WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB EM Validation Summary Report (i)

May 2, 2023 – 08:14 PM EDT

PDB ID	:	7UJA
EMDB ID	:	EMD-26562
Title	:	Cryo-EM structure of Human respiratory syncytial virus F variant (construct pXCS847A)
Authors	:	Lees, J.A.; Ammirati, M.; Han, S.
Deposited on	:	2022-03-30
Resolution	:	3.70 Å(reported)

This is a wwPDB EM Validation Summary 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 (i) 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 (i)) were used in the production of this report:
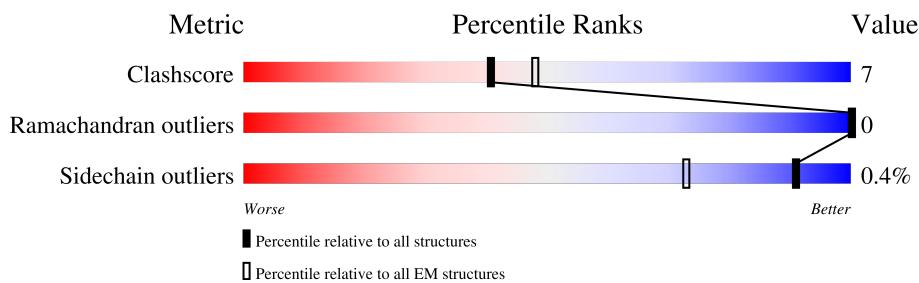
|		
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1   Overall quality at a glance   ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY
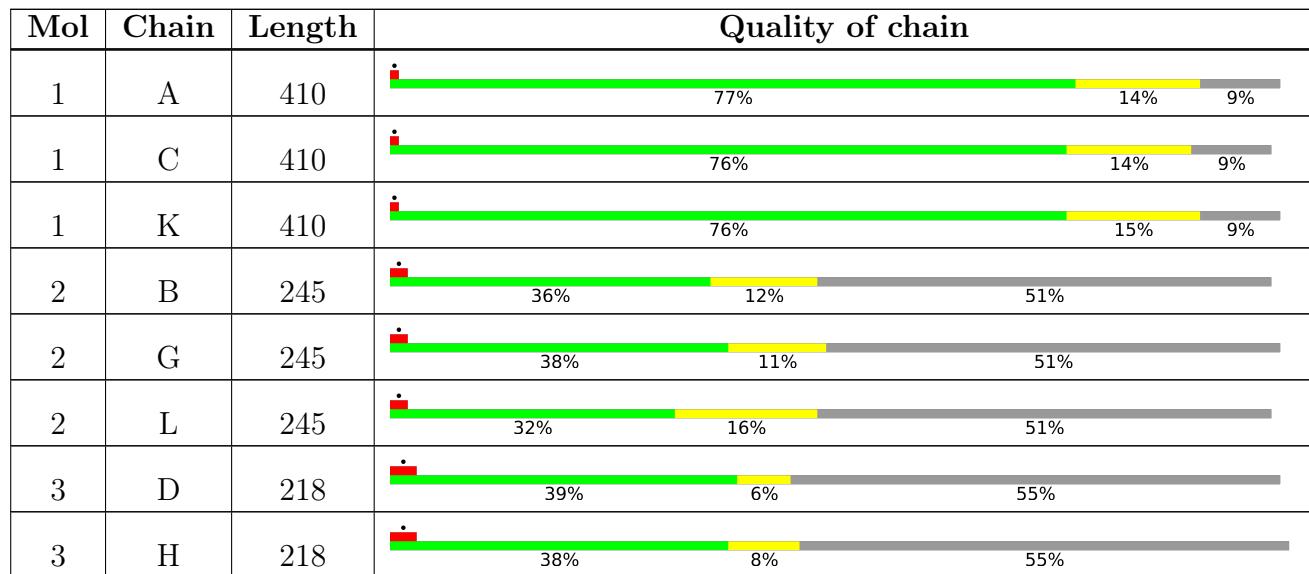
The reported resolution of this entry is 3.70 Å.

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	Percentile Ranks	Value
Clashscore		7
Ramachandran outliers		0
Sidechain outliers		0.4%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures
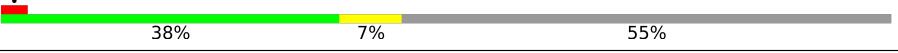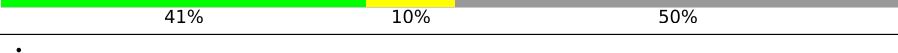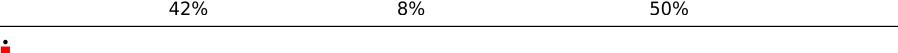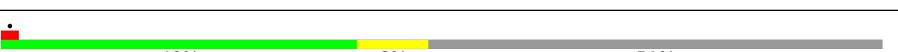
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	410	77% 14% 9%
1	C	410	76% 14% 9%
1	K	410	76% 15% 9%
2	B	245	36% 12% 51%
2	G	245	38% 11% 51%
2	L	245	32% 16% 51%
3	D	218	39% 6% 55%
3	H	218	38% 8% 55%

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Mol	Chain	Length	Quality of chain
3	M	218	38% 7% 55%
4	E	246	6% 40% 10% 50%
4	I	246	5% 41% 10% 50%
4	N	246	42% 8% 50%
5	F	215	39% 10% 51%
5	J	215	45% . 51%
5	O	215	40% 8% 51%
6	P	109	6% 63% 9% 28%
6	Q	109	60% 13% 28%
6	R	109	62% 10% 28%

2   Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 20748 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 RSV variant (construct pXCS847A) F1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	372	Total 2859	C 1804	N 474	O 562	S 19	0	0
1	C	372	Total 2859	C 1804	N 474	O 562	S 19	0	0
1	K	372	Total 2859	C 1804	N 474	O 562	S 19	0	0

