



Full wwPDB EM Validation Report ⓘ

Nov 3, 2024 – 01:12 PM EST

PDB ID : 7L0L
EMDB ID : EMD-23098
Title : Cryo-EM structure of the VRC316 clinical trial, vaccine-elicited, human antibody 316-310-1B11 in complex with an H2 CAN05 HA trimer
Authors : Gorman, J.; Kwong, P.D.
Deposited on : 2020-12-11
Resolution : 2.85 Å (reported)
Based on initial models : 3KU3, ?

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) : 2.39

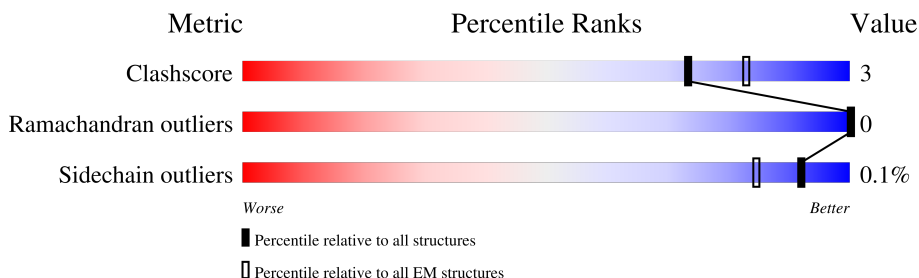
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.85 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	J	215	<div> <div>7%</div> <div>48%</div> <div>50%</div> </div>
1	K	215	<div> <div>6%</div> <div>47%</div> <div>50%</div> </div>
1	L	215	<div> <div>7%</div> <div>47%</div> <div>50%</div> </div>
2	A	345	<div> <div>84%</div> <div>9%</div> <div>7%</div> </div>
2	C	345	<div> <div>85%</div> <div>8%</div> <div>7%</div> </div>
2	D	345	<div> <div>87%</div> <div>6%</div> <div>7%</div> </div>
3	B	222	<div> <div>68%</div> <div>9%</div> <div>23%</div> </div>
3	E	222	<div> <div>71%</div> <div>6%</div> <div>23%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	222	<div><div></div><div>73%5%23%</div></div>
4	G	236	<div><div></div><div>45%6%49%</div></div>
4	H	236	<div><div></div><div>46%5%49%</div></div>
4	I	236	<div><div></div><div>46%5%49%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17211 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 316-310-1B11 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	108	Total	C	N	O	S	0	0
			824	518	143	161	2		
1	J	108	Total	C	N	O	S	0	0
			824	518	143	161	2		
1	K	108	Total	C	N	O	S	0	0
			824	518	143	161	2		

- Molecule 2 is a protein called Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	322	Total	C	N	O	S	0	0
			2521	1583	439	483	16		
2	C	322	Total	C	N	O	S	0	0
			2521	1583	439	483	16		
2	D	322	Total	C	N	O	S	0	0
			2521	1583	439	483	16		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	CYS	LEU	conflict	UNP Q4ZH98
A	330	ARG	-	expression tag	UNP Q4ZH98
A	331	ARG	-	expression tag	UNP Q4ZH98
A	332	ARG	-	expression tag	UNP Q4ZH98
A	333	ARG	-	expression tag	UNP Q4ZH98
A	334	ARG	-	expression tag	UNP Q4ZH98
C	30	CYS	LEU	conflict	UNP Q4ZH98
C	330	ARG	-	expression tag	UNP Q4ZH98
C	331	ARG	-	expression tag	UNP Q4ZH98
C	332	ARG	-	expression tag	UNP Q4ZH98
C	333	ARG	-	expression tag	UNP Q4ZH98
C	334	ARG	-	expression tag	UNP Q4ZH98
D	30	CYS	LEU	conflict	UNP Q4ZH98

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Chain	Residue	Modelled	Actual	Comment	Reference
D	330	ARG	-	expression tag	UNP Q4ZH98
D	331	ARG	-	expression tag	UNP Q4ZH98
D	332	ARG	-	expression tag	UNP Q4ZH98
D	333	ARG	-	expression tag	UNP Q4ZH98
D	334	ARG	-	expression tag	UNP Q4ZH98

- Molecule 3 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	172	Total	C	N	O	S	0	0
			1398	872	237	279	10		
3	E	172	Total	C	N	O	S	0	0
			1398	872	237	279	10		
3	F	172	Total	C	N	O	S	0	0
			1398	872	237	279	10		

There are 138 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	47	CYS	GLY	conflict	UNP Q4ZH98
B	178	GLY	-	expression tag	UNP Q4ZH98
B	179	ARG	-	expression tag	UNP Q4ZH98
B	180	LEU	-	expression tag	UNP Q4ZH98
B	181	VAL	-	expression tag	UNP Q4ZH98
B	182	PRO	-	expression tag	UNP Q4ZH98
B	183	ARG	-	expression tag	UNP Q4ZH98
B	184	GLY	-	expression tag	UNP Q4ZH98
B	185	SER	-	expression tag	UNP Q4ZH98
B	186	PRO	-	expression tag	UNP Q4ZH98
B	187	GLY	-	expression tag	UNP Q4ZH98
B	188	SER	-	expression tag	UNP Q4ZH98
B	189	GLY	-	expression tag	UNP Q4ZH98
B	190	TYR	-	expression tag	UNP Q4ZH98
B	191	ILE	-	expression tag	UNP Q4ZH98
B	192	PRO	-	expression tag	UNP Q4ZH98
B	193	GLU	-	expression tag	UNP Q4ZH98
B	194	ALA	-	expression tag	UNP Q4ZH98
B	195	PRO	-	expression tag	UNP Q4ZH98
B	196	ARG	-	expression tag	UNP Q4ZH98
B	197	ASP	-	expression tag	UNP Q4ZH98
B	198	GLY	-	expression tag	UNP Q4ZH98
B	199	GLN	-	expression tag	UNP Q4ZH98

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Chain	Residue	Modelled	Actual	Comment	Reference
B	200	ALA	-	expression tag	UNP Q4ZH98
B	201	TYR	-	expression tag	UNP Q4ZH98
B	202	VAL	-	expression tag	UNP Q4ZH98
B	203	ARG	-	expression tag	UNP Q4ZH98
B	204	LYS	-	expression tag	UNP Q4ZH98
B	205	ASP	-	expression tag	UNP Q4ZH98
B	206	GLY	-	expression tag	UNP Q4ZH98
B	207	GLU	-	expression tag	UNP Q4ZH98
B	208	TRP	-	expression tag	UNP Q4ZH98
B	209	VAL	-	expression tag	UNP Q4ZH98
B	210	LEU	-	expression tag	UNP Q4ZH98
B	211	LEU	-	expression tag	UNP Q4ZH98
B	212	SER	-	expression tag	UNP Q4ZH98
B	213	THR	-	expression tag	UNP Q4ZH98
B	214	PHE	-	expression tag	UNP Q4ZH98
B	215	LEU	-	expression tag	UNP Q4ZH98
B	216	GLY	-	expression tag	UNP Q4ZH98
B	217	HIS	-	expression tag	UNP Q4ZH98
B	218	HIS	-	expression tag	UNP Q4ZH98
B	219	HIS	-	expression tag	UNP Q4ZH98
B	220	HIS	-	expression tag	UNP Q4ZH98
B	221	HIS	-	expression tag	UNP Q4ZH98
B	222	HIS	-	expression tag	UNP Q4ZH98
E	47	CYS	GLY	conflict	UNP Q4ZH98
E	178	GLY	-	expression tag	UNP Q4ZH98
E	179	ARG	-	expression tag	UNP Q4ZH98
E	180	LEU	-	expression tag	UNP Q4ZH98
E	181	VAL	-	expression tag	UNP Q4ZH98
E	182	PRO	-	expression tag	UNP Q4ZH98
E	183	ARG	-	expression tag	UNP Q4ZH98
E	184	GLY	-	expression tag	UNP Q4ZH98
E	185	SER	-	expression tag	UNP Q4ZH98
E	186	PRO	-	expression tag	UNP Q4ZH98
E	187	GLY	-	expression tag	UNP Q4ZH98
E	188	SER	-	expression tag	UNP Q4ZH98
E	189	GLY	-	expression tag	UNP Q4ZH98
E	190	TYR	-	expression tag	UNP Q4ZH98
E	191	ILE	-	expression tag	UNP Q4ZH98
E	192	PRO	-	expression tag	UNP Q4ZH98
E	193	GLU	-	expression tag	UNP Q4ZH98
E	194	ALA	-	expression tag	UNP Q4ZH98
E	195	PRO	-	expression tag	UNP Q4ZH98

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Chain	Residue	Modelled	Actual	Comment	Reference
E	196	ARG	-	expression tag	UNP Q4ZH98
E	197	ASP	-	expression tag	UNP Q4ZH98
E	198	GLY	-	expression tag	UNP Q4ZH98
E	199	GLN	-	expression tag	UNP Q4ZH98
E	200	ALA	-	expression tag	UNP Q4ZH98
E	201	TYR	-	expression tag	UNP Q4ZH98
E	202	VAL	-	expression tag	UNP Q4ZH98
E	203	ARG	-	expression tag	UNP Q4ZH98
E	204	LYS	-	expression tag	UNP Q4ZH98
E	205	ASP	-	expression tag	UNP Q4ZH98
E	206	GLY	-	expression tag	UNP Q4ZH98
E	207	GLU	-	expression tag	UNP Q4ZH98
E	208	TRP	-	expression tag	UNP Q4ZH98
E	209	VAL	-	expression tag	UNP Q4ZH98
E	210	LEU	-	expression tag	UNP Q4ZH98
E	211	LEU	-	expression tag	UNP Q4ZH98
E	212	SER	-	expression tag	UNP Q4ZH98
E	213	THR	-	expression tag	UNP Q4ZH98
E	214	PHE	-	expression tag	UNP Q4ZH98
E	215	LEU	-	expression tag	UNP Q4ZH98
E	216	GLY	-	expression tag	UNP Q4ZH98
E	217	HIS	-	expression tag	UNP Q4ZH98
E	218	HIS	-	expression tag	UNP Q4ZH98
E	219	HIS	-	expression tag	UNP Q4ZH98
E	220	HIS	-	expression tag	UNP Q4ZH98
E	221	HIS	-	expression tag	UNP Q4ZH98
E	222	HIS	-	expression tag	UNP Q4ZH98
F	47	CYS	GLY	conflict	UNP Q4ZH98
F	178	GLY	-	expression tag	UNP Q4ZH98
F	179	ARG	-	expression tag	UNP Q4ZH98
F	180	LEU	-	expression tag	UNP Q4ZH98
F	181	VAL	-	expression tag	UNP Q4ZH98
F	182	PRO	-	expression tag	UNP Q4ZH98
F	183	ARG	-	expression tag	UNP Q4ZH98
F	184	GLY	-	expression tag	UNP Q4ZH98
F	185	SER	-	expression tag	UNP Q4ZH98
F	186	PRO	-	expression tag	UNP Q4ZH98
F	187	GLY	-	expression tag	UNP Q4ZH98
F	188	SER	-	expression tag	UNP Q4ZH98
F	189	GLY	-	expression tag	UNP Q4ZH98
F	190	TYR	-	expression tag	UNP Q4ZH98
F	191	ILE	-	expression tag	UNP Q4ZH98

