.41
1:B:405:ASN:N	1:B:504:GLY:O	2.37	0.41
1:C:87:PHE:N	1:C:236:THR:O	2.50	0.41
1:C:792:ILE:HG23	1:C:880:ALA:HB2	2.01	0.41
1:B:417:ASN:OD1	1:B:417:ASN:N	2.53	0.41
1:A:202:LYS:NZ	1:A:228:ASP:OD2	2.50	0.41
1:A:504:GLY:HA3	1:B:373:PRO:HD3	2.02	0.41
3:E:41:TRP:CG	3:E:89:LEU:HD11	2.56	0.41
1:B:350:VAL:HG12	1:B:422:ASN:HB3	2.02	0.41
1:C:226:LEU:HG	1:C:227:VAL:HG23	2.01	0.41
1:A:65:TRP:HE1	1:A:264:ALA:HB1	1.85	0.41
1:B:193:VAL:HB	1:B:204:TYR:HB2	2.02	0.41
1:A:379:CYS:HA	1:A:432:CYS:HA	2.03	0.41
1:A:763:PHE:CD2	1:A:1005:LEU:HD21	2.56	0.41
1:A:135:GLN:HB3	1:A:161:SER:HB3	2.01	0.41
1:A:988:LEU:HA	1:C:383:SER:HB2	2.03	0.41
2:D:161:TYR:HB3	2:D:162:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:LEU:HG	1:A:520:ALA:H	1.85	0.41
1:A:613:GLN:HA	1:A:648:GLY:HA3	2.02	0.41
1:A:870:THR:HG21	1:C:646:ARG:HH11	1.86	0.41
1:A:910:PHE:HA	1:A:913:ILE:HG12	2.03	0.41
1:A:917:GLN:NE2	1:C:1094:PRO:O	2.54	0.41
3:G:9:ALA:HB1	3:G:124:VAL:HA	2.02	0.41
2:H:170:LYS:N	2:H:213:SER:O	2.49	0.41
1:C:666:ILE:HG12	1:C:671:CYS:HA	2.03	0.41
1:A:988:LEU:HB3	1:A:992:GLU:HG3	2.02	0.41
2:D:116:VAL:HB	3:E:52:TRP:CG	2.56	0.41
3:I:41:TRP:CG	3:I:89:LEU:HD11	2.56	0.41
1:C:22:LEU:HB3	1:C:70:HIS:CE1	2.55	0.41
2:H:138:LEU:HD11	2:H:153:LEU:HD11	2.03	0.40
3:I:45:MET:HG2	3:I:100:ALA:HB2	2.02	0.40
1:B:533:LEU:HD21	1:B:585:LEU:HD11	2.01	0.40
1:A:339:HIS:O	1:A:339:HIS:ND1	2.54	0.40
2:F:126:VAL:O	2:F:161:TYR:OH	2.38	0.40
1:B:744:MET:HE3	1:B:861:GLY:HA2	2.04	0.40
1:C:430:THR:HG21	1:C:517:LEU:HD11	2.03	0.40
1:B:393:THR:O	1:B:523:THR:OG1	2.35	0.40
1:B:409:GLN:OE1	1:B:419:ALA:N	2.50	0.40
1:B:480:CYS:SG	1:B:481:ASN:N	2.94	0.40
1:B:646:ARG:HH11	1:C:870:THR:HG21	1.87	0.40
1:C:613:GLN:HA	1:C:648:GLY:HA3	2.02	0.40
1:C:902:PHE:N	1:C:903:PRO:HD2	2.37	0.40
1:A:350:VAL:HG11	1:A:418:ILE:HD12	2.03	0.40
1:A:393:THR:HG22	1:A:394:ASN:HD22	1.87	0.40
1:A:567:ARG:NH2	1:A:571:ASP:O	2.54	0.40
1:B:468:ILE:H	1:B:468:ILE:HD13	1.86	0.40
1:B:763:PHE:CD2	1:B:1005:LEU:HD21	2.57	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	A	1027/1299 (79%)	999 (97%)	27 (3%)	1 (0%)	48 75
1	B	1024/1299 (79%)	992 (97%)	32 (3%)	0	100 100
1	C	1027/1299 (79%)	995 (97%)	31 (3%)	1 (0%)	48 75
2	D	181/215 (84%)	176 (97%)	5 (3%)	0	100 100
2	F	182/215 (85%)	179 (98%)	3 (2%)	0	100 100
2	H	182/215 (85%)	179 (98%)	3 (2%)	0	100 100
3	E	194/451 (43%)	186 (96%)	8 (4%)	0	100 100
3	G	190/451 (42%)	181 (95%)	9 (5%)	0	100 100
3	I	194/451 (43%)	186 (96%)	8 (4%)	0	100 100
All	All	4201/5895 (71%)	4073 (97%)	126 (3%)	2 (0%)	100 100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	486	PRO
1	A	486	PRO

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	A	919/1122 (82%)	901 (98%)	18 (2%)	50 78
1	B	918/1122 (82%)	906 (99%)	12 (1%)	65 86
1	C	919/1122 (82%)	902 (98%)	17 (2%)	54 80
2	D	161/181 (89%)	161 (100%)	0	100 100
2	F	162/181 (90%)	162 (100%)	0	100 100
2	H	162/181 (90%)	162 (100%)	0	100 100
3	E	171/399 (43%)	167 (98%)	4 (2%)	45 75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	G	167/399 (42%)	165 (99%)	2 (1%)	67 87
3	I	171/399 (43%)	169 (99%)	2 (1%)	67 87
All	All	3750/5106 (73%)	3695 (98%)	55 (2%)	60 84

