



Full wwPDB EM Validation Report ⓘ

Oct 14, 2024 – 05:49 PM EDT

PDB ID : 8T7A
EMDB ID : EMD-41089
Title : Cryo-EM structure of RSV preF in complex with Fab 2.4K
Authors : McCool, R.S.; McLellan, J.S.
Deposited on : 2023-06-20
Resolution : 2.80 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) : 2.39

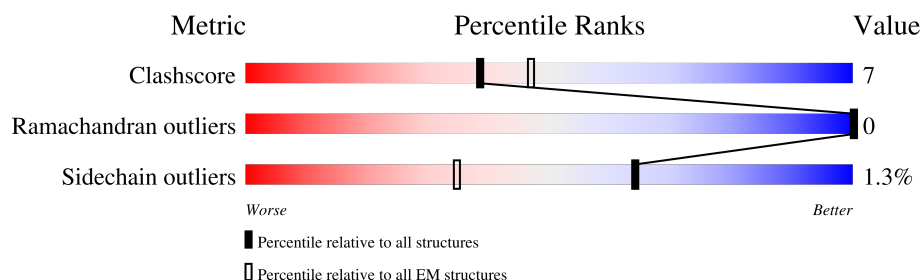
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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	84	
1	B	84	
1	C	84	
2	a	436	
2	b	436	
2	c	436	
3	D	125	
3	F	125	

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Mol	Chain	Length	Quality of chain
3	H	125	
4	E	113	
4	G	113	
4	I	113	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15819 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 Fusion glycoprotein F2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	72	Total	C	N	O	S	0	0
			571	363	92	113	3		
1	B	72	Total	C	N	O	S	0	0
			571	363	92	113	3		
1	C	72	Total	C	N	O	S	0	0
			571	363	92	113	3		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	ILE	ASN	conflict	UNP P12568
A	80	LYS	ASN	conflict	UNP P12568
A	101	PRO	THR	conflict	UNP P12568
B	67	ILE	ASN	conflict	UNP P12568
B	80	LYS	ASN	conflict	UNP P12568
B	101	PRO	THR	conflict	UNP P12568
C	67	ILE	ASN	conflict	UNP P12568
C	80	LYS	ASN	conflict	UNP P12568
C	101	PRO	THR	conflict	UNP P12568

- Molecule 2 is a protein called Fusion glycoprotein F1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	370	Total	C	N	O	S	0	0
			2847	1800	469	560	18		
2	b	370	Total	C	N	O	S	0	0
			2847	1800	469	560	18		
2	c	370	Total	C	N	O	S	0	0
			2847	1800	469	560	18		

There are 186 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	152	VAL	ILE	conflict	UNP P12568
a	213	SER	ARG	conflict	UNP P12568
a	215	PRO	SER	conflict	UNP P12568
a	514	GLY	-	expression tag	UNP P12568
a	515	SER	-	expression tag	UNP P12568
a	516	GLY	-	expression tag	UNP P12568
a	517	TYR	-	expression tag	UNP P12568
a	518	ILE	-	expression tag	UNP P12568
a	519	PRO	-	expression tag	UNP P12568
a	520	GLU	-	expression tag	UNP P12568
a	521	ALA	-	expression tag	UNP P12568
a	522	PRO	-	expression tag	UNP P12568
a	523	ARG	-	expression tag	UNP P12568
a	524	ASP	-	expression tag	UNP P12568
a	525	GLY	-	expression tag	UNP P12568
a	526	GLN	-	expression tag	UNP P12568
a	527	ALA	-	expression tag	UNP P12568
a	528	TYR	-	expression tag	UNP P12568
a	529	VAL	-	expression tag	UNP P12568
a	530	ARG	-	expression tag	UNP P12568
a	531	LYS	-	expression tag	UNP P12568
a	532	ASP	-	expression tag	UNP P12568
a	533	GLY	-	expression tag	UNP P12568
a	534	GLU	-	expression tag	UNP P12568
a	535	TRP	-	expression tag	UNP P12568
a	536	VAL	-	expression tag	UNP P12568
a	537	LEU	-	expression tag	UNP P12568
a	538	LEU	-	expression tag	UNP P12568
a	539	SER	-	expression tag	UNP P12568
a	540	THR	-	expression tag	UNP P12568
a	541	PHE	-	expression tag	UNP P12568
a	542	LEU	-	expression tag	UNP P12568
a	543	GLY	-	expression tag	UNP P12568
a	544	ARG	-	expression tag	UNP P12568
a	545	SER	-	expression tag	UNP P12568
a	546	LEU	-	expression tag	UNP P12568
a	547	GLU	-	expression tag	UNP P12568
a	548	VAL	-	expression tag	UNP P12568
a	549	LEU	-	expression tag	UNP P12568
a	550	PHE	-	expression tag	UNP P12568
a	551	GLN	-	expression tag	UNP P12568
a	552	GLY	-	expression tag	UNP P12568
a	553	PRO	-	expression tag	UNP P12568

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Chain	Residue	Modelled	Actual	Comment	Reference
a	554	GLY	-	expression tag	UNP P12568
a	555	HIS	-	expression tag	UNP P12568
a	556	HIS	-	expression tag	UNP P12568
a	557	HIS	-	expression tag	UNP P12568
a	558	HIS	-	expression tag	UNP P12568
a	559	HIS	-	expression tag	UNP P12568
a	560	HIS	-	expression tag	UNP P12568
a	561	HIS	-	expression tag	UNP P12568
a	562	HIS	-	expression tag	UNP P12568
a	563	SER	-	expression tag	UNP P12568
a	564	ALA	-	expression tag	UNP P12568
a	565	TRP	-	expression tag	UNP P12568
a	566	SER	-	expression tag	UNP P12568
a	567	HIS	-	expression tag	UNP P12568
a	568	PRO	-	expression tag	UNP P12568
a	569	GLN	-	expression tag	UNP P12568
a	570	PHE	-	expression tag	UNP P12568
a	571	GLU	-	expression tag	UNP P12568
a	572	LYS	-	expression tag	UNP P12568
b	152	VAL	ILE	conflict	UNP P12568
b	213	SER	ARG	conflict	UNP P12568
b	215	PRO	SER	conflict	UNP P12568
b	514	GLY	-	expression tag	UNP P12568
b	515	SER	-	expression tag	UNP P12568
b	516	GLY	-	expression tag	UNP P12568
b	517	TYR	-	expression tag	UNP P12568
b	518	ILE	-	expression tag	UNP P12568
b	519	PRO	-	expression tag	UNP P12568
b	520	GLU	-	expression tag	UNP P12568
b	521	ALA	-	expression tag	UNP P12568
b	522	PRO	-	expression tag	UNP P12568
b	523	ARG	-	expression tag	UNP P12568
b	524	ASP	-	expression tag	UNP P12568
b	525	GLY	-	expression tag	UNP P12568
b	526	GLN	-	expression tag	UNP P12568
b	527	ALA	-	expression tag	UNP P12568
b	528	TYR	-	expression tag	UNP P12568
b	529	VAL	-	expression tag	UNP P12568
b	530	ARG	-	expression tag	UNP P12568
b	531	LYS	-	expression tag	UNP P12568
b	532	ASP	-	expression tag	UNP P12568
b	533	GLY	-	expression tag	UNP P12568

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Chain	Residue	Modelled	Actual	Comment	Reference
b	534	GLU	-	expression tag	UNP P12568
b	535	TRP	-	expression tag	UNP P12568
b	536	VAL	-	expression tag	UNP P12568
b	537	LEU	-	expression tag	UNP P12568
b	538	LEU	-	expression tag	UNP P12568
b	539	SER	-	expression tag	UNP P12568
b	540	THR	-	expression tag	UNP P12568
b	541	PHE	-	expression tag	UNP P12568
b	542	LEU	-	expression tag	UNP P12568
b	543	GLY	-	expression tag	UNP P12568
b	544	ARG	-	expression tag	UNP P12568
b	545	SER	-	expression tag	UNP P12568
b	546	LEU	-	expression tag	UNP P12568
b	547	GLU	-	expression tag	UNP P12568
b	548	VAL	-	expression tag	UNP P12568
b	549	LEU	-	expression tag	UNP P12568
b	550	PHE	-	expression tag	UNP P12568
b	551	GLN	-	expression tag	UNP P12568
b	552	GLY	-	expression tag	UNP P12568
b	553	PRO	-	expression tag	UNP P12568
b	554	GLY	-	expression tag	UNP P12568
b	555	HIS	-	expression tag	UNP P12568
b	556	HIS	-	expression tag	UNP P12568
b	557	HIS	-	expression tag	UNP P12568
b	558	HIS	-	expression tag	UNP P12568
b	559	HIS	-	expression tag	UNP P12568
b	560	HIS	-	expression tag	UNP P12568
b	561	HIS	-	expression tag	UNP P12568
b	562	HIS	-	expression tag	UNP P12568
b	563	SER	-	expression tag	UNP P12568
b	564	ALA	-	expression tag	UNP P12568
b	565	TRP	-	expression tag	UNP P12568
b	566	SER	-	expression tag	UNP P12568
b	567	HIS	-	expression tag	UNP P12568
b	568	PRO	-	expression tag	UNP P12568
b	569	GLN	-	expression tag	UNP P12568
b	570	PHE	-	expression tag	UNP P12568
b	571	GLU	-	expression tag	UNP P12568
b	572	LYS	-	expression tag	UNP P12568
c	152	VAL	ILE	conflict	UNP P12568
c	213	SER	ARG	conflict	UNP P12568
c	215	PRO	SER	conflict	UNP P12568

