



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 02:43 AM UTC

PDB ID : 8Z6S / pdb_00008z6s
EMDB ID : EMD-39803
Title : Structure of XBB.1.16 S trimer with 2 down-RBDs complex with antibody CYFN1006-1.
Authors : Wang, Y.J.; Sun, L.
Deposited on : 2024-04-19
Resolution : 2.84 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:

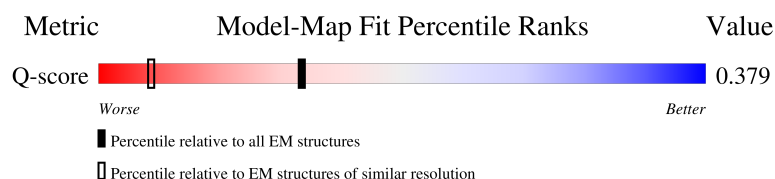
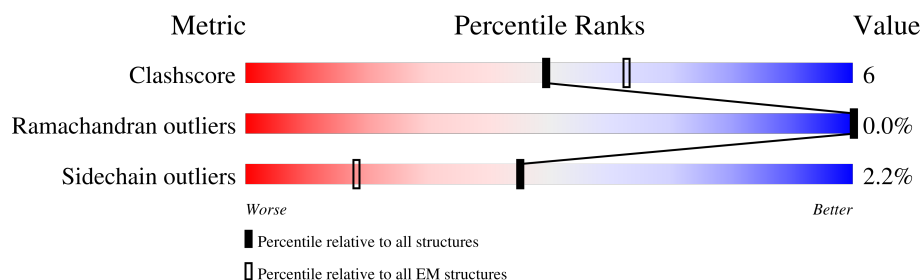
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.84 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11884 (2.34 - 3.34)

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	D	215	
1	F	215	
1	H	215	
2	E	451	

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Mol	Chain	Length	Quality of chain
2	G	451	
2	I	451	
3	A	1299	
3	B	1299	
3	C	1299	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 35014 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 CYFN1006-1 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	194	Total	C	N	O	S	0	0
			1443	904	240	292	7		
1	F	192	Total	C	N	O	S	0	0
			1429	895	237	290	7		
1	H	192	Total	C	N	O	S	0	0
			1429	895	237	290	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	202	Total	C	N	O	S	0	0
			1544	992	251	293	8		
2	G	202	Total	C	N	O	S	0	0
			1544	992	251	293	8		
2	I	202	Total	C	N	O	S	0	0
			1544	992	251	293	8		

- Molecule 3 is a protein called Spike glycoprotein,Fibritin,Expression Tag.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	1106	Total	C	N	O	S	0	0
			8662	5534	1445	1643	40		
3	B	1103	Total	C	N	O	S	0	0
			8650	5533	1440	1637	40		
3	A	1119	Total	C	N	O	S	0	0
			8769	5607	1462	1660	40		

There are 243 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	MET	-	initiating methionine	UNP P0DTC2
C	-5	PRO	-	expression tag	UNP P0DTC2
C	-4	MET	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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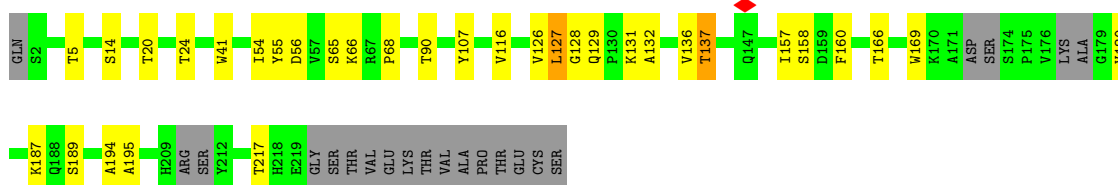
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A	478	ARG	THR	conflict	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	486	PRO	PHE	variant	UNP P0DTC2
A	490	SER	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	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
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

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.

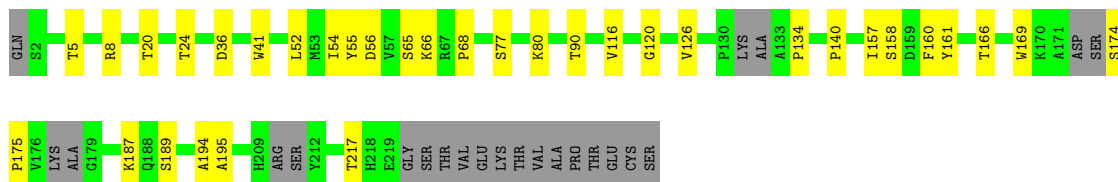
- Molecule 1: CYFN1006-1 light chain

Chain D: 



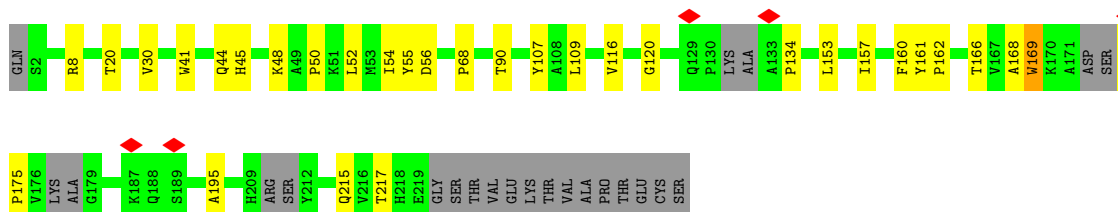
- Molecule 1: CYFN1006-1 light chain

Chain F: 



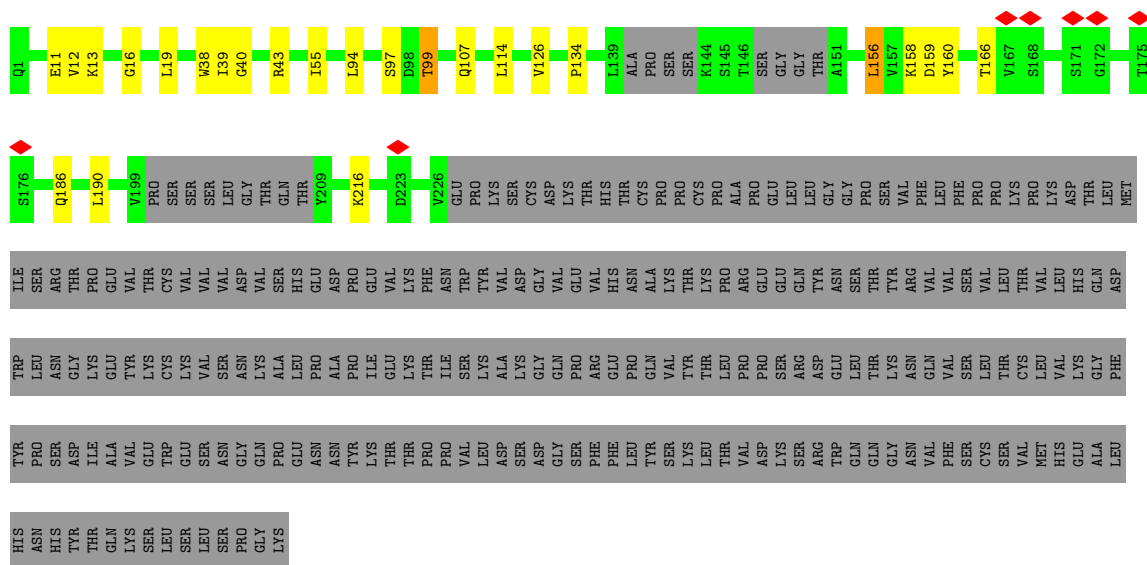
- Molecule 1: CYFN1006-1 light chain

Chain H: 



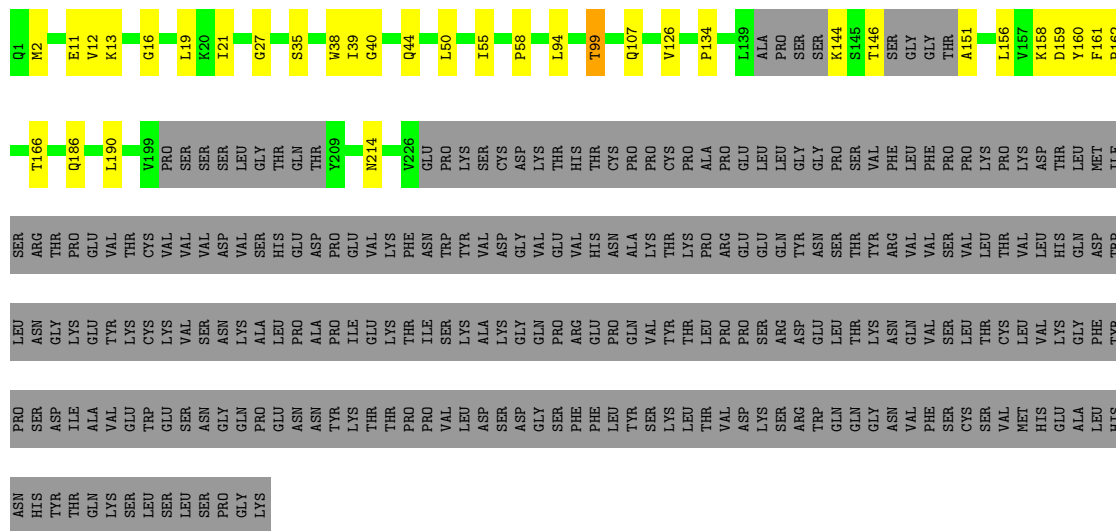
- Molecule 2: CYFN1006-1 heavy chain

Chain E: 