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	148	CYS	ILE	engineered mutation	UNP A0A7D5GVC1
A	190	ILE	SER	engineered mutation	UNP A0A7D5GVC1
A	486	SER	ASP	engineered mutation	UNP A0A7D5GVC1
A	514	SER	-	expression tag	UNP A0A7D5GVC1
A	515	ALA	-	expression tag	UNP A0A7D5GVC1
A	516	ILE	-	expression tag	UNP A0A7D5GVC1
A	517	GLY	-	expression tag	UNP A0A7D5GVC1
A	518	GLY	-	expression tag	UNP A0A7D5GVC1
A	519	TYR	-	expression tag	UNP A0A7D5GVC1
A	520	ILE	-	expression tag	UNP A0A7D5GVC1
A	521	PRO	-	expression tag	UNP A0A7D5GVC1
A	522	GLU	-	expression tag	UNP A0A7D5GVC1
A	523	ALA	-	expression tag	UNP A0A7D5GVC1
A	524	PRO	-	expression tag	UNP A0A7D5GVC1
A	525	ARG	-	expression tag	UNP A0A7D5GVC1
A	526	ASP	-	expression tag	UNP A0A7D5GVC1
A	527	GLY	-	expression tag	UNP A0A7D5GVC1
A	528	GLN	-	expression tag	UNP A0A7D5GVC1
A	529	ALA	-	expression tag	UNP A0A7D5GVC1
A	530	TYR	-	expression tag	UNP A0A7D5GVC1
A	531	VAL	-	expression tag	UNP A0A7D5GVC1
A	532	ARG	-	expression tag	UNP A0A7D5GVC1
A	533	LYS	-	expression tag	UNP A0A7D5GVC1
A	534	ASP	-	expression tag	UNP A0A7D5GVC1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	535	GLY	-	expression tag	UNP A0A7D5GVC1
A	536	GLU	-	expression tag	UNP A0A7D5GVC1
A	537	TRP	-	expression tag	UNP A0A7D5GVC1
A	538	VAL	-	expression tag	UNP A0A7D5GVC1
A	539	LEU	-	expression tag	UNP A0A7D5GVC1
A	540	LEU	-	expression tag	UNP A0A7D5GVC1
A	541	SER	-	expression tag	UNP A0A7D5GVC1
A	542	THR	-	expression tag	UNP A0A7D5GVC1
A	543	PHE	-	expression tag	UNP A0A7D5GVC1
A	544	LEU	-	expression tag	UNP A0A7D5GVC1
A	545	GLY	-	expression tag	UNP A0A7D5GVC1
A	546	GLY	-	expression tag	UNP A0A7D5GVC1
C	148	CYS	ILE	engineered mutation	UNP A0A7D5GVC1
C	190	ILE	SER	engineered mutation	UNP A0A7D5GVC1
C	486	SER	ASP	engineered mutation	UNP A0A7D5GVC1
C	514	SER	-	expression tag	UNP A0A7D5GVC1
C	515	ALA	-	expression tag	UNP A0A7D5GVC1
C	516	ILE	-	expression tag	UNP A0A7D5GVC1
C	517	GLY	-	expression tag	UNP A0A7D5GVC1
C	518	GLY	-	expression tag	UNP A0A7D5GVC1
C	519	TYR	-	expression tag	UNP A0A7D5GVC1
C	520	ILE	-	expression tag	UNP A0A7D5GVC1
C	521	PRO	-	expression tag	UNP A0A7D5GVC1
C	522	GLU	-	expression tag	UNP A0A7D5GVC1
C	523	ALA	-	expression tag	UNP A0A7D5GVC1
C	524	PRO	-	expression tag	UNP A0A7D5GVC1
C	525	ARG	-	expression tag	UNP A0A7D5GVC1
C	526	ASP	-	expression tag	UNP A0A7D5GVC1
C	527	GLY	-	expression tag	UNP A0A7D5GVC1
C	528	GLN	-	expression tag	UNP A0A7D5GVC1
C	529	ALA	-	expression tag	UNP A0A7D5GVC1
C	530	TYR	-	expression tag	UNP A0A7D5GVC1
C	531	VAL	-	expression tag	UNP A0A7D5GVC1
C	532	ARG	-	expression tag	UNP A0A7D5GVC1
C	533	LYS	-	expression tag	UNP A0A7D5GVC1
C	534	ASP	-	expression tag	UNP A0A7D5GVC1
C	535	GLY	-	expression tag	UNP A0A7D5GVC1
C	536	GLU	-	expression tag	UNP A0A7D5GVC1
C	537	TRP	-	expression tag	UNP A0A7D5GVC1
C	538	VAL	-	expression tag	UNP A0A7D5GVC1
C	539	LEU	-	expression tag	UNP A0A7D5GVC1
C	540	LEU	-	expression tag	UNP A0A7D5GVC1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	541	SER	-	expression tag	UNP A0A7D5GVC1
C	542	THR	-	expression tag	UNP A0A7D5GVC1
C	543	PHE	-	expression tag	UNP A0A7D5GVC1
C	544	LEU	-	expression tag	UNP A0A7D5GVC1
C	545	GLY	-	expression tag	UNP A0A7D5GVC1
C	546	GLY	-	expression tag	UNP A0A7D5GVC1
K	148	CYS	ILE	engineered mutation	UNP A0A7D5GVC1
K	190	ILE	SER	engineered mutation	UNP A0A7D5GVC1
K	486	SER	ASP	engineered mutation	UNP A0A7D5GVC1
K	514	SER	-	expression tag	UNP A0A7D5GVC1
K	515	ALA	-	expression tag	UNP A0A7D5GVC1
K	516	ILE	-	expression tag	UNP A0A7D5GVC1
K	517	GLY	-	expression tag	UNP A0A7D5GVC1
K	518	GLY	-	expression tag	UNP A0A7D5GVC1
K	519	TYR	-	expression tag	UNP A0A7D5GVC1
K	520	ILE	-	expression tag	UNP A0A7D5GVC1
K	521	PRO	-	expression tag	UNP A0A7D5GVC1
K	522	GLU	-	expression tag	UNP A0A7D5GVC1
K	523	ALA	-	expression tag	UNP A0A7D5GVC1
K	524	PRO	-	expression tag	UNP A0A7D5GVC1
K	525	ARG	-	expression tag	UNP A0A7D5GVC1
K	526	ASP	-	expression tag	UNP A0A7D5GVC1
K	527	GLY	-	expression tag	UNP A0A7D5GVC1
K	528	GLN	-	expression tag	UNP A0A7D5GVC1
K	529	ALA	-	expression tag	UNP A0A7D5GVC1
K	530	TYR	-	expression tag	UNP A0A7D5GVC1
K	531	VAL	-	expression tag	UNP A0A7D5GVC1
K	532	ARG	-	expression tag	UNP A0A7D5GVC1
K	533	LYS	-	expression tag	UNP A0A7D5GVC1
K	534	ASP	-	expression tag	UNP A0A7D5GVC1
K	535	GLY	-	expression tag	UNP A0A7D5GVC1
K	536	GLU	-	expression tag	UNP A0A7D5GVC1
K	537	TRP	-	expression tag	UNP A0A7D5GVC1
K	538	VAL	-	expression tag	UNP A0A7D5GVC1
K	539	LEU	-	expression tag	UNP A0A7D5GVC1
K	540	LEU	-	expression tag	UNP A0A7D5GVC1
K	541	SER	-	expression tag	UNP A0A7D5GVC1
K	542	THR	-	expression tag	UNP A0A7D5GVC1
K	543	PHE	-	expression tag	UNP A0A7D5GVC1
K	544	LEU	-	expression tag	UNP A0A7D5GVC1
K	545	GLY	-	expression tag	UNP A0A7D5GVC1
K	546	GLY	-	expression tag	UNP A0A7D5GVC1

- Molecule 2 is a protein called AM14 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	119	Total 934	C 587	N 162	O 180	S 5	0	0
2	G	119	Total 934	C 587	N 162	O 180	S 5	0	0
2	L	119	Total 934	C 587	N 162	O 180	S 5	0	0

- Molecule 3 is a protein called AM14 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	99	Total 769	C 483	N 129	O 153	S 4	0	0
3	H	99	Total 769	C 483	N 129	O 153	S 4	0	0
3	M	99	Total 769	C 483	N 129	O 153	S 4	0	0

- Molecule 4 is a protein called AM22 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	124	Total 940	C 598	N 155	O 183	S 4	0	0
4	I	124	Total 940	C 598	N 155	O 183	S 4	0	0
4	N	124	Total 940	C 598	N 155	O 183	S 4	0	0

- Molecule 5 is a protein called AM22 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	105	Total 785	C 497	N 135	O 151	S 2	0	0
5	J	105	Total 785	C 497	N 135	O 151	S 2	0	0
5	O	105	Total 785	C 497	N 135	O 151	S 2	0	0
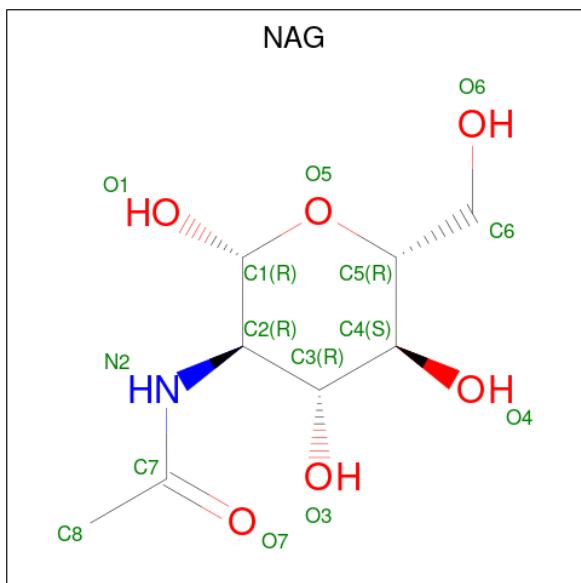
- Molecule 6 is a protein called RSV variant (construct pXCS847A) F2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	79	Total	C	N	O	S	0	0
			615	386	101	124	4		
6	Q	79	Total	C	N	O	S	0	0
			615	386	101	124	4		
6	R	79	Total	C	N	O	S	0	0
			615	386	101	124	4		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	1	MET	-	initiating methionine	UNP A0A7D5GVC1
P	2	GLU	-	expression tag	UNP A0A7D5GVC1
P	3	LEU	-	expression tag	UNP A0A7D5GVC1
P	103	CYS	ALA	engineered mutation	UNP A0A7D5GVC1
Q	1	MET	-	initiating methionine	UNP A0A7D5GVC1
Q	2	GLU	-	expression tag	UNP A0A7D5GVC1
Q	3	LEU	-	expression tag	UNP A0A7D5GVC1
Q	103	CYS	ALA	engineered mutation	UNP A0A7D5GVC1
R	1	MET	-	initiating methionine	UNP A0A7D5GVC1
R	2	GLU	-	expression tag	UNP A0A7D5GVC1
R	3	LEU	-	expression tag	UNP A0A7D5GVC1
R	103	CYS	ALA	engineered mutation	UNP A0A7D5GVC1