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	LEU
1	A	159	VAL
1	A	200	TYR
1	A	244	LEU
1	A	336	CYS
1	A	361	CYS
1	A	362	VAL
1	A	377	PHE
1	A	395	VAL
1	A	468	ILE
1	A	471	GLU
1	A	473	TYR
1	A	480	CYS
1	A	481	ASN
1	A	483	VAL
1	A	517	LEU
1	A	558	LYS
1	A	1014	GLN
3	E	19	LEU
3	E	39	ILE
3	E	45	MET
3	E	99	THR
3	G	39	ILE
3	G	99	THR
3	I	39	ILE
3	I	99	THR
1	B	118	LEU
1	B	131	VAL
1	B	200	TYR
1	B	244	LEU
1	B	273	ARG
1	B	361	CYS
1	B	362	VAL
1	B	377	PHE

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Mol	Chain	Res	Type
1	B	395	VAL
1	B	468	ILE
1	B	517	LEU
1	B	1129	ASN
1	C	118	LEU
1	C	244	LEU
1	C	336	CYS
1	C	361	CYS
1	C	362	VAL
1	C	377	PHE
1	C	395	VAL
1	C	468	ILE
1	C	480	CYS
1	C	481	ASN
1	C	483	VAL
1	C	487	ASN
1	C	488	CYS
1	C	489	TYR
1	C	517	LEU
1	C	658	ASN
1	C	1129	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	188	ASN
1	A	321	GLN
1	A	394	ASN
1	A	519	HIS
1	A	641	ASN
1	A	644	GLN
1	A	876	GLN
1	A	917	GLN
1	A	1015	GLN
1	A	1092	HIS
1	A	1139	ASN
2	D	95	GLN
3	E	3	GLN
3	E	72	GLN
3	E	179	HIS
2	F	95	GLN

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Mol	Chain	Res	Type
3	G	179	HIS
3	G	186	GLN
2	H	6	GLN
2	H	95	GLN
3	I	3	GLN
3	I	120	GLN
3	I	179	HIS
1	B	88	ASN
1	B	188	ASN
1	B	239	GLN
1	B	370	ASN
1	B	394	ASN
1	B	519	HIS
1	B	613	GLN
1	B	641	ASN
1	B	876	GLN
1	B	917	GLN
1	B	1015	GLN
1	B	1129	ASN
1	B	1139	ASN
1	C	88	ASN
1	C	321	GLN
1	C	370	ASN
1	C	394	ASN
1	C	519	HIS
1	C	641	ASN
1	C	644	GLN
1	C	876	GLN
1	C	917	GLN
1	C	1015	GLN
1	C	1075	GLN
1	C	1129	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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

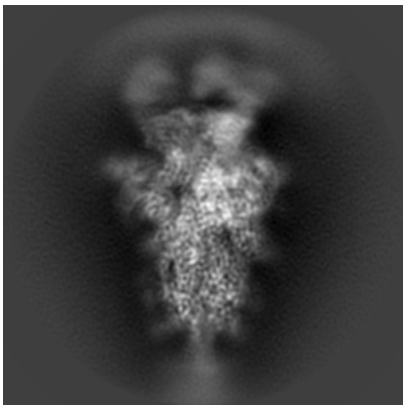
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-39802. These allow visual inspection of the internal detail of the map and identification of artifacts.

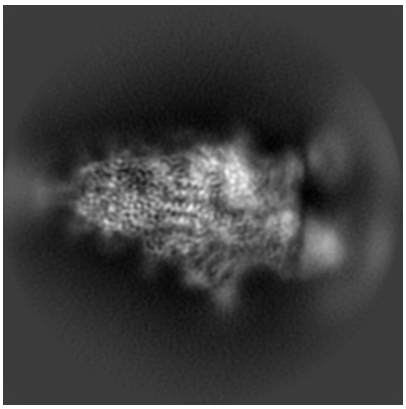
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