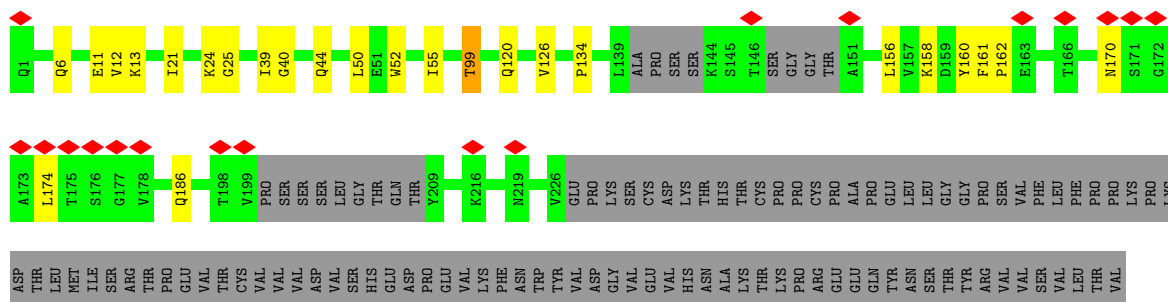
• Molecule 2: CYFN1006-1 heavy chain

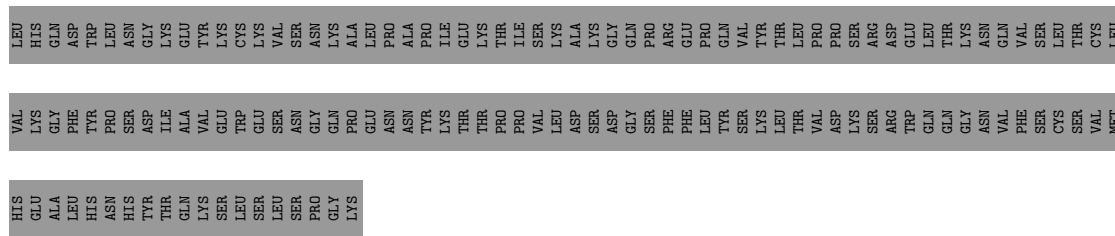
Chain G: 37% 7% 55%



• Molecule 2: CYFN1006-1 heavy chain

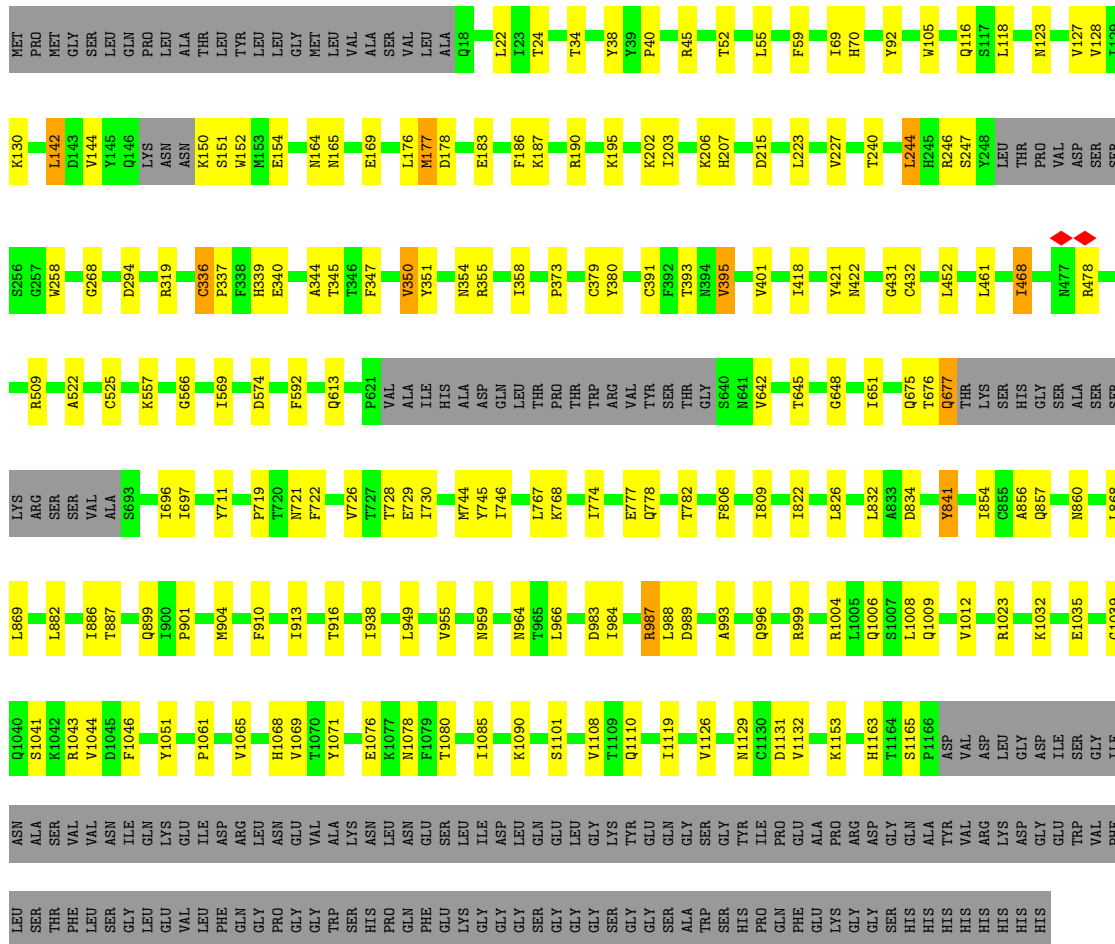
Chain I: 39% 5% 55%





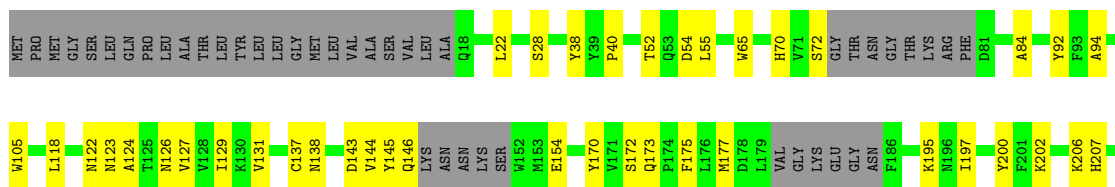
• Molecule 3: Spike glycoprotein,Fibritin,Expression Tag

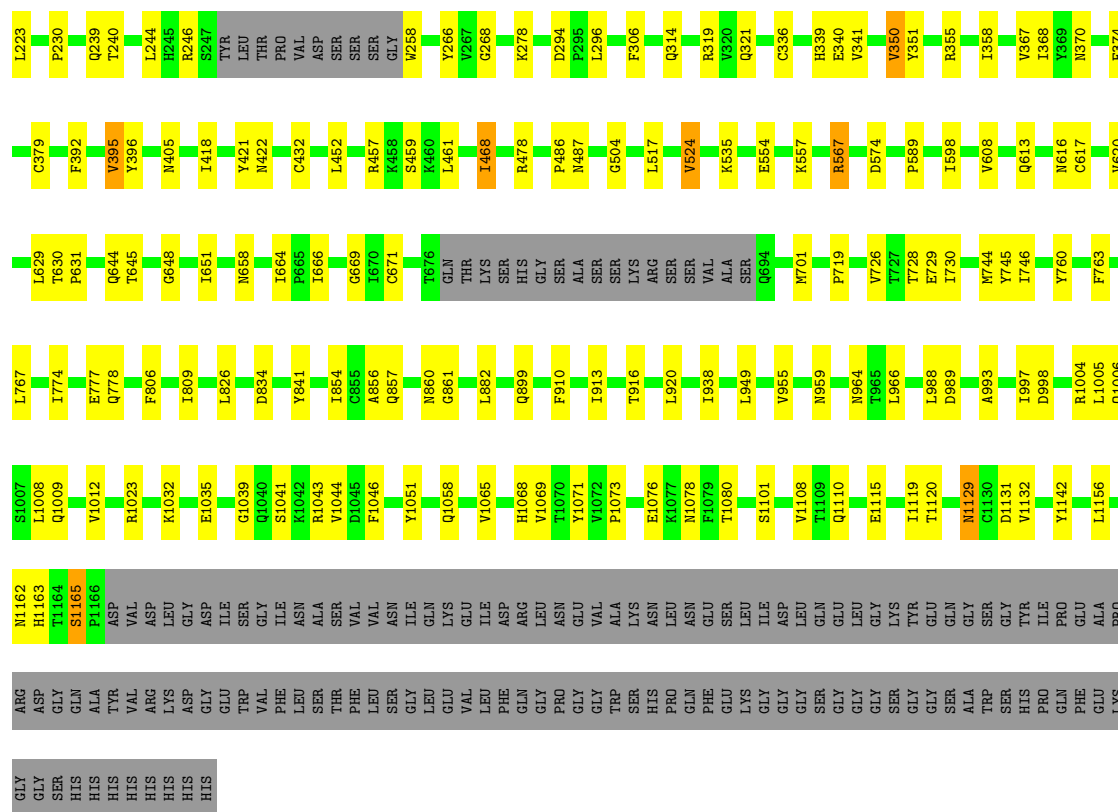
Chain C: 71% 14% 15%



• Molecule 3: Spike glycoprotein,Fibritin,Expression Tag

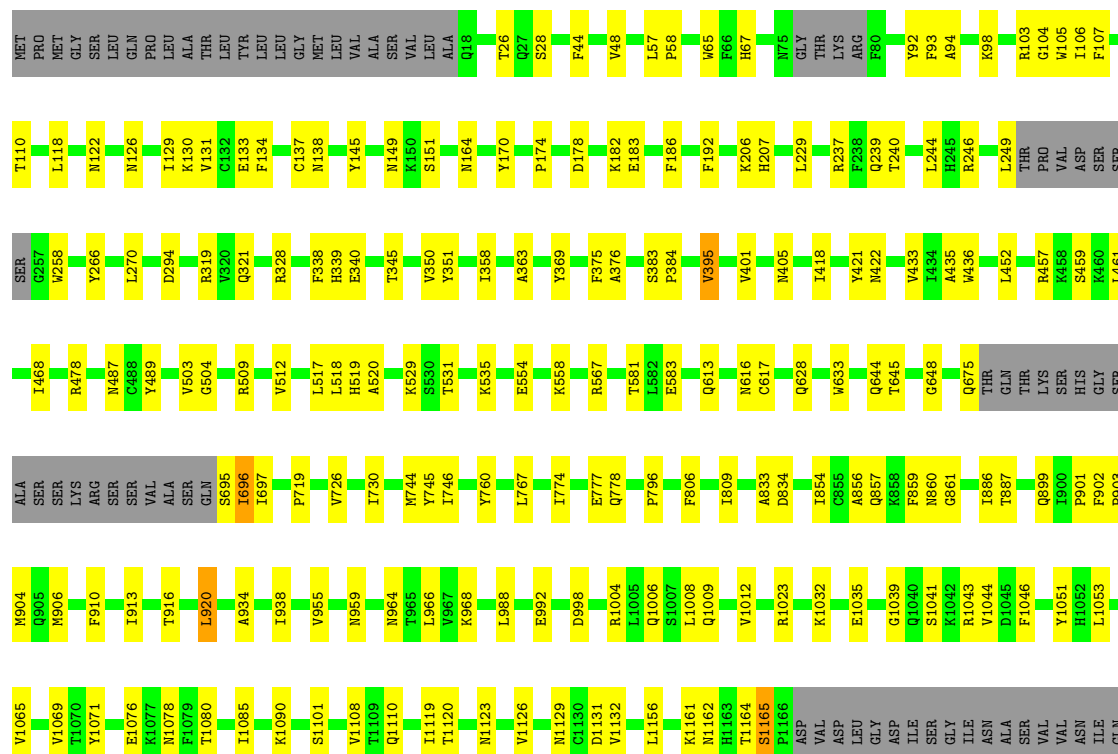
Chain B: 70% 14% 15%





• Molecule 3: Spike glycoprotein, Fibrin, Expression Tag

Chain A: 71% 15% 14%



LYS	GLU
GLU	VAL
ILE	LEU
ASP	PHE
ARG	GLN
LEU	GLY
ASN	PRO
GLU	GLY
VAL	GLY
ALA	TRP
LYS	SER
ASN	HIS
LEU	PRO
ASN	GLN
GLU	PHE
SER	GLU
LEU	LYS
ILE	GLY
ASP	GLY
LEU	GLY
GLN	SER
GLU	GLY
LEU	GLY
GLY	GLY
LYS	SER
TYR	GLY
GLU	GLY
GLN	GLY
GLY	ALA
SER	TRP
GLY	SER
TYR	HIS
ILE	PRO
PRO	GLN
GLU	PHE
ALA	GLU
PRO	LYS
ARG	GLY
ASP	GLY
GLN	SER
GLN	HIS
ALA	HIS
TYR	HIS
VAL	HIS
ARG	HIS
LYS	HIS
ASP	HIS
GLY	HIS
GLU	
TRP	
VAL	
PHE	
LEU	
SER	
THR	
PHE	
LEU	
SER	
GLY	
LEU	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	936842	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	1.086	Depositor
Minimum map value	-0.344	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.04	Depositor
Map size ($\text{\AA}$)	298.24, 298.24, 298.24	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.932, 0.932, 0.932	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	D	0.16	0/1475	0.38	0/2007
1	F	0.13	0/1460	0.31	0/1986
1	H	0.12	0/1460	0.30	0/1986
2	E	0.11	0/1584	0.33	0/2151
2	G	0.12	0/1584	0.35	0/2151
2	I	0.12	0/1584	0.32	0/2151
3	A	0.12	0/8983	0.32	0/12230
3	B	0.12	0/8860	0.32	0/12064
3	C	0.14	0/8870	0.34	0/12069
All	All	0.13	0/35860	0.33	0/48795

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1443	0	1394	15	0
1	F	1429	0	1375	20	0
1	H	1429	0	1375	19	0
2	E	1544	0	1519	12	0
2	G	1544	0	1519	16	0
2	I	1544	0	1519	11	0
3	A	8769	0	8563	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	8650	0	8445	115	0
3	C	8662	0	8458	114	0
All	All	35014	0	34167	396	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 6.

