



Full wwPDB EM Validation Report ⓘ

Dec 14, 2024 – 08:13 AM EST

PDB ID : 8UME
EMDB ID : EMD-42377
Title : Influenza A virus Hemagglutinin H5/Vietnam/1204/2004 in complex with D04 Fab
Authors : Ferreira Ramos, A.S.; Bajic, G.
Deposited on : 2023-10-17
Resolution : 3.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

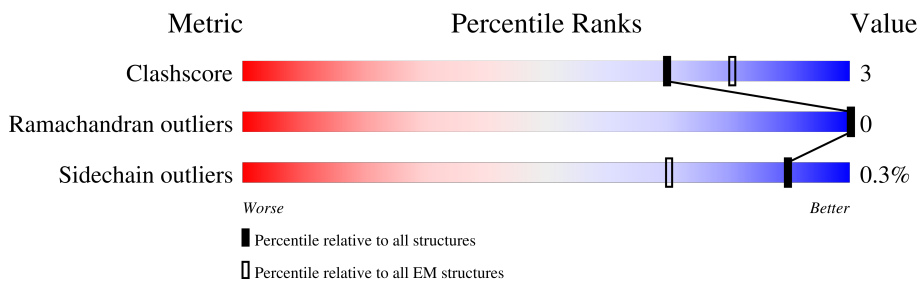
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 Å.

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




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

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

Mol	Chain	Length	Quality of chain
1	A	547	
1	B	547	
1	C	547	
2	D	228	
2	E	228	
2	H	228	
3	F	221	
3	G	221	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	L	221	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into two segments: a green segment on the left labeled '49%' and a grey segment on the right labeled '48%'. A small red dot is at the far left end, and a small black dot is at the boundary between the green and grey segments.</p>

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 16671 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	466	3729	2342	648	718	21	0	0
1	C	466	3729	2342	648	718	21	0	0
1	A	466	3729	2342	648	718	21	0	0

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	98	PHE	TYR	conflict	UNP A0A076G8X7
B	?	-	THR	deletion	UNP A0A076G8X7
B	475	ARG	-	expression tag	UNP A0A076G8X7
B	476	SER	-	expression tag	UNP A0A076G8X7
B	477	GLY	-	expression tag	UNP A0A076G8X7
B	478	ALA	-	expression tag	UNP A0A076G8X7
B	479	GLY	-	expression tag	UNP A0A076G8X7
B	480	SER	-	expression tag	UNP A0A076G8X7
B	481	SER	-	expression tag	UNP A0A076G8X7
B	482	GLY	-	expression tag	UNP A0A076G8X7
B	483	SER	-	expression tag	UNP A0A076G8X7
B	484	GLY	-	expression tag	UNP A0A076G8X7
B	485	ARG	-	expression tag	UNP A0A076G8X7
B	486	MET	-	expression tag	UNP A0A076G8X7
B	487	LYS	-	expression tag	UNP A0A076G8X7
B	488	GLN	-	expression tag	UNP A0A076G8X7
B	489	ILE	-	expression tag	UNP A0A076G8X7
B	490	GLU	-	expression tag	UNP A0A076G8X7
B	491	ASP	-	expression tag	UNP A0A076G8X7
B	492	LYS	-	expression tag	UNP A0A076G8X7
B	493	ILE	-	expression tag	UNP A0A076G8X7
B	494	GLU	-	expression tag	UNP A0A076G8X7
B	495	GLU	-	expression tag	UNP A0A076G8X7
B	496	ILE	-	expression tag	UNP A0A076G8X7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	497	LEU	-	expression tag	UNP A0A076G8X7
B	498	SER	-	expression tag	UNP A0A076G8X7
B	499	LYS	-	expression tag	UNP A0A076G8X7
B	500	ILE	-	expression tag	UNP A0A076G8X7
B	501	TYR	-	expression tag	UNP A0A076G8X7
B	502	HIS	-	expression tag	UNP A0A076G8X7
B	503	ILE	-	expression tag	UNP A0A076G8X7
B	504	GLU	-	expression tag	UNP A0A076G8X7
B	505	ASN	-	expression tag	UNP A0A076G8X7
B	506	GLU	-	expression tag	UNP A0A076G8X7
B	507	ILE	-	expression tag	UNP A0A076G8X7
B	508	ALA	-	expression tag	UNP A0A076G8X7
B	509	ARG	-	expression tag	UNP A0A076G8X7
B	510	ILE	-	expression tag	UNP A0A076G8X7
B	511	LYS	-	expression tag	UNP A0A076G8X7
B	512	LYS	-	expression tag	UNP A0A076G8X7
B	513	LEU	-	expression tag	UNP A0A076G8X7
B	514	ILE	-	expression tag	UNP A0A076G8X7
B	515	GLY	-	expression tag	UNP A0A076G8X7
B	516	GLU	-	expression tag	UNP A0A076G8X7
B	517	ARG	-	expression tag	UNP A0A076G8X7
B	518	SER	-	expression tag	UNP A0A076G8X7
B	519	GLY	-	expression tag	UNP A0A076G8X7
B	520	GLY	-	expression tag	UNP A0A076G8X7
C	98	PHE	TYR	conflict	UNP A0A076G8X7
C	?	-	THR	deletion	UNP A0A076G8X7
C	475	ARG	-	expression tag	UNP A0A076G8X7
C	476	SER	-	expression tag	UNP A0A076G8X7
C	477	GLY	-	expression tag	UNP A0A076G8X7
C	478	ALA	-	expression tag	UNP A0A076G8X7
C	479	GLY	-	expression tag	UNP A0A076G8X7
C	480	SER	-	expression tag	UNP A0A076G8X7
C	481	SER	-	expression tag	UNP A0A076G8X7
C	482	GLY	-	expression tag	UNP A0A076G8X7
C	483	SER	-	expression tag	UNP A0A076G8X7
C	484	GLY	-	expression tag	UNP A0A076G8X7
C	485	ARG	-	expression tag	UNP A0A076G8X7
C	486	MET	-	expression tag	UNP A0A076G8X7
C	487	LYS	-	expression tag	UNP A0A076G8X7
C	488	GLN	-	expression tag	UNP A0A076G8X7
C	489	ILE	-	expression tag	UNP A0A076G8X7
C	490	GLU	-	expression tag	UNP A0A076G8X7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	491	ASP	-	expression tag	UNP A0A076G8X7
C	492	LYS	-	expression tag	UNP A0A076G8X7
C	493	ILE	-	expression tag	UNP A0A076G8X7
C	494	GLU	-	expression tag	UNP A0A076G8X7
C	495	GLU	-	expression tag	UNP A0A076G8X7
C	496	ILE	-	expression tag	UNP A0A076G8X7
C	497	LEU	-	expression tag	UNP A0A076G8X7
C	498	SER	-	expression tag	UNP A0A076G8X7
C	499	LYS	-	expression tag	UNP A0A076G8X7
C	500	ILE	-	expression tag	UNP A0A076G8X7
C	501	TYR	-	expression tag	UNP A0A076G8X7
C	502	HIS	-	expression tag	UNP A0A076G8X7
C	503	ILE	-	expression tag	UNP A0A076G8X7
C	504	GLU	-	expression tag	UNP A0A076G8X7
C	505	ASN	-	expression tag	UNP A0A076G8X7
C	506	GLU	-	expression tag	UNP A0A076G8X7
C	507	ILE	-	expression tag	UNP A0A076G8X7
C	508	ALA	-	expression tag	UNP A0A076G8X7
C	509	ARG	-	expression tag	UNP A0A076G8X7
C	510	ILE	-	expression tag	UNP A0A076G8X7
C	511	LYS	-	expression tag	UNP A0A076G8X7
C	512	LYS	-	expression tag	UNP A0A076G8X7
C	513	LEU	-	expression tag	UNP A0A076G8X7
C	514	ILE	-	expression tag	UNP A0A076G8X7
C	515	GLY	-	expression tag	UNP A0A076G8X7
C	516	GLU	-	expression tag	UNP A0A076G8X7
C	517	ARG	-	expression tag	UNP A0A076G8X7
C	518	SER	-	expression tag	UNP A0A076G8X7
C	519	GLY	-	expression tag	UNP A0A076G8X7
C	520	GLY	-	expression tag	UNP A0A076G8X7
A	98	PHE	TYR	conflict	UNP A0A076G8X7
A	?	-	THR	deletion	UNP A0A076G8X7
A	475	ARG	-	expression tag	UNP A0A076G8X7
A	476	SER	-	expression tag	UNP A0A076G8X7
A	477	GLY	-	expression tag	UNP A0A076G8X7
A	478	ALA	-	expression tag	UNP A0A076G8X7
A	479	GLY	-	expression tag	UNP A0A076G8X7
A	480	SER	-	expression tag	UNP A0A076G8X7
A	481	SER	-	expression tag	UNP A0A076G8X7
A	482	GLY	-	expression tag	UNP A0A076G8X7
A	483	SER	-	expression tag	UNP A0A076G8X7
A	484	GLY	-	expression tag	UNP A0A076G8X7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	485	ARG	-	expression tag	UNP A0A076G8X7
A	486	MET	-	expression tag	UNP A0A076G8X7
A	487	LYS	-	expression tag	UNP A0A076G8X7
A	488	GLN	-	expression tag	UNP A0A076G8X7
A	489	ILE	-	expression tag	UNP A0A076G8X7
A	490	GLU	-	expression tag	UNP A0A076G8X7
A	491	ASP	-	expression tag	UNP A0A076G8X7
A	492	LYS	-	expression tag	UNP A0A076G8X7
A	493	ILE	-	expression tag	UNP A0A076G8X7
A	494	GLU	-	expression tag	UNP A0A076G8X7
A	495	GLU	-	expression tag	UNP A0A076G8X7
A	496	ILE	-	expression tag	UNP A0A076G8X7
A	497	LEU	-	expression tag	UNP A0A076G8X7
A	498	SER	-	expression tag	UNP A0A076G8X7
A	499	LYS	-	expression tag	UNP A0A076G8X7
A	500	ILE	-	expression tag	UNP A0A076G8X7
A	501	TYR	-	expression tag	UNP A0A076G8X7
A	502	HIS	-	expression tag	UNP A0A076G8X7
A	503	ILE	-	expression tag	UNP A0A076G8X7
A	504	GLU	-	expression tag	UNP A0A076G8X7
A	505	ASN	-	expression tag	UNP A0A076G8X7
A	506	GLU	-	expression tag	UNP A0A076G8X7
A	507	ILE	-	expression tag	UNP A0A076G8X7
A	508	ALA	-	expression tag	UNP A0A076G8X7
A	509	ARG	-	expression tag	UNP A0A076G8X7
A	510	ILE	-	expression tag	UNP A0A076G8X7
A	511	LYS	-	expression tag	UNP A0A076G8X7
A	512	LYS	-	expression tag	UNP A0A076G8X7
A	513	LEU	-	expression tag	UNP A0A076G8X7
A	514	ILE	-	expression tag	UNP A0A076G8X7
A	515	GLY	-	expression tag	UNP A0A076G8X7
A	516	GLU	-	expression tag	UNP A0A076G8X7
A	517	ARG	-	expression tag	UNP A0A076G8X7
A	518	SER	-	expression tag	UNP A0A076G8X7
A	519	GLY	-	expression tag	UNP A0A076G8X7
A	520	GLY	-	expression tag	UNP A0A076G8X7