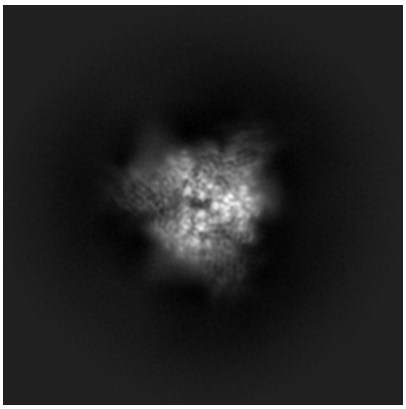
6.1.1 Primary map



X

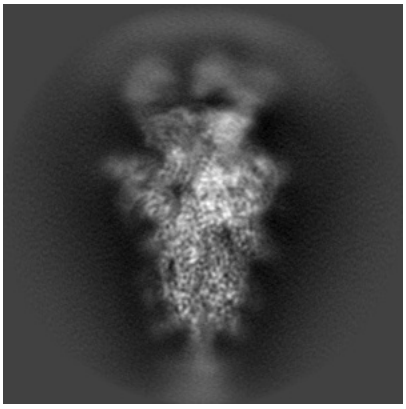


Y

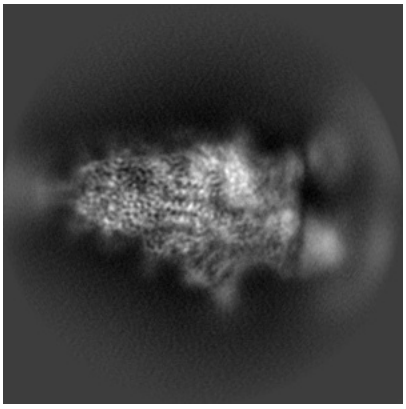


Z

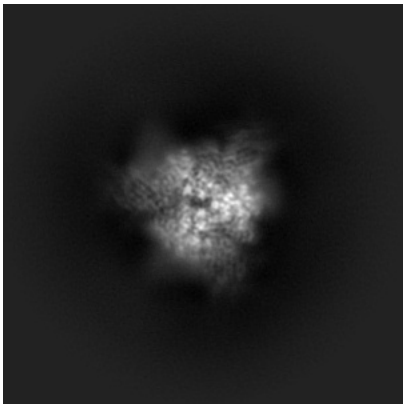
6.1.2 Raw map



X



Y

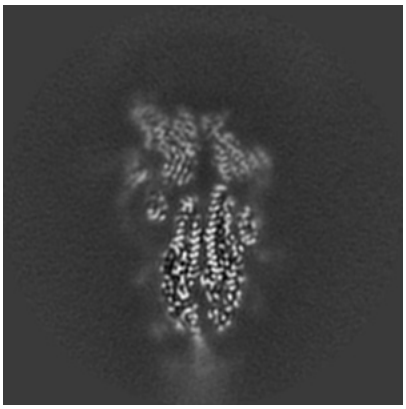


Z

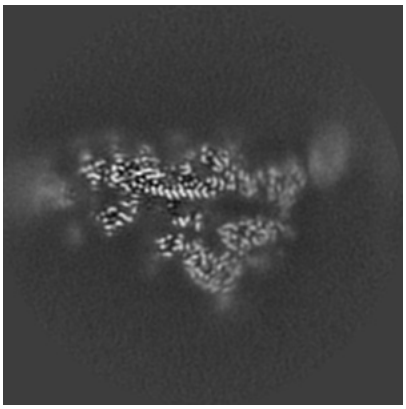
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

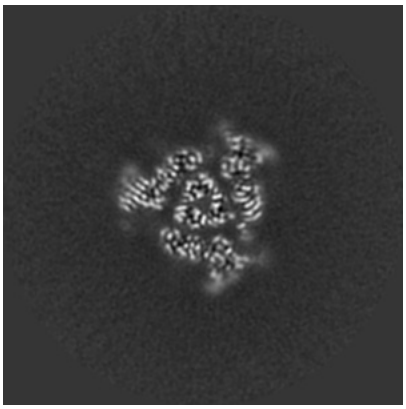
6.2.1 Primary map



X Index: 160

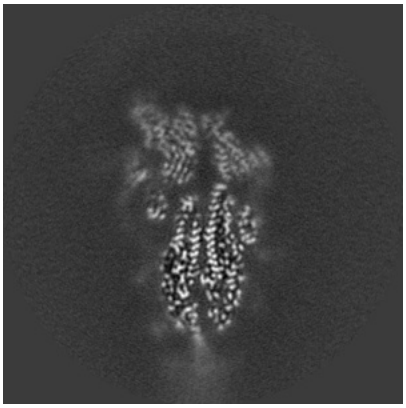


Y Index: 160

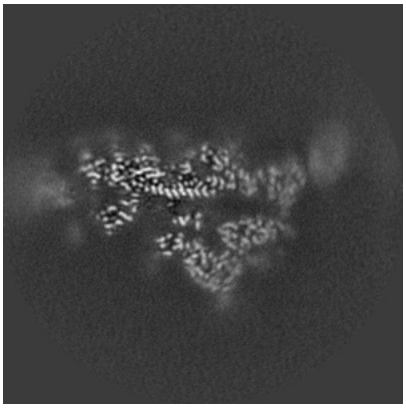


Z Index: 160

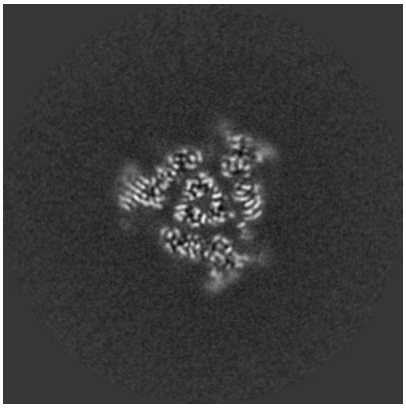
6.2.2 Raw map



X Index: 160



Y Index: 160

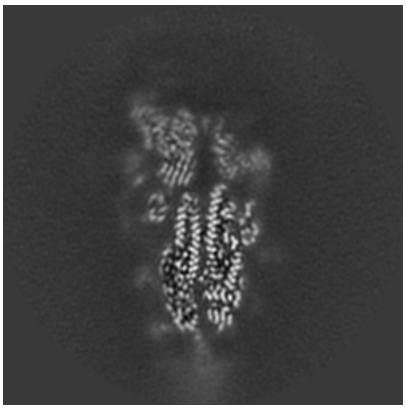


Z Index: 160

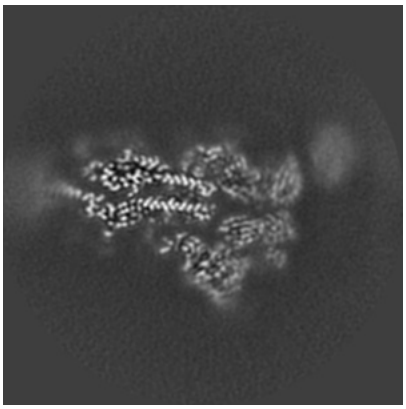
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