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Chain	Residue	Modelled	Actual	Comment	Reference
c	514	GLY	-	expression tag	UNP P12568
c	515	SER	-	expression tag	UNP P12568
c	516	GLY	-	expression tag	UNP P12568
c	517	TYR	-	expression tag	UNP P12568
c	518	ILE	-	expression tag	UNP P12568
c	519	PRO	-	expression tag	UNP P12568
c	520	GLU	-	expression tag	UNP P12568
c	521	ALA	-	expression tag	UNP P12568
c	522	PRO	-	expression tag	UNP P12568
c	523	ARG	-	expression tag	UNP P12568
c	524	ASP	-	expression tag	UNP P12568
c	525	GLY	-	expression tag	UNP P12568
c	526	GLN	-	expression tag	UNP P12568
c	527	ALA	-	expression tag	UNP P12568
c	528	TYR	-	expression tag	UNP P12568
c	529	VAL	-	expression tag	UNP P12568
c	530	ARG	-	expression tag	UNP P12568
c	531	LYS	-	expression tag	UNP P12568
c	532	ASP	-	expression tag	UNP P12568
c	533	GLY	-	expression tag	UNP P12568
c	534	GLU	-	expression tag	UNP P12568
c	535	TRP	-	expression tag	UNP P12568
c	536	VAL	-	expression tag	UNP P12568
c	537	LEU	-	expression tag	UNP P12568
c	538	LEU	-	expression tag	UNP P12568
c	539	SER	-	expression tag	UNP P12568
c	540	THR	-	expression tag	UNP P12568
c	541	PHE	-	expression tag	UNP P12568
c	542	LEU	-	expression tag	UNP P12568
c	543	GLY	-	expression tag	UNP P12568
c	544	ARG	-	expression tag	UNP P12568
c	545	SER	-	expression tag	UNP P12568
c	546	LEU	-	expression tag	UNP P12568
c	547	GLU	-	expression tag	UNP P12568
c	548	VAL	-	expression tag	UNP P12568
c	549	LEU	-	expression tag	UNP P12568
c	550	PHE	-	expression tag	UNP P12568
c	551	GLN	-	expression tag	UNP P12568
c	552	GLY	-	expression tag	UNP P12568
c	553	PRO	-	expression tag	UNP P12568
c	554	GLY	-	expression tag	UNP P12568
c	555	HIS	-	expression tag	UNP P12568

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Chain	Residue	Modelled	Actual	Comment	Reference
c	556	HIS	-	expression tag	UNP P12568
c	557	HIS	-	expression tag	UNP P12568
c	558	HIS	-	expression tag	UNP P12568
c	559	HIS	-	expression tag	UNP P12568
c	560	HIS	-	expression tag	UNP P12568
c	561	HIS	-	expression tag	UNP P12568
c	562	HIS	-	expression tag	UNP P12568
c	563	SER	-	expression tag	UNP P12568
c	564	ALA	-	expression tag	UNP P12568
c	565	TRP	-	expression tag	UNP P12568
c	566	SER	-	expression tag	UNP P12568
c	567	HIS	-	expression tag	UNP P12568
c	568	PRO	-	expression tag	UNP P12568
c	569	GLN	-	expression tag	UNP P12568
c	570	PHE	-	expression tag	UNP P12568
c	571	GLU	-	expression tag	UNP P12568
c	572	LYS	-	expression tag	UNP P12568

- Molecule 3 is a protein called 2.4K Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	125	Total	C	N	O	S	0	0
			963	605	161	192	5		
3	F	125	Total	C	N	O	S	0	0
			963	605	161	192	5		
3	H	125	Total	C	N	O	S	0	0
			963	605	161	192	5		

- Molecule 4 is a protein called 2.4K Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	113	Total	C	N	O	S	0	0
			878	554	149	173	2		
4	G	113	Total	C	N	O	S	0	0
			878	554	149	173	2		
4	I	113	Total	C	N	O	S	0	0
			878	554	149	173	2		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

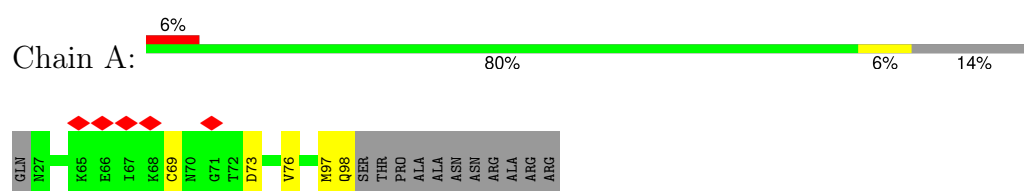


Mol	Chain	Residues	Atoms				AltConf
5	a	1	Total	C	N	O	0
			14	8	1	5	
5	b	1	Total	C	N	O	0
			14	8	1	5	
5	c	1	Total	C	N	O	0
			14	8	1	5	

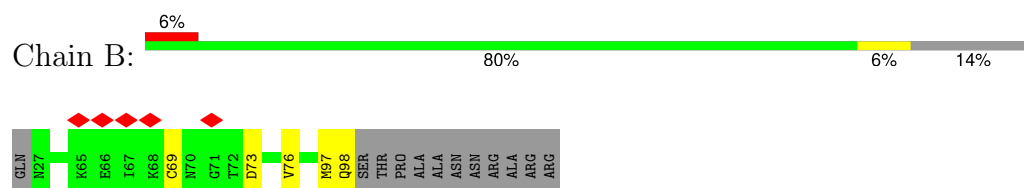
3 Residue-property plots [i](#)

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.

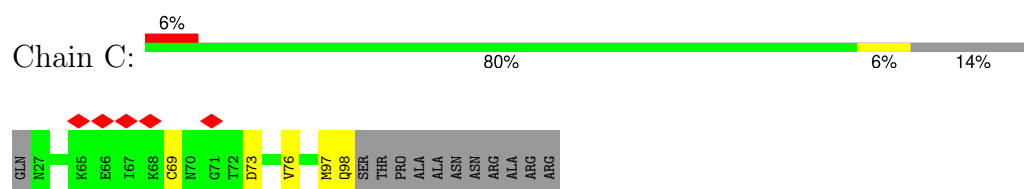
- Molecule 1: Fusion glycoprotein F2



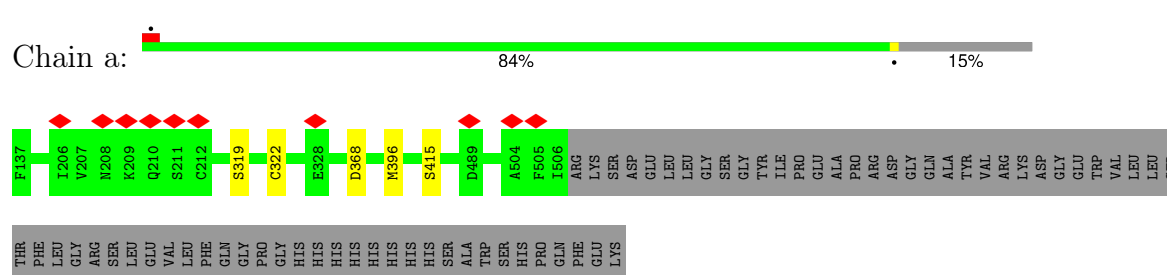
- Molecule 1: Fusion glycoprotein F2



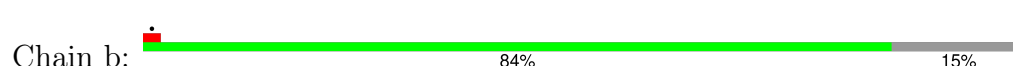
- Molecule 1: Fusion glycoprotein F2

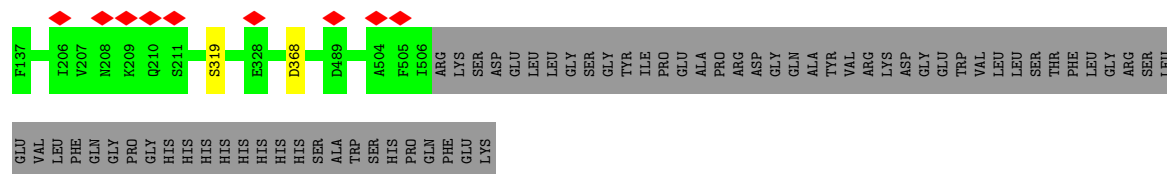


- Molecule 2: Fusion glycoprotein F1

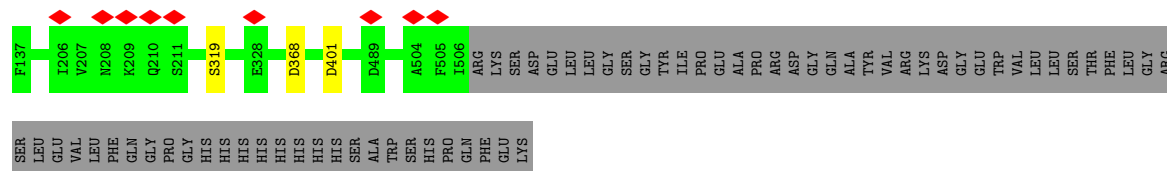
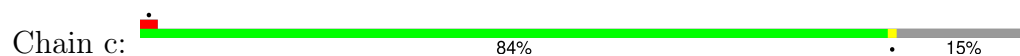


- Molecule 2: Fusion glycoprotein F1

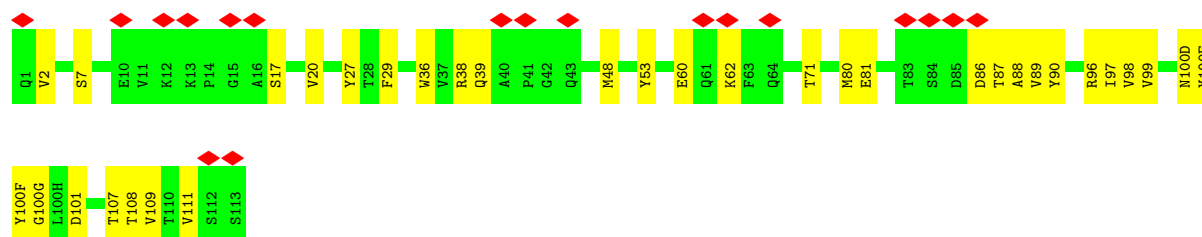




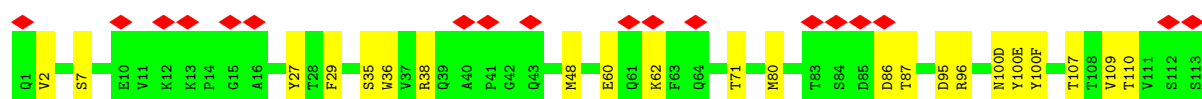
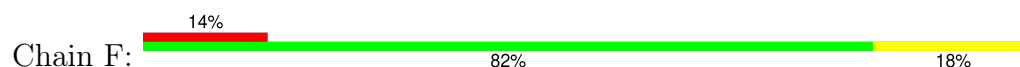
• Molecule 2: Fusion glycoprotein F1



