



Full wwPDB EM Validation Report ⓘ

Jun 2, 2026 – 10:56 PM JST

PDB ID : 24KR / pdb_000024kr
EMDB ID : EMD-69590
Title : Structural basis of influenza A virus neutralization by broadly active single-domain antibody G2.3 recognizing glycosylated epitope within hemagglutinin stem
Authors : Ilyasov, I.O.; Baymukhametov, T.N.; Voronina, D.V.; Vorobiev, I.I.; Khodak, Y.A.; Burtseva, A.D.; Popov, V.O.; Sluchanko, N.N.; Shcheblyakov, D.V.; Boyko, K.M.
Deposited on : 2026-03-08
Resolution : 2.53 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:

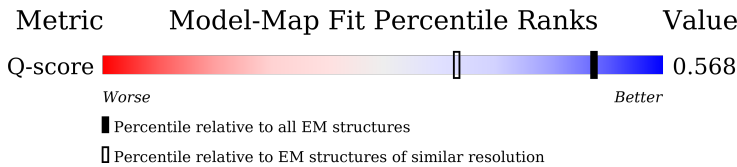
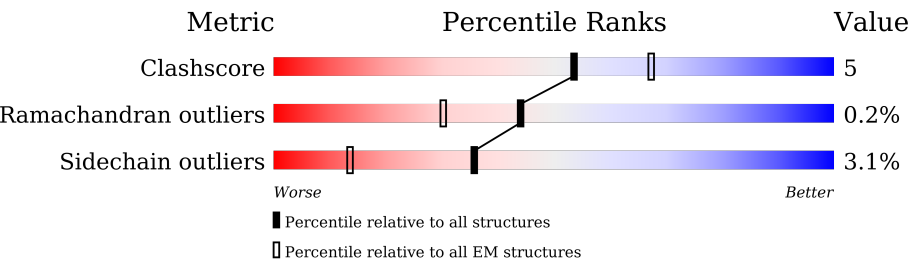
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.53 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7309 (2.03 - 3.03)

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	567	
1	B	567	
1	C	567	
2	D	400	

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Mol	Chain	Length	Quality of chain
2	E	400	<div><div></div><div>25%6%70%</div></div>
2	F	400	<div><div></div><div>25%5%70%</div></div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13938 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	498	Total	C	N	O	S	0	0
			3720	2366	638	699	17		
1	B	498	Total	C	N	O	S	0	0
			3720	2366	638	699	17		
1	C	498	Total	C	N	O	S	0	0
			3720	2366	638	699	17		

There are 147 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	502	SER	-	expression tag	UNP C3W5S1
A	503	GLY	-	expression tag	UNP C3W5S1
A	504	GLY	-	expression tag	UNP C3W5S1
A	505	GLY	-	expression tag	UNP C3W5S1
A	506	GLY	-	expression tag	UNP C3W5S1
A	507	ARG	-	expression tag	UNP C3W5S1
A	508	LEU	-	expression tag	UNP C3W5S1
A	509	VAL	-	expression tag	UNP C3W5S1
A	510	PRO	-	expression tag	UNP C3W5S1
A	511	ARG	-	expression tag	UNP C3W5S1
A	512	GLY	-	expression tag	UNP C3W5S1
A	513	SER	-	expression tag	UNP C3W5S1
A	514	PRO	-	expression tag	UNP C3W5S1
A	515	GLY	-	expression tag	UNP C3W5S1
A	516	SER	-	expression tag	UNP C3W5S1
A	517	GLY	-	expression tag	UNP C3W5S1
A	518	TYR	-	expression tag	UNP C3W5S1
A	519	ILE	-	expression tag	UNP C3W5S1
A	520	PRO	-	expression tag	UNP C3W5S1
A	521	GLU	-	expression tag	UNP C3W5S1
A	522	ALA	-	expression tag	UNP C3W5S1
A	523	PRO	-	expression tag	UNP C3W5S1
A	524	ARG	-	expression tag	UNP C3W5S1
A	525	ASP	-	expression tag	UNP C3W5S1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	526	GLY	-	expression tag	UNP C3W5S1
A	527	GLN	-	expression tag	UNP C3W5S1
A	528	ALA	-	expression tag	UNP C3W5S1
A	529	TYR	-	expression tag	UNP C3W5S1
A	530	VAL	-	expression tag	UNP C3W5S1
A	531	ARG	-	expression tag	UNP C3W5S1
A	532	LYS	-	expression tag	UNP C3W5S1
A	533	ASP	-	expression tag	UNP C3W5S1
A	534	GLY	-	expression tag	UNP C3W5S1
A	535	GLU	-	expression tag	UNP C3W5S1
A	536	TRP	-	expression tag	UNP C3W5S1
A	537	VAL	-	expression tag	UNP C3W5S1
A	538	LEU	-	expression tag	UNP C3W5S1
A	539	LEU	-	expression tag	UNP C3W5S1
A	540	SER	-	expression tag	UNP C3W5S1
A	541	THR	-	expression tag	UNP C3W5S1
A	542	PHE	-	expression tag	UNP C3W5S1
A	543	LEU	-	expression tag	UNP C3W5S1
A	544	GLY	-	expression tag	UNP C3W5S1
A	545	HIS	-	expression tag	UNP C3W5S1
A	546	HIS	-	expression tag	UNP C3W5S1
A	547	HIS	-	expression tag	UNP C3W5S1
A	548	HIS	-	expression tag	UNP C3W5S1
A	549	HIS	-	expression tag	UNP C3W5S1
A	550	HIS	-	expression tag	UNP C3W5S1
B	502	SER	-	expression tag	UNP C3W5S1
B	503	GLY	-	expression tag	UNP C3W5S1
B	504	GLY	-	expression tag	UNP C3W5S1
B	505	GLY	-	expression tag	UNP C3W5S1
B	506	GLY	-	expression tag	UNP C3W5S1
B	507	ARG	-	expression tag	UNP C3W5S1
B	508	LEU	-	expression tag	UNP C3W5S1
B	509	VAL	-	expression tag	UNP C3W5S1
B	510	PRO	-	expression tag	UNP C3W5S1
B	511	ARG	-	expression tag	UNP C3W5S1
B	512	GLY	-	expression tag	UNP C3W5S1
B	513	SER	-	expression tag	UNP C3W5S1
B	514	PRO	-	expression tag	UNP C3W5S1
B	515	GLY	-	expression tag	UNP C3W5S1
B	516	SER	-	expression tag	UNP C3W5S1
B	517	GLY	-	expression tag	UNP C3W5S1
B	518	TYR	-	expression tag	UNP C3W5S1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	519	ILE	-	expression tag	UNP C3W5S1
B	520	PRO	-	expression tag	UNP C3W5S1
B	521	GLU	-	expression tag	UNP C3W5S1
B	522	ALA	-	expression tag	UNP C3W5S1
B	523	PRO	-	expression tag	UNP C3W5S1
B	524	ARG	-	expression tag	UNP C3W5S1
B	525	ASP	-	expression tag	UNP C3W5S1
B	526	GLY	-	expression tag	UNP C3W5S1
B	527	GLN	-	expression tag	UNP C3W5S1
B	528	ALA	-	expression tag	UNP C3W5S1
B	529	TYR	-	expression tag	UNP C3W5S1
B	530	VAL	-	expression tag	UNP C3W5S1
B	531	ARG	-	expression tag	UNP C3W5S1
B	532	LYS	-	expression tag	UNP C3W5S1
B	533	ASP	-	expression tag	UNP C3W5S1
B	534	GLY	-	expression tag	UNP C3W5S1
B	535	GLU	-	expression tag	UNP C3W5S1
B	536	TRP	-	expression tag	UNP C3W5S1
B	537	VAL	-	expression tag	UNP C3W5S1
B	538	LEU	-	expression tag	UNP C3W5S1
B	539	LEU	-	expression tag	UNP C3W5S1
B	540	SER	-	expression tag	UNP C3W5S1
B	541	THR	-	expression tag	UNP C3W5S1
B	542	PHE	-	expression tag	UNP C3W5S1
B	543	LEU	-	expression tag	UNP C3W5S1
B	544	GLY	-	expression tag	UNP C3W5S1
B	545	HIS	-	expression tag	UNP C3W5S1
B	546	HIS	-	expression tag	UNP C3W5S1
B	547	HIS	-	expression tag	UNP C3W5S1
B	548	HIS	-	expression tag	UNP C3W5S1
B	549	HIS	-	expression tag	UNP C3W5S1
B	550	HIS	-	expression tag	UNP C3W5S1
C	502	SER	-	expression tag	UNP C3W5S1
C	503	GLY	-	expression tag	UNP C3W5S1
C	504	GLY	-	expression tag	UNP C3W5S1
C	505	GLY	-	expression tag	UNP C3W5S1
C	506	GLY	-	expression tag	UNP C3W5S1
C	507	ARG	-	expression tag	UNP C3W5S1
C	508	LEU	-	expression tag	UNP C3W5S1
C	509	VAL	-	expression tag	UNP C3W5S1
C	510	PRO	-	expression tag	UNP C3W5S1
C	511	ARG	-	expression tag	UNP C3W5S1

