Full wwPDB EM Validation Report

Aug 18, 2026 – 12:25 PM EDT

PDB ID	:	9MQ7 / pdb_00009mq7
EMDB ID	:	EMD-48515
Title	:	Cryo-EM structure of hemagglutinin H5N1 in complex with Fab 326-366.26
Authors	:	Malla, T.N.; Tsybovsky, Y.; Zhou, T.
Deposited on	:	2025-01-02
Resolution	:	3.63 Å(reported)
Based on initial model	:	.

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:

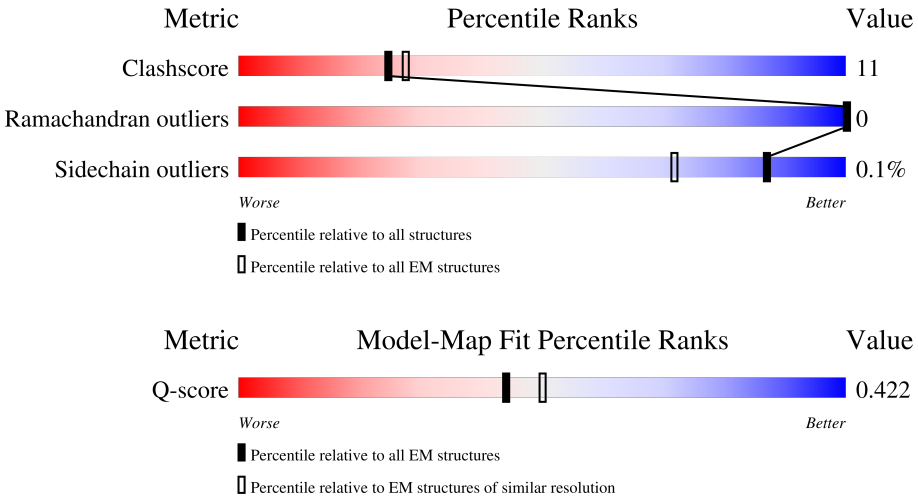
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 3.63 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.



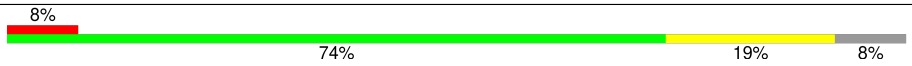
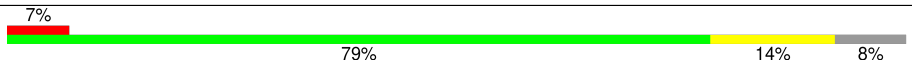
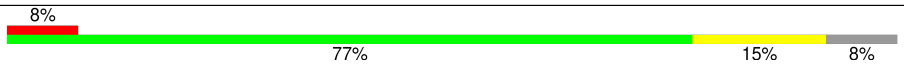
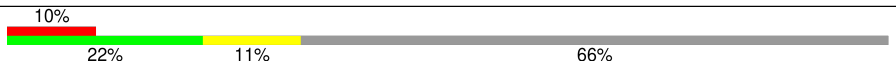
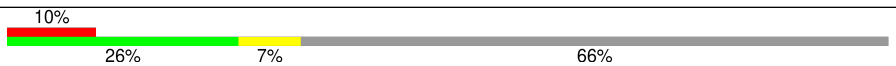
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11696 (3.13 - 4.13)

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	H	123	39% 68% 28%
1	I	123	41% 70% 28%
1	J	123	41% 72% 25%
2	L	108	54% 76% 23%

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Mol	Chain	Length	Quality of chain
2	M	108	
2	N	108	
3	A	342	
3	C	342	
3	E	342	
4	B	227	
4	D	227	
4	F	227	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14625 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 326-366.26 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	120	Total	C	N	O	S	0	0
			919	583	157	175	4		
1	I	120	Total	C	N	O	S	0	0
			919	583	157	175	4		
1	J	120	Total	C	N	O	S	0	0
			919	583	157	175	4		

- Molecule 2 is a protein called 326-366.26 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	107	Total	C	N	O	S	0	0
			808	510	137	158	3		
2	M	107	Total	C	N	O	S	0	0
			808	510	137	158	3		
2	N	107	Total	C	N	O	S	0	0
			808	510	137	158	3		

- Molecule 3 is a protein called Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	316	Total	C	N	O	S	0	0
			2503	1588	435	465	15		
3	C	316	Total	C	N	O	S	0	0
			2503	1588	435	465	15		
3	E	316	Total	C	N	O	S	0	0
			2503	1588	435	465	15		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	98	PHE	TYR	conflict	UNP A0AAX6NN08
A	199	ILE	THR	conflict	UNP A0AAX6NN08
C	98	PHE	TYR	conflict	UNP A0AAX6NN08

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Chain	Residue	Modelled	Actual	Comment	Reference
C	199	ILE	THR	conflict	UNP A0AAX6NN08
E	98	PHE	TYR	conflict	UNP A0AAX6NN08
E	199	ILE	THR	conflict	UNP A0AAX6NN08

- Molecule 4 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	77	Total	C	N	O	S	0	0
			645	404	113	125	3		
4	D	77	Total	C	N	O	S	0	0
			645	404	113	125	3		
4	F	77	Total	C	N	O	S	0	0
			645	404	113	125	3		

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	174	SER	-	expression tag	UNP A0A5Q2MJY3
B	175	GLY	-	expression tag	UNP A0A5Q2MJY3
B	176	TYR	-	expression tag	UNP A0A5Q2MJY3
B	177	ILE	-	expression tag	UNP A0A5Q2MJY3
B	178	PRO	-	expression tag	UNP A0A5Q2MJY3
B	179	GLU	-	expression tag	UNP A0A5Q2MJY3
B	180	ALA	-	expression tag	UNP A0A5Q2MJY3
B	181	PRO	-	expression tag	UNP A0A5Q2MJY3
B	182	ARG	-	expression tag	UNP A0A5Q2MJY3
B	183	ASP	-	expression tag	UNP A0A5Q2MJY3
B	184	GLY	-	expression tag	UNP A0A5Q2MJY3
B	185	GLN	-	expression tag	UNP A0A5Q2MJY3
B	186	ALA	-	expression tag	UNP A0A5Q2MJY3
B	187	TYR	-	expression tag	UNP A0A5Q2MJY3
B	188	VAL	-	expression tag	UNP A0A5Q2MJY3
B	189	ARG	-	expression tag	UNP A0A5Q2MJY3
B	190	LYS	-	expression tag	UNP A0A5Q2MJY3
B	191	ASP	-	expression tag	UNP A0A5Q2MJY3
B	192	GLY	-	expression tag	UNP A0A5Q2MJY3
B	193	GLU	-	expression tag	UNP A0A5Q2MJY3
B	194	TRP	-	expression tag	UNP A0A5Q2MJY3
B	195	VAL	-	expression tag	UNP A0A5Q2MJY3
B	196	LEU	-	expression tag	UNP A0A5Q2MJY3
B	197	LEU	-	expression tag	UNP A0A5Q2MJY3
B	198	SER	-	expression tag	UNP A0A5Q2MJY3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	199	THR	-	expression tag	UNP A0A5Q2MJY3
B	200	PHE	-	expression tag	UNP A0A5Q2MJY3
B	201	LEU	-	expression tag	UNP A0A5Q2MJY3
B	202	GLY	-	expression tag	UNP A0A5Q2MJY3
B	203	SER	-	expression tag	UNP A0A5Q2MJY3
B	204	GLY	-	expression tag	UNP A0A5Q2MJY3
B	205	LEU	-	expression tag	UNP A0A5Q2MJY3
B	206	ASN	-	expression tag	UNP A0A5Q2MJY3
B	207	ASP	-	expression tag	UNP A0A5Q2MJY3
B	208	ILE	-	expression tag	UNP A0A5Q2MJY3
B	209	PHE	-	expression tag	UNP A0A5Q2MJY3
B	210	GLU	-	expression tag	UNP A0A5Q2MJY3
B	211	ALA	-	expression tag	UNP A0A5Q2MJY3
B	212	GLN	-	expression tag	UNP A0A5Q2MJY3
B	213	LYS	-	expression tag	UNP A0A5Q2MJY3
B	214	ILE	-	expression tag	UNP A0A5Q2MJY3
B	215	GLU	-	expression tag	UNP A0A5Q2MJY3
B	216	TRP	-	expression tag	UNP A0A5Q2MJY3
B	217	HIS	-	expression tag	UNP A0A5Q2MJY3
B	218	GLU	-	expression tag	UNP A0A5Q2MJY3
B	219	GLY	-	expression tag	UNP A0A5Q2MJY3
B	220	HIS	-	expression tag	UNP A0A5Q2MJY3
B	221	HIS	-	expression tag	UNP A0A5Q2MJY3
B	222	HIS	-	expression tag	UNP A0A5Q2MJY3
B	223	HIS	-	expression tag	UNP A0A5Q2MJY3
B	224	HIS	-	expression tag	UNP A0A5Q2MJY3
B	225	HIS	-	expression tag	UNP A0A5Q2MJY3
D	174	SER	-	expression tag	UNP A0A5Q2MJY3
D	175	GLY	-	expression tag	UNP A0A5Q2MJY3
D	176	TYR	-	expression tag	UNP A0A5Q2MJY3
D	177	ILE	-	expression tag	UNP A0A5Q2MJY3
D	178	PRO	-	expression tag	UNP A0A5Q2MJY3
D	179	GLU	-	expression tag	UNP A0A5Q2MJY3
D	180	ALA	-	expression tag	UNP A0A5Q2MJY3
D	181	PRO	-	expression tag	UNP A0A5Q2MJY3
D	182	ARG	-	expression tag	UNP A0A5Q2MJY3
D	183	ASP	-	expression tag	UNP A0A5Q2MJY3
D	184	GLY	-	expression tag	UNP A0A5Q2MJY3
D	185	GLN	-	expression tag	UNP A0A5Q2MJY3
D	186	ALA	-	expression tag	UNP A0A5Q2MJY3
D	187	TYR	-	expression tag	UNP A0A5Q2MJY3
D	188	VAL	-	expression tag	UNP A0A5Q2MJY3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	189	ARG	-	expression tag	UNP A0A5Q2MJY3
D	190	LYS	-	expression tag	UNP A0A5Q2MJY3
D	191	ASP	-	expression tag	UNP A0A5Q2MJY3
D	192	GLY	-	expression tag	UNP A0A5Q2MJY3
D	193	GLU	-	expression tag	UNP A0A5Q2MJY3
D	194	TRP	-	expression tag	UNP A0A5Q2MJY3
D	195	VAL	-	expression tag	UNP A0A5Q2MJY3
D	196	LEU	-	expression tag	UNP A0A5Q2MJY3
D	197	LEU	-	expression tag	UNP A0A5Q2MJY3
D	198	SER	-	expression tag	UNP A0A5Q2MJY3
D	199	THR	-	expression tag	UNP A0A5Q2MJY3
D	200	PHE	-	expression tag	UNP A0A5Q2MJY3
D	201	LEU	-	expression tag	UNP A0A5Q2MJY3
D	202	GLY	-	expression tag	UNP A0A5Q2MJY3
D	203	SER	-	expression tag	UNP A0A5Q2MJY3
D	204	GLY	-	expression tag	UNP A0A5Q2MJY3
D	205	LEU	-	expression tag	UNP A0A5Q2MJY3
D	206	ASN	-	expression tag	UNP A0A5Q2MJY3
D	207	ASP	-	expression tag	UNP A0A5Q2MJY3
D	208	ILE	-	expression tag	UNP A0A5Q2MJY3
D	209	PHE	-	expression tag	UNP A0A5Q2MJY3
D	210	GLU	-	expression tag	UNP A0A5Q2MJY3
D	211	ALA	-	expression tag	UNP A0A5Q2MJY3
D	212	GLN	-	expression tag	UNP A0A5Q2MJY3
D	213	LYS	-	expression tag	UNP A0A5Q2MJY3
D	214	ILE	-	expression tag	UNP A0A5Q2MJY3
D	215	GLU	-	expression tag	UNP A0A5Q2MJY3
D	216	TRP	-	expression tag	UNP A0A5Q2MJY3
D	217	HIS	-	expression tag	UNP A0A5Q2MJY3
D	218	GLU	-	expression tag	UNP A0A5Q2MJY3
D	219	GLY	-	expression tag	UNP A0A5Q2MJY3
D	220	HIS	-	expression tag	UNP A0A5Q2MJY3
D	221	HIS	-	expression tag	UNP A0A5Q2MJY3
D	222	HIS	-	expression tag	UNP A0A5Q2MJY3
D	223	HIS	-	expression tag	UNP A0A5Q2MJY3
D	224	HIS	-	expression tag	UNP A0A5Q2MJY3
D	225	HIS	-	expression tag	UNP A0A5Q2MJY3
F	174	SER	-	expression tag	UNP A0A5Q2MJY3
F	175	GLY	-	expression tag	UNP A0A5Q2MJY3
F	176	TYR	-	expression tag	UNP A0A5Q2MJY3
F	177	ILE	-	expression tag	UNP A0A5Q2MJY3
F	178	PRO	-	expression tag	UNP A0A5Q2MJY3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	179	GLU	-	expression tag	UNP A0A5Q2MJY3
F	180	ALA	-	expression tag	UNP A0A5Q2MJY3
F	181	PRO	-	expression tag	UNP A0A5Q2MJY3
F	182	ARG	-	expression tag	UNP A0A5Q2MJY3
F	183	ASP	-	expression tag	UNP A0A5Q2MJY3
F	184	GLY	-	expression tag	UNP A0A5Q2MJY3
F	185	GLN	-	expression tag	UNP A0A5Q2MJY3
F	186	ALA	-	expression tag	UNP A0A5Q2MJY3
F	187	TYR	-	expression tag	UNP A0A5Q2MJY3
F	188	VAL	-	expression tag	UNP A0A5Q2MJY3
F	189	ARG	-	expression tag	UNP A0A5Q2MJY3
F	190	LYS	-	expression tag	UNP A0A5Q2MJY3
F	191	ASP	-	expression tag	UNP A0A5Q2MJY3
F	192	GLY	-	expression tag	UNP A0A5Q2MJY3
F	193	GLU	-	expression tag	UNP A0A5Q2MJY3
F	194	TRP	-	expression tag	UNP A0A5Q2MJY3
F	195	VAL	-	expression tag	UNP A0A5Q2MJY3
F	196	LEU	-	expression tag	UNP A0A5Q2MJY3
F	197	LEU	-	expression tag	UNP A0A5Q2MJY3
F	198	SER	-	expression tag	UNP A0A5Q2MJY3
F	199	THR	-	expression tag	UNP A0A5Q2MJY3
F	200	PHE	-	expression tag	UNP A0A5Q2MJY3
F	201	LEU	-	expression tag	UNP A0A5Q2MJY3
F	202	GLY	-	expression tag	UNP A0A5Q2MJY3
F	203	SER	-	expression tag	UNP A0A5Q2MJY3
F	204	GLY	-	expression tag	UNP A0A5Q2MJY3
F	205	LEU	-	expression tag	UNP A0A5Q2MJY3
F	206	ASN	-	expression tag	UNP A0A5Q2MJY3
F	207	ASP	-	expression tag	UNP A0A5Q2MJY3
F	208	ILE	-	expression tag	UNP A0A5Q2MJY3
F	209	PHE	-	expression tag	UNP A0A5Q2MJY3
F	210	GLU	-	expression tag	UNP A0A5Q2MJY3
F	211	ALA	-	expression tag	UNP A0A5Q2MJY3
F	212	GLN	-	expression tag	UNP A0A5Q2MJY3
F	213	LYS	-	expression tag	UNP A0A5Q2MJY3
F	214	ILE	-	expression tag	UNP A0A5Q2MJY3
F	215	GLU	-	expression tag	UNP A0A5Q2MJY3
F	216	TRP	-	expression tag	UNP A0A5Q2MJY3
F	217	HIS	-	expression tag	UNP A0A5Q2MJY3
F	218	GLU	-	expression tag	UNP A0A5Q2MJY3
F	219	GLY	-	expression tag	UNP A0A5Q2MJY3
F	220	HIS	-	expression tag	UNP A0A5Q2MJY3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	221	HIS	-	expression tag	UNP A0A5Q2MJY3
F	222	HIS	-	expression tag	UNP A0A5Q2MJY3
F	223	HIS	-	expression tag	UNP A0A5Q2MJY3
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F	225	HIS	-	expression tag	UNP A0A5Q2MJY3

