



Full wwPDB EM Validation Report ⓘ

Oct 5, 2026 – 04:21 pm BST

PDB ID : 33SD / pdb_000033sd
EMDB ID : EMD-59533
Title : Immune complex comprising the HRSV preF trimer (SC-DM) and the monoclonal antibody Lor69 - Obtained by cryo-EM
Authors : Ols, S.; Cerveira, R.A.; Borst, A.J.; Bermudez-Mendez, E.; Gegenfurtner, F.; Eray, E.; Weidle, C.; Miranda, M.C.; Peng, Z.; Carr, K.D.; Skotheim, R.; Kochmann, J.; Brunette, N.; Lenart, K.; Hanke, L.; Karlsson Hedestam, G.B.; Perez, L.; Antanasijevic, A.; King, N.P.; Lore, K.
Deposited on : 2026-08-21
Resolution : 3.30 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.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.2
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) : 2.51

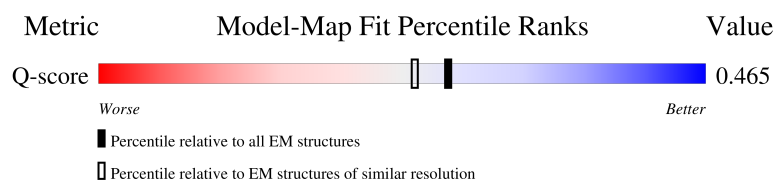
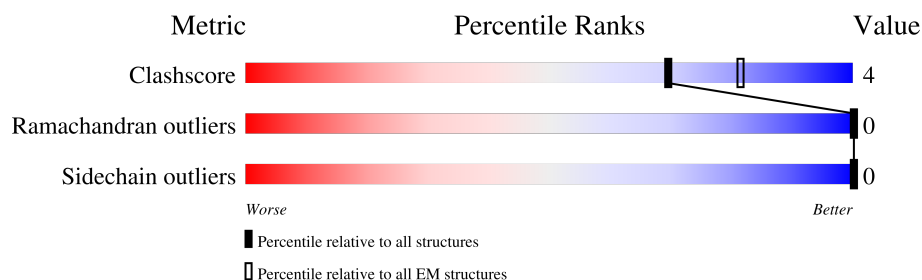
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	522	 75% 11% 14%
1	B	522	 75% 10% 14%
1	C	522	 75% 11% 14%

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Mol	Chain	Length	Quality of chain
2	D	121	92% 6% ..
2	E	121	92% 6% ..
2	H	121	92% 6% ..
3	F	107	86% 12% .
3	G	107	86% 12% .
3	L	107	87% 11% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15687 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 F0.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	448	Total	C	N	O	S	0	0
			3461	2181	573	686	21		
1	B	448	Total	C	N	O	S	0	0
			3461	2181	573	686	21		
1	C	448	Total	C	N	O	S	0	0
			3461	2181	573	686	21		

There are 189 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	LYS	GLU	conflict	UNP P03420
A	67	ILE	ASN	conflict	UNP P03420
A	76	ILE	VAL	conflict	UNP P03420
A	102	ALA	PRO	conflict	UNP P03420
A	106	GLN	ARG	conflict	UNP P03420
A	?	-	ARG	deletion	UNP P03420
A	?	-	GLU	deletion	UNP P03420
A	?	-	LEU	deletion	UNP P03420
A	?	-	PRO	deletion	UNP P03420
A	?	-	ARG	deletion	UNP P03420
A	?	-	PHE	deletion	UNP P03420
A	?	-	MET	deletion	UNP P03420
A	?	-	ASN	deletion	UNP P03420
A	?	-	TYR	deletion	UNP P03420
A	?	-	THR	deletion	UNP P03420
A	?	-	LEU	deletion	UNP P03420
A	?	-	ASN	deletion	UNP P03420
A	?	-	ASN	deletion	UNP P03420
A	?	-	ALA	deletion	UNP P03420
A	?	-	LYS	deletion	UNP P03420
A	?	-	LYS	deletion	UNP P03420
A	?	-	THR	deletion	UNP P03420
A	?	-	ASN	deletion	UNP P03420
A	?	-	VAL	deletion	UNP P03420

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP P03420
A	?	-	LEU	deletion	UNP P03420
A	?	-	SER	deletion	UNP P03420
A	109	GLY	LYS	linker	UNP P03420
A	110	SER	LYS	linker	UNP P03420
A	111	GLY	ARG	linker	UNP P03420
A	112	SER	LYS	linker	UNP P03420
A	113	GLY	ARG	linker	UNP P03420
A	115	SER	PHE	conflict	UNP P03420
A	193	PRO	SER	conflict	UNP P03420
A	357	VAL	ILE	conflict	UNP P03420
A	425	VAL	MET	conflict	UNP P03420
A	492	SER	-	insertion	UNP P03420
A	493	ALA	HIS	conflict	UNP P03420
A	494	ILE	ASN	conflict	UNP P03420
A	495	GLY	VAL	conflict	UNP P03420
A	496	GLY	ASN	conflict	UNP P03420
A	497	TYR	ALA	conflict	UNP P03420
A	498	ILE	GLY	conflict	UNP P03420
A	499	PRO	LYS	conflict	UNP P03420
A	500	GLU	SER	conflict	UNP P03420
A	501	ALA	THR	conflict	UNP P03420
A	502	PRO	THR	conflict	UNP P03420
A	503	ARG	ASN	conflict	UNP P03420
A	504	ASP	ILE	conflict	UNP P03420
A	505	GLY	MET	conflict	UNP P03420
A	506	GLN	ILE	conflict	UNP P03420
A	507	ALA	THR	conflict	UNP P03420
A	508	TYR	THR	conflict	UNP P03420
A	509	VAL	ILE	conflict	UNP P03420
A	510	ARG	ILE	conflict	UNP P03420
A	511	LYS	ILE	conflict	UNP P03420
A	512	ASP	VAL	conflict	UNP P03420
A	513	GLY	ILE	conflict	UNP P03420
A	514	GLU	ILE	conflict	UNP P03420
A	515	TRP	VAL	conflict	UNP P03420
A	516	VAL	ILE	conflict	UNP P03420
A	520	THR	-	insertion	UNP P03420
A	521	PHE	-	insertion	UNP P03420
B	66	LYS	GLU	conflict	UNP P03420
B	67	ILE	ASN	conflict	UNP P03420
B	76	ILE	VAL	conflict	UNP P03420

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Chain	Residue	Modelled	Actual	Comment	Reference
B	102	ALA	PRO	conflict	UNP P03420
B	106	GLN	ARG	conflict	UNP P03420
B	?	-	ARG	deletion	UNP P03420
B	?	-	GLU	deletion	UNP P03420
B	?	-	LEU	deletion	UNP P03420
B	?	-	PRO	deletion	UNP P03420
B	?	-	ARG	deletion	UNP P03420
B	?	-	PHE	deletion	UNP P03420
B	?	-	MET	deletion	UNP P03420
B	?	-	ASN	deletion	UNP P03420
B	?	-	TYR	deletion	UNP P03420
B	?	-	THR	deletion	UNP P03420
B	?	-	LEU	deletion	UNP P03420
B	?	-	ASN	deletion	UNP P03420
B	?	-	ASN	deletion	UNP P03420
B	?	-	ALA	deletion	UNP P03420
B	?	-	LYS	deletion	UNP P03420
B	?	-	LYS	deletion	UNP P03420
B	?	-	THR	deletion	UNP P03420
B	?	-	ASN	deletion	UNP P03420
B	?	-	VAL	deletion	UNP P03420
B	?	-	THR	deletion	UNP P03420
B	?	-	LEU	deletion	UNP P03420
B	?	-	SER	deletion	UNP P03420
B	109	GLY	LYS	linker	UNP P03420
B	110	SER	LYS	linker	UNP P03420
B	111	GLY	ARG	linker	UNP P03420
B	112	SER	LYS	linker	UNP P03420
B	113	GLY	ARG	linker	UNP P03420
B	115	SER	PHE	conflict	UNP P03420
B	193	PRO	SER	conflict	UNP P03420
B	357	VAL	ILE	conflict	UNP P03420
B	425	VAL	MET	conflict	UNP P03420
B	492	SER	-	insertion	UNP P03420
B	493	ALA	HIS	conflict	UNP P03420
B	494	ILE	ASN	conflict	UNP P03420
B	495	GLY	VAL	conflict	UNP P03420
B	496	GLY	ASN	conflict	UNP P03420
B	497	TYR	ALA	conflict	UNP P03420
B	498	ILE	GLY	conflict	UNP P03420
B	499	PRO	LYS	conflict	UNP P03420
B	500	GLU	SER	conflict	UNP P03420

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Chain	Residue	Modelled	Actual	Comment	Reference
B	501	ALA	THR	conflict	UNP P03420
B	502	PRO	THR	conflict	UNP P03420
B	503	ARG	ASN	conflict	UNP P03420
B	504	ASP	ILE	conflict	UNP P03420
B	505	GLY	MET	conflict	UNP P03420
B	506	GLN	ILE	conflict	UNP P03420
B	507	ALA	THR	conflict	UNP P03420
B	508	TYR	THR	conflict	UNP P03420
B	509	VAL	ILE	conflict	UNP P03420
B	510	ARG	ILE	conflict	UNP P03420
B	511	LYS	ILE	conflict	UNP P03420
B	512	ASP	VAL	conflict	UNP P03420
B	513	GLY	ILE	conflict	UNP P03420
B	514	GLU	ILE	conflict	UNP P03420
B	515	TRP	VAL	conflict	UNP P03420
B	516	VAL	ILE	conflict	UNP P03420
B	520	THR	-	insertion	UNP P03420
B	521	PHE	-	insertion	UNP P03420
C	66	LYS	GLU	conflict	UNP P03420
C	67	ILE	ASN	conflict	UNP P03420
C	76	ILE	VAL	conflict	UNP P03420
C	102	ALA	PRO	conflict	UNP P03420
C	106	GLN	ARG	conflict	UNP P03420
C	?	-	ARG	deletion	UNP P03420
C	?	-	GLU	deletion	UNP P03420
C	?	-	LEU	deletion	UNP P03420
C	?	-	PRO	deletion	UNP P03420
C	?	-	ARG	deletion	UNP P03420
C	?	-	PHE	deletion	UNP P03420
C	?	-	MET	deletion	UNP P03420
C	?	-	ASN	deletion	UNP P03420
C	?	-	TYR	deletion	UNP P03420
C	?	-	THR	deletion	UNP P03420
C	?	-	LEU	deletion	UNP P03420
C	?	-	ASN	deletion	UNP P03420
C	?	-	ASN	deletion	UNP P03420
C	?	-	ALA	deletion	UNP P03420
C	?	-	LYS	deletion	UNP P03420
C	?	-	LYS	deletion	UNP P03420
C	?	-	THR	deletion	UNP P03420
C	?	-	ASN	deletion	UNP P03420
C	?	-	VAL	deletion	UNP P03420

