



Full wwPDB EM Validation Report ⓘ

Sep 12, 2024 – 04:14 PM EDT

PDB ID : 9ATP
EMDB ID : EMD-43832
Title : local refinement of XBB.1.5 spike/Nanosota-3C complex
Authors : Ye, G.; Bu, F.; Liu, B.; Li, F.
Deposited on : 2024-02-27
Resolution : 3.50 Å (reported)
Based on initial model : 8vkl

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:

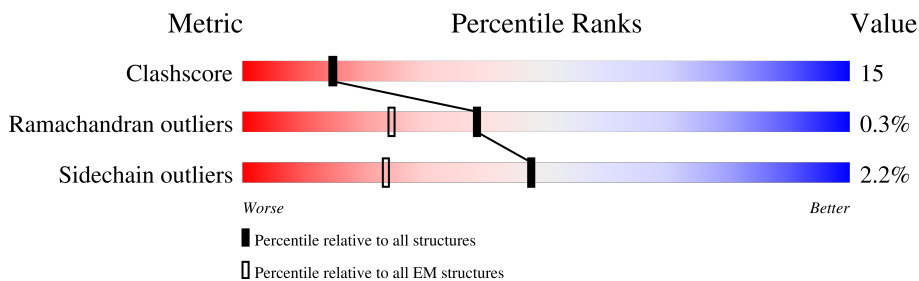
EMDB validation analysis : 0.0.1.dev112
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.3

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 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	1230	
1	B	1230	
1	C	1230	
2	D	136	
2	E	136	
2	L	136	

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 13004 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	438	3513	2278	575	646	14	0	0
1	B	436	3498	2267	573	644	14	0	0
1	C	417	3356	2181	546	617	12	0	0