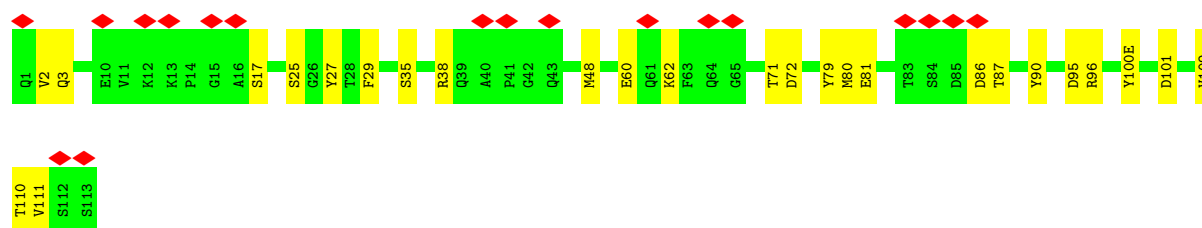
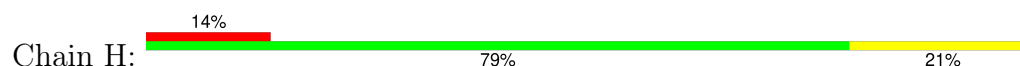
• Molecule 3: 2.4K Fab Heavy Chain



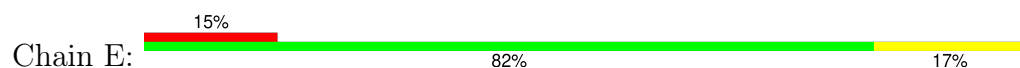
• Molecule 3: 2.4K Fab Heavy Chain



• Molecule 3: 2.4K Fab Heavy Chain

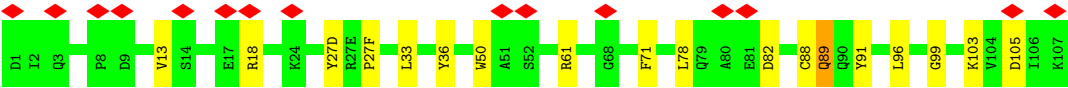
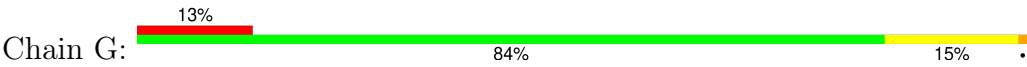


• Molecule 4: 2.4K Fab Light Chain

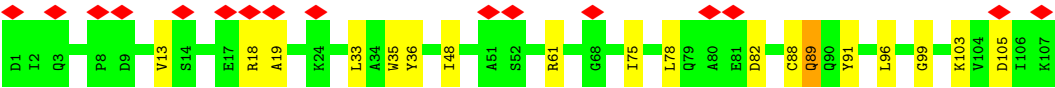
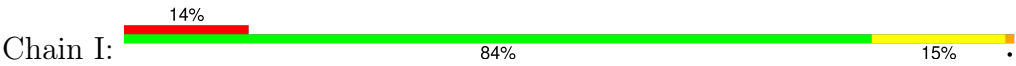




• Molecule 4: 2.4K Fab Light Chain



• Molecule 4: 2.4K Fab Light Chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	268139	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.977	Depositor
Minimum map value	-2.330	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.324	Depositor
Map size (\AA)	360.96, 360.96, 360.96	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.94, 0.94, 0.94	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	A	0.28	0/577	0.54	0/777
1	B	0.28	0/577	0.52	0/777
1	C	0.28	0/577	0.52	0/777
2	a	0.35	0/2891	0.50	0/3924
2	b	0.38	0/2891	0.53	0/3924
2	c	0.40	0/2891	0.53	0/3924
3	D	0.26	0/984	0.52	0/1338
3	F	0.26	0/984	0.50	0/1338
3	H	0.27	0/984	0.51	0/1338
4	E	0.29	0/899	0.47	0/1222
4	G	0.25	0/899	0.47	0/1222
4	I	0.26	0/899	0.47	0/1222
All	All	0.33	0/16053	0.51	0/21783

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	A	571	0	586	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	571	0	586	2	0
1	C	571	0	586	2	0
2	a	2847	0	2879	0	0
2	b	2847	0	2879	0	0
2	c	2847	0	2879	0	0
3	D	963	0	922	30	0
3	F	963	0	922	17	0
3	H	963	0	922	21	0
4	E	878	0	857	16	0
4	G	878	0	857	11	0
4	I	878	0	857	10	0
5	a	14	0	13	0	0
5	b	14	0	13	0	0
5	c	14	0	13	0	0
All	All	15819	0	15771	109	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 7.

All (109) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:87:THR:HG23	3:H:110:THR:HA	1.29	1.09
3:D:87:THR:HG22	3:D:111:VAL:H	0.91	1.07
3:D:87:THR:HG22	3:D:111:VAL:N	1.72	1.02
3:D:87:THR:CG2	3:D:111:VAL:H	1.73	1.00
3:D:96:ARG:HD3	3:D:100(E):TYR:CE1	2.07	0.89
3:H:87:THR:CG2	3:H:110:THR:HA	2.05	0.86
3:F:38:ARG:HB2	3:F:48:MET:SD	2.21	0.81
3:D:38:ARG:HB2	3:D:48:MET:SD	2.21	0.81
3:H:38:ARG:HB2	3:H:48:MET:SD	2.21	0.80
4:E:33:LEU:HD12	4:E:89:GLN:O	1.83	0.78
4:E:36:TYR:HE1	4:E:89:GLN:HG2	1.54	0.71
3:F:87:THR:HG23	3:F:110:THR:HA	1.71	0.71
3:D:80:MET:HE3	3:D:90:TYR:CG	2.27	0.69
3:D:20:VAL:HG21	3:D:80:MET:CE	2.23	0.69
3:D:20:VAL:HG21	3:D:80:MET:HE2	1.77	0.66
3:F:36:TRP:CG	3:F:80:MET:SD	2.90	0.65
3:D:97:ILE:CG2	3:D:99:VAL:HG22	2.27	0.65
3:D:20:VAL:CG2	3:D:80:MET:HE2	2.26	0.65
3:D:89:VAL:HG22	3:D:108:THR:HG22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:48:MET:HE2	3:F:80:MET:SD	2.39	0.63
3:D:97:ILE:HG22	3:D:99:VAL:H	1.66	0.59
3:D:96:ARG:HD3	3:D:100(E):TYR:CD1	2.38	0.58
3:H:87:THR:HG23	3:H:109:VAL:O	2.04	0.57
3:D:100(D):ASN:HB3	3:D:100(F):TYR:CE1	2.40	0.56
3:D:36:TRP:CE3	3:D:80:MET:SD	3.00	0.55
3:D:20:VAL:HB	3:D:80:MET:HB3	1.88	0.55
4:G:36:TYR:HE1	4:G:89:GLN:HG2	1.72	0.55
3:H:3:GLN:CG	3:H:25:SER:OG	2.54	0.55
4:I:36:TYR:HE1	4:I:89:GLN:HG2	1.72	0.54
3:H:87:THR:OG1	3:H:111:VAL:N	2.29	0.54
3:F:36:TRP:CE3	3:F:80:MET:CE	2.91	0.53
3:H:3:GLN:HG2	3:H:25:SER:OG	2.09	0.53
3:D:100(E):TYR:HD2	3:D:100(G):GLY:H	1.57	0.53
1:B:97:MET:HE3	1:B:98:GLN:HG3	1.91	0.52
3:F:36:TRP:CB	3:F:80:MET:SD	2.97	0.52
4:G:103:LYS:NZ	4:G:105:ASP:OD1	2.43	0.52
3:H:80:MET:HE3	3:H:90:TYR:CD2	2.45	0.52
3:F:35:SER:OG	3:F:95:ASP:OD2	2.27	0.52
4:E:19:ALA:HB3	4:E:75:ILE:HB	1.92	0.52
3:F:87:THR:HA	3:F:109:VAL:O	2.11	0.51
3:D:101:ASP:OD1	3:D:101:ASP:N	2.39	0.51
4:G:36:TYR:CE1	4:G:89:GLN:HG2	2.45	0.51
1:A:97:MET:HE3	1:A:98:GLN:HG3	1.93	0.51
4:G:33:LEU:HD12	4:G:89:GLN:O	2.11	0.50
4:E:103:LYS:NZ	4:E:105:ASP:OD1	2.43	0.50
3:F:36:TRP:HB3	3:F:80:MET:SD	2.52	0.49
3:H:48:MET:CE	3:H:80:MET:SD	3.01	0.49
3:D:97:ILE:HG23	3:D:99:VAL:HG22	1.93	0.48
4:E:91:TYR:HA	4:E:96:LEU:HD22	1.96	0.48
3:H:35:SER:OG	3:H:95:ASP:OD2	2.27	0.48
4:I:91:TYR:HA	4:I:96:LEU:HD22	1.95	0.48
4:G:91:TYR:HA	4:G:96:LEU:HD22	1.95	0.48
1:C:97:MET:HE2	1:C:98:GLN:HG3	1.95	0.47
3:D:80:MET:HE3	3:D:90:TYR:CD2	2.49	0.47
3:D:29:PHE:HE2	3:D:71:THR:HG23	1.80	0.47
4:I:103:LYS:NZ	4:I:105:ASP:OD1	2.43	0.47
3:H:17:SER:HB2	3:H:81:GLU:OE2	2.14	0.47
3:H:29:PHE:HE2	3:H:71:THR:HG23	1.79	0.47
3:F:29:PHE:HE2	3:F:71:THR:HG23	1.80	0.47
4:E:90:GLN:HE21	4:E:97:THR:H	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:33:LEU:HD22	4:E:71:PHE:CD1	2.50	0.47
3:D:87:THR:HA	3:D:109:VAL:O	2.15	0.46
4:E:18:ARG:NE	4:E:76:SER:HA	2.30	0.46
3:D:53:TYR:HB2	3:D:98:VAL:HG23	1.98	0.46
3:F:7:SER:O	3:F:107:THR:OG1	2.26	0.46
3:D:17:SER:HB2	3:D:81:GLU:OE2	2.16	0.46
4:I:88:CYS:O	4:I:99:GLY:N	2.49	0.46
3:H:101:ASP:OD1	3:H:101:ASP:N	2.39	0.45
4:G:88:CYS:O	4:G:99:GLY:N	2.49	0.45
4:I:18:ARG:HA	4:I:75:ILE:O	2.16	0.45
1:A:73:ASP:HB3	1:A:76:VAL:HG12	1.98	0.45
1:B:73:ASP:HB3	1:B:76:VAL:HG12	1.98	0.45
4:E:61:ARG:NE	4:E:82:ASP:OD2	2.46	0.45
3:H:48:MET:HE1	3:H:80:MET:SD	2.57	0.45
3:F:36:TRP:CE3	3:F:80:MET:HE2	2.51	0.44
3:F:36:TRP:CD2	3:F:80:MET:SD	3.10	0.44
4:I:13:VAL:HB	4:I:78:LEU:HD22	1.99	0.44
4:E:13:VAL:HB	4:E:78:LEU:HD22	1.99	0.44
1:C:73:ASP:HB3	1:C:76:VAL:HG12	1.98	0.44
3:F:100(D):ASN:HB3	3:F:100(F):TYR:CE1	2.52	0.44
4:E:18:ARG:HA	4:E:75:ILE:O	2.17	0.44
3:D:2:VAL:HG13	3:D:27:TYR:CD1	2.54	0.43
4:G:33:LEU:HD22	4:G:71:PHE:CD1	2.54	0.43
3:H:60:GLU:HG3	3:H:62:LYS:H	1.84	0.43
3:F:60:GLU:HG3	3:F:62:LYS:H	1.84	0.43
4:G:13:VAL:HB	4:G:78:LEU:HD22	1.99	0.43
3:H:2:VAL:HG13	3:H:27:TYR:CD1	2.54	0.43
4:I:19:ALA:HB3	4:I:75:ILE:HB	2.00	0.43
4:E:89:GLN:O	4:E:89:GLN:HG3	2.14	0.43
3:F:2:VAL:HG13	3:F:27:TYR:CD1	2.54	0.43
3:F:100(F):TYR:HE1	4:G:50:TRP:CH2	2.37	0.43
4:G:61:ARG:NE	4:G:82:ASP:OD2	2.46	0.43
3:D:60:GLU:HG3	3:D:62:LYS:H	1.84	0.42
3:H:72:ASP:HB2	3:H:79:TYR:HE1	1.84	0.42
3:D:7:SER:O	3:D:107:THR:OG1	2.26	0.42
3:D:38:ARG:HH22	3:D:86:ASP:HA	1.84	0.42
4:E:61:ARG:NH1	4:E:82:ASP:OD1	2.49	0.42
4:I:61:ARG:NE	4:I:82:ASP:OD2	2.46	0.41
3:H:3:GLN:HG3	3:H:25:SER:OG	2.18	0.41
3:H:48:MET:HE2	3:H:80:MET:SD	2.61	0.41
3:H:3:GLN:HG2	3:H:25:SER:HG	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:35:TRP:HB2	4:I:48:ILE:HB	2.03	0.41
4:G:27(D):TYR:CE2	4:G:27(F):PRO:HG2	2.57	0.40
3:D:39:GLN:O	3:D:88:ALA:HB1	2.22	0.40
3:H:100(E):TYR:CE1	4:I:91:TYR:CD2	3.10	0.40
3:D:80:MET:CE	3:D:90:TYR:CG	3.01	0.40
4:E:18:ARG:CZ	4:E:76:SER:HA	2.51	0.40
4:E:27(D):TYR:CE2	4:E:27(F):PRO:HG2	2.57	0.40
4:E:33:LEU:HD23	4:E:71:PHE:CG	2.56	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	70/84 (83%)	69 (99%)	1 (1%)	0	100	100
1	B	70/84 (83%)	69 (99%)	1 (1%)	0	100	100
1	C	70/84 (83%)	69 (99%)	1 (1%)	0	100	100
2	a	368/436 (84%)	363 (99%)	5 (1%)	0	100	100
2	b	368/436 (84%)	363 (99%)	5 (1%)	0	100	100
2	c	368/436 (84%)	364 (99%)	4 (1%)	0	100	100
3	D	123/125 (98%)	118 (96%)	5 (4%)	0	100	100
3	F	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
3	H	123/125 (98%)	122 (99%)	1 (1%)	0	100	100
4	E	111/113 (98%)	106 (96%)	5 (4%)	0	100	100
4	G	111/113 (98%)	106 (96%)	5 (4%)	0	100	100
4	I	111/113 (98%)	106 (96%)	5 (4%)	0	100	100
All	All	2016/2274 (89%)	1976 (98%)	40 (2%)	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	65/74 (88%)	64 (98%)	1 (2%)	60	86
1	B	65/74 (88%)	64 (98%)	1 (2%)	60	86
1	C	65/74 (88%)	64 (98%)	1 (2%)	60	86
2	a	338/394 (86%)	333 (98%)	5 (2%)	60	86
2	b	338/394 (86%)	336 (99%)	2 (1%)	84	95
2	c	338/394 (86%)	335 (99%)	3 (1%)	75	92
3	D	102/102 (100%)	102 (100%)	0	100	100
3	F	102/102 (100%)	99 (97%)	3 (3%)	37	71
3	H	102/102 (100%)	100 (98%)	2 (2%)	50	81
4	E	98/98 (100%)	97 (99%)	1 (1%)	73	91
4	G	98/98 (100%)	96 (98%)	2 (2%)	50	81
4	I	98/98 (100%)	96 (98%)	2 (2%)	50	81
All	All	1809/2004 (90%)	1786 (99%)	23 (1%)	64	88