All (396) 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)
3:A:767:LEU:HG	3:A:1012:VAL:HG21	1.74	0.70
3:B:629:LEU:HG	3:B:631:PRO:HD2	1.72	0.70
1:H:41:TRP:HB2	1:H:54:ILE:HB	1.75	0.69
3:B:767:LEU:HG	3:B:1012:VAL:HG21	1.75	0.68
3:B:478:ARG:HE	3:B:487:ASN:HD21	1.41	0.67
1:D:41:TRP:HB2	1:D:54:ILE:HB	1.76	0.67
1:F:41:TRP:HB2	1:F:54:ILE:HB	1.76	0.67
3:C:105:TRP:HA	3:C:240:THR:HA	1.77	0.67
3:C:767:LEU:HG	3:C:1012:VAL:HG21	1.77	0.67
3:C:1129:ASN:ND2	3:C:1131:ASP:OD1	2.29	0.66
3:B:1032:LYS:NZ	3:B:1046:PHE:O	2.29	0.65
3:B:1129:ASN:ND2	3:B:1131:ASP:OD1	2.29	0.65
3:A:1129:ASN:ND2	3:A:1131:ASP:OD1	2.29	0.65
2:I:170:ASN:HD22	2:I:174:LEU:HD23	1.62	0.65
3:C:152:TRP:HH2	3:C:247:SER:HA	1.62	0.65
3:A:1051:TYR:HB2	3:A:1071:TYR:HB3	1.79	0.65
1:D:107:TYR:HB3	1:D:116:VAL:HG12	1.79	0.65
2:G:134:PRO:HB3	2:G:160:TYR:HB3	1.78	0.64
3:A:1108:VAL:HG23	3:A:1119:ILE:HG12	1.80	0.63
1:F:157:ILE:HB	1:F:195:ALA:HB3	1.80	0.63
3:B:105:TRP:HA	3:B:240:THR:HA	1.80	0.63
1:F:52:LEU:HD11	1:F:55:TYR:HB3	1.81	0.62
3:C:1035:GLU:HB3	3:C:1041:SER:HB2	1.80	0.62
3:B:1051:TYR:HB2	3:B:1071:TYR:HB3	1.80	0.62
3:C:832:LEU:HD11	3:C:1061:PRO:HB3	1.82	0.62
3:B:1035:GLU:HB3	3:B:1041:SER:HB2	1.81	0.62
3:B:123:ASN:ND2	3:B:126:ASN:O	2.33	0.61
3:A:746:ILE:O	3:A:1004:ARG:NH2	2.32	0.61
3:A:1035:GLU:HB3	3:A:1041:SER:HB2	1.83	0.61
2:E:16:GLY:H	2:E:94:LEU:HB2	1.65	0.61
3:A:1032:LYS:NZ	3:A:1046:PHE:O	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:730:ILE:HG13	3:B:1065:VAL:HG22	1.83	0.60
3:C:1090:LYS:HE2	3:C:1126:VAL:HG11	1.83	0.60
3:B:988:LEU:HA	3:A:383:SER:HB2	1.83	0.60
3:A:955:VAL:O	3:A:959:ASN:ND2	2.35	0.60
2:E:13:LYS:HB2	2:E:19:LEU:HD23	1.83	0.60
3:A:105:TRP:HA	3:A:240:THR:HA	1.82	0.60
3:C:1051:TYR:HB2	3:C:1071:TYR:HB3	1.83	0.60
3:A:857:GLN:NE2	3:A:964:ASN:OD1	2.35	0.60
3:B:746:ILE:O	3:B:1004:ARG:NH2	2.35	0.59
3:B:777:GLU:OE2	3:B:1023:ARG:NE	2.33	0.59
1:D:157:ILE:HB	1:D:195:ALA:HB3	1.85	0.59
3:A:137:CYS:SG	3:A:138:ASN:N	2.75	0.59
3:C:984:ILE:HG23	3:C:988:LEU:HD12	1.83	0.59
3:C:1032:LYS:NZ	3:C:1046:PHE:O	2.34	0.59
3:C:744:MET:SD	3:B:319:ARG:NH2	2.76	0.59
3:B:955:VAL:O	3:B:959:ASN:ND2	2.35	0.59
3:A:149:ASN:ND2	3:A:151:SER:OG	2.36	0.59
2:G:158:LYS:NZ	2:G:186:GLN:OE1	2.36	0.58
3:C:339:HIS:HD2	3:C:340:GLU:HG3	1.68	0.58
3:B:126:ASN:ND2	3:B:172:SER:O	2.36	0.58
1:D:56:ASP:O	1:D:66:LYS:N	2.34	0.58
2:G:11:GLU:OE1	2:G:13:LYS:NZ	2.37	0.58
3:C:777:GLU:OE2	3:C:1023:ARG:NE	2.33	0.58
3:A:104:GLY:O	3:A:240:THR:OG1	2.21	0.58
2:I:99:THR:HB	2:I:126:VAL:H	1.69	0.58
3:C:319:ARG:NH2	3:A:744:MET:SD	2.77	0.58
2:E:11:GLU:OE1	2:E:13:LYS:NZ	2.36	0.58
3:B:137:CYS:SG	3:B:138:ASN:N	2.77	0.58
3:B:726:VAL:HG22	3:B:1069:VAL:HG22	1.86	0.58
1:H:134:PRO:HB3	1:H:160:PHE:HB3	1.85	0.57
3:B:856:ALA:O	3:B:860:ASN:ND2	2.37	0.57
3:B:368:ILE:HG22	3:B:374:PHE:HZ	1.68	0.57
3:A:57:LEU:HD12	3:A:58:PRO:HD2	1.85	0.57
3:C:834:ASP:HB2	3:C:854:ILE:HG12	1.85	0.57
3:A:613:GLN:HA	3:A:648:GLY:HA3	1.86	0.57
1:D:166:THR:HB	1:D:217:THR:HB	1.86	0.57
3:A:1129:ASN:HD21	3:A:1132:VAL:HG23	1.69	0.57
3:A:988:LEU:HB3	3:A:992:GLU:HG3	1.87	0.57
3:C:746:ILE:O	3:C:1004:ARG:NH2	2.37	0.57
3:A:130:LYS:HE3	3:A:134:PHE:HZ	1.69	0.57
3:B:916:THR:OG1	3:B:1110:GLN:NE2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:777:GLU:OE2	3:A:1023:ARG:NE	2.30	0.56
3:B:857:GLN:NE2	3:B:964:ASN:OD1	2.38	0.56
3:C:726:VAL:HG22	3:C:1069:VAL:HG22	1.86	0.56
3:C:856:ALA:O	3:C:860:ASN:ND2	2.35	0.56
1:F:5:THR:OG1	1:F:24:THR:OG1	2.24	0.56
3:B:1156:LEU:HD13	3:A:1156:LEU:HD11	1.87	0.56
3:A:916:THR:OG1	3:A:1110:GLN:NE2	2.39	0.56
1:F:134:PRO:HB3	1:F:160:PHE:HB3	1.88	0.56
1:H:56:ASP:OD1	1:H:107:TYR:OH	2.23	0.56
1:D:5:THR:OG1	1:D:24:THR:OG1	2.24	0.55
3:A:726:VAL:HG22	3:A:1069:VAL:HG22	1.87	0.55
3:C:1035:GLU:OE2	3:B:1043:ARG:NE	2.37	0.55
2:E:158:LYS:NZ	2:E:186:GLN:OE1	2.35	0.55
3:C:730:ILE:HG13	3:C:1065:VAL:HG22	1.87	0.55
3:C:1080:THR:HB	3:C:1101:SER:HB3	1.87	0.55
1:H:166:THR:HB	1:H:217:THR:HB	1.88	0.55
3:C:955:VAL:O	3:C:959:ASN:ND2	2.36	0.55
3:B:644:GLN:NE2	3:B:645:THR:O	2.40	0.55
3:A:535:LYS:NZ	3:A:554:GLU:OE2	2.35	0.55
3:A:126:ASN:H	3:A:174:PRO:HD3	1.72	0.55
3:A:339:HIS:HD2	3:A:340:GLU:HG3	1.72	0.55
3:A:1090:LYS:HE2	3:A:1126:VAL:HG11	1.88	0.55
1:F:36:ASP:O	1:F:80:LYS:NZ	2.40	0.54
3:C:246:ARG:HG3	3:C:258:TRP:HA	1.90	0.54
3:C:899:GLN:NE2	3:B:1078:ASN:OD1	2.40	0.54
1:F:56:ASP:O	1:F:66:LYS:N	2.30	0.54
3:B:1009:GLN:OE1	3:A:1006:GLN:NE2	2.40	0.54
3:A:730:ILE:HG12	3:A:1065:VAL:HG22	1.90	0.54
3:C:177:MET:SD	3:C:177:MET:N	2.75	0.54
3:C:557:LYS:NZ	3:C:574:ASP:OD1	2.40	0.54
3:C:645:THR:OG1	3:C:648:GLY:O	2.24	0.54
3:C:401:VAL:HG22	3:C:509:ARG:HG2	1.89	0.54
3:C:745:TYR:OH	3:C:966:LEU:O	2.26	0.54
3:C:916:THR:OG1	3:C:1110:GLN:NE2	2.40	0.54
3:B:84:ALA:HA	3:B:239:GLN:HE21	1.72	0.54
3:B:339:HIS:HD2	3:B:340:GLU:HG3	1.72	0.54
3:B:744:MET:SD	3:A:319:ARG:NH2	2.82	0.53
3:C:613:GLN:HA	3:C:648:GLY:HA3	1.89	0.53
3:C:1009:GLN:OE1	3:B:1006:GLN:NE2	2.36	0.53
2:E:134:PRO:HB3	2:E:160:TYR:HB3	1.90	0.53
2:I:6:GLN:H	2:I:120:GLN:HE22	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:899:GLN:NE2	3:A:1078:ASN:OD1	2.41	0.53
3:A:94:ALA:HB3	3:A:266:TYR:HB2	1.91	0.53
3:A:644:GLN:NE2	3:A:645:THR:O	2.42	0.53
1:H:20:THR:HG22	1:H:90:THR:HG22	1.91	0.53
3:C:195:LYS:HD2	3:C:202:LYS:HD2	1.91	0.53
1:F:166:THR:HB	1:F:217:THR:HB	1.90	0.53
3:A:457:ARG:NH2	3:A:459:SER:O	2.40	0.53
3:C:566:GLY:HA2	3:A:44:PHE:HB3	1.91	0.53
3:C:391:CYS:HA	3:C:525:CYS:HA	1.92	0.52
3:A:886:ILE:HG13	3:A:887:THR:HG23	1.91	0.52
3:A:1120:THR:OG1	3:A:1123:ASN:OD1	2.27	0.52
3:C:468:ILE:HD13	3:C:468:ILE:H	1.74	0.52
3:C:768:LYS:NZ	3:B:314:GLN:O	2.40	0.52
3:C:857:GLN:NE2	3:C:964:ASN:OD1	2.43	0.52
3:C:1043:ARG:NE	3:A:1035:GLU:OE2	2.38	0.52
3:C:901:PRO:HB2	3:C:904:MET:HG3	1.91	0.52
3:B:367:VAL:HA	3:B:370:ASN:HD21	1.74	0.52
3:A:616:ASN:OD1	3:A:617:CYS:N	2.42	0.52
1:D:20:THR:HG22	1:D:90:THR:HG22	1.92	0.52
3:B:206:LYS:NZ	3:B:207:HIS:O	2.40	0.52
3:B:468:ILE:HD13	3:B:468:ILE:H	1.74	0.52
3:B:744:MET:HE3	3:B:861:GLY:HA2	1.91	0.52
3:B:760:TYR:OH	3:B:998:ASP:OD1	2.27	0.52
3:B:1108:VAL:HG23	3:B:1119:ILE:HG12	1.93	0.51
2:G:38:TRP:H	2:G:107:GLN:HE21	1.56	0.51
1:D:158:SER:HA	1:D:194:ALA:HA	1.93	0.51
3:C:24:THR:OG1	3:C:69:ILE:O	2.26	0.51
3:A:358:ILE:HB	3:A:395:VAL:HG13	1.93	0.51
3:C:1006:GLN:NE2	3:A:1009:GLN:OE1	2.39	0.51
3:B:535:LYS:NZ	3:B:554:GLU:OE2	2.38	0.51
3:A:369:TYR:OH	3:A:384:PRO:O	2.26	0.51
2:I:158:LYS:NZ	2:I:186:GLN:OE1	2.36	0.51
3:C:130:LYS:HG3	3:C:169:GLU:HG2	1.93	0.51
1:D:187:LYS:NZ	1:D:189:SER:OG	2.43	0.51
1:H:168:ALA:HB3	1:H:215:GLN:HB3	1.93	0.51
3:A:98:LYS:NZ	3:A:186:PHE:O	2.43	0.51
3:C:164:ASN:ND2	3:C:165:ASN:OD1	2.44	0.50
3:A:774:ILE:O	3:A:778:GLN:HG2	2.11	0.50
3:C:393:THR:HA	3:C:522:ALA:HA	1.93	0.50
3:B:129:ILE:HB	3:B:170:TYR:HB3	1.92	0.50
3:B:321:GLN:NE2	3:B:630:THR:OG1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1035:GLU:OE2	3:A:1043:ARG:NE	2.42	0.50
2:G:35:SER:HA	2:G:58:PRO:HB2	1.92	0.50
3:C:206:LYS:NZ	3:C:207:HIS:O	2.39	0.50
3:C:719:PRO:HA	3:C:1076:GLU:HA	1.94	0.50
3:A:345:THR:O	3:A:509:ARG:NH1	2.44	0.50
3:C:989:ASP:O	3:C:993:ALA:N	2.44	0.50
3:B:55:LEU:HD11	3:B:197:ILE:HD11	1.93	0.50
3:B:745:TYR:OH	3:B:966:LEU:O	2.28	0.50
1:H:52:LEU:HD11	1:H:55:TYR:HB3	1.93	0.50
3:C:1078:ASN:OD1	3:A:899:GLN:NE2	2.44	0.50
3:A:966:LEU:HD11	3:A:1008:LEU:HD23	1.94	0.50
2:E:40:GLY:HA3	2:E:55:ILE:HG22	1.93	0.49
3:C:421:TYR:HA	3:C:461:LEU:HD13	1.94	0.49
3:A:107:PHE:HB2	3:A:118:LEU:HB3	1.94	0.49
3:B:124:ALA:HA	3:B:177:MET:HE1	1.94	0.49
3:A:719:PRO:HA	3:A:1076:GLU:HA	1.93	0.49
1:F:158:SER:HA	1:F:194:ALA:HA	1.94	0.49
3:C:379:CYS:HA	3:C:432:CYS:HA	1.94	0.49
3:C:806:PHE:HD1	3:C:809:ILE:HD11	1.77	0.49
1:D:56:ASP:O	1:D:65:SER:N	2.46	0.49
3:A:376:ALA:HB3	3:A:435:ALA:HB3	1.93	0.49
3:C:774:ILE:O	3:C:778:GLN:HG2	2.12	0.49
3:B:246:ARG:HA	3:B:258:TRP:HA	1.94	0.49
3:B:966:LEU:HD11	3:B:1008:LEU:HD23	1.94	0.49
3:A:745:TYR:OH	3:A:966:LEU:O	2.27	0.49
3:B:719:PRO:HA	3:B:1076:GLU:HA	1.95	0.48
3:A:834:ASP:HB2	3:A:854:ILE:HG12	1.94	0.48
3:C:1129:ASN:HD21	3:C:1132:VAL:HG23	1.78	0.48
3:B:1080:THR:HB	3:B:1101:SER:HB3	1.94	0.48
3:A:246:ARG:HG3	3:A:258:TRP:HA	1.95	0.48
1:F:157:ILE:O	1:F:195:ALA:N	2.41	0.48
3:C:782:THR:HG22	3:C:869:LEU:HD12	1.96	0.48
3:A:103:ARG:HB3	3:A:122:ASN:HB3	1.94	0.48
1:H:109:LEU:HD11	3:C:339:HIS:HB2	1.96	0.48
3:A:129:ILE:O	3:A:170:TYR:N	2.47	0.48
3:A:806:PHE:HD1	3:A:809:ILE:HD11	1.78	0.48
3:B:1162:ASN:O	3:B:1165:SER:OG	2.31	0.48
3:A:110:THR:O	3:A:237:ARG:NH1	2.45	0.48
1:F:8:ARG:NH2	1:F:120:GLY:O	2.46	0.48
3:C:569:ILE:HG13	3:A:48:VAL:HB	1.96	0.48
3:B:774:ILE:O	3:B:778:GLN:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1120:THR:HG22	3:B:1142:TYR:HD2	1.78	0.48
3:A:401:VAL:HG22	3:A:509:ARG:HG2	1.95	0.48
3:A:421:TYR:HA	3:A:461:LEU:HD13	1.96	0.48
1:F:56:ASP:O	1:F:65:SER:N	2.47	0.48
3:B:92:TYR:N	3:B:268:GLY:O	2.39	0.48
3:A:321:GLN:HG3	3:A:628:GLN:HG3	1.95	0.48
3:C:350:VAL:HG11	3:C:418:ILE:HD12	1.94	0.47
3:C:841:TYR:OH	3:B:589:PRO:O	2.30	0.47
3:A:206:LYS:NZ	3:A:207:HIS:O	2.41	0.47