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	THR	deletion	UNP P03420
C	?	-	LEU	deletion	UNP P03420
C	?	-	SER	deletion	UNP P03420
C	109	GLY	LYS	linker	UNP P03420
C	110	SER	LYS	linker	UNP P03420
C	111	GLY	ARG	linker	UNP P03420
C	112	SER	LYS	linker	UNP P03420
C	113	GLY	ARG	linker	UNP P03420
C	115	SER	PHE	conflict	UNP P03420
C	193	PRO	SER	conflict	UNP P03420
C	357	VAL	ILE	conflict	UNP P03420
C	425	VAL	MET	conflict	UNP P03420
C	492	SER	-	insertion	UNP P03420
C	493	ALA	HIS	conflict	UNP P03420
C	494	ILE	ASN	conflict	UNP P03420
C	495	GLY	VAL	conflict	UNP P03420
C	496	GLY	ASN	conflict	UNP P03420
C	497	TYR	ALA	conflict	UNP P03420
C	498	ILE	GLY	conflict	UNP P03420
C	499	PRO	LYS	conflict	UNP P03420
C	500	GLU	SER	conflict	UNP P03420
C	501	ALA	THR	conflict	UNP P03420
C	502	PRO	THR	conflict	UNP P03420
C	503	ARG	ASN	conflict	UNP P03420
C	504	ASP	ILE	conflict	UNP P03420
C	505	GLY	MET	conflict	UNP P03420
C	506	GLN	ILE	conflict	UNP P03420
C	507	ALA	THR	conflict	UNP P03420
C	508	TYR	THR	conflict	UNP P03420
C	509	VAL	ILE	conflict	UNP P03420
C	510	ARG	ILE	conflict	UNP P03420
C	511	LYS	ILE	conflict	UNP P03420
C	512	ASP	VAL	conflict	UNP P03420
C	513	GLY	ILE	conflict	UNP P03420
C	514	GLU	ILE	conflict	UNP P03420
C	515	TRP	VAL	conflict	UNP P03420
C	516	VAL	ILE	conflict	UNP P03420
C	520	THR	-	insertion	UNP P03420
C	521	PHE	-	insertion	UNP P03420

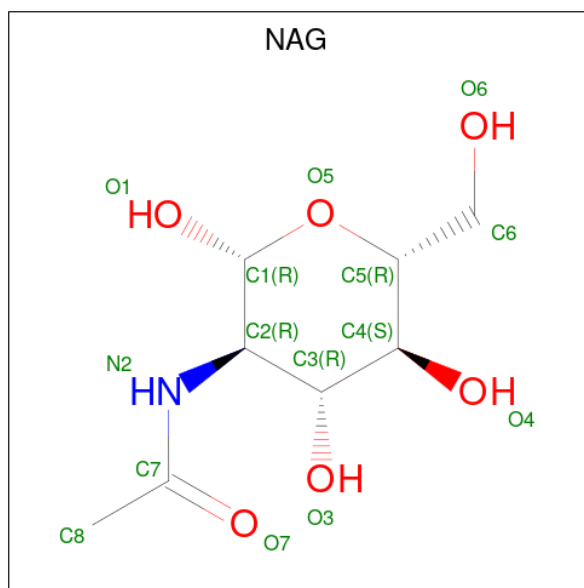
- Molecule 2 is a protein called Lor69 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	119	Total	C	N	O	S	0	0
			911	573	154	182	2		
2	D	119	Total	C	N	O	S	0	0
			911	573	154	182	2		
2	E	119	Total	C	N	O	S	0	0
			911	573	154	182	2		

- Molecule 3 is a protein called Lor69 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	105	Total	C	N	O	S	0	0
			815	515	139	158	3		
3	F	105	Total	C	N	O	S	0	0
			815	515	139	158	3		
3	G	105	Total	C	N	O	S	0	0
			815	515	139	158	3		

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



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

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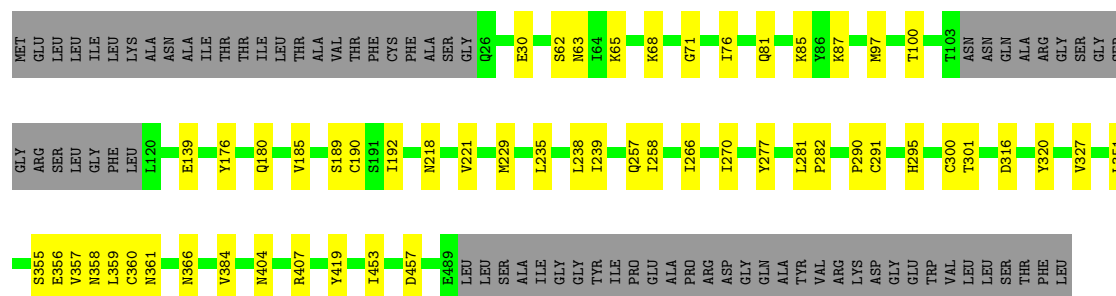
Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	

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.

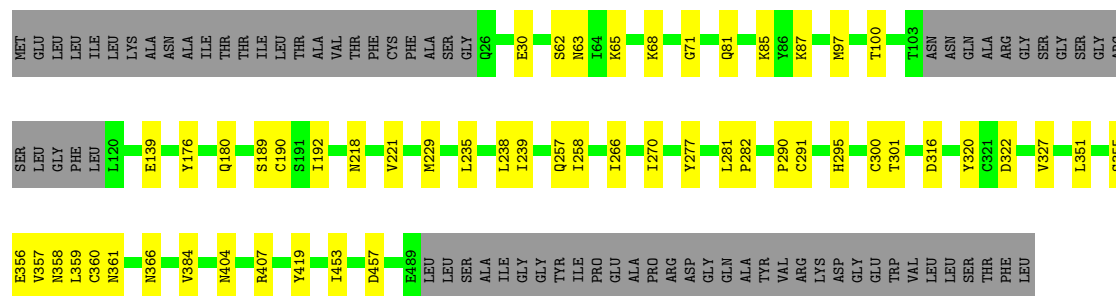
• Molecule 1: Fusion glycoprotein F0

Chain A: 



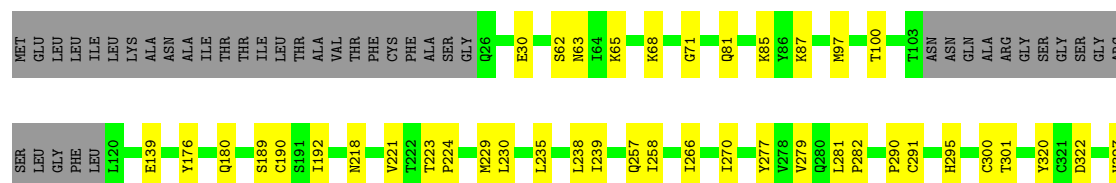
• Molecule 1: Fusion glycoprotein F0

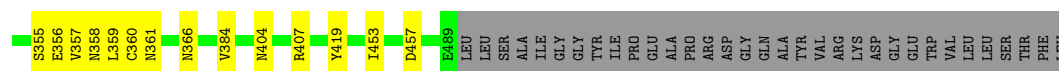
Chain B: 



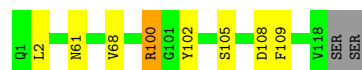
• Molecule 1: Fusion glycoprotein F0

Chain C: 





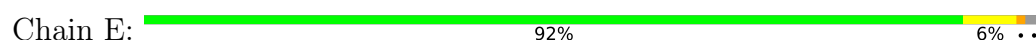
• Molecule 2: Lor69 Heavy Chain



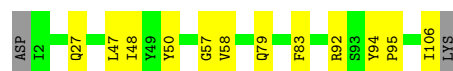
• Molecule 2: Lor69 Heavy Chain



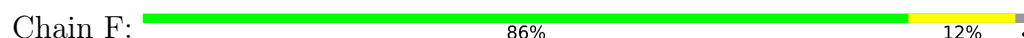
• Molecule 2: Lor69 Heavy Chain



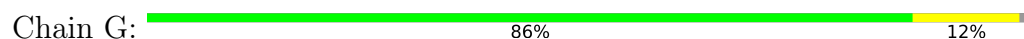
• Molecule 3: Lor69 Light Chain



• Molecule 3: Lor69 Light Chain



• Molecule 3: Lor69 Light Chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	128395	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)	250	Depositor
Maximum defocus (nm)	500	Depositor
Magnification	150000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.028	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.003	Depositor
Map size ($\text{\AA}$)	277.8, 277.8, 277.8	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.92599994, 0.92599994, 0.92599994	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	1.06	2/3510 (0.1%)	1.20	16/4757 (0.3%)
1	B	1.06	2/3510 (0.1%)	1.20	16/4757 (0.3%)
1	C	1.06	2/3510 (0.1%)	1.20	16/4757 (0.3%)
2	D	1.03	0/932	1.19	3/1269 (0.2%)
2	E	1.03	0/932	1.19	3/1269 (0.2%)
2	H	1.03	0/932	1.19	3/1269 (0.2%)
3	F	1.03	1/837 (0.1%)	1.27	9/1140 (0.8%)
3	G	1.03	1/837 (0.1%)	1.27	9/1140 (0.8%)
3	L	1.03	1/837 (0.1%)	1.27	9/1140 (0.8%)
All	All	1.05	9/15837 (0.1%)	1.21	84/21498 (0.4%)

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	D	0	1
2	E	0	1
2	H	0	1
All	All	0	3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	404	ASN	CB-CG	-5.67	1.37	1.52
1	A	404	ASN	CB-CG	-5.66	1.38	1.52
1	C	404	ASN	CB-CG	-5.65	1.38	1.52
3	F	106	ILE	CB-CG1	5.58	1.64	1.53
3	G	106	ILE	CB-CG1	5.56	1.64	1.53
3	L	106	ILE	CB-CG1	5.56	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	295	HIS	CB-CG	-5.54	1.42	1.50
1	A	295	HIS	CB-CG	-5.54	1.42	1.50
1	C	295	HIS	CB-CG	-5.54	1.42	1.50