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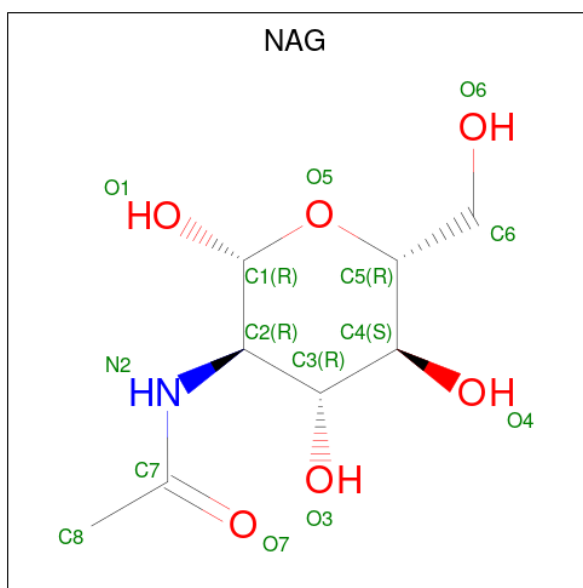
Chain	Residue	Modelled	Actual	Comment	Reference
F	192	PRO	-	expression tag	UNP Q4ZH98
F	193	GLU	-	expression tag	UNP Q4ZH98
F	194	ALA	-	expression tag	UNP Q4ZH98
F	195	PRO	-	expression tag	UNP Q4ZH98
F	196	ARG	-	expression tag	UNP Q4ZH98
F	197	ASP	-	expression tag	UNP Q4ZH98
F	198	GLY	-	expression tag	UNP Q4ZH98
F	199	GLN	-	expression tag	UNP Q4ZH98
F	200	ALA	-	expression tag	UNP Q4ZH98
F	201	TYR	-	expression tag	UNP Q4ZH98
F	202	VAL	-	expression tag	UNP Q4ZH98
F	203	ARG	-	expression tag	UNP Q4ZH98
F	204	LYS	-	expression tag	UNP Q4ZH98
F	205	ASP	-	expression tag	UNP Q4ZH98
F	206	GLY	-	expression tag	UNP Q4ZH98
F	207	GLU	-	expression tag	UNP Q4ZH98
F	208	TRP	-	expression tag	UNP Q4ZH98
F	209	VAL	-	expression tag	UNP Q4ZH98
F	210	LEU	-	expression tag	UNP Q4ZH98
F	211	LEU	-	expression tag	UNP Q4ZH98
F	212	SER	-	expression tag	UNP Q4ZH98
F	213	THR	-	expression tag	UNP Q4ZH98
F	214	PHE	-	expression tag	UNP Q4ZH98
F	215	LEU	-	expression tag	UNP Q4ZH98
F	216	GLY	-	expression tag	UNP Q4ZH98
F	217	HIS	-	expression tag	UNP Q4ZH98
F	218	HIS	-	expression tag	UNP Q4ZH98
F	219	HIS	-	expression tag	UNP Q4ZH98
F	220	HIS	-	expression tag	UNP Q4ZH98
F	221	HIS	-	expression tag	UNP Q4ZH98
F	222	HIS	-	expression tag	UNP Q4ZH98

- Molecule 4 is a protein called 316-310-1B11 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	120	Total	C	N	O	S	0	0
			924	581	161	178	4		
4	G	120	Total	C	N	O	S	0	0
			924	581	161	178	4		
4	I	120	Total	C	N	O	S	0	0
			924	581	161	178	4		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

C₈H₁₅NO₆).




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

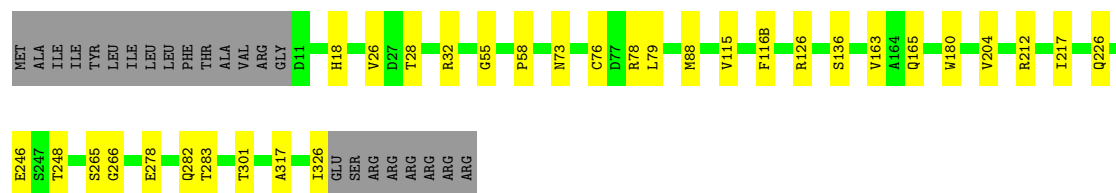
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Mol	Chain	Residues	Atoms				AltConf
5	D	1	Total	C	N	O	0
			14	8	1	5	
5	F	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 2: Hemagglutinin HA1 chain