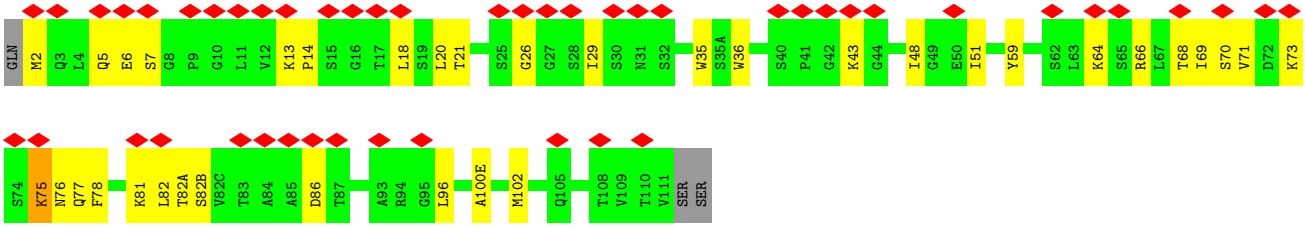
3 Residue-property plots (i)

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: 326-366.26 Fab heavy chain

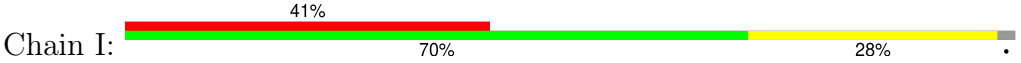
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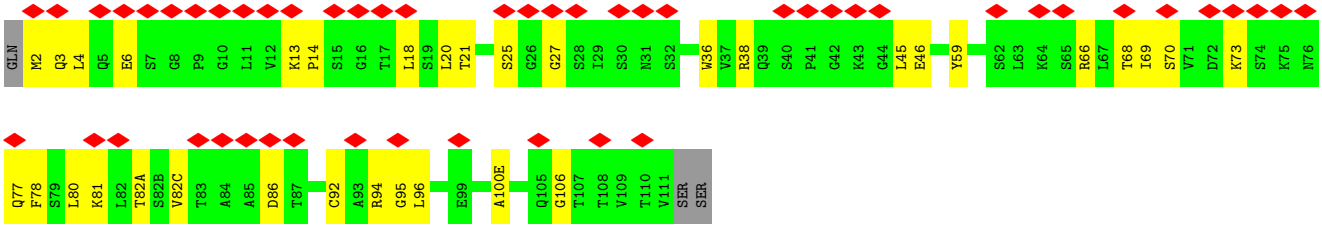




• Molecule 1: 326-366.26 Fab heavy chain

Chain I:

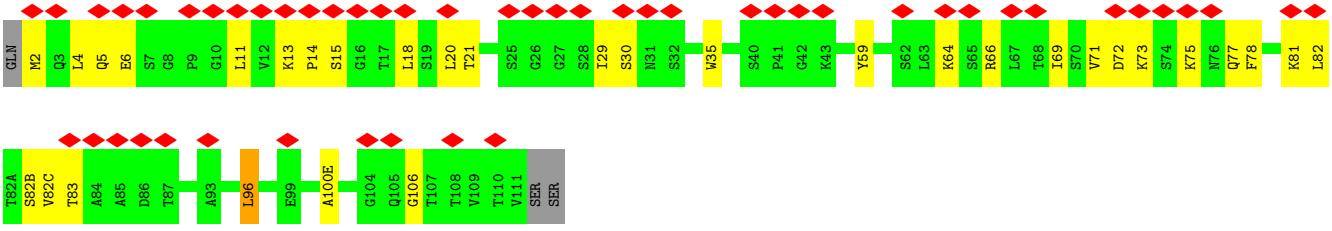




• Molecule 1: 326-366.26 Fab heavy chain

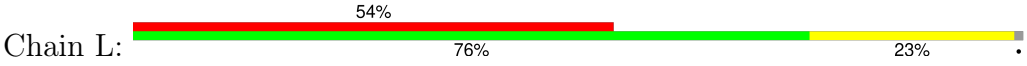
Chain J:

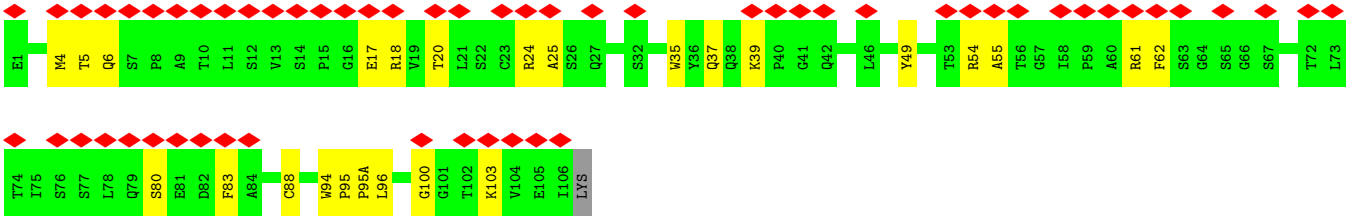




• Molecule 2: 326-366.26 Fab light chain

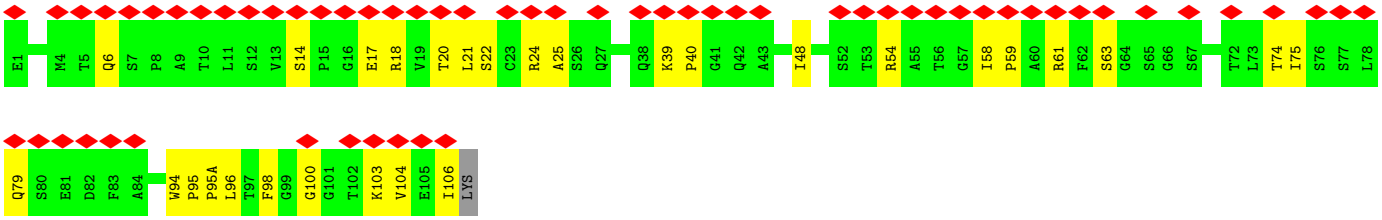
Chain L:





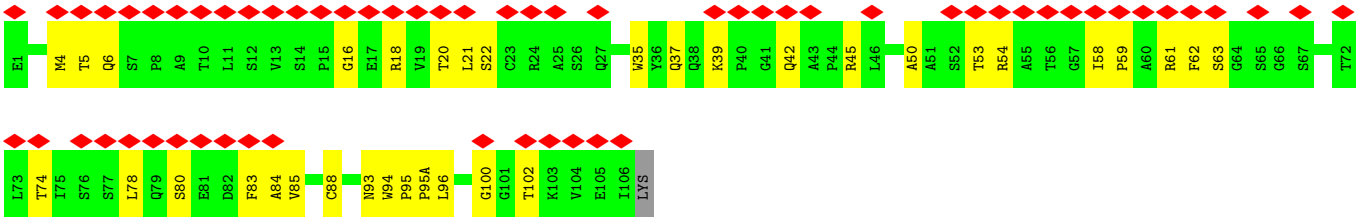
• Molecule 2: 326-366.26 Fab light chain





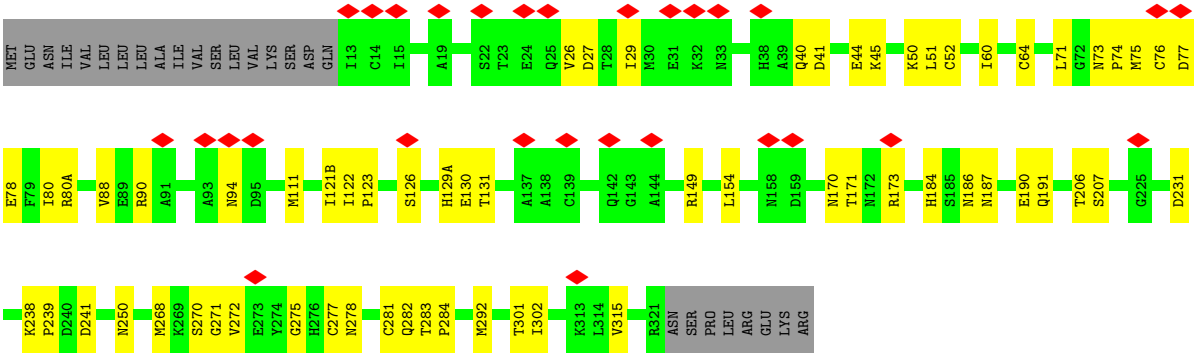
• Molecule 2: 326-366.26 Fab light chain