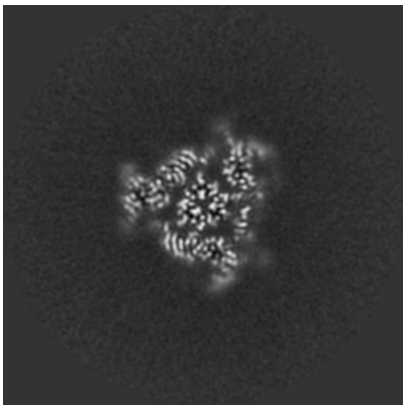
6.3.1 Primary map



X Index: 158

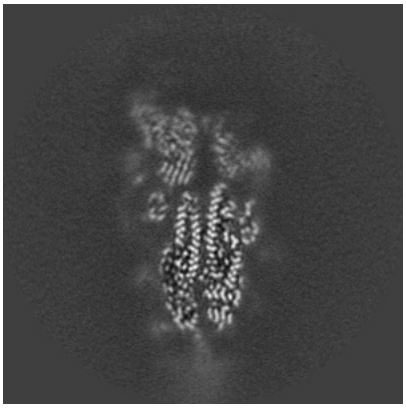


Y Index: 166

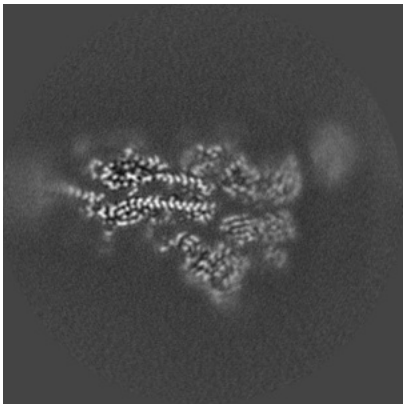


Z Index: 156

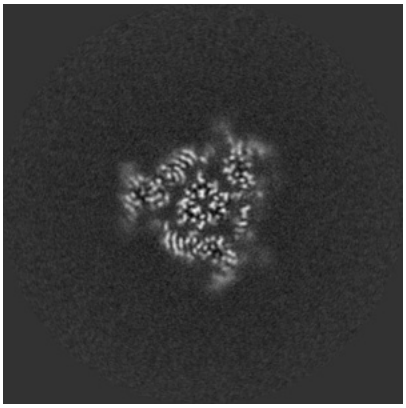
6.3.2 Raw map



X Index: 158



Y Index: 167

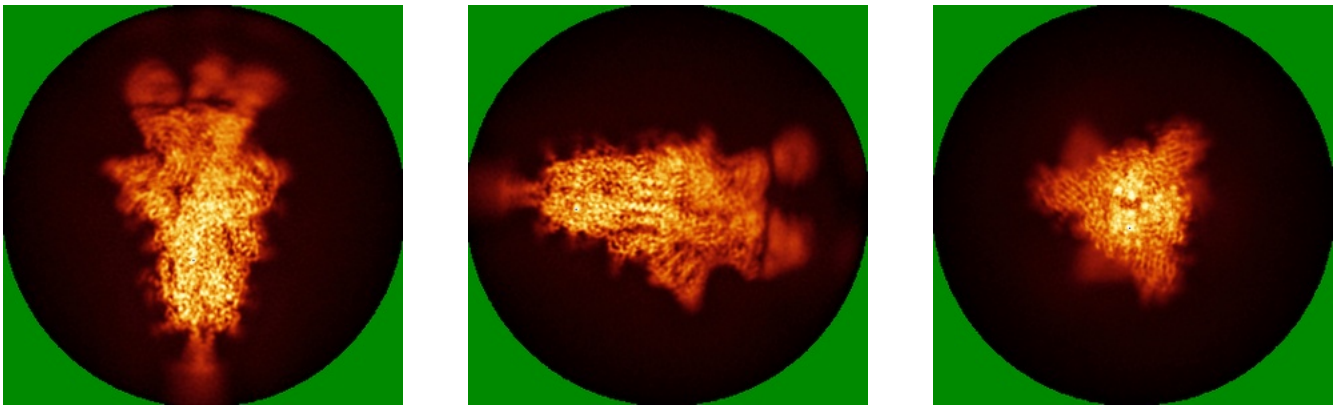


Z Index: 156

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

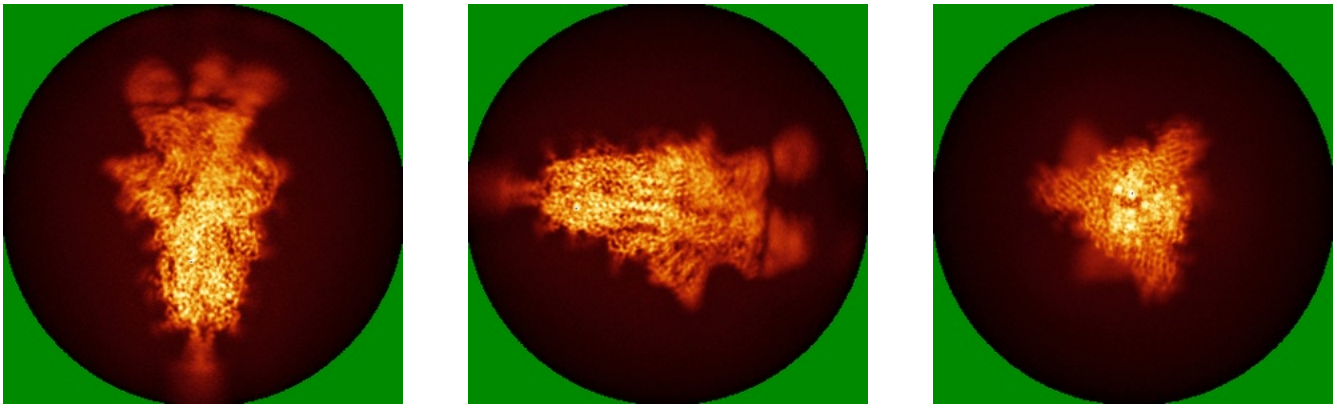
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

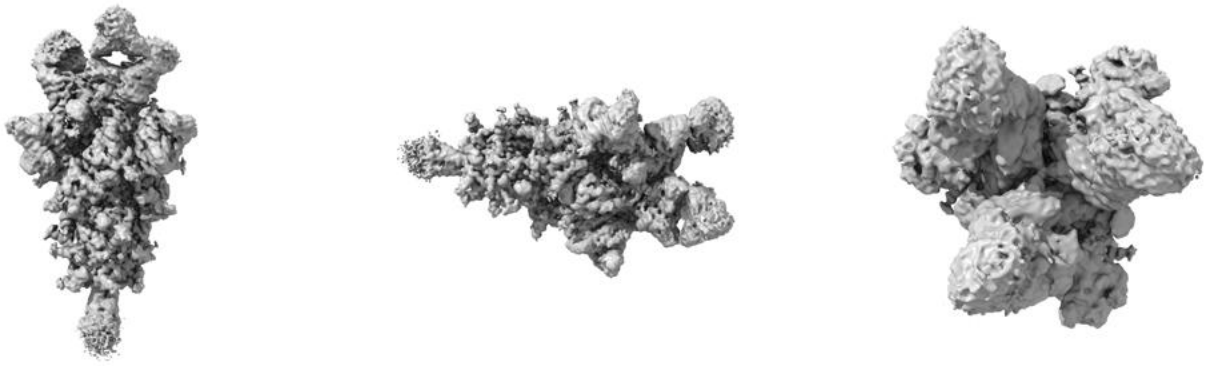


X Y Z

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 0.004. 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.