2:G:146:THR:HG22	2:G:151:ALA:HB1	1.96	0.47
3:B:94:ALA:HB3	3:B:266:TYR:HB2	1.96	0.47
3:C:345:THR:O	3:C:509:ARG:NH1	2.46	0.47
3:C:354:ASN:OD1	3:C:355:ARG:N	2.47	0.47
3:A:328:ARG:NH2	3:A:531:THR:O	2.47	0.47
3:A:901:PRO:HB2	3:A:904:MET:HG3	1.96	0.47
2:I:24:LYS:NZ	2:I:25:GLY:O	2.43	0.47
3:C:38:TYR:HA	3:C:223:LEU:H	1.78	0.47
3:C:350:VAL:HG12	3:C:422:ASN:HB3	1.96	0.47
3:B:719:PRO:HG3	3:B:1073:PRO:HB3	1.95	0.47
2:G:16:GLY:H	2:G:94:LEU:HB2	1.79	0.47
2:I:134:PRO:HB3	2:I:160:TYR:HB3	1.95	0.47
3:C:123:ASN:H	3:C:127:VAL:HG12	1.79	0.47
3:A:183:GLU:HG3	3:A:186:PHE:HB2	1.96	0.47
1:F:20:THR:HG22	1:F:90:THR:HG22	1.97	0.47
1:F:55:TYR:HD1	1:F:68:PRO:HG3	1.80	0.47
3:B:620:VAL:HG11	3:B:651:ILE:HD11	1.97	0.47
3:C:711:TYR:HB3	3:A:796:PRO:HG2	1.97	0.47
1:H:157:ILE:HB	1:H:195:ALA:HB3	1.96	0.46
3:B:421:TYR:HA	3:B:461:LEU:HD13	1.97	0.46
3:C:358:ILE:HB	3:C:395:VAL:HG13	1.97	0.46
3:C:729:GLU:OE1	3:C:1068:HIS:NE2	2.48	0.46
1:D:127:LEU:HD22	1:D:127:LEU:HA	1.78	0.46
3:A:133:GLU:HB2	3:A:164:ASN:HB3	1.96	0.46
3:A:350:VAL:HG11	3:A:418:ILE:HD12	1.97	0.46
2:I:40:GLY:HA3	2:I:55:ILE:HG22	1.98	0.46
3:C:40:PRO:HG3	3:C:52:THR:HG21	1.98	0.46
3:C:203:ILE:HB	3:C:227:VAL:HB	1.98	0.46
3:C:809:ILE:HG22	3:C:822:ILE:HD12	1.97	0.46
1:F:187:LYS:NZ	1:F:189:SER:OG	2.42	0.46
3:C:187:LYS:NZ	3:C:215:ASP:OD1	2.49	0.46
3:B:557:LYS:NZ	3:B:574:ASP:OD1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:910:PHE:HA	3:B:913:ILE:HG12	1.98	0.46
1:F:140:PRO:HG3	2:G:144:LYS:HG3	1.97	0.46
3:B:38:TYR:HA	3:B:223:LEU:H	1.81	0.46
3:A:478:ARG:HB3	3:A:487:ASN:HD21	1.81	0.46
3:B:728:THR:HG23	3:B:938:ILE:HD12	1.98	0.46
3:B:1039:GLY:HA3	3:A:1044:VAL:HG21	1.96	0.46
2:G:13:LYS:HB2	2:G:19:LEU:HD23	1.99	0.45
3:B:613:GLN:HA	3:B:648:GLY:HA3	1.98	0.45
1:H:55:TYR:HD1	1:H:68:PRO:HG3	1.80	0.45
3:C:176:LEU:HD21	3:C:207:HIS:HD2	1.81	0.45
3:B:358:ILE:HB	3:B:395:VAL:HG13	1.98	0.45
3:A:92:TYR:HB2	3:A:270:LEU:HD21	1.98	0.45
2:G:166:THR:OG1	2:G:214:ASN:O	2.33	0.45
3:A:645:THR:OG1	3:A:648:GLY:O	2.26	0.45
1:H:107:TYR:HB3	1:H:116:VAL:HG12	1.98	0.45
3:C:868:LEU:HG	3:B:701:MET:HE1	1.98	0.45
3:B:379:CYS:HA	3:B:432:CYS:HA	1.99	0.45
3:A:178:ASP:HB3	3:A:182:LYS:HE2	1.99	0.45
1:F:126:VAL:O	1:F:161:TYR:OH	2.33	0.45
2:G:159:ASP:HA	2:G:190:LEU:HD13	1.97	0.45
2:G:2:MET:HA	2:G:27:GLY:HA3	1.98	0.45
1:F:77:SER:HG	1:F:90:THR:HG1	1.62	0.45
1:H:153:LEU:HD23	1:H:169:TRP:HE1	1.81	0.45
3:B:173:GLN:HG2	3:B:175:PHE:H	1.81	0.45
3:B:806:PHE:HD1	3:B:809:ILE:HD11	1.80	0.45
3:A:519:HIS:CE1	3:A:567:ARG:HH11	2.34	0.45
3:B:729:GLU:OE1	3:B:1068:HIS:NE2	2.48	0.45
3:B:1110:GLN:NE2	3:B:1115:GLU:OE1	2.50	0.45
3:A:1161:LYS:O	3:A:1164:THR:OG1	2.34	0.45
1:H:8:ARG:NH2	1:H:120:GLY:O	2.50	0.45
3:C:45:ARG:HG2	3:B:567:ARG:HB3	2.00	0.44
2:E:43:ARG:NH1	2:E:97:SER:O	2.50	0.44
3:C:569:ILE:O	3:A:968:LYS:NZ	2.50	0.44
3:A:433:VAL:HG12	3:A:512:VAL:HG22	1.98	0.44
3:C:92:TYR:N	3:C:268:GLY:O	2.37	0.44
3:B:1129:ASN:HD21	3:B:1132:VAL:HG23	1.82	0.44
1:H:30:VAL:HG13	3:C:354:ASN:HB3	1.98	0.44
3:C:1039:GLY:HA3	3:B:1044:VAL:HG21	2.00	0.44
3:C:1044:VAL:HG21	3:A:1039:GLY:HA3	1.98	0.44
3:B:457:ARG:NH2	3:B:459:SER:O	2.46	0.44
1:F:55:TYR:CD1	1:F:68:PRO:HG3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:161:PHE:HB3	2:G:162:PRO:HD3	1.99	0.44
3:C:478:ARG:NE	3:C:487:ASN:HD21	2.15	0.44
3:C:910:PHE:HA	3:C:913:ILE:HG12	1.99	0.44
2:G:40:GLY:HA3	2:G:55:ILE:HG22	1.99	0.44
3:C:642:VAL:HG13	3:C:651:ILE:HG12	1.99	0.44
3:C:183:GLU:HB3	3:C:186:PHE:HB2	2.00	0.44
3:C:1108:VAL:HG23	3:C:1119:ILE:HG12	1.99	0.44
3:B:405:ASN:N	3:B:504:GLY:O	2.51	0.44
3:C:294:ASP:OD1	3:C:294:ASP:N	2.50	0.43
3:A:405:ASN:N	3:A:504:GLY:O	2.50	0.43
1:H:55:TYR:CD1	1:H:68:PRO:HG3	2.53	0.43
3:B:350:VAL:HG12	3:B:422:ASN:HB3	2.00	0.43
3:B:1131:ASP:OD1	3:B:1131:ASP:N	2.50	0.43
3:A:518:LEU:HG	3:A:520:ALA:H	1.82	0.43
3:C:373:PRO:HB3	3:B:486:PRO:HG3	2.00	0.43
3:B:54:ASP:OD1	3:B:55:LEU:N	2.44	0.43
3:A:294:ASP:OD1	3:A:294:ASP:N	2.51	0.43
1:D:55:TYR:CD1	1:D:68:PRO:HG3	2.52	0.43
3:C:144:VAL:HG22	3:C:152:TRP:HE3	1.83	0.43
3:C:380:TYR:N	3:C:431:GLY:O	2.42	0.43
3:B:22:LEU:HB3	3:B:70:HIS:HE1	1.83	0.43
3:A:350:VAL:HG12	3:A:422:ASN:HB3	1.99	0.43
2:E:159:ASP:HA	2:E:190:LEU:HD13	2.01	0.43
3:C:677:GLN:H	3:C:677:GLN:HG3	1.52	0.43
3:B:616:ASN:OD1	3:B:617:CYS:N	2.51	0.43
3:B:989:ASP:O	3:B:993:ALA:N	2.50	0.43
1:H:44:GLN:HA	1:H:50:PRO:HA	2.01	0.43
3:C:34:THR:HG22	3:C:59:PHE:HE2	1.83	0.43
3:A:934:ALA:O	3:A:938:ILE:HG12	2.18	0.43
3:C:22:LEU:HB3	3:C:70:HIS:CE1	2.53	0.43
3:C:116:GLN:HB2	3:B:468:ILE:HD11	2.00	0.43
3:A:744:MET:HE3	3:A:861:GLY:HA2	1.99	0.43
1:D:55:TYR:HD1	1:D:68:PRO:HG3	1.84	0.43
3:C:721:ASN:OD1	3:C:722:PHE:N	2.45	0.43
3:C:728:THR:HG23	3:C:938:ILE:HD12	2.00	0.43
3:B:170:TYR:HE2	3:B:172:SER:HB2	1.84	0.43
2:E:156:LEU:HD22	2:E:158:LYS:HG3	2.01	0.42
3:A:418:ILE:HA	3:A:422:ASN:HD22	1.84	0.42
3:C:344:ALA:HB3	3:C:347:PHE:HE1	1.84	0.42
3:A:910:PHE:HA	3:A:913:ILE:HG12	2.00	0.42
2:E:99:THR:HB	2:E:126:VAL:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:993:ALA:O	3:B:997:ILE:HG12	2.20	0.42
3:A:26:THR:O	3:A:67:HIS:N	2.47	0.42
3:A:106:ILE:HD12	3:A:239:GLN:HB2	2.01	0.42
3:A:696:ILE:H	3:A:696:ILE:HG12	1.53	0.42
2:E:166:THR:OG1	2:E:216:LYS:NZ	2.52	0.42
3:B:669:GLY:HA2	3:B:701:MET:HE3	2.01	0.42
3:B:988:LEU:HB2	3:B:993:ALA:HB2	2.02	0.42
3:A:581:THR:HG23	3:A:583:GLU:HG2	2.00	0.42
3:A:913:ILE:HD13	3:A:1053:LEU:HD21	2.02	0.42
2:G:44:GLN:HB2	2:G:50:LEU:HD23	2.02	0.42
3:C:178:ASP:OD1	3:C:190:ARG:NH1	2.39	0.42
3:B:129:ILE:O	3:B:170:TYR:N	2.52	0.42
3:C:337:PRO:HB3	3:C:339:HIS:CE1	2.55	0.42
3:C:966:LEU:HD11	3:C:1008:LEU:HD23	2.02	0.42
3:B:355:ARG:HG3	3:B:396:TYR:HB3	2.01	0.42
3:A:93:PHE:HB3	3:A:192:PHE:HB2	2.02	0.42
3:B:294:ASP:OD1	3:B:294:ASP:N	2.52	0.42
3:B:350:VAL:HG11	3:B:418:ILE:HD12	2.00	0.42
3:B:351:TYR:HE1	3:B:452:LEU:HB2	1.85	0.42
3:A:28:SER:N	3:A:65:TRP:O	2.50	0.42
3:B:763:PHE:HD2	3:B:1005:LEU:HD21	1.85	0.41
3:A:760:TYR:OH	3:A:998:ASP:OD1	2.30	0.41
3:C:1163:HIS:CE1	3:B:1163:HIS:HD2	2.38	0.41
3:B:40:PRO:HG3	3:B:52:THR:HG21	2.02	0.41
3:B:598:ILE:HG23	3:B:664:ILE:HG21	2.02	0.41
3:A:338:PHE:HE1	3:A:363:ALA:HA	1.84	0.41
1:F:174:SER:HA	1:F:175:PRO:HD3	1.97	0.41
1:H:161:TYR:HB3	1:H:162:PRO:HD3	2.02	0.41
3:C:592:PHE:HZ	3:A:859:PHE:HA	1.85	0.41
3:A:1162:ASN:O	3:A:1165:SER:OG	2.37	0.41
1:D:14:SER:HA	1:D:127:LEU:HB2	2.01	0.41
1:D:132:ALA:HB1	1:D:160:PHE:HA	2.01	0.41
1:H:174:SER:HA	1:H:175:PRO:HD3	1.97	0.41
3:C:38:TYR:OH	3:C:55:LEU:O	2.29	0.41
3:C:996:GLN:OE1	3:C:999:ARG:NH1	2.35	0.41
3:C:809:ILE:HG13	3:C:882:LEU:HD21	2.03	0.41
3:B:296:LEU:HB2	3:B:608:VAL:HG11	2.02	0.41
2:I:11:GLU:OE1	2:I:13:LYS:NZ	2.51	0.41
3:C:826:LEU:HD22	3:C:949:LEU:HD21	2.03	0.41
3:B:339:HIS:CD2	3:B:340:GLU:HG3	2.52	0.41
3:A:375:PHE:H	3:A:436:TRP:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:45:HIS:HB2	1:H:48:LYS:HB2	2.03	0.41
2:I:52:TRP:HE1	2:I:55:ILE:HG23	1.85	0.41
3:B:28:SER:N	3:B:65:TRP:O	2.52	0.41
3:B:122:ASN:HA	3:B:127:VAL:HG12	2.01	0.41
3:B:195:LYS:HE3	3:B:202:LYS:HD2	2.03	0.41
3:B:645:THR:OG1	3:B:648:GLY:O	2.27	0.41
3:A:833:ALA:HB1	3:A:854:ILE:HD11	2.02	0.41
2:I:161:PHE:HB3	2:I:162:PRO:HD3	2.03	0.41
3:C:336:CYS:SG	3:C:358:ILE:HG23	2.61	0.41
3:C:351:TYR:HE1	3:C:452:LEU:HB2	1.85	0.41
3:C:1153:LYS:HE2	3:C:1153:LYS:HB3	1.92	0.41
3:B:278:LYS:HB2	3:B:306:PHE:CZ	2.55	0.41
3:A:902:PHE:N	3:A:903:PRO:HD2	2.36	0.41
2:E:38:TRP:H	2:E:107:GLN:HE21	1.69	0.40
3:C:886:ILE:HG13	3:C:887:THR:HG23	2.03	0.40
3:C:983:ASP:O	3:C:987:ARG:HG3	2.21	0.40
3:B:146:GLN:HE21	3:B:146:GLN:HB2	1.65	0.40
3:B:392:PHE:HB2	3:B:524:VAL:HG13	2.03	0.40
3:A:906:MET:HB3	3:A:920:LEU:HD11	2.03	0.40
2:I:44:GLN:HB2	2:I:50:LEU:HD23	2.02	0.40
3:C:244:LEU:HD13	3:C:246:ARG:HB2	2.04	0.40
3:B:70:HIS:CE1	3:B:72:SER:HB2	2.56	0.40
3:B:666:ILE:HG12	3:B:671:CYS:HA	2.03	0.40
3:B:809:ILE:HG13	3:B:882:LEU:HD21	2.03	0.40
3:B:826:LEU:HD22	3:B:949:LEU:HD21	2.02	0.40
3:A:351:TYR:HE1	3:A:452:LEU:HB2	1.86	0.40
3:C:418:ILE:HA	3:C:422:ASN:HD22	1.87	0.40
3:B:200:TYR:HA	3:B:230:PRO:HA	2.03	0.40
3:B:418:ILE:HA	3:B:422:ASN:HD22	1.86	0.40
3:B:834:ASP:HB2	3:B:854:ILE:HG12	2.03	0.40
2:G:99:THR:HB	2:G:126:VAL:H	1.86	0.40
3:A:856:ALA:O	3:A:860:ASN:ND2	2.53	0.40
3:C:142:LEU:HD13	3:C:142:LEU:HA	1.93	0.40
3:C:938:ILE:HD13	3:C:938:ILE:HA	1.96	0.40
3:C:1131:ASP:OD1	3:C:1131:ASP:N	2.49	0.40
3:B:809:ILE:HB	3:B:1058:GLN:HE22	1.86	0.40
3:A:1080:THR:HB	3:A:1101:SER:HB3	2.02	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	D	186/215 (86%)	178 (96%)	6 (3%)	2 (1%)	11	23
1	F	182/215 (85%)	176 (97%)	6 (3%)	0	100	100
1	H	182/215 (85%)	179 (98%)	3 (2%)	0	100	100
2	E	194/451 (43%)	187 (96%)	7 (4%)	0	100	100
2	G	194/451 (43%)	186 (96%)	8 (4%)	0	100	100
2	I	194/451 (43%)	186 (96%)	8 (4%)	0	100	100
3	A	1111/1299 (86%)	1074 (97%)	37 (3%)	0	100	100
3	B	1091/1299 (84%)	1066 (98%)	25 (2%)	0	100	100
3	C	1096/1299 (84%)	1060 (97%)	36 (3%)	0	100	100
All	All	4430/5895 (75%)	4292 (97%)	136 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	137	THR
1	D	128	GLY