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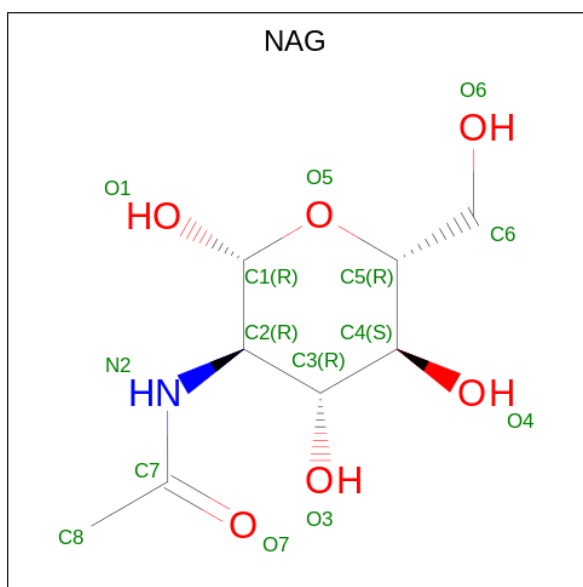
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Chain	Residue	Modelled	Actual	Comment	Reference
C	512	GLY	-	expression tag	UNP C3W5S1
C	513	SER	-	expression tag	UNP C3W5S1
C	514	PRO	-	expression tag	UNP C3W5S1
C	515	GLY	-	expression tag	UNP C3W5S1
C	516	SER	-	expression tag	UNP C3W5S1
C	517	GLY	-	expression tag	UNP C3W5S1
C	518	TYR	-	expression tag	UNP C3W5S1
C	519	ILE	-	expression tag	UNP C3W5S1
C	520	PRO	-	expression tag	UNP C3W5S1
C	521	GLU	-	expression tag	UNP C3W5S1
C	522	ALA	-	expression tag	UNP C3W5S1
C	523	PRO	-	expression tag	UNP C3W5S1
C	524	ARG	-	expression tag	UNP C3W5S1
C	525	ASP	-	expression tag	UNP C3W5S1
C	526	GLY	-	expression tag	UNP C3W5S1
C	527	GLN	-	expression tag	UNP C3W5S1
C	528	ALA	-	expression tag	UNP C3W5S1
C	529	TYR	-	expression tag	UNP C3W5S1
C	530	VAL	-	expression tag	UNP C3W5S1
C	531	ARG	-	expression tag	UNP C3W5S1
C	532	LYS	-	expression tag	UNP C3W5S1
C	533	ASP	-	expression tag	UNP C3W5S1
C	534	GLY	-	expression tag	UNP C3W5S1
C	535	GLU	-	expression tag	UNP C3W5S1
C	536	TRP	-	expression tag	UNP C3W5S1
C	537	VAL	-	expression tag	UNP C3W5S1
C	538	LEU	-	expression tag	UNP C3W5S1
C	539	LEU	-	expression tag	UNP C3W5S1
C	540	SER	-	expression tag	UNP C3W5S1
C	541	THR	-	expression tag	UNP C3W5S1
C	542	PHE	-	expression tag	UNP C3W5S1
C	543	LEU	-	expression tag	UNP C3W5S1
C	544	GLY	-	expression tag	UNP C3W5S1
C	545	HIS	-	expression tag	UNP C3W5S1
C	546	HIS	-	expression tag	UNP C3W5S1
C	547	HIS	-	expression tag	UNP C3W5S1
C	548	HIS	-	expression tag	UNP C3W5S1
C	549	HIS	-	expression tag	UNP C3W5S1
C	550	HIS	-	expression tag	UNP C3W5S1

- Molecule 2 is a protein called Heavy chain antibody G2.3-Fc.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	121	Total	C	N	O	S	0	0
			856	541	154	156	5		
2	E	121	Total	C	N	O	S	0	0
			856	541	154	156	5		
2	F	121	Total	C	N	O	S	0	0
			856	541	154	156	5		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

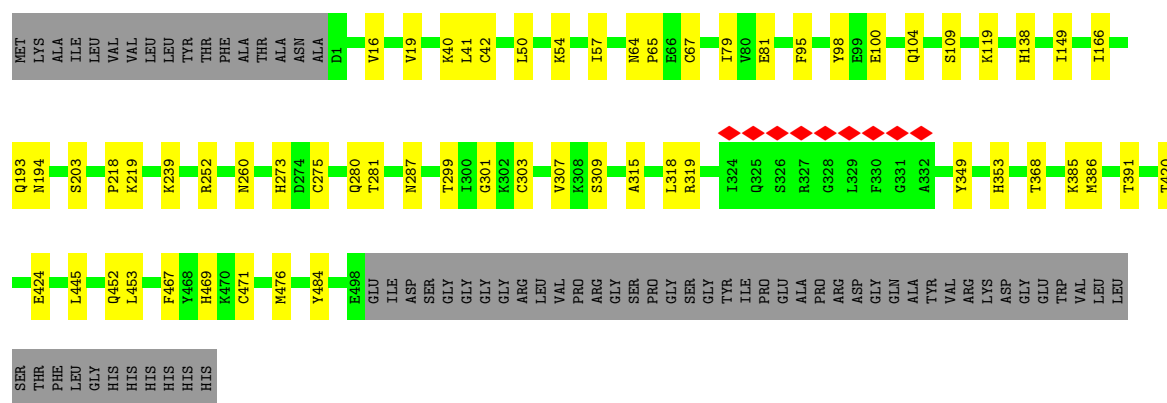


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	

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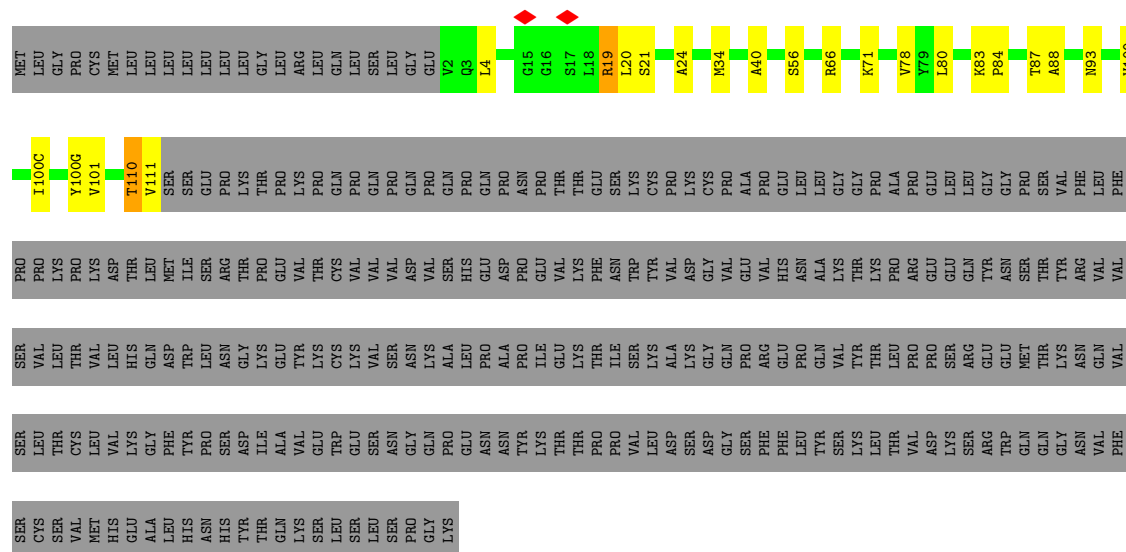
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Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	



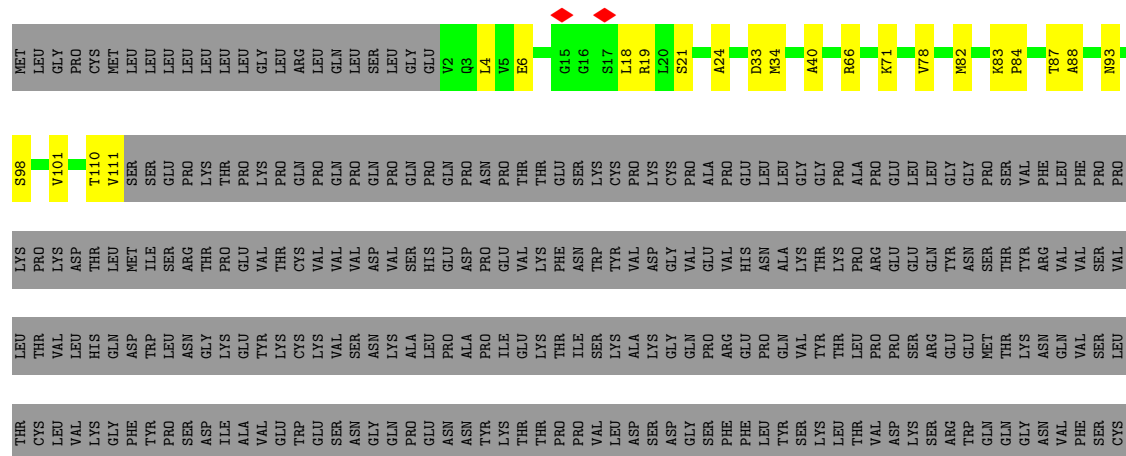
• Molecule 2: Heavy chain antibody G2.3-Fc

Chain D: 24% 5% 70%



• Molecule 2: Heavy chain antibody G2.3-Fc

Chain E: 25% 6% 70%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	96191	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	66	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.201	Depositor
Minimum map value	-0.086	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.039	Depositor
Map size (\AA)	261.0, 261.0, 261.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.87, 0.87, 0.87	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	0.19	0/3811	0.32	0/5195
1	B	0.21	0/3811	0.39	4/5195 (0.1%)
1	C	0.19	0/3811	0.32	0/5195
2	D	0.26	0/876	0.44	0/1190
2	E	0.22	0/876	0.39	0/1190
2	F	0.29	0/876	0.44	0/1190
All	All	0.21	0/14061	0.36	4/19155 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	374	GLU	CA-C-N	-8.07	109.40	120.46
1	B	374	GLU	C-N-CA	-8.07	109.40	120.46
1	B	373	ASP	N-CA-C	-7.06	101.18	110.43
1	B	374	GLU	N-CA-CB	6.27	121.09	110.49

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	30	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3720	0	3417	36	0
1	B	3720	0	3417	39	0
1	C	3720	0	3417	37	0
2	D	856	0	756	10	0
2	E	856	0	756	11	0
2	F	856	0	756	10	0
3	A	70	0	65	0	0
3	B	70	0	65	0	0
3	C	70	0	65	1	0
All	All	13938	0	12714	137	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 5.