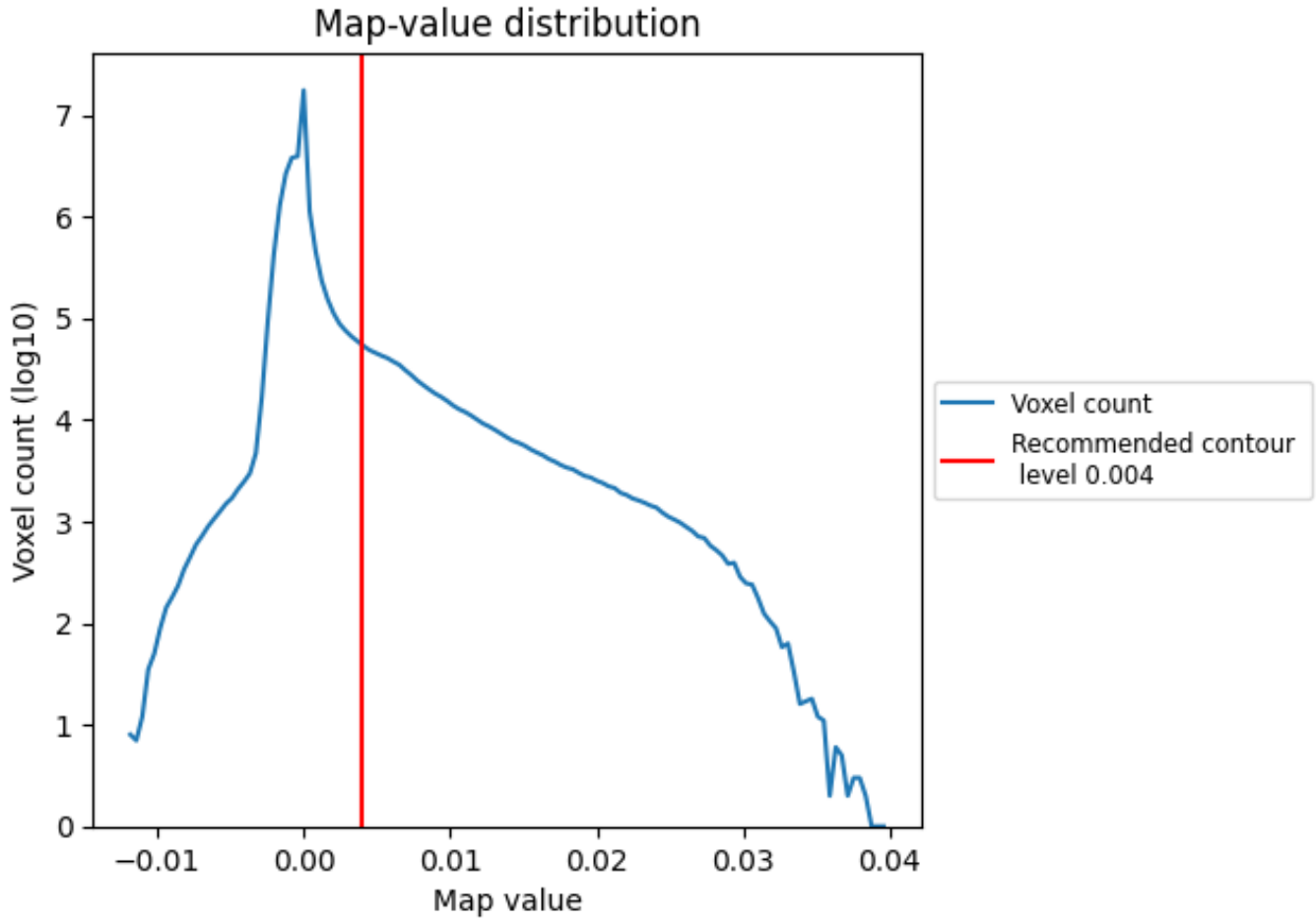
6.6 Mask visualisation (i)