Chain A:  84% 9% 7%




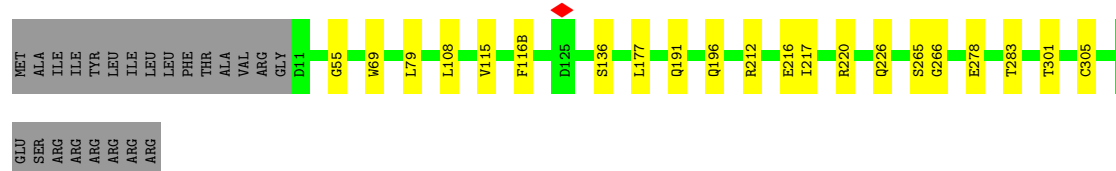
- Molecule 2: Hemagglutinin HA1 chain

Chain C:  85% 8% 7%



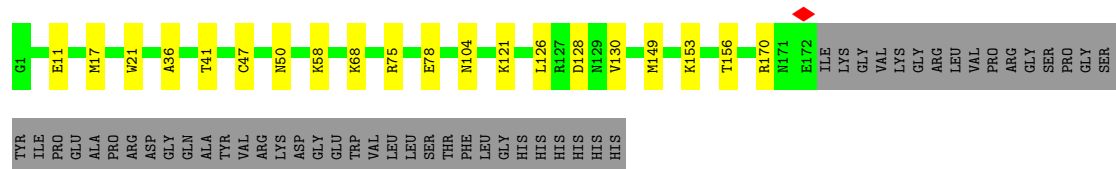
- Molecule 2: Hemagglutinin HA1 chain

Chain D:  87% 6% 7%



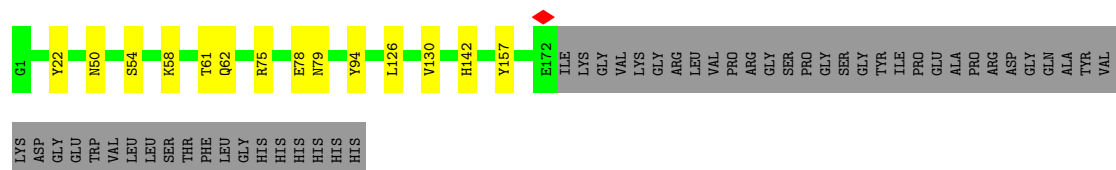
- Molecule 3: Hemagglutinin HA2 chain

Chain B:  68% 9% 23%



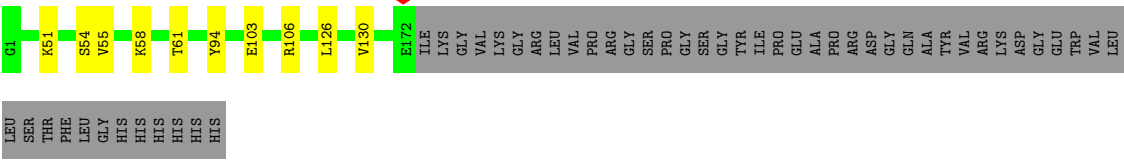
- Molecule 3: Hemagglutinin HA2 chain

Chain E:  71% 6% 23%



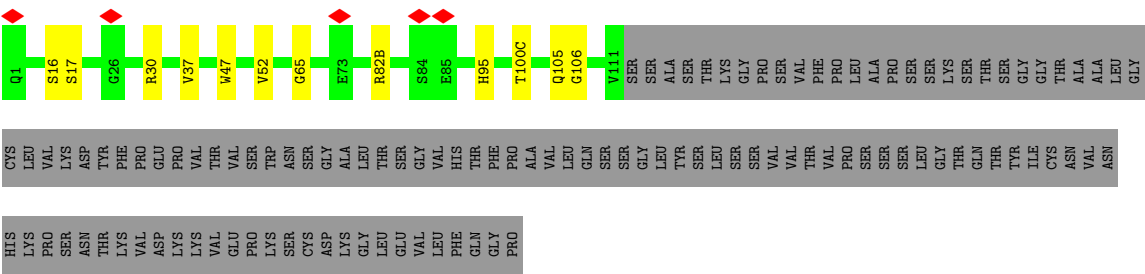
• Molecule 3: Hemagglutinin HA2 chain

Chain F:  73% 5% 23%



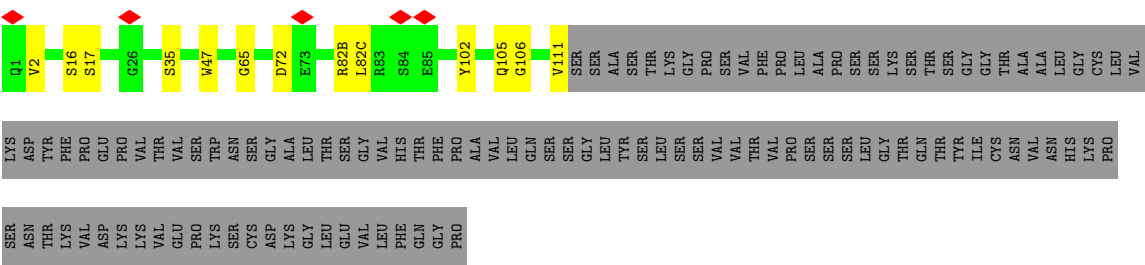
• Molecule 4: 316-310-1B11 Heavy Chain

Chain H:  46% 5% 49%



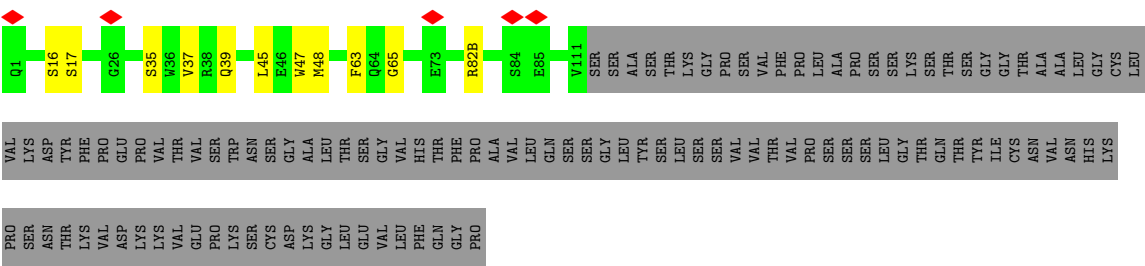
• Molecule 4: 316-310-1B11 Heavy Chain

Chain G:  45% 6% 49%



• Molecule 4: 316-310-1B11 Heavy Chain

Chain I:  46% 5% 49%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	115194	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.16	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.943	Depositor
Minimum map value	-1.581	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.3	Depositor
Map size (\AA)	346.56, 346.56, 346.56	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.083, 1.083, 1.083	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	J	0.27	0/845	0.46	0/1147
1	K	0.26	0/845	0.45	0/1147
1	L	0.26	0/845	0.46	0/1147
2	A	0.25	0/2580	0.44	0/3502
2	C	0.25	0/2580	0.44	0/3502
2	D	0.25	0/2580	0.44	0/3502
3	B	0.27	0/1426	0.40	0/1915
3	E	0.26	0/1426	0.40	0/1915
3	F	0.26	0/1426	0.40	0/1915
4	G	0.26	0/944	0.45	0/1280
4	H	0.26	0/944	0.45	0/1280
4	I	0.26	0/944	0.45	0/1280
All	All	0.26	0/17385	0.44	0/23532

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	824	0	802	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	824	0	802	4	0
1	L	824	0	802	4	0
2	A	2521	0	2468	21	0
2	C	2521	0	2468	20	0
2	D	2521	0	2468	14	0
3	B	1398	0	1299	14	0
3	E	1398	0	1299	10	0
3	F	1398	0	1299	7	0
4	G	924	0	893	7	0
4	H	924	0	893	6	0
4	I	924	0	893	7	0
5	A	56	0	52	0	0
5	B	14	0	13	0	0
5	C	56	0	52	0	0
5	D	56	0	52	0	0
5	E	14	0	13	0	0
5	F	14	0	13	0	0
All	All	17211	0	16581	103	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 (103) 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:D:283:THR:HG22	2:D:301:THR:HG22	1.72	0.70
2:A:126:ARG:NH2	2:A:165:GLN:O	2.25	0.69
3:B:68:LYS:HZ1	3:E:79:ASN:HB3	1.60	0.67
1:L:54:ARG:NH1	1:L:58:ILE:O	2.28	0.67
1:J:54:ARG:NH2	1:J:58:ILE:O	2.29	0.66
2:A:283:THR:HG22	2:A:301:THR:HG22	1.78	0.65
2:A:217:ILE:O	2:D:212:ARG:NH2	2.30	0.65
2:A:32:ARG:NH2	3:F:54:SER:OG	2.31	0.62
2:A:28:THR:O	2:A:32:ARG:NH1	2.32	0.62
2:C:283:THR:HG22	2:C:301:THR:HG22	1.81	0.62
2:D:108:LEU:HD11	2:D:177:LEU:HD11	1.82	0.61
2:C:74:PRO:HB3	2:C:149:ARG:HH21	1.65	0.61
1:K:54:ARG:NH2	1:K:58:ILE:O	2.34	0.61
2:A:212:ARG:NH2	2:C:217:ILE:O	2.33	0.60
3:F:126:LEU:HD13	3:F:130:VAL:HG11	1.83	0.60
2:A:136:SER:OG	2:A:226:GLN:NE2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:78:ARG:HG3	2:A:79:LEU:HD12	1.83	0.59
2:C:212:ARG:NH2	2:D:217:ILE:O	2.35	0.59
3:E:75:ARG:NH2	3:E:78:GLU:OE2	2.37	0.58
4:G:65:GLY:O	4:G:82(B):ARG:NH2	2.35	0.58
3:B:75:ARG:NH2	3:B:78:GLU:OE1	2.37	0.57
4:I:65:GLY:O	4:I:82(B):ARG:NH2	2.38	0.57
2:D:136:SER:OG	2:D:226:GLN:NE2	2.38	0.57
4:I:37:VAL:HG12	4:I:47:TRP:HA	1.87	0.56
2:A:58:PRO:HG2	2:A:88:MET:HE2	1.88	0.56
3:E:126:LEU:HD13	3:E:130:VAL:HG11	1.86	0.56
2:C:78:ARG:HG3	2:C:79:LEU:HD12	1.89	0.55
3:B:17:MET:HE1	3:B:36:ALA:HA	1.89	0.54
2:A:165:GLN:NE2	2:A:246:GLU:OE1	2.41	0.54
4:H:65:GLY:O	4:H:82(B):ARG:NH2	2.40	0.54
2:A:265:SER:OG	2:A:266:GLY:N	2.41	0.54
4:H:37:VAL:HG12	4:H:47:TRP:HA	1.90	0.53
3:B:126:LEU:HD13	3:B:130:VAL:HG11	1.89	0.53
2:C:115:VAL:HG11	2:C:116(B):PHE:CE1	2.42	0.53
1:K:90:GLN:HE21	1:K:97:THR:H	1.56	0.53
2:C:265:SER:OG	2:C:266:GLY:N	2.42	0.51
2:D:191:GLN:HE21	2:D:217:ILE:HD11	1.76	0.51
2:A:115:VAL:HG11	2:A:116(B):PHE:CE1	2.46	0.50
2:D:69:TRP:CD1	2:D:79:LEU:HB3	2.45	0.50
4:H:30:ARG:NH2	4:H:52:VAL:O	2.44	0.50
2:D:216:GLU:O	2:D:220:ARG:NH2	2.45	0.50
2:A:326:ILE:HD11	3:B:11:GLU:HB2	1.94	0.50
2:D:265:SER:OG	2:D:266:GLY:N	2.44	0.49
4:I:39:GLN:HB2	4:I:45:LEU:HD23	1.94	0.49
3:B:128:ASP:OD2	3:B:170:ARG:NH1	2.45	0.49
2:A:282:GLN:NE2	2:A:283:THR:O	2.46	0.49
4:H:16:SER:OG	4:H:17:SER:N	2.45	0.48
2:D:196:GLN:O	2:D:196:GLN:HG3	2.13	0.48
3:F:103:GLU:OE2	3:F:106:ARG:NH2	2.42	0.48
3:E:142:HIS:HE2	3:E:157:TYR:HH	1.57	0.48
1:K:37:ARG:HB2	1:K:47:LEU:HD11	1.96	0.48
2:D:115:VAL:HG11	2:D:116(B):PHE:CE1	2.48	0.48
4:I:48:MET:HG2	4:I:63:PHE:CE2	2.49	0.47
2:C:180:TRP:CE2	2:C:204:VAL:HG21	2.49	0.47
2:A:18:HIS:ND1	3:B:17:MET:O	2.46	0.47
2:D:115:VAL:HG11	2:D:116(B):PHE:HE1	1.80	0.46
4:G:105:GLN:NE2	4:G:106:GLY:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:26:VAL:HG21	2:A:317:ALA:HB2	1.98	0.46
4:H:105:GLN:NE2	4:H:106:GLY:O	2.48	0.46
4:I:35:SER:OG	4:I:47:TRP:NE1	2.49	0.46
2:C:55:GLY:N	2:C:278:GLU:OE2	2.49	0.46
4:G:16:SER:OG	4:G:17:SER:N	2.49	0.46
2:C:307:LYS:HD2	3:E:62:GLN:HB3	1.98	0.46
1:J:37:ARG:HB2	1:J:47:LEU:HD11	1.98	0.45
3:F:61:THR:HG22	3:F:61:THR:O	2.17	0.45
1:L:37:ARG:HB2	1:L:47:LEU:HD11	1.99	0.45
3:E:54:SER:O	3:E:58:LYS:HG2	2.17	0.45
2:C:196:GLN:O	2:C:196:GLN:HG2	2.17	0.45
4:I:16:SER:OG	4:I:17:SER:N	2.49	0.45
4:G:35:SER:OG	4:G:47:TRP:NE1	2.50	0.44
4:H:95:HIS:ND1	4:H:100(C):THR:OG1	2.48	0.44
3:E:61:THR:HG22	3:E:61:THR:O	2.18	0.44
2:A:28:THR:HG22	3:B:104:ASN:HB3	1.98	0.44
2:C:26:VAL:HG21	2:C:317:ALA:HB2	2.00	0.44
4:G:72:ASP:OD1	4:G:72:ASP:N	2.49	0.44
3:B:156:THR:O	3:B:156:THR:HG22	2.19	0.43
2:C:71:LEU:HD21	2:C:102:PHE:HE1	1.83	0.43
2:A:163:VAL:HG12	2:A:248:THR:HG22	2.01	0.43
3:B:58:LYS:HB3	3:E:94:TYR:CD1	2.53	0.43
2:C:320:LEU:H	2:C:320:LEU:HD23	1.84	0.43
1:L:45:ARG:HH12	1:L:58:ILE:HD13	1.82	0.42
2:C:29:ILE:HD12	2:C:29:ILE:HA	1.92	0.42
2:C:320:LEU:HD13	3:E:22:TYR:HE1	1.85	0.42
3:B:121:LYS:HB3	3:B:121:LYS:HE3	1.82	0.42
2:C:137:ARG:HD3	2:C:137:ARG:HA	1.88	0.42
2:D:55:GLY:N	2:D:278:GLU:OE2	2.52	0.42
3:B:47:CYS:O	2:C:30:CYS:HB2	2.18	0.42
3:F:51:LYS:O	3:F:55:VAL:HG23	2.20	0.42
4:I:48:MET:HG2	4:I:63:PHE:CD2	2.55	0.42
3:B:149:MET:O	3:B:153:LYS:HG3	2.20	0.42
4:G:2:VAL:HB	4:G:102:TYR:CE1	2.55	0.41
2:C:307:LYS:HA	2:C:307:LYS:HD3	1.91	0.41
2:A:73:ASN:HB3	2:A:76:CYS:SG	2.61	0.41
3:B:21:TRP:CD1	3:B:41:THR:HG23	2.55	0.41
2:C:163:VAL:HG22	2:C:248:THR:HG22	2.01	0.41
3:E:58:LYS:HB3	3:F:94:TYR:CE1	2.56	0.41
4:G:82(C):LEU:HD13	4:G:111:VAL:HG12	2.02	0.41
1:L:90:GLN:HE21	1:L:97:THR:H	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:55:GLY:N	2:A:278:GLU:OE2	2.54	0.41
2:A:180:TRP:CE2	2:A:204:VAL:HG21	2.56	0.41
2:D:301:THR:HB	2:D:305:CYS:SG	2.62	0.40
1:K:19:ALA:HB3	1:K:75:ILE:HB	2.03	0.40
3:F:54:SER:O	3:F:58:LYS:HG2	2.21	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	J	106/215 (49%)	100 (94%)	6 (6%)	0	100	100
1	K	106/215 (49%)	99 (93%)	7 (7%)	0	100	100
1	L	106/215 (49%)	99 (93%)	7 (7%)	0	100	100
2	A	320/345 (93%)	311 (97%)	9 (3%)	0	100	100
2	C	320/345 (93%)	314 (98%)	6 (2%)	0	100	100
2	D	320/345 (93%)	311 (97%)	9 (3%)	0	100	100
3	B	170/222 (77%)	167 (98%)	3 (2%)	0	100	100
3	E	170/222 (77%)	165 (97%)	5 (3%)	0	100	100
3	F	170/222 (77%)	167 (98%)	3 (2%)	0	100	100
4	G	118/236 (50%)	117 (99%)	1 (1%)	0	100	100
4	H	118/236 (50%)	117 (99%)	1 (1%)	0	100	100
4	I	118/236 (50%)	117 (99%)	1 (1%)	0	100	100
All	All	2142/3054 (70%)	2084 (97%)	58 (3%)	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	J	90/186 (48%)	90 (100%)	0	100	100
1	K	90/186 (48%)	90 (100%)	0	100	100
1	L	90/186 (48%)	90 (100%)	0	100	100
2	A	284/304 (93%)	284 (100%)	0	100	100
2	C	284/304 (93%)	284 (100%)	0	100	100
2	D	284/304 (93%)	284 (100%)	0	100	100
3	B	150/190 (79%)	149 (99%)	1 (1%)	81	91
3	E	150/190 (79%)	149 (99%)	1 (1%)	81	91
3	F	150/190 (79%)	150 (100%)	0	100	100
4	G	99/199 (50%)	99 (100%)	0	100	100
4	H	99/199 (50%)	99 (100%)	0	100	100
4	I	99/199 (50%)	99 (100%)	0	100	100
All	All	1869/2637 (71%)	1867 (100%)	2 (0%)	92	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	50	ASN
3	E	50	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	226	GLN
3	B	79	ASN
3	E	79	ASN
2	D	226	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