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	366	ASN	CA-C-N	7.11	126.79	119.82
1	B	366	ASN	C-N-CA	7.11	126.79	119.82
1	C	366	ASN	CA-C-N	7.09	126.77	119.82
1	C	366	ASN	C-N-CA	7.09	126.77	119.82
1	A	366	ASN	CA-C-N	7.07	126.75	119.82
1	A	366	ASN	C-N-CA	7.07	126.75	119.82
1	C	457	ASP	CA-C-N	7.04	126.74	119.56
1	C	457	ASP	C-N-CA	7.04	126.74	119.56
1	A	457	ASP	CA-C-N	7.01	126.72	119.56
1	A	457	ASP	C-N-CA	7.01	126.72	119.56
1	B	384	VAL	CA-C-N	-7.00	113.73	122.48
1	B	384	VAL	C-N-CA	-7.00	113.73	122.48
1	C	384	VAL	CA-C-N	-6.99	113.75	122.48
1	C	384	VAL	C-N-CA	-6.99	113.75	122.48
1	A	384	VAL	CA-C-N	-6.97	113.76	122.48
1	A	384	VAL	C-N-CA	-6.97	113.76	122.48
1	B	457	ASP	CA-C-N	6.97	126.67	119.56
1	B	457	ASP	C-N-CA	6.97	126.67	119.56
3	F	79	GLN	CA-C-N	6.63	126.32	119.56
3	F	79	GLN	C-N-CA	6.63	126.32	119.56
3	G	79	GLN	CA-C-N	6.62	126.31	119.56
3	G	79	GLN	C-N-CA	6.62	126.31	119.56
3	L	79	GLN	CA-C-N	6.60	126.30	119.56
3	L	79	GLN	C-N-CA	6.60	126.30	119.56
1	A	189	SER	CA-C-N	6.15	131.48	122.63
1	A	189	SER	C-N-CA	6.15	131.48	122.63
1	C	189	SER	CA-C-N	6.14	131.48	122.63
1	C	189	SER	C-N-CA	6.14	131.48	122.63
1	B	189	SER	CA-C-N	6.14	131.47	122.63
1	B	189	SER	C-N-CA	6.14	131.47	122.63
3	G	57	GLY	CA-C-N	-6.13	117.40	123.04
3	G	57	GLY	C-N-CA	-6.13	117.40	123.04
3	F	57	GLY	CA-C-N	-6.12	117.41	123.04
3	F	57	GLY	C-N-CA	-6.12	117.41	123.04
3	L	57	GLY	CA-C-N	-6.11	117.42	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	57	GLY	C-N-CA	-6.11	117.42	123.04
1	B	100	THR	CA-C-N	6.05	126.01	119.78
1	B	100	THR	C-N-CA	6.05	126.01	119.78
1	A	100	THR	CA-C-N	6.03	125.99	119.78
1	A	100	THR	C-N-CA	6.03	125.99	119.78
3	F	58	VAL	CA-C-N	6.03	125.99	119.78
3	F	58	VAL	C-N-CA	6.03	125.99	119.78
3	L	58	VAL	CA-C-N	6.03	125.99	119.78
3	L	58	VAL	C-N-CA	6.03	125.99	119.78
3	G	58	VAL	CA-C-N	6.03	125.99	119.78
3	G	58	VAL	C-N-CA	6.03	125.99	119.78
1	C	100	THR	CA-C-N	6.01	125.97	119.78
1	C	100	THR	C-N-CA	6.01	125.97	119.78
1	C	139	GLU	CA-C-N	-5.89	111.47	121.85
1	C	139	GLU	C-N-CA	-5.89	111.47	121.85
1	A	139	GLU	CA-C-N	-5.89	111.48	121.85
1	A	139	GLU	C-N-CA	-5.89	111.48	121.85
1	B	139	GLU	CA-C-N	-5.89	111.48	121.85
1	B	139	GLU	C-N-CA	-5.89	111.48	121.85
2	H	61	ASN	CA-C-N	5.86	126.27	119.47
2	H	61	ASN	C-N-CA	5.86	126.27	119.47
2	D	61	ASN	CA-C-N	5.84	126.25	119.47
2	D	61	ASN	C-N-CA	5.84	126.25	119.47
2	E	61	ASN	CA-C-N	5.81	126.21	119.47
2	E	61	ASN	C-N-CA	5.81	126.21	119.47
1	A	266	ILE	N-CA-C	5.65	115.99	107.80
1	B	266	ILE	N-CA-C	5.64	115.98	107.80
1	C	266	ILE	N-CA-C	5.63	115.97	107.80
2	D	68	VAL	N-CA-C	5.43	115.71	108.11
2	H	68	VAL	N-CA-C	5.42	115.70	108.11
2	E	68	VAL	N-CA-C	5.41	115.69	108.11
3	F	83	PHE	CA-CB-CG	-5.37	108.43	113.80
3	L	83	PHE	CA-CB-CG	-5.36	108.44	113.80
3	G	83	PHE	CA-CB-CG	-5.34	108.46	113.80
3	F	27	GLN	CA-C-N	-5.32	114.89	120.31
3	F	27	GLN	C-N-CA	-5.32	114.89	120.31
3	G	27	GLN	CA-C-N	-5.31	114.89	120.31
3	G	27	GLN	C-N-CA	-5.31	114.89	120.31
3	L	27	GLN	CA-C-N	-5.31	114.89	120.31
3	L	27	GLN	C-N-CA	-5.31	114.89	120.31
1	B	192	ILE	CA-C-N	5.31	124.92	119.56
1	B	192	ILE	C-N-CA	5.31	124.92	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	ILE	N-CA-C	-5.31	105.95	111.58
1	C	239	ILE	N-CA-C	-5.30	105.96	111.58
1	C	192	ILE	CA-C-N	5.30	124.91	119.56
1	C	192	ILE	C-N-CA	5.30	124.91	119.56
1	A	192	ILE	CA-C-N	5.29	124.91	119.56
1	A	192	ILE	C-N-CA	5.29	124.91	119.56
1	B	239	ILE	N-CA-C	-5.28	105.98	111.58

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	100	ARG	Sidechain
2	E	100	ARG	Sidechain
2	H	100	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	3461	0	3509	30	0
1	B	3461	0	3509	31	0
1	C	3461	0	3509	29	0
2	D	911	0	880	5	0
2	E	911	0	880	5	0
2	H	911	0	880	5	0
3	F	815	0	786	6	0
3	G	815	0	786	6	0
3	L	815	0	786	4	0
4	A	42	0	39	1	0
4	B	42	0	39	1	0
4	C	42	0	39	1	0
All	All	15687	0	15642	113	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 4.