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	CYS
2	a	319	SER
2	a	322	CYS
2	a	368	ASP
2	a	396	MET
2	a	415	SER
1	B	69	CYS
2	b	319	SER
2	b	368	ASP
1	C	69	CYS
2	c	319	SER

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Mol	Chain	Res	Type
2	c	368	ASP
2	c	401	ASP
4	E	89	GLN
3	F	86	ASP
3	F	96	ARG
3	F	100(E)	TYR
4	G	18	ARG
4	G	89	GLN
3	H	86	ASP
3	H	96	ARG
4	I	33	LEU
4	I	89	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
4	I	38	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](#)

3 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	a	601	2	14,14,15	0.27	0	17,19,21	0.55	0
5	NAG	b	601	2	14,14,15	0.29	0	17,19,21	0.55	0
5	NAG	c	601	2	14,14,15	0.29	0	17,19,21	0.54	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	a	601	2	-	4/6/23/26	0/1/1/1
5	NAG	b	601	2	-	4/6/23/26	0/1/1/1
5	NAG	c	601	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	a	601	NAG	C4-C5-C6-O6
5	b	601	NAG	C4-C5-C6-O6
5	c	601	NAG	C4-C5-C6-O6
5	a	601	NAG	C3-C2-N2-C7
5	b	601	NAG	C3-C2-N2-C7
5	c	601	NAG	C3-C2-N2-C7
5	a	601	NAG	C1-C2-N2-C7
5	b	601	NAG	C1-C2-N2-C7
5	c	601	NAG	C1-C2-N2-C7
5	a	601	NAG	O5-C5-C6-O6
5	b	601	NAG	O5-C5-C6-O6
5	c	601	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.

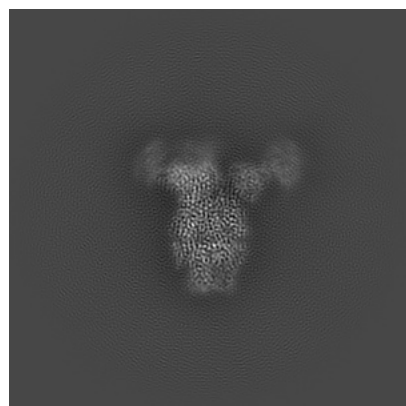
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41089. These allow visual inspection of the internal detail of the map and identification of artifacts.

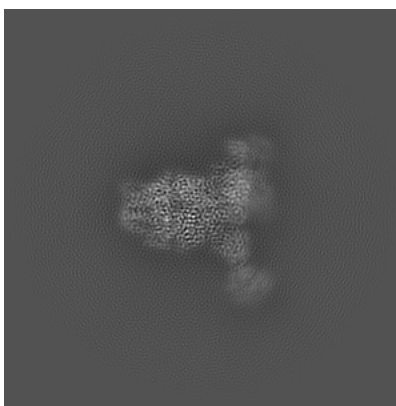
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

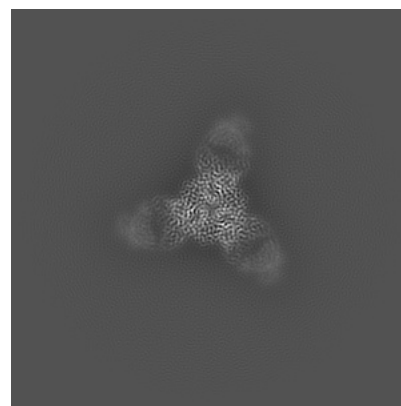
6.1.1 Primary map



X

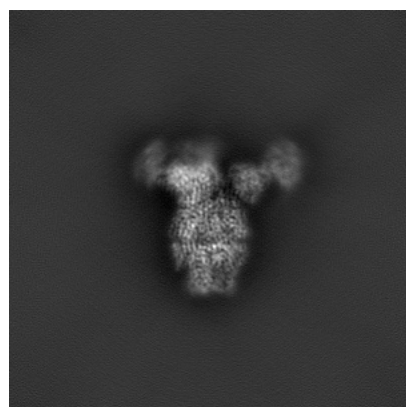


Y

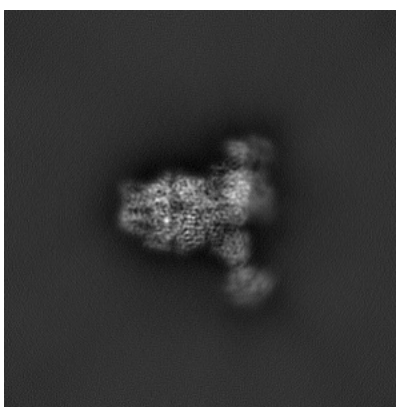


Z

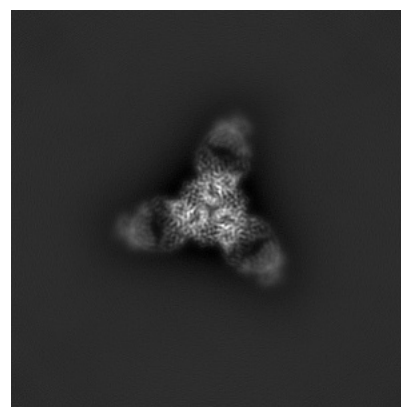
6.1.2 Raw map



X



Y

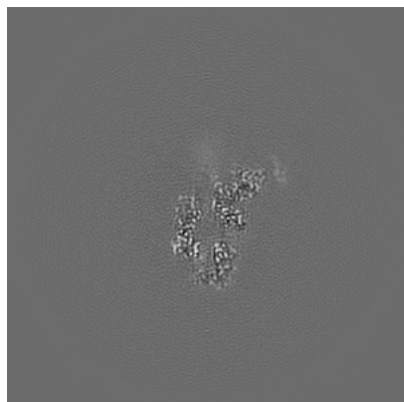


Z

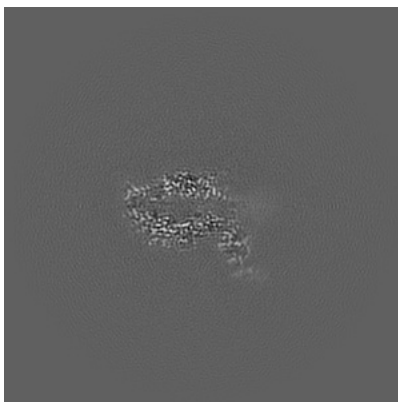
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