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	D	163/181 (90%)	155 (95%)	8 (5%)	22	45
1	F	162/181 (90%)	160 (99%)	2 (1%)	63	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	162/181 (90%)	161 (99%)	1 (1%)	78	89
2	E	171/399 (43%)	166 (97%)	5 (3%)	37	61
2	G	171/399 (43%)	166 (97%)	5 (3%)	37	61
2	I	171/399 (43%)	166 (97%)	5 (3%)	37	61
3	A	977/1122 (87%)	957 (98%)	20 (2%)	48	72
3	B	965/1122 (86%)	945 (98%)	20 (2%)	47	70
3	C	966/1122 (86%)	945 (98%)	21 (2%)	45	69
All	All	3908/5106 (76%)	3821 (98%)	87 (2%)	45	69

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	126	VAL
1	D	127	LEU
1	D	129	GLN
1	D	131	LYS
1	D	136	VAL
1	D	137	THR
1	D	169	TRP
1	D	180	VAL
2	E	12	VAL
2	E	39	ILE
2	E	99	THR
2	E	114	LEU
2	E	156	LEU
1	F	116	VAL
1	F	169	TRP
2	G	12	VAL
2	G	21	ILE
2	G	39	ILE
2	G	99	THR
2	G	156	LEU
1	H	169	TRP
2	I	12	VAL
2	I	21	ILE
2	I	39	ILE
2	I	99	THR
2	I	156	LEU
3	C	118	LEU
3	C	128	VAL

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Mol	Chain	Res	Type
3	C	142	LEU
3	C	150	LYS
3	C	151	SER
3	C	154	GLU
3	C	177	MET
3	C	244	LEU
3	C	336	CYS
3	C	350	VAL
3	C	395	VAL
3	C	468	ILE
3	C	675	GLN
3	C	676	THR
3	C	677	GLN
3	C	696	ILE
3	C	697	ILE
3	C	841	TYR
3	C	987	ARG
3	C	1085	ILE
3	C	1165	SER
3	B	118	LEU
3	B	131	VAL
3	B	143	ASP
3	B	144	VAL
3	B	145	TYR
3	B	154	GLU
3	B	244	LEU
3	B	336	CYS
3	B	341	VAL
3	B	350	VAL
3	B	395	VAL
3	B	468	ILE
3	B	517	LEU
3	B	524	VAL
3	B	567	ARG
3	B	658	ASN
3	B	841	TYR
3	B	920	LEU
3	B	1129	ASN
3	B	1165	SER
3	A	131	VAL
3	A	145	TYR
3	A	229	LEU

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Mol	Chain	Res	Type
3	A	244	LEU
3	A	249	LEU
3	A	395	VAL
3	A	468	ILE
3	A	489	TYR
3	A	503	VAL
3	A	517	LEU
3	A	529	LYS
3	A	558	LYS
3	A	633	TRP
3	A	675	GLN
3	A	695	SER
3	A	696	ILE
3	A	697	ILE
3	A	920	LEU
3	A	1085	ILE
3	A	1165	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	44	GLN
1	D	45	HIS
2	E	3	GLN
2	E	44	GLN
2	E	107	GLN
2	E	179	HIS
1	F	95	GLN
2	G	107	GLN
2	I	179	HIS
3	C	21	ASN
3	C	138	ASN
3	C	188	ASN
3	C	207	HIS
3	C	245	HIS
3	C	339	HIS
3	C	343	ASN
3	C	394	ASN
3	C	474	GLN
3	C	536	ASN
3	C	540	ASN
3	C	580	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	644	GLN
3	C	658	ASN
3	C	694	GLN
3	C	707	ASN
3	C	788	GLN
3	C	876	GLN
3	C	905	GLN
3	C	911	ASN
3	C	1015	GLN
3	C	1075	GLN
3	C	1110	GLN
3	C	1123	ASN
3	C	1129	ASN
3	B	27	GLN
3	B	146	GLN
3	B	239	GLN
3	B	339	HIS
3	B	360	ASN
3	B	370	ASN
3	B	394	ASN
3	B	414	GLN
3	B	474	GLN
3	B	519	HIS
3	B	580	GLN
3	B	707	ASN
3	B	876	GLN
3	B	911	ASN
3	B	917	GLN
3	B	969	GLN
3	B	1015	GLN
3	B	1075	GLN
3	B	1110	GLN
3	B	1123	ASN
3	B	1129	ASN
3	A	50	HIS
3	A	148	ASN
3	A	149	ASN
3	A	188	ASN
3	A	339	HIS
3	A	394	ASN
3	A	474	GLN
3	A	519	HIS

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Mol	Chain	Res	Type
3	A	536	ASN
3	A	580	GLN
3	A	613	GLN
3	A	644	GLN
3	A	658	ASN
3	A	675	GLN
3	A	791	GLN
3	A	876	GLN
3	A	1015	GLN
3	A	1110	GLN
3	A	1129	ASN
3	A	1139	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.

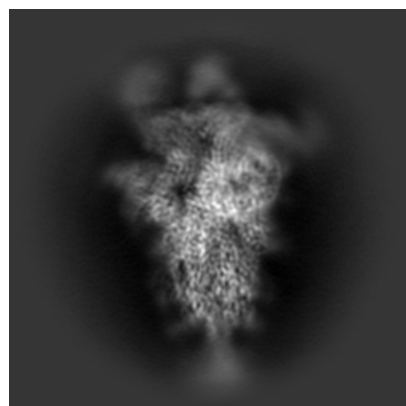
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39803. These allow visual inspection of the internal detail of the map and identification of artifacts.

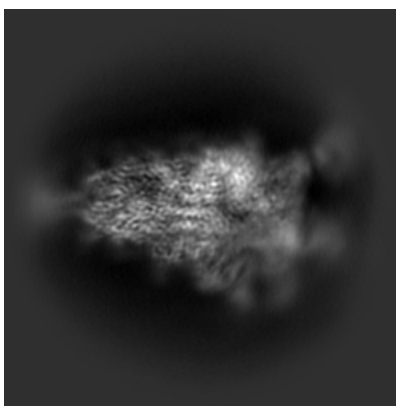
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