- Molecule 2 is a protein called Fab Heavy chain.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			S
2	H	120	909	573	153	178	5	0	0

Continued on next page...

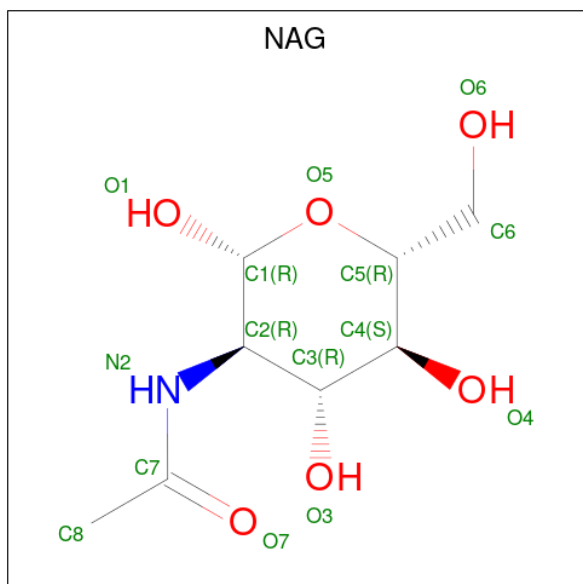
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	120	Total	C	N	O	S	0	0
			909	573	153	178	5		
2	E	120	Total	C	N	O	S	0	0
			909	573	153	178	5		

- Molecule 3 is a protein called Fab Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	114	Total	C	N	O	S	0	0
			877	554	143	177	3		
3	F	114	Total	C	N	O	S	0	0
			877	554	143	177	3		
3	G	114	Total	C	N	O	S	0	0
			877	554	143	177	3		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	

Continued on next page...

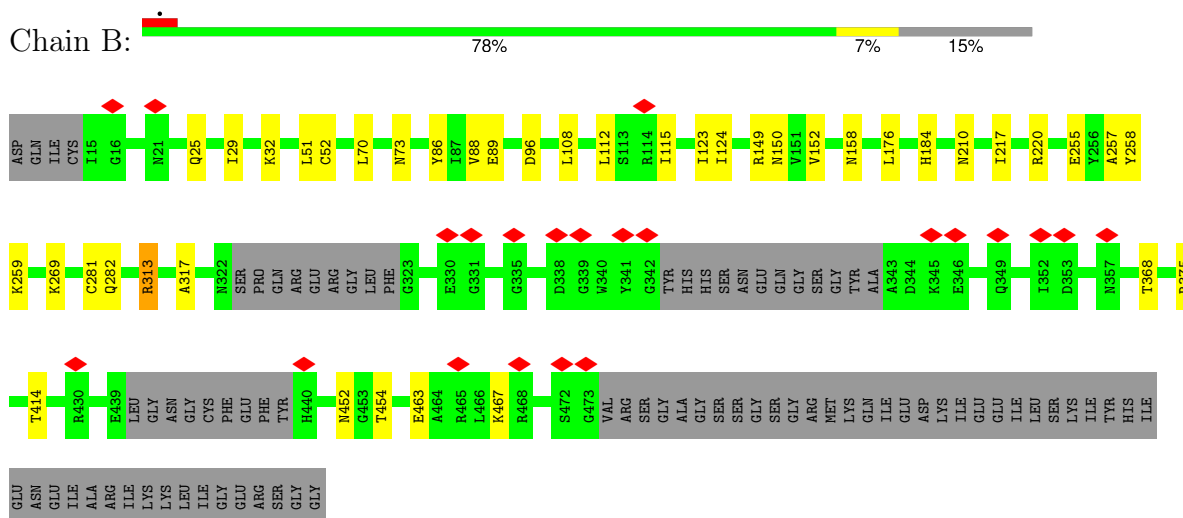
Continued from previous page...

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

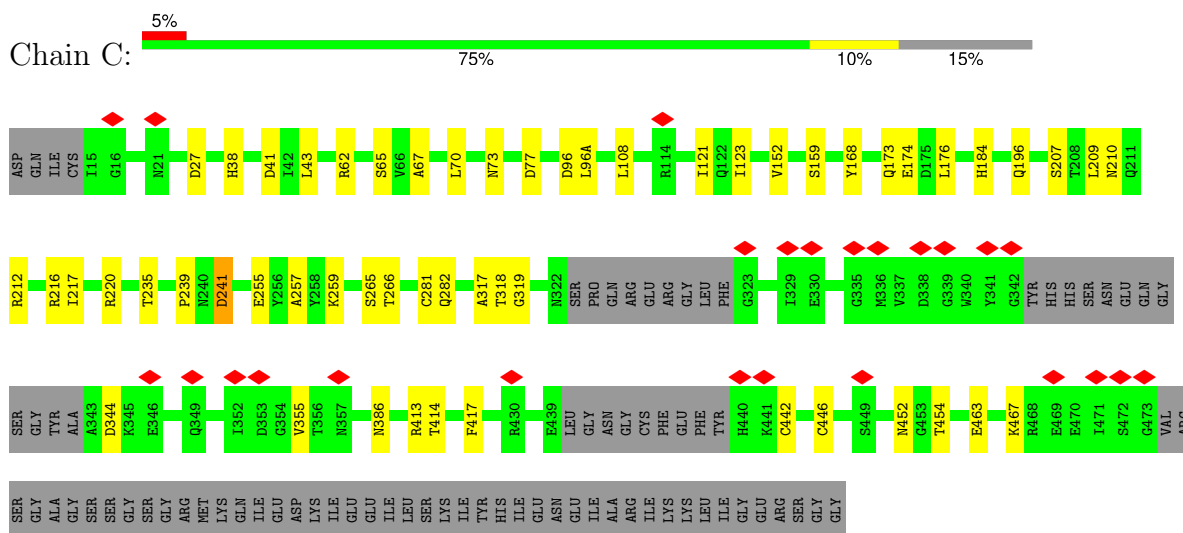
3 Residue-property plots [i](#)