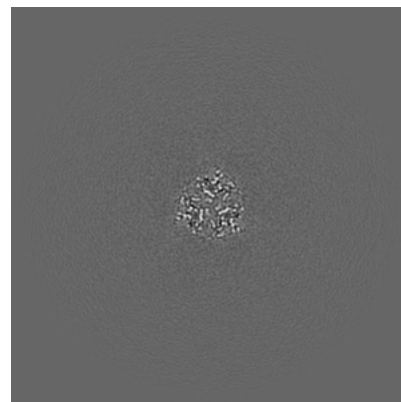
6.2.1 Primary map



X Index: 192

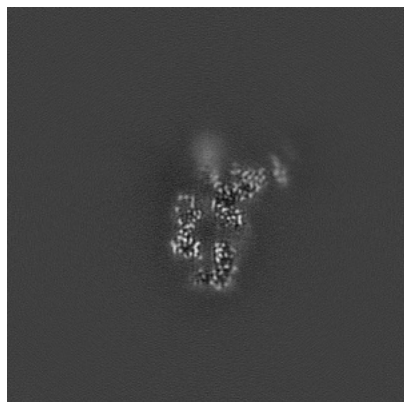


Y Index: 192

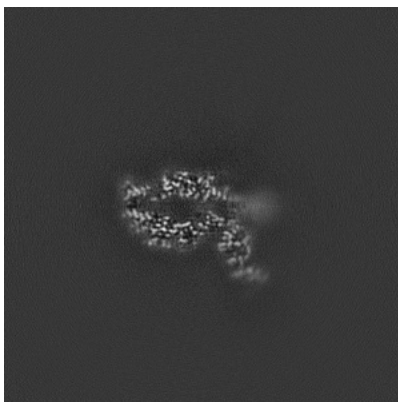


Z Index: 192

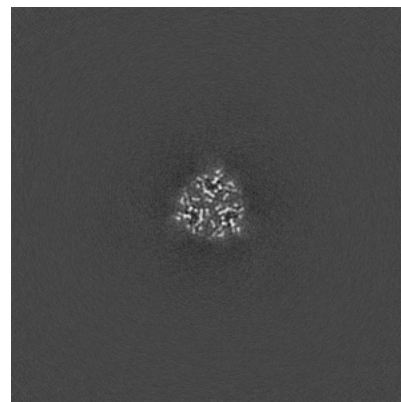
6.2.2 Raw map



X Index: 192



Y Index: 192

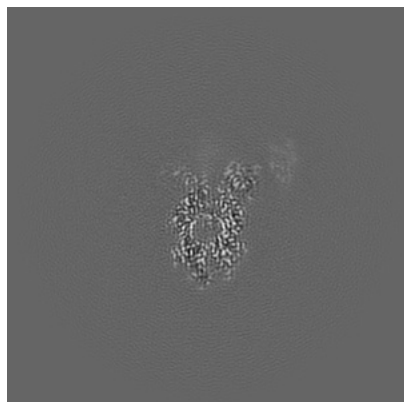


Z Index: 192

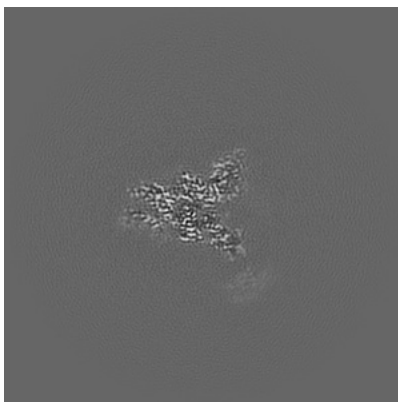
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

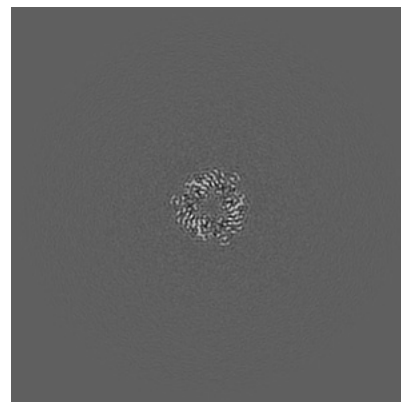
6.3.1 Primary map



X Index: 201

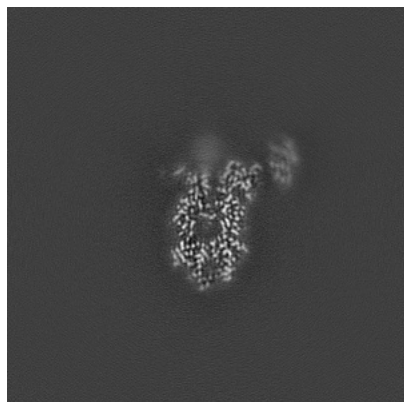


Y Index: 177

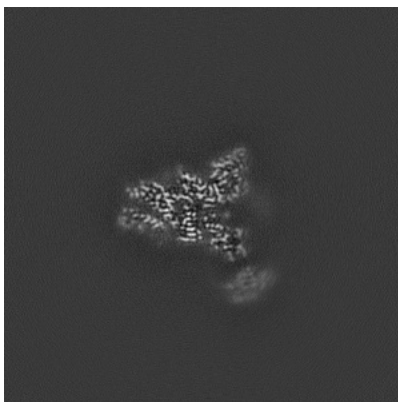


Z Index: 177

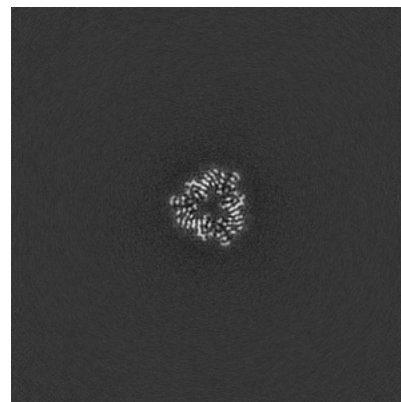
6.3.2 Raw map



X Index: 200



Y Index: 177

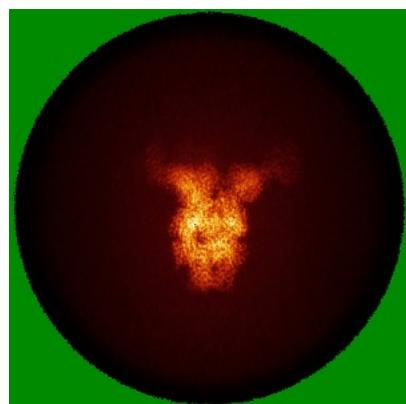


Z Index: 177

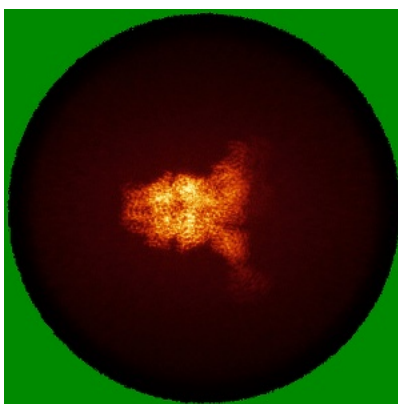
The images above show the largest variance slices of the map in three orthogonal directions.