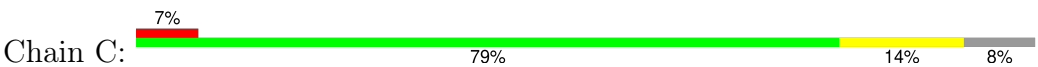


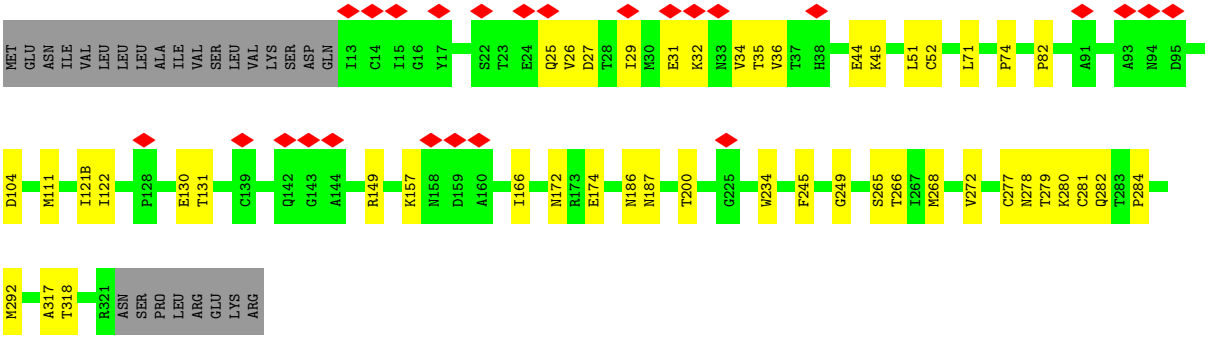
• Molecule 3: Hemagglutinin HA1 chain





• Molecule 3: Hemagglutinin HA1 chain

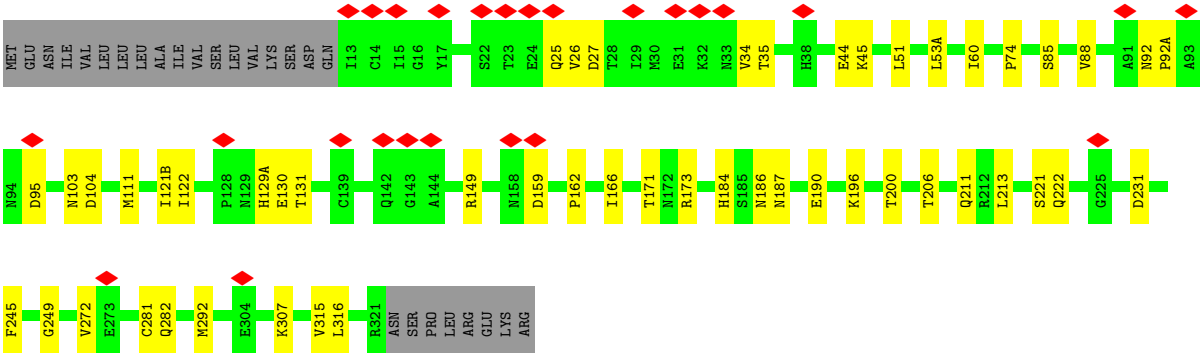




• Molecule 3: Hemagglutinin HA1 chain

Chain E:

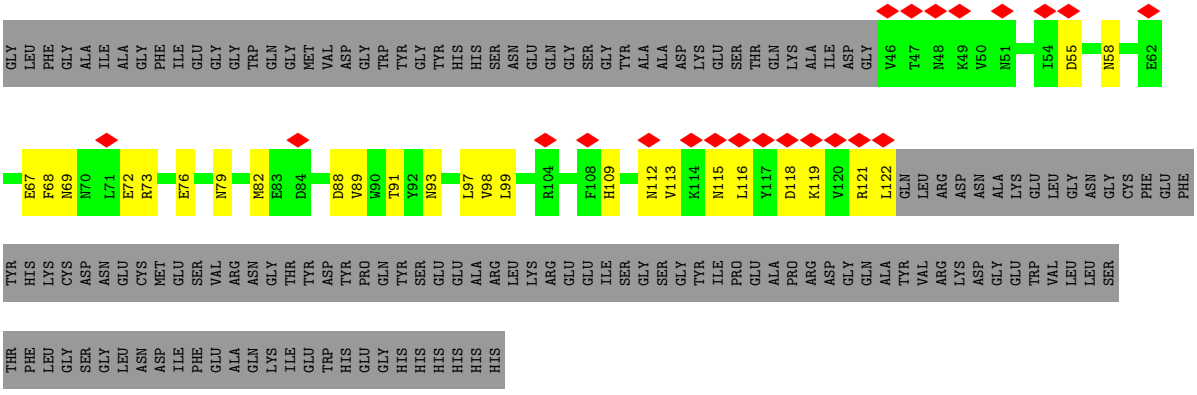




• Molecule 4: Hemagglutinin HA2 chain

Chain B:

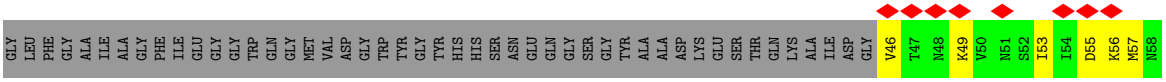


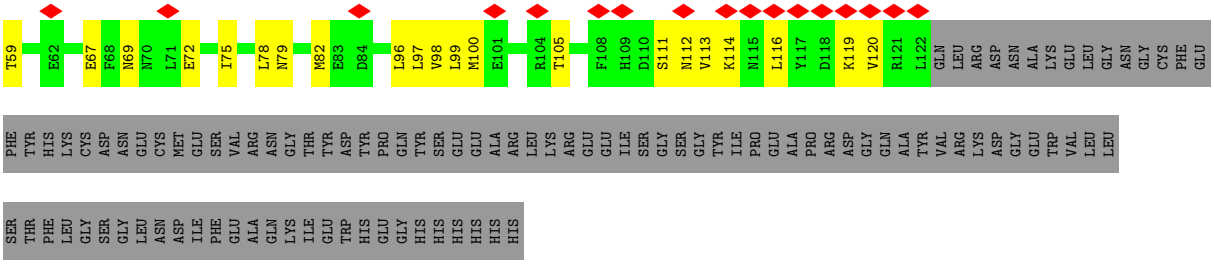


• Molecule 4: Hemagglutinin HA2 chain

Chain D:



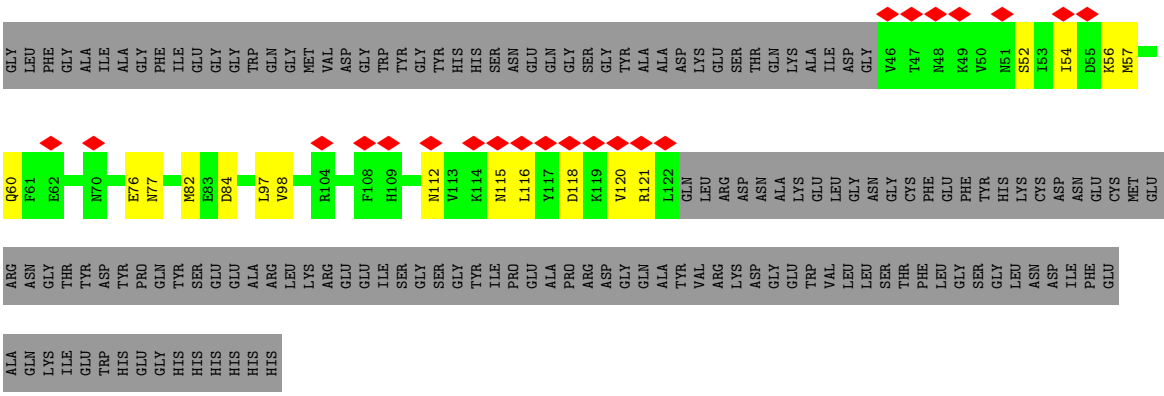




• Molecule 4: Hemagglutinin HA2 chain

Chain F:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	410566	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	DIRECT ELECTRON APOLLO (4k x 4k)	Depositor
Maximum map value	1.973	Depositor
Minimum map value	-1.497	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.236	Depositor
Map size (Å)	400.0, 400.0, 400.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	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	H	0.18	0/944	0.54	1/1282 (0.1%)
1	I	0.17	0/944	0.47	0/1282
1	J	0.17	0/944	0.49	0/1282
2	L	0.18	0/828	0.48	0/1128
2	M	0.18	0/828	0.46	0/1128
2	N	0.16	0/828	0.51	2/1128 (0.2%)
3	A	0.15	0/2566	0.35	0/3487
3	C	0.15	0/2566	0.34	0/3487
3	E	0.15	0/2566	0.33	0/3487
4	B	0.20	0/653	0.49	0/878
4	D	0.15	0/653	0.45	0/878
4	F	0.16	0/653	0.50	0/878
All	All	0.16	0/14973	0.42	3/20325 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	93	ASN	CA-C-N	-5.67	116.50	122.28
2	N	93	ASN	C-N-CA	-5.67	116.50	122.28
1	H	75	LYS	CA-CB-CG	5.65	125.41	114.10

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	H	919	0	887	29	0
1	I	919	0	887	28	0
1	J	919	0	887	30	0
2	L	808	0	788	19	0
2	M	808	0	788	25	0
2	N	808	0	788	23	0
3	A	2503	0	2462	45	0
3	C	2503	0	2462	30	0
3	E	2503	0	2462	30	0
4	B	645	0	635	20	0
4	D	645	0	635	23	0
4	F	645	0	635	14	0
All	All	14625	0	14316	307	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 11.