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

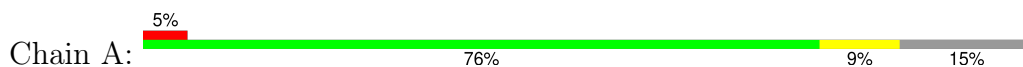
- Molecule 1: Hemagglutinin

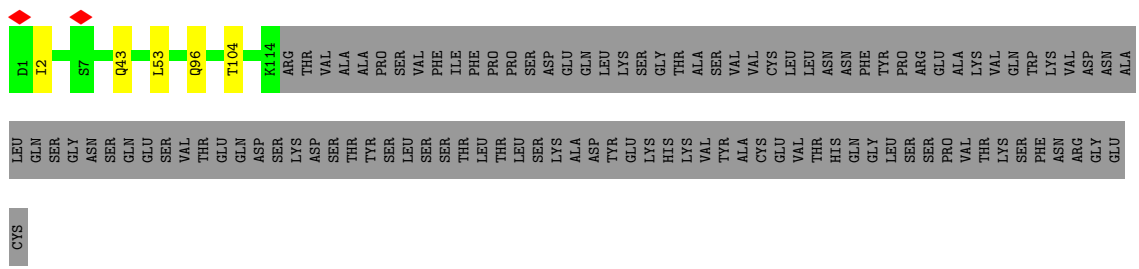


- Molecule 1: Hemagglutinin

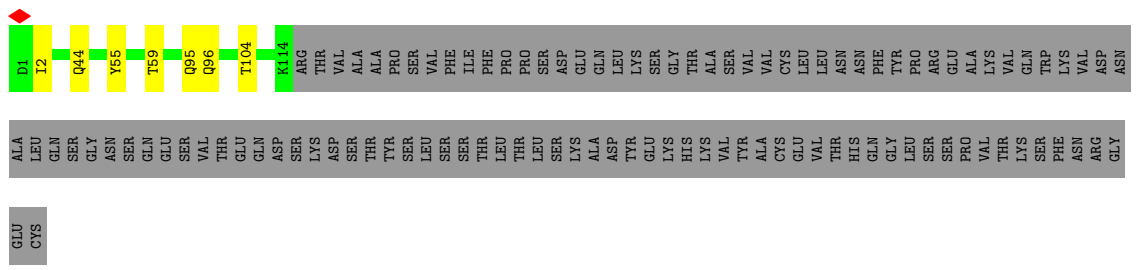


- Molecule 1: Hemagglutinin

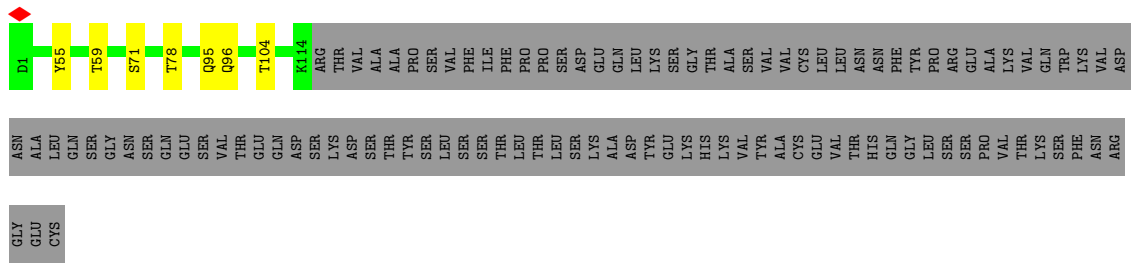




• Molecule 3: Fab Light chain



• Molecule 3: Fab Light chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	77276	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58.49	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.862	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.1	Depositor
Map size (\AA)	338.4, 338.4, 338.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.84599996, 0.84599996, 0.84599996	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.34	0/3808	0.66	1/5150 (0.0%)
1	B	0.33	0/3808	0.65	0/5150
1	C	0.35	0/3808	0.67	2/5150 (0.0%)
2	D	0.33	0/929	0.67	0/1258
2	E	0.33	0/929	0.65	0/1258
2	H	0.33	0/929	0.64	0/1258
3	F	0.34	0/897	0.61	0/1220
3	G	0.33	0/897	0.62	0/1220
3	L	0.34	0/897	0.64	0/1220
All	All	0.34	0/16902	0.65	3/22884 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	27	ASP	CB-CG-OD1	7.63	125.17	118.30
1	A	41	ASP	CB-CG-OD1	7.46	125.01	118.30
1	C	241	ASP	CB-CG-OD1	6.87	124.49	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3729	0	3615	32	0
1	B	3729	0	3615	26	0
1	C	3729	0	3615	34	0
2	D	909	0	882	5	0
2	E	909	0	882	2	0
2	H	909	0	882	8	0
3	F	877	0	851	6	0
3	G	877	0	851	4	0
3	L	877	0	851	3	0
4	A	42	0	39	1	0
4	B	42	0	39	1	0
4	C	42	0	39	0	0
All	All	16671	0	16161	110	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (110) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ASN:ND2	1:B:258:TYR:OH	1.98	0.96
1:B:217:ILE:O	1:C:212:ARG:NH1	2.27	0.68
1:A:44:GLU:OE2	1:A:290:SER:OG	2.08	0.66
1:B:73:ASN:ND2	1:B:96:ASP:O	2.29	0.66
1:A:176:LEU:HD11	1:A:257:ALA:HB1	1.77	0.65
3:G:55:TYR:O	3:G:59:THR:OG1	2.10	0.64
1:B:210:ASN:O	1:A:216:ARG:NH1	2.32	0.63
1:C:173:GLN:HA	1:C:239:PRO:HB3	1.82	0.62
1:B:184:HIS:O	1:B:220:ARG:NH2	2.32	0.62
1:C:184:HIS:O	1:C:220:ARG:NH2	2.33	0.61
1:C:217:ILE:O	1:A:212:ARG:NH2	2.33	0.61
1:C:38:HIS:O	1:C:319:GLY:N	2.33	0.61
3:F:96:GLN:NE2	3:F:104:THR:OG1	2.35	0.59
1:A:41:ASP:OD2	1:A:45:LYS:NZ	2.36	0.59
1:A:184:HIS:O	1:A:220:ARG:NH2	2.37	0.57
1:A:316:LEU:HD21	1:A:362:ILE:HD11	1.86	0.57
1:B:52:CYS:O	1:B:86:TYR:OH	2.23	0.55
3:G:96:GLN:NE2	3:G:104:THR:OG1	2.39	0.55
1:C:73:ASN:ND2	1:C:96:ASP:O	2.39	0.55
1:B:375:ARG:NH1	1:A:386:ASN:OD1	2.41	0.53
1:B:70:LEU:HD13	1:B:108:LEU:HD21	1.91	0.53
1:C:65:SER:OG	1:C:96:ASP:HA	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:LEU:HD11	1:B:88:VAL:HG21	1.91	0.53
3:L:96:GLN:NE2	3:L:104:THR:OG1	2.42	0.52
1:C:123:ILE:HG23	1:C:168:TYR:CG	2.43	0.52
2:D:52:SER:O	2:D:72:ARG:NH1	2.43	0.51
2:D:67:ARG:NH2	2:D:90:ASP:OD2	2.42	0.51
1:C:216:ARG:NH1	1:A:210:ASN:O	2.42	0.51
1:A:281:CYS:SG	1:A:282:GLN:N	2.83	0.51
1:B:368:THR:HG22	1:A:397:ASP:HB3	1.93	0.51
1:B:123:ILE:HG22	1:B:124:ILE:HG13	1.93	0.51
1:A:176:LEU:HD11	1:A:257:ALA:CB	2.41	0.51
1:A:413:ARG:O	1:A:417:PHE:N	2.43	0.50
1:A:158:ASN:HB3	4:A:603:NAG:O5	2.12	0.50
1:C:209:LEU:HD22	1:C:235:THR:HG21	1.94	0.49
2:H:29:PHE:O	2:H:72:ARG:NH2	2.45	0.49
1:B:29:ILE:HG21	1:C:413:ARG:NH2	2.27	0.49
1:B:112:LEU:HD12	1:B:115:ILE:HD11	1.93	0.49
1:B:32:LYS:HB2	4:B:602:NAG:H82	1.95	0.48
1:B:176:LEU:HD12	1:B:259:LYS:HA	1.95	0.48
1:A:452:ASN:ND2	1:A:454:THR:OG1	2.47	0.48
1:A:52:CYS:O	1:A:282:GLN:NE2	2.46	0.48
1:A:121:ILE:O	1:A:257:ALA:N	2.45	0.48
1:C:41:ASP:OD1	1:C:43:LEU:N	2.46	0.48
1:C:281:CYS:SG	1:C:282:GLN:N	2.87	0.47
1:B:123:ILE:CG1	1:B:257:ALA:HB2	2.45	0.47
3:L:2:ILE:O	3:L:96:GLN:NE2	2.45	0.47
2:H:63:SER:O	2:H:67:ARG:NH1	2.48	0.47
1:A:27:ASP:N	1:A:27:ASP:OD1	2.48	0.47
1:A:156:LYS:HD2	1:A:159:SER:HA	1.98	0.46
1:B:452:ASN:ND2	1:B:454:THR:OG1	2.48	0.46
1:C:70:LEU:HD13	1:C:108:LEU:HD21	1.98	0.46
1:B:152:VAL:HG23	1:B:255:GLU:HB2	1.97	0.46
1:B:317:ALA:O	1:B:414:THR:HG21	2.15	0.46
3:F:55:TYR:O	3:F:59:THR:OG1	2.24	0.46
1:A:97:CYS:SG	1:A:98:PHE:N	2.88	0.45
1:B:89:GLU:OE1	1:B:269:LYS:NZ	2.43	0.45
1:A:317:ALA:O	1:A:414:THR:HG21	2.16	0.45
1:A:38:HIS:O	1:A:318:THR:OG1	2.18	0.45
2:H:47:TRP:NE1	2:H:49:SER:O	2.49	0.45
3:G:95:GLN:NE2	3:G:96:GLN:O	2.49	0.45
1:A:158:ASN:O	1:A:159:SER:C	2.55	0.45
1:B:25:GLN:O	1:B:313:ARG:NH2	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:63:SER:O	2:E:67:ARG:NH1	2.50	0.45
2:H:35:ASN:N	2:H:97:ALA:O	2.48	0.44
2:H:52:SER:O	2:H:72:ARG:NH1	2.49	0.44
3:F:95:GLN:NE2	3:F:96:GLN:O	2.50	0.44
1:B:220:ARG:NH1	1:C:210:ASN:OD1	2.50	0.44
1:C:123:ILE:HD11	1:C:257:ALA:HB2	1.99	0.44
1:C:265:SER:OG	1:C:266:THR:N	2.51	0.44
1:C:386:ASN:OD1	1:A:375:ARG:NH1	2.48	0.44
2:D:39:GLN:OE1	3:F:44:GLN:NE2	2.50	0.44
1:C:452:ASN:ND2	1:C:454:THR:OG1	2.51	0.43
2:D:91:THR:HG22	2:D:118:VAL:H	1.83	0.43
1:C:152:VAL:HG23	1:C:255:GLU:HB2	2.00	0.43
1:A:316:LEU:HD21	1:A:362:ILE:CD1	2.48	0.43
1:C:174:GLU:HB2	1:C:259:LYS:HD3	2.01	0.43
1:B:463:GLU:O	1:B:467:LYS:N	2.48	0.43
2:D:63:SER:O	2:D:67:ARG:NH1	2.52	0.43
1:C:463:GLU:O	1:C:467:LYS:N	2.47	0.43
2:H:86:LEU:HB3	2:H:118:VAL:HG21	2.00	0.42
1:C:67:ALA:HB1	1:C:96(A):LEU:HD21	2.01	0.42
1:C:121:ILE:O	1:C:257:ALA:N	2.49	0.42
3:G:71:SER:OG	3:G:78:THR:OG1	2.35	0.42
1:C:413:ARG:O	1:C:417:PHE:N	2.48	0.42
1:B:32:LYS:HA	1:B:32:LYS:HD3	1.88	0.42
2:H:67:ARG:NH2	2:H:90:ASP:OD2	2.49	0.42
1:C:317:ALA:O	1:C:414:THR:HG21	2.19	0.42
1:A:344:ASP:N	1:A:344:ASP:OD1	2.52	0.42
2:H:6:GLU:HB2	2:H:114:THR:HG23	2.02	0.42
1:A:209:LEU:HD22	1:A:235:THR:HG21	2.01	0.42
1:A:152:VAL:HG23	1:A:255:GLU:HB2	2.02	0.41
1:C:159:SER:HB3	1:C:196:GLN:NE2	2.35	0.41
1:C:454:THR:OG1	1:C:454:THR:O	2.36	0.41
1:B:281:CYS:SG	1:B:282:GLN:N	2.93	0.41
1:C:62:ARG:NH2	1:C:77:ASP:OD1	2.53	0.41
1:C:318:THR:HG23	1:C:355:VAL:HG22	2.03	0.41
3:L:43:GLN:HB2	3:L:53:LEU:HD11	2.01	0.41
1:C:207:SER:OG	1:C:241:ASP:OD2	2.32	0.41
1:C:344:ASP:N	1:C:344:ASP:OD1	2.54	0.41
3:F:2:ILE:HG23	3:F:96:GLN:NE2	2.36	0.41
2:E:67:ARG:NH2	2:E:90:ASP:OD2	2.50	0.41
1:C:442:CYS:SG	1:C:446:CYS:N	2.94	0.41
1:A:265:SER:OG	1:A:266:THR:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LEU:HD13	1:A:108:LEU:HD21	2.03	0.41
1:A:154:LEU:HB2	1:A:161:TYR:OH	2.21	0.41
1:C:176:LEU:HG	1:C:257:ALA:HB1	2.03	0.40
3:F:2:ILE:O	3:F:96:GLN:NE2	2.52	0.40
1:B:108:LEU:O	1:B:112:LEU:N	2.51	0.40
1:A:159:SER:HB3	1:A:196:GLN:OE1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	460/547 (84%)	433 (94%)	27 (6%)	0	100	100
1	B	460/547 (84%)	438 (95%)	22 (5%)	0	100	100
1	C	460/547 (84%)	435 (95%)	25 (5%)	0	100	100
2	D	118/228 (52%)	113 (96%)	5 (4%)	0	100	100
2	E	118/228 (52%)	115 (98%)	3 (2%)	0	100	100
2	H	118/228 (52%)	114 (97%)	4 (3%)	0	100	100
3	F	112/221 (51%)	107 (96%)	5 (4%)	0	100	100
3	G	112/221 (51%)	107 (96%)	5 (4%)	0	100	100
3	L	112/221 (51%)	108 (96%)	4 (4%)	0	100	100
All	All	2070/2988 (69%)	1970 (95%)	100 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	414/480 (86%)	412 (100%)	2 (0%)	86	92
1	B	414/480 (86%)	411 (99%)	3 (1%)	81	90
1	C	414/480 (86%)	414 (100%)	0	100	100
2	D	97/190 (51%)	97 (100%)	0	100	100
2	E	97/190 (51%)	97 (100%)	0	100	100
2	H	97/190 (51%)	97 (100%)	0	100	100
3	F	98/194 (50%)	98 (100%)	0	100	100
3	G	98/194 (50%)	98 (100%)	0	100	100
3	L	98/194 (50%)	98 (100%)	0	100	100
All	All	1827/2592 (70%)	1822 (100%)	5 (0%)	90	95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	149	ARG
1	B	158	ASN
1	B	313	ARG
1	A	149	ARG
1	A	382	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	95	ASN
1	B	150	ASN
1	B	211	GLN
3	G	37	ASN
1	C	81	ASN
1	C	196	GLN
1	A	282	GLN
1	A	379	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	603	1	14,14,15	0.39	0	17,19,21	0.89	1 (5%)
4	NAG	C	603	1	14,14,15	0.38	0	17,19,21	1.20	2 (11%)
4	NAG	B	601	1	14,14,15	0.38	0	17,19,21	1.41	2 (11%)
4	NAG	C	602	1	14,14,15	0.37	0	17,19,21	1.09	2 (11%)
4	NAG	B	602	1	14,14,15	0.38	0	17,19,21	0.59	0
4	NAG	A	601	1	14,14,15	0.38	0	17,19,21	0.67	1 (5%)
4	NAG	B	603	1	14,14,15	0.39	0	17,19,21	0.83	1 (5%)
4	NAG	C	601	1	14,14,15	0.37	0	17,19,21	0.98	1 (5%)
4	NAG	A	602	1	14,14,15	0.39	0	17,19,21	0.52	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	603	1	-	1/6/23/26	0/1/1/1
4	NAG	C	603	1	-	4/6/23/26	0/1/1/1
4	NAG	B	601	1	-	3/6/23/26	0/1/1/1
4	NAG	C	602	1	-	4/6/23/26	0/1/1/1
4	NAG	B	602	1	-	1/6/23/26	0/1/1/1
4	NAG	A	601	1	-	2/6/23/26	0/1/1/1
4	NAG	B	603	1	-	5/6/23/26	0/1/1/1
4	NAG	C	601	1	-	1/6/23/26	0/1/1/1
4	NAG	A	602	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	NAG	C2-N2-C7	4.85	129.40	122.90
4	C	602	NAG	C2-N2-C7	3.43	127.50	122.90
4	C	601	NAG	C2-N2-C7	3.39	127.44	122.90
4	C	603	NAG	C1-C2-N2	3.30	115.63	110.43
4	C	603	NAG	C2-N2-C7	3.19	127.17	122.90
4	B	601	NAG	C1-C2-N2	-2.63	106.29	110.43
4	A	603	NAG	O5-C1-C2	2.56	115.26	111.29
4	B	603	NAG	C1-O5-C5	2.51	115.56	112.19
4	C	602	NAG	C1-C2-N2	-2.30	106.80	110.43
4	A	601	NAG	C1-O5-C5	2.09	114.98	112.19