All (137) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:HIS:HB2	1:B:476:MET:HE1	1.71	0.73
1:C:353:HIS:HB2	1:C:476:MET:HE1	1.74	0.70
1:C:301:GLY:HA2	1:C:391:THR:HG22	1.76	0.67
1:A:307:VAL:HG12	1:A:309:SER:H	1.59	0.66
1:A:301:GLY:HA2	1:A:391:THR:HG22	1.78	0.66
1:B:307:VAL:HG12	1:B:309:SER:H	1.61	0.66
1:B:281:THR:HG22	1:B:299:THR:HG22	1.78	0.66
1:C:307:VAL:HG12	1:C:309:SER:H	1.61	0.65
1:A:281:THR:HG22	1:A:299:THR:HG22	1.79	0.64
1:B:301:GLY:HA2	1:B:391:THR:HG22	1.77	0.64
1:C:281:THR:HG22	1:C:299:THR:HG22	1.79	0.64
2:F:40:ALA:H	2:F:88:ALA:HB1	1.63	0.64
1:A:65:PRO:HB3	1:A:138:HIS:HB2	1.80	0.62
2:E:82:MET:HA	2:E:82:MET:HE2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:PRO:HB3	1:C:138:HIS:HB2	1.82	0.61
1:A:277:THR:HG21	1:A:285:ALA:HB1	1.82	0.61
1:B:65:PRO:HB3	1:B:138:HIS:HB2	1.83	0.60
2:E:71:LYS:HG2	2:E:78:VAL:HG22	1.84	0.60
2:D:40:ALA:H	2:D:88:ALA:HB1	1.67	0.59
1:B:307:VAL:HG13	1:B:420:THR:HG22	1.84	0.59
2:E:83:LYS:HB3	2:E:83:LYS:HZ2	1.68	0.59
2:F:66:ARG:HH12	2:F:83:LYS:HG2	1.67	0.59
1:C:307:VAL:HG13	1:C:420:THR:HG22	1.83	0.59
1:B:277:THR:HG21	1:B:285:ALA:HB1	1.84	0.58
2:E:40:ALA:H	2:E:88:ALA:HB1	1.68	0.57
1:A:307:VAL:HG13	1:A:420:THR:HG22	1.84	0.57
2:D:83:LYS:HZ2	2:D:83:LYS:HB3	1.68	0.57
1:C:16:VAL:HG21	1:C:315:ALA:HB2	1.87	0.56
1:A:257:MET:HE2	1:A:259:ARG:HD3	1.86	0.55
2:F:83:LYS:HZ2	2:F:83:LYS:HB3	1.72	0.55
1:B:50:LEU:HD23	1:B:79:ILE:HG12	1.89	0.55
1:C:469:HIS:CE1	1:C:471:CYS:HB2	2.44	0.53
2:D:19:ARG:HA	2:D:80:LEU:O	2.08	0.53
1:C:50:LEU:HD23	1:C:79:ILE:HG12	1.90	0.52
2:F:71:LYS:HG2	2:F:78:VAL:HG22	1.91	0.52
1:C:149:ILE:HD11	1:C:252:ARG:HD3	1.91	0.52
1:C:166:ILE:HG12	1:C:239:LYS:HE3	1.92	0.51
2:D:66:ARG:HH12	2:D:83:LYS:HG2	1.76	0.51
2:F:19:ARG:HA	2:F:80:LEU:O	2.09	0.51
1:A:424:GLU:HB3	1:B:385:LYS:HD2	1.93	0.51
1:A:149:ILE:HD11	1:A:252:ARG:HD3	1.92	0.51
1:B:197:THR:HG22	1:B:245:THR:HG22	1.94	0.50
1:B:149:ILE:HD11	1:B:252:ARG:HD3	1.93	0.50
1:A:50:LEU:HD23	1:A:79:ILE:HG12	1.92	0.50
2:F:4:LEU:HD23	2:F:24:ALA:HB2	1.93	0.50
1:B:166:ILE:HG12	1:B:239:LYS:HE3	1.94	0.49
2:E:4:LEU:HD23	2:E:24:ALA:HB2	1.93	0.49
1:A:385:LYS:HD2	1:C:424:GLU:HB3	1.95	0.49
1:A:166:ILE:HG12	1:A:239:LYS:HE3	1.93	0.49
1:B:424:GLU:HB3	1:C:385:LYS:HD2	1.93	0.49
1:B:469:HIS:CE1	1:B:471:CYS:HB2	2.48	0.49
1:A:353:HIS:HB2	1:A:476:MET:SD	2.52	0.48
2:D:4:LEU:HD23	2:D:24:ALA:HB2	1.94	0.48
1:A:41:LEU:HD23	1:A:280:GLN:NE2	2.29	0.48
2:E:33:ASP:OD2	2:E:98:SER:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:LEU:HD23	1:C:280:GLN:NE2	2.29	0.48
1:C:100:GLU:O	1:C:104:GLN:HG2	2.14	0.48
2:D:71:LYS:HG2	2:D:78:VAL:HG22	1.96	0.48
1:B:64:ASN:HB3	1:B:67:CYS:SG	2.54	0.48
2:E:66:ARG:HH12	2:E:83:LYS:HG2	1.78	0.48
1:A:40:LYS:HD2	1:A:273:HIS:CG	2.49	0.47
1:B:41:LEU:HD23	1:B:280:GLN:NE2	2.28	0.47
1:B:40:LYS:HD2	1:B:273:HIS:CG	2.49	0.47
1:A:100:GLU:O	1:A:104:GLN:HG2	2.13	0.47
1:C:42:CYS:HB3	1:C:275:CYS:HB2	1.52	0.47
1:C:385:LYS:HD3	1:C:385:LYS:HA	1.68	0.47
2:D:84:PRO:HA	2:D:111:VAL:HG13	1.97	0.47
1:A:64:ASN:HB3	1:A:67:CYS:SG	2.55	0.47
1:C:40:LYS:HD2	1:C:273:HIS:CG	2.50	0.47
1:C:64:ASN:HB3	1:C:67:CYS:SG	2.55	0.47
1:C:353:HIS:HB2	1:C:476:MET:CE	2.43	0.47
1:B:452:GLN:HE22	1:B:484:TYR:H	1.63	0.47
1:A:452:GLN:HE22	1:A:484:TYR:H	1.63	0.46
1:C:349:TYR:H	1:C:368:THR:HG22	1.80	0.46
1:C:119:LYS:HB2	1:C:149:ILE:HD11	1.98	0.46
2:F:34:MET:HB2	2:F:78:VAL:HG21	1.98	0.46
1:A:203:SER:HA	1:C:218:PRO:HG2	1.98	0.46
1:B:95:PHE:HB3	1:B:98:TYR:HB2	1.98	0.46
1:B:385:LYS:HA	1:B:385:LYS:HD3	1.66	0.46
1:B:349:TYR:H	1:B:368:THR:HG22	1.82	0.45
1:B:182:PRO:HB2	1:B:187:ASP:HB3	1.99	0.45
1:C:445:LEU:HD12	1:C:445:LEU:HA	1.83	0.45
1:C:95:PHE:HB3	1:C:98:TYR:HB2	1.99	0.45
1:C:219:LYS:HE2	1:C:219:LYS:HB2	1.78	0.45
1:C:452:GLN:HE22	1:C:484:TYR:H	1.65	0.45
2:E:84:PRO:HA	2:E:111:VAL:HG13	1.99	0.45
1:A:95:PHE:HB3	1:A:98:TYR:HB2	1.98	0.45
1:A:453:LEU:HD11	1:A:467:PHE:CE2	2.52	0.45
1:A:119:LYS:HB2	1:A:149:ILE:HD11	1.98	0.44
1:A:70:LEU:HD23	1:A:70:LEU:HA	1.78	0.44
1:B:386:MET:HE2	1:B:386:MET:HB2	1.73	0.44
1:A:349:TYR:H	1:A:368:THR:HG22	1.81	0.44
1:A:42:CYS:HB3	1:A:275:CYS:HB2	1.53	0.44
1:B:57:ILE:HG12	1:B:81:GLU:OE2	2.17	0.44
2:F:34:MET:HA	2:F:93:ASN:O	2.18	0.44
1:C:453:LEU:HD12	1:C:453:LEU:HA	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LYS:HB2	1:B:149:ILE:HD11	1.99	0.44
1:A:385:LYS:HA	1:A:385:LYS:HD3	1.67	0.44
1:B:100:GLU:O	1:B:104:GLN:HG2	2.18	0.44
1:A:218:PRO:HG2	1:B:203:SER:HA	1.98	0.43
2:D:34:MET:HA	2:D:93:ASN:O	2.18	0.43
1:C:287:ASN:HD22	3:C:603:NAG:H83	1.82	0.43
1:C:453:LEU:HD11	1:C:467:PHE:CE2	2.53	0.43
1:B:42:CYS:HB3	1:B:275:CYS:HB2	1.53	0.43
1:B:218:PRO:HG2	1:C:203:SER:HA	1.99	0.43
1:A:57:ILE:HG12	1:A:81:GLU:OE2	2.19	0.43
1:A:305:LYS:HD2	1:A:305:LYS:HA	1.76	0.42
2:D:20:LEU:HD23	2:D:80:LEU:HD23	2.00	0.42
2:E:34:MET:HA	2:E:93:ASN:O	2.20	0.42
2:E:87:THR:OG1	2:E:110:THR:HA	2.19	0.42
1:C:299:THR:HB	1:C:303:CYS:SG	2.59	0.42
2:F:6:GLU:HG3	2:F:107:THR:HG23	2.02	0.42
1:C:57:ILE:HG12	1:C:81:GLU:OE2	2.18	0.42
1:B:305:LYS:HA	1:B:305:LYS:HD2	1.75	0.42
1:C:54:LYS:H	1:C:54:LYS:HG3	1.57	0.42
1:B:16:VAL:HG11	1:B:315:ALA:HB2	2.02	0.42
1:A:299:THR:HB	1:A:303:CYS:SG	2.59	0.42
1:B:132:VAL:HG13	1:B:142:LYS:HD3	2.02	0.42
2:D:87:THR:OG1	2:D:110:THR:HA	2.20	0.41
1:B:299:THR:HB	1:B:303:CYS:SG	2.60	0.41
1:C:57:ILE:HD11	1:C:79:ILE:HG21	2.02	0.41
1:A:151:LEU:HD23	1:A:151:LEU:HA	1.82	0.41
1:A:109:SER:OG	1:A:260:ASN:HB2	2.21	0.41
1:B:219:LYS:HE2	1:B:219:LYS:HB2	1.79	0.41
1:B:40:LYS:HE2	1:B:40:LYS:HB2	1.83	0.41
1:B:453:LEU:HD11	1:B:467:PHE:CE2	2.55	0.41
1:A:40:LYS:HE2	1:A:40:LYS:HB2	1.83	0.41
2:F:84:PRO:HA	2:F:111:VAL:HG13	2.01	0.41
1:B:386:MET:HE1	1:B:419:TRP:CZ3	2.56	0.41
2:E:18:LEU:H	2:E:82:MET:HB2	1.86	0.41
1:C:109:SER:OG	1:C:260:ASN:HB2	2.21	0.41
1:A:122:SER:HG	1:A:123:TRP:CD1	2.38	0.41
1:B:61:ILE:HD12	1:B:61:ILE:HA	1.93	0.41
1:B:193:GLN:O	1:B:194:ASN:C	2.64	0.40
1:A:219:LYS:HE2	1:A:219:LYS:HB2	1.79	0.40
1:A:193:GLN:O	1:A:194:ASN:C	2.64	0.40
1:C:386:MET:HB2	1:C:386:MET:HE2	1.83	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	496/567 (88%)	471 (95%)	24 (5%)	1 (0%)	43	62
1	B	496/567 (88%)	471 (95%)	24 (5%)	1 (0%)	43	62
1	C	496/567 (88%)	470 (95%)	25 (5%)	1 (0%)	43	62
2	D	119/400 (30%)	116 (98%)	3 (2%)	0	100	100
2	E	119/400 (30%)	116 (98%)	3 (2%)	0	100	100
2	F	119/400 (30%)	115 (97%)	4 (3%)	0	100	100
All	All	1845/2901 (64%)	1759 (95%)	83 (4%)	3 (0%)	44	62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	GLN
1	C	193	GLN
1	B	193	GLN