There are 255 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	24	SER	ALA	variant	UNP P0DTC2
A	80	ALA	VAL	variant	UNP P0DTC2
A	139	ASP	GLY	variant	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	142	GLN	HIS	variant	UNP P0DTC2
A	179	GLU	GLN	variant	UNP P0DTC2
A	209	GLU	VAL	variant	UNP P0DTC2
A	335	HIS	GLY	variant	UNP P0DTC2
A	342	THR	ARG	variant	UNP P0DTC2
A	364	ILE	LEU	variant	UNP P0DTC2
A	367	PHE	SER	variant	UNP P0DTC2
A	369	PRO	SER	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	372	ALA	THR	variant	UNP P0DTC2
A	401	ASN	ASP	variant	UNP P0DTC2
A	404	SER	ARG	variant	UNP P0DTC2
A	413	ASN	LYS	variant	UNP P0DTC2
A	436	LYS	ASN	variant	UNP P0DTC2
A	441	PRO	VAL	variant	UNP P0DTC2
A	442	SER	GLY	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	456	LYS	ASN	variant	UNP P0DTC2
A	473	ASN	SER	variant	UNP P0DTC2
A	474	LYS	THR	variant	UNP P0DTC2
A	480	ALA	GLU	variant	UNP P0DTC2
A	482	PRO	PHE	variant	UNP P0DTC2
A	486	SER	PHE	variant	UNP P0DTC2
A	494	ARG	GLN	variant	UNP P0DTC2
A	497	TYR	ASN	variant	UNP P0DTC2
A	501	HIS	TYR	variant	UNP P0DTC2
A	610	GLY	ASP	variant	UNP P0DTC2
A	651	TYR	HIS	variant	UNP P0DTC2
A	675	LYS	ASN	variant	UNP P0DTC2
A	677	HIS	PRO	variant	UNP P0DTC2
A	678	ALA	ARG	engineered mutation	UNP P0DTC2
A	679	GLY	ARG	engineered mutation	UNP P0DTC2
A	760	LYS	ASN	variant	UNP P0DTC2
A	792	TYR	ASP	variant	UNP P0DTC2
A	813	PRO	PHE	engineered mutation	UNP P0DTC2
A	888	PRO	ALA	engineered mutation	UNP P0DTC2
A	895	PRO	ALA	engineered mutation	UNP P0DTC2
A	938	PRO	ALA	engineered mutation	UNP P0DTC2
A	950	HIS	GLN	variant	UNP P0DTC2
A	965	LYS	ASN	variant	UNP P0DTC2
A	982	PRO	LYS	engineered mutation	UNP P0DTC2
A	983	PRO	VAL	engineered mutation	UNP P0DTC2
A	1208	GLY	-	expression tag	UNP P0DTC2
A	1209	SER	-	expression tag	UNP P0DTC2
A	1210	GLY	-	expression tag	UNP P0DTC2
A	1211	TYR	-	expression tag	UNP P0DTC2
A	1212	ILE	-	expression tag	UNP P0DTC2
A	1213	PRO	-	expression tag	UNP P0DTC2
A	1214	GLU	-	expression tag	UNP P0DTC2
A	1215	ALA	-	expression tag	UNP P0DTC2
A	1216	PRO	-	expression tag	UNP P0DTC2
A	1217	ARG	-	expression tag	UNP P0DTC2
A	1218	ASP	-	expression tag	UNP P0DTC2
A	1219	GLY	-	expression tag	UNP P0DTC2
A	1220	GLN	-	expression tag	UNP P0DTC2
A	1221	ALA	-	expression tag	UNP P0DTC2
A	1222	TYR	-	expression tag	UNP P0DTC2
A	1223	VAL	-	expression tag	UNP P0DTC2
A	1224	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1225	LYS	-	expression tag	UNP P0DTC2
A	1226	ASP	-	expression tag	UNP P0DTC2
A	1227	GLY	-	expression tag	UNP P0DTC2
A	1228	GLU	-	expression tag	UNP P0DTC2
A	1229	TRP	-	expression tag	UNP P0DTC2
A	1230	VAL	-	expression tag	UNP P0DTC2
A	1231	LEU	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	SER	-	expression tag	UNP P0DTC2
A	1234	THR	-	expression tag	UNP P0DTC2
A	1235	PHE	-	expression tag	UNP P0DTC2
A	1236	LEU	-	expression tag	UNP P0DTC2
A	1237	GLY	-	expression tag	UNP P0DTC2
A	1238	HIS	-	expression tag	UNP P0DTC2
A	1239	HIS	-	expression tag	UNP P0DTC2
A	1240	HIS	-	expression tag	UNP P0DTC2
A	1241	HIS	-	expression tag	UNP P0DTC2
A	1242	HIS	-	expression tag	UNP P0DTC2
A	1243	HIS	-	expression tag	UNP P0DTC2
B	19	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	24	SER	ALA	variant	UNP P0DTC2
B	80	ALA	VAL	variant	UNP P0DTC2
B	139	ASP	GLY	variant	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	142	GLN	HIS	variant	UNP P0DTC2
B	179	GLU	GLN	variant	UNP P0DTC2
B	209	GLU	VAL	variant	UNP P0DTC2
B	335	HIS	GLY	variant	UNP P0DTC2
B	342	THR	ARG	variant	UNP P0DTC2
B	364	ILE	LEU	variant	UNP P0DTC2
B	367	PHE	SER	variant	UNP P0DTC2
B	369	PRO	SER	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	372	ALA	THR	variant	UNP P0DTC2
B	401	ASN	ASP	variant	UNP P0DTC2
B	404	SER	ARG	variant	UNP P0DTC2
B	413	ASN	LYS	variant	UNP P0DTC2
B	436	LYS	ASN	variant	UNP P0DTC2
B	441	PRO	VAL	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	442	SER	GLY	variant	UNP P0DTC2
B	456	LYS	ASN	variant	UNP P0DTC2
B	473	ASN	SER	variant	UNP P0DTC2
B	474	LYS	THR	variant	UNP P0DTC2
B	480	ALA	GLU	variant	UNP P0DTC2
B	482	PRO	PHE	variant	UNP P0DTC2
B	486	SER	PHE	variant	UNP P0DTC2
B	494	ARG	GLN	variant	UNP P0DTC2
B	497	TYR	ASN	variant	UNP P0DTC2
B	501	HIS	TYR	variant	UNP P0DTC2
B	610	GLY	ASP	variant	UNP P0DTC2
B	651	TYR	HIS	variant	UNP P0DTC2
B	675	LYS	ASN	variant	UNP P0DTC2
B	677	HIS	PRO	variant	UNP P0DTC2
B	678	ALA	ARG	engineered mutation	UNP P0DTC2
B	679	GLY	ARG	engineered mutation	UNP P0DTC2
B	760	LYS	ASN	variant	UNP P0DTC2
B	792	TYR	ASP	variant	UNP P0DTC2
B	813	PRO	PHE	engineered mutation	UNP P0DTC2
B	888	PRO	ALA	engineered mutation	UNP P0DTC2
B	895	PRO	ALA	engineered mutation	UNP P0DTC2
B	938	PRO	ALA	engineered mutation	UNP P0DTC2
B	950	HIS	GLN	variant	UNP P0DTC2
B	965	LYS	ASN	variant	UNP P0DTC2
B	982	PRO	LYS	engineered mutation	UNP P0DTC2
B	983	PRO	VAL	engineered mutation	UNP P0DTC2
B	1208	GLY	-	expression tag	UNP P0DTC2
B	1209	SER	-	expression tag	UNP P0DTC2
B	1210	GLY	-	expression tag	UNP P0DTC2
B	1211	TYR	-	expression tag	UNP P0DTC2
B	1212	ILE	-	expression tag	UNP P0DTC2
B	1213	PRO	-	expression tag	UNP P0DTC2
B	1214	GLU	-	expression tag	UNP P0DTC2
B	1215	ALA	-	expression tag	UNP P0DTC2
B	1216	PRO	-	expression tag	UNP P0DTC2
B	1217	ARG	-	expression tag	UNP P0DTC2
B	1218	ASP	-	expression tag	UNP P0DTC2
B	1219	GLY	-	expression tag	UNP P0DTC2
B	1220	GLN	-	expression tag	UNP P0DTC2
B	1221	ALA	-	expression tag	UNP P0DTC2
B	1222	TYR	-	expression tag	UNP P0DTC2
B	1223	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1224	ARG	-	expression tag	UNP P0DTC2
B	1225	LYS	-	expression tag	UNP P0DTC2
B	1226	ASP	-	expression tag	UNP P0DTC2
B	1227	GLY	-	expression tag	UNP P0DTC2
B	1228	GLU	-	expression tag	UNP P0DTC2
B	1229	TRP	-	expression tag	UNP P0DTC2
B	1230	VAL	-	expression tag	UNP P0DTC2
B	1231	LEU	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	SER	-	expression tag	UNP P0DTC2
B	1234	THR	-	expression tag	UNP P0DTC2
B	1235	PHE	-	expression tag	UNP P0DTC2
B	1236	LEU	-	expression tag	UNP P0DTC2
B	1237	GLY	-	expression tag	UNP P0DTC2
B	1238	HIS	-	expression tag	UNP P0DTC2
B	1239	HIS	-	expression tag	UNP P0DTC2
B	1240	HIS	-	expression tag	UNP P0DTC2
B	1241	HIS	-	expression tag	UNP P0DTC2
B	1242	HIS	-	expression tag	UNP P0DTC2
B	1243	HIS	-	expression tag	UNP P0DTC2
C	19	ILE	THR	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	24	SER	ALA	variant	UNP P0DTC2
C	80	ALA	VAL	variant	UNP P0DTC2
C	139	ASP	GLY	variant	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	142	GLN	HIS	variant	UNP P0DTC2
C	179	GLU	GLN	variant	UNP P0DTC2
C	209	GLU	VAL	variant	UNP P0DTC2
C	335	HIS	GLY	variant	UNP P0DTC2
C	342	THR	ARG	variant	UNP P0DTC2
C	364	ILE	LEU	variant	UNP P0DTC2
C	367	PHE	SER	variant	UNP P0DTC2
C	369	PRO	SER	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	372	ALA	THR	variant	UNP P0DTC2
C	401	ASN	ASP	variant	UNP P0DTC2
C	404	SER	ARG	variant	UNP P0DTC2
C	413	ASN	LYS	variant	UNP P0DTC2
C	436	LYS	ASN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	441	PRO	VAL	variant	UNP P0DTC2
C	442	SER	GLY	variant	UNP P0DTC2
C	456	LYS	ASN	variant	UNP P0DTC2
C	473	ASN	SER	variant	UNP P0DTC2
C	474	LYS	THR	variant	UNP P0DTC2
C	480	ALA	GLU	variant	UNP P0DTC2
C	482	PRO	PHE	variant	UNP P0DTC2
C	486	SER	PHE	variant	UNP P0DTC2
C	494	ARG	GLN	variant	UNP P0DTC2
C	497	TYR	ASN	variant	UNP P0DTC2
C	501	HIS	TYR	variant	UNP P0DTC2
C	610	GLY	ASP	variant	UNP P0DTC2
C	651	TYR	HIS	variant	UNP P0DTC2
C	675	LYS	ASN	variant	UNP P0DTC2
C	677	HIS	PRO	variant	UNP P0DTC2
C	678	ALA	ARG	engineered mutation	UNP P0DTC2
C	679	GLY	ARG	engineered mutation	UNP P0DTC2
C	760	LYS	ASN	variant	UNP P0DTC2
C	792	TYR	ASP	variant	UNP P0DTC2
C	813	PRO	PHE	engineered mutation	UNP P0DTC2
C	888	PRO	ALA	engineered mutation	UNP P0DTC2
C	895	PRO	ALA	engineered mutation	UNP P0DTC2
C	938	PRO	ALA	engineered mutation	UNP P0DTC2
C	950	HIS	GLN	variant	UNP P0DTC2
C	965	LYS	ASN	variant	UNP P0DTC2
C	982	PRO	LYS	engineered mutation	UNP P0DTC2
C	983	PRO	VAL	engineered mutation	UNP P0DTC2
C	1208	GLY	-	expression tag	UNP P0DTC2
C	1209	SER	-	expression tag	UNP P0DTC2
C	1210	GLY	-	expression tag	UNP P0DTC2
C	1211	TYR	-	expression tag	UNP P0DTC2
C	1212	ILE	-	expression tag	UNP P0DTC2
C	1213	PRO	-	expression tag	UNP P0DTC2
C	1214	GLU	-	expression tag	UNP P0DTC2
C	1215	ALA	-	expression tag	UNP P0DTC2
C	1216	PRO	-	expression tag	UNP P0DTC2
C	1217	ARG	-	expression tag	UNP P0DTC2
C	1218	ASP	-	expression tag	UNP P0DTC2
C	1219	GLY	-	expression tag	UNP P0DTC2
C	1220	GLN	-	expression tag	UNP P0DTC2
C	1221	ALA	-	expression tag	UNP P0DTC2
C	1222	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1223	VAL	-	expression tag	UNP P0DTC2
C	1224	ARG	-	expression tag	UNP P0DTC2
C	1225	LYS	-	expression tag	UNP P0DTC2
C	1226	ASP	-	expression tag	UNP P0DTC2
C	1227	GLY	-	expression tag	UNP P0DTC2
C	1228	GLU	-	expression tag	UNP P0DTC2
C	1229	TRP	-	expression tag	UNP P0DTC2
C	1230	VAL	-	expression tag	UNP P0DTC2
C	1231	LEU	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression tag	UNP P0DTC2
C	1233	SER	-	expression tag	UNP P0DTC2
C	1234	THR	-	expression tag	UNP P0DTC2
C	1235	PHE	-	expression tag	UNP P0DTC2
C	1236	LEU	-	expression tag	UNP P0DTC2
C	1237	GLY	-	expression tag	UNP P0DTC2
C	1238	HIS	-	expression tag	UNP P0DTC2
C	1239	HIS	-	expression tag	UNP P0DTC2
C	1240	HIS	-	expression tag	UNP P0DTC2
C	1241	HIS	-	expression tag	UNP P0DTC2
C	1242	HIS	-	expression tag	UNP P0DTC2
C	1243	HIS	-	expression tag	UNP P0DTC2