15 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	$\# Z > 2$
5	NAG	C	401	2	14,14,15	0.21	0	17,19,21	0.44	0
5	NAG	A	401	2	14,14,15	0.21	0	17,19,21	0.43	0
5	NAG	A	404	2	14,14,15	0.24	0	17,19,21	0.47	0
5	NAG	C	402	2	14,14,15	0.21	0	17,19,21	0.48	0
5	NAG	A	402	2	14,14,15	0.21	0	17,19,21	0.48	0
5	NAG	E	301	3	14,14,15	0.22	0	17,19,21	0.44	0
5	NAG	D	404	2	14,14,15	0.24	0	17,19,21	0.47	0
5	NAG	D	401	2	14,14,15	0.22	0	17,19,21	0.45	0
5	NAG	C	403	2	14,14,15	0.20	0	17,19,21	0.41	0
5	NAG	F	301	3	14,14,15	0.20	0	17,19,21	0.43	0
5	NAG	D	402	2	14,14,15	0.21	0	17,19,21	0.49	0
5	NAG	B	301	3	14,14,15	0.21	0	17,19,21	0.43	0
5	NAG	A	403	2	14,14,15	0.21	0	17,19,21	0.42	0
5	NAG	C	404	2	14,14,15	0.24	0	17,19,21	0.47	0
5	NAG	D	403	2	14,14,15	0.22	0	17,19,21	0.42	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
5	NAG	C	401	2	-	2/6/23/26	0/1/1/1
5	NAG	A	401	2	-	2/6/23/26	0/1/1/1
5	NAG	A	404	2	-	2/6/23/26	0/1/1/1
5	NAG	C	402	2	-	2/6/23/26	0/1/1/1
5	NAG	A	402	2	-	2/6/23/26	0/1/1/1
5	NAG	E	301	3	-	2/6/23/26	0/1/1/1
5	NAG	D	404	2	-	0/6/23/26	0/1/1/1
5	NAG	D	401	2	-	2/6/23/26	0/1/1/1
5	NAG	C	403	2	-	0/6/23/26	0/1/1/1
5	NAG	F	301	3	-	2/6/23/26	0/1/1/1
5	NAG	D	402	2	-	2/6/23/26	0/1/1/1
5	NAG	B	301	3	-	2/6/23/26	0/1/1/1
5	NAG	A	403	2	-	0/6/23/26	0/1/1/1
5	NAG	C	404	2	-	2/6/23/26	0/1/1/1
5	NAG	D	403	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	404	NAG	O5-C5-C6-O6
5	B	301	NAG	O5-C5-C6-O6
5	A	404	NAG	C4-C5-C6-O6
5	E	301	NAG	C4-C5-C6-O6
5	E	301	NAG	O5-C5-C6-O6
5	B	301	NAG	C4-C5-C6-O6
5	F	301	NAG	O5-C5-C6-O6
5	F	301	NAG	C4-C5-C6-O6
5	C	401	NAG	O5-C5-C6-O6
5	A	401	NAG	O5-C5-C6-O6
5	C	401	NAG	C4-C5-C6-O6
5	A	401	NAG	C4-C5-C6-O6
5	D	402	NAG	C4-C5-C6-O6
5	D	402	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	402	NAG	O5-C5-C6-O6
5	A	402	NAG	C4-C5-C6-O6
5	C	402	NAG	O5-C5-C6-O6
5	C	402	NAG	C4-C5-C6-O6
5	D	401	NAG	O5-C5-C6-O6
5	D	401	NAG	C4-C5-C6-O6
5	C	404	NAG	C4-C5-C6-O6
5	C	404	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

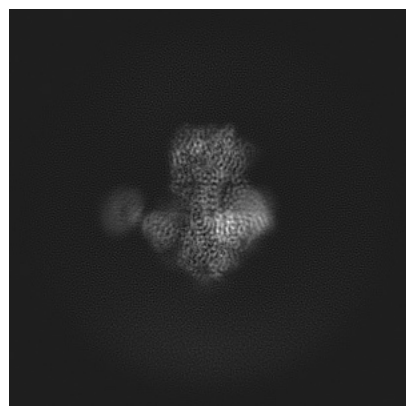
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23098. These allow visual inspection of the internal detail of the map and identification of artifacts.

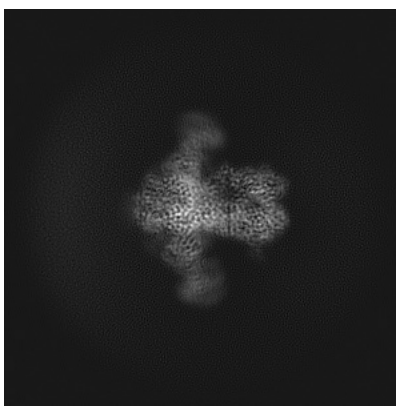
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