All (113) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:100:ARG:HB3	2:D:105:SER:HB3	1.82	0.61
2:E:100:ARG:HB3	2:E:105:SER:HB3	1.82	0.61
2:H:100:ARG:HB3	2:H:105:SER:HB3	1.82	0.60
1:C:97:MET:SD	1:C:270:ILE:HG22	2.45	0.57
1:B:97:MET:SD	1:B:270:ILE:HG22	2.45	0.57
1:A:97:MET:SD	1:A:270:ILE:HG22	2.45	0.56
1:C:291:CYS:SG	1:C:320:TYR:O	2.65	0.55
1:B:291:CYS:SG	1:B:320:TYR:O	2.65	0.54
1:A:291:CYS:SG	1:A:320:TYR:O	2.65	0.54
1:C:327:VAL:HG23	1:C:355:SER:HA	1.90	0.54
1:C:238:LEU:HD23	1:C:281:LEU:HD12	1.90	0.54
1:A:238:LEU:HD23	1:A:281:LEU:HD12	1.90	0.53
1:A:327:VAL:HG23	1:A:355:SER:HA	1.90	0.53
2:H:2:LEU:HD23	2:H:109:PHE:HD2	1.74	0.53
1:B:327:VAL:HG23	1:B:355:SER:HA	1.90	0.53
3:F:48:ILE:HG22	3:F:50:TYR:O	2.09	0.53
1:B:238:LEU:HD23	1:B:281:LEU:HD12	1.90	0.52
2:E:2:LEU:HD23	2:E:109:PHE:HD2	1.74	0.52
3:G:48:ILE:HG22	3:G:50:TYR:O	2.09	0.52
3:L:47:LEU:C	3:L:48:ILE:HG13	2.36	0.51
3:L:48:ILE:HG22	3:L:50:TYR:O	2.09	0.51
3:F:47:LEU:C	3:F:48:ILE:HG13	2.36	0.51
2:D:2:LEU:HD23	2:D:109:PHE:HD2	1.74	0.51
1:B:257:GLN:HG2	1:B:258:ILE:N	2.26	0.51
3:G:47:LEU:C	3:G:48:ILE:HG13	2.36	0.50
1:A:257:GLN:HG2	1:A:258:ILE:N	2.26	0.50
1:C:407:ARG:HG2	1:C:407:ARG:O	2.12	0.50
1:B:358:ASN:OD1	1:B:361:ASN:ND2	2.42	0.50
1:C:257:GLN:HG2	1:C:258:ILE:N	2.26	0.50
1:A:320:TYR:CE2	1:A:357:VAL:HG11	2.47	0.50
1:C:358:ASN:OD1	1:C:361:ASN:ND2	2.42	0.49
1:B:65:LYS:O	1:B:87:LYS:HD3	2.12	0.49
1:B:320:TYR:CE2	1:B:357:VAL:HG11	2.47	0.49
1:C:320:TYR:CE2	1:C:357:VAL:HG11	2.47	0.49
1:A:407:ARG:O	1:A:407:ARG:HG2	2.12	0.49
1:B:30:GLU:OE1	1:B:419:TYR:OH	2.31	0.49
1:A:65:LYS:O	1:A:87:LYS:HD3	2.12	0.49
1:B:407:ARG:O	1:B:407:ARG:HG2	2.12	0.49
1:C:65:LYS:O	1:C:87:LYS:HD3	2.12	0.49
2:H:108:ASP:OD1	2:H:109:PHE:N	2.46	0.48
1:C:229:MET:O	1:C:277:TYR:OH	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:GLU:OE1	1:A:419:TYR:OH	2.31	0.48
1:A:358:ASN:OD1	1:A:361:ASN:ND2	2.42	0.48
2:D:108:ASP:OD1	2:D:109:PHE:N	2.46	0.48
1:C:30:GLU:OE1	1:C:419:TYR:OH	2.31	0.47
1:B:229:MET:O	1:B:277:TYR:OH	2.32	0.47
2:E:108:ASP:OD1	2:E:109:PHE:N	2.46	0.47
1:A:229:MET:O	1:A:277:TYR:OH	2.32	0.47
1:A:358:ASN:O	1:A:359:LEU:C	2.58	0.47
1:B:235:LEU:CD1	1:B:281:LEU:HD11	2.46	0.46
1:C:358:ASN:O	1:C:359:LEU:C	2.58	0.46
1:C:218:ASN:HB3	1:C:221:VAL:O	2.16	0.46
1:B:300:CYS:O	1:B:453:ILE:HG21	2.16	0.46
1:A:218:ASN:HB3	1:A:221:VAL:O	2.16	0.46
1:A:235:LEU:CD1	1:A:281:LEU:HD11	2.46	0.46
1:A:290:PRO:HD3	3:L:92:ARG:HG2	1.98	0.46
1:A:81:GLN:O	1:A:85:LYS:HG2	2.16	0.45
1:C:81:GLN:O	1:C:85:LYS:HG2	2.16	0.45
3:G:94:TYR:N	3:G:95:PRO:HD2	2.31	0.45
2:E:2:LEU:HD23	2:E:109:PHE:CD2	2.52	0.45
1:B:235:LEU:HD11	1:B:281:LEU:HD21	1.99	0.45
1:A:301:THR:HG22	1:A:301:THR:O	2.16	0.45
1:B:218:ASN:HB3	1:B:221:VAL:O	2.16	0.45
1:C:235:LEU:CD1	1:C:281:LEU:HD11	2.46	0.45
1:C:235:LEU:HD11	1:C:281:LEU:HD21	1.99	0.45
1:A:235:LEU:HD11	1:A:281:LEU:HD21	1.99	0.45
3:F:94:TYR:N	3:F:95:PRO:HD2	2.31	0.45
1:C:300:CYS:O	1:C:453:ILE:HG21	2.16	0.45
1:A:300:CYS:O	1:A:453:ILE:HG21	2.16	0.45
1:B:62:SER:OG	1:B:63:ASN:N	2.50	0.45
1:B:290:PRO:HD3	3:F:92:ARG:HG2	1.98	0.45
1:C:62:SER:OG	1:C:63:ASN:N	2.50	0.44
1:A:62:SER:OG	1:A:63:ASN:N	2.50	0.44
1:B:281:LEU:CD2	1:B:282:PRO:HD2	2.48	0.44
1:B:301:THR:HG22	1:B:301:THR:O	2.16	0.44
1:B:81:GLN:O	1:B:85:LYS:HG2	2.16	0.44
3:L:94:TYR:N	3:L:95:PRO:HD2	2.31	0.44
2:D:2:LEU:HD23	2:D:109:PHE:CD2	2.52	0.44
1:A:281:LEU:CD2	1:A:282:PRO:HD2	2.48	0.44
1:B:176:TYR:HA	1:B:180:GLN:HG3	2.00	0.44
1:C:290:PRO:HD3	3:G:92:ARG:HG2	1.98	0.44
1:B:358:ASN:O	1:B:359:LEU:C	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:LYS:HA	4:C:603:NAG:H62	2.00	0.43
1:B:68:LYS:HA	4:B:603:NAG:H62	2.00	0.43
1:A:68:LYS:HA	4:A:603:NAG:H62	2.00	0.43
1:A:358:ASN:C	1:A:360:CYS:N	2.76	0.43
2:H:2:LEU:HD23	2:H:109:PHE:CD2	2.52	0.43
1:C:301:THR:O	1:C:301:THR:HG22	2.16	0.43
1:C:281:LEU:CD2	1:C:282:PRO:HD2	2.48	0.43
1:A:176:TYR:HA	1:A:180:GLN:HG3	2.00	0.43
1:A:257:GLN:H	1:A:257:GLN:CD	2.26	0.43
1:B:316:ASP:OD1	1:B:316:ASP:N	2.51	0.43
1:C:358:ASN:C	1:C:360:CYS:N	2.76	0.43
1:A:351:LEU:HD23	1:A:351:LEU:HA	1.87	0.42
1:B:351:LEU:HD23	1:B:351:LEU:HA	1.87	0.42
1:B:356:GLU:HG3	2:D:102:TYR:CD2	2.54	0.42
1:A:356:GLU:HG3	2:H:102:TYR:CD2	2.54	0.42
1:B:257:GLN:H	1:B:257:GLN:CD	2.26	0.42
1:C:176:TYR:HA	1:C:180:GLN:HG3	2.00	0.42
1:B:358:ASN:C	1:B:360:CYS:N	2.76	0.42
1:A:71:GLY:HA3	1:A:190:CYS:HB3	2.02	0.42
1:C:356:GLU:HG3	2:E:102:TYR:CD2	2.54	0.42
1:C:71:GLY:HA3	1:C:190:CYS:HB3	2.02	0.41
1:B:322:ASP:O	3:F:32:TYR:OH	2.39	0.41
1:C:223:THR:HB	1:C:224:PRO:HD3	2.03	0.41
1:C:322:ASP:O	3:G:32:TYR:OH	2.39	0.41
1:B:71:GLY:HA3	1:B:190:CYS:HB3	2.02	0.40
3:G:47:LEU:O	3:G:48:ILE:HG13	2.21	0.40
3:F:47:LEU:O	3:F:48:ILE:HG13	2.21	0.40
1:A:76:ILE:HD11	1:A:185:VAL:HG13	2.04	0.40
1:B:65:LYS:HB3	1:B:87:LYS:HG3	2.03	0.40
1:C:230:LEU:HD11	1:C:279:VAL:HG21	2.03	0.40
1:A:316:ASP:OD1	1:A:316:ASP:N	2.51	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	444/522 (85%)	431 (97%)	13 (3%)	0	100	100
1	B	444/522 (85%)	431 (97%)	13 (3%)	0	100	100
1	C	444/522 (85%)	431 (97%)	13 (3%)	0	100	100
2	D	117/121 (97%)	113 (97%)	4 (3%)	0	100	100
2	E	117/121 (97%)	113 (97%)	4 (3%)	0	100	100
2	H	117/121 (97%)	113 (97%)	4 (3%)	0	100	100
3	F	103/107 (96%)	98 (95%)	5 (5%)	0	100	100
3	G	103/107 (96%)	98 (95%)	5 (5%)	0	100	100
3	L	103/107 (96%)	98 (95%)	5 (5%)	0	100	100
All	All	1992/2250 (88%)	1926 (97%)	66 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	409/466 (88%)	409 (100%)	0	100	100
1	B	409/466 (88%)	409 (100%)	0	100	100
1	C	409/466 (88%)	409 (100%)	0	100	100
2	D	101/103 (98%)	101 (100%)	0	100	100
2	E	101/103 (98%)	101 (100%)	0	100	100
2	H	101/103 (98%)	101 (100%)	0	100	100
3	F	90/92 (98%)	90 (100%)	0	100	100
3	G	90/92 (98%)	90 (100%)	0	100	100
3	L	90/92 (98%)	90 (100%)	0	100	100
All	All	1800/1983 (91%)	1800 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	248	GLN
2	H	3	GLN
3	L	27	GLN
3	L	89	GLN
3	L	90	GLN
3	L	91	HIS
1	B	248	GLN
2	D	3	GLN
3	F	89	GLN
3	F	90	GLN
3	F	91	HIS
1	C	248	GLN
2	E	3	GLN
3	G	27	GLN
3	G	89	GLN
3	G	90	GLN
3	G	91	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	602	1	14,14,15	2.13	5 (35%)	17,19,21	0.99	1 (5%)
4	NAG	A	601	1	14,14,15	2.06	5 (35%)	17,19,21	0.94	1 (5%)
4	NAG	B	601	1	14,14,15	2.07	5 (35%)	17,19,21	0.94	1 (5%)
4	NAG	A	602	1	14,14,15	2.12	5 (35%)	17,19,21	0.99	0
4	NAG	C	602	1	14,14,15	2.12	5 (35%)	17,19,21	0.99	1 (5%)
4	NAG	C	601	1	14,14,15	2.06	5 (35%)	17,19,21	0.93	1 (5%)
4	NAG	C	603	1	14,14,15	0.45	0	17,19,21	0.65	0
4	NAG	B	603	1	14,14,15	0.46	0	17,19,21	0.66	0
4	NAG	A	603	1	14,14,15	0.45	0	17,19,21	0.66	0

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

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

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	602	NAG	C1-C2	5.41	1.60	1.52
4	A	602	NAG	C1-C2	5.37	1.60	1.52
4	C	602	NAG	C1-C2	5.36	1.60	1.52
4	B	601	NAG	C1-C2	5.16	1.60	1.52
4	A	601	NAG	C1-C2	5.12	1.60	1.52
4	C	601	NAG	C1-C2	5.10	1.60	1.52
4	C	601	NAG	O5-C5	3.21	1.50	1.43

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	602	NAG	O5-C5	3.21	1.49	1.43
4	A	601	NAG	O5-C5	3.20	1.49	1.43
4	B	601	NAG	O5-C5	3.20	1.49	1.43
4	A	602	NAG	O5-C5	3.18	1.49	1.43
4	B	602	NAG	O5-C5	3.18	1.49	1.43
4	B	602	NAG	O5-C1	2.87	1.48	1.43
4	A	602	NAG	O5-C1	2.82	1.48	1.43
4	C	602	NAG	O5-C1	2.81	1.48	1.43
4	A	601	NAG	O5-C1	2.53	1.47	1.43
4	B	601	NAG	O5-C1	2.52	1.47	1.43
4	C	601	NAG	O5-C1	2.49	1.47	1.43
4	B	601	NAG	C4-C5	2.34	1.58	1.53
4	A	601	NAG	C4-C5	2.32	1.57	1.53
4	C	601	NAG	C4-C5	2.29	1.57	1.53
4	B	602	NAG	C4-C5	2.20	1.57	1.53
4	A	602	NAG	C4-C5	2.20	1.57	1.53
4	C	602	NAG	C4-C5	2.19	1.57	1.53
4	C	601	NAG	C3-C2	2.13	1.57	1.52
4	C	602	NAG	C3-C2	2.13	1.57	1.52
4	B	601	NAG	C3-C2	2.12	1.57	1.52
4	A	601	NAG	C3-C2	2.12	1.57	1.52
4	A	602	NAG	C3-C2	2.10	1.57	1.52
4	B	602	NAG	C3-C2	2.10	1.57	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	NAG	C8-C7-N2	2.05	119.57	116.10
4	C	601	NAG	C8-C7-N2	2.05	119.56	116.10
4	A	601	NAG	C8-C7-N2	2.04	119.56	116.10
4	B	602	NAG	C8-C7-N2	2.02	119.51	116.10
4	C	602	NAG	C8-C7-N2	2.01	119.50	116.10

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	NAG	O5-C5-C6-O6
4	B	601	NAG	O5-C5-C6-O6
4	C	601	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

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

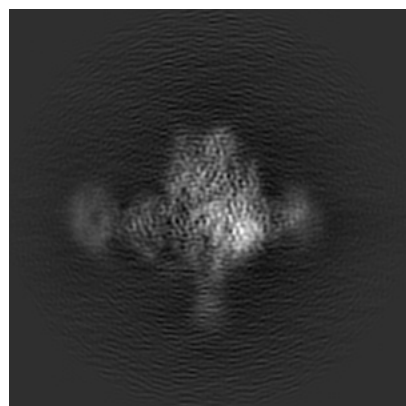
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-59533. These allow visual inspection of the internal detail of the map and identification of artifacts.