All (307) 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)
2:M:39:LYS:NZ	2:M:40:PRO:O	2.12	0.83
3:E:307:LYS:HG3	4:F:57:MET:HE1	1.62	0.81
2:L:18:ARG:HH22	2:L:20:THR:HB	1.45	0.80
1:H:68:THR:HG22	1:H:81:LYS:HZ1	1.46	0.79
4:B:79:ASN:O	4:B:82:MET:HB2	1.83	0.78
4:B:109:HIS:O	4:B:112:ASN:ND2	2.17	0.78
4:B:55:ASP:O	4:B:58:ASN:ND2	2.17	0.77
1:H:5:GLN:OE1	1:H:6:GLU:N	2.18	0.76
1:I:6:GLU:OE1	1:I:6:GLU:N	2.23	0.72
1:H:59:TYR:HE1	1:H:69:ILE:HG12	1.55	0.71
3:C:186:ASN:OD1	3:C:187:ASN:ND2	2.23	0.71
1:I:6:GLU:OE2	1:I:106:GLY:N	2.25	0.70
3:E:186:ASN:OD1	3:E:187:ASN:ND2	2.24	0.70
1:I:18:LEU:HD11	1:I:82(C):VAL:HA	1.74	0.67
1:J:6:GLU:OE1	1:J:106:GLY:N	2.26	0.67
2:N:18:ARG:NH2	2:N:20:THR:OG1	2.27	0.67
4:B:113:VAL:HA	4:B:116:LEU:HD12	1.77	0.67
2:N:4:MET:HE3	2:N:5:THR:H	1.60	0.67
3:C:25:GLN:HA	3:C:35:THR:HA	1.77	0.66
3:C:277:CYS:SG	3:C:278:ASN:N	2.69	0.66
1:H:2:MET:N	1:H:102:MET:SD	2.68	0.66
3:A:90:ARG:HH12	3:A:271:GLY:HA2	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:292:MET:SD	3:C:292:MET:N	2.68	0.66
3:C:172:ASN:ND2	3:C:174:GLU:OE1	2.28	0.66
3:E:111:MET:HE2	3:E:111:MET:HA	1.77	0.66
3:E:281:CYS:SG	3:E:282:GLN:N	2.69	0.65
3:A:171:THR:O	3:A:173:ARG:NH2	2.29	0.65
2:N:42:GLN:N	2:N:42:GLN:OE1	2.31	0.65
2:N:54:ARG:HH21	2:N:59:PRO:HA	1.61	0.65
4:D:111:SER:HA	4:D:114:LYS:HE2	1.79	0.64
3:A:281:CYS:SG	3:A:282:GLN:N	2.71	0.64
1:H:70:SER:OG	1:H:81:LYS:NZ	2.28	0.64
1:J:59:TYR:HB2	1:J:64:LYS:HG3	1.80	0.63
3:A:277:CYS:SG	3:A:278:ASN:N	2.72	0.63
3:A:73:ASN:HB3	3:A:76:CYS:HB2	1.81	0.62
3:A:123:PRO:HG2	3:A:126:SER:HB3	1.82	0.62
1:H:73:LYS:HE2	1:H:73:LYS:N	2.15	0.61
3:E:74:PRO:HA	3:E:149:ARG:HH21	1.66	0.61
2:N:50:ALA:HB3	2:N:53:THR:HG22	1.80	0.61
1:J:13:LYS:HE2	1:J:13:LYS:HA	1.82	0.61
1:J:96:LEU:HD11	1:J:100(E):ALA:HB3	1.82	0.61
2:M:18:ARG:NH2	2:M:20:THR:OG1	2.33	0.61
4:F:54:ILE:HD12	4:F:54:ILE:H	1.66	0.60
3:C:74:PRO:HA	3:C:149:ARG:HH21	1.66	0.60
4:F:118:ASP:OD1	4:F:121:ARG:NH2	2.35	0.60
1:J:77:GLN:OE1	1:J:78:PHE:N	2.34	0.59
3:A:60:ILE:HG22	3:A:88:VAL:HB	1.85	0.59
2:L:17:GLU:OE1	2:L:18:ARG:N	2.35	0.59
3:E:316:LEU:HD21	4:F:98:VAL:HG22	1.83	0.59
1:J:14:PRO:HA	1:J:82(C):VAL:HB	1.84	0.59
1:J:5:GLN:NE2	1:J:6:GLU:O	2.36	0.58
1:I:20:LEU:HD12	1:I:21:THR:H	1.68	0.58
1:J:59:TYR:HE1	1:J:69:ILE:HG12	1.68	0.58
3:A:50:LYS:HA	3:A:272:VAL:HG11	1.85	0.58
1:J:6:GLU:N	1:J:6:GLU:OE2	2.37	0.57
1:J:11:LEU:HD13	1:J:18:LEU:HB3	1.86	0.57
3:C:104:ASP:OD2	3:C:234:TRP:NE1	2.32	0.57
1:J:20:LEU:HD12	1:J:21:THR:H	1.70	0.57
1:H:51:ILE:HG21	1:H:69:ILE:HG21	1.86	0.57
2:N:54:ARG:HH22	2:N:62:PHE:HB2	1.70	0.57
3:E:92(A):PRO:HG2	3:E:95:ASP:HB2	1.86	0.57
1:H:2:MET:HE2	1:H:26:GLY:HA3	1.87	0.56
3:A:26:VAL:HG23	3:A:315:VAL:HB	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:25:GLN:HA	3:E:35:THR:HA	1.87	0.56
1:I:2:MET:HE3	1:I:2:MET:HA	1.87	0.56
1:I:2:MET:HE1	1:I:27:GLY:HA3	1.87	0.56
3:E:44:GLU:OE1	3:E:45:LYS:N	2.38	0.56
3:A:186:ASN:OD1	3:A:187:ASN:ND2	2.38	0.56
2:N:95:PRO:HB2	2:N:95(A):PRO:HD3	1.87	0.56
2:M:39:LYS:HD2	2:M:40:PRO:HD2	1.86	0.56
3:A:80:ILE:HG13	3:A:80(A):ARG:H	1.71	0.56
3:C:268:MET:HG2	3:C:284:PRO:HB3	1.88	0.56
1:J:66:ARG:HD2	1:J:82(B):SER:HB2	1.86	0.55
3:C:281:CYS:SG	3:C:282:GLN:N	2.79	0.55
3:A:44:GLU:OE1	3:A:45:LYS:N	2.39	0.55
4:F:112:ASN:HA	4:F:115:ASN:ND2	2.22	0.55
3:C:36:VAL:HG21	3:C:317:ALA:HB1	1.88	0.55
4:D:57:MET:O	4:D:57:MET:HE2	2.06	0.55
2:N:58:ILE:HD11	2:N:61:ARG:HG3	1.89	0.55
1:H:7:SER:OG	1:H:21:THR:OG1	2.22	0.55
2:N:16:GLY:H	2:N:78:LEU:HD23	1.72	0.54
3:E:166:ILE:HG22	3:E:245:PHE:HB2	1.89	0.54
1:H:2:MET:HE3	1:H:2:MET:HA	1.90	0.54
2:M:61:ARG:HH22	2:M:79:GLN:HG3	1.72	0.54
3:C:27:ASP:OD1	3:C:27:ASP:N	2.35	0.54
1:J:29:ILE:HG22	1:J:30:SER:H	1.72	0.54
2:N:63:SER:HB3	2:N:74:THR:HG23	1.89	0.54
4:D:96:LEU:O	4:D:100:MET:HG2	2.08	0.54
3:C:44:GLU:OE2	3:C:45:LYS:N	2.40	0.53
4:B:115:ASN:O	4:B:119:LYS:N	2.40	0.53
4:D:116:LEU:O	4:D:120:VAL:HG22	2.08	0.53
4:F:116:LEU:O	4:F:120:VAL:HG22	2.08	0.53
1:I:68:THR:HG22	1:I:81:LYS:HZ3	1.74	0.53
3:A:90:ARG:NH1	3:A:271:GLY:HA2	2.23	0.53
4:F:52:SER:O	4:F:56:LYS:HG2	2.07	0.53
1:H:96:LEU:HD11	1:H:100(E):ALA:HB3	1.90	0.53
3:A:75:MET:HE2	3:A:75:MET:HA	1.91	0.53
1:J:18:LEU:HD13	1:J:82:LEU:HB3	1.90	0.53
1:J:2:MET:HB3	1:J:4:LEU:HD23	1.91	0.53
1:I:77:GLN:OE1	1:I:78:PHE:N	2.42	0.52
3:A:88:VAL:HG22	3:A:268:MET:HG2	1.91	0.52
4:B:69:ASN:N	4:B:72:GLU:OE2	2.39	0.52
2:N:35:TRP:NE1	2:N:88:CYS:SG	2.82	0.52
1:J:18:LEU:HG	1:J:82(C):VAL:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:184:HIS:NE2	3:A:231:ASP:OD2	2.41	0.51
3:C:111:MET:HE2	3:C:111:MET:HA	1.91	0.51
1:H:71:VAL:HB	1:H:73:LYS:HZ3	1.76	0.51
1:I:3:GLN:HB3	1:I:25:SER:HB3	1.91	0.51
1:I:3:GLN:OE1	1:I:4:LEU:N	2.43	0.51
1:I:96:LEU:HD21	1:I:100(E):ALA:HB3	1.92	0.51
4:B:118:ASP:HA	4:B:121:ARG:HB3	1.92	0.51
3:E:51:LEU:HD23	3:E:272:VAL:HB	1.92	0.51
4:B:122:LEU:H	4:B:122:LEU:HD23	1.75	0.51
1:H:75:LYS:HD2	1:H:75:LYS:O	2.11	0.51
3:E:60:ILE:HG22	3:E:88:VAL:HB	1.91	0.51
4:F:112:ASN:HA	4:F:115:ASN:HD21	1.76	0.51
1:H:66:ARG:HD2	1:H:82(B):SER:HB2	1.92	0.51
1:I:70:SER:OG	1:I:81:LYS:NZ	2.37	0.51
4:B:88:ASP:OD2	4:D:59:THR:OG1	2.28	0.51
1:I:73:LYS:HD2	1:I:73:LYS:N	2.26	0.51
1:J:59:TYR:CE1	1:J:69:ILE:HG12	2.44	0.51
3:C:29:ILE:HG12	4:D:99:LEU:HD23	1.93	0.51
1:J:72:ASP:OD1	1:J:72:ASP:N	2.44	0.51
2:M:24:ARG:HD2	2:M:25:ALA:N	2.26	0.50
3:E:184:HIS:NE2	3:E:231:ASP:OD2	2.44	0.50
1:J:20:LEU:HD12	1:J:21:THR:N	2.26	0.50
3:C:26:VAL:N	3:C:34:VAL:O	2.45	0.50
4:D:67:GLU:N	4:D:67:GLU:OE1	2.43	0.50
3:A:51:LEU:HD13	3:A:272:VAL:HB	1.94	0.50
3:E:53(A):LEU:HD23	3:E:85:SER:HB2	1.92	0.50
4:F:76:GLU:OE1	4:F:77:ASN:ND2	2.44	0.50
2:M:14:SER:HG	2:M:17:GLU:CD	2.20	0.50
3:A:130:GLU:OE2	3:A:131:THR:N	2.44	0.50
1:J:29:ILE:O	1:J:30:SER:OG	2.28	0.49
1:J:75:LYS:NZ	1:J:77:GLN:HE21	2.09	0.49
1:H:36:TRP:HB2	1:H:48:ILE:HB	1.93	0.49
3:A:270:SER:OG	3:A:284:PRO:O	2.25	0.49
3:C:318:THR:HG22	4:D:105:THR:HG21	1.94	0.49
1:I:13:LYS:HD3	1:I:14:PRO:O	2.12	0.49
2:L:54:ARG:NH1	2:L:62:PHE:O	2.45	0.49
2:M:6:GLN:NE2	2:M:100:GLY:O	2.45	0.49
1:I:21:THR:OG1	1:I:21:THR:O	2.31	0.49
2:L:61:ARG:C	2:L:62:PHE:HD1	2.20	0.49
2:L:103:LYS:HE2	2:L:103:LYS:HA	1.95	0.49
3:C:166:ILE:HG22	3:C:245:PHE:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:171:THR:O	3:E:173:ARG:NH2	2.39	0.49
1:H:59:TYR:HB2	1:H:64:LYS:HG3	1.95	0.49
4:F:97:LEU:HD12	4:F:98:VAL:N	2.28	0.49
2:L:80:SER:HA	2:L:83:PHE:HE1	1.78	0.49
2:N:6:GLN:N	2:N:6:GLN:OE1	2.46	0.49
3:A:88:VAL:HA	3:A:268:MET:HB3	1.94	0.48
4:B:112:ASN:HA	4:B:115:ASN:ND2	2.28	0.48
3:E:159:ASP:O	3:E:196:LYS:NZ	2.39	0.48
4:D:55:ASP:OD1	4:D:56:LYS:HD2	2.14	0.48
3:A:40:GLN:NE2	3:A:41:ASP:O	2.40	0.48
2:M:54:ARG:NH1	2:M:59:PRO:O	2.47	0.48
1:J:2:MET:N	1:J:2:MET:HE2	2.27	0.48
1:J:81:LYS:N	1:J:81:LYS:HD3	2.29	0.48
2:N:6:GLN:HE22	2:N:100:GLY:N	2.11	0.48
1:J:35:TRP:H	1:J:35:TRP:CD1	2.31	0.48
1:H:13:LYS:HD3	1:H:14:PRO:O	2.13	0.48
3:E:27:ASP:OD1	3:E:27:ASP:N	2.35	0.48
4:D:46:VAL:HA	4:D:49:LYS:HG2	1.96	0.48
1:H:75:LYS:HZ2	1:H:77:GLN:HB2	1.79	0.47
3:C:130:GLU:H	3:C:157:LYS:HB2	1.78	0.47
2:N:39:LYS:NZ	2:N:83:PHE:O	2.47	0.47
3:C:51:LEU:HG	3:C:272:VAL:HB	1.96	0.47
3:A:29:ILE:HG12	4:B:99:LEU:HD23	1.95	0.47
2:N:39:LYS:NZ	2:N:84:ALA:HB2	2.30	0.47
3:C:31:GLU:OE1	3:C:32:LYS:N	2.45	0.47
3:E:130:GLU:OE2	3:E:131:THR:N	2.47	0.47
2:M:63:SER:HB3	2:M:74:THR:HG23	1.96	0.47
3:A:206:THR:OG1	3:A:207:SER:N	2.46	0.47
3:E:26:VAL:N	3:E:34:VAL:O	2.46	0.46
2:M:95:PRO:HD2	2:M:95(A):PRO:HD3	1.97	0.46
2:N:39:LYS:HA	2:N:39:LYS:HD3	1.70	0.46
2:N:85:VAL:HA	2:N:102:THR:O	2.16	0.46
2:N:4:MET:HE3	2:N:4:MET:HA	1.97	0.46
4:F:57:MET:SD	4:F:60:GLN:HB2	2.55	0.46
1:J:18:LEU:HD11	1:J:82(C):VAL:HA	1.97	0.46
3:E:292:MET:SD	3:E:292:MET:N	2.89	0.46
1:I:38:ARG:HG2	1:I:46:GLU:HB3	1.97	0.46
2:L:94:TRP:CD1	2:L:96:LEU:HD11	2.50	0.46
2:L:49:TYR:HE1	2:L:55:ALA:HB3	1.80	0.45
4:D:97:LEU:HD12	4:D:98:VAL:N	2.32	0.45
4:D:72:GLU:HB2	4:D:75:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:112:ASN:O	4:D:116:LEU:HG	2.16	0.45
3:A:74:PRO:HA	3:A:149:ARG:HH21	1.80	0.45
3:C:200:THR:HB	3:C:249:GLY:HA3	1.99	0.45
3:C:121(B):ILE:HG13	3:C:122:ILE:HG12	1.99	0.45
4:D:49:LYS:O	4:D:53:ILE:HG12	2.17	0.45
4:D:112:ASN:OD1	4:D:113:VAL:N	2.50	0.45
2:L:95:PRO:HD2	2:L:95(A):PRO:HD3	1.98	0.45
3:A:111:MET:HA	3:A:111:MET:HE2	1.99	0.45
3:A:123:PRO:O	3:A:126:SER:OG	2.30	0.45
3:A:292:MET:SD	3:A:292:MET:N	2.89	0.45
3:A:171:THR:C	3:A:173:ARG:HH21	2.25	0.44
3:E:92:ASN:ND2	3:E:92:ASN:O	2.50	0.44
1:H:81:LYS:HD3	1:H:81:LYS:N	2.32	0.44
1:J:13:LYS:HD3	1:J:14:PRO:O	2.17	0.44
3:A:191:GLN:HE22	3:A:250:ASN:CG	2.25	0.44
3:A:283:THR:HG22	3:A:301:THR:HG22	2.00	0.44
1:I:14:PRO:HA	1:I:82(C):VAL:HG21	1.99	0.44
3:A:71:LEU:HD13	3:A:71:LEU:HA	1.87	0.44
3:A:90:ARG:HH22	3:A:271:GLY:HA2	1.81	0.44
3:A:64:CYS:HA	3:A:94:ASN:HB3	2.00	0.44
3:E:186:ASN:N	3:E:190:GLU:OE1	2.43	0.44
1:H:20:LEU:HG	1:H:36:TRP:CH2	2.53	0.44
2:M:95:PRO:O	2:M:96:LEU:N	2.51	0.44
3:C:52:CYS:HB2	3:C:277:CYS:HB3	1.32	0.44
3:C:130:GLU:N	3:C:157:LYS:HB2	2.33	0.44
2:M:39:LYS:HD2	2:M:40:PRO:CD	2.48	0.44
3:C:265:SER:OG	3:C:266:THR:N	2.51	0.44
4:B:67:GLU:OE2	4:B:67:GLU:N	2.51	0.44
4:B:93:ASN:O	4:B:97:LEU:HG	2.18	0.44
1:J:71:VAL:HG23	1:J:78:PHE:HB3	2.00	0.43
2:N:21:LEU:HD23	2:N:22:SER:H	1.83	0.43
3:A:80:ILE:HD12	3:A:80(A):ARG:HD2	2.00	0.43
3:A:238:LYS:HB2	3:A:241:ASP:OD2	2.18	0.43
3:E:200:THR:HB	3:E:249:GLY:HA3	1.98	0.43
4:B:97:LEU:O	4:B:98:VAL:C	2.61	0.43
3:C:279:THR:O	3:C:280:LYS:HD2	2.18	0.43
1:H:18:LEU:HD13	1:H:82:LEU:HB3	2.00	0.43
1:I:86:ASP:N	1:I:86:ASP:OD1	2.51	0.43
1:J:75:LYS:HZ1	1:J:77:GLN:HE21	1.67	0.43
2:L:4:MET:HA	2:L:4:MET:HE3	2.00	0.43
1:H:13:LYS:HE2	1:H:13:LYS:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:58:ILE:CD1	2:M:61:ARG:HG3	2.49	0.43
3:E:221:SER:OG	3:E:222:GLN:N	2.51	0.43
4:B:119:LYS:O	4:B:119:LYS:HD3	2.19	0.43
3:A:77:ASP:OD1	3:A:78:GLU:N	2.52	0.43
1:I:66:ARG:HG3	1:I:82(A):THR:OG1	2.19	0.43
3:A:129(A):HIS:HD1	3:A:154:LEU:HD23	1.83	0.43
3:A:191:GLN:NE2	3:A:250:ASN:OD1	2.47	0.43
4:D:69:ASN:ND2	4:D:72:GLU:OE2	2.52	0.43
2:M:18:ARG:NH1	2:M:75:ILE:H	2.16	0.43
3:A:52:CYS:HB2	3:A:277:CYS:HB3	1.25	0.43
3:E:129(A):HIS:CE1	3:E:162:PRO:HG2	2.54	0.43
2:L:35:TRP:NE1	2:L:88:CYS:SG	2.92	0.42
3:C:71:LEU:HD13	3:C:71:LEU:HA	1.89	0.42
4:D:59:THR:OG1	4:D:59:THR:O	2.37	0.42
3:A:282:GLN:HB3	3:A:302:ILE:HG23	2.00	0.42
3:E:121(B):ILE:HG13	3:E:122:ILE:HG12	2.01	0.42
4:B:112:ASN:HA	4:B:115:ASN:HD21	1.85	0.42
1:H:18:LEU:HD12	1:H:18:LEU:H	1.84	0.42
2:L:4:MET:HE3	2:L:5:THR:H	1.85	0.42
2:M:94:TRP:CZ3	3:C:82:PRO:HD3	2.54	0.42
4:D:79:ASN:HA	4:D:82:MET:HG2	2.02	0.42
1:H:71:VAL:HG12	1:H:78:PHE:HB2	2.00	0.42
2:L:6:GLN:NE2	2:L:100:GLY:O	2.49	0.42
2:N:80:SER:HA	2:N:83:PHE:HE1	1.85	0.42
4:D:72:GLU:OE1	4:D:72:GLU:N	2.53	0.42
1:I:68:THR:HG22	1:I:81:LYS:NZ	2.35	0.42
2:M:58:ILE:HA	2:M:59:PRO:HD3	1.83	0.42
3:E:103:ASN:HB3	3:E:104:ASP:OD1	2.20	0.42
2:L:24:ARG:HD2	2:L:24:ARG:C	2.45	0.42
3:C:130:GLU:OE2	3:C:131:THR:N	2.51	0.42
3:E:211:GLN:NE2	3:E:213:LEU:HD12	2.35	0.42
2:L:24:ARG:HD2	2:L:25:ALA:N	2.35	0.42
2:M:103:LYS:HD3	2:M:104:VAL:N	2.35	0.42
2:N:37:GLN:OE1	2:N:45:ARG:NH2	2.48	0.42
2:N:96:LEU:HD12	2:N:96:LEU:HA	1.88	0.42
4:F:112:ASN:O	4:F:116:LEU:HG	2.20	0.42
1:J:15:SER:H	1:J:83:THR:HG23	1.84	0.41
2:N:94:TRP:O	2:N:94:TRP:CD1	2.73	0.41
4:D:78:LEU:O	4:D:82:MET:HG2	2.20	0.41
4:D:119:LYS:HD3	4:D:120:VAL:HG13	2.01	0.41
1:H:43:LYS:NZ	1:H:86:ASP:OD2	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:29:ILE:HG21	1:J:73:LYS:NZ	2.34	0.41
2:M:21:LEU:HD23	2:M:22:SER:N	2.35	0.41
1:I:36:TRP:CZ3	1:I:92:CYS:HB3	2.54	0.41
1:H:35:TRP:CD1	1:H:35:TRP:H	2.37	0.41
1:I:45:LEU:HB2	2:M:98:PHE:CD2	2.56	0.41
3:A:170:ASN:ND2	3:A:239:PRO:HA	2.35	0.41
3:A:186:ASN:N	3:A:190:GLU:OE1	2.45	0.41
3:E:206:THR:O	3:E:206:THR:OG1	2.28	0.41
4:B:68:PHE:HB2	4:B:76:GLU:HB2	2.02	0.41
1:I:13:LYS:NZ	1:I:14:PRO:HD2	2.35	0.41
2:M:58:ILE:HD11	2:M:61:ARG:HG3	2.03	0.41
1:H:29:ILE:HG12	1:H:76:ASN:HB2	2.02	0.41
3:A:50:LYS:HD3	3:A:275:GLY:HA3	2.03	0.41
1:I:36:TRP:CD1	1:I:80:LEU:HD12	2.56	0.41
1:I:81:LYS:HD3	1:I:81:LYS:N	2.36	0.41
2:L:62:PHE:N	2:L:62:PHE:CD1	2.88	0.41
2:M:103:LYS:HA	2:M:103:LYS:HE2	2.03	0.41
4:D:82:MET:HE1	4:F:82:MET:HE2	2.03	0.41
2:L:37:GLN:HE22	2:L:39:LYS:HE2	1.86	0.41
2:M:48:ILE:HD13	2:M:48:ILE:HA	1.89	0.41
2:M:103:LYS:HD3	2:M:104:VAL:O	2.21	0.41
1:I:59:TYR:CE1	1:I:69:ILE:HG12	2.56	0.40
2:M:61:ARG:NH1	2:M:79:GLN:OE1	2.53	0.40
3:A:27:ASP:OD1	3:A:27:ASP:N	2.39	0.40
2:L:83:PHE:CD1	2:L:83:PHE:N	2.89	0.40
3:C:279:THR:OG1	3:C:280:LYS:N	2.54	0.40
4:B:88:ASP:O	4:B:91:THR:HG22	2.21	0.40
4:F:84:ASP:N	4:F:84:ASP:OD1	2.53	0.40
1:H:66:ARG:HG3	1:H:82(A):THR:OG1	2.21	0.40
1:I:94:ARG:HD2	1:I:95:GLY:H	1.86	0.40
2:L:18:ARG:NH2	2:L:20:THR:HB	2.25	0.40
1:H:86:ASP:OD1	1:H:86:ASP:N	2.50	0.40
1:I:80:LEU:C	1:I:81:LYS:HD3	2.46	0.40
2:M:106:ILE:H	2:M:106:ILE:HG12	1.71	0.40
4:B:72:GLU:O	4:B:73:ARG:C	2.64	0.40
4:D:69:ASN:N	4:D:72:GLU:OE2	2.50	0.40
3:A:121(B):ILE:HG13	3:A:122:ILE:N	2.37	0.40
3:E:26:VAL:HG23	3:E:315:VAL:HB	2.03	0.40
4:B:88:ASP:O	4:B:89:VAL:C	2.65	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	H	118/123 (96%)	114 (97%)	4 (3%)	0	100	100
1	I	118/123 (96%)	108 (92%)	10 (8%)	0	100	100
1	J	118/123 (96%)	112 (95%)	6 (5%)	0	100	100
2	L	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	M	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
2	N	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
3	A	314/342 (92%)	287 (91%)	27 (9%)	0	100	100
3	C	314/342 (92%)	290 (92%)	24 (8%)	0	100	100
3	E	314/342 (92%)	295 (94%)	19 (6%)	0	100	100
4	B	75/227 (33%)	68 (91%)	7 (9%)	0	100	100
4	D	75/227 (33%)	71 (95%)	4 (5%)	0	100	100
4	F	75/227 (33%)	72 (96%)	3 (4%)	0	100	100
All	All	1836/2400 (76%)	1701 (93%)	135 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	99/102 (97%)	99 (100%)	0	100	100
1	I	99/102 (97%)	99 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	J	99/102 (97%)	98 (99%)	1 (1%)	68 72
2	L	88/89 (99%)	88 (100%)	0	100 100
2	M	88/89 (99%)	88 (100%)	0	100 100
2	N	88/89 (99%)	88 (100%)	0	100 100
3	A	280/305 (92%)	280 (100%)	0	100 100
3	C	280/305 (92%)	280 (100%)	0	100 100
3	E	280/305 (92%)	280 (100%)	0	100 100
4	B	73/192 (38%)	73 (100%)	0	100 100
4	D	73/192 (38%)	73 (100%)	0	100 100
4	F	73/192 (38%)	73 (100%)	0	100 100
All	All	1620/2064 (78%)	1619 (100%)	1 (0%)	87 87