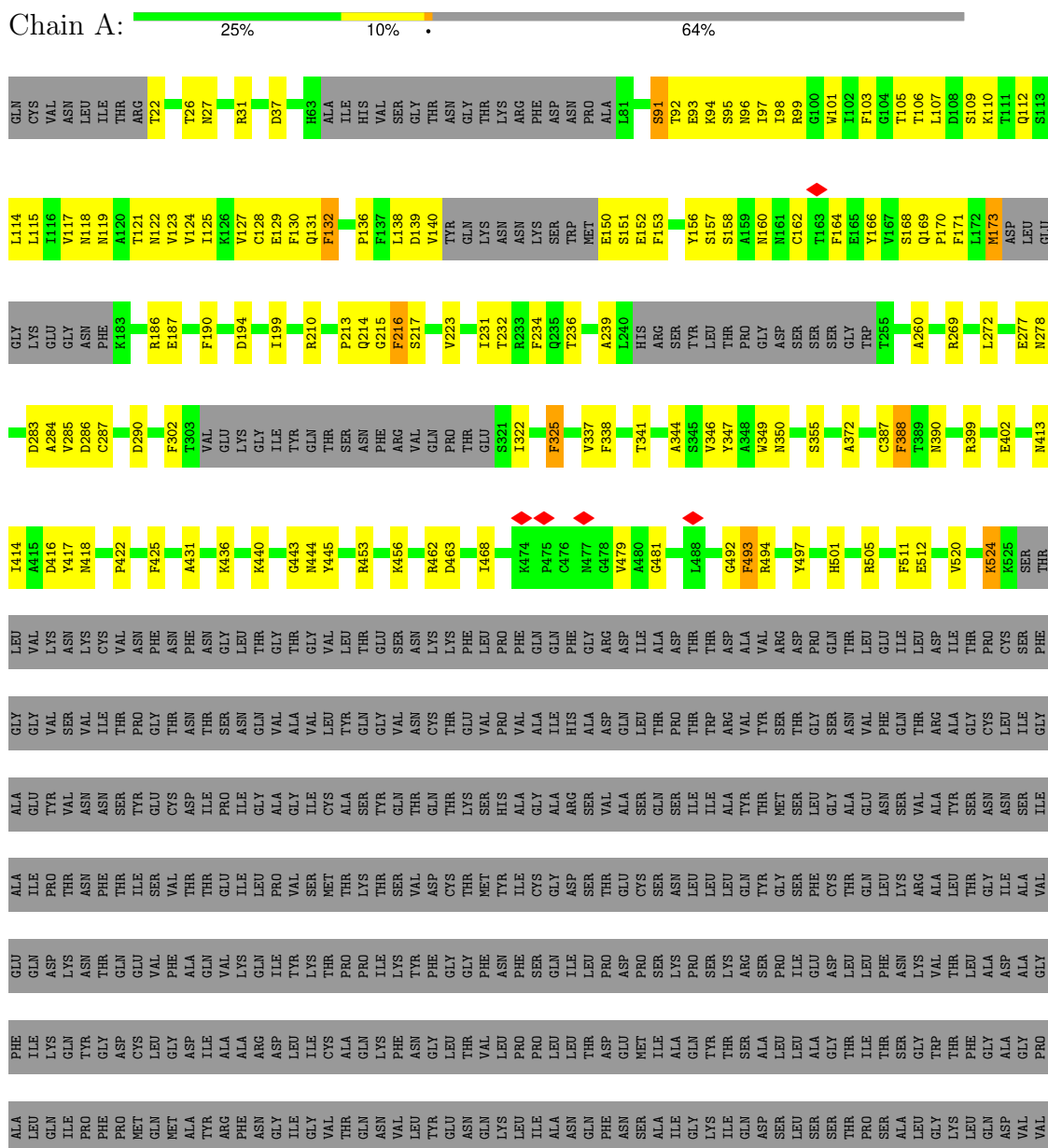
- Molecule 2 is a protein called Nanosota-3C.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	115	Total	C	N	O	S	0	0
			879	551	153	171	4		
2	E	115	Total	C	N	O	S	0	0
			879	551	153	171	4		
2	L	115	Total	C	N	O	S	0	0
			879	551	153	171	4		