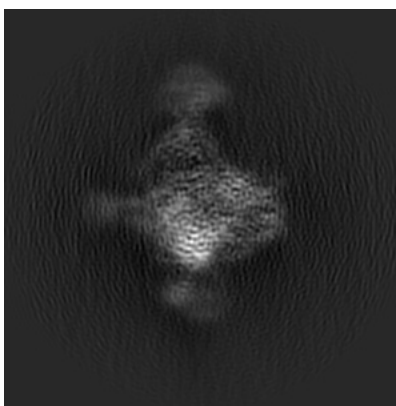
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

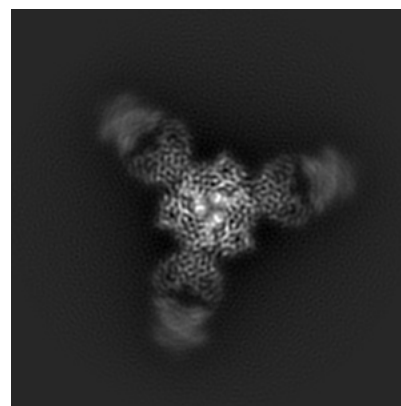
6.1.1 Primary map



X

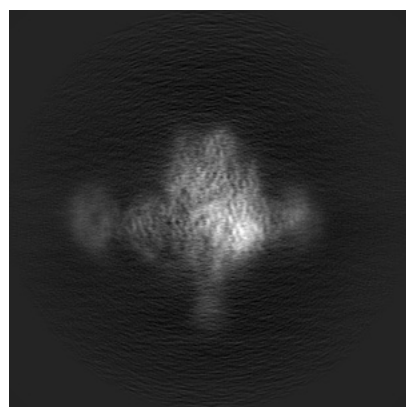


Y

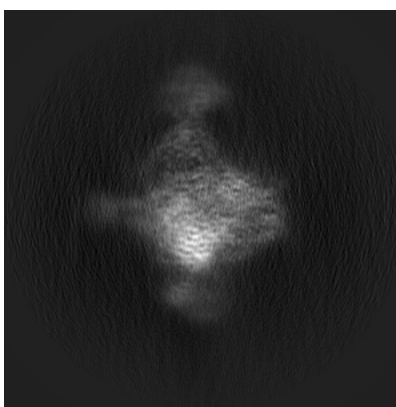


Z

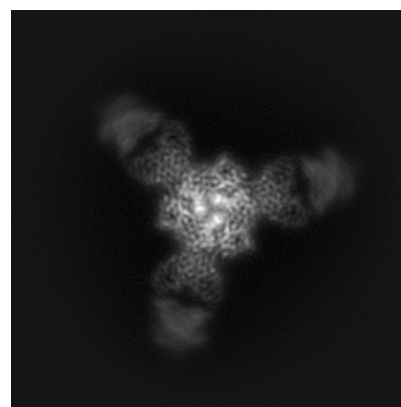
6.1.2 Raw map



X



Y

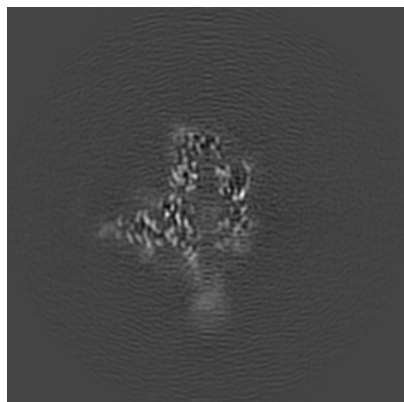


Z

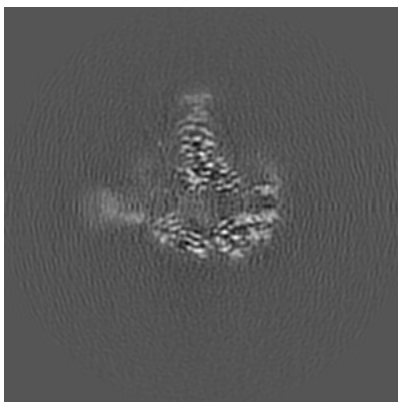
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

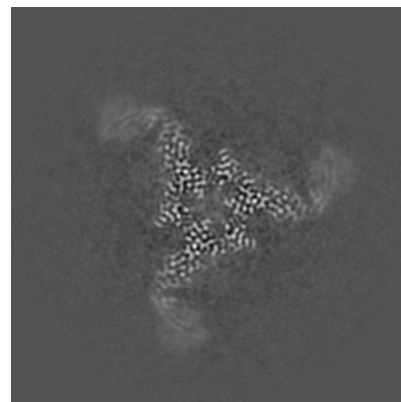
6.2.1 Primary map



X Index: 150

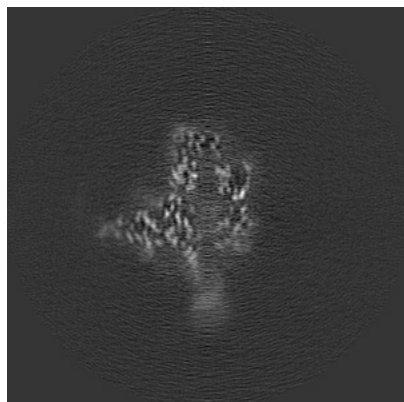


Y Index: 150

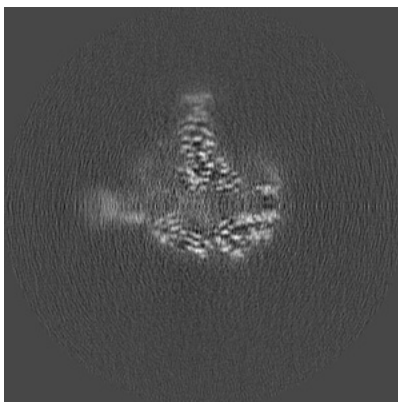


Z Index: 150

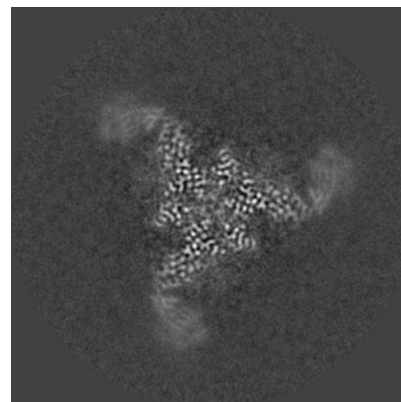
6.2.2 Raw map



X Index: 150



Y Index: 150

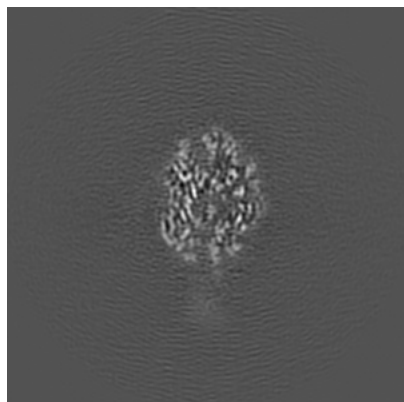


Z Index: 150

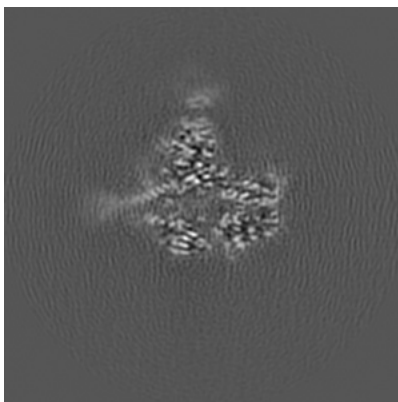
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

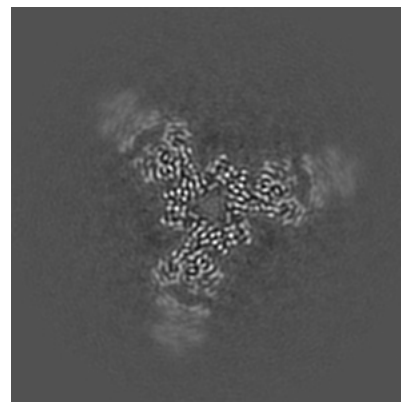
6.3.1 Primary map



X Index: 162

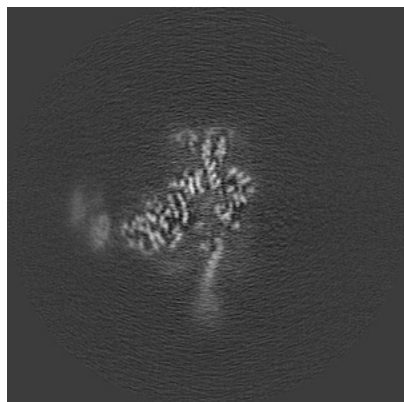


Y Index: 156

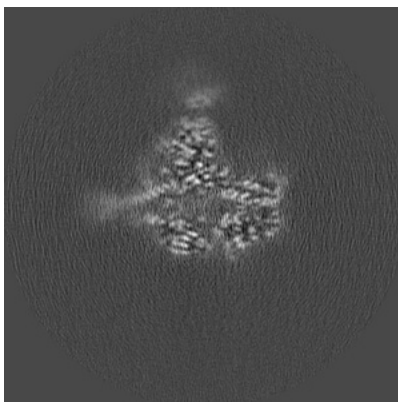


Z Index: 140

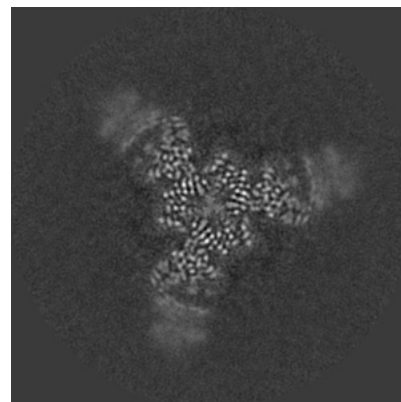
6.3.2 Raw map



X Index: 141



Y Index: 156

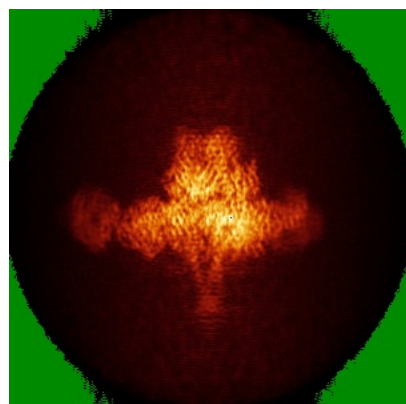


Z Index: 142

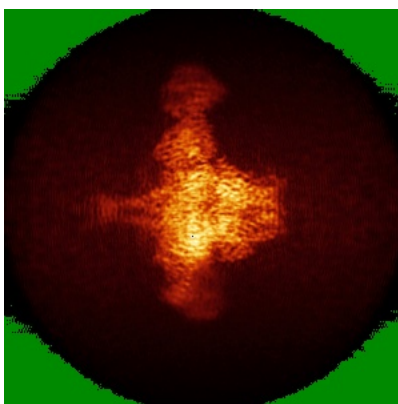
The images above show the largest variance slices of the map in three orthogonal directions.