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

Mol	Chain	Res	Type
1	J	96	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	105	GLN
1	J	39	GLN
2	N	27	GLN
2	N	38	GLN
2	N	93	ASN
3	A	47	HIS
3	A	116	ASN
3	A	187	ASN
3	A	276	HIS
3	A	278	ASN
3	C	38	HIS
3	C	116	ASN
3	C	197	ASN
3	C	282	GLN
3	E	25	GLN
3	E	116	ASN
3	E	170	ASN

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Mol	Chain	Res	Type
3	E	276	HIS
4	B	102	ASN
4	D	77	ASN
4	F	77	ASN
4	F	102	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.

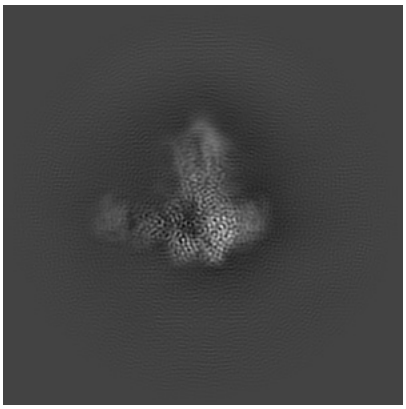
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-48515. These allow visual inspection of the internal detail of the map and identification of artifacts.

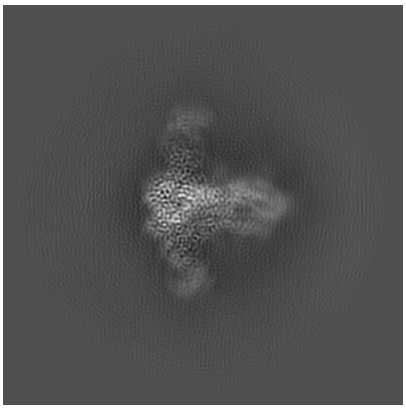
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

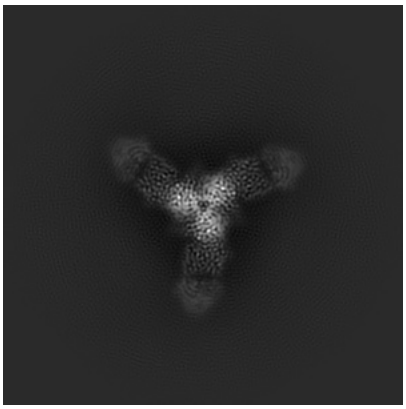
6.1.1 Primary map



X

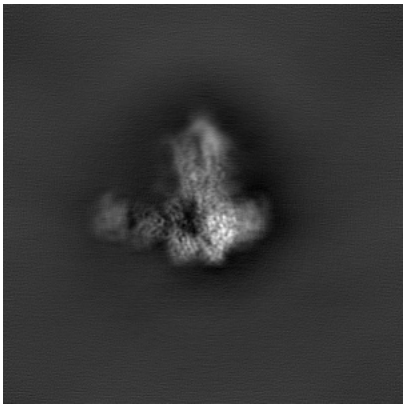


Y

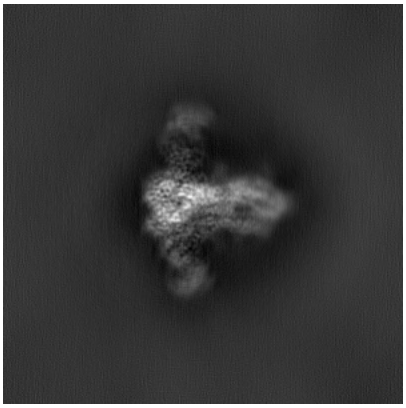


Z

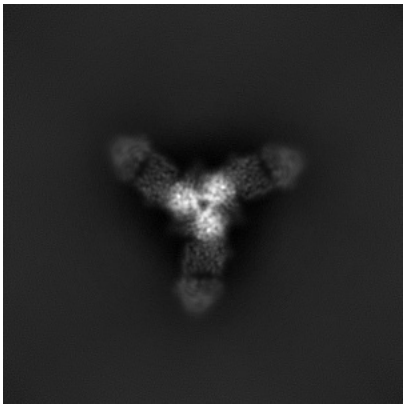
6.1.2 Raw map



X



Y

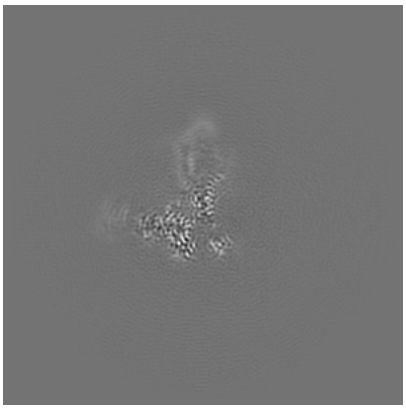


Z

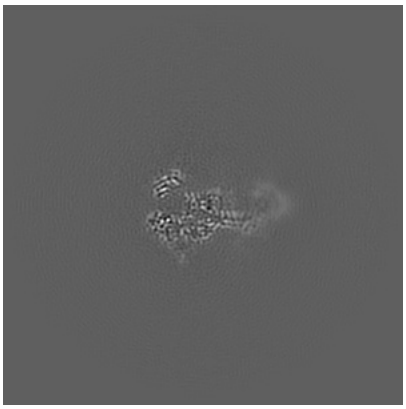
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