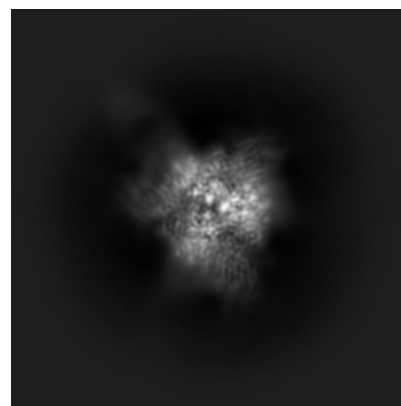
6.1.1 Primary map



X

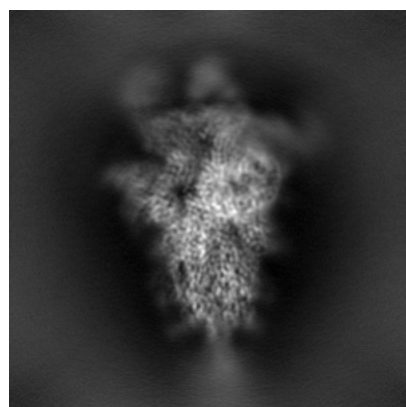


Y

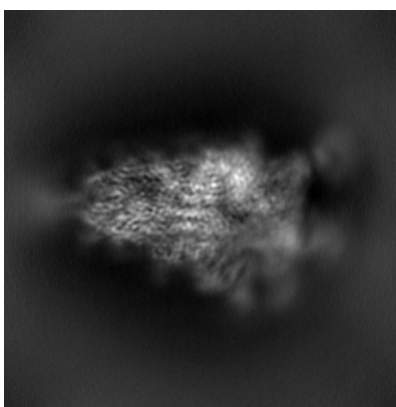


Z

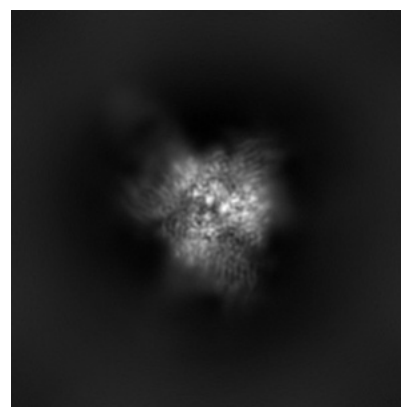
6.1.2 Raw map



X



Y

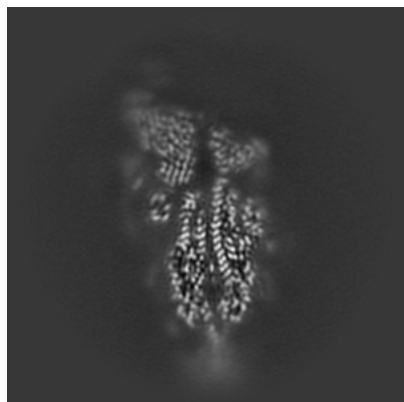


Z

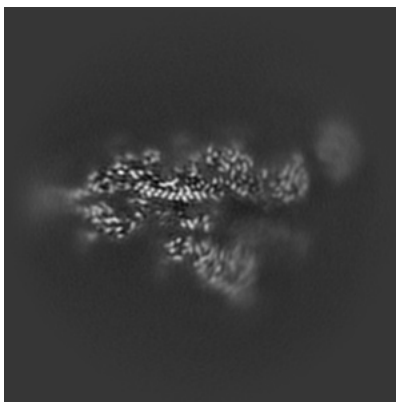
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

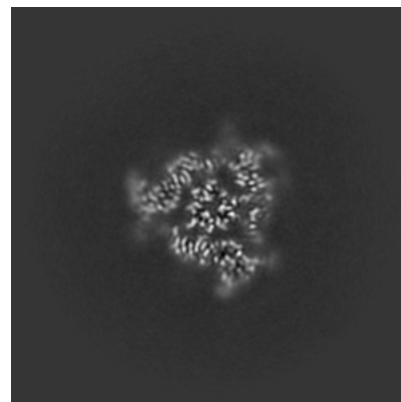
6.2.1 Primary map



X Index: 160

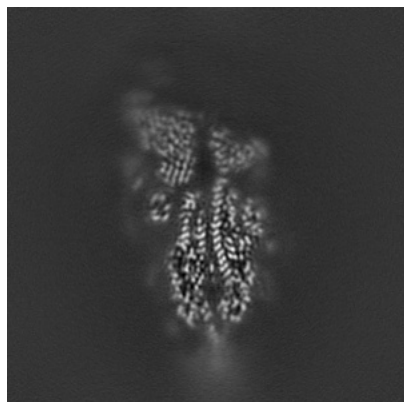


Y Index: 160

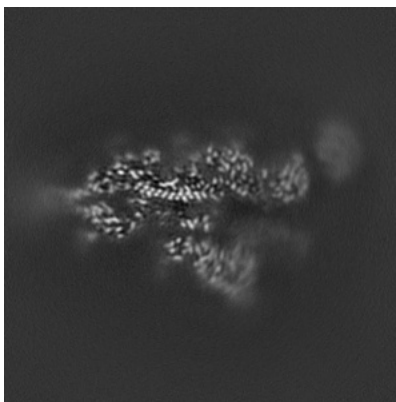


Z Index: 160

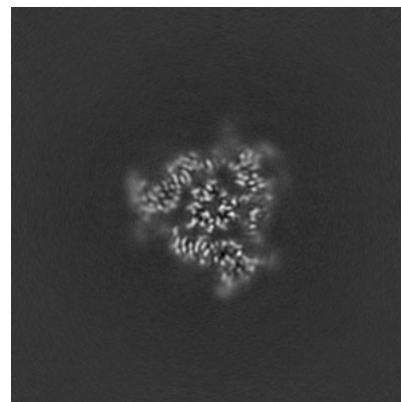
6.2.2 Raw map



X Index: 160



Y Index: 160

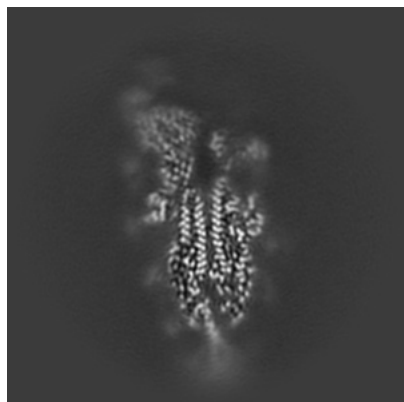


Z Index: 160

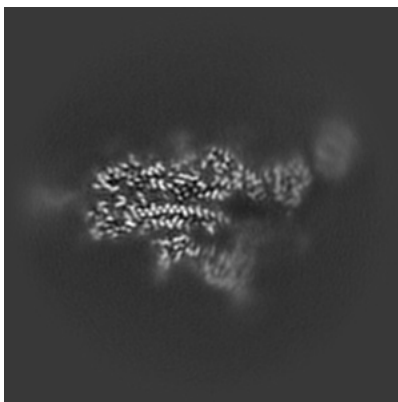
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

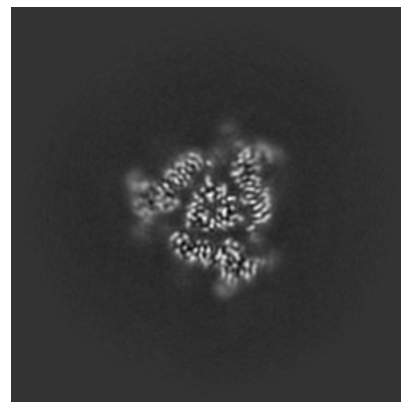
6.3.1 Primary map



X Index: 157

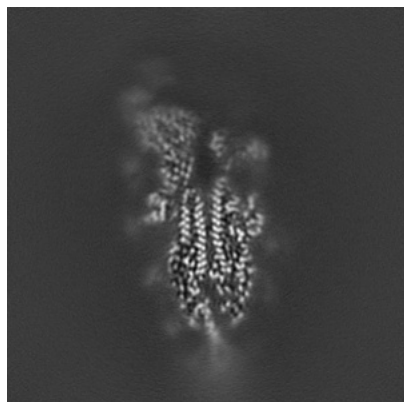


Y Index: 155

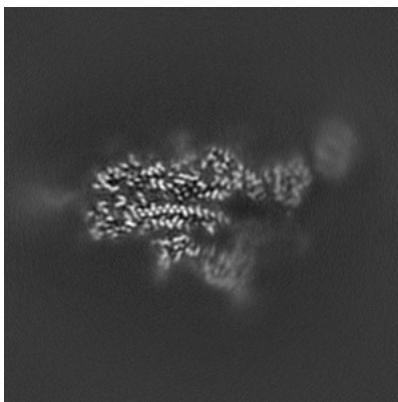


Z Index: 163

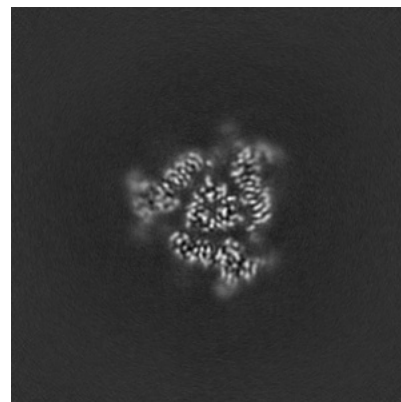
6.3.2 Raw map



X Index: 157



Y Index: 155

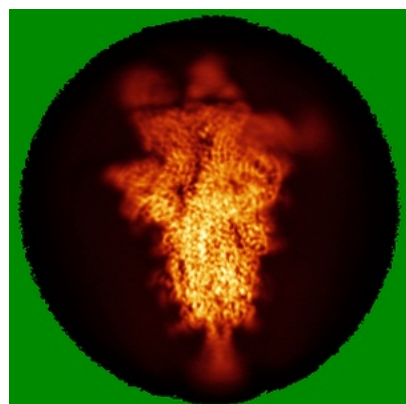


Z Index: 163

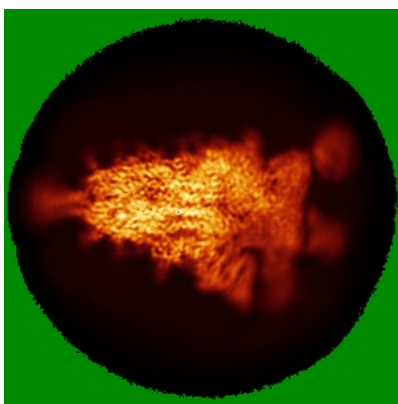
The images above show the largest variance slices of the map in three orthogonal directions.

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

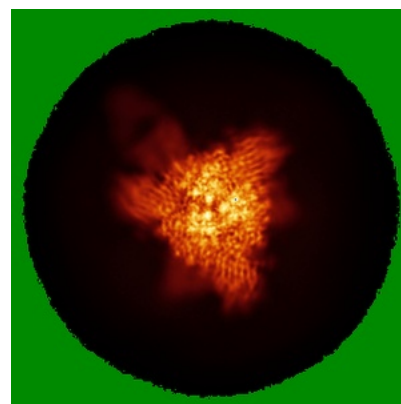
6.4.1 Primary map



X

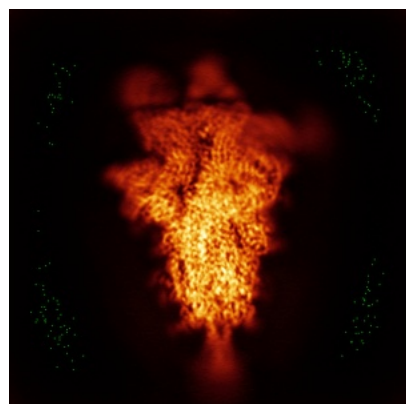


Y

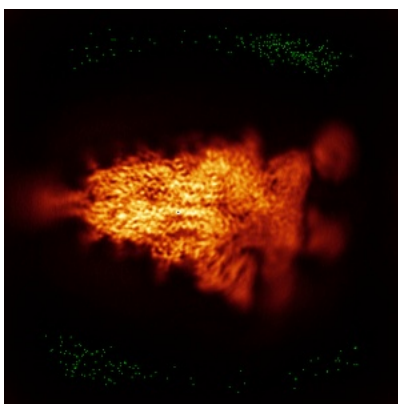


Z

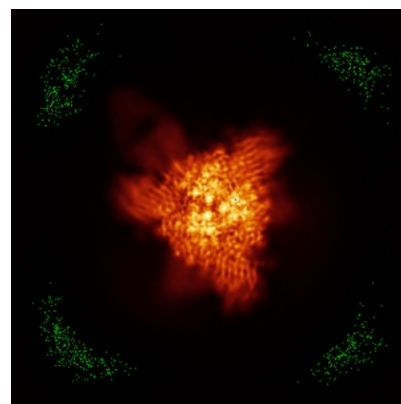
6.4.2 Raw map



X



Y

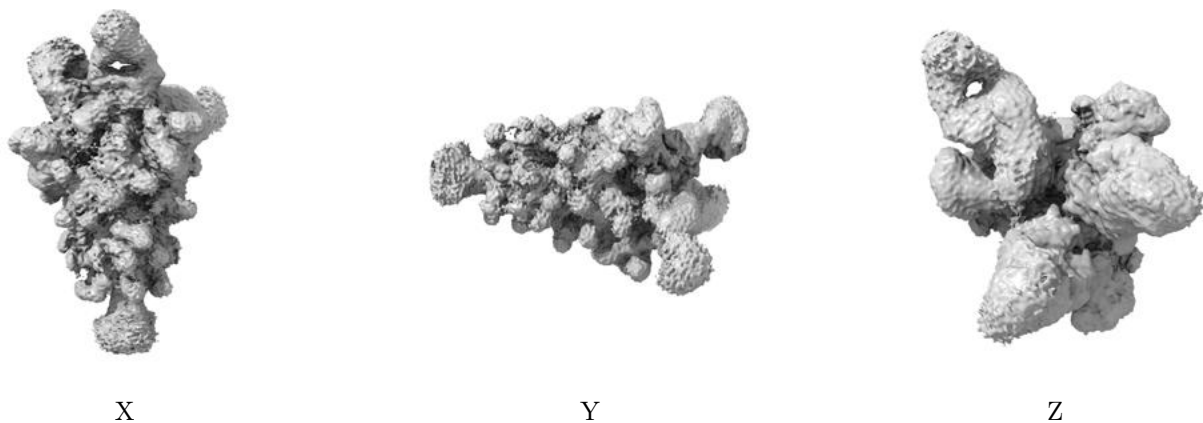


Z

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.