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

7 Map analysis

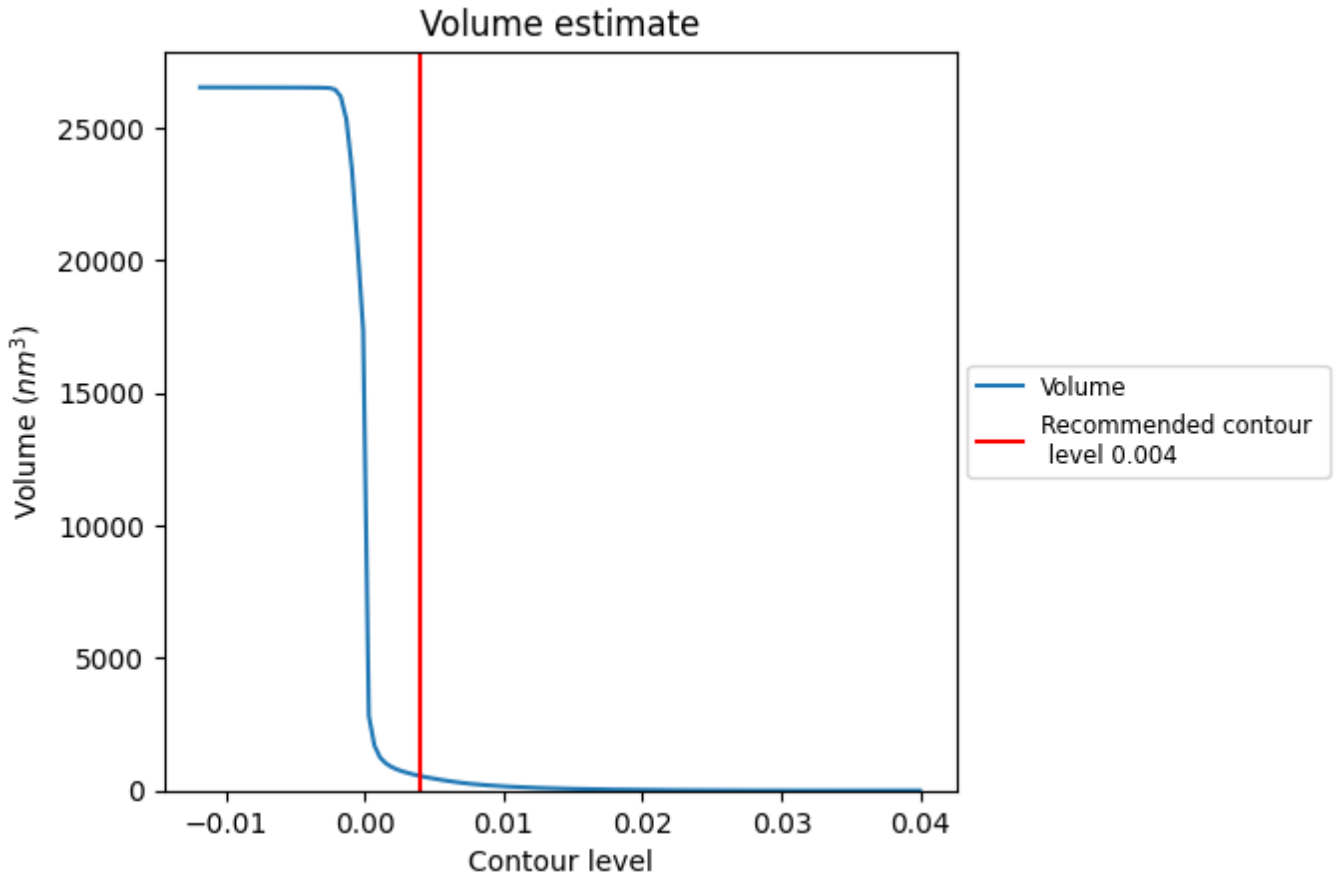
This section contains the results of statistical analysis of the map.

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.

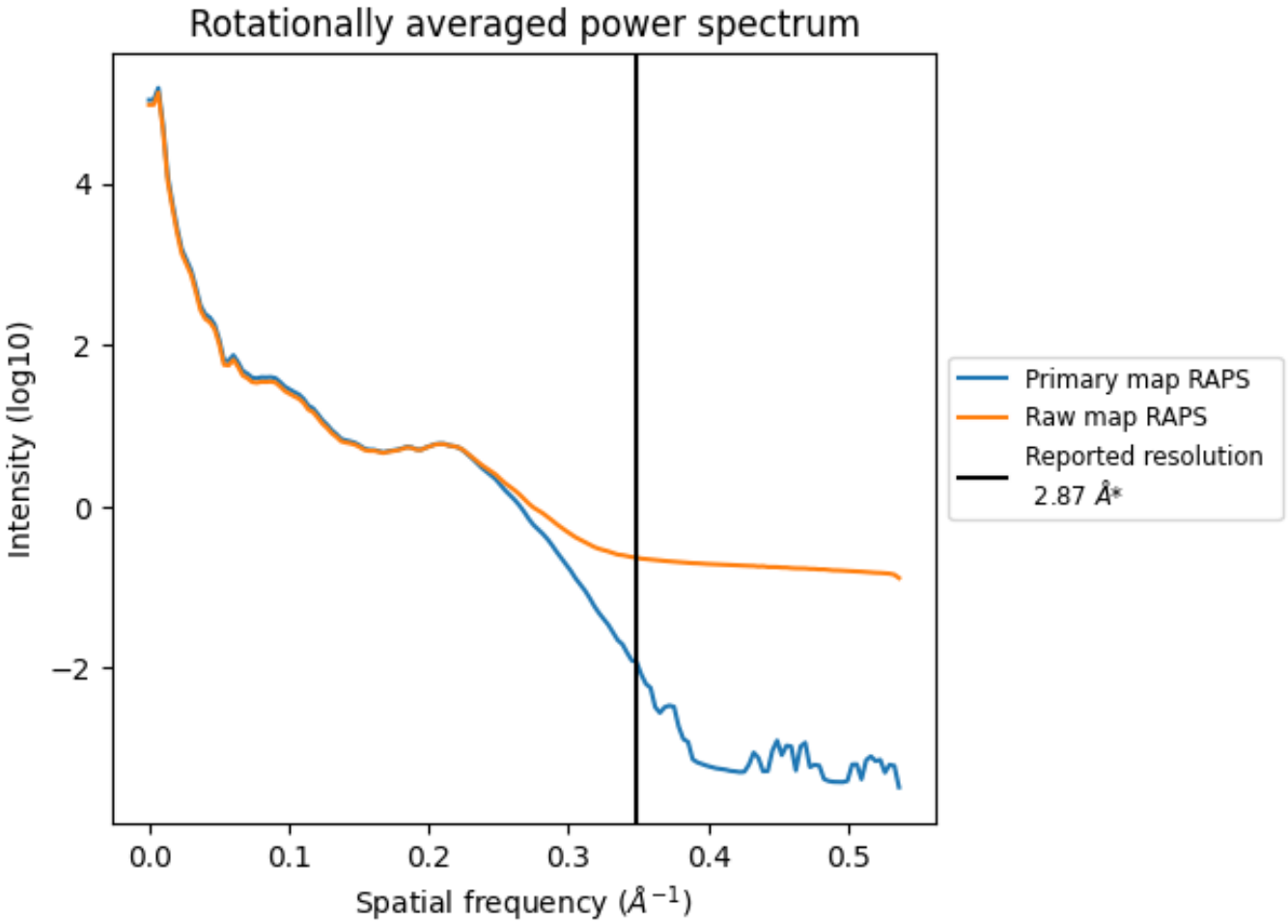
7.2 Volume estimate (i)