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	365/488 (75%)	357 (98%)	8 (2%)	45	71
1	B	365/488 (75%)	355 (97%)	10 (3%)	39	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	365/488 (75%)	361 (99%)	4 (1%)	65 83
2	D	71/350 (20%)	63 (89%)	8 (11%)	5 11
2	E	71/350 (20%)	67 (94%)	4 (6%)	19 37
2	F	71/350 (20%)	65 (92%)	6 (8%)	10 20
All	All	1308/2514 (52%)	1268 (97%)	40 (3%)	36 60

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	187	ASP
1	A	194	ASN
1	A	245	THR
1	A	318	LEU
1	A	372	ILE
1	A	475	CYS
1	A	476	MET
2	D	19	ARG
2	D	21	SER
2	D	56	SER
2	D	100	VAL
2	D	100(C)	ILE
2	D	100(G)	TYR
2	D	101	VAL
2	D	110	THR
1	B	16	VAL
1	B	66	GLU
1	B	108	VAL
1	B	187	ASP
1	B	194	ASN
1	B	318	LEU
1	B	319	ARG
1	B	372	ILE
1	B	373	ASP
1	B	475	CYS
2	E	6	GLU
2	E	19	ARG
2	E	21	SER
2	E	101	VAL
1	C	19	VAL
1	C	194	ASN

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Mol	Chain	Res	Type
1	C	318	LEU
1	C	319	ARG
2	F	19	ARG
2	F	21	SER
2	F	30	ARG
2	F	100	VAL
2	F	100(C)	ILE
2	F	100(G)	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	ASN
1	A	147	ASN
1	A	273	HIS
1	A	280	GLN
1	A	369	GLN
1	A	452	GLN
2	D	3	GLN
1	B	129	ASN
1	B	147	ASN
1	B	273	HIS
1	B	280	GLN
1	B	369	GLN
2	E	3	GLN
1	C	129	ASN
1	C	147	ASN
1	C	280	GLN
1	C	369	GLN
2	F	3	GLN

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 [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	$\# Z > 2$
3	NAG	A	604	1	14,14,15	0.70	0	17,19,21	1.29	2 (11%)
3	NAG	C	602	1	14,14,15	0.73	0	17,19,21	0.81	0
3	NAG	C	603	1	14,14,15	0.74	0	17,19,21	0.89	0
3	NAG	B	601	1	14,14,15	0.72	0	17,19,21	0.84	0
3	NAG	A	602	1	14,14,15	0.75	0	17,19,21	0.96	1 (5%)
3	NAG	B	605	1	14,14,15	0.72	0	17,19,21	0.83	0
3	NAG	C	601	1	14,14,15	0.73	0	17,19,21	0.85	0
3	NAG	C	605	1	14,14,15	0.77	0	17,19,21	0.78	0
3	NAG	A	603	1	14,14,15	0.70	0	17,19,21	1.27	1 (5%)
3	NAG	B	604	1	14,14,15	0.76	0	17,19,21	0.78	0
3	NAG	C	604	1	14,14,15	0.76	0	17,19,21	0.97	1 (5%)
3	NAG	A	601	1	14,14,15	0.73	0	17,19,21	0.84	0
3	NAG	B	602	1	14,14,15	0.75	0	17,19,21	0.98	1 (5%)
3	NAG	A	605	1	14,14,15	0.76	0	17,19,21	0.78	0
3	NAG	B	603	1	14,14,15	0.74	0	17,19,21	0.83	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
3	NAG	A	604	1	-	2/6/23/26	0/1/1/1
3	NAG	C	602	1	-	0/6/23/26	0/1/1/1
3	NAG	C	603	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	601	1	-	0/6/23/26	0/1/1/1
3	NAG	A	602	1	-	1/6/23/26	0/1/1/1
3	NAG	B	605	1	-	0/6/23/26	0/1/1/1
3	NAG	C	601	1	-	0/6/23/26	0/1/1/1
3	NAG	C	605	1	-	0/6/23/26	0/1/1/1
3	NAG	A	603	1	-	2/6/23/26	0/1/1/1
3	NAG	B	604	1	-	0/6/23/26	0/1/1/1
3	NAG	C	604	1	-	1/6/23/26	0/1/1/1
3	NAG	A	601	1	-	0/6/23/26	0/1/1/1
3	NAG	B	602	1	-	0/6/23/26	0/1/1/1
3	NAG	A	605	1	-	0/6/23/26	0/1/1/1
3	NAG	B	603	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	604	NAG	C2-N2-C7	3.35	127.68	122.90
3	A	603	NAG	C2-N2-C7	3.23	127.50	122.90
3	B	602	NAG	C1-O5-C5	2.72	115.88	112.19
3	C	604	NAG	C1-O5-C5	2.61	115.73	112.19
3	A	602	NAG	C1-O5-C5	2.58	115.69	112.19
3	A	604	NAG	O5-C1-C2	-2.26	107.73	111.29

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	603	NAG	C8-C7-N2-C2
3	C	603	NAG	O7-C7-N2-C2
3	A	603	NAG	O5-C5-C6-O6
3	A	603	NAG	C3-C2-N2-C7
3	A	604	NAG	C3-C2-N2-C7
3	A	604	NAG	C1-C2-N2-C7
3	A	602	NAG	O5-C5-C6-O6
3	C	604	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	603	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

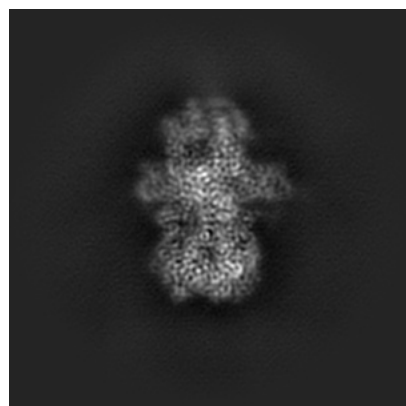
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-69590. These allow visual inspection of the internal detail of the map and identification of artifacts.

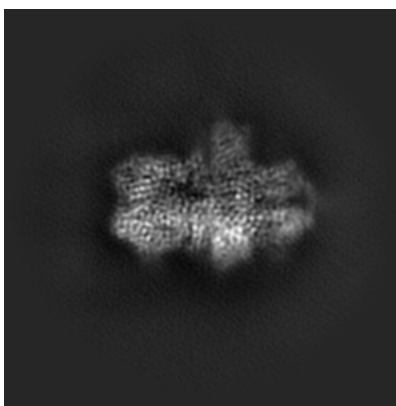
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