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

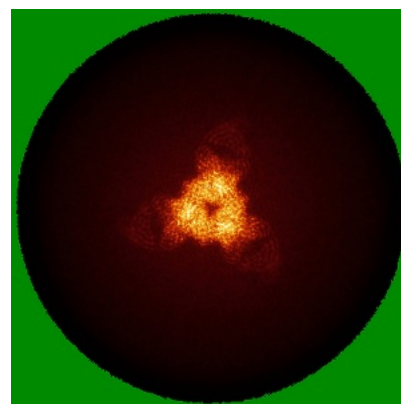
6.4.1 Primary map



X

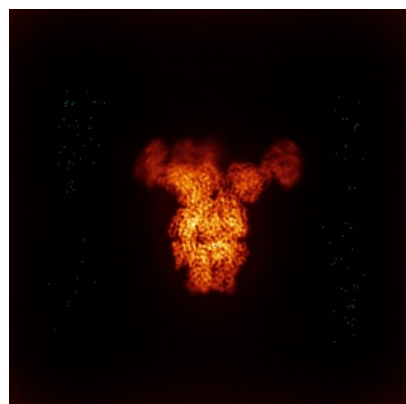


Y

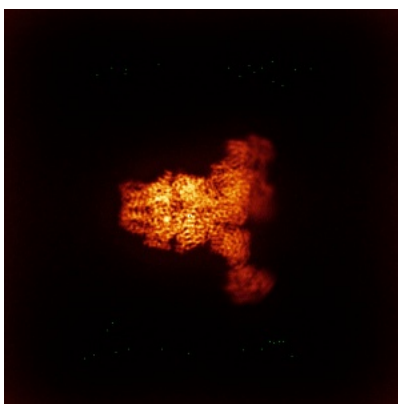


Z

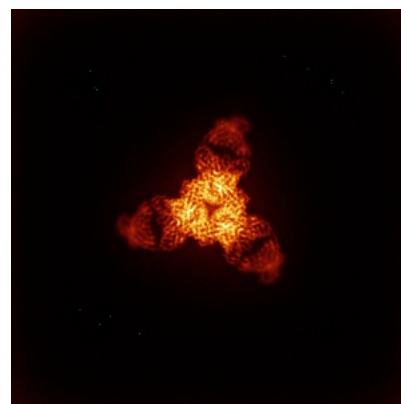
6.4.2 Raw map



X



Y

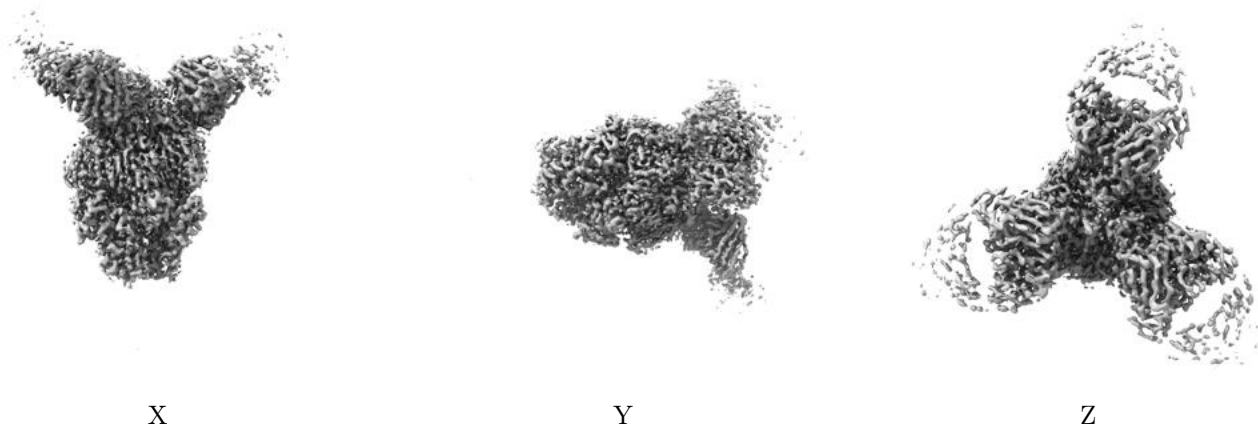


Z

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

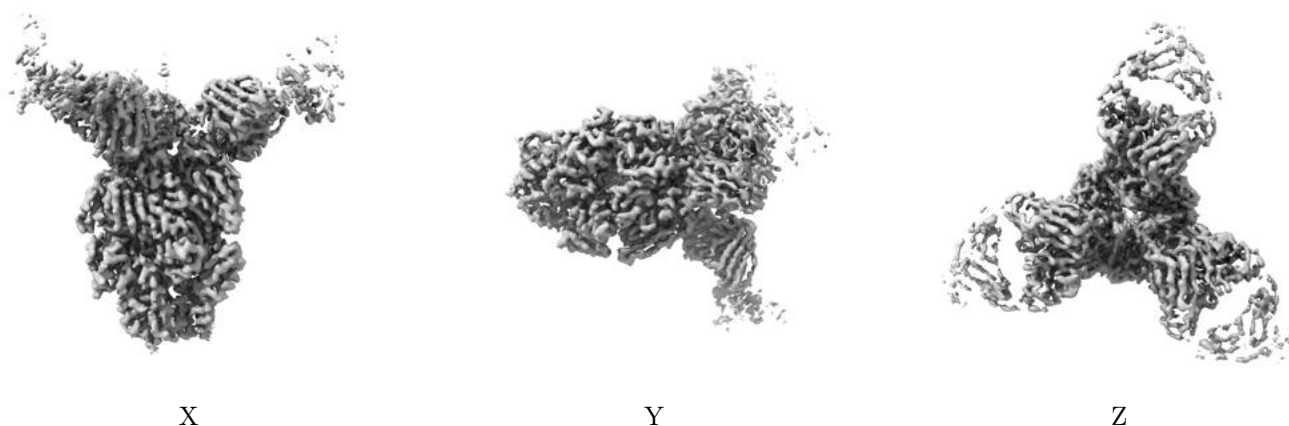
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.324. 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.

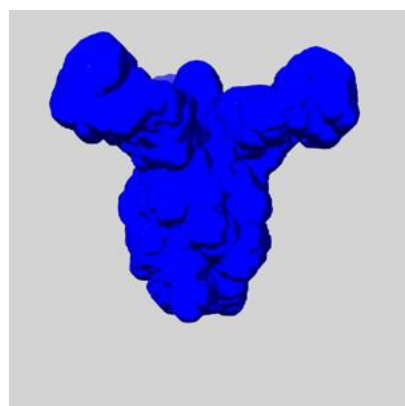
6.6 Mask visualisation [i](#)

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

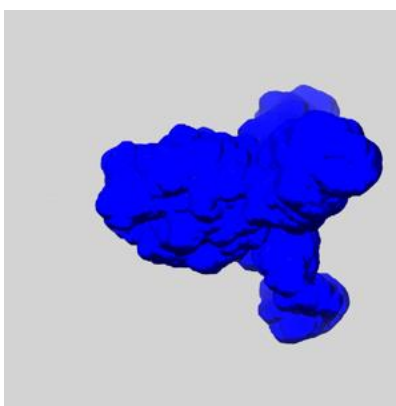
A mask typically either:

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

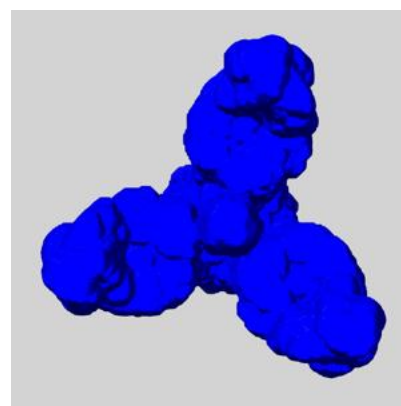
6.6.1 emd_41089_msk_1.map [i](#)