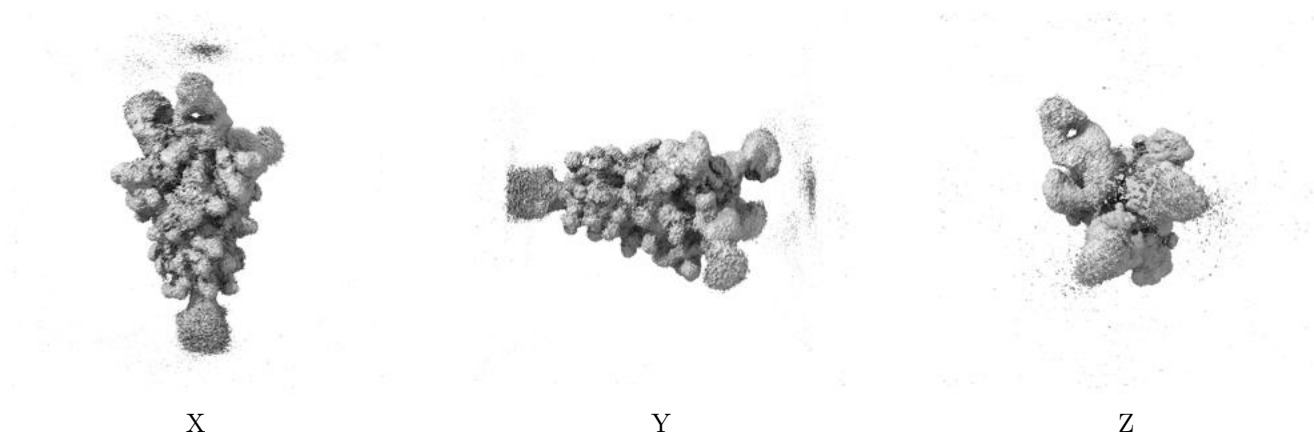
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

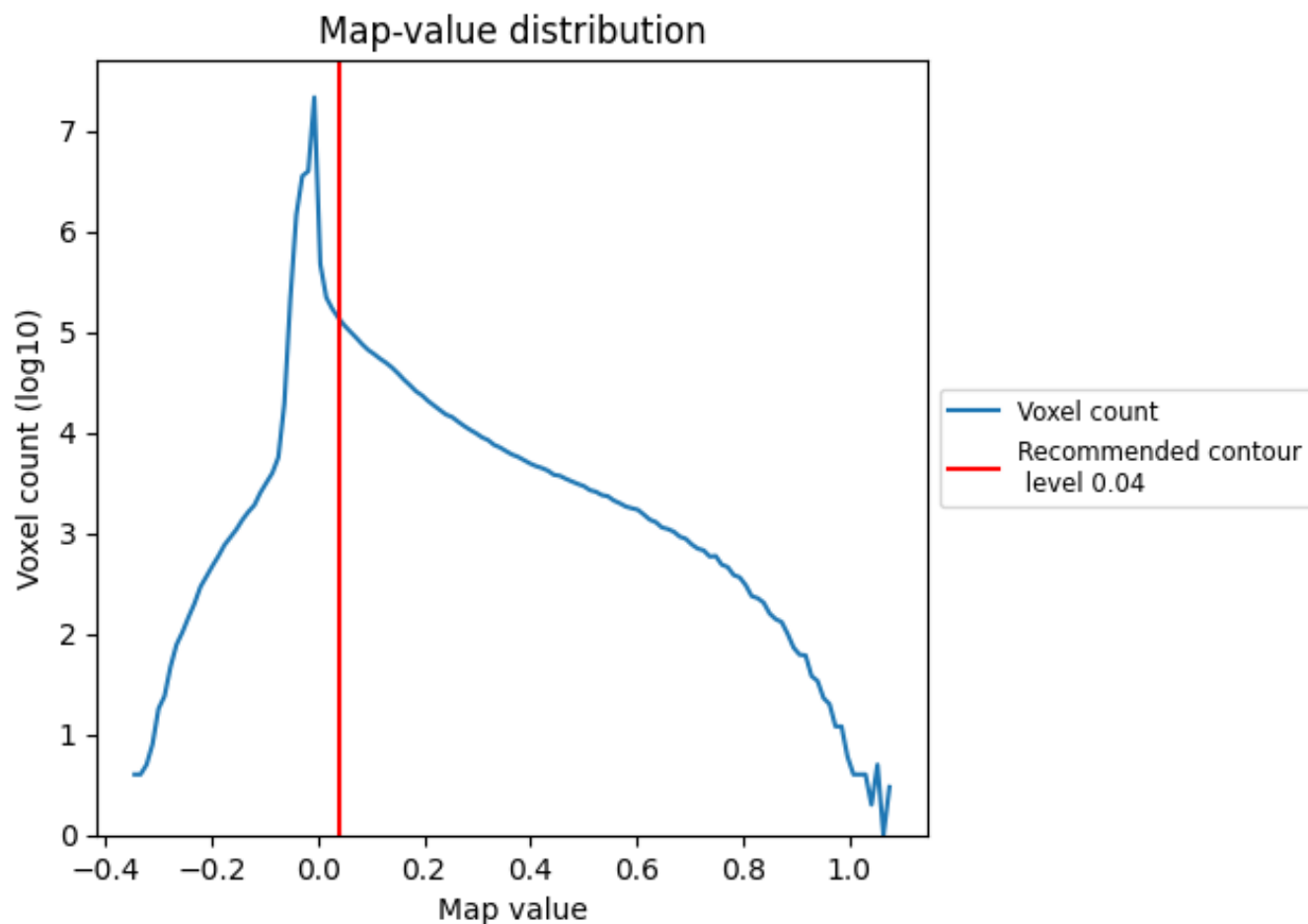
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

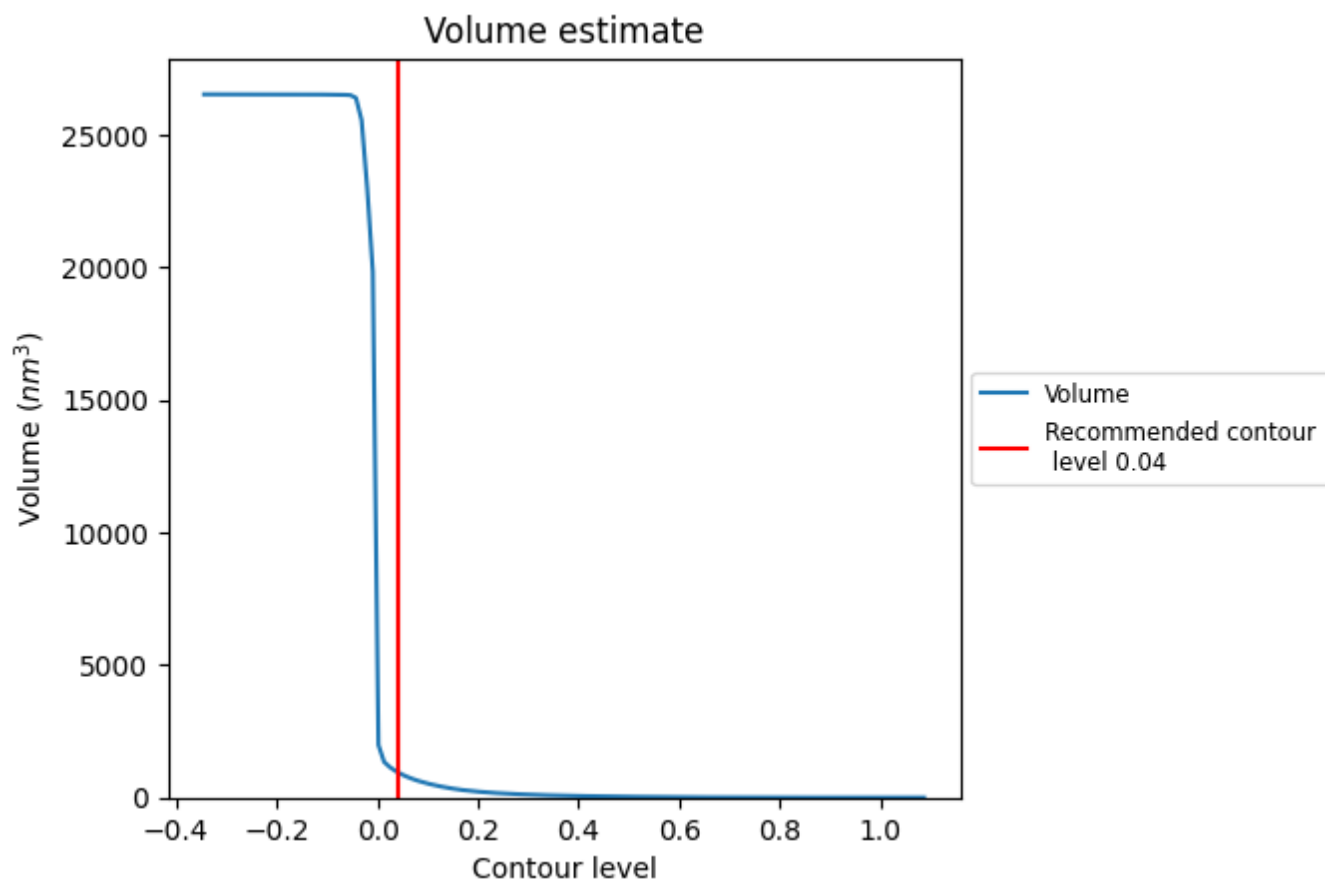
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

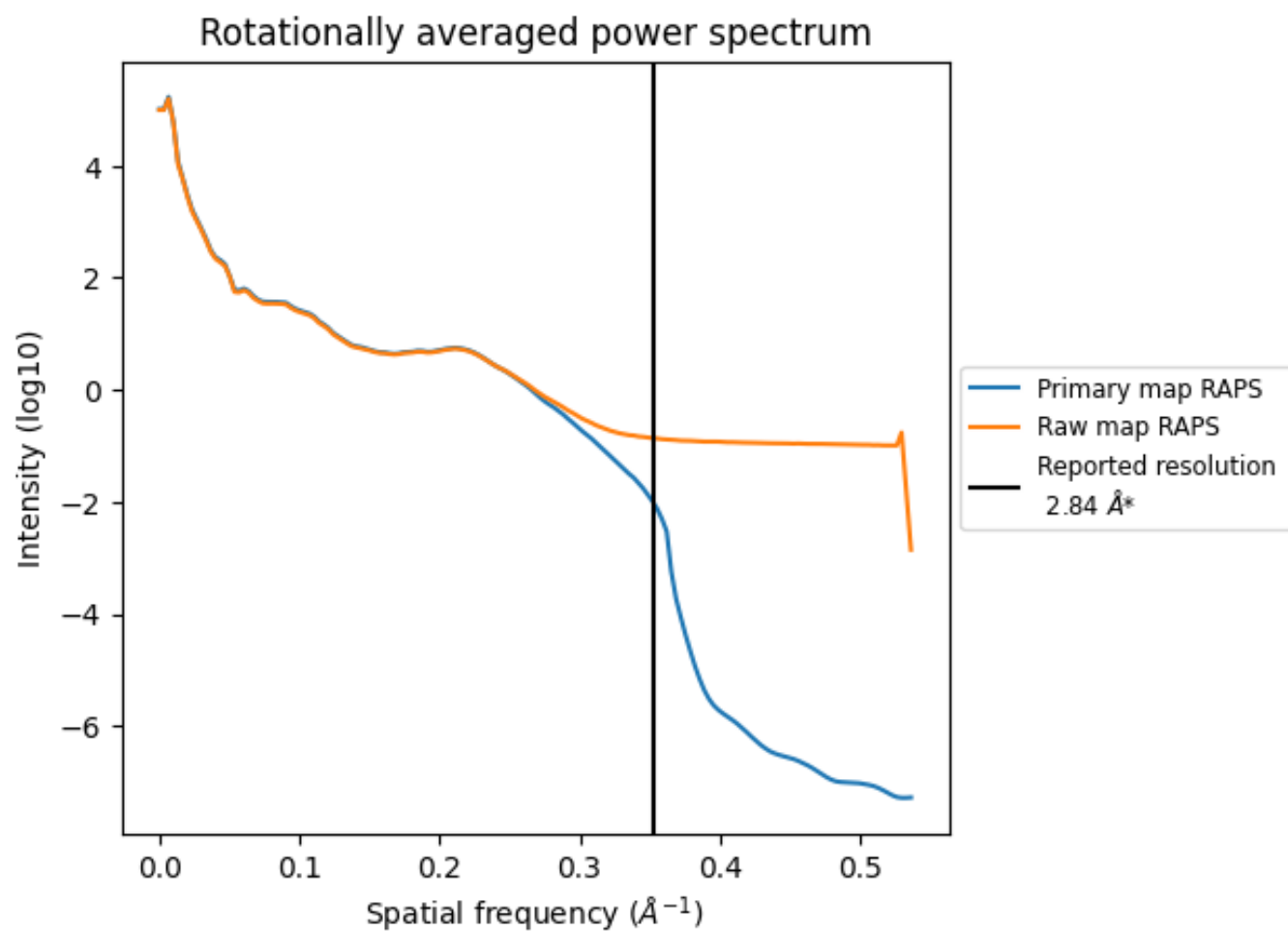
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 962 nm³; this corresponds to an approximate mass of 869 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 ⓘ