3 Residue-property plots i

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

- Molecule 1: Spike glycoprotein



I85	I86	P87	T90	A91	V92	Y93	Y94	D99	K100	G108	T112	V113	S114	S115	GLY	GLY	GLN	HIS	HIS	HIS	HIS	HIS	HIS	HIS	GLY	ALA	TYR	PRO	TYR	ASP	VAL	PRO	ASP	TYR	ALA	SER
-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	225916	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.655	Depositor
Minimum map value	-0.362	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0311	Depositor
Map size (\AA)	339.96786, 339.96786, 339.96786	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.885333, 0.885333, 0.885333	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.34	0/3611	0.53	1/4911 (0.0%)
1	B	0.34	0/3595	0.53	0/4888
1	C	0.32	0/3448	0.51	0/4688
2	D	0.30	0/897	0.57	0/1216
2	E	0.28	0/897	0.59	0/1216
2	L	0.35	0/897	0.68	0/1216
All	All	0.33	0/13345	0.54	1/18135 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	ASP	CB-CG-OD1	5.87	123.58	118.30

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	3513	0	3396	102	0
1	B	3498	0	3378	105	0
1	C	3356	0	3251	76	0
2	D	879	0	855	46	0
2	E	879	0	855	28	0
2	L	879	0	855	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13004	0	12590	381	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 15.