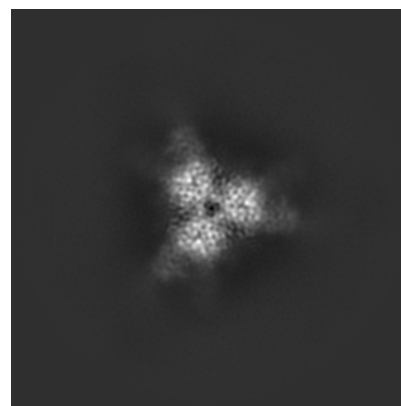
6.1.1 Primary map



X

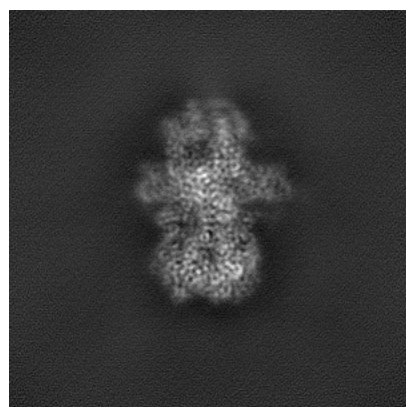


Y

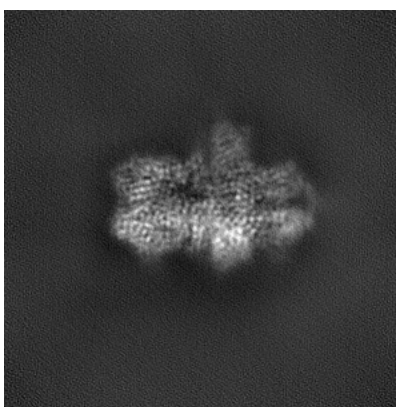


Z

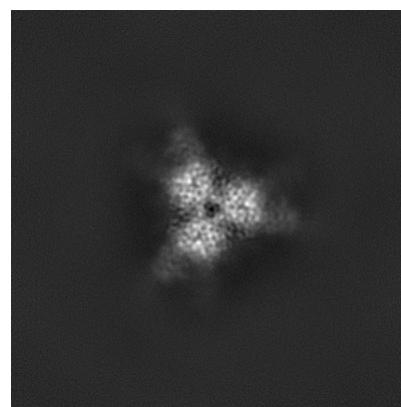
6.1.2 Raw map



X



Y

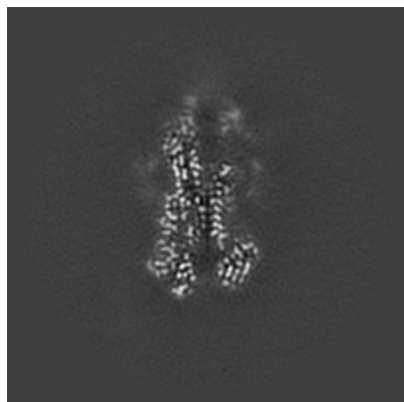


Z

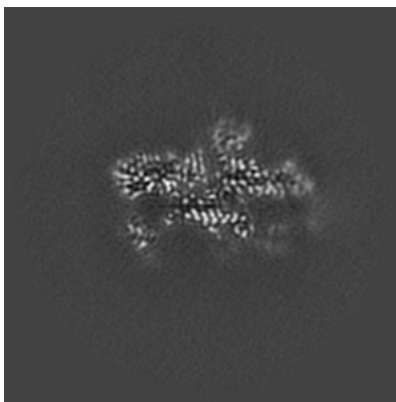
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

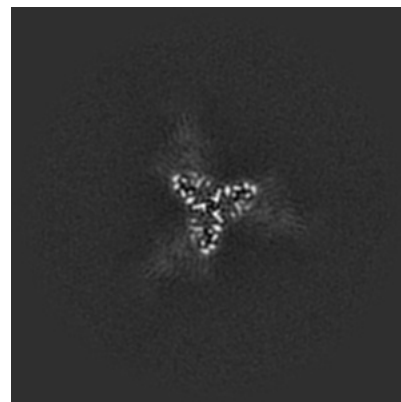
6.2.1 Primary map



X Index: 150

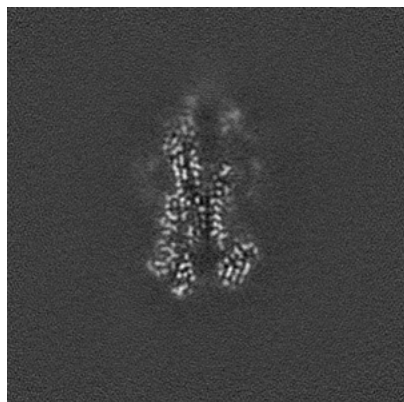


Y Index: 150

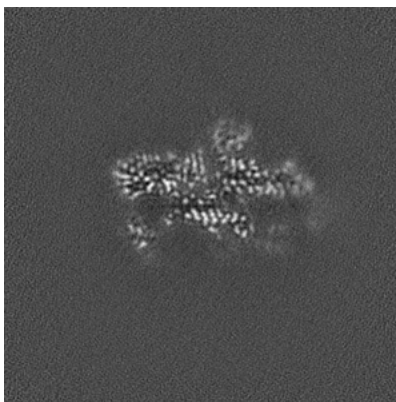


Z Index: 150

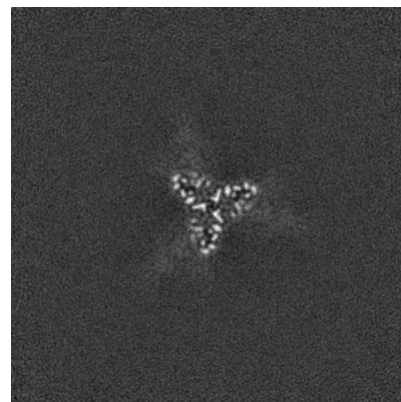
6.2.2 Raw map



X Index: 150



Y Index: 150

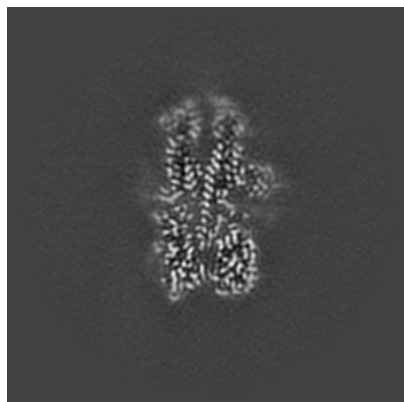


Z Index: 150

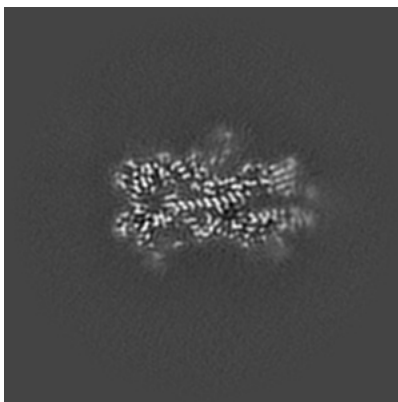
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

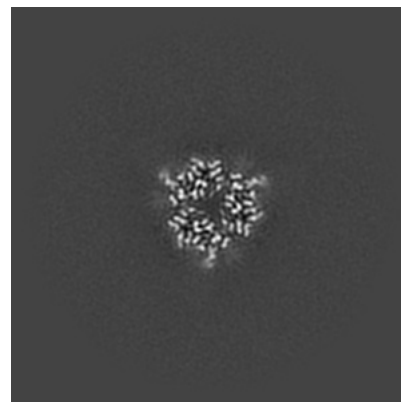
6.3.1 Primary map



X Index: 140

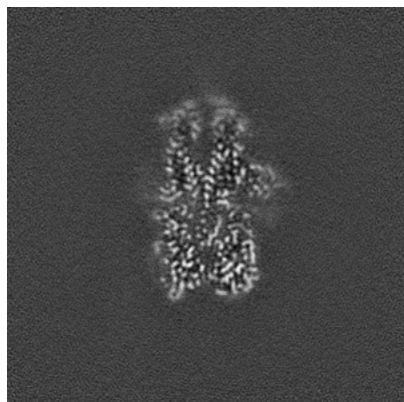


Y Index: 159

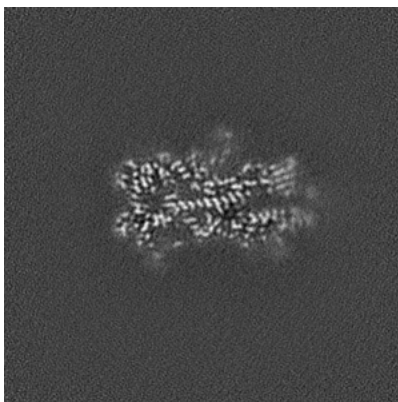


Z Index: 107

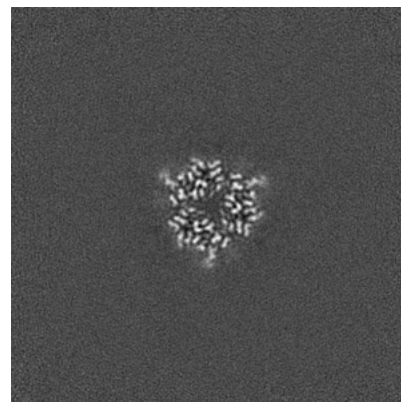
6.3.2 Raw map



X Index: 139



Y Index: 159

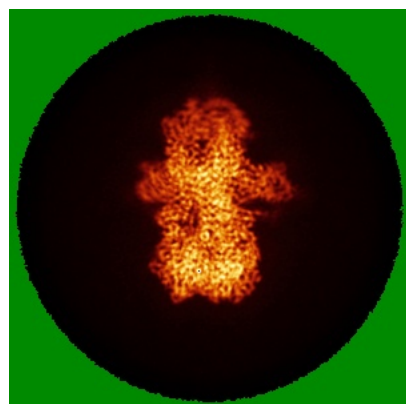


Z Index: 107

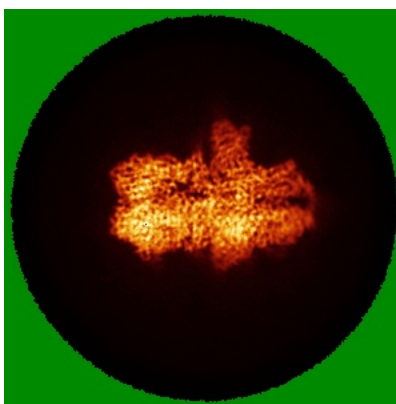
The images above show the largest variance slices of the map in three orthogonal directions.