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
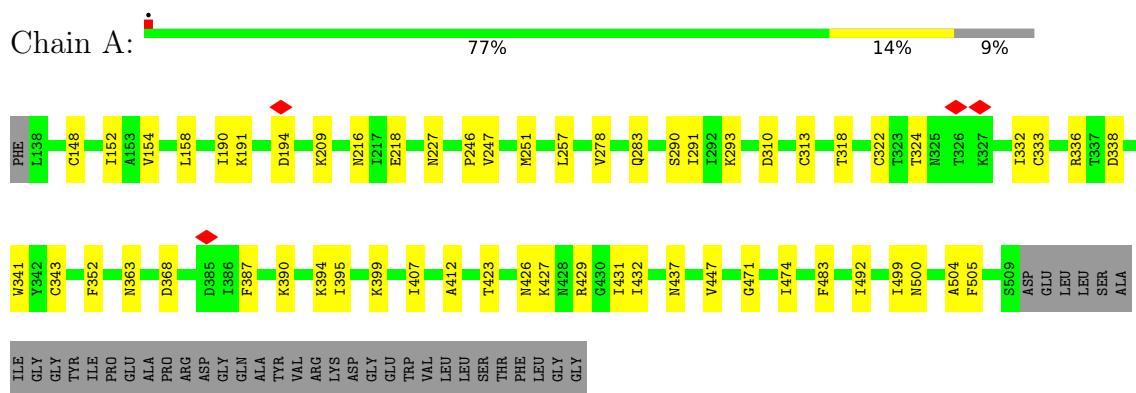
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total 14	C 8	N 1	O 5	0
7	C	1	Total 14	C 8	N 1	O 5	0
7	K	1	Total 14	C 8	N 1	O 5	0
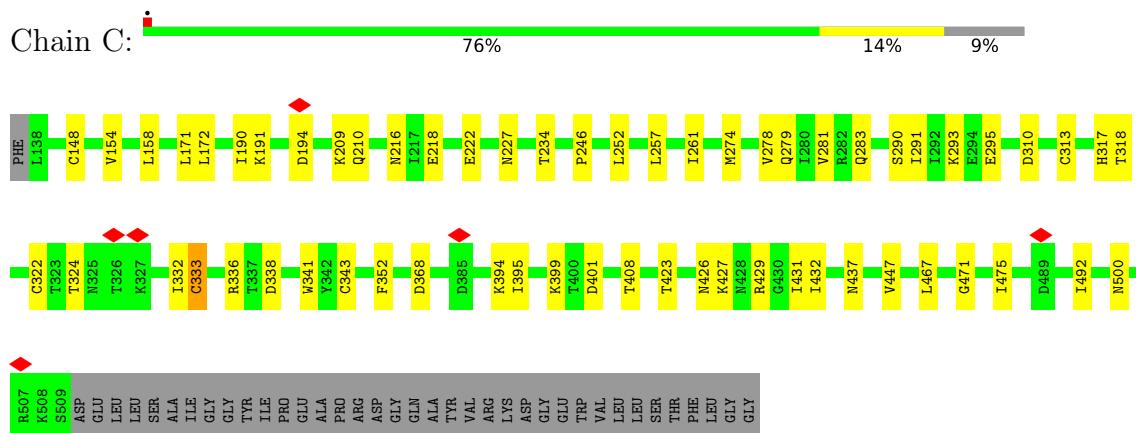
3 Residue-property plots ⓘ

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

- Molecule 1: RSV variant (construct pXCS847A) F1

Chain A:

- Molecule 1: RSV variant (construct pXCS847A) F1

Chain C:

- Molecule 1: RSV variant (construct pXCS847A) F1

Chain K:

• Molecule 2: AM14 Fab heavy chain

Chain B:

• Molecule 2: AM14 Fab heavy chain

Chain G:

• Molecule 2: AM14 Fab heavy chain

Chain L:

• Molecule 3: AM14 Fab light chain

Chain D:

• Molecule 3: AM14 Fab light chain

Chain H:

• Molecule 3: AM14 Fab light chain

Chain M:

• Molecule 4: AM22 Fab heavy chain

Chain E:

ASP ASP ASP LYS

• Molecule 4: AM22 Fab heavy chain

Chain I:

5%

41%　　10%　　50%

• Molecule 4: AM22 Fab heavy chain

Chain N:

42%　　8%　　50%

• Molecule 5: AM22 Fab light chain

Chain F:

39%　　10%　　51%

• Molecule 5: AM22 Fab light chain

Chain J:

45%　　·　　51%

SER PRO VAL THR LYS SER PHE ASN ARG GLY GLU CYS

• Molecule 5: AM22 Fab light chain

Chain O:

40%   8%   51%

GLU ILE V3 G9 T10 L11 S12 L13 S14 E17 L21 K40 L47 N77 G78 L79 A80 P81 E82 D83 F84 A85 V86 C89 D93 T103 K104 V105 D106 F107 LYS ARG THR VAL ALA ALA PRO SER VAL PHE ILE PHE PRO PRO SER ASP GLU GLN LEU LYS SER

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

LYS HIS LYS VAL TYR ALA CYS GLU VAL THR HIS GLN GLY LEU SER SER PRO VAL THR LYS SER PHE ASN ARG GLY GLU CYS

• Molecule 6: RSV variant (construct pXCS847A) F2

6%

Chain P:

63%   9%   28%

MET GLU LEU PRO ILE LEU LYS THR ASN ALA ILE THR THR ILE LEU ALA ALA VAL THR LEU CYS PHE ALA SER S25 Q26 Q34 L45 S46 T54 T72 D73 V76 E82 E92 S99 T100 P101 A102 C103 ASN SER ARG ALA ARG ARG

• Molecule 6: RSV variant (construct pXCS847A) F2

Chain Q:

60%   13%   28%

MET GLU LEU PRO ILE LEU LYS THR ASN ALA ILE THR THR ILE LEU ALA ALA VAL THR LEU CYS PHE ALA SER S25 E31 Q34 L45 S46 T54 N63 C69 T72 D73 V76 K77 L78 L93 M97 Q98 C103 ASN SER ARG ALA ARG ARG

• Molecule 6: RSV variant (construct pXCS847A) F2

Chain R:

62%   10%   28%

MET GLU LEU PRO ILE LEU LYS THR ASN ALA ILE THR THR ILE LEU ALA ALA VAL THR LEU CYS PHE ALA SER S25 Q34 L45 S46 T54 T72 D73 V76 E82 L83 L93 M97 C103 ASN SER ARG ALA ARG ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	183713	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 $(e^-/\text{Å}^2)$	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.299	Depositor
Minimum map value	-0.178	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	383.6, 383.6, 383.6	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	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	0.25	0/2901	0.47	0/3933
1	C	0.25	0/2901	0.48	0/3933
1	K	0.25	0/2901	0.48	0/3933
2	B	0.26	0/957	0.55	0/1298
2	G	0.26	0/957	0.54	0/1298
2	L	0.26	0/957	0.58	0/1298
3	D	0.27	0/786	0.51	0/1066
3	H	0.26	0/786	0.50	0/1066
3	M	0.26	0/786	0.49	0/1066
4	E	0.24	0/958	0.54	1/1301 (0.1%)
4	I	0.24	0/958	0.53	0/1301
4	N	0.24	0/958	0.51	0/1301
5	F	0.25	0/804	0.50	0/1093
5	J	0.25	0/804	0.50	0/1093
5	O	0.26	0/804	0.51	0/1093
6	P	0.25	0/622	0.45	0/839
6	Q	0.24	0/622	0.47	0/839
6	R	0.24	0/622	0.44	0/839
All	All	0.25	0/21084	0.50	1/28590 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	29	LEU	CA-CB-CG	5.50	127.94	115.30

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	2859	0	2902	40	0
1	C	2859	0	2902	44	0
1	K	2859	0	2902	50	0
2	B	934	0	878	20	0
2	G	934	0	878	20	0
2	L	934	0	878	27	0
3	D	769	0	749	11	0
3	H	769	0	749	13	0
3	M	769	0	749	12	0
4	E	940	0	928	20	0
4	I	940	0	930	15	0
4	N	940	0	930	13	0
5	F	785	0	768	14	0
5	J	785	0	768	7	0
5	O	785	0	768	10	0
6	P	615	0	618	11	0
6	Q	615	0	618	12	0
6	R	615	0	618	15	0
7	A	14	0	13	2	0
7	C	14	0	13	1	0
7	K	14	0	13	2	0
All	All	20748	0	20572	308	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.

The worst 5 of 308 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:C:313:CYS:HA	1:C:343:CYS:HB3	1.44	0.98
5:F:13:LEU:HD11	5:F:79:LEU:HD13	1.49	0.93
4:E:6:GLN:NE2	4:E:96:CYS:SG	2.45	0.90
1:A:313:CYS:HA	1:A:343:CYS:HB3	1.54	0.90
1:K:313:CYS:HA	1:K:343:CYS:HB3	1.57	0.87

There are no symmetry-related clashes.

5.3   Torsion angles ⓘ

5.3.1   Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	370/410 (90%)	355 (96%)	15 (4%)	0	100	100
1	C	370/410 (90%)	352 (95%)	18 (5%)	0	100	100
1	K	370/410 (90%)	355 (96%)	15 (4%)	0	100	100
2	B	117/245 (48%)	112 (96%)	5 (4%)	0	100	100
2	G	117/245 (48%)	111 (95%)	6 (5%)	0	100	100
2	L	117/245 (48%)	112 (96%)	5 (4%)	0	100	100
3	D	95/218 (44%)	83 (87%)	12 (13%)	0	100	100
3	H	95/218 (44%)	83 (87%)	12 (13%)	0	100	100
3	M	95/218 (44%)	87 (92%)	8 (8%)	0	100	100
4	E	122/246 (50%)	116 (95%)	6 (5%)	0	100	100
4	I	122/246 (50%)	114 (93%)	8 (7%)	0	100	100
4	N	122/246 (50%)	112 (92%)	10 (8%)	0	100	100
5	F	103/215 (48%)	96 (93%)	7 (7%)	0	100	100
5	J	103/215 (48%)	96 (93%)	7 (7%)	0	100	100
5	O	103/215 (48%)	94 (91%)	9 (9%)	0	100	100
6	P	77/109 (71%)	75 (97%)	2 (3%)	0	100	100
6	Q	77/109 (71%)	75 (97%)	2 (3%)	0	100	100
6	R	77/109 (71%)	75 (97%)	2 (3%)	0	100	100
All	All	2652/4329 (61%)	2503 (94%)	149 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2   Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	340/369 (92%)	339 (100%)	1 (0%)	92	96
1	C	340/369 (92%)	339 (100%)	1 (0%)	92	96
1	K	340/369 (92%)	340 (100%)	0	100	100
2	B	98/206 (48%)	95 (97%)	3 (3%)	40	65
2	G	98/206 (48%)	97 (99%)	1 (1%)	76	86
2	L	98/206 (48%)	96 (98%)	2 (2%)	55	74
3	D	88/194 (45%)	88 (100%)	0	100	100
3	H	88/194 (45%)	88 (100%)	0	100	100
3	M	88/194 (45%)	88 (100%)	0	100	100
4	E	100/205 (49%)	100 (100%)	0	100	100
4	I	100/205 (49%)	100 (100%)	0	100	100
4	N	100/205 (49%)	100 (100%)	0	100	100
5	F	86/185 (46%)	86 (100%)	0	100	100
5	J	86/185 (46%)	85 (99%)	1 (1%)	71	84
5	O	86/185 (46%)	85 (99%)	1 (1%)	71	84
6	P	70/96 (73%)	70 (100%)	0	100	100
6	Q	70/96 (73%)	70 (100%)	0	100	100
6	R	70/96 (73%)	70 (100%)	0	100	100
All	All	2346/3765 (62%)	2336 (100%)	10 (0%)	91	95