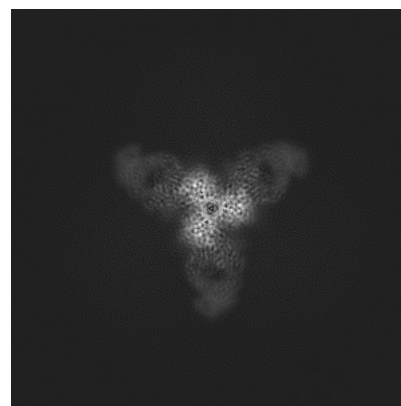
6.1.1 Primary map



X

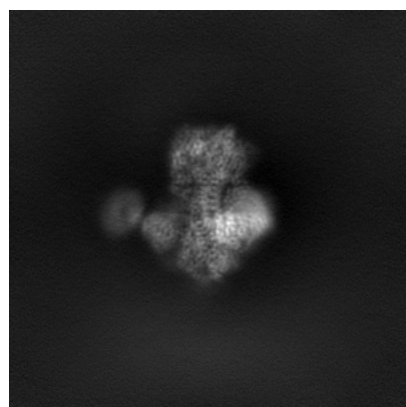


Y

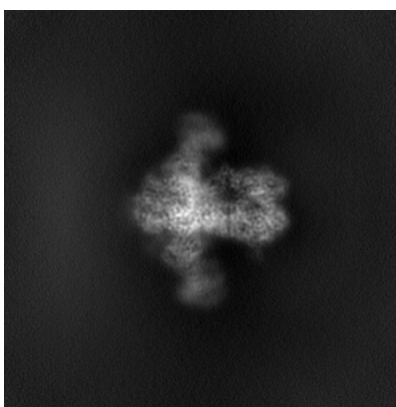


Z

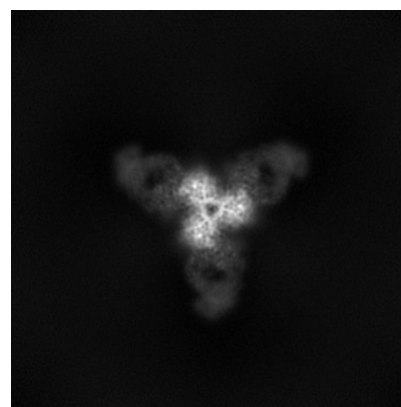
6.1.2 Raw map



X



Y

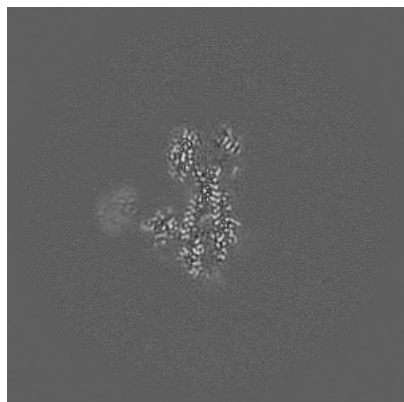


Z

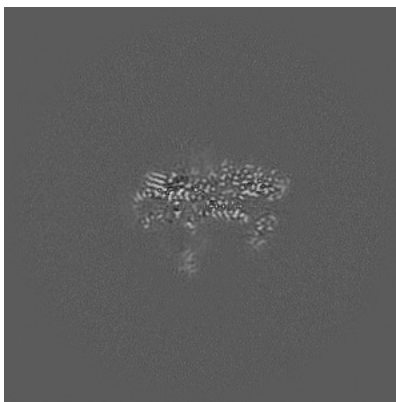
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

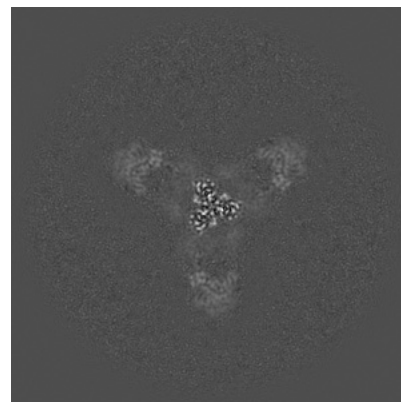
6.2.1 Primary map



X Index: 160

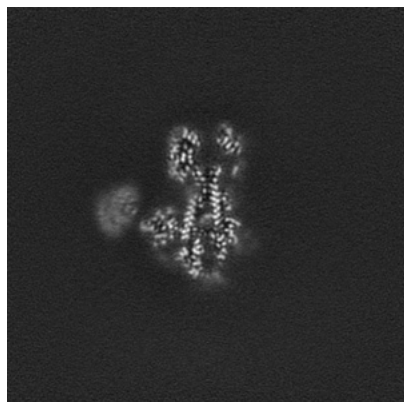


Y Index: 160

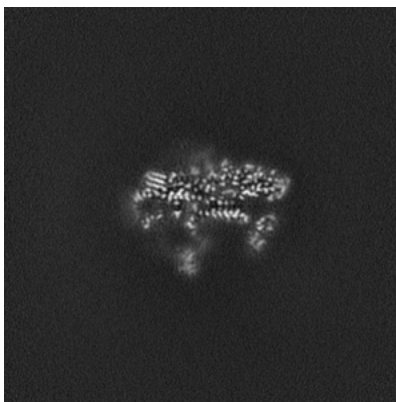


Z Index: 160

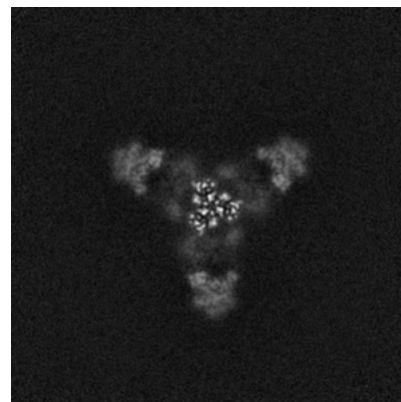
6.2.2 Raw map



X Index: 160



Y Index: 160

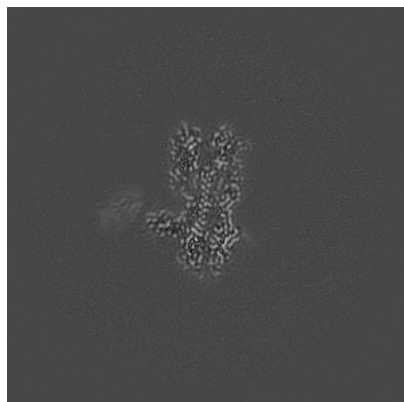


Z Index: 160

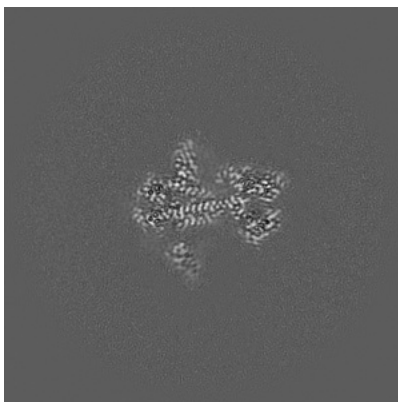
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

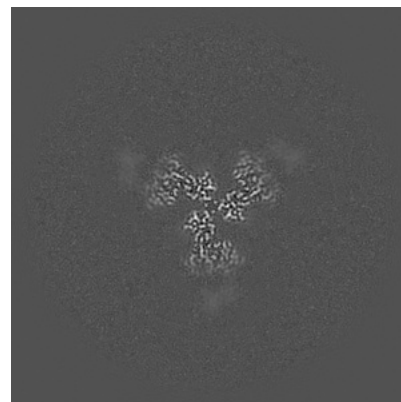
6.3.1 Primary map



X Index: 154

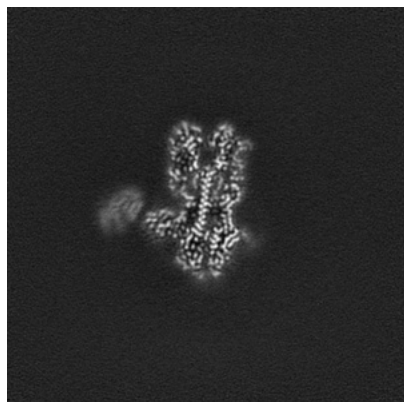


Y Index: 166

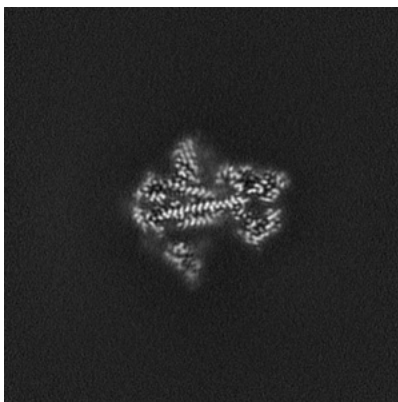


Z Index: 141

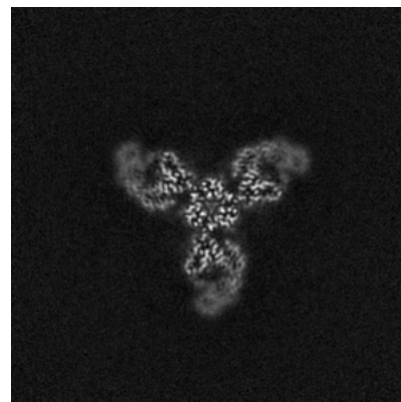
6.3.2 Raw map



X Index: 154



Y Index: 166

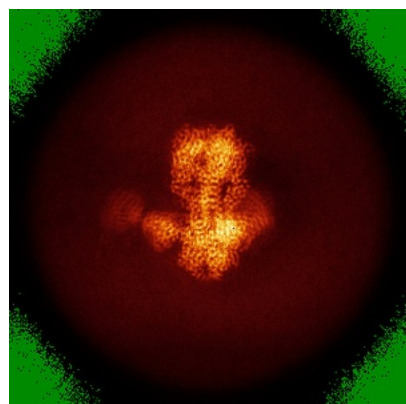


Z Index: 149

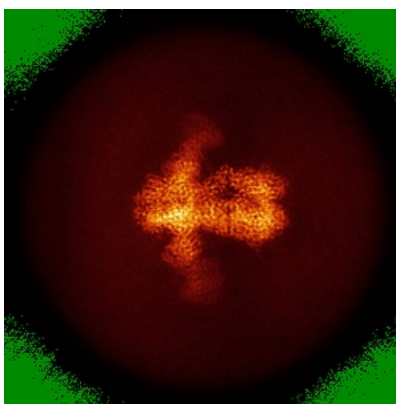
The images above show the largest variance slices of the map in three orthogonal directions.