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

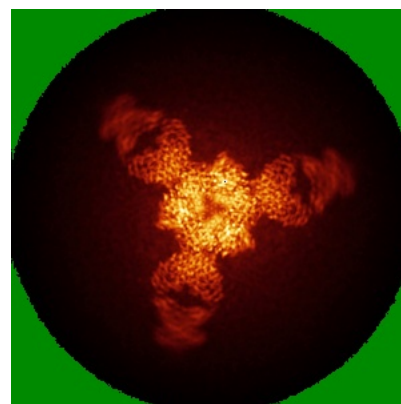
6.4.1 Primary map



X

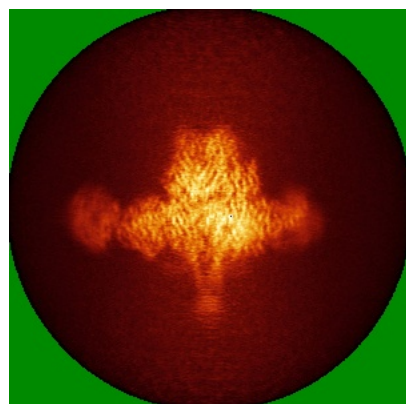


Y

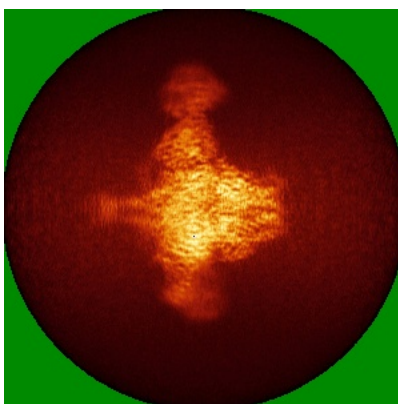


Z

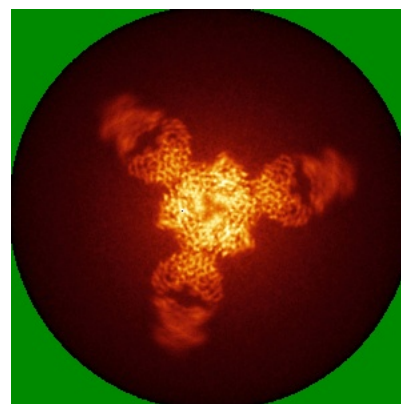
6.4.2 Raw map



X



Y

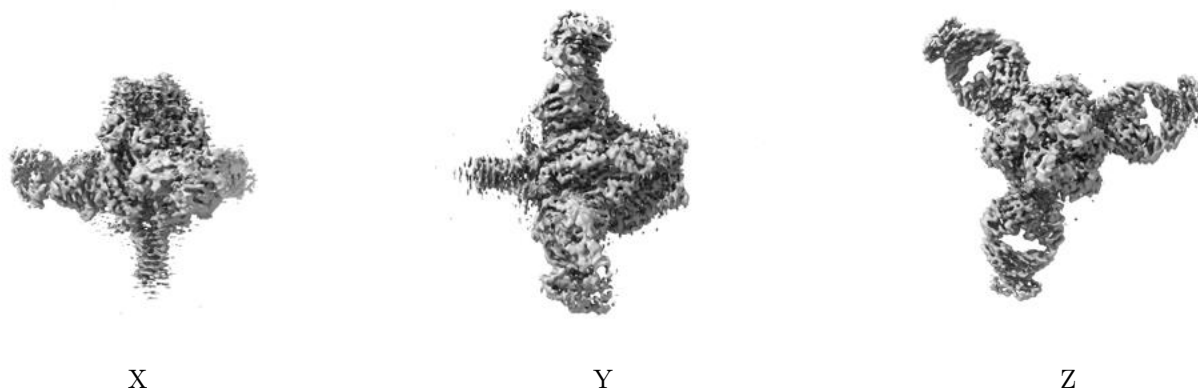


Z

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.

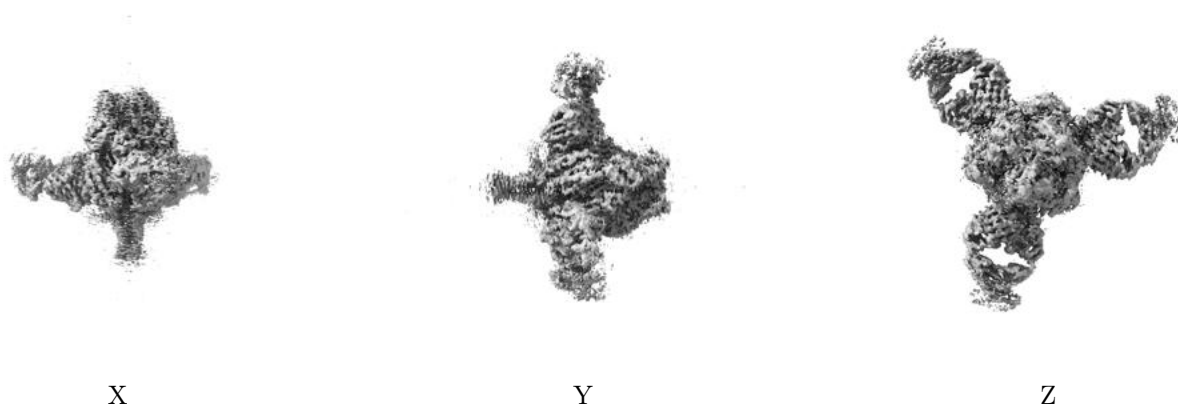
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.003. 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.

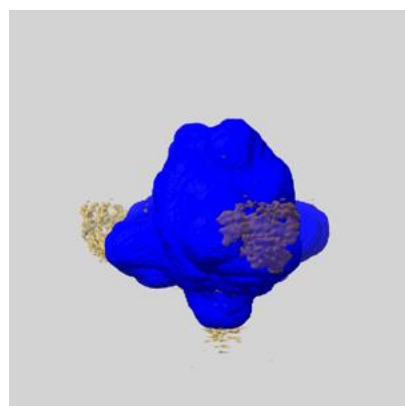
6.6 Mask visualisation [i](#)

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

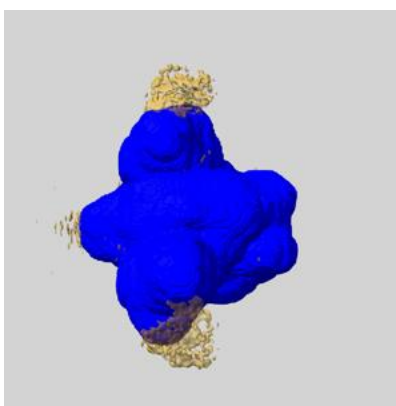
A mask typically either:

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

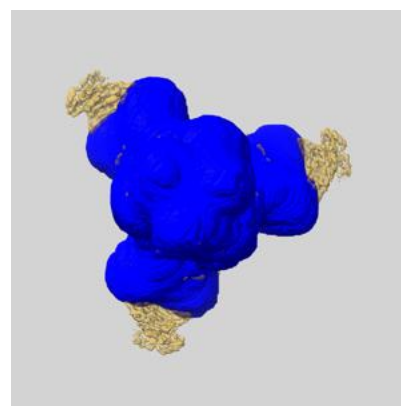
6.6.1 emd_59533_msk_1.map [i](#)