All (381) 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:L:99:ASP:OD1	2:L:100:LYS:N	2.04	0.89
1:A:94:LYS:HE2	1:A:186:ARG:HH22	1.39	0.82
1:B:136:PRO:HD2	1:B:235:GLN:HE22	1.45	0.81
2:L:66:ARG:NH2	2:L:84:SER:O	2.13	0.81
2:E:2:VAL:HG12	2:E:27:SER:H	1.46	0.81
1:B:31:ARG:NH2	1:B:213:PRO:O	2.17	0.78
1:B:358:VAL:HG22	1:B:522:GLY:HA3	1.67	0.77
2:D:5:GLN:O	2:D:22:CYS:HA	1.86	0.76
1:C:373:PHE:HE1	1:C:380:PRO:HB3	1.52	0.75
2:D:19:ARG:HH12	2:D:79:HIS:HB3	1.52	0.74
2:D:72:ASP:O	2:D:76:ASN:HA	1.88	0.73
2:L:90:THR:HG23	2:L:112:THR:HA	1.68	0.73
1:C:172:LEU:HD12	1:C:186:ARG:HH11	1.55	0.71
1:B:413:ASN:O	1:B:417:TYR:HB2	1.91	0.70
1:C:394:ASP:HB2	1:C:508:VAL:HG12	1.73	0.70
1:A:93:GLU:HB3	1:A:97:ILE:HD12	1.73	0.69
1:A:128:CYS:HA	1:A:162:CYS:HB3	1.72	0.69
2:L:44:GLN:OE1	2:L:44:GLN:N	2.22	0.69
1:C:387:CYS:HA	1:C:521:CYS:HB3	1.76	0.68
2:E:19:ARG:HH21	2:E:81:GLN:HB2	1.59	0.68
1:A:129:GLU:HG2	1:A:160:ASN:HB3	1.75	0.68
2:L:35:GLY:HA3	2:L:50:PHE:HD2	1.59	0.67
2:E:99:ASP:OD1	2:E:100:LYS:N	2.28	0.67
1:B:339:ASN:HB3	1:B:367:PHE:HZ	1.59	0.67
1:B:128:CYS:HA	1:B:162:CYS:HB3	1.75	0.66
2:D:19:ARG:NH1	2:D:79:HIS:HB3	2.10	0.66
2:L:6:GLU:N	2:L:6:GLU:OE2	2.28	0.66
1:C:114:LEU:HD21	1:C:227:ILE:HD13	1.78	0.65
1:A:103:PHE:HD1	1:A:234:PHE:HB2	1.61	0.65
1:B:402:GLU:O	1:B:405:GLN:HB2	1.96	0.65
2:D:96:TYR:HE1	2:D:103:ASP:HB3	1.62	0.65
1:B:114:LEU:HD21	1:B:227:ILE:HG21	1.78	0.65
2:D:68:THR:OG1	2:D:81:GLN:NE2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:ASN:HB3	1:A:493:PHE:HD2	1.61	0.64
1:B:164:PHE:HE1	1:B:166:TYR:HB2	1.63	0.64
1:C:269:ARG:NH1	1:C:286:ASP:OD2	2.31	0.64
1:A:468:ILE:HD11	2:D:58:SER:HB2	1.80	0.64
1:B:122:ASN:HA	1:B:170:PRO:HD3	1.77	0.64
1:A:347:TYR:HH	2:D:96:TYR:HH	1.46	0.64
1:C:429:VAL:HG22	1:C:508:VAL:HG23	1.80	0.64
1:C:195:GLY:HA2	1:C:228:GLY:HA2	1.79	0.63
1:B:522:GLY:N	1:B:523:PRO:HD3	2.13	0.63
1:C:486:SER:O	1:C:489:GLN:NE2	2.32	0.63
2:D:72:ASP:O	2:D:76:ASN:CA	2.47	0.62
1:A:269:ARG:NH1	1:A:286:ASP:OD2	2.32	0.62
1:C:201:SER:HB3	1:C:222:LEU:HD22	1.82	0.62
1:B:100:GLY:HA2	1:B:116:ILE:O	1.99	0.62
2:D:10:GLY:N	2:D:110:GLN:O	2.33	0.62
2:L:87:PRO:HA	2:L:113:VAL:HG13	1.81	0.62
1:C:346:VAL:HG21	1:C:398:ILE:HD13	1.81	0.61
2:D:72:ASP:OD2	2:D:79:HIS:NE2	2.33	0.61
1:B:112:GLN:HA	1:B:129:GLU:HG2	1.83	0.61
1:B:129:GLU:O	1:B:160:ASN:ND2	2.27	0.61
1:A:152:GLU:HG3	1:A:156:TYR:CZ	2.35	0.61
1:A:199:ILE:HB	1:A:223:VAL:HG22	1.82	0.61
1:A:341:THR:HA	1:A:505:ARG:HH22	1.65	0.61
1:B:387:CYS:HA	1:B:521:CYS:HB3	1.84	0.60
1:C:129:GLU:HB2	1:C:160:ASN:HD21	1.66	0.60
1:B:98:ILE:HD11	1:B:236:THR:HG21	1.82	0.60
1:A:453:ARG:NH1	1:A:463:ASP:OD2	2.34	0.60
1:C:392:TYR:HB2	1:C:510:SER:HB3	1.82	0.60
2:D:71:ARG:NH2	2:D:76:ASN:OD1	2.33	0.60
1:A:169:GLN:HG2	1:A:170:PRO:HD2	1.83	0.60
1:B:61:TRP:HE1	1:B:260:ALA:HB1	1.66	0.60
1:B:273:LEU:HD22	1:B:281:ILE:HD13	1.84	0.60
1:B:199:ILE:HB	1:B:223:VAL:HG22	1.84	0.59
1:C:49:GLN:OE1	1:C:270:THR:OG1	2.18	0.59
1:B:397:VAL:O	1:B:398:ILE:HD13	2.02	0.59
1:A:173:MET:SD	1:A:173:MET:N	2.75	0.59
2:E:39:GLN:HB3	2:E:92:VAL:HG23	1.84	0.59
2:E:88:GLU:OE1	2:E:88:GLU:N	2.34	0.59
1:C:128:CYS:HA	1:C:162:CYS:HB3	1.85	0.59
1:C:26:THR:HG23	1:C:59:VAL:HG23	1.84	0.58
2:L:5:GLN:O	2:L:22:CYS:HA	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:ARG:HH12	1:B:212:LEU:HB3	1.68	0.58
2:L:53:SER:HA	2:L:71:ARG:HH21	1.68	0.58
1:C:522:GLY:N	1:C:523:PRO:HD3	2.18	0.58
2:D:72:ASP:OD2	2:D:77:THR:OG1	2.21	0.58
1:A:344:ALA:HB2	2:D:102:GLN:HA	1.85	0.58
1:A:443:GLY:HA2	1:A:494:ARG:HH11	1.69	0.58
1:B:445:TYR:O	1:B:447:TYR:N	2.37	0.58
2:L:39:GLN:HB3	2:L:92:VAL:HG23	1.85	0.58
2:L:11:LEU:HD22	2:L:112:THR:OG1	2.03	0.58