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	96	CYS
2	L	108	TYR
5	O	89	CYS
2	B	108	TYR
1	C	333	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	227	ASN
2	L	82	GLN
3	M	6	GLN
1	C	279	GLN
1	C	183	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\#|Z| > 2$
7	NAG	C	601	1	14,14,15	0.36	0	17,19,21	0.51	0
7	NAG	A	601	1	14,14,15	0.35	0	17,19,21	0.50	0
7	NAG	K	601	1	14,14,15	0.36	0	17,19,21	0.49	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
7	NAG	C	601	1	-	2/6/23/26	0/1/1/1
7	NAG	A	601	1	-	3/6/23/26	0/1/1/1
7	NAG	K	601	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	601	NAG	O5-C5-C6-O6
7	K	601	NAG	O5-C5-C6-O6
7	A	601	NAG	O5-C5-C6-O6
7	C	601	NAG	C4-C5-C6-O6
7	K	601	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	601	NAG	1	0
7	A	601	NAG	2	0
7	K	601	NAG	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.
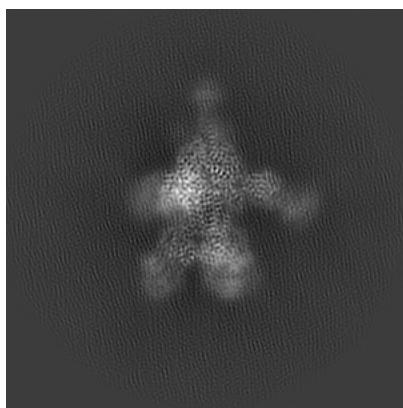
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-26562. These allow visual inspection of the internal detail of the map and identification of artifacts.
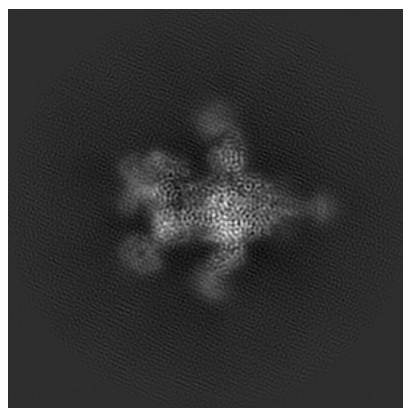
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections ⓘ
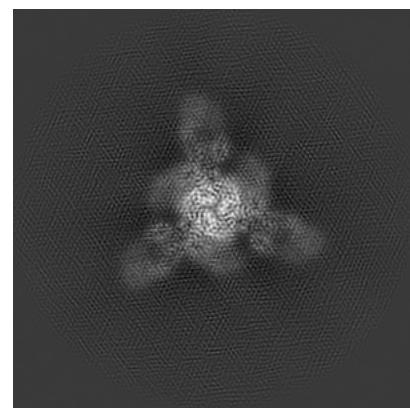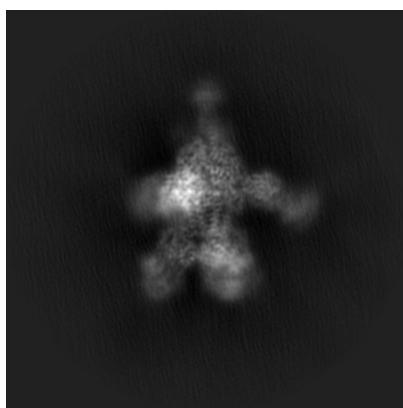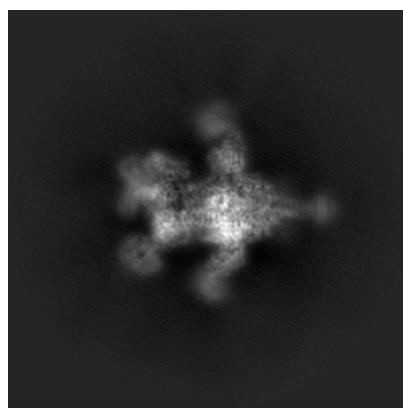
6.1.1 Primary map