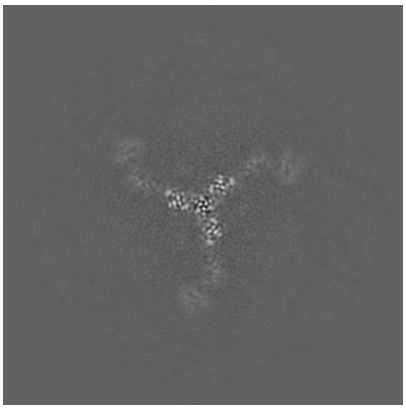
6.2.1 Primary map



X Index: 200

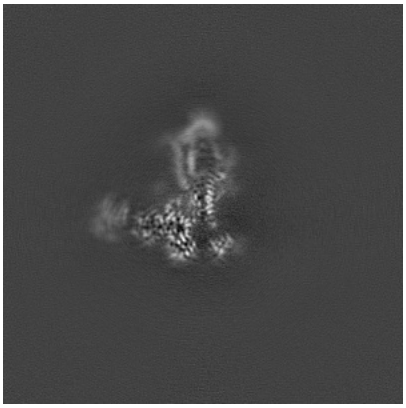


Y Index: 200

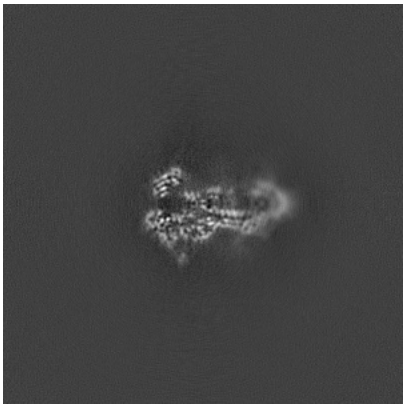


Z Index: 200

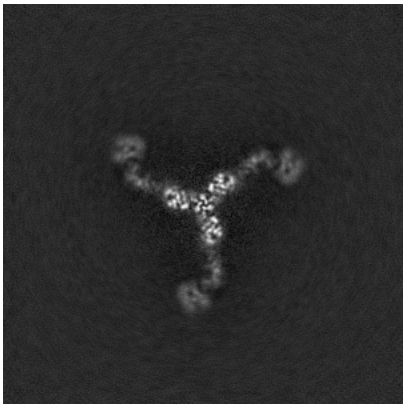
6.2.2 Raw map



X Index: 200



Y Index: 200

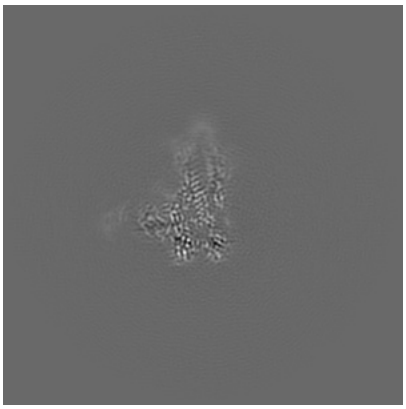


Z Index: 200

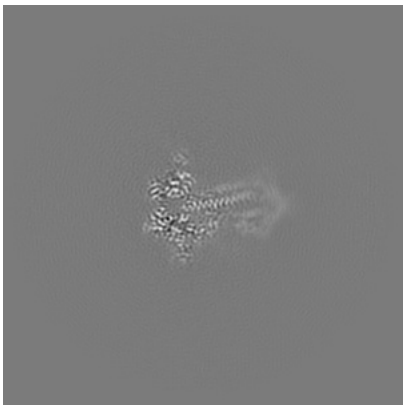
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

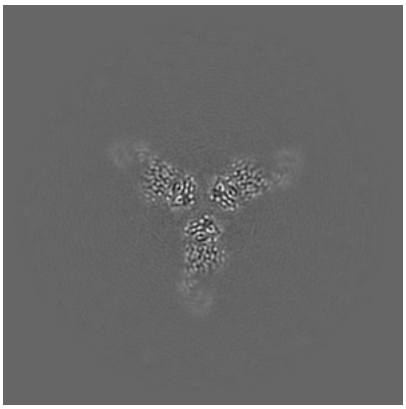
6.3.1 Primary map



X Index: 207

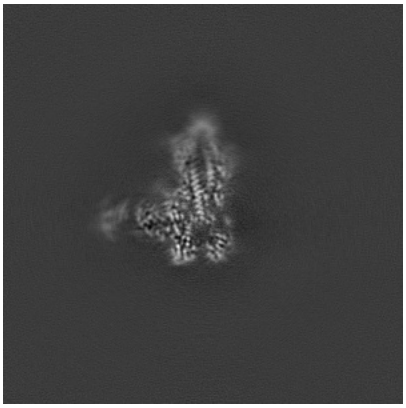


Y Index: 206

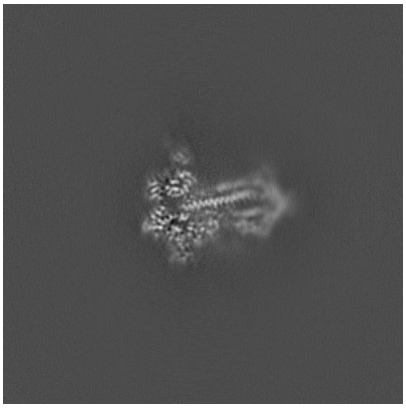


Z Index: 174

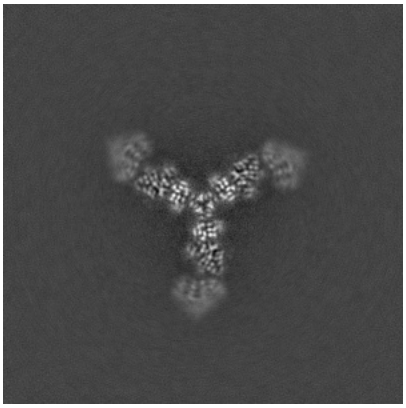
6.3.2 Raw map



X Index: 206



Y Index: 206

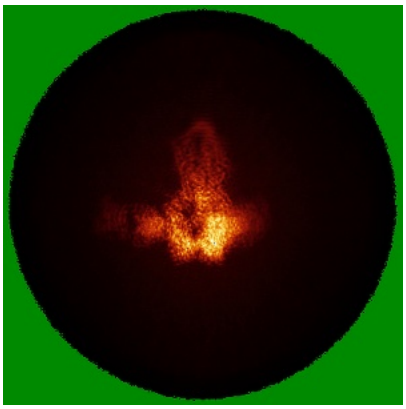


Z Index: 186

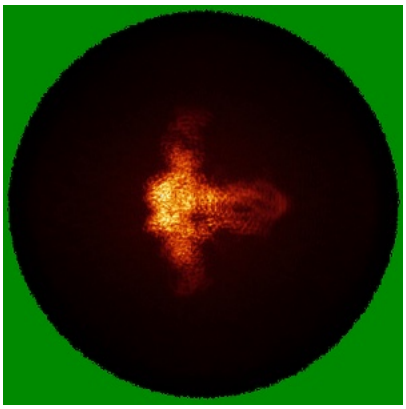
The images above show the largest variance slices of the map in three orthogonal directions.

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

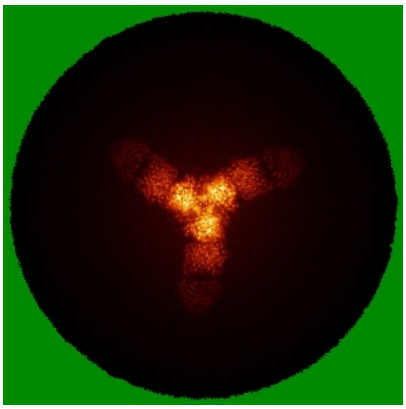
6.4.1 Primary map



X

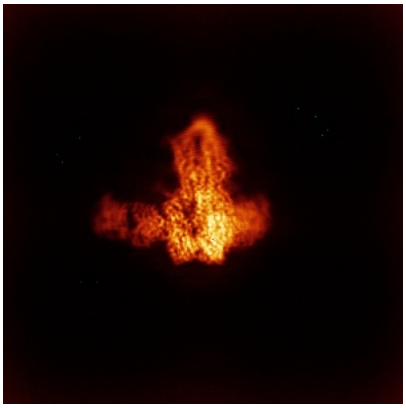


Y

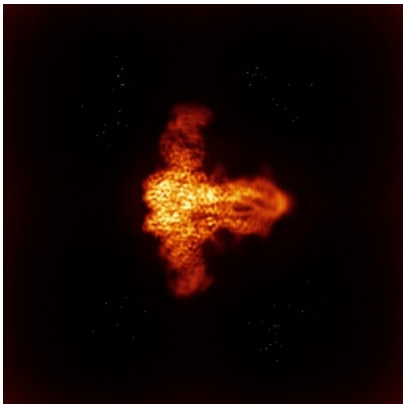


Z

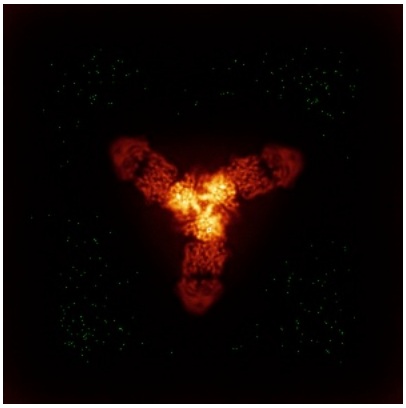
6.4.2 Raw map



X



Y

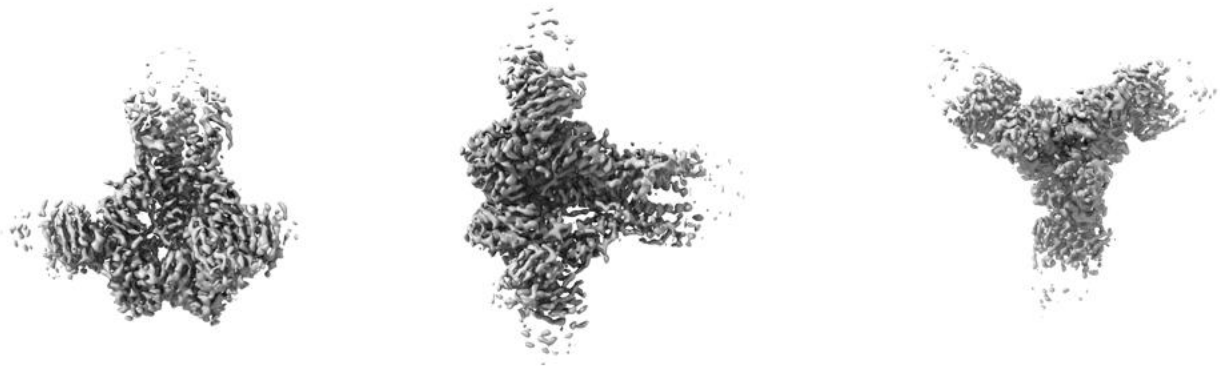


Z

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 0.236. 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.