1:A:350:ASN:HD21	2:D:102:GLN:HB2	1.69	0.57
2:L:1:GLN:HG3	2:L:3:GLN:HE22	1.68	0.57
1:B:93:GLU:OE1	1:B:93:GLU:N	2.34	0.57
1:A:130:PHE:HB3	1:A:156:TYR:CB	2.34	0.57
1:C:61:TRP:HD1	1:C:262:TYR:CE2	2.21	0.57
2:D:85:LEU:HB3	2:D:113:VAL:HG21	1.85	0.57
2:E:90:THR:HG23	2:E:112:THR:HA	1.85	0.57
1:A:103:PHE:CD1	1:A:234:PHE:HB2	2.40	0.57
1:C:488:LEU:HB2	2:E:60:TRP:HH2	1.69	0.57
1:C:112:GLN:HA	1:C:129:GLU:HG2	1.86	0.57
1:C:117:VAL:HG22	1:C:124:VAL:HB	1.84	0.57
1:B:168:SER:OG	1:B:169:GLN:N	2.38	0.57
1:C:50:ASP:OD1	1:C:51:LEU:N	2.29	0.57
1:A:128:CYS:HB2	1:A:130:PHE:CE1	2.40	0.56
1:A:139:ASP:OD2	1:A:151:SER:OG	2.23	0.56
1:A:346:VAL:HG11	1:A:414:ILE:HD11	1.86	0.56
2:L:35:GLY:HA3	2:L:50:PHE:CD2	2.40	0.56
2:E:72:ASP:O	2:E:76:ASN:N	2.39	0.56
2:L:46:GLU:N	2:L:46:GLU:OE1	2.39	0.56
1:B:208:LEU:C	1:B:210:ARG:HH21	2.09	0.56
1:B:452:PHE:HB3	1:B:469:TYR:CD2	2.41	0.56
2:E:63:VAL:HG22	2:E:66:ARG:HB2	1.88	0.56
1:A:290:ASP:N	1:A:290:ASP:OD1	2.38	0.56
1:C:210:ARG:O	1:C:210:ARG:NH1	2.37	0.55
2:L:39:GLN:HB2	2:L:45:ARG:HD3	1.87	0.55
1:C:93:GLU:OE1	1:C:96:ASN:N	2.39	0.55
2:E:39:GLN:HB2	2:E:45:ARG:HD3	1.89	0.55
1:A:91:SER:OG	1:A:92:THR:N	2.40	0.55
1:A:414:ILE:HD12	1:A:418:ASN:HD22	1.71	0.55
1:C:123:VAL:HB	1:C:170:PRO:HA	1.89	0.54
1:C:272:LEU:HB3	1:C:285:VAL:HG23	1.89	0.54
1:A:272:LEU:HB3	1:A:285:VAL:HG12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:66:ARG:HH22	2:E:86:ILE:HG12	1.71	0.54
1:C:96:ASN:O	1:C:99:ARG:NH2	2.34	0.54
1:A:123:VAL:HG11	1:A:171:PHE:CE1	2.43	0.54
1:A:110:LYS:O	2:L:30:SER:OG	2.26	0.54
2:D:32:ASN:ND2	2:D:76:ASN:HD21	2.05	0.54
1:B:105:THR:OG1	1:B:230:ASN:O	2.26	0.54
1:A:109:SER:HB3	1:A:131:GLN:HB2	1.89	0.54
1:B:101:TRP:CD1	1:B:190:PHE:HE2	2.25	0.54
1:B:272:LEU:HB3	1:B:285:VAL:HG23	1.89	0.54
1:C:427:GLY:HA3	1:C:509:LEU:O	2.08	0.53
1:A:95:SER:O	1:A:96:ASN:ND2	2.41	0.53
1:A:103:PHE:HB3	1:A:231:ILE:HG21	1.90	0.53
1:A:325:PHE:CD2	1:A:524:LYS:HD3	2.44	0.53
2:D:12:VAL:HG13	2:D:113:VAL:HG22	1.90	0.53
1:A:26:THR:OG1	1:A:27:ASN:N	2.42	0.53
1:A:118:ASN:ND2	1:A:171:PHE:HB2	2.24	0.53
1:B:139:ASP:OD2	1:B:151:SER:OG	2.21	0.53
1:B:164:PHE:CE1	1:B:166:TYR:HB2	2.44	0.53
1:B:350:ASN:OD1	1:B:351:ARG:N	2.41	0.53
1:B:201:SER:HB3	1:B:222:LEU:HD22	1.91	0.52
1:A:118:ASN:HD21	1:A:171:PHE:HB2	1.73	0.52
2:D:32:ASN:HD21	2:D:76:ASN:HD21	1.57	0.52
1:A:440:LYS:HG3	1:A:443:GLY:H	1.75	0.52
1:C:81:LEU:N	1:C:233:ARG:HE	2.08	0.52
1:A:346:VAL:HG22	1:A:418:ASN:HB3	1.91	0.52
2:D:6:GLU:H	2:D:107:GLN:HE22	1.58	0.52
1:B:209:GLU:N	1:B:210:ARG:HH21	2.08	0.52
1:B:405:GLN:NE2	1:B:411:THR:O	2.39	0.51
2:E:5:GLN:HG3	2:E:23:ALA:HB3	1.93	0.51
2:E:102:GLN:NE2	2:E:103:ASP:O	2.43	0.51
1:B:488:LEU:HB2	2:L:60:TRP:HH2	1.76	0.51
1:C:227:ILE:HG13	1:C:228:GLY:N	2.26	0.51
1:B:105:THR:HA	1:B:232:THR:HG22	1.91	0.51
1:B:500:GLY:O	1:B:501:HIS:ND1	2.42	0.51
1:C:87:VAL:HG21	1:C:234:PHE:CZ	2.45	0.51
2:D:49:ALA:HB1	2:D:69:ILE:HD11	1.93	0.51
1:B:522:GLY:H	1:B:523:PRO:HD3	1.75	0.51
1:A:22:THR:O	1:A:22:THR:OG1	2.28	0.51
1:C:494:ARG:H	1:C:497:TYR:HD2	1.57	0.51
1:A:214:GLN:OE1	1:A:215:GLY:N	2.44	0.51
1:B:339:ASN:HB3	1:B:367:PHE:CZ	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:ALA:HB3	1:B:483:ASN:OD1	2.11	0.51
1:C:168:SER:OG	1:C:169:GLN:N	2.43	0.51
1:A:115:LEU:HD21	1:A:117:VAL:HG23	1.93	0.51
1:B:385:ASP:OD2	1:B:385:ASP:N	2.44	0.51
1:A:286:ASP:OD1	1:A:287:CYS:N	2.44	0.50
1:B:421:LEU:HD23	1:B:422:PRO:HD2	1.93	0.50
1:B:478:GLY:HA2	2:L:64:LYS:CE	2.42	0.50
1:C:343:PHE:CD2	1:C:505:ARG:HG2	2.47	0.50
1:C:290:ASP:OD1	1:C:290:ASP:N	2.43	0.50
2:L:70:THR:OG1	2:L:79:HIS:HB2	2.11	0.50
1:B:451:LEU:HG	1:B:452:PHE:CD1	2.45	0.50
1:C:102:ILE:HD11	1:C:237:LEU:HD21	1.93	0.50