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	601	NAG	C3-C2-N2-C7
4	B	601	NAG	O7-C7-N2-C2
4	B	603	NAG	C1-C2-N2-C7
4	B	603	NAG	C8-C7-N2-C2
4	B	603	NAG	O7-C7-N2-C2
4	C	602	NAG	C3-C2-N2-C7
4	C	602	NAG	C8-C7-N2-C2
4	C	602	NAG	O7-C7-N2-C2
4	C	603	NAG	C1-C2-N2-C7
4	C	603	NAG	C8-C7-N2-C2
4	C	603	NAG	O7-C7-N2-C2
4	B	601	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	601	NAG	C8-C7-N2-C2
4	B	603	NAG	O5-C5-C6-O6
4	C	603	NAG	O5-C5-C6-O6
4	A	603	NAG	O5-C5-C6-O6
4	C	602	NAG	O5-C5-C6-O6
4	A	602	NAG	O5-C5-C6-O6
4	B	602	NAG	O5-C5-C6-O6
4	B	603	NAG	C3-C2-N2-C7
4	A	601	NAG	O7-C7-N2-C2
4	C	601	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	NAG	1	0
4	B	602	NAG	1	0

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.

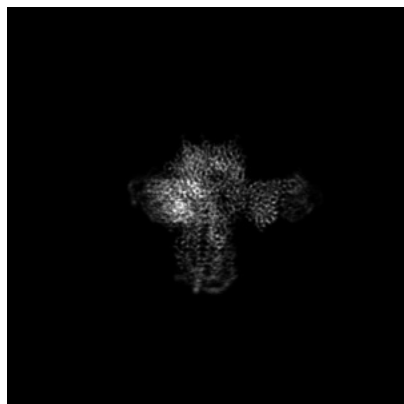
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42377. These allow visual inspection of the internal detail of the map and identification of artifacts.