X



Y

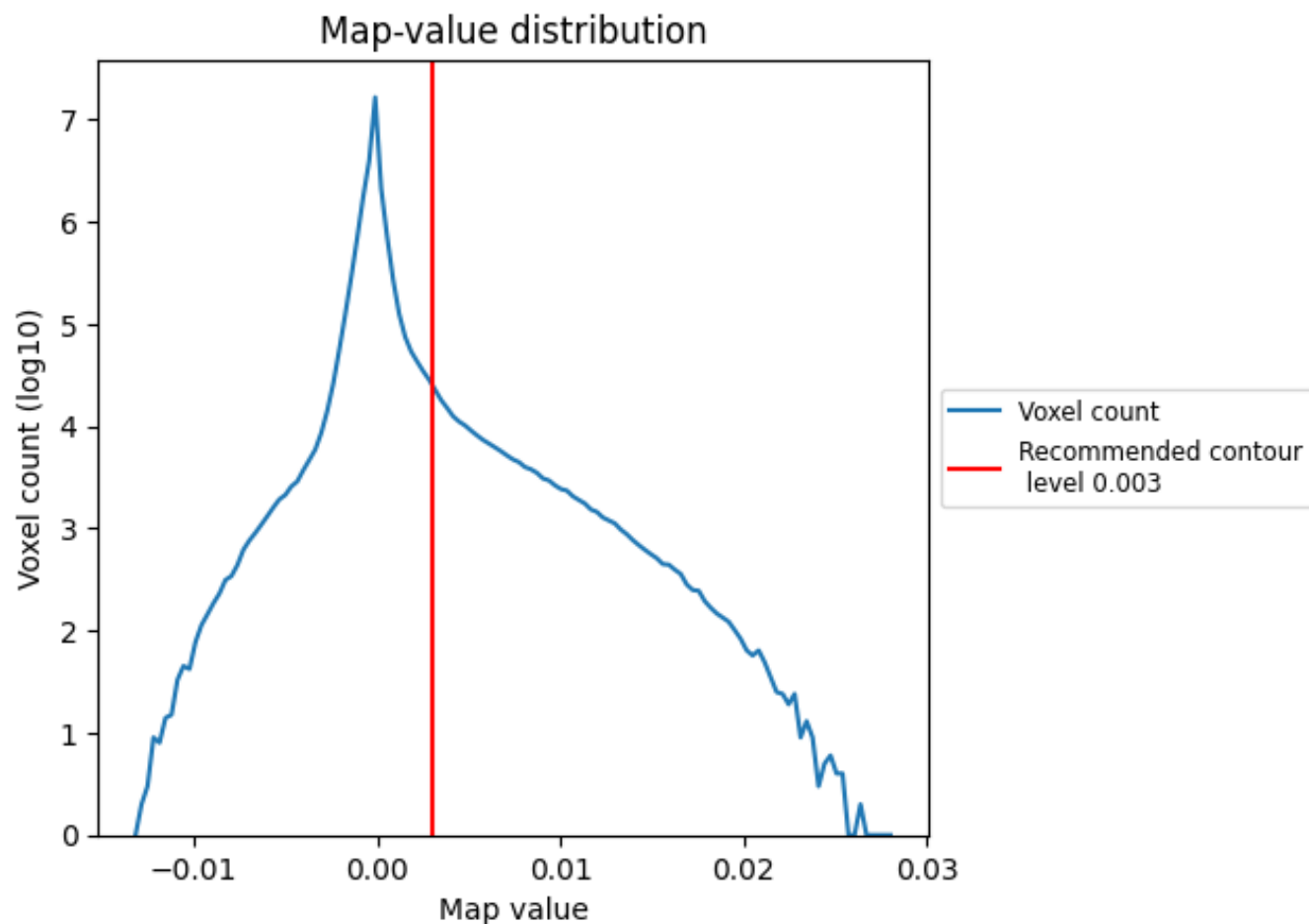


Z

7 Map analysis [i](#)

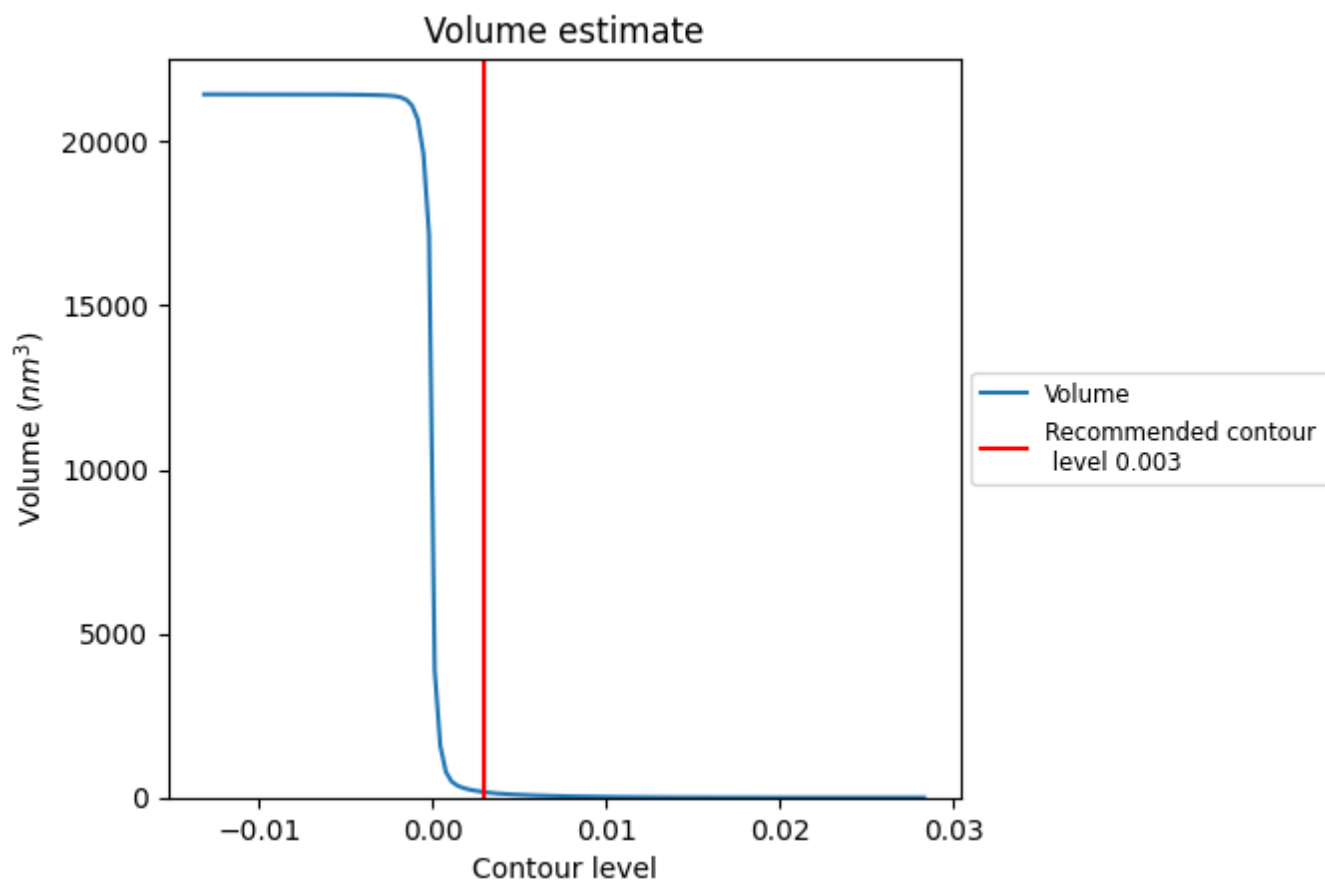
This section contains the results of statistical analysis of the map.

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.

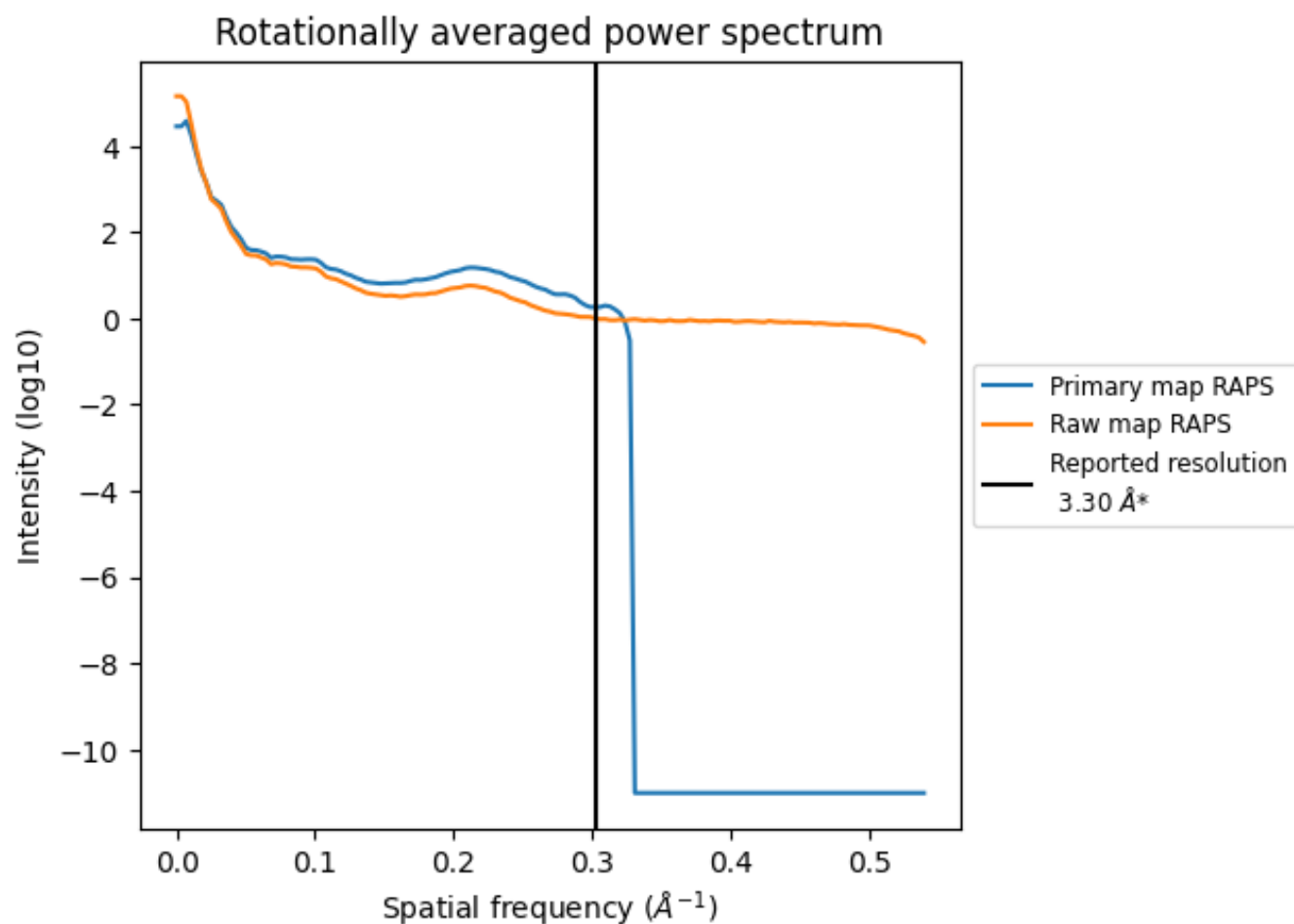
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 164 nm^3 ; this corresponds to an approximate mass of 148 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 ⓘ

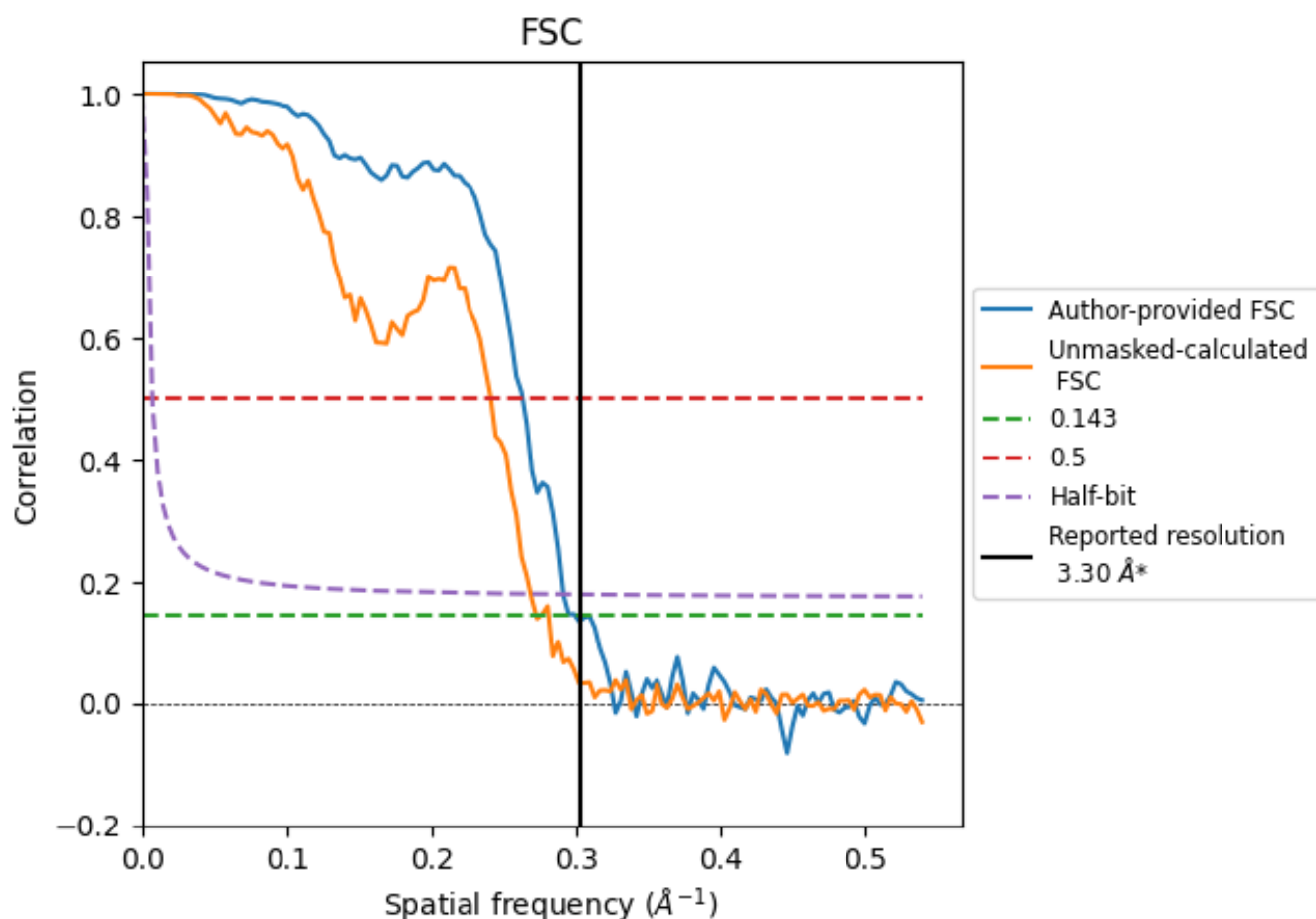


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 $0.303 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