| X | Y | Z |
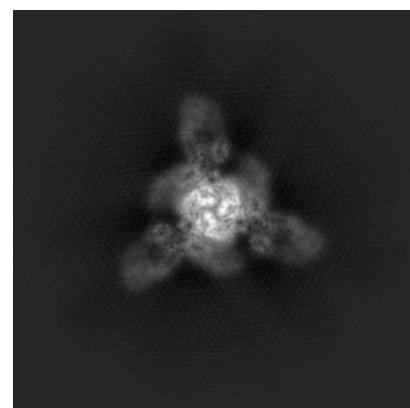
6.1.2 Raw map

| X | Y | Z |
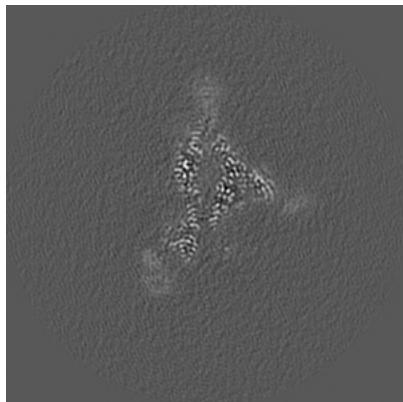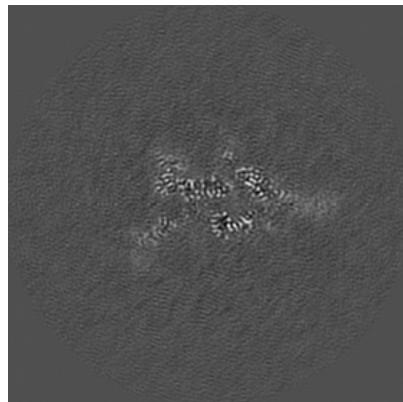
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)
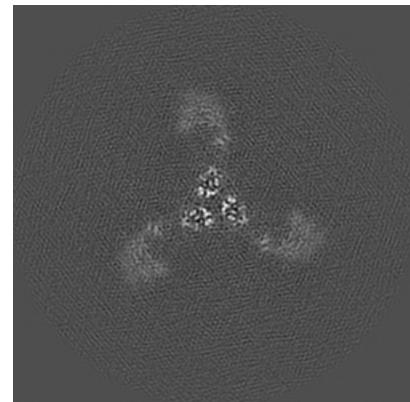
6.2.1 Primary map
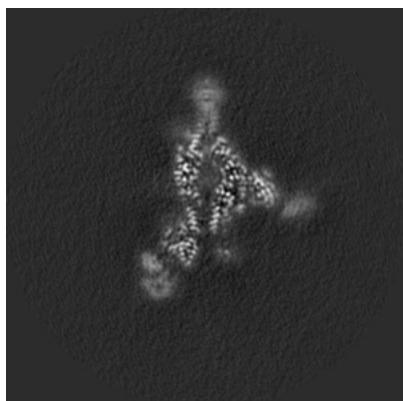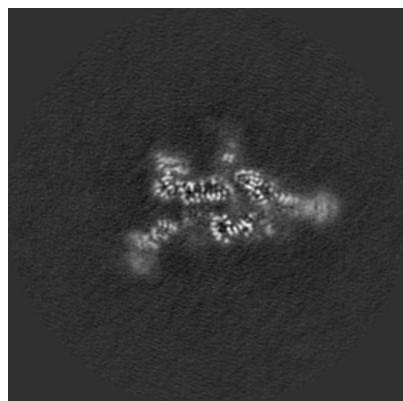
| X Index: 140 | Y Index: 140 | Z Index: 140 |
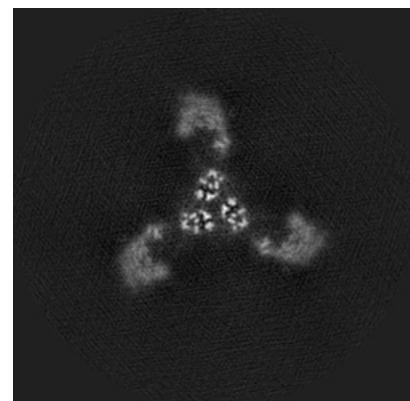
6.2.2 Raw map
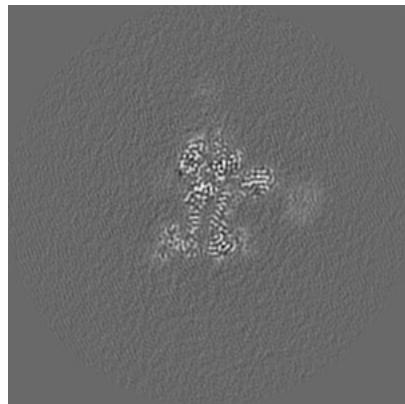
| X Index: 140 | Y Index: 140 | Z Index: 140 |
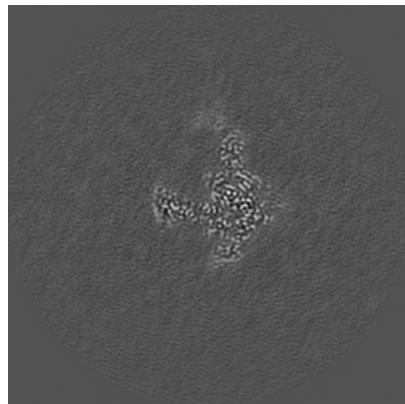
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ
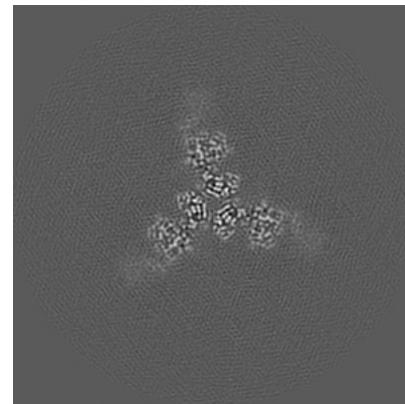
6.3.1 Primary map
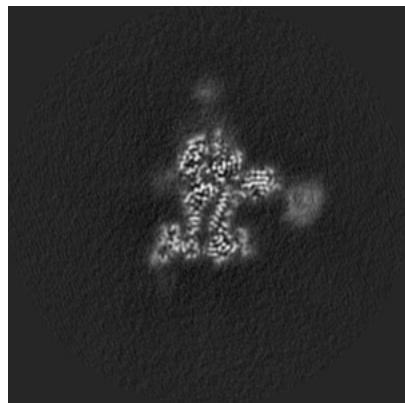
| X Index: 130 | Y Index: 127 | Z Index: 152 |
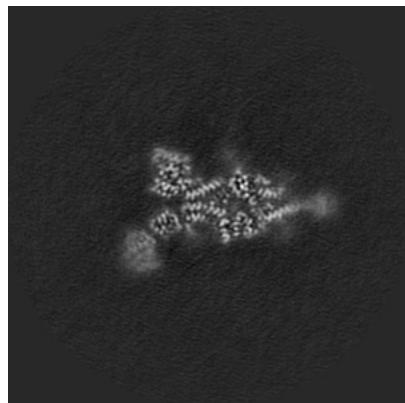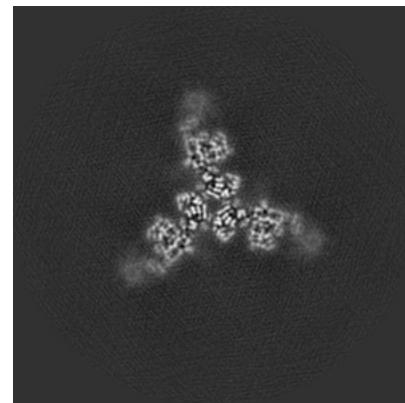
6.3.2 Raw map

| X Index: 130 | Y Index: 145 | Z Index: 152 |
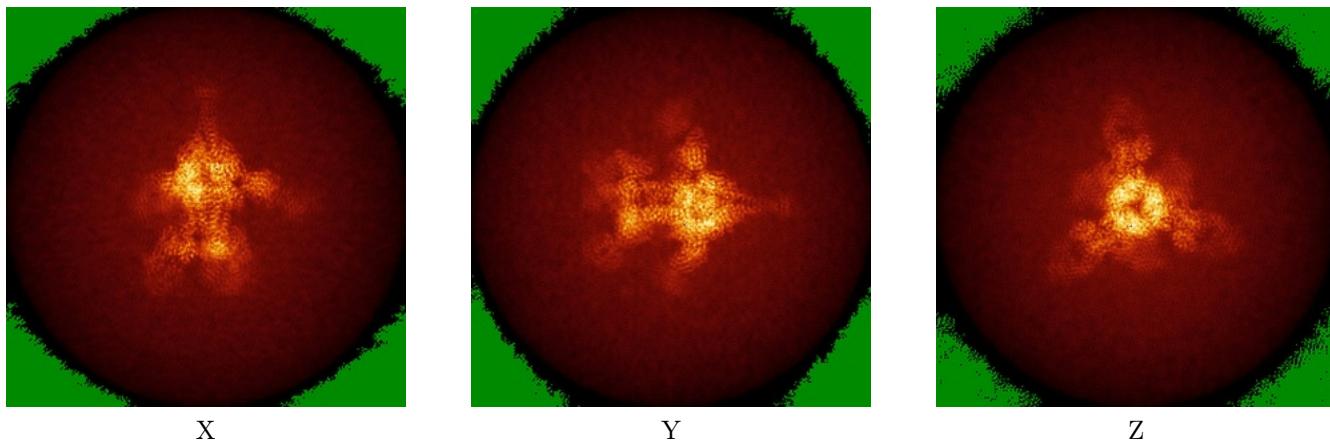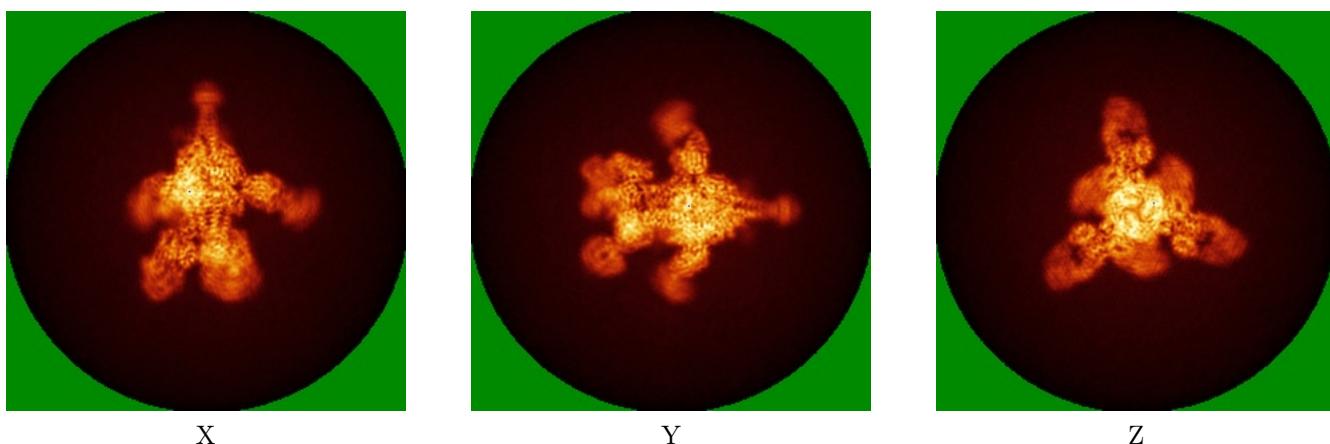
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map