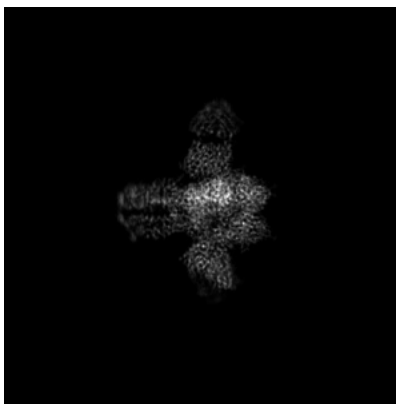
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

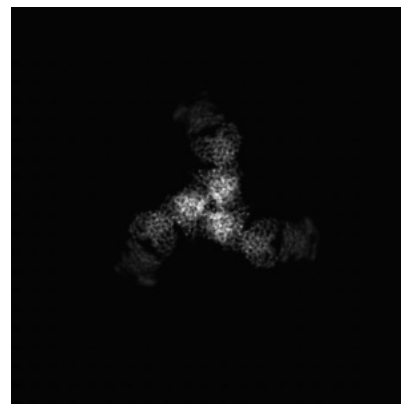
6.1.1 Primary map



X

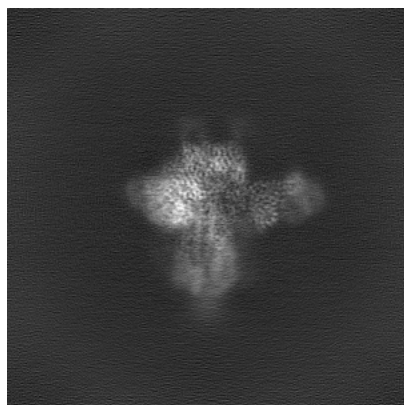


Y

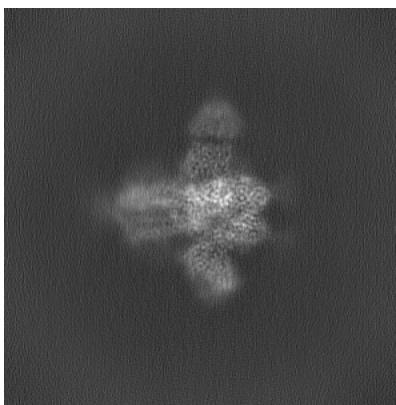


Z

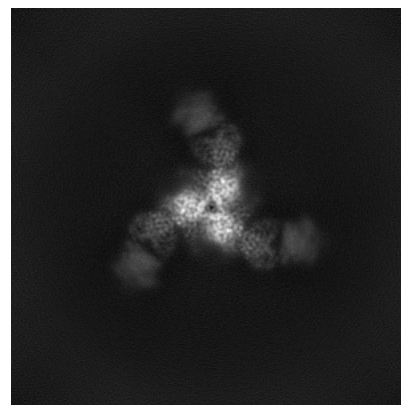
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

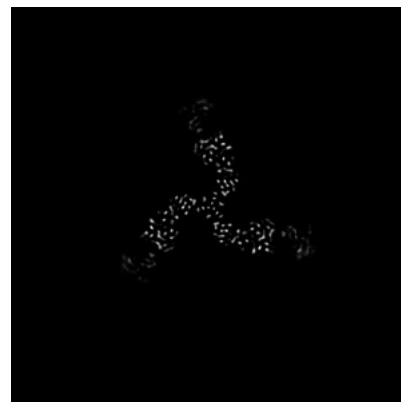
6.2.1 Primary map



X Index: 200

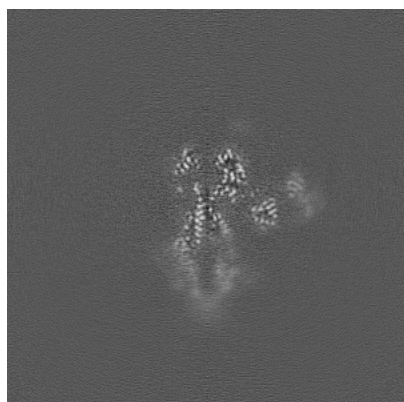


Y Index: 200

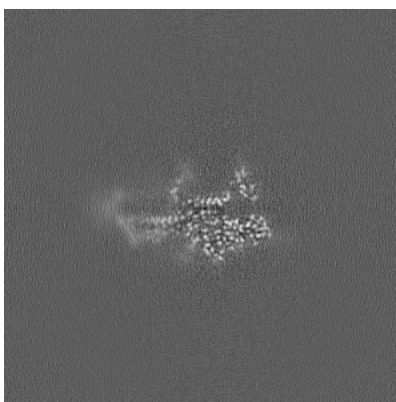


Z Index: 200

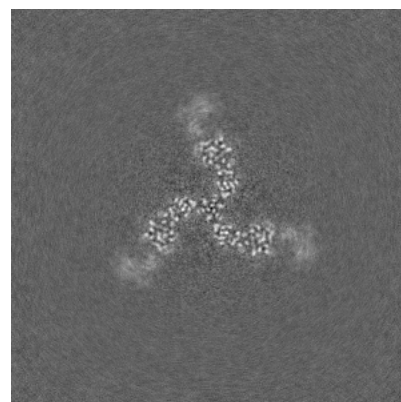
6.2.2 Raw map



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](#)

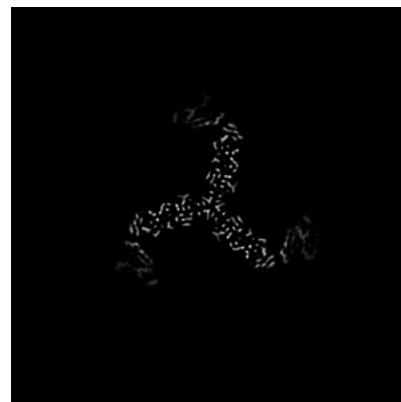
6.3.1 Primary map



X Index: 209

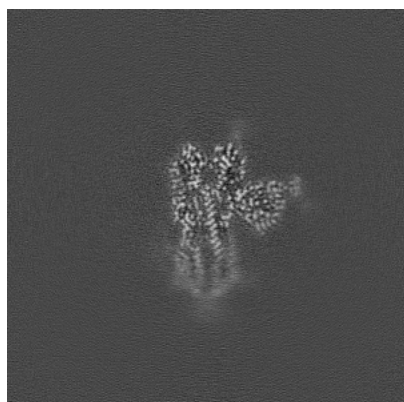


Y Index: 181

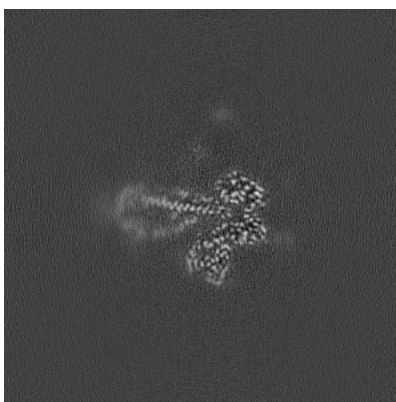


Z Index: 215

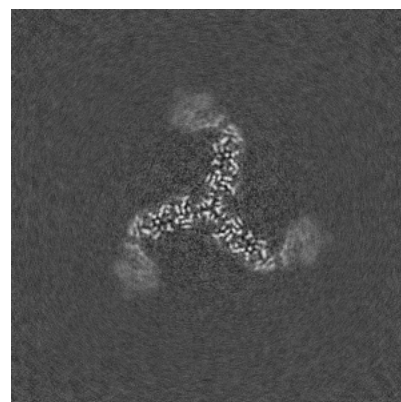
6.3.2 Raw map



X Index: 208



Y Index: 190

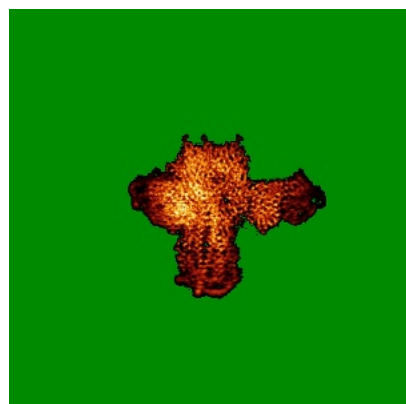


Z Index: 215

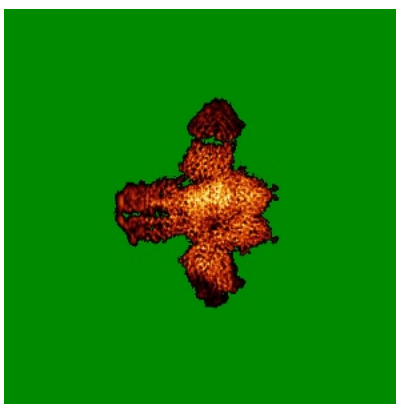
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