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

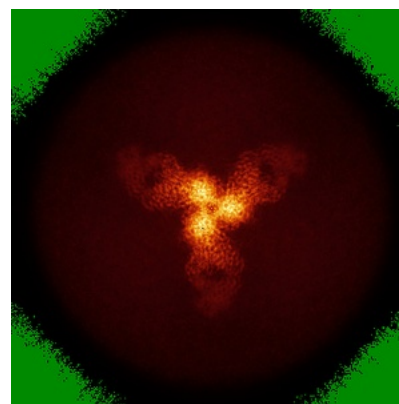
6.4.1 Primary map



X

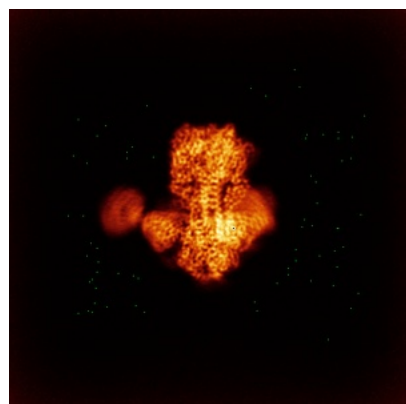


Y

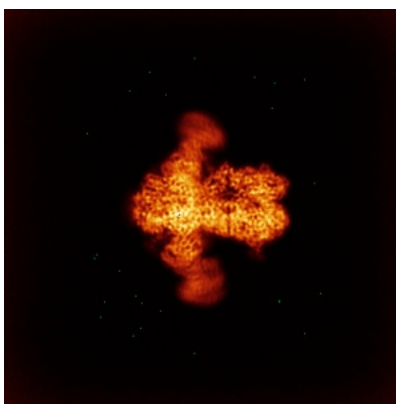


Z

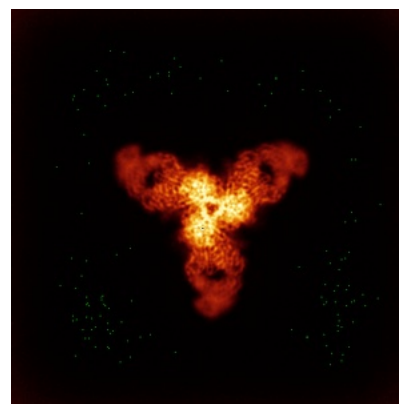
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



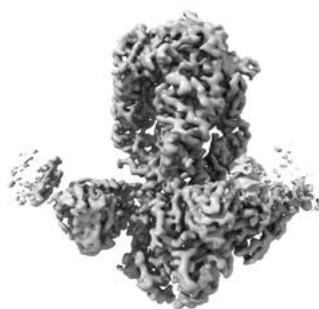
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

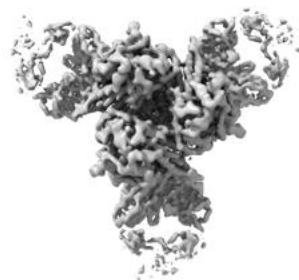
6.5.2 Raw map



X



Y



Z

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

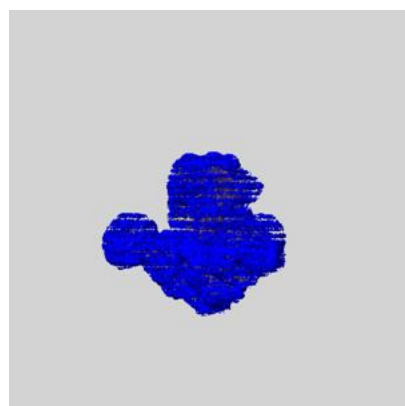
6.6 Mask visualisation [i](#)

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

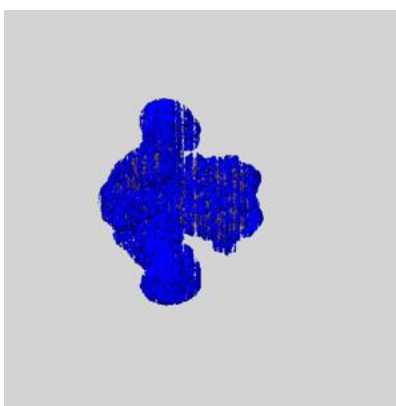
A mask typically either:

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

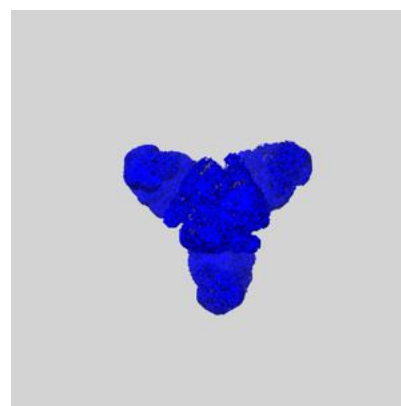
6.6.1 emd_23098_msk_1.map [i](#)