X   Y   Z

6.4.2 Raw map

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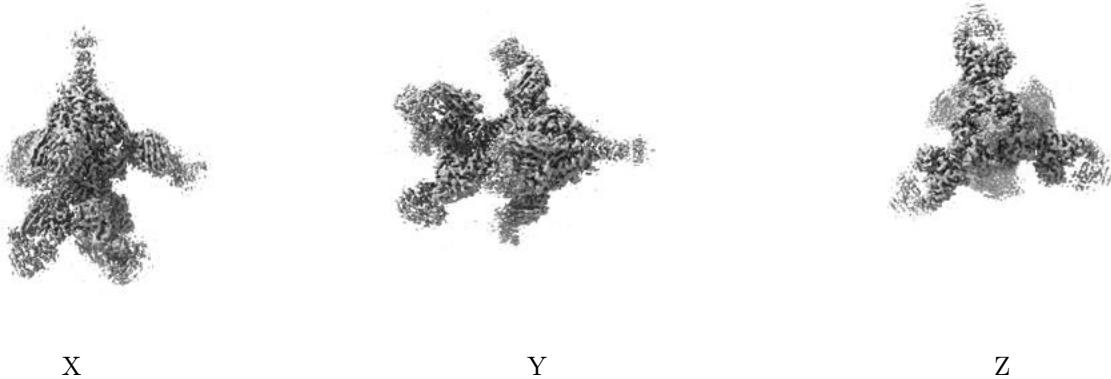
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.
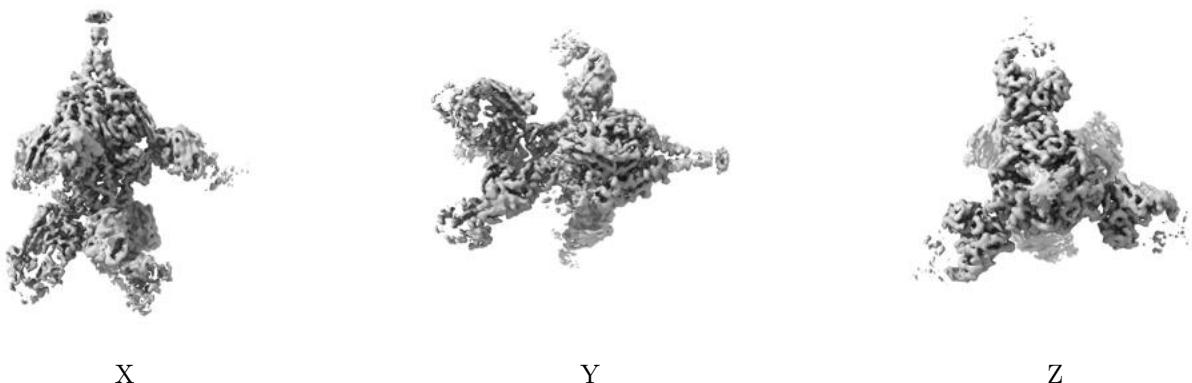
6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

X Y Z

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

6.5.2 Raw map

X Y Z

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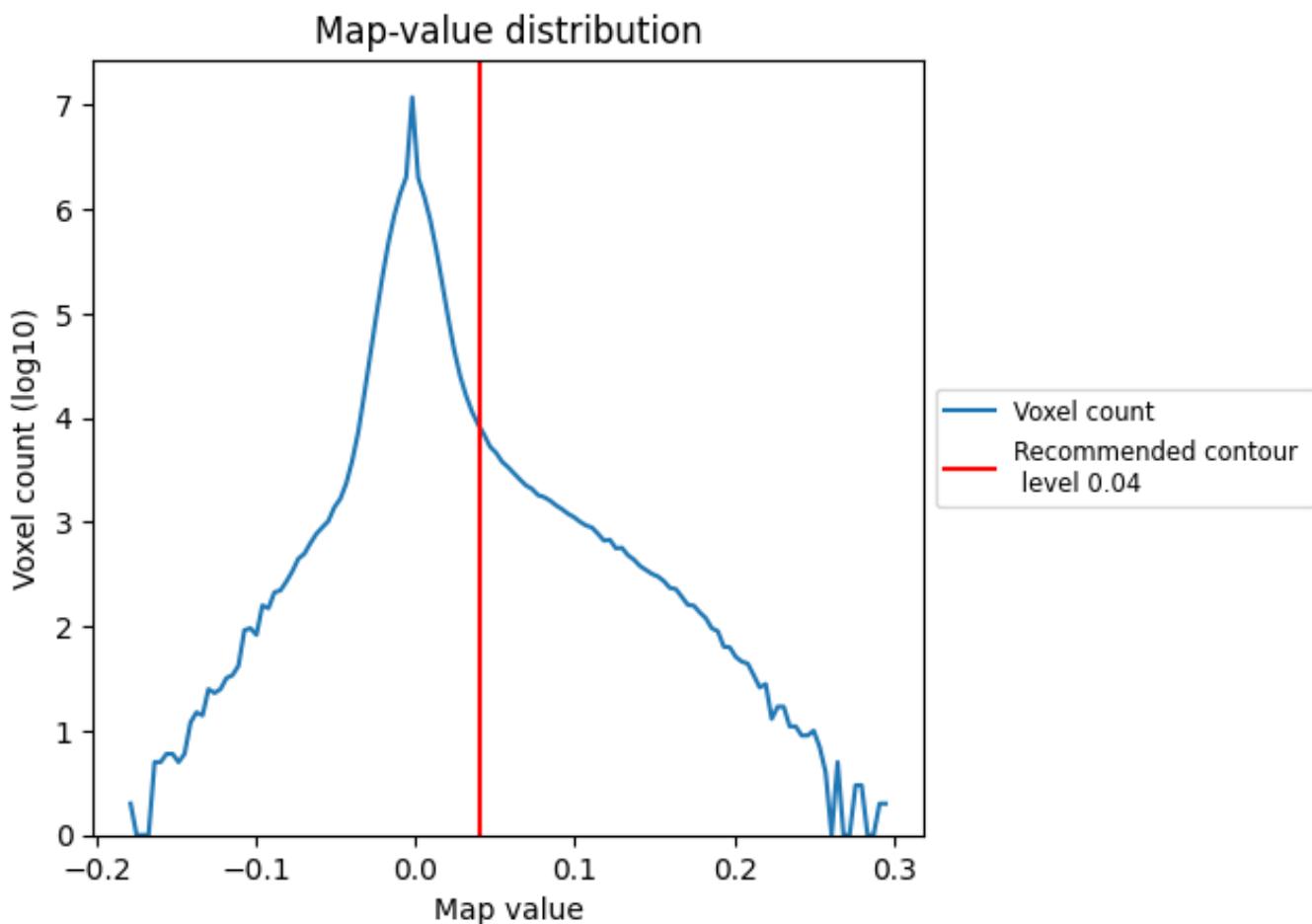
6.6 Mask visualisation ⓘ

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

7   Map analysis ⓘ
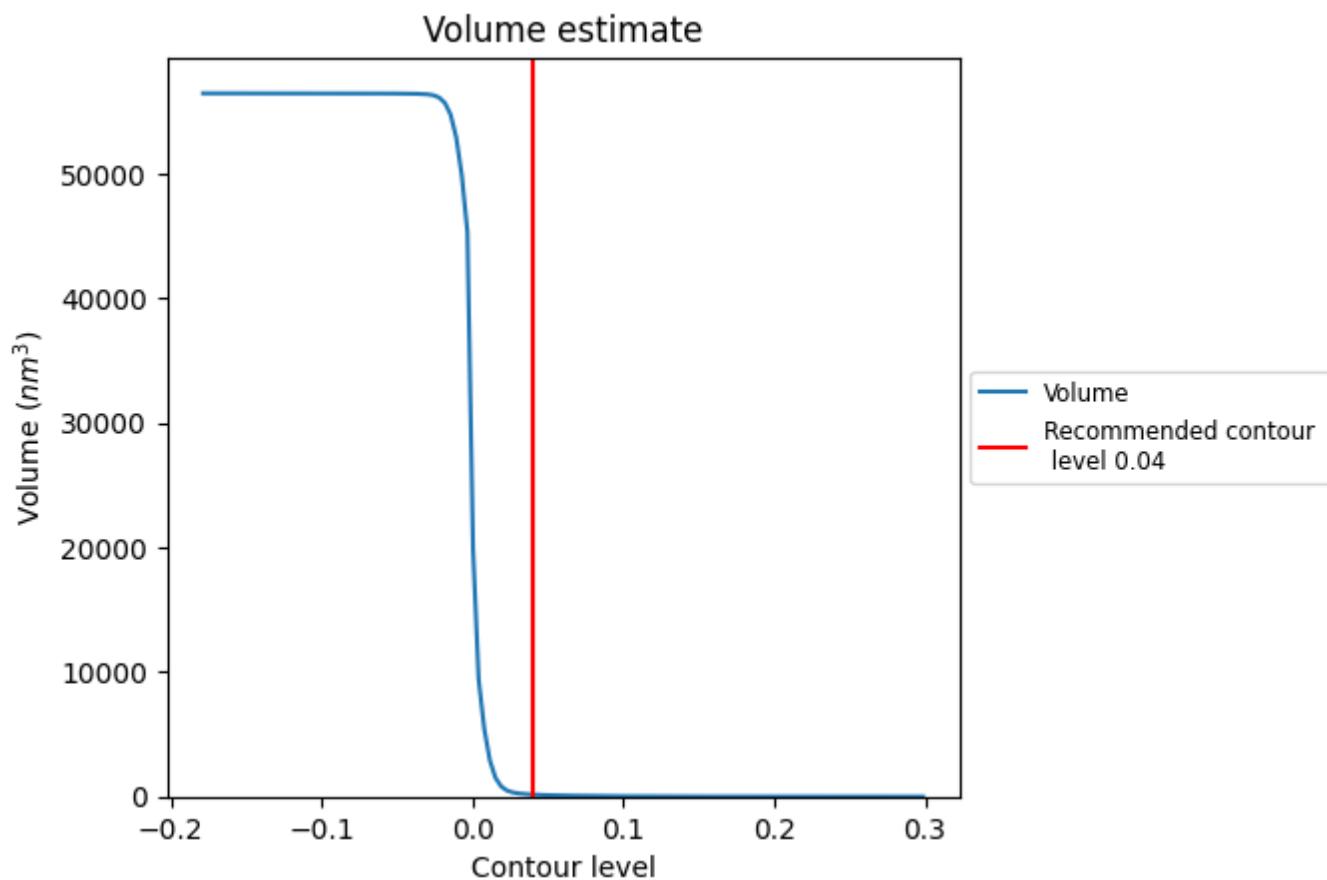
This section contains the results of statistical analysis of the map.