1:A:127:VAL:HG11	1:A:164:PHE:HB3	1.94	0.50
1:A:129:GLU:O	1:A:129:GLU:HG3	2.12	0.49
1:C:172:LEU:HD12	1:C:186:ARG:HD3	1.93	0.49
1:B:413:ASN:OD1	1:B:413:ASN:N	2.45	0.49
2:D:72:ASP:O	2:D:76:ASN:N	2.45	0.49
2:L:68:THR:OG1	2:L:81:GLN:HB3	2.12	0.49
1:B:173:MET:SD	1:B:186:ARG:NH1	2.85	0.49
1:C:349:TRP:CE2	1:C:462:ARG:HD3	2.48	0.49
2:L:1:GLN:OE1	2:L:2:VAL:N	2.45	0.49
1:C:103:PHE:HB3	1:C:231:ILE:HG12	1.93	0.49
1:A:372:ALA:HB3	1:A:431:ALA:HB3	1.93	0.49
2:D:67:PHE:CD1	2:D:82:MET:HA	2.48	0.49
2:E:66:ARG:NH2	2:E:84:SER:O	2.43	0.49
1:B:478:GLY:HA2	2:L:64:LYS:HE3	1.94	0.49
2:L:3:GLN:N	2:L:3:GLN:OE1	2.46	0.49
1:A:416:ASP:HB2	1:A:456:LYS:HD2	1.95	0.49
1:B:96:ASN:O	1:B:99:ARG:NH2	2.41	0.49
1:B:103:PHE:HB3	1:B:231:ILE:HD12	1.95	0.48
1:B:354:ILE:HB	1:B:391:VAL:HG23	1.94	0.48
2:D:19:ARG:NH2	2:D:21:SER:HB3	2.28	0.48
1:A:130:PHE:HB3	1:A:156:TYR:CG	2.49	0.48
2:D:18:LEU:HD12	2:D:111:VAL:HG13	1.95	0.48
1:C:363:VAL:O	1:C:367:PHE:HB2	2.14	0.48
2:D:67:PHE:HD1	2:D:82:MET:HA	1.78	0.48
1:A:99:ARG:HH21	1:A:138:LEU:HB2	1.78	0.48
1:A:190:PHE:HD1	1:A:199:ILE:HG12	1.78	0.48
1:C:125:ILE:HB	1:C:166:TYR:HB3	1.95	0.48
1:C:432:TRP:NE1	1:C:505:ARG:HB2	2.28	0.48
1:A:105:THR:HA	1:A:232:THR:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:LEU:HD12	1:B:222:LEU:HA	1.73	0.48
1:C:127:VAL:HG12	1:C:127:VAL:O	2.13	0.48
2:E:5:GLN:O	2:E:22:CYS:HA	2.13	0.48
2:L:61:LEU:O	2:L:63:VAL:HG12	2.14	0.48
1:A:128:CYS:CA	1:A:162:CYS:HB3	2.43	0.48
1:B:163:THR:HG22	1:C:461:GLU:HB3	1.95	0.48
1:C:372:ALA:HB3	1:C:431:ALA:HB3	1.96	0.48
2:E:68:THR:OG1	2:E:81:GLN:HB3	2.14	0.48
2:L:38:ARG:HB2	2:L:48:VAL:HG23	1.96	0.48
2:L:66:ARG:HH22	2:L:86:ILE:HG12	1.78	0.48
1:A:124:VAL:C	1:A:125:ILE:HD12	2.35	0.47
1:B:494:ARG:HB2	1:B:497:TYR:CE1	2.49	0.47
2:D:102:GLN:NE2	2:D:103:ASP:O	2.45	0.47
1:B:454:LYS:HE2	1:B:454:LYS:HB3	1.68	0.47
1:C:422:PRO:HG2	1:C:425:PHE:HB2	1.96	0.47
1:A:98:ILE:HD11	1:A:236:THR:OG1	2.14	0.47
2:D:51:ILE:HD11	2:D:78:VAL:HG22	1.97	0.47
2:D:61:LEU:O	2:D:64:LYS:HG2	2.14	0.47
2:L:69:ILE:HG12	2:L:80:LEU:HD13	1.97	0.47
1:A:337:VAL:HG23	1:A:338:PHE:HD2	1.79	0.47
1:A:168:SER:OG	1:A:169:GLN:N	2.48	0.47
1:C:230:ASN:OD1	1:C:231:ILE:N	2.48	0.47
2:D:39:GLN:HA	2:D:43:LYS:HZ1	1.79	0.47
2:L:12:VAL:O	2:L:113:VAL:HA	2.14	0.47
1:C:104:GLY:N	1:C:231:ILE:HD11	2.30	0.47
1:C:350:ASN:O	1:C:394:ASP:HA	2.15	0.47
1:A:349:TRP:O	1:A:462:ARG:NH1	2.47	0.47
1:A:492:GLY:O	1:A:501:HIS:NE2	2.38	0.47
1:B:398:ILE:HG22	1:B:399:ARG:O	2.15	0.47
1:A:119:ASN:ND2	1:A:121:THR:OG1	2.46	0.47
1:B:28:SER:N	1:B:57:SER:O	2.40	0.47
1:C:31:ARG:NH2	1:C:187:GLU:OE2	2.32	0.47
1:B:494:ARG:HD3	1:B:497:TYR:HE1	1.80	0.46
1:C:377:GLY:HA3	1:C:426:THR:HG23	1.96	0.46
1:B:235:GLN:HG2	1:B:236:THR:N	2.29	0.46
1:C:116:ILE:HG13	1:C:125:ILE:HG12	1.97	0.46
1:B:188:PHE:HB3	1:B:190:PHE:CE1	2.51	0.46
2:E:11:LEU:HD22	2:E:112:THR:OG1	2.15	0.46
1:C:30:THR:HG23	1:C:30:THR:O	2.15	0.46
2:D:82:MET:SD	2:D:82:MET:N	2.88	0.46
1:B:28:SER:HG	1:B:57:SER:H	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ASN:OD1	1:B:184:ASN:N	2.48	0.46
1:B:130:PHE:CE1	1:B:159:ALA:HA	2.51	0.46
1:B:169:GLN:NE2	1:B:170:PRO:HD2	2.31	0.46
1:B:450:ARG:NH2	1:B:465:SER:O	2.49	0.46
1:B:399:ARG:HG3	1:B:402:GLU:HB2	1.97	0.45
2:E:70:THR:OG1	2:E:79:HIS:HB2	2.15	0.45
1:A:399:ARG:HG2	1:A:501:HIS:HA	1.98	0.45
2:E:87:PRO:HA	2:E:113:VAL:HG13	1.98	0.45
1:B:31:ARG:HG2	1:B:31:ARG:HH11	1.82	0.45
1:B:114:LEU:HD23	1:B:229:ILE:HG21	1.98	0.45
2:E:10:GLY:N	2:E:110:GLN:O	2.49	0.45
1:B:392:TYR:HB2	1:B:510:SER:OG	2.16	0.45
1:C:82:PRO:O	1:C:265:TYR:OH	2.21	0.45
2:D:19:ARG:HH12	2:D:79:HIS:CB	2.27	0.45
1:B:154:ARG:HA	1:B:154:ARG:HD3	1.83	0.45