X



Y

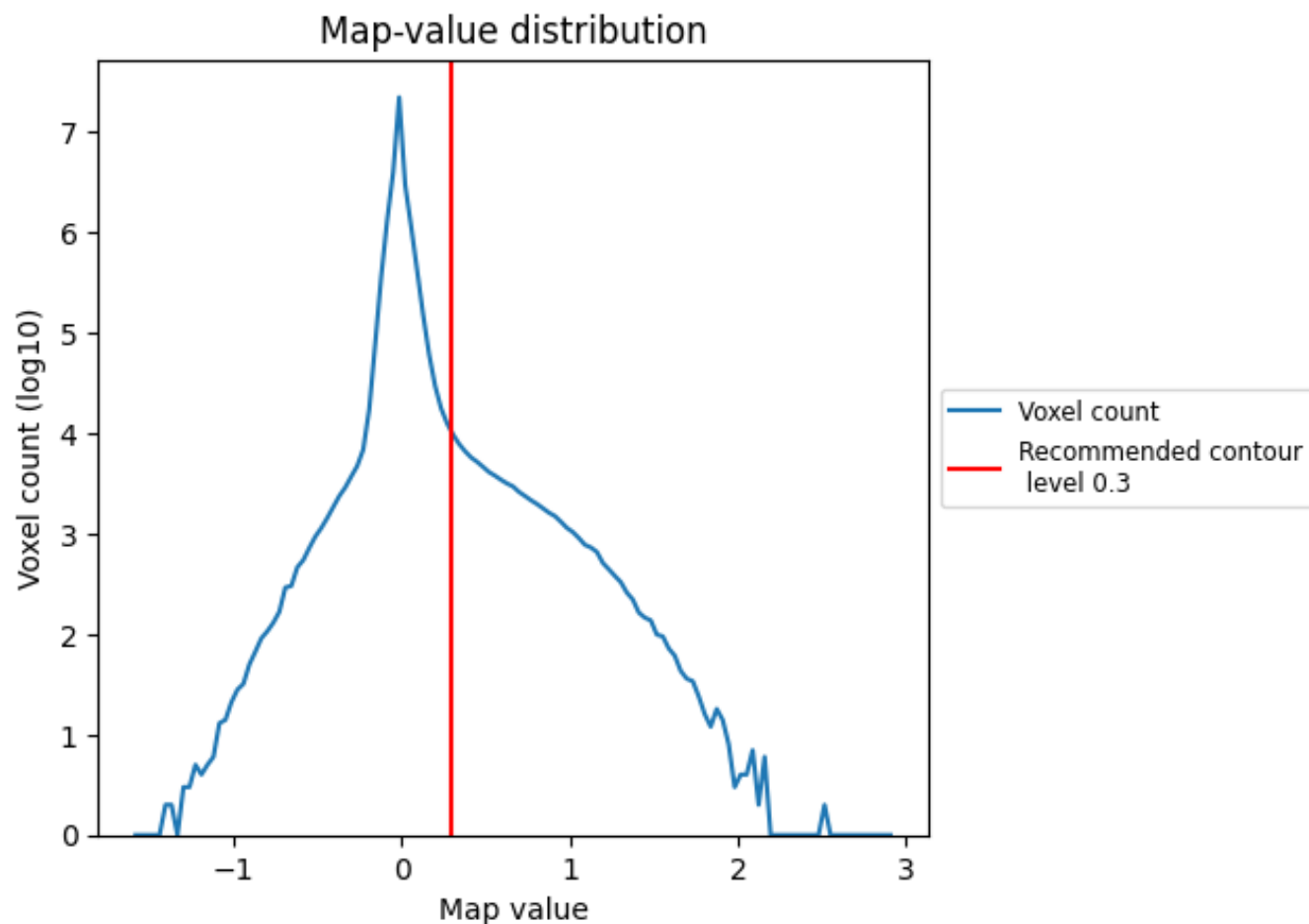


Z

7 Map analysis [i](#)

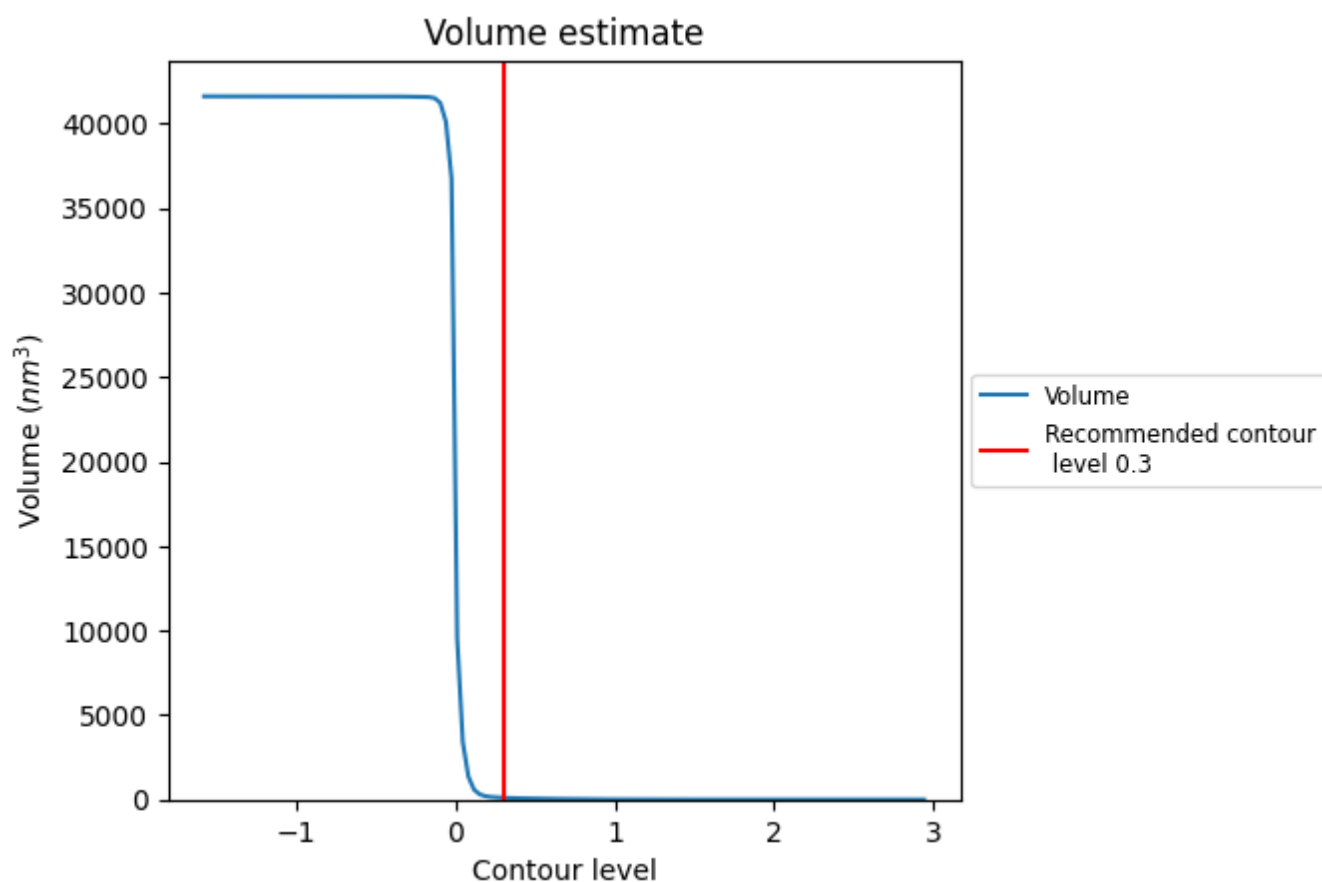
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

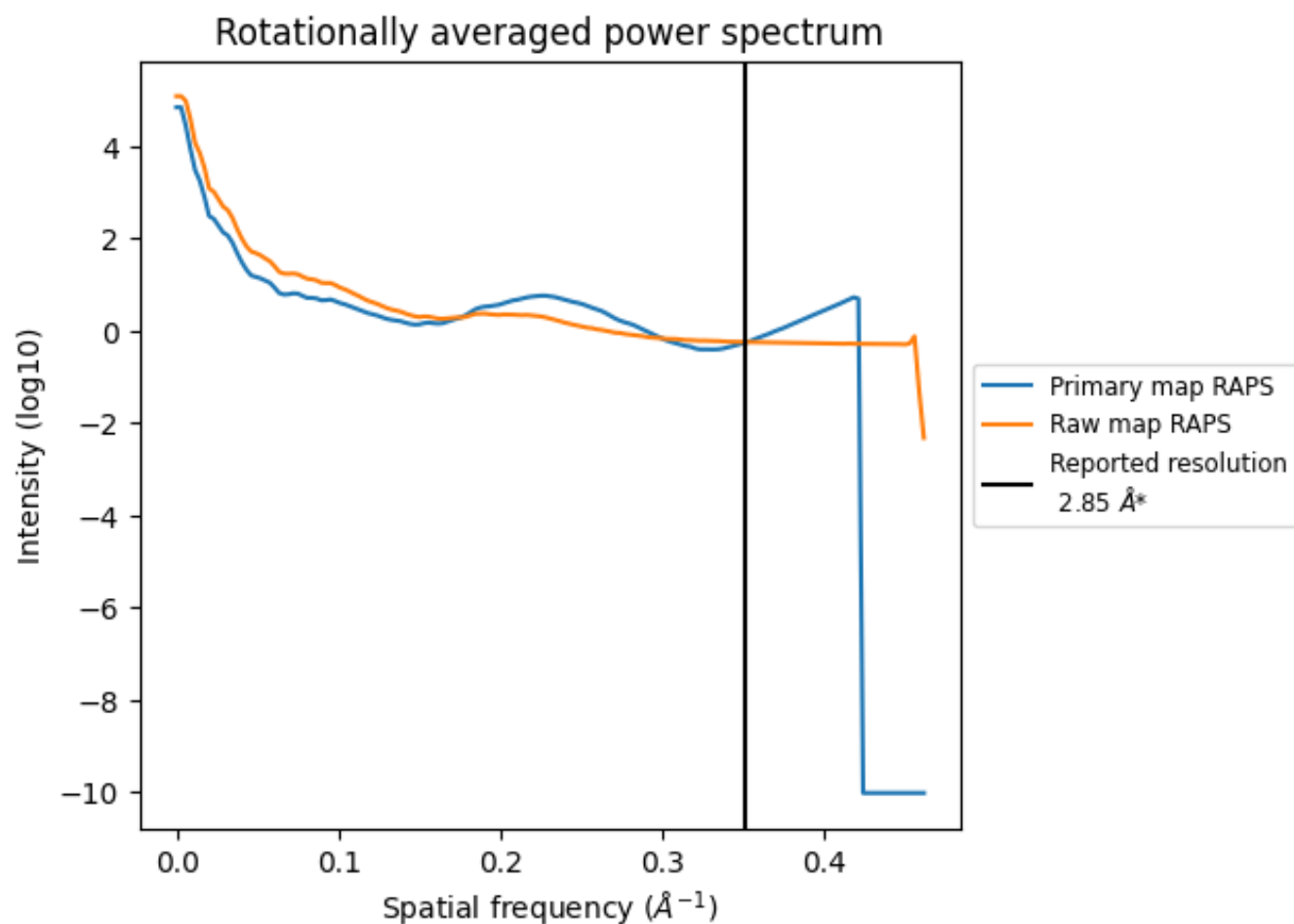
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 106 nm^3 ; this corresponds to an approximate mass of 96 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