X



Y

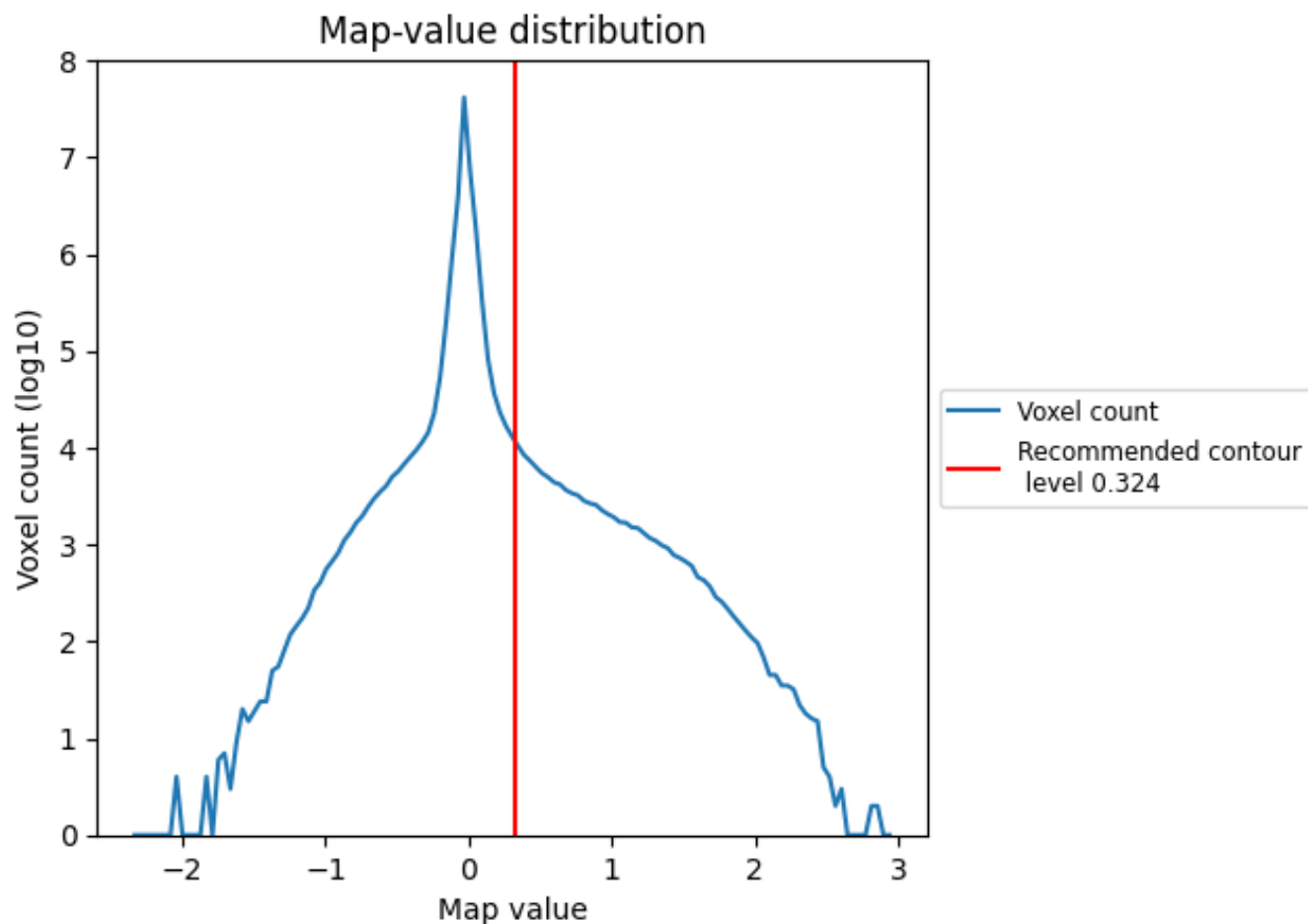


Z

7 Map analysis [i](#)

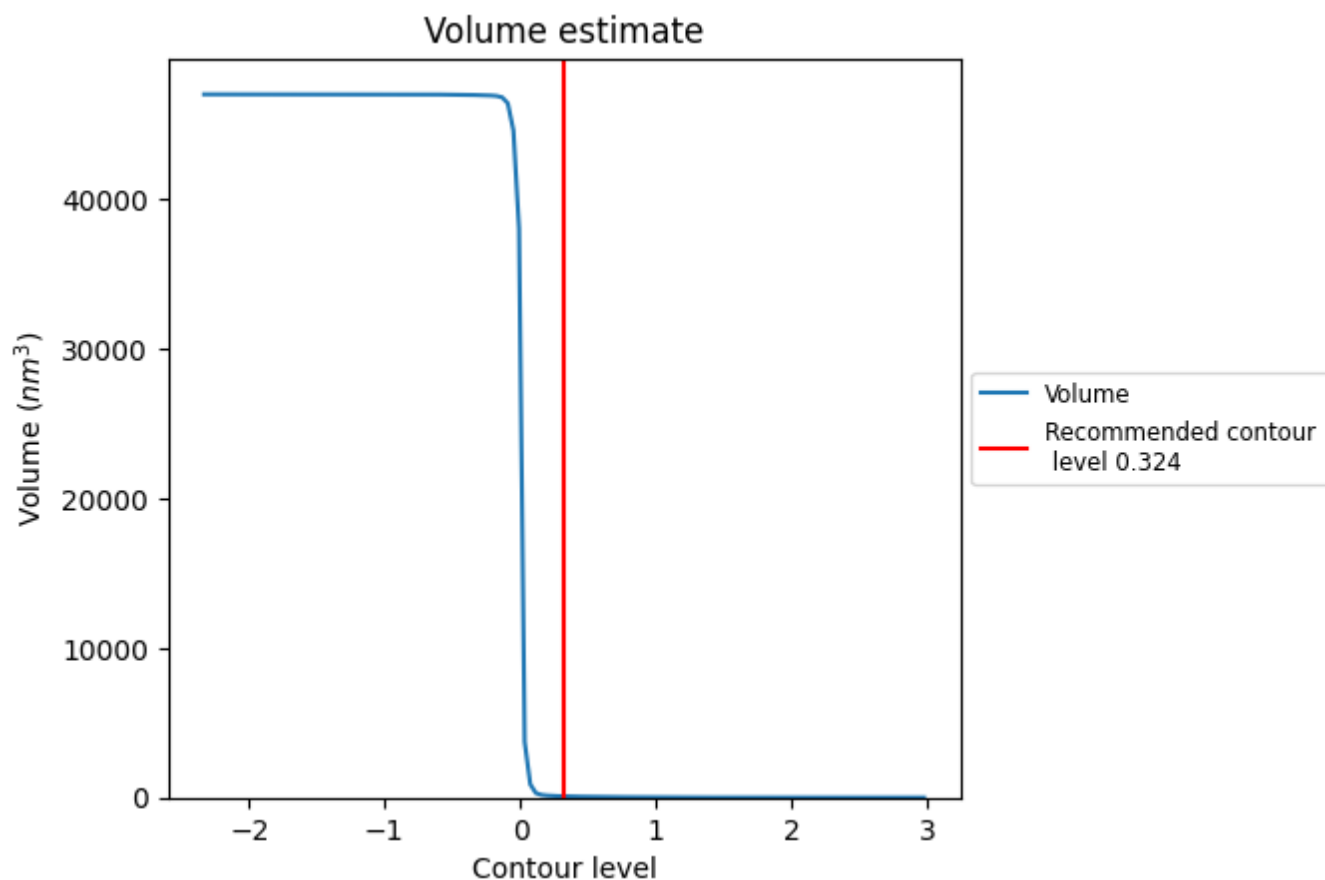
This section contains the results of statistical analysis of the map.

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.

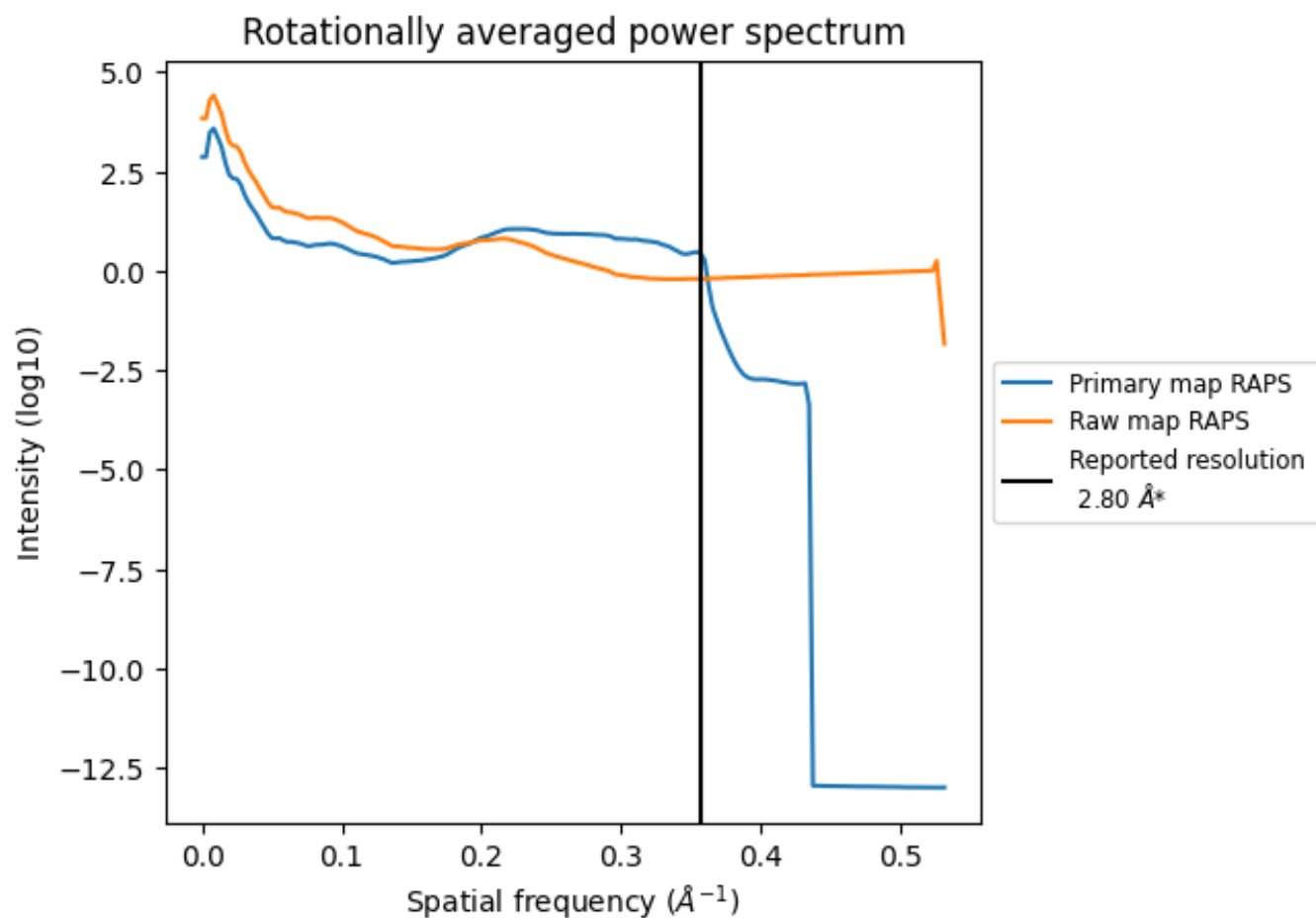
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 83 nm³; this corresponds to an approximate mass of 75 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 ⓘ