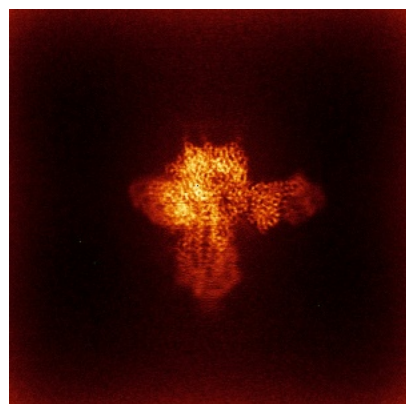


Y

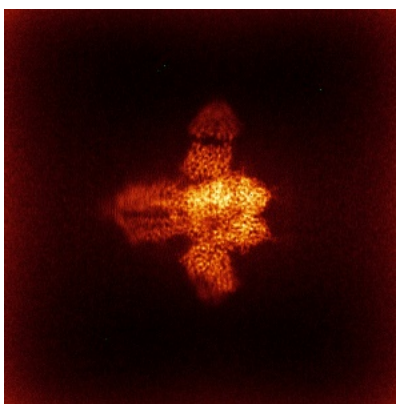


Z

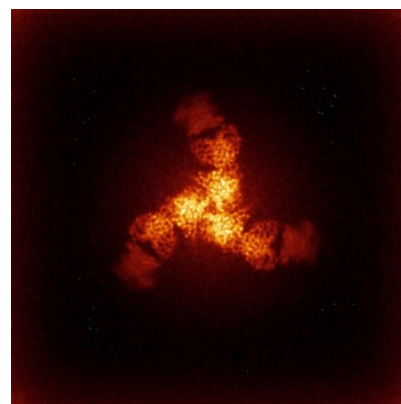
6.4.2 Raw map



X



Y

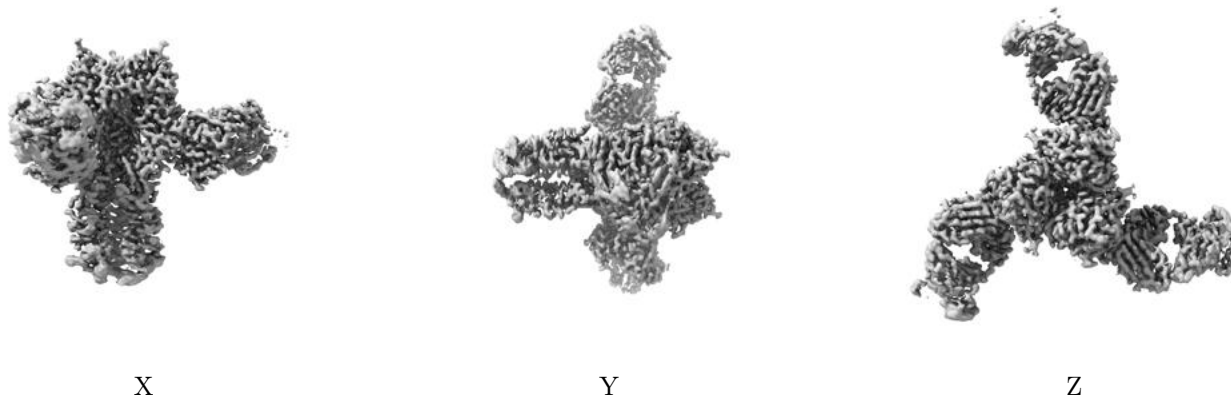


Z

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

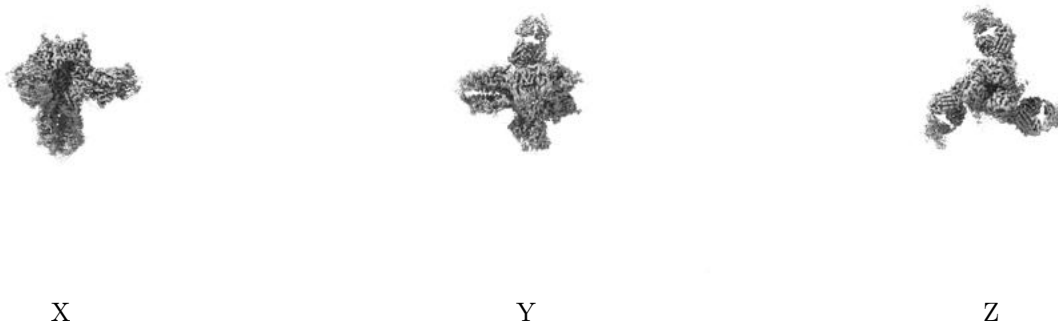
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

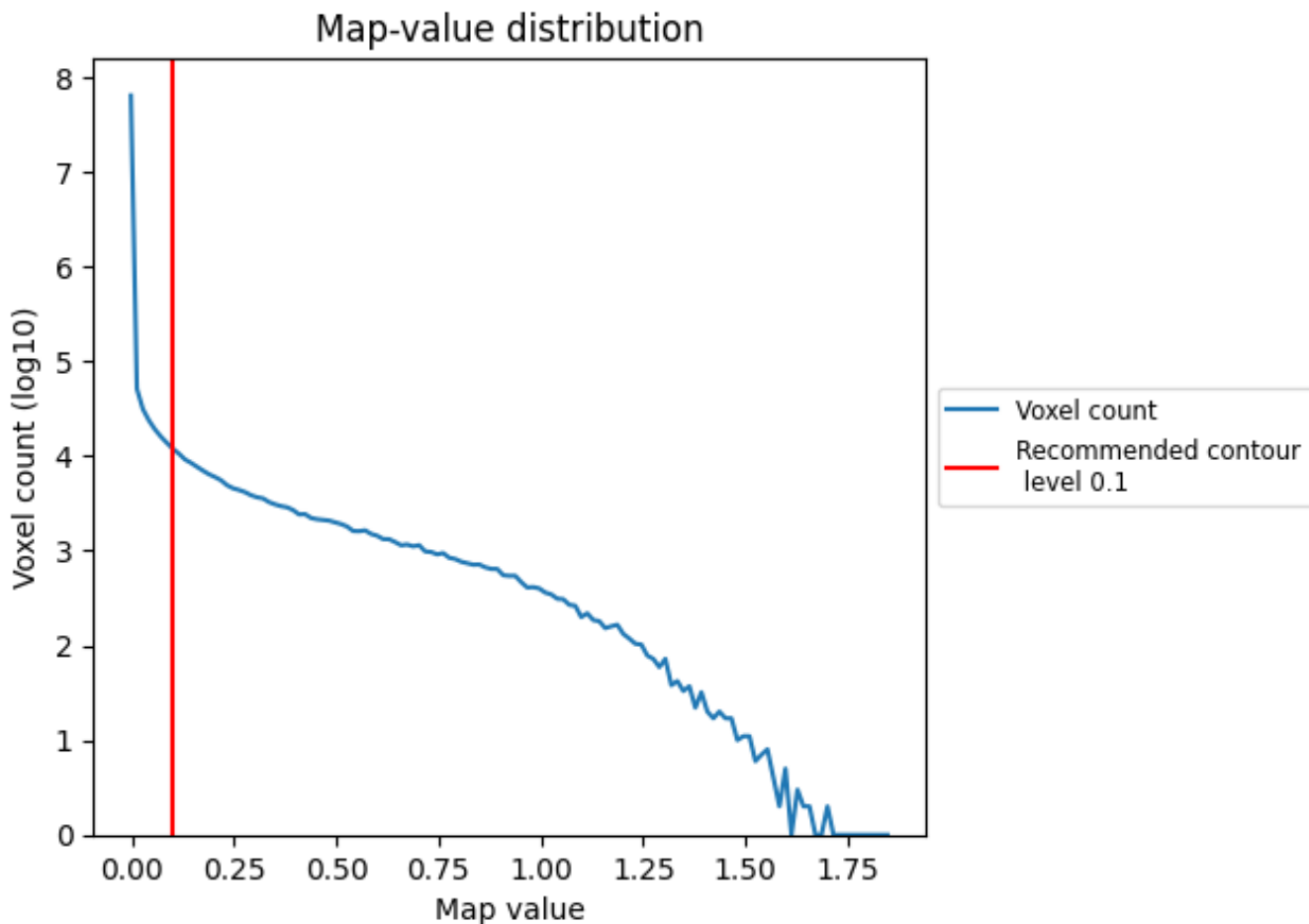
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

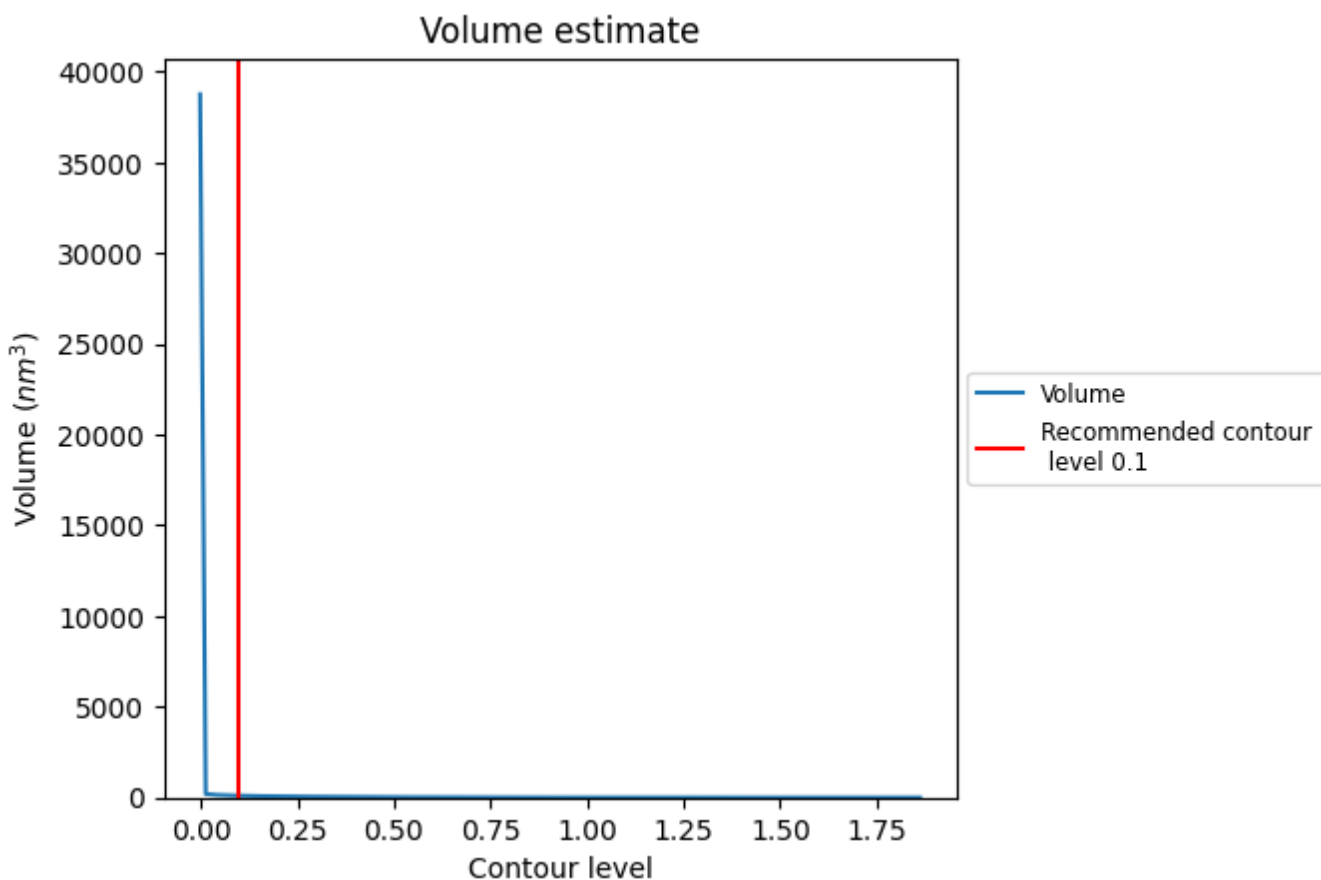
This section contains the results of statistical analysis of the map.