The volume at the recommended contour level is 549 nm^3; this corresponds to an approximate mass of 496 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)

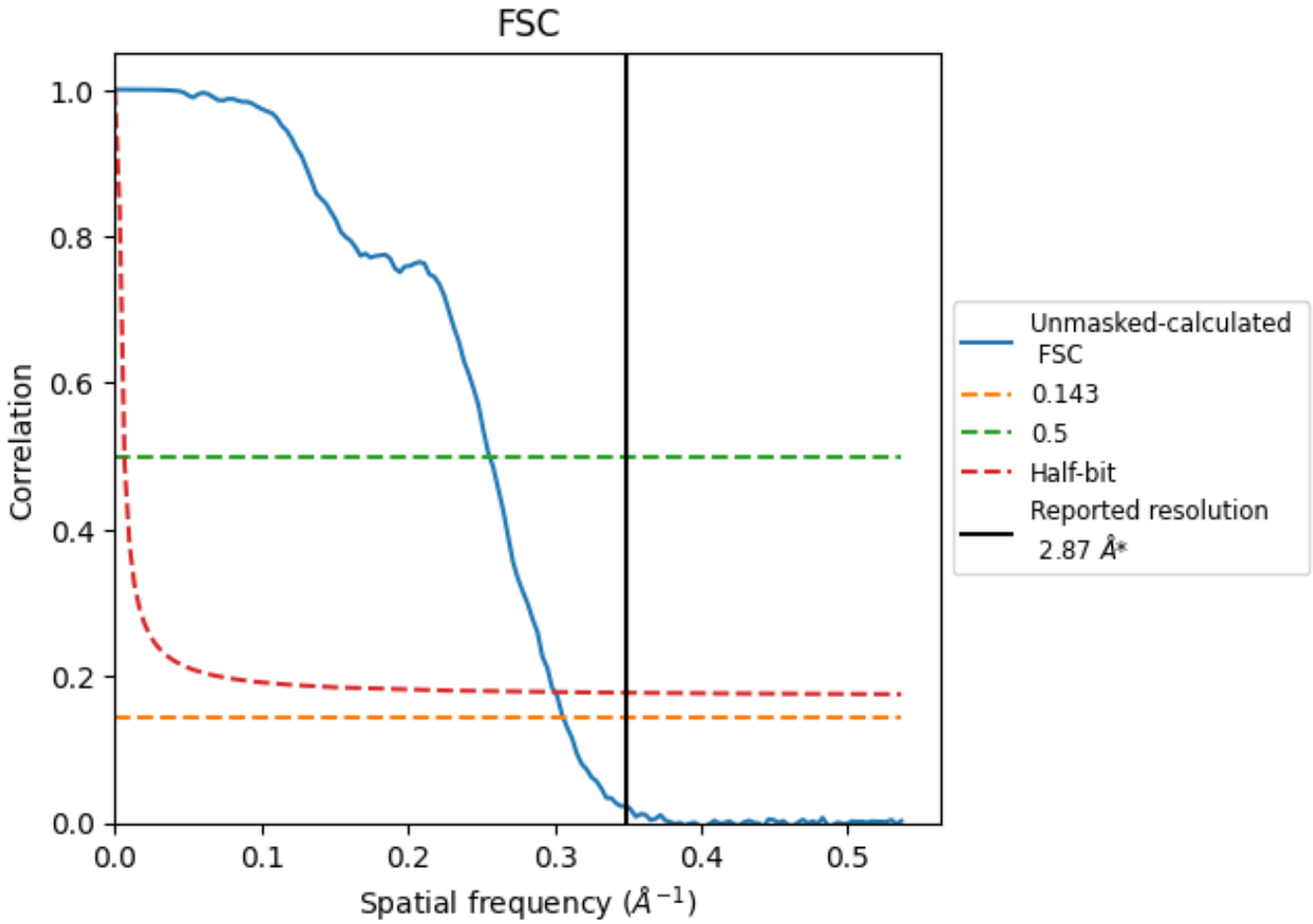


*Reported resolution corresponds to spatial frequency of 0.348 $Å^{-1}$

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 0.348 Å^{-1}

8.2 Resolution estimates (i)

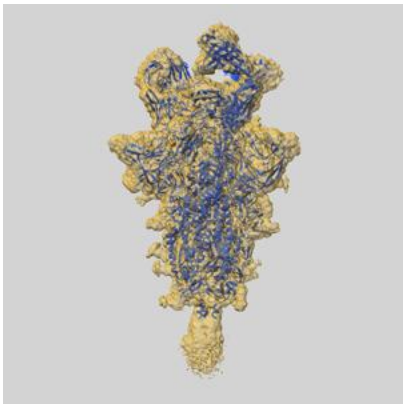
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.87	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.27	3.91	3.33

*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 3.27 differs from the reported value 2.87 by more than 10 %

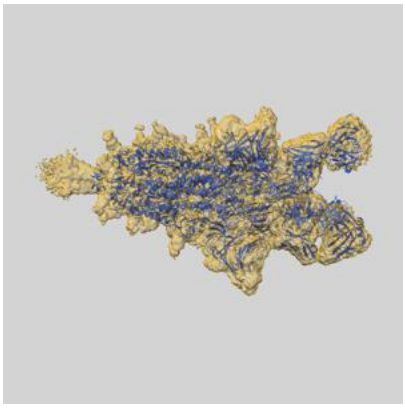
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-39802 and PDB model 8Z6R. Per-residue inclusion information can be found in section 3 on page 11.