2:L:66:ARG:NH2	2:L:86:ILE:HG23	2.32	0.45
1:A:114:LEU:HD12	1:A:115:LEU:N	2.32	0.45
1:A:501:HIS:O	1:A:501:HIS:CD2	2.70	0.45
1:B:440:LYS:O	1:B:494:ARG:HG3	2.16	0.45
1:A:388:PHE:CD2	1:A:511:PHE:HB3	2.52	0.45
1:A:157:SER:OG	1:A:158:SER:N	2.50	0.44
1:A:272:LEU:HD23	1:A:302:PHE:HE1	1.82	0.44
1:B:330:ASN:O	1:B:358:VAL:HB	2.17	0.44
1:C:416:ASP:HB2	1:C:456:LYS:HG3	1.98	0.44
2:L:39:GLN:O	2:L:91:ALA:HB1	2.16	0.44
1:A:121:THR:OG1	1:A:122:ASN:N	2.50	0.44
1:B:123:VAL:HB	1:B:170:PRO:HA	1.99	0.44
1:B:97:ILE:HG13	1:B:238:LEU:HD12	1.99	0.44
1:B:118:ASN:OD1	1:B:119:ASN:N	2.51	0.44
1:B:163:THR:OG1	1:B:164:PHE:N	2.51	0.44
1:A:479:VAL:HB	2:D:64:LYS:NZ	2.32	0.44
1:B:88:TYR:OH	1:B:187:GLU:OE1	2.26	0.44
2:L:63:VAL:HG22	2:L:66:ARG:HB2	1.99	0.44
1:A:422:PRO:HG2	1:A:425:PHE:HB2	1.99	0.44
1:C:103:PHE:C	1:C:231:ILE:HD11	2.38	0.44
1:C:363:VAL:HA	1:C:366:ASN:OD1	2.17	0.44
1:A:524:LYS:O	1:A:524:LYS:HG3	2.18	0.44
1:B:290:ASP:OD1	1:B:290:ASP:N	2.48	0.44
2:D:28:ILE:O	2:D:28:ILE:HG22	2.18	0.44
1:A:164:PHE:CZ	1:A:166:TYR:HB2	2.53	0.44
1:A:445:TYR:CZ	2:D:44:GLN:HG3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:LYS:NZ	1:C:353:ARG:O	2.51	0.44
1:C:389:THR:HG21	1:C:515:HIS:HB2	2.00	0.44
1:A:106:THR:HG21	1:A:110:LYS:HB2	2.00	0.44
1:B:210:ARG:N	1:B:210:ARG:NE	2.66	0.44
1:C:123:VAL:HG21	1:C:171:PHE:CE1	2.52	0.44
2:D:33:THR:HB	2:D:98:VAL:HB	1.99	0.44
1:A:119:ASN:OD1	1:A:122:ASN:N	2.50	0.43
1:B:101:TRP:HB3	1:B:103:PHE:CE1	2.53	0.43
1:C:222:LEU:HD12	1:C:222:LEU:HA	1.75	0.43
1:A:93:GLU:OE2	1:A:260:ALA:N	2.51	0.43
1:A:112:GLN:HA	1:A:129:GLU:HA	2.00	0.43
2:L:74:THR:OG1	2:L:75:LYS:HD2	2.17	0.43
1:A:37:ASP:OD1	1:A:37:ASP:N	2.48	0.43
1:B:103:PHE:HB2	1:B:114:LEU:HB2	2.01	0.43
1:C:458:LYS:HG2	1:C:459:PRO:HD2	2.00	0.43
2:D:40:ALA:H	2:D:43:LYS:HG2	1.83	0.43
2:E:38:ARG:HH22	2:E:89:ASP:HA	1.82	0.43
1:B:470:GLN:HE22	1:B:476:CYS:N	2.16	0.43
1:A:132:PHE:CE1	1:A:136:PRO:HB3	2.53	0.43
1:A:277:GLU:HG2	1:A:278:ASN:N	2.34	0.43
1:A:436:LYS:HE2	1:A:436:LYS:HB2	1.83	0.43
1:A:31:ARG:NH2	1:A:187:GLU:OE2	2.35	0.43
1:A:216:PHE:HD1	1:A:217:SER:N	2.15	0.43
1:A:127:VAL:O	1:A:127:VAL:HG22	2.19	0.43
2:E:72:ASP:O	2:E:76:ASN:CA	2.67	0.43
2:L:51:ILE:HB	2:L:69:ILE:HG21	2.00	0.43
1:A:322:ILE:HD12	1:A:322:ILE:HA	1.82	0.43
1:B:157:SER:OG	1:B:158:SER:N	2.52	0.43
1:B:415:ALA:O	1:B:420:LYS:HD2	2.19	0.43
1:A:387:CYS:HB2	1:A:520:VAL:O	2.19	0.43
1:B:35:TYR:HE2	1:B:220:GLU:HG3	1.84	0.42
1:B:402:GLU:HG2	1:B:405:GLN:HG3	2.01	0.42
1:C:432:TRP:CD1	1:C:505:ARG:HB2	2.54	0.42
2:D:72:ASP:OD2	2:D:75:LYS:HE3	2.18	0.42
1:A:107:LEU:HB3	1:A:132:PHE:HD2	1.85	0.42
1:A:399:ARG:HB3	1:A:402:GLU:HG3	2.00	0.42
1:B:130:PHE:HE1	1:B:159:ALA:HA	1.84	0.42
1:B:394:ASP:O	1:B:507:VAL:HA	2.19	0.42
1:B:488:LEU:HB2	2:L:60:TRP:CH2	2.54	0.42
2:E:12:VAL:O	2:E:113:VAL:HA	2.18	0.42
2:E:36:TRP:O	2:E:48:VAL:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:38:ARG:HD3	2:D:93:TYR:HE1	1.83	0.42
2:E:38:ARG:HG2	2:E:46:GLU:O	2.20	0.42
1:C:123:VAL:HG21	1:C:171:PHE:CD1	2.54	0.42
1:C:193:ILE:HG13	1:C:194:ASP:OD2	2.20	0.42
2:D:90:THR:HG22	2:D:113:VAL:H	1.82	0.42
1:A:101:TRP:HB3	1:A:103:PHE:CE1	2.55	0.42
1:B:479:VAL:HG21	2:L:62:PRO:CD	2.50	0.42
2:D:107:GLN:OE1	2:D:107:GLN:N	2.51	0.42
1:B:355:SER:HB3	1:B:390:ASN:OD1	2.19	0.42
1:C:102:ILE:HD11	1:C:237:LEU:CD2	2.50	0.42
1:B:206:ILE:HG12	1:B:207:ASN:O	2.20	0.42
2:E:34:MET:HB3	2:E:78:VAL:HG21	2.01	0.42
1:A:130:PHE:HB3	1:A:156:TYR:HB2	2.02	0.42
1:A:355:SER:HA	1:A:520:VAL:HG21	2.02	0.42
1:B:264:GLY:C	1:B:265:TYR:HD1	2.23	0.42
1:B:333:PRO:HD2	1:B:354:ILE:HD12	2.01	0.42
1:B:453:ARG:NE	1:B:463:ASP:OD2	2.53	0.42
1:C:102:ILE:O	1:C:234:PHE:HA	