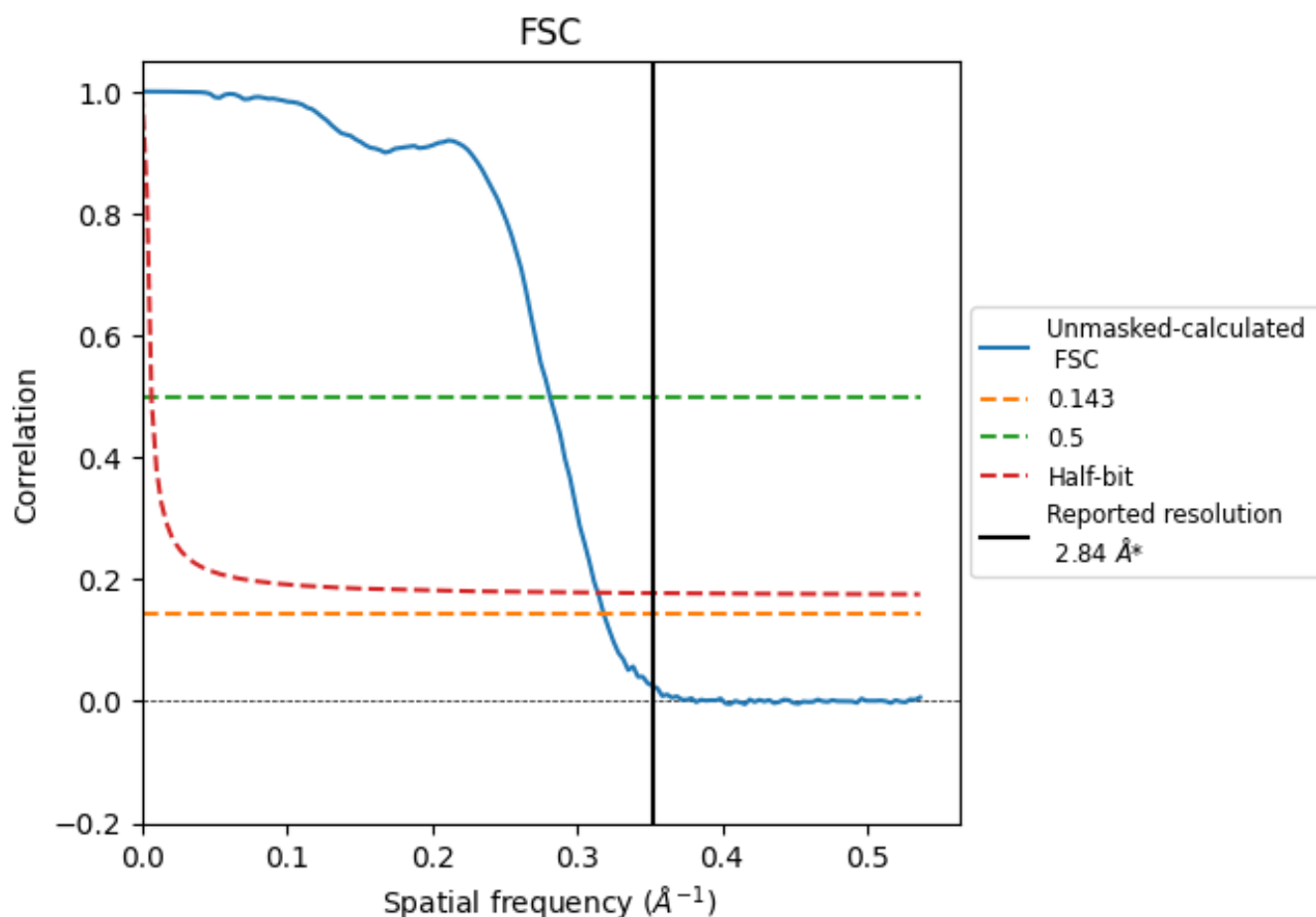


*Reported resolution corresponds to spatial frequency of 0.352 Å⁻¹

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 $0.352 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

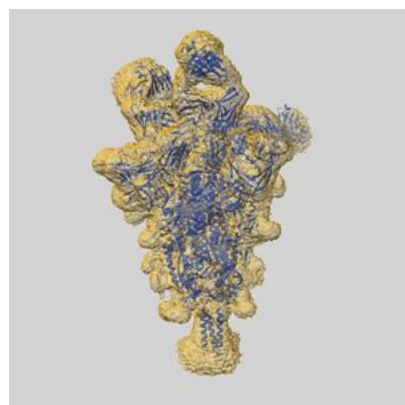
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.14	3.55	3.18

*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 3.14 differs from the reported value 2.84 by more than 10 %

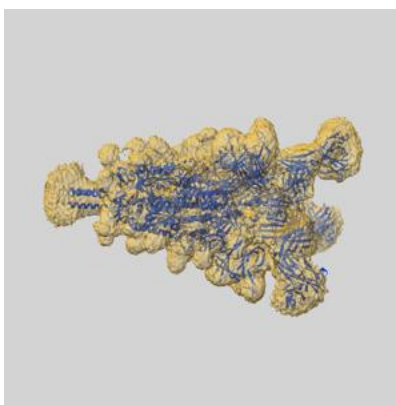
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39803 and PDB model 8Z6S. Per-residue inclusion information can be found in section 3 on page 11.

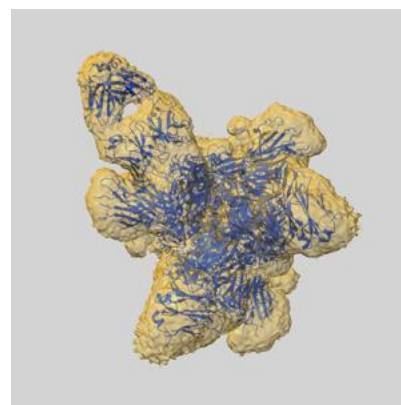
9.1 Map-model overlay [i](#)



X



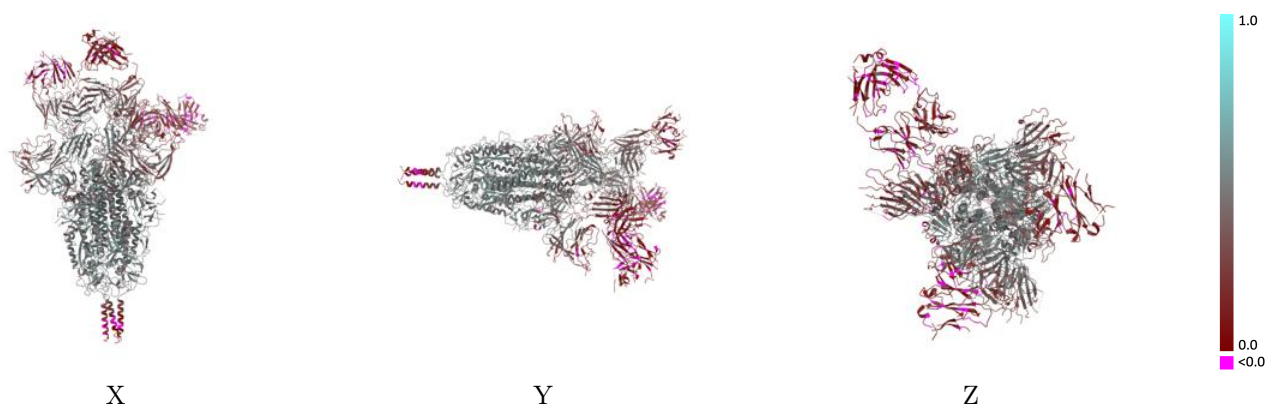
Y



Z

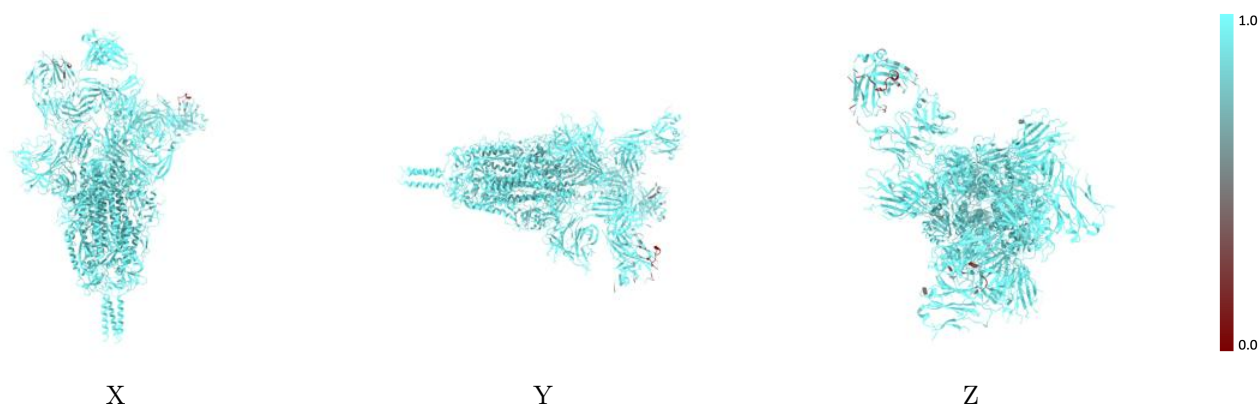
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



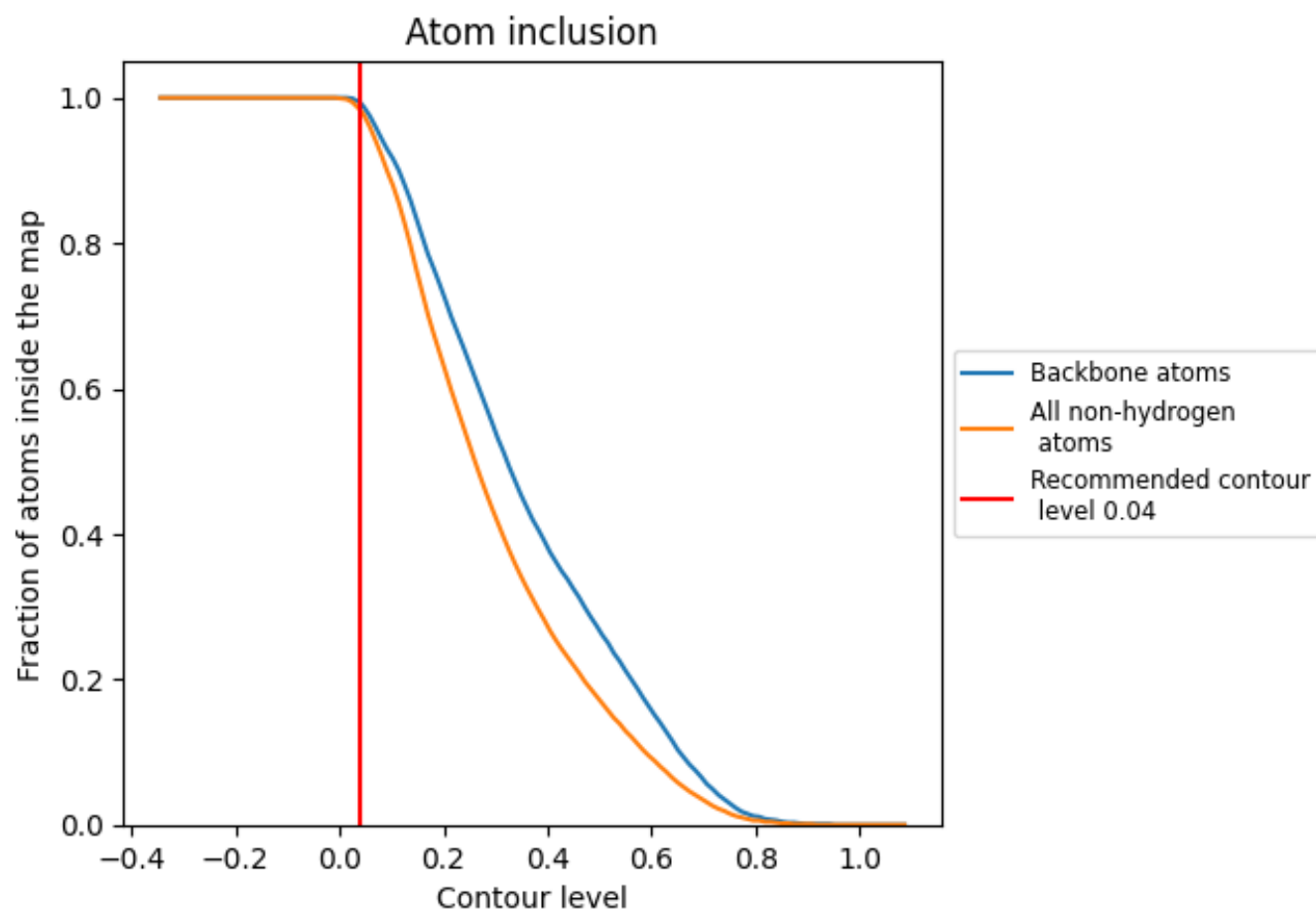
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 98% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9830	0.3790
A	0.9940	0.4310
B	0.9950	0.4550
C	0.9910	0.4050
D	0.9730	0.2590
E	0.9260	0.2900
F	0.9950	0.2780
G	0.9830	0.3040
H	0.9490	0.1230
I	0.8950	0.1120

1.0

0.0

<0.0