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

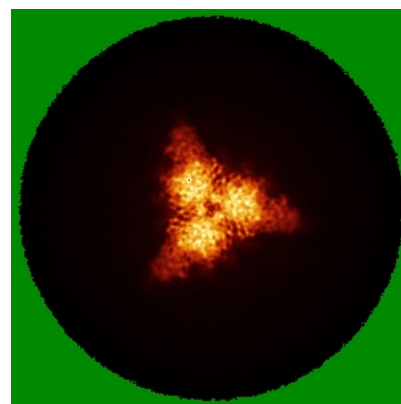
6.4.1 Primary map



X

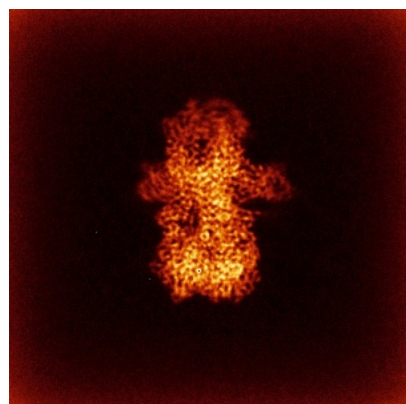


Y

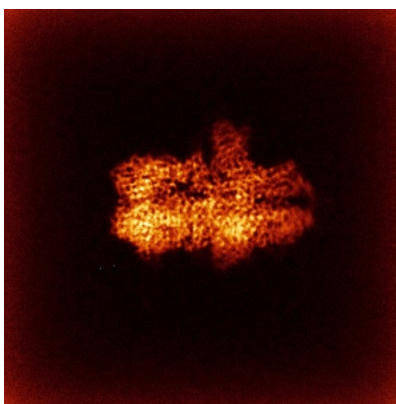


Z

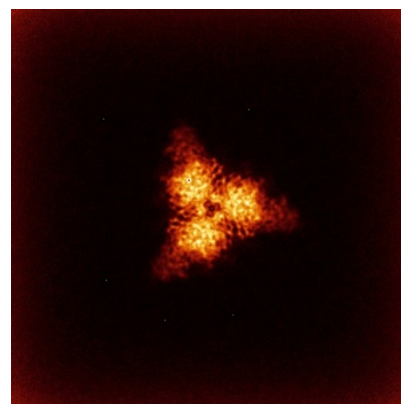
6.4.2 Raw map



X



Y

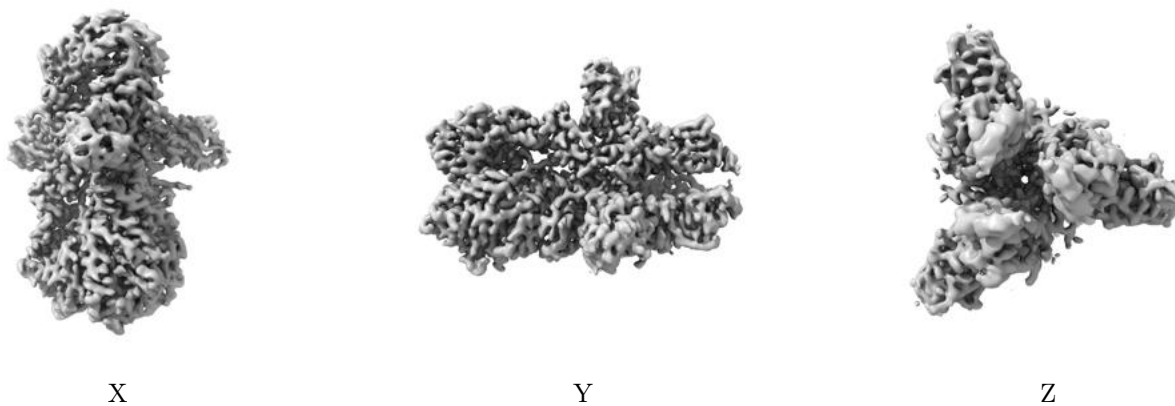


Z

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

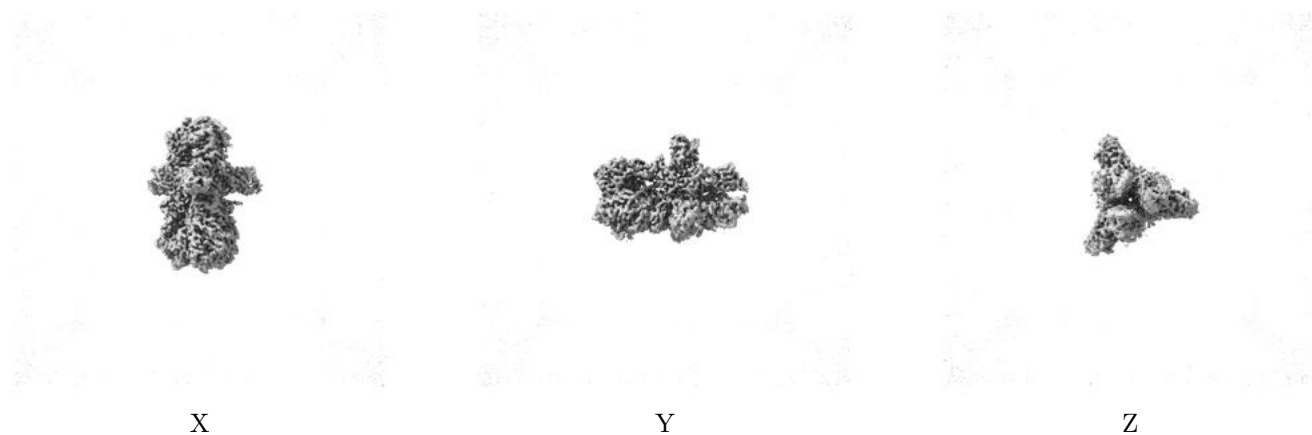
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.039. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

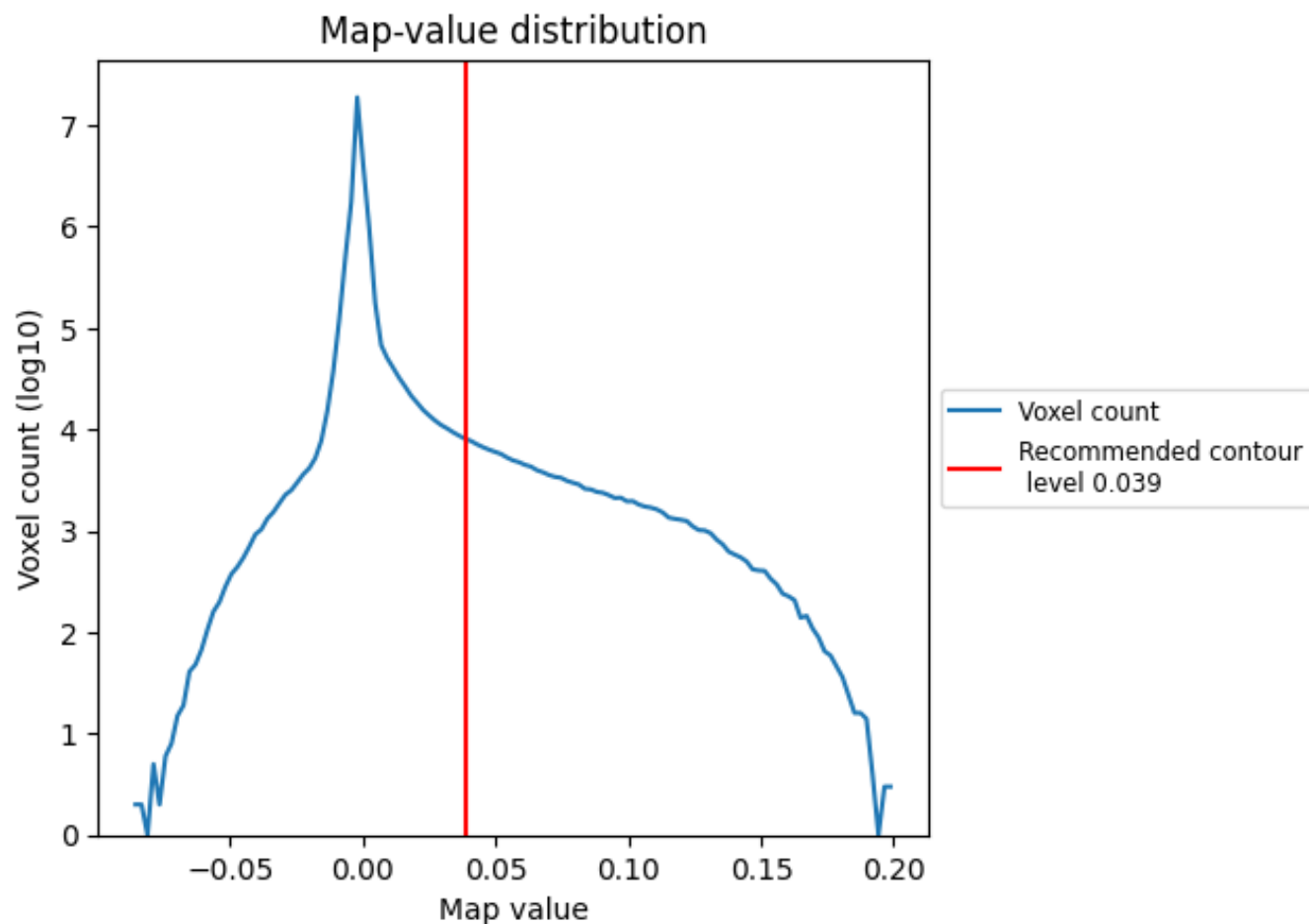
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