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.

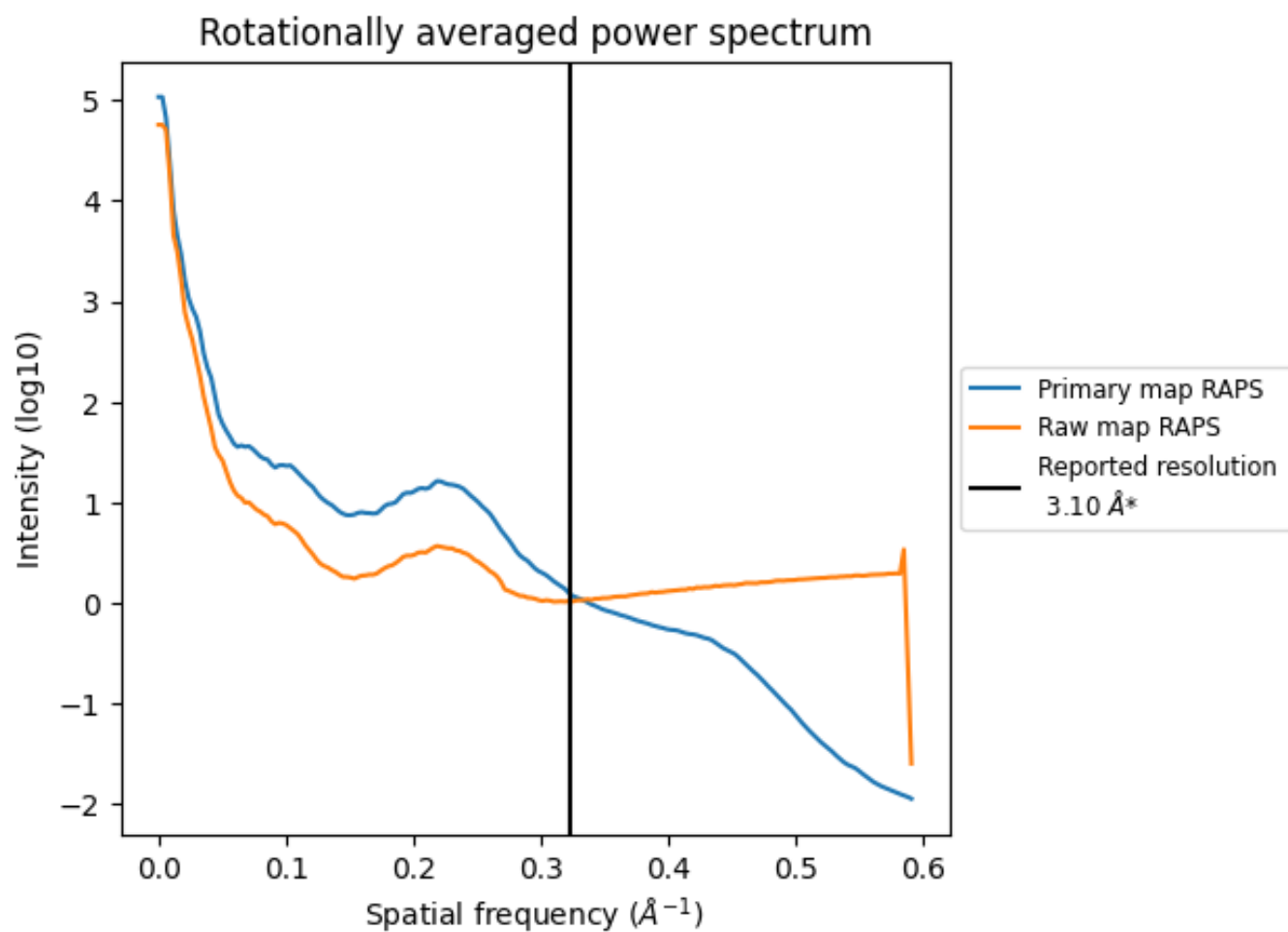
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 103 nm³; this corresponds to an approximate mass of 93 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