7.1   Map-value distribution ⓘ

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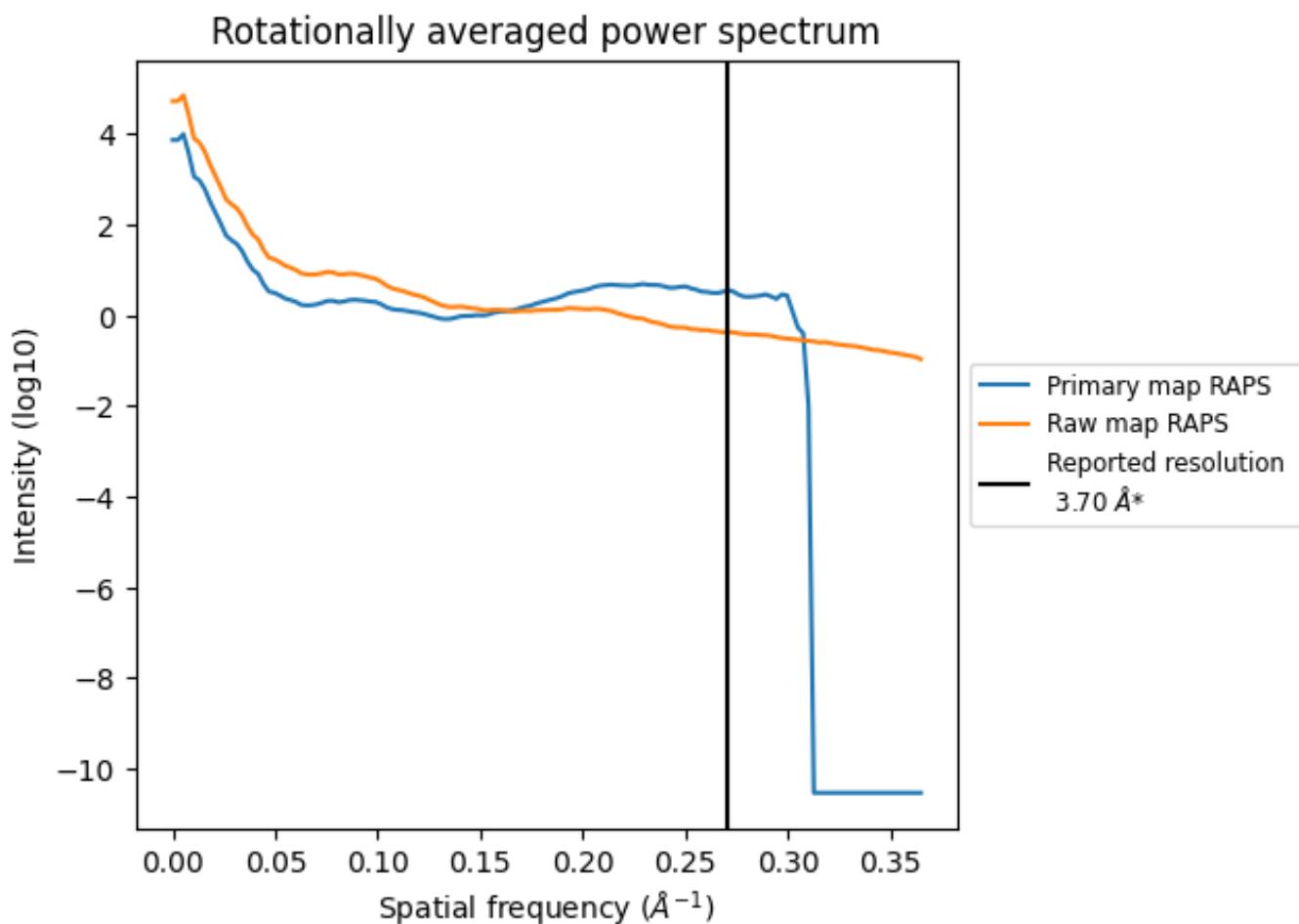
7.2   Volume estimate ⓘ

The volume at the recommended contour level is 159 nm^3; this corresponds to an approximate mass of 144 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   ⓘ
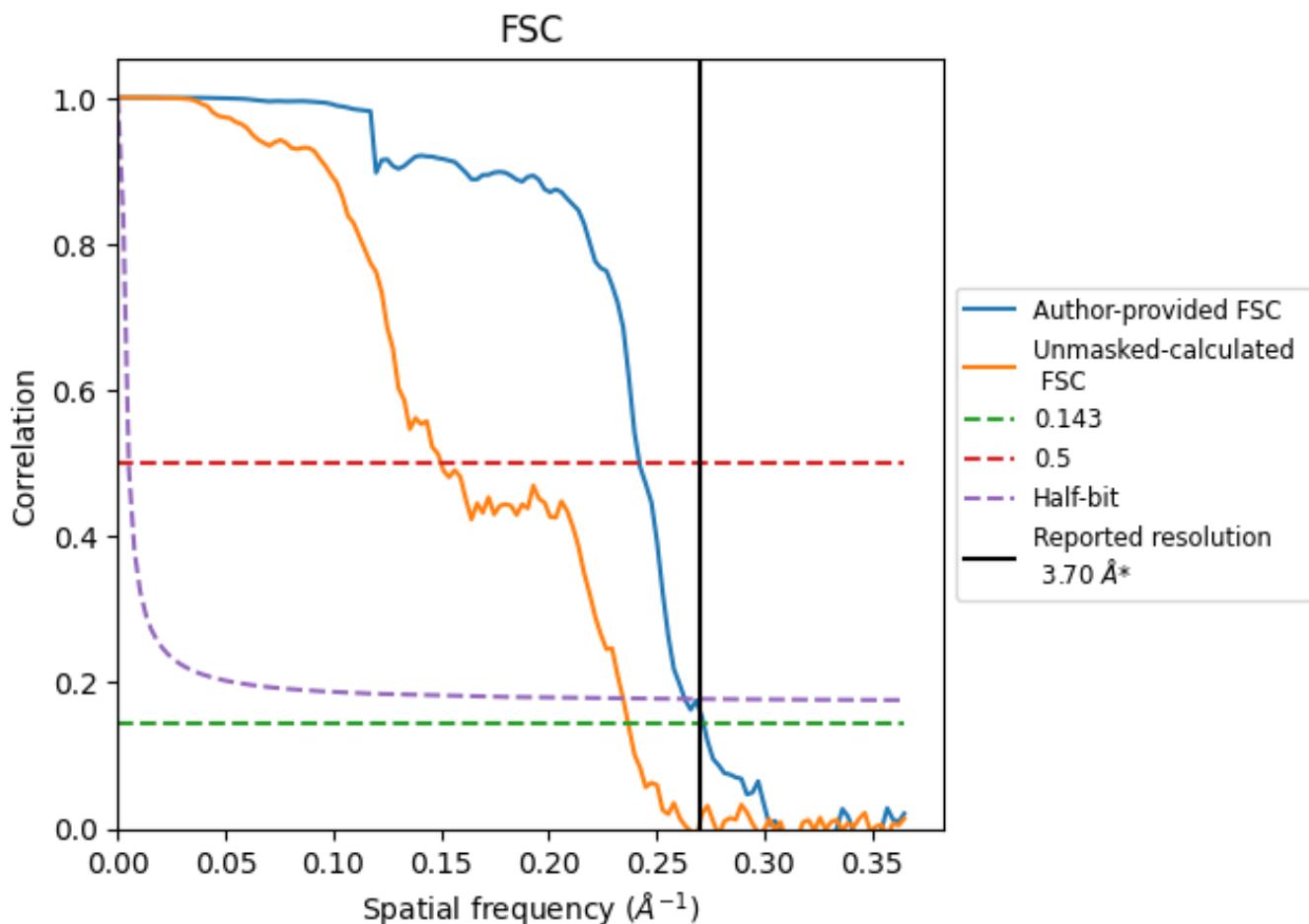
*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ

*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8.2   Resolution estimates ⓘ
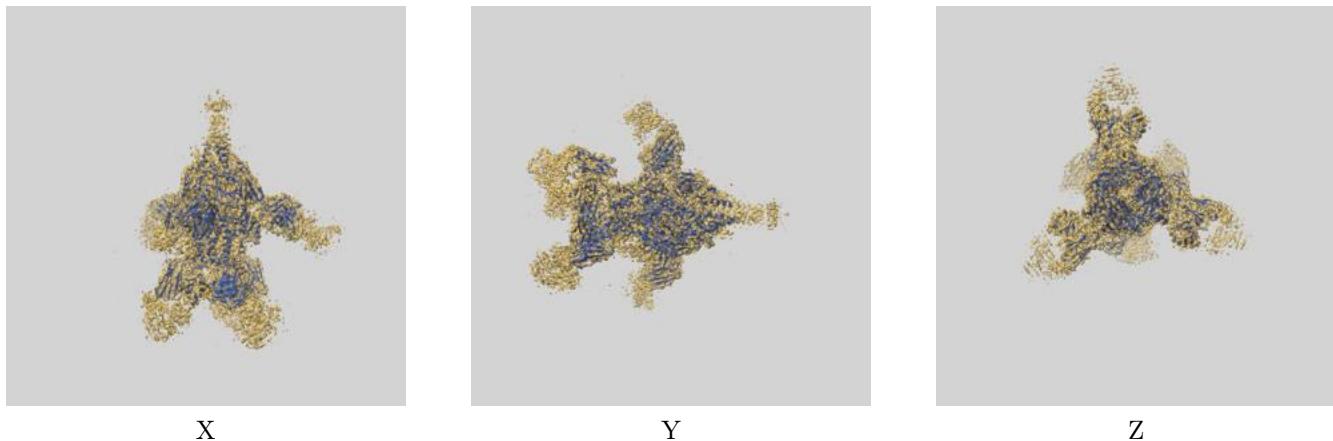
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.68	4.13	3.80
Unmasked-calculated*	4.22	6.67	4.26