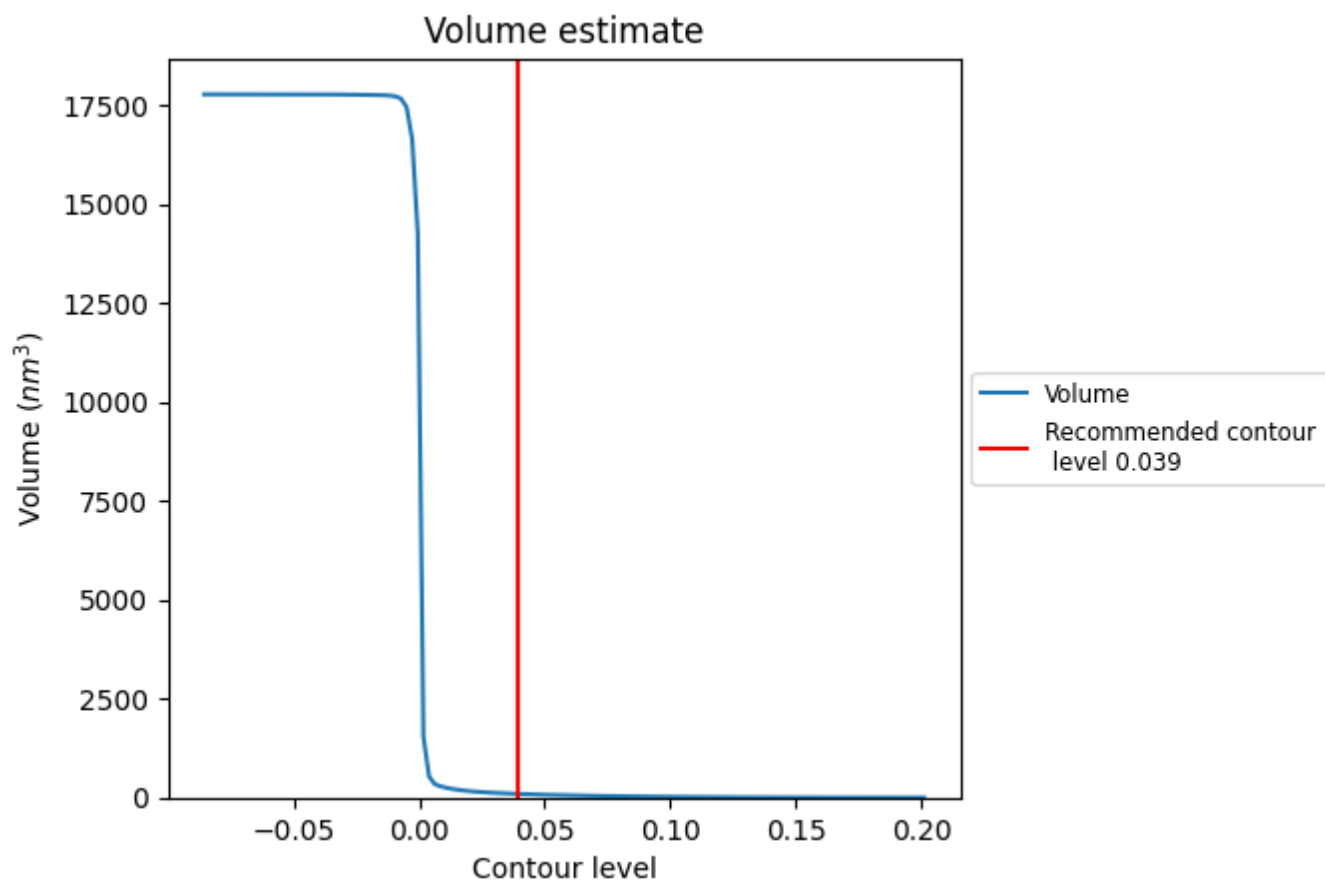
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

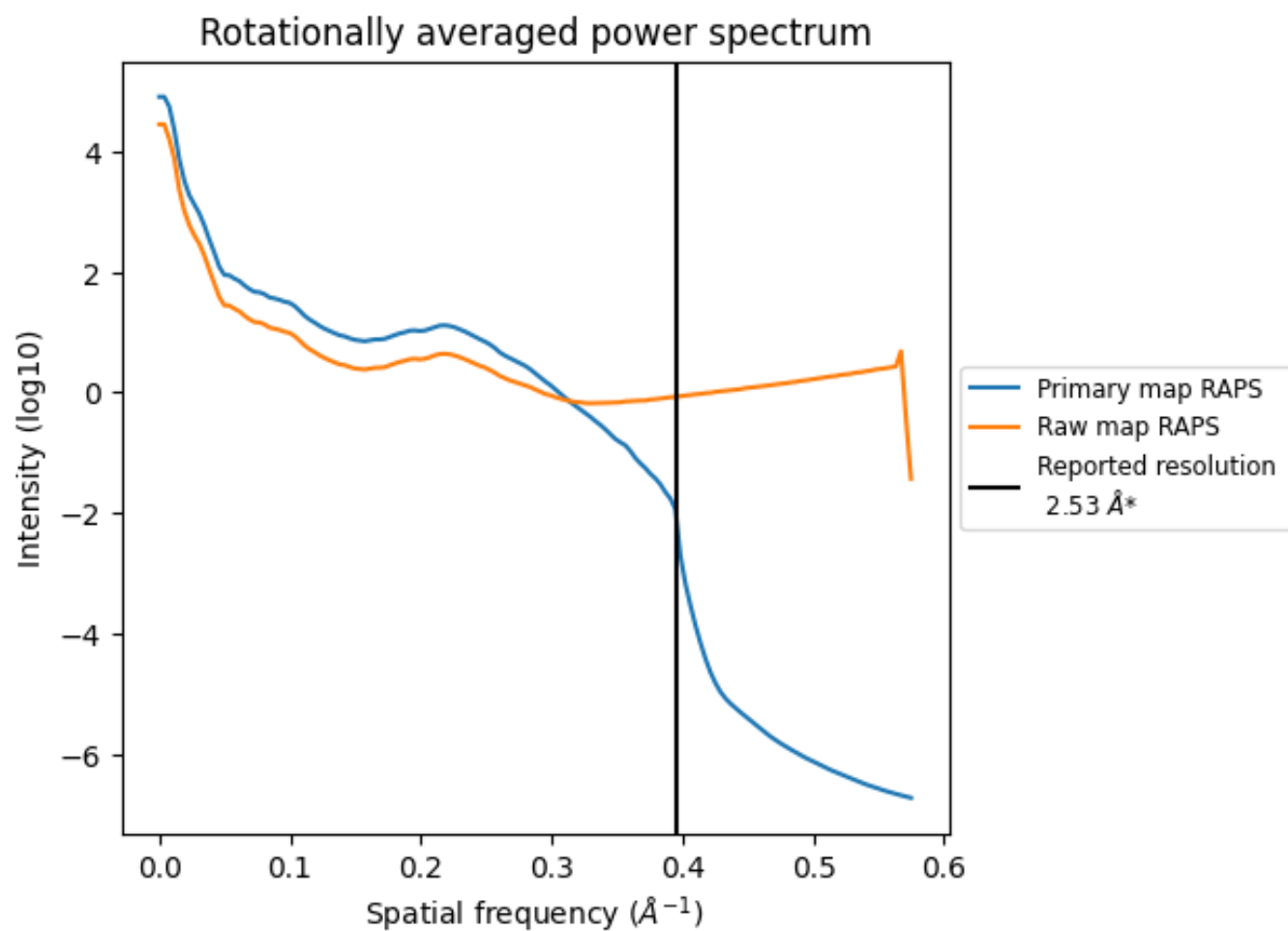
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 93 nm^3 ; this corresponds to an approximate mass of 84 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 ⓘ

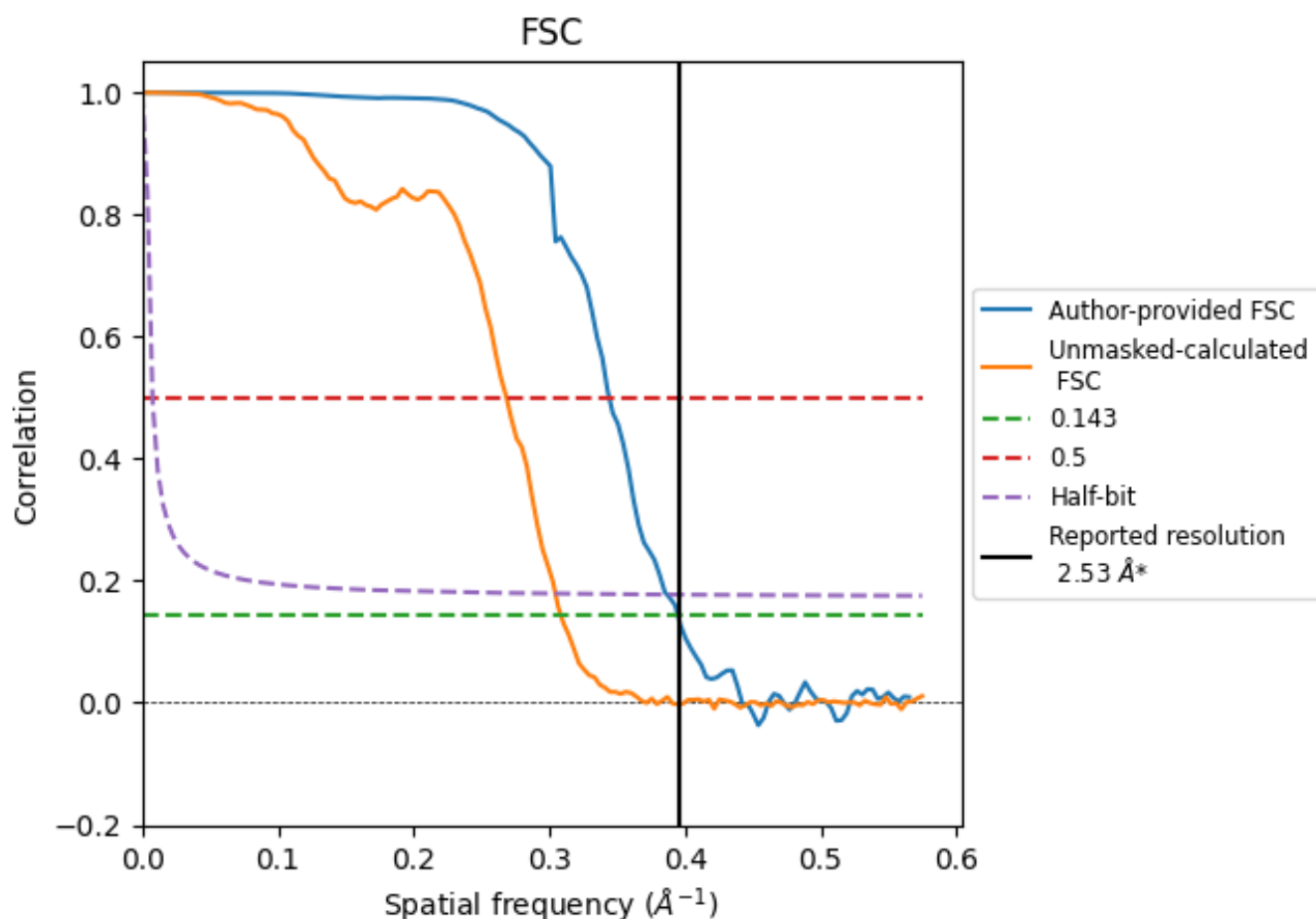


*Reported resolution corresponds to spatial frequency of 0.395 \AA^{-1}

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 0.395 \AA^{-1}

8.2 Resolution estimates [i](#)

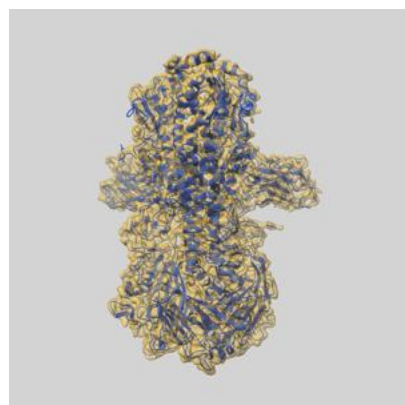
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.53	-	-
Author-provided FSC curve	2.53	2.91	2.59
Unmasked-calculated*	3.24	3.73	3.28