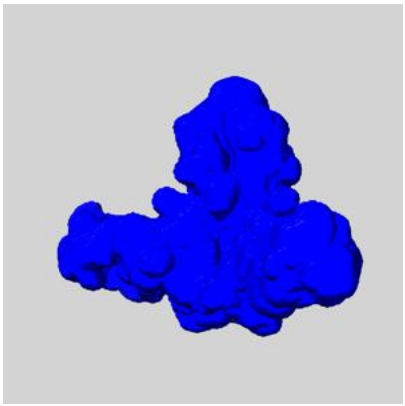
6.6 Mask visualisation

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

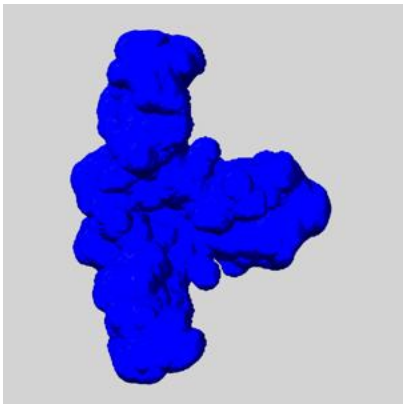
A mask typically either:

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

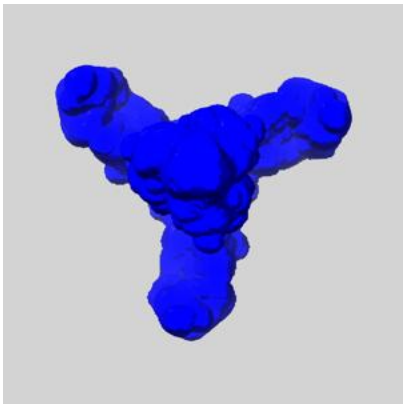
6.6.1 emd_48515_msk_1.map



X



Y

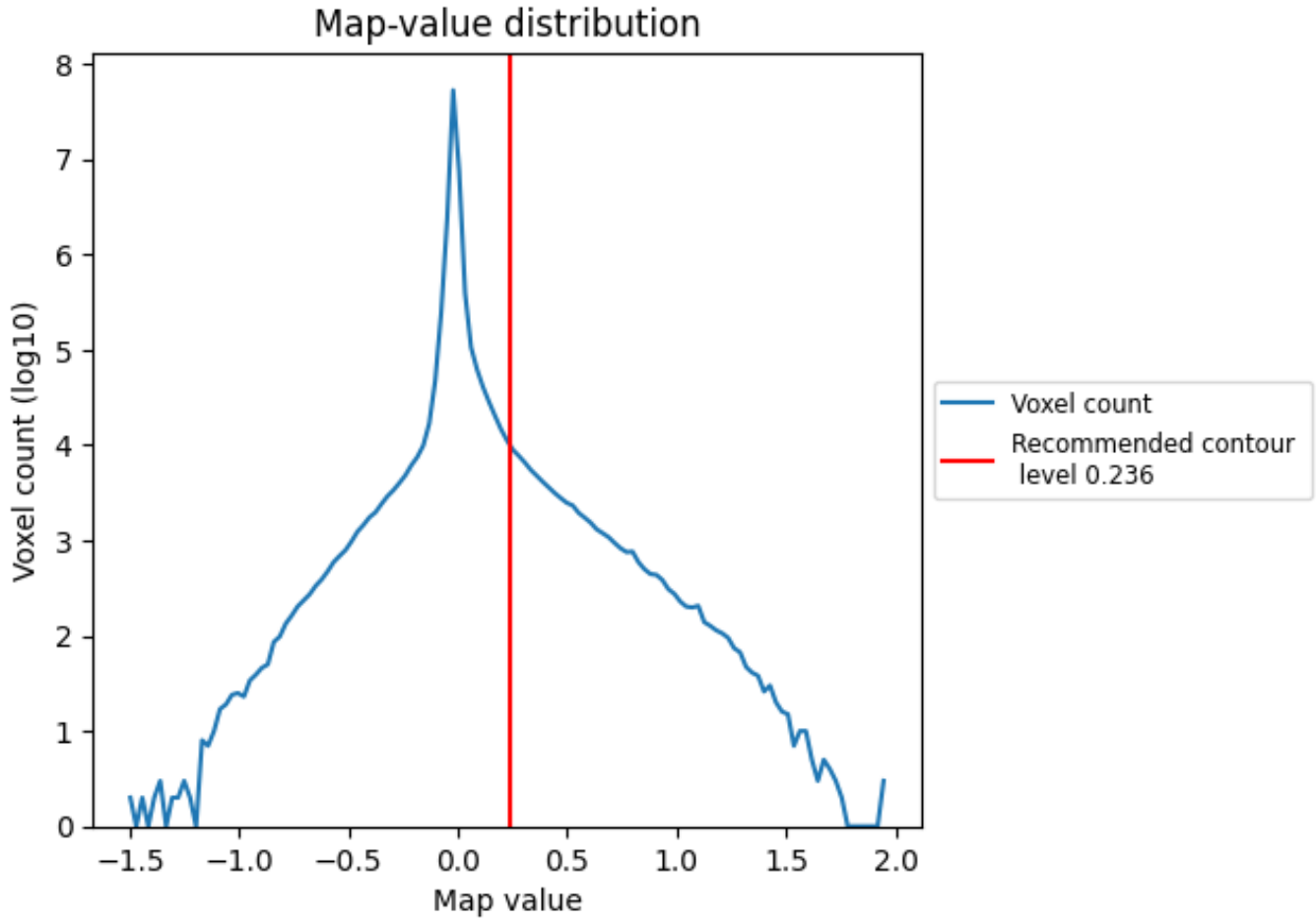


Z

7 Map analysis

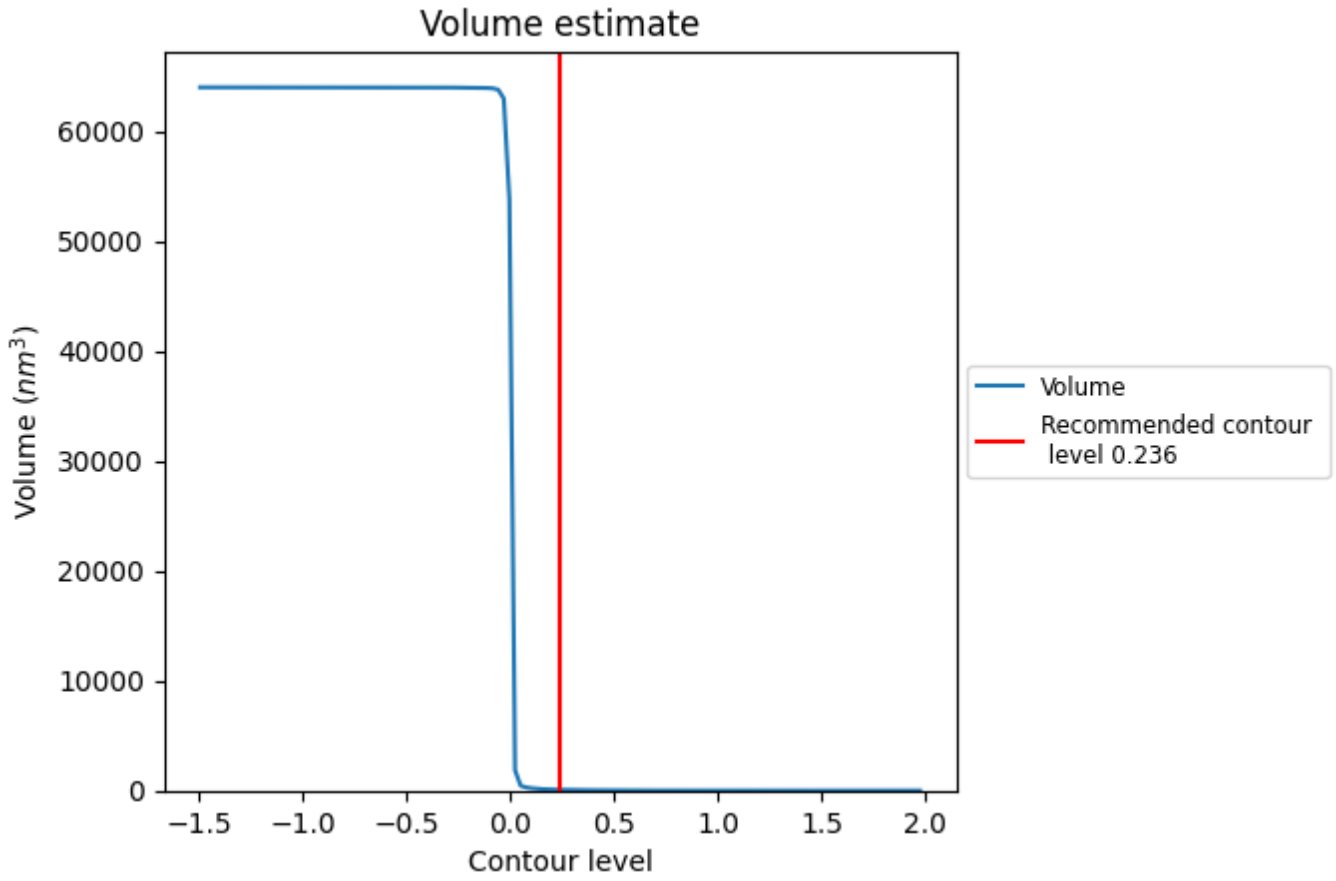
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

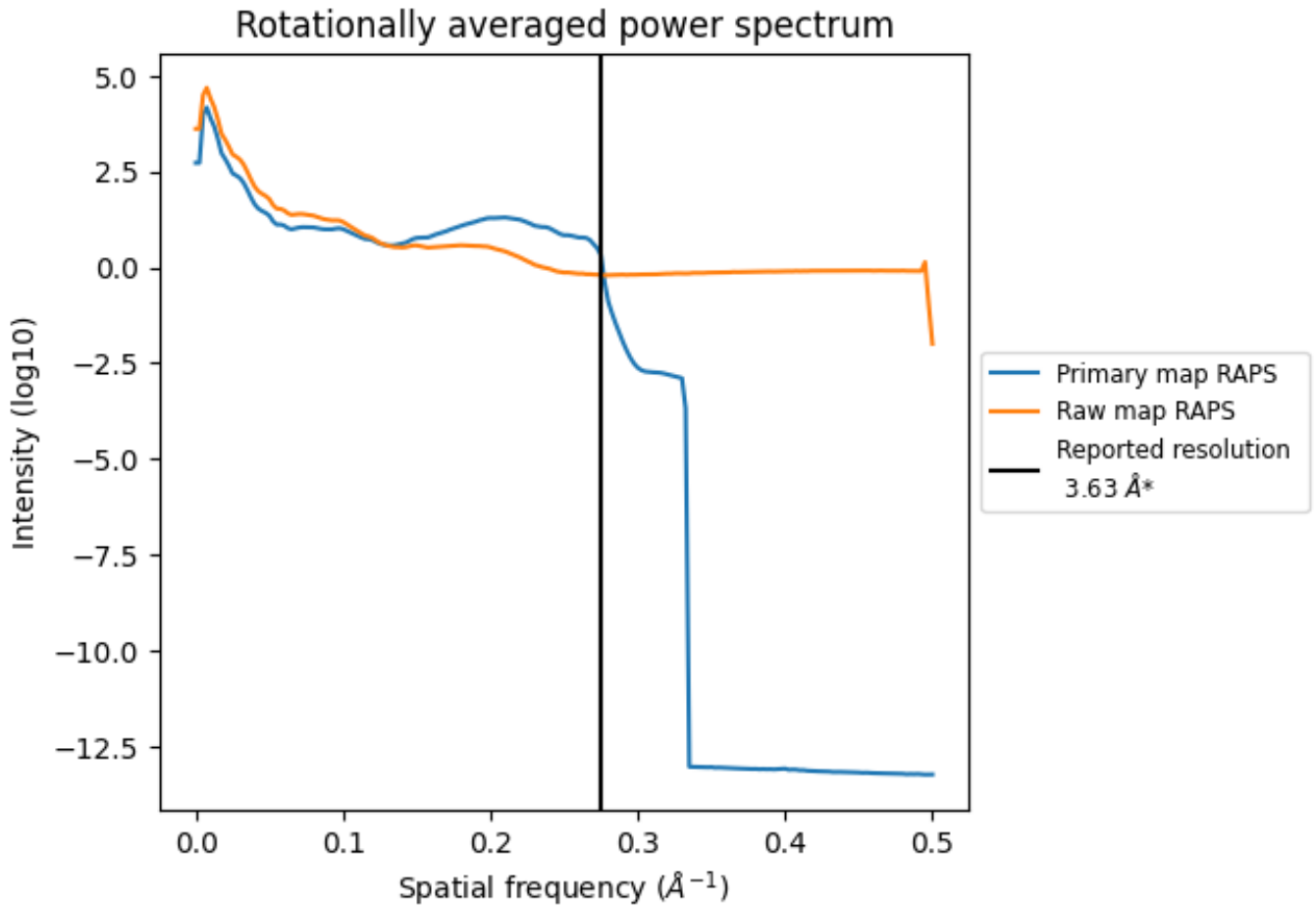
7.2 Volume estimate



The volume at the recommended contour level is 75 nm^3; this corresponds to an approximate mass of 68 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)