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.22 differs from the reported value 3.7 by more than 10 %

9   Map-model fit ⓘ
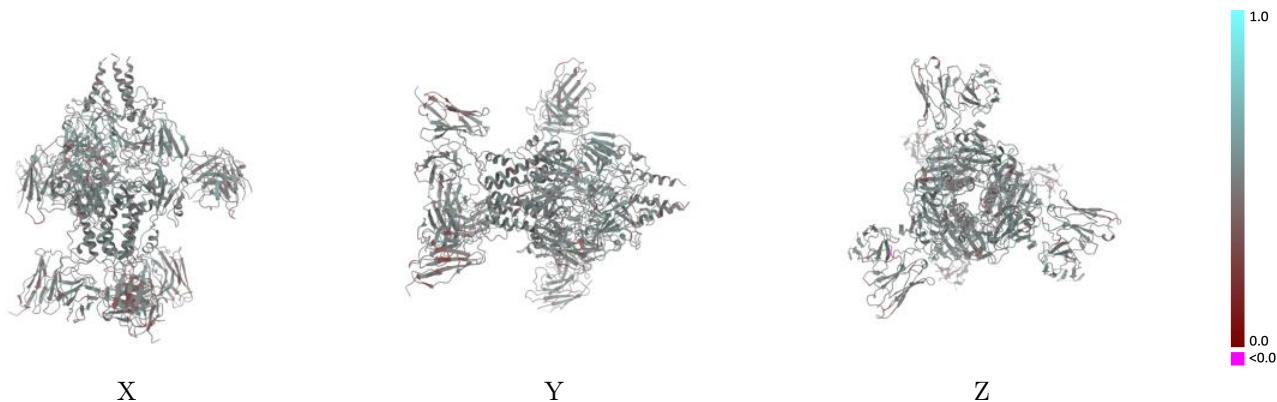
This section contains information regarding the fit between EMDB map EMD-26562 and PDB model 7UJA. Per-residue inclusion information can be found in section 3 on page 10.

9.1   Map-model overlay ⓘ

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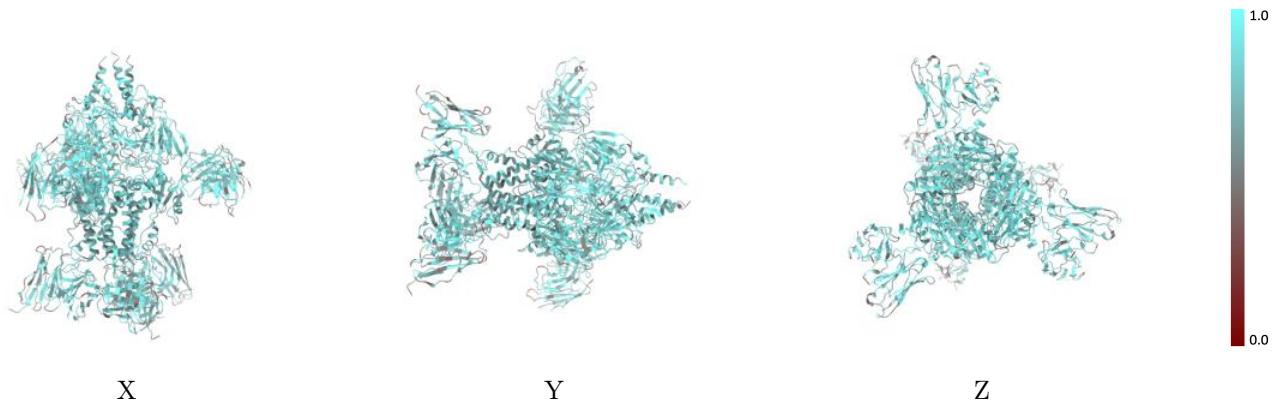
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ

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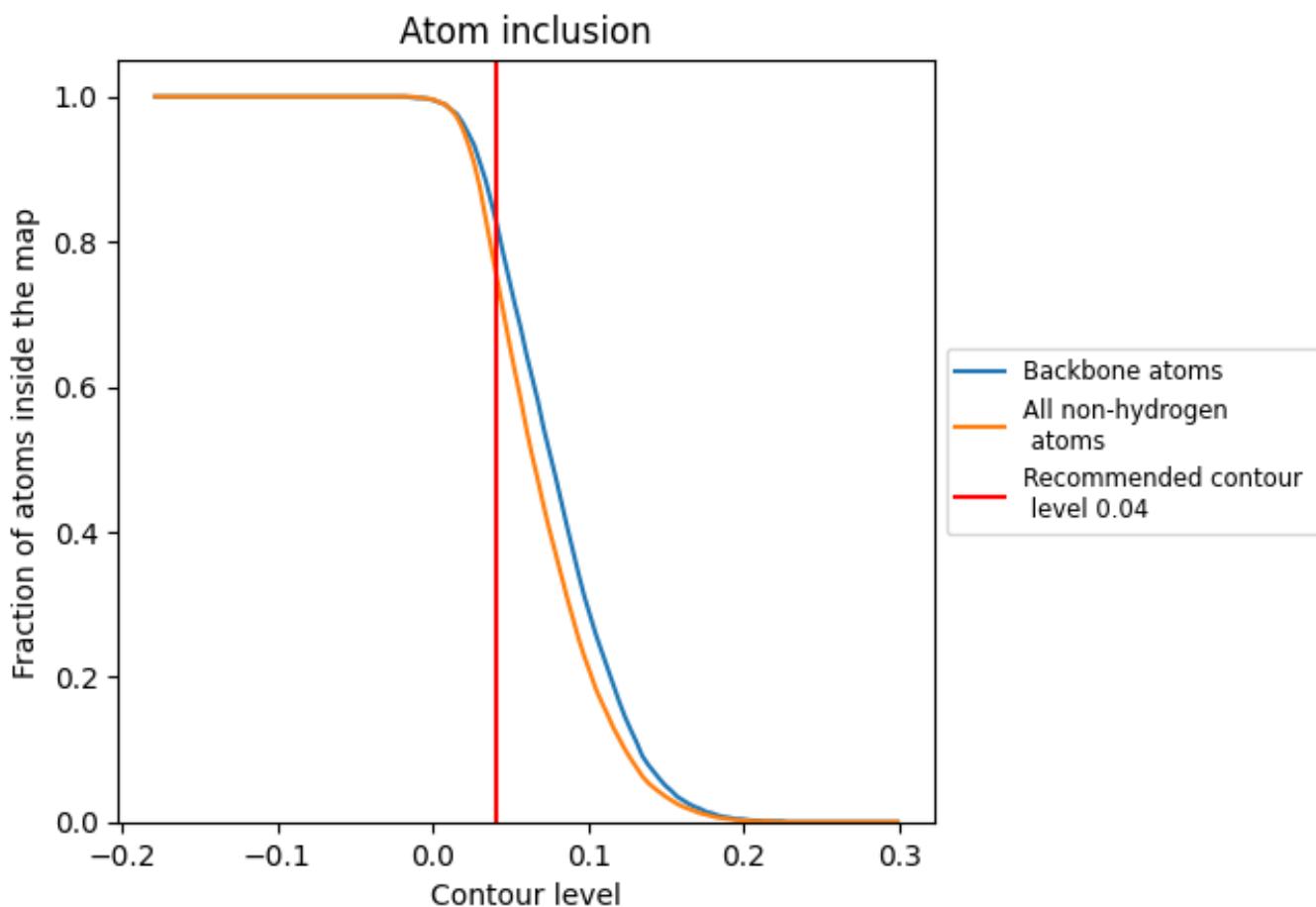
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3   Atom inclusion mapped to coordinate model ⓘ

X   Y   Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion ⓘ

At the recommended contour level, 83% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5　Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7620	0.4920
A	0.7920	0.5090
B	0.7690	0.4760
C	0.7880	0.5100
D	0.7400	0.4810
E	0.6840	0.4540
F	0.7530	0.4960
G	0.7700	0.4800
H	0.7310	0.4760
I	0.6920	0.4630
J	0.7620	0.4930
K	0.7930	0.5090
L	0.7650	0.4750
M	0.7320	0.4740
N	0.6900	0.4610
O	0.7570	0.4970
P	0.7680	0.5030
Q	0.7730	0.4990
R	0.7760	0.5010

1.0

0.0
<0.0