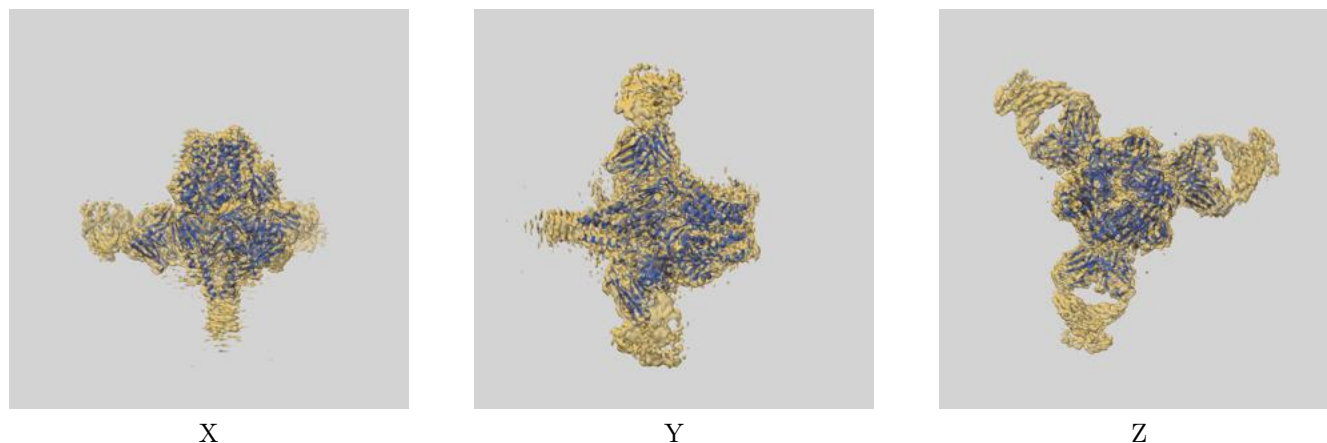
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.34	3.80	3.43
Unmasked-calculated*	3.66	4.14	3.72

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.66 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

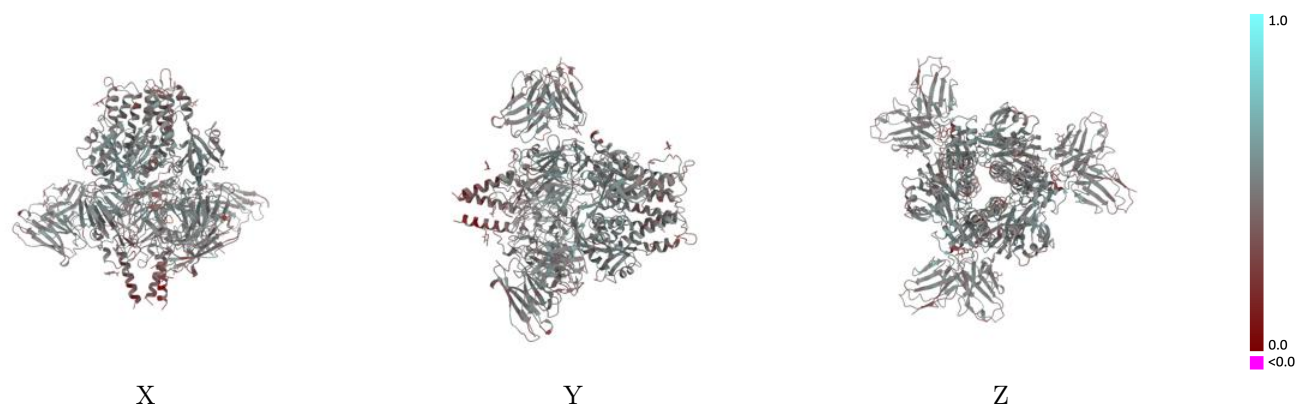
This section contains information regarding the fit between EMDB map EMD-59533 and PDB model 33SD. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



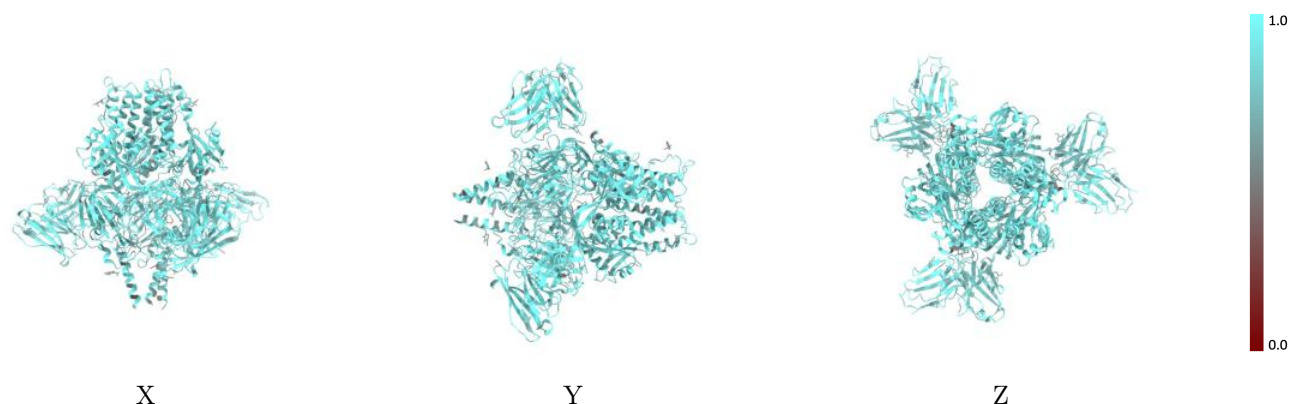
The images above show the 3D surface view of the map at the recommended contour level 0.003 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



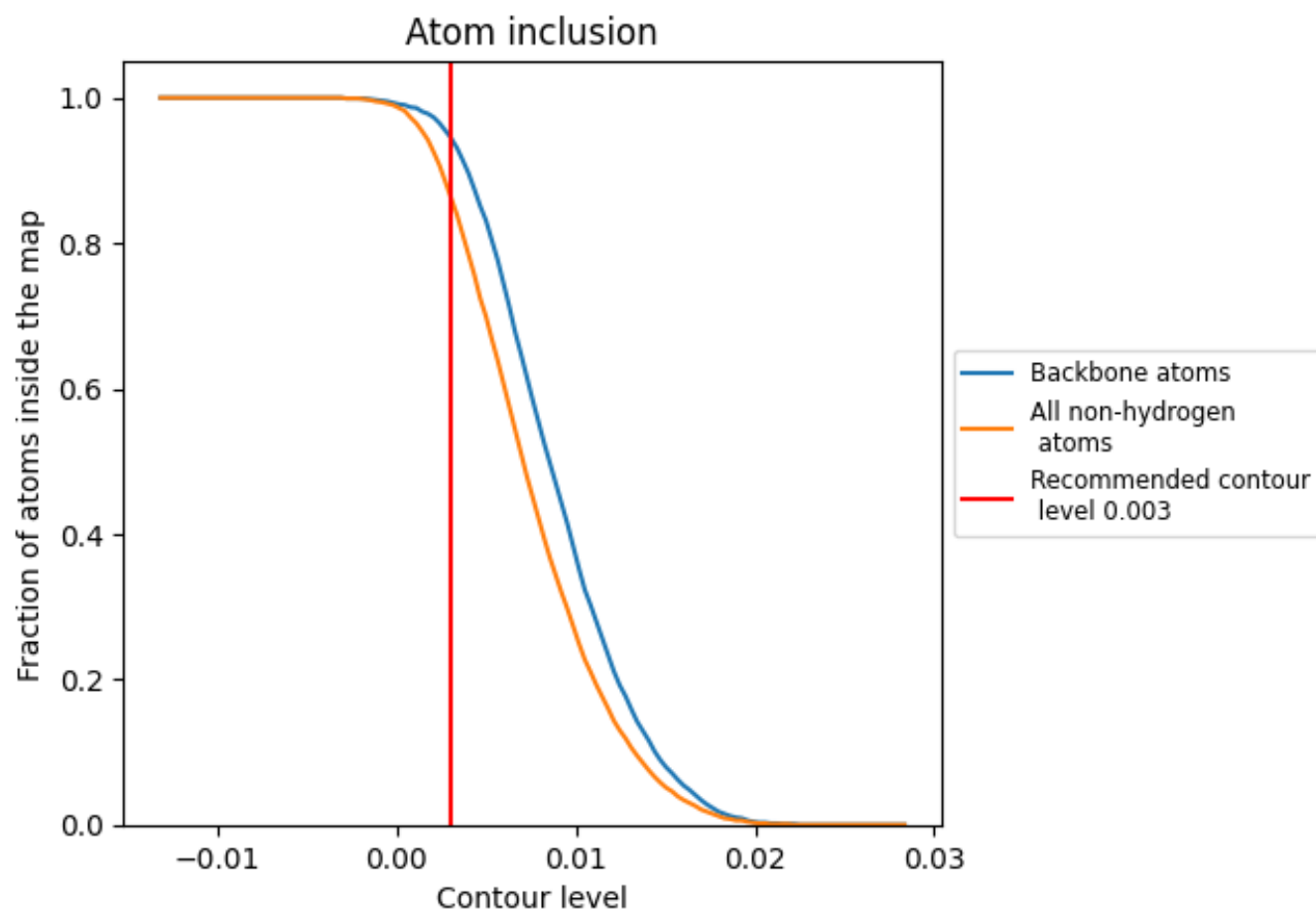
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.003).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 86% 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 (0.003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8650	0.4650
A	0.8650	0.4660
B	0.8640	0.4650
C	0.8650	0.4660
D	0.8700	0.4690
E	0.8700	0.4640
F	0.8560	0.4570
G	0.8570	0.4550
H	0.8690	0.4670
L	0.8620	0.4580

1.0

0.0

<0.0