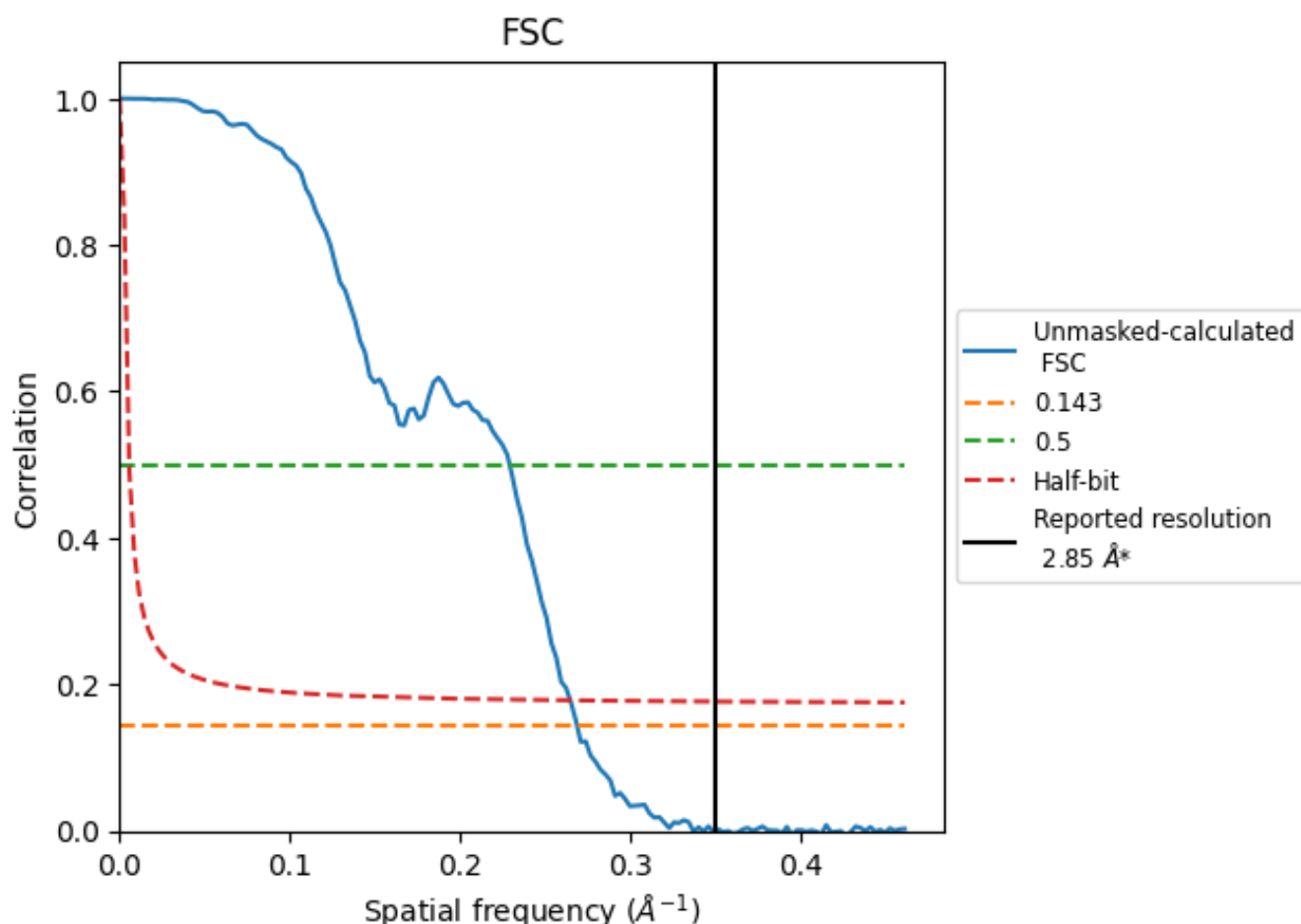


*Reported resolution corresponds to spatial frequency of 0.351 Å⁻¹

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 0.351 \AA^{-1}

8.2 Resolution estimates [i](#)

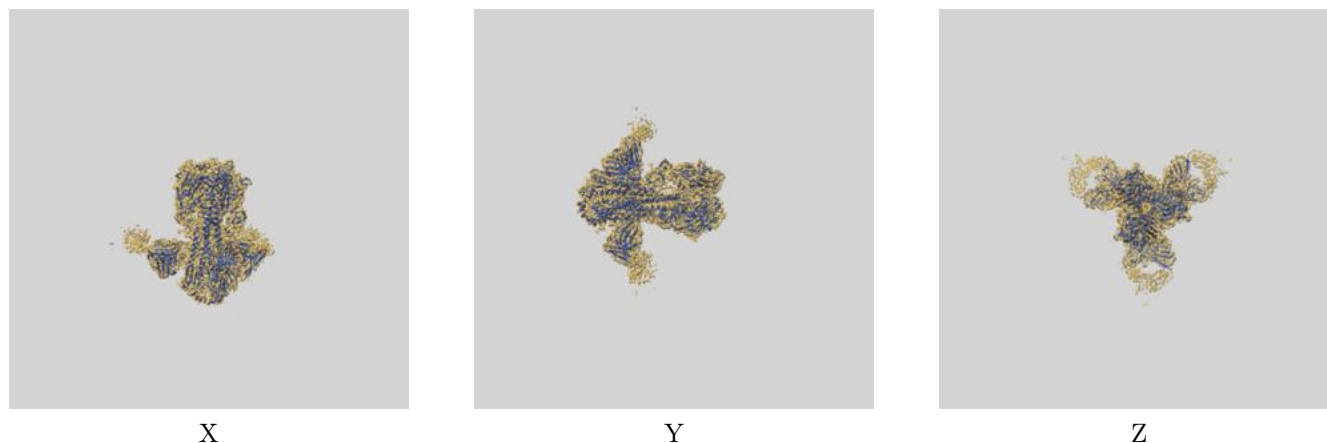
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.85	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.72	4.36	3.77

*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 3.72 differs from the reported value 2.85 by more than 10 %

9 Map-model fit [i](#)

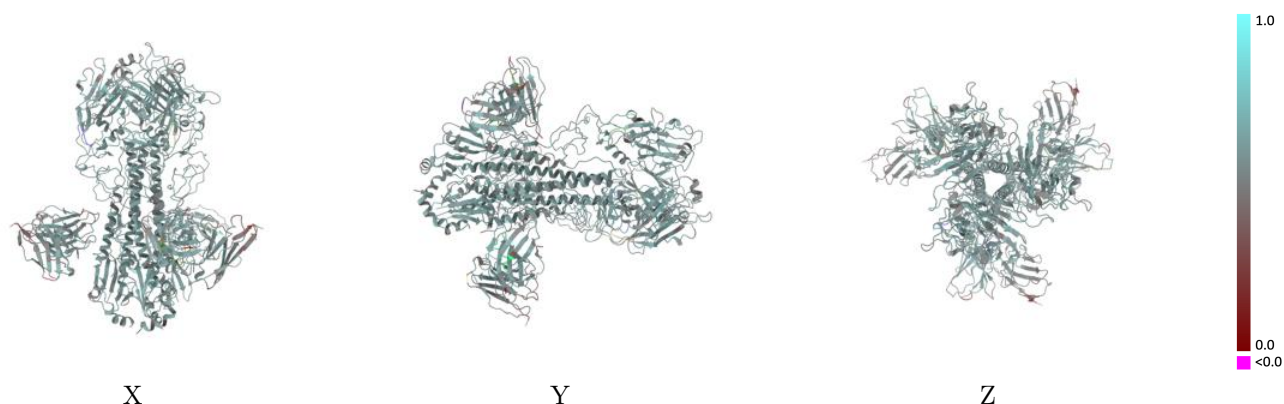
This section contains information regarding the fit between EMDB map EMD-23098 and PDB model 7L0L. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



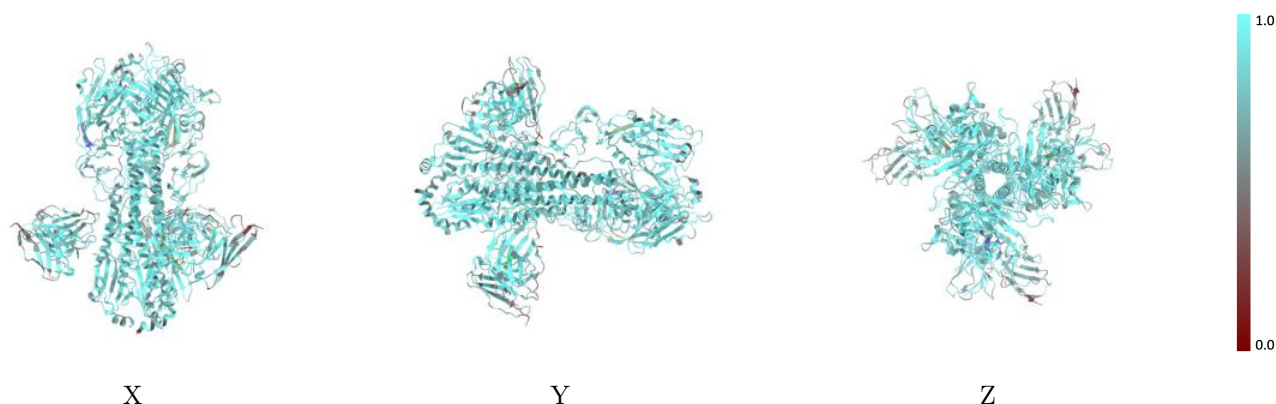
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



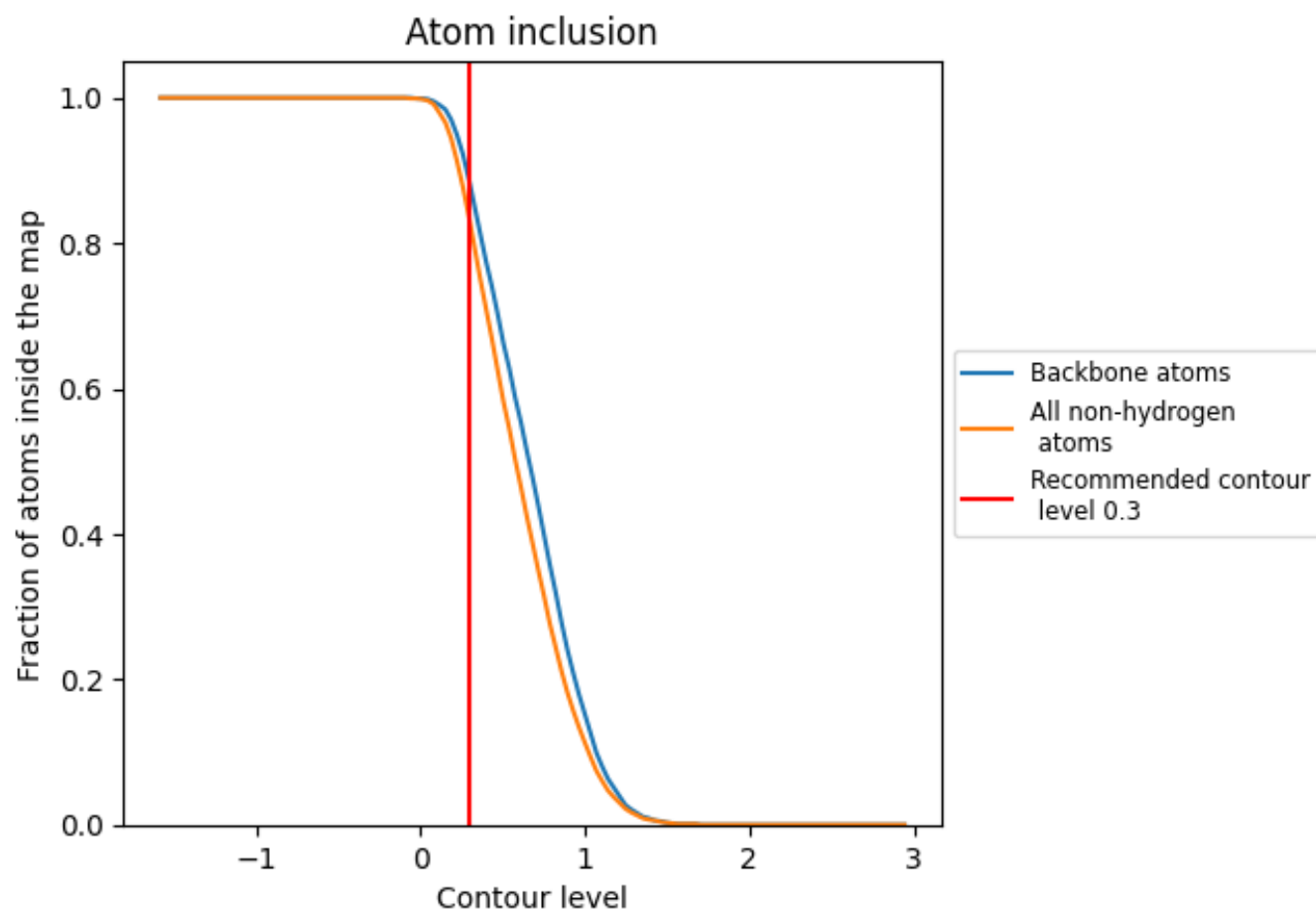
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8300</div>	<div><div></div>0.5550</div>
A	<div><div></div>0.8520</div>	<div><div></div>0.5670</div>
B	<div><div></div>0.8620</div>	<div><div></div>0.5730</div>
C	<div><div></div>0.8590</div>	<div><div></div>0.5650</div>
D	<div><div></div>0.8550</div>	<div><div></div>0.5640</div>
E	<div><div></div>0.8620</div>	<div><div></div>0.5670</div>
F	<div><div></div>0.8670</div>	<div><div></div>0.5740</div>
G	<div><div></div>0.7980</div>	<div><div></div>0.5450</div>
H	<div><div></div>0.7920</div>	<div><div></div>0.5430</div>
I	<div><div></div>0.7970</div>	<div><div></div>0.5400</div>
J	<div><div></div>0.7210</div>	<div><div></div>0.5020</div>
K	<div><div></div>0.7290</div>	<div><div></div>0.5090</div>
L	<div><div></div>0.7300</div>	<div><div></div>0.5060</div>