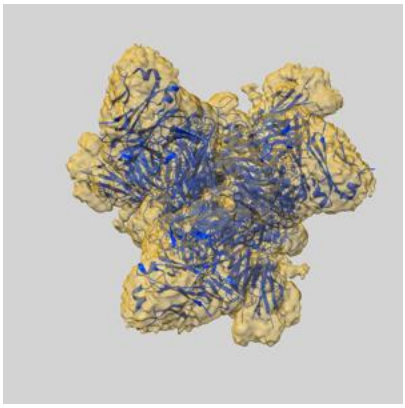
9.1 Map-model overlay



X



Y



Z

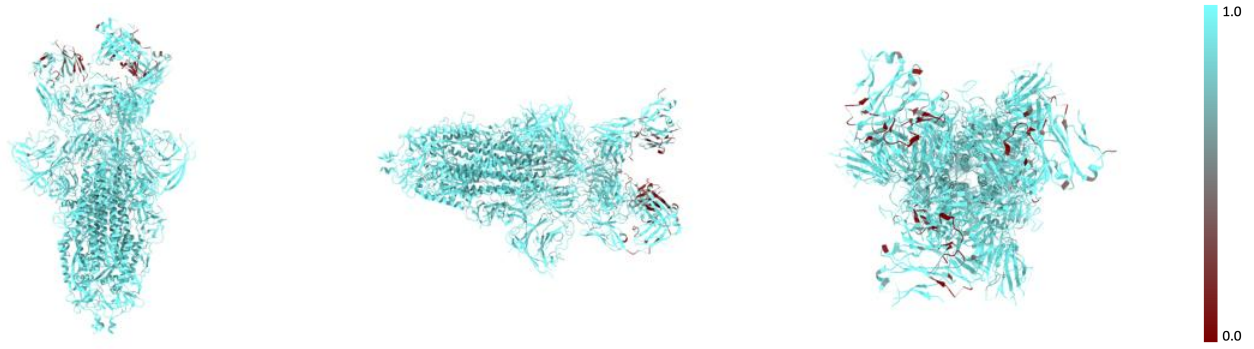
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

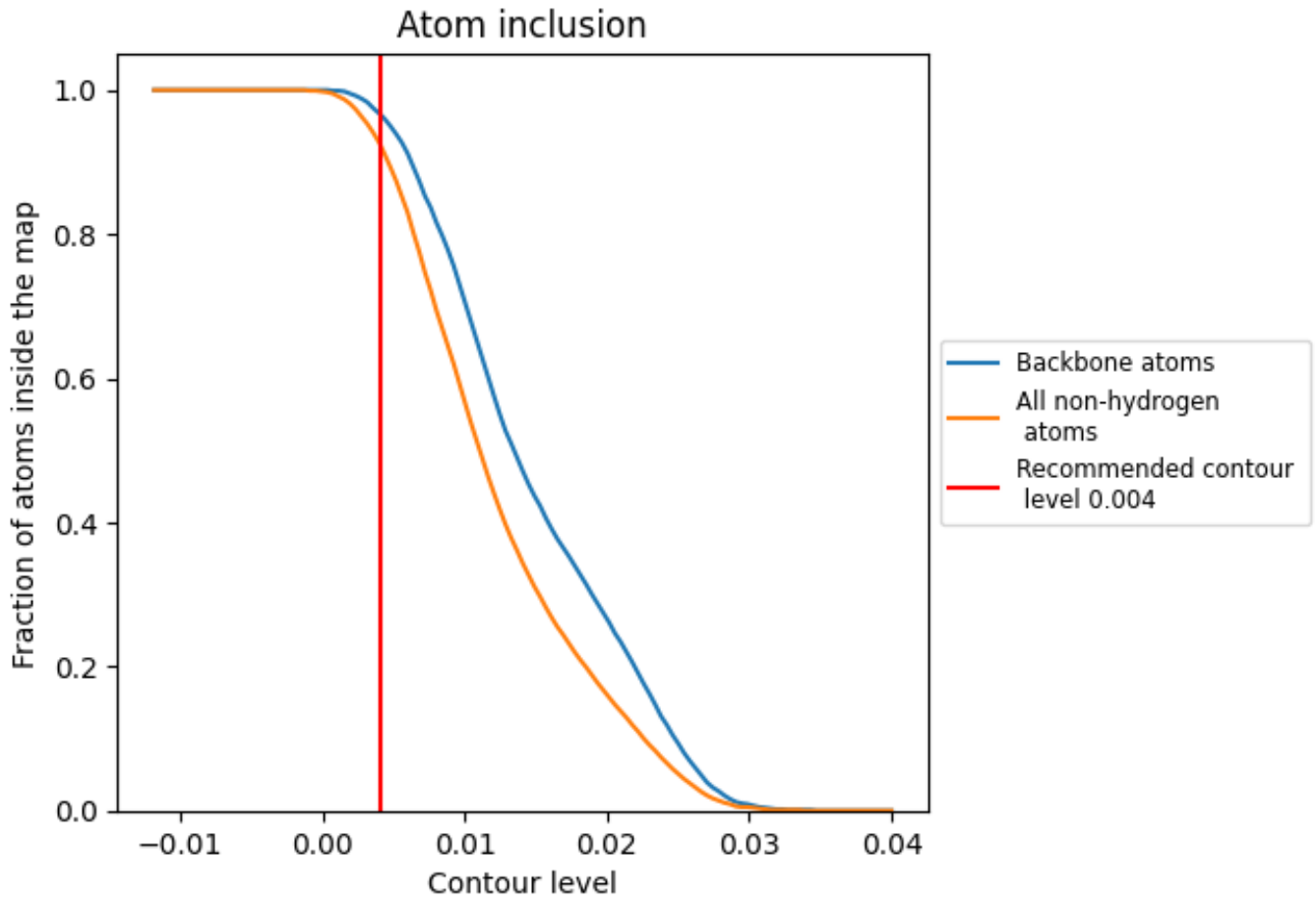
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.004).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 93% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9260	0.4100
A	0.9600	0.4710
B	0.9590	0.4680
C	0.9580	0.4690
D	0.8710	0.2390
E	0.7780	0.2420
F	0.8800	0.2330
G	0.8400	0.2290
H	0.8660	0.2470
I	0.7730	0.2730