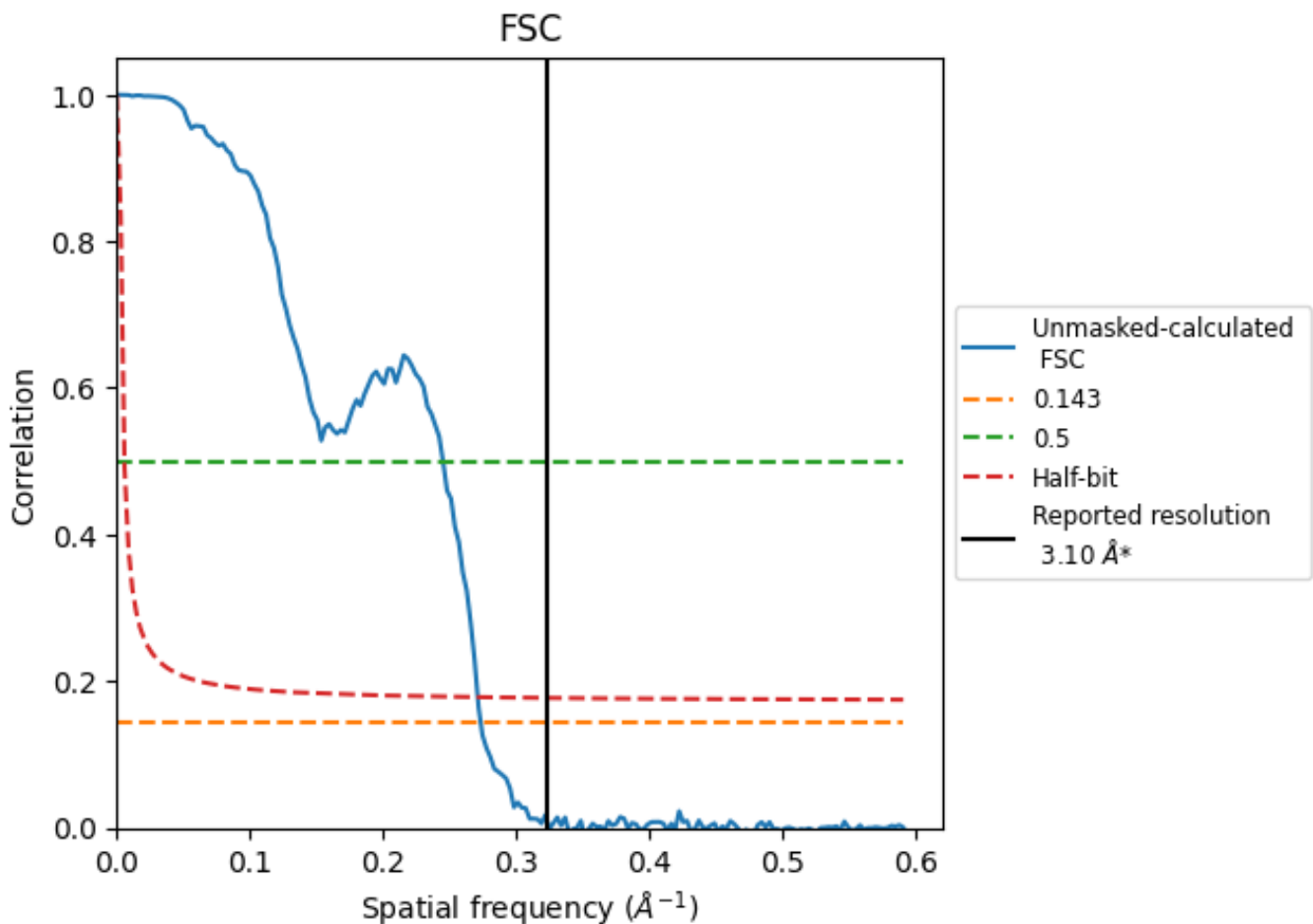


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

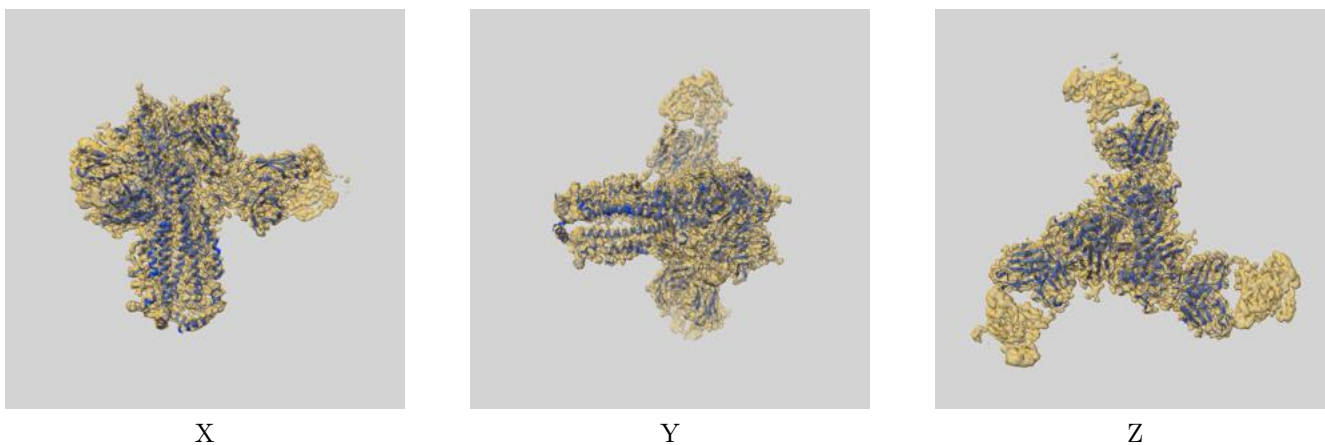
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.66	4.08	3.69

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

9 Map-model fit [i](#)

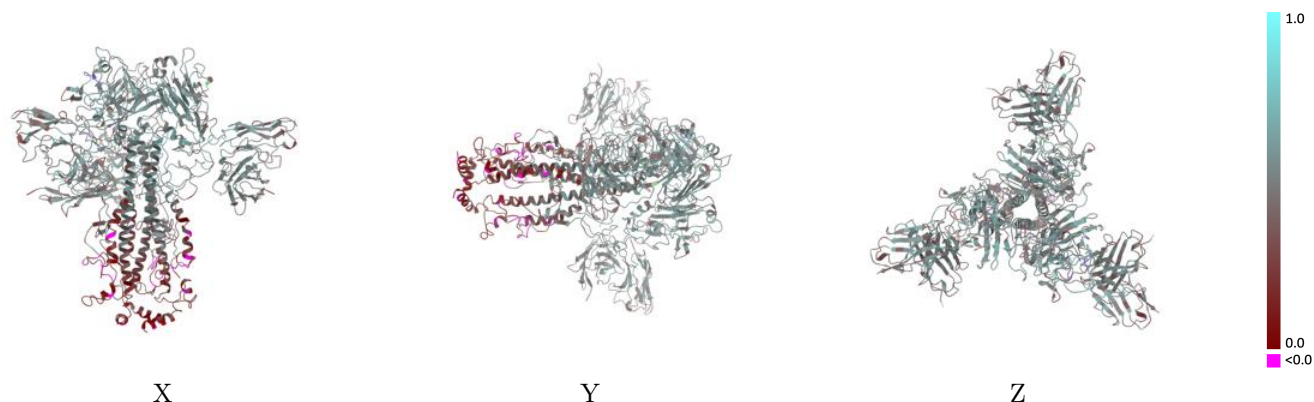
This section contains information regarding the fit between EMDB map EMD-42377 and PDB model 8UME. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



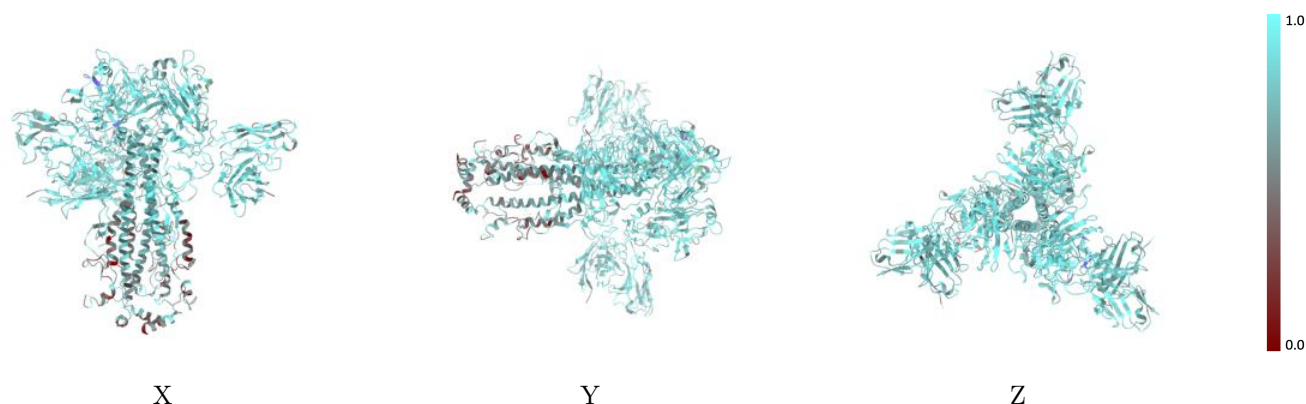
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



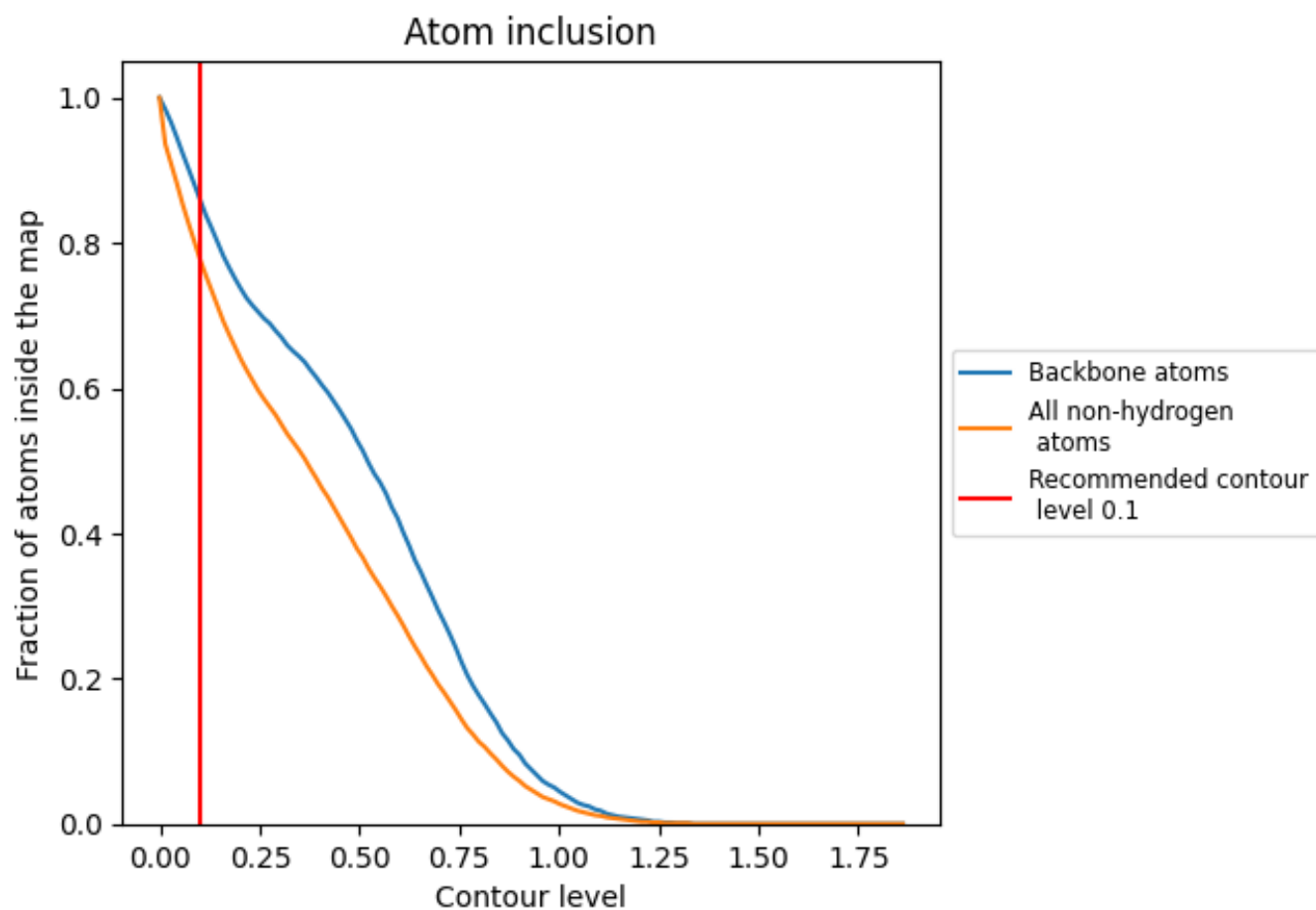
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).





















9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 78% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7770	 0.4620
A	 0.7640	 0.4500
B	 0.7640	 0.4510
C	 0.7580	 0.4470
D	 0.8090	 0.4810
E	 0.8070	 0.4820
F	 0.8130	 0.4990
G	 0.8060	 0.4970
H	 0.8120	 0.4790
L	 0.8030	 0.5000