*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 3.24 differs from the reported value 2.53 by more than 10 %

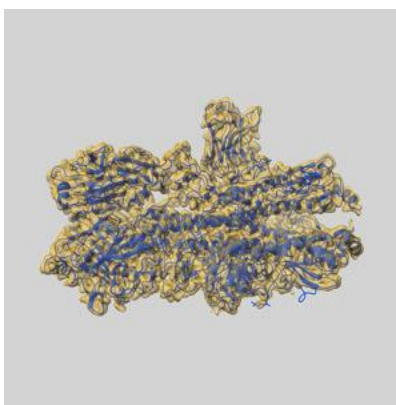
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-69590 and PDB model 24KR. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

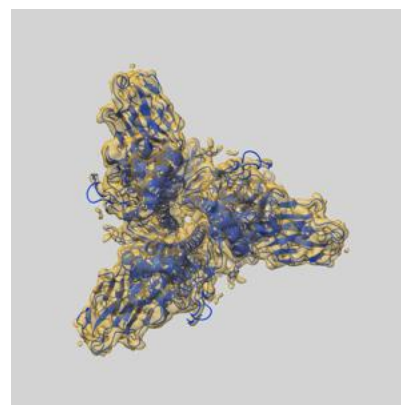
9.1 Map-model overlay [i](#)



X



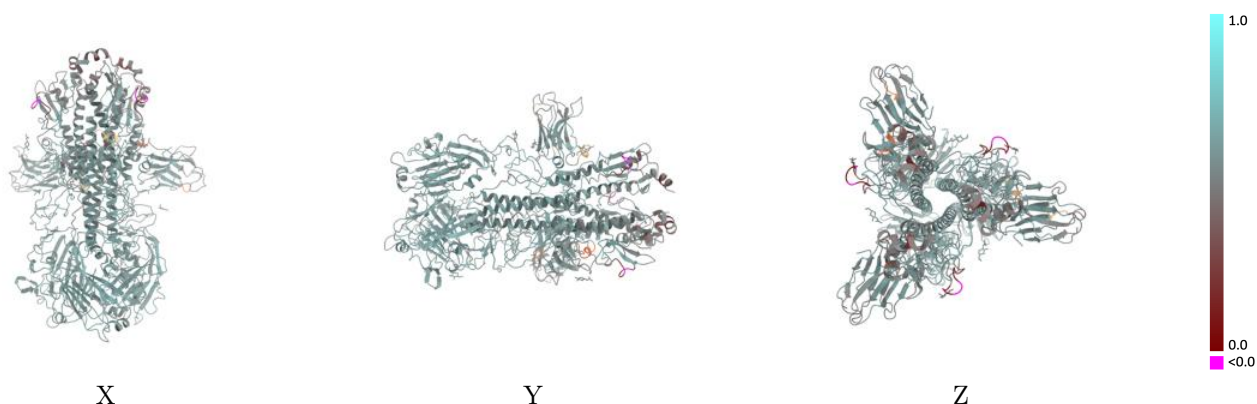
Y



Z

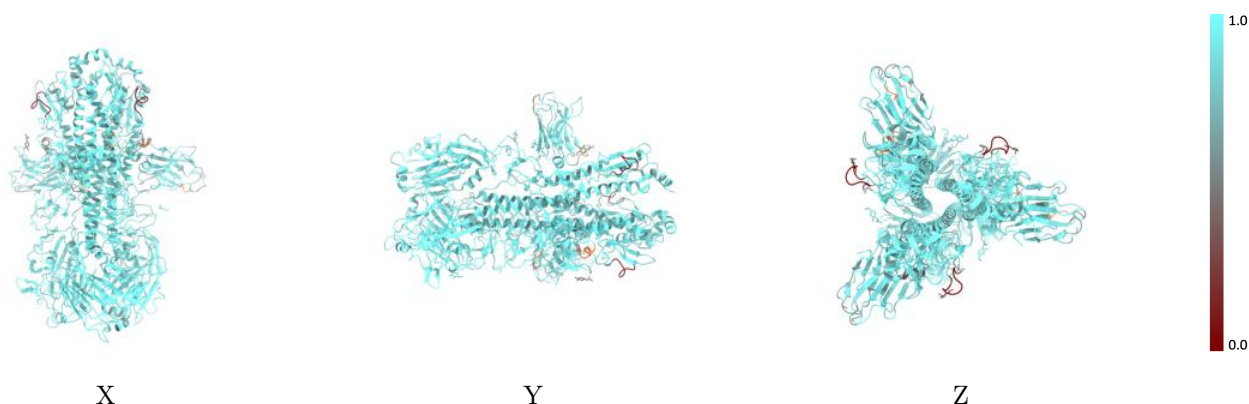
The images above show the 3D surface view of the map at the recommended contour level 0.039 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



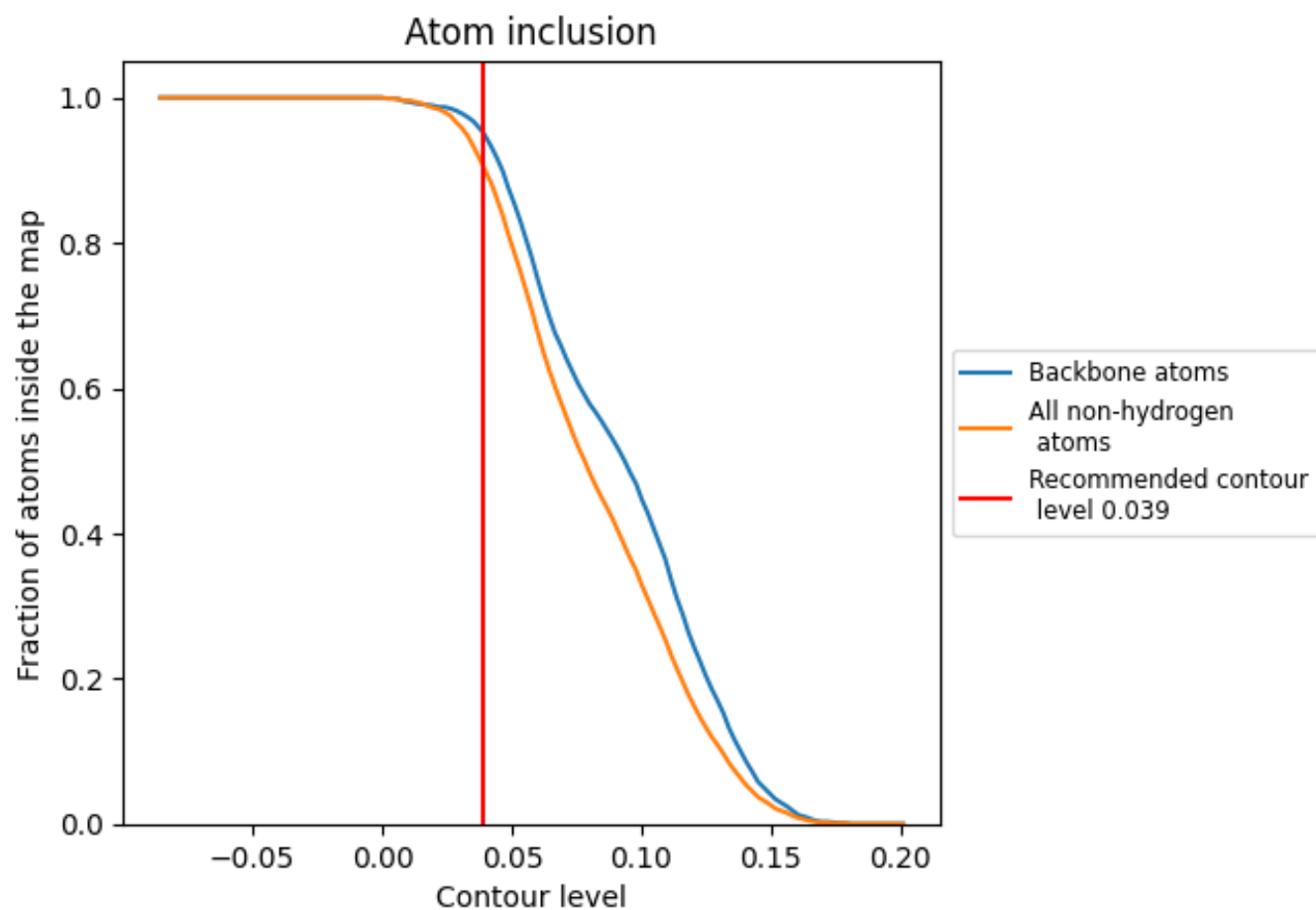
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.039).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 91% 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 (0.039) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9060	<div><div></div></div> 0.5680
A	<div><div></div></div> 0.9120	<div><div></div></div> 0.5710
B	<div><div></div></div> 0.9130	<div><div></div></div> 0.5710
C	<div><div></div></div> 0.9120	<div><div></div></div> 0.5700
D	<div><div></div></div> 0.8770	<div><div></div></div> 0.5520
E	<div><div></div></div> 0.8790	<div><div></div></div> 0.5530
F	<div><div></div></div> 0.8730	<div><div></div></div> 0.5520