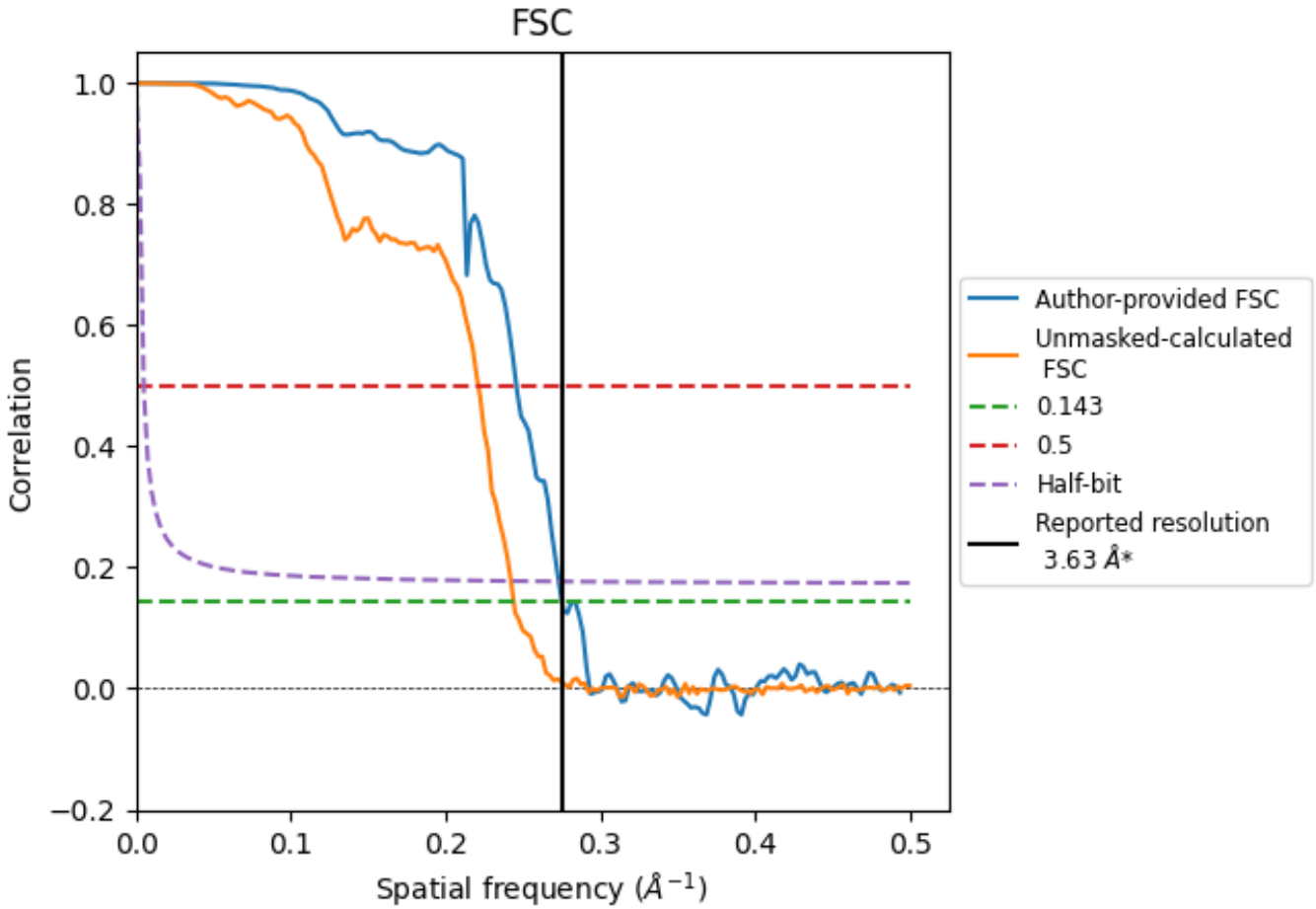


*Reported resolution corresponds to spatial frequency of 0.275 $Å^{-1}$

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 0.275 Å^{-1}

8.2 Resolution estimates (i)

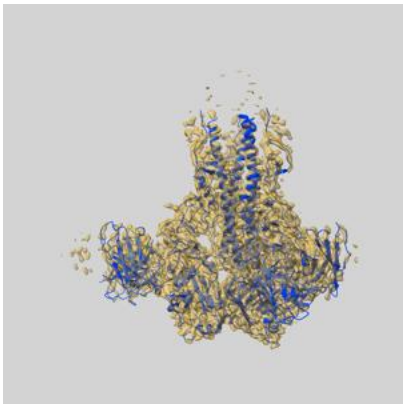
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.63	-	-
Author-provided FSC curve	3.63	4.07	3.66
Unmasked-calculated*	4.10	4.52	4.13

*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 4.10 differs from the reported value 3.63 by more than 10 %

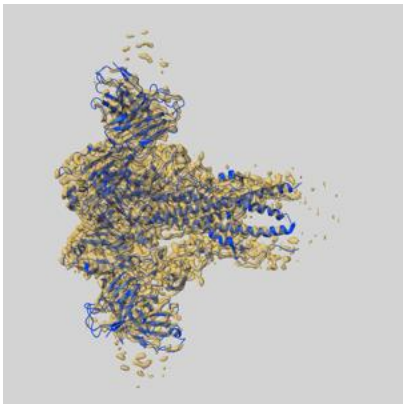
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-48515 and PDB model 9MQ7. Per-residue inclusion information can be found in section 3 on page 10.

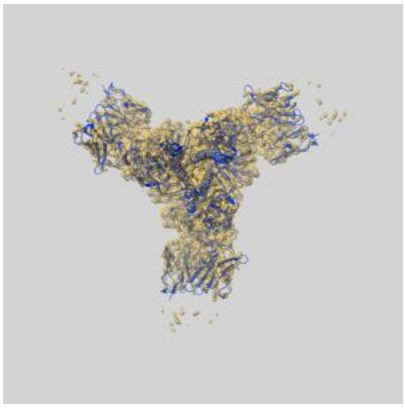
9.1 Map-model overlay



X



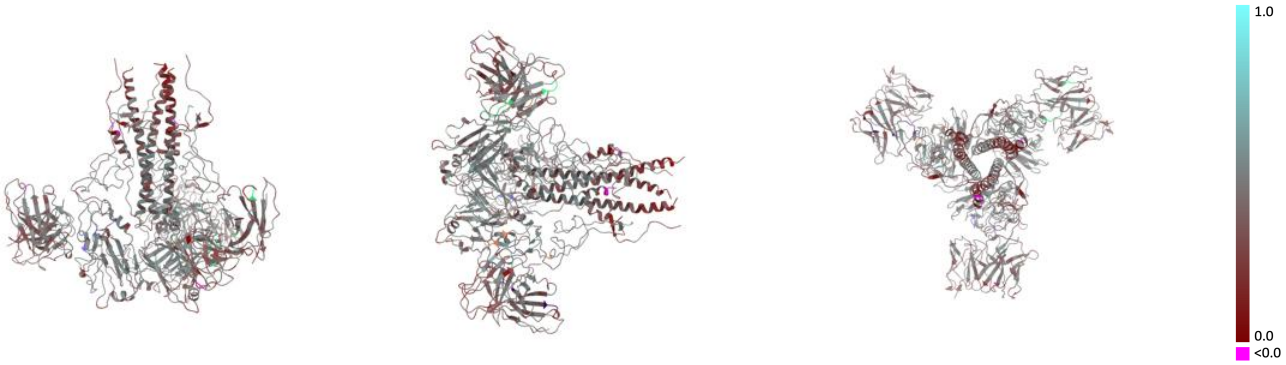
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.236 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.

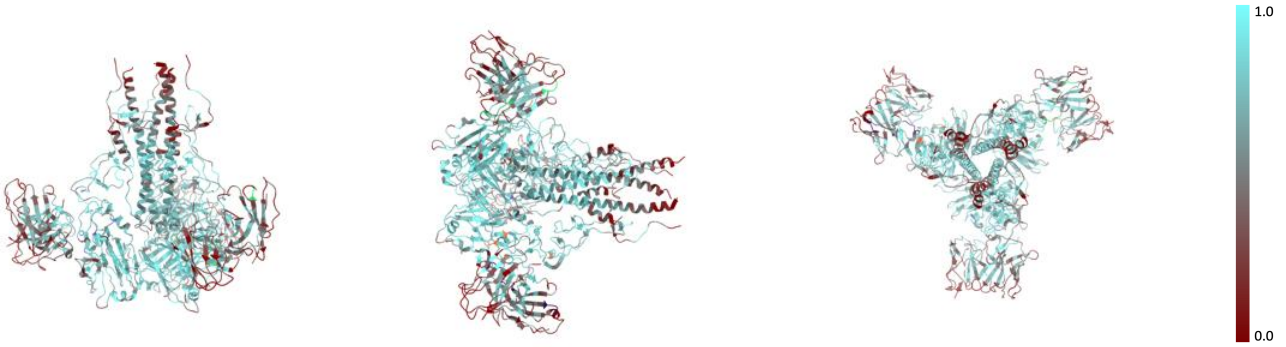
9.2 Q-score mapped to coordinate model (i)



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.

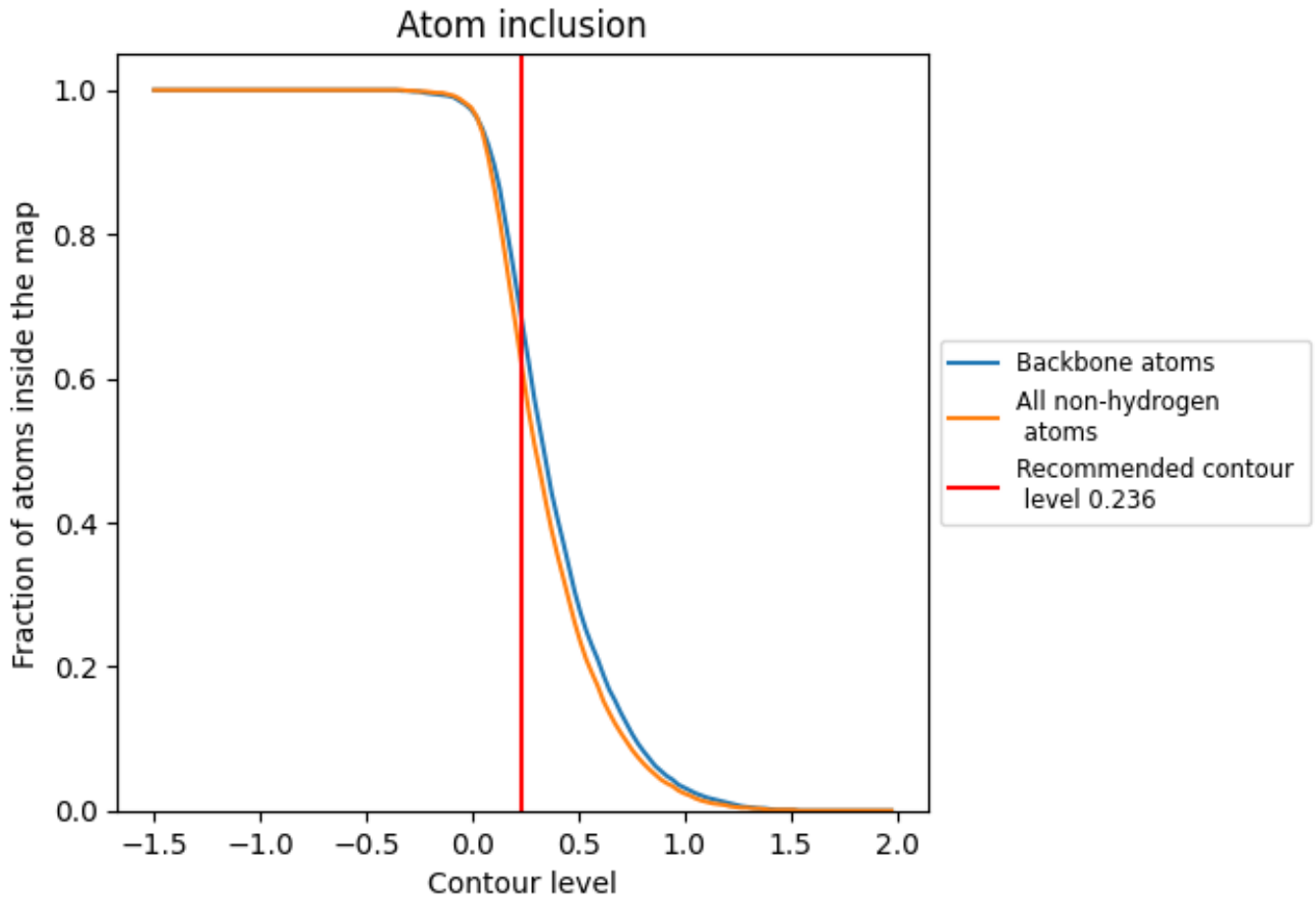
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.236).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 61% 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 (0.236) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6110	0.4220
A	0.7280	0.4480
B	0.5440	0.3640
C	0.7330	0.4550
D	0.5600	0.3530
E	0.7350	0.4560
F	0.5650	0.3740
H	0.4800	0.4110
I	0.4920	0.4210
J	0.4920	0.4170
L	0.4250	0.3790
M	0.4110	0.3730
N	0.4130	0.3810