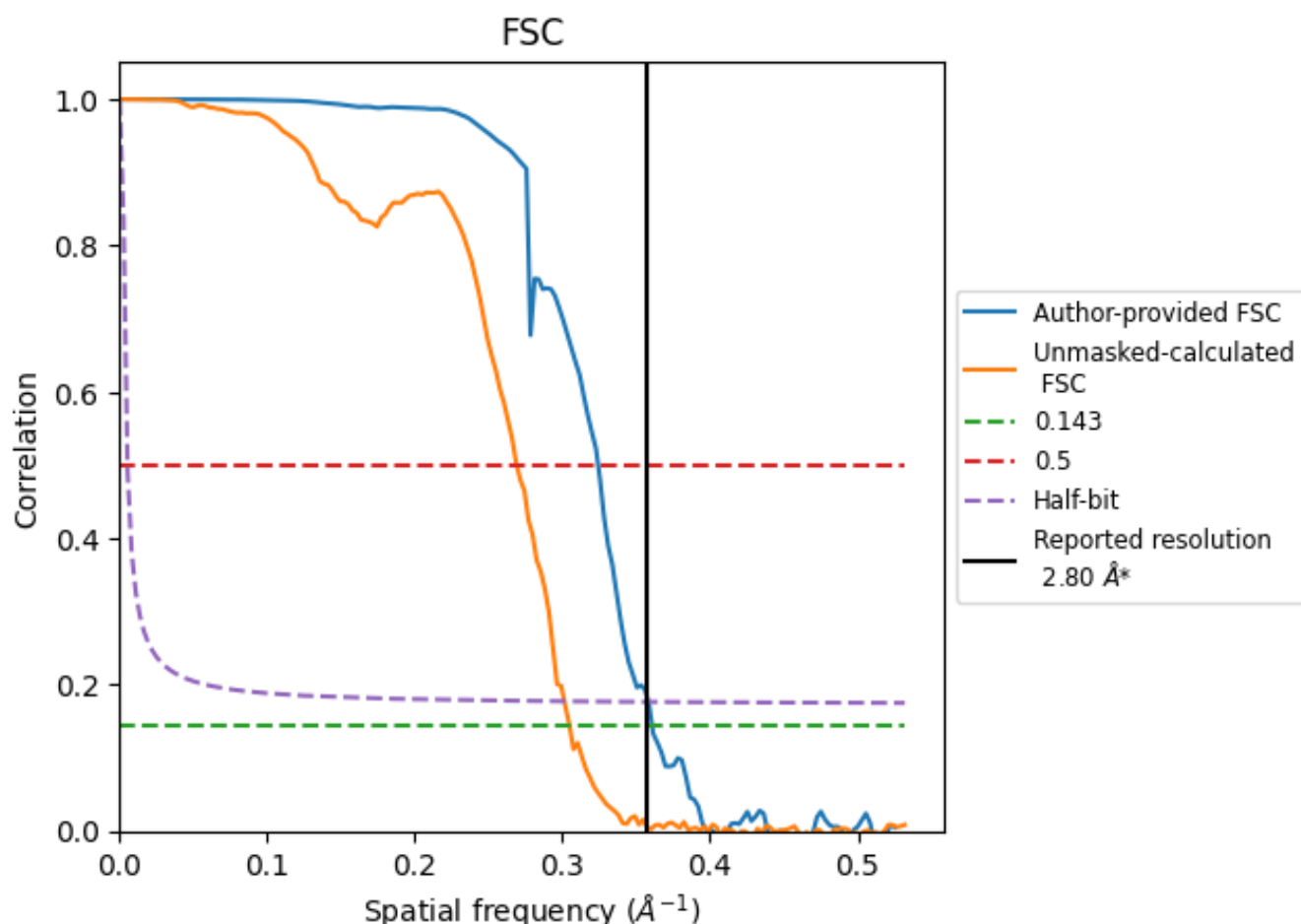


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 \AA^{-1}

8.2 Resolution estimates [i](#)

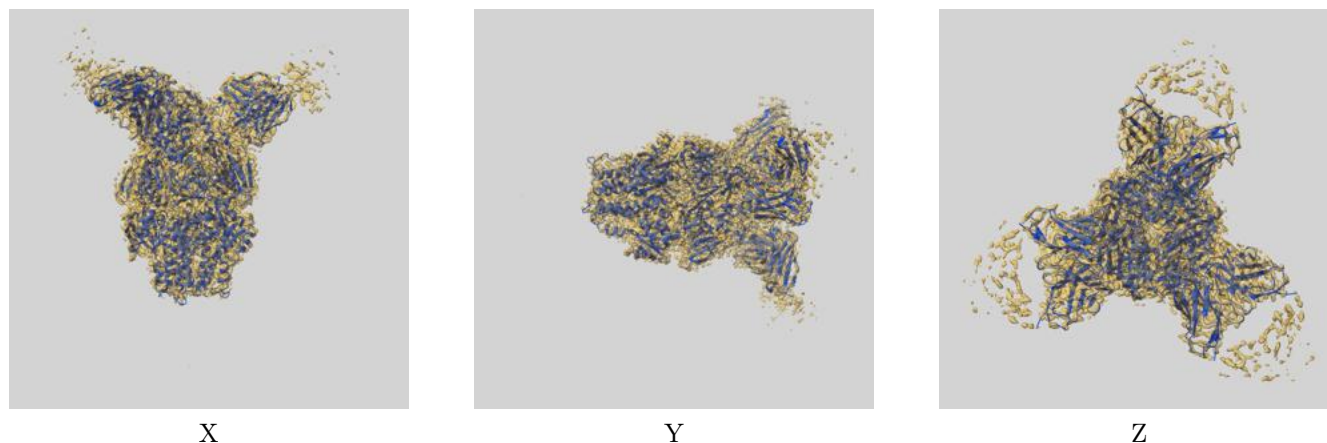
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.77	3.08	2.79
Unmasked-calculated*	3.28	3.72	3.32

*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 3.28 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

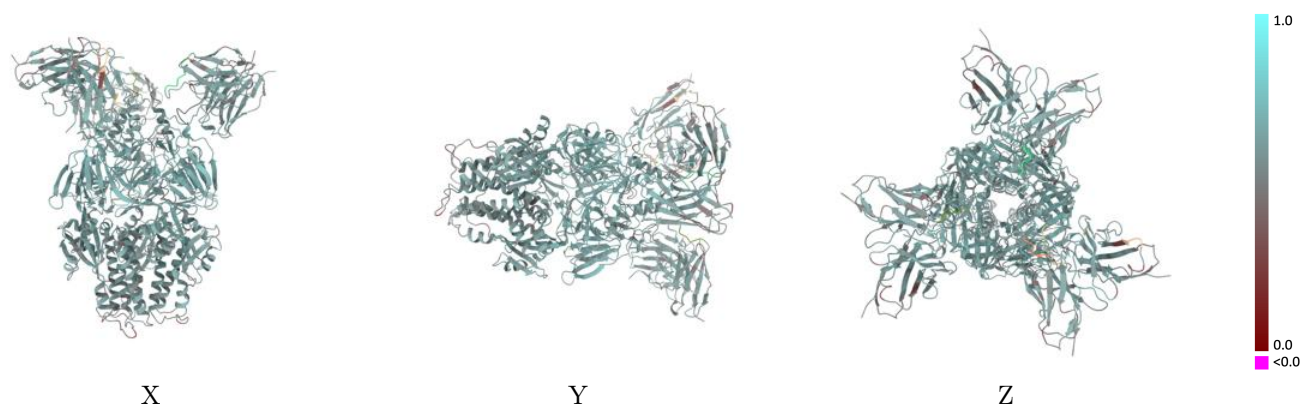
This section contains information regarding the fit between EMDB map EMD-41089 and PDB model 8T7A. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



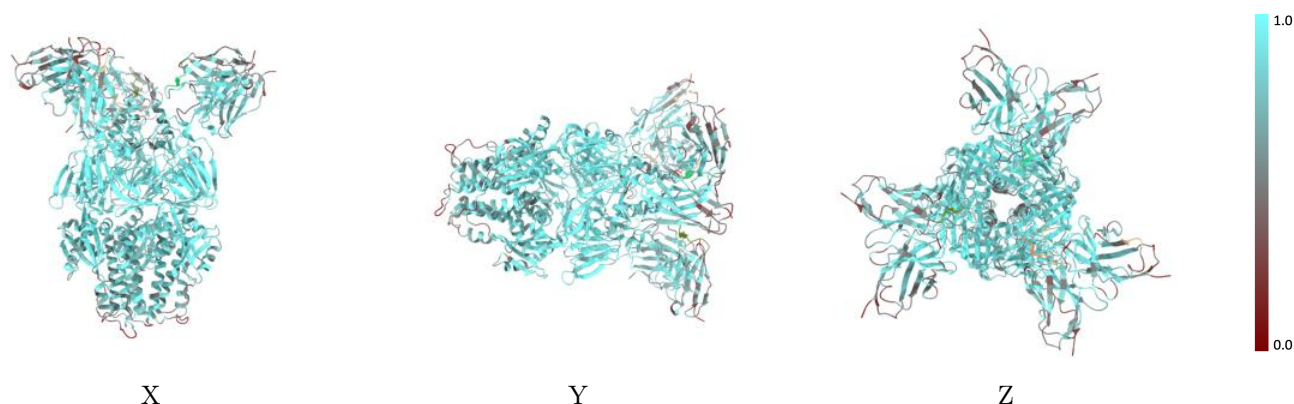
The images above show the 3D surface view of the map at the recommended contour level 0.324 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



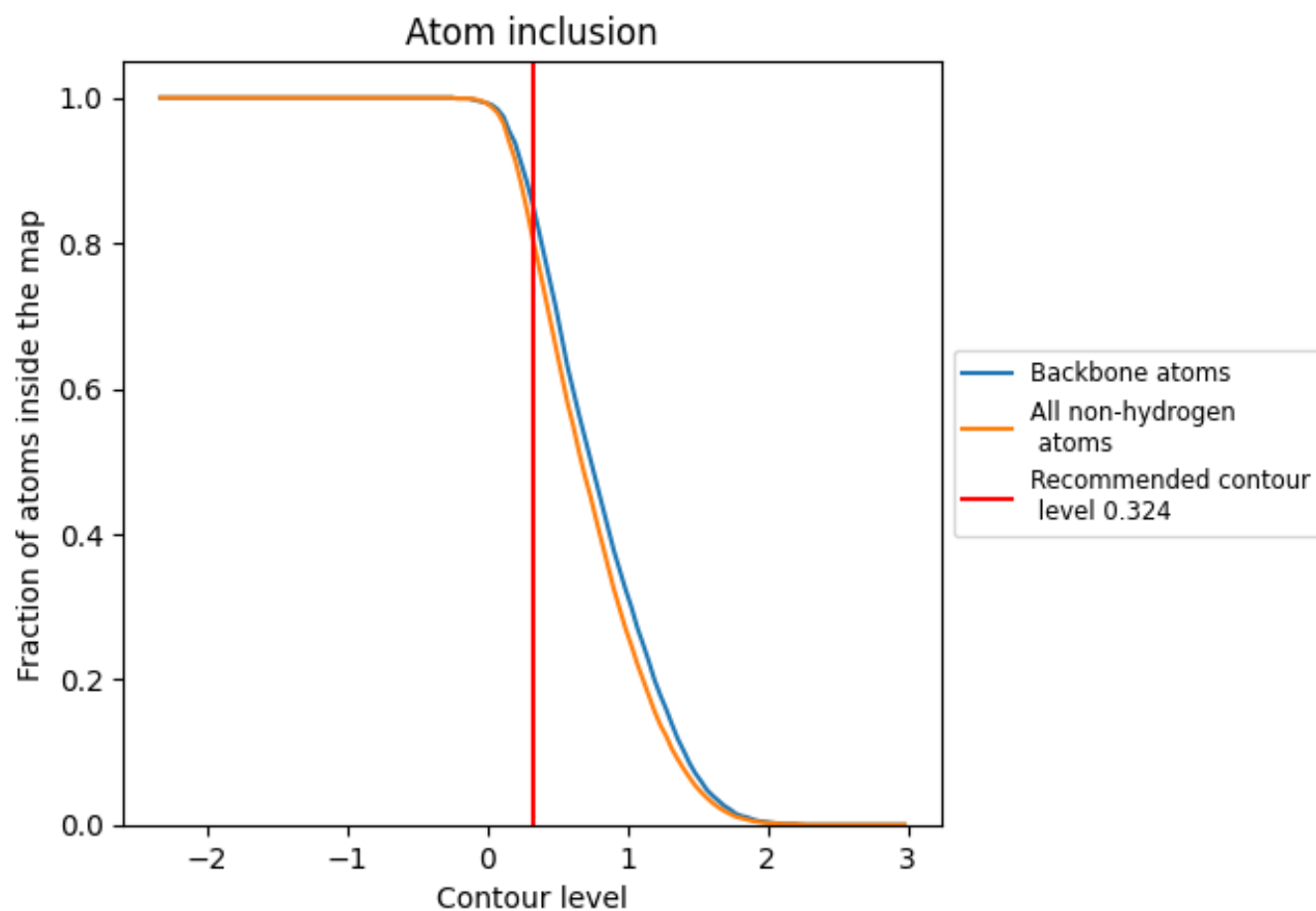
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.324).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 81% 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 (0.324) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8070	<div><div></div></div> 0.5870
A	<div><div></div></div> 0.8250	<div><div></div></div> 0.5860
B	<div><div></div></div> 0.8140	<div><div></div></div> 0.5870
C	<div><div></div></div> 0.8210	<div><div></div></div> 0.5870
D	<div><div></div></div> 0.7330	<div><div></div></div> 0.5570
E	<div><div></div></div> 0.6800	<div><div></div></div> 0.5560
F	<div><div></div></div> 0.7360	<div><div></div></div> 0.5680
G	<div><div></div></div> 0.6750	<div><div></div></div> 0.5610
H	<div><div></div></div> 0.7380	<div><div></div></div> 0.5650
I	<div><div></div></div> 0.6790	<div><div></div></div> 0.5600
a	<div><div></div></div> 0.8680	<div><div></div></div> 0.6040
b	<div><div></div></div> 0.8660	<div><div></div></div> 0.6030
c	<div><div></div></div> 0.8700	<div><div></div></div> 0.6040

1.0

0.0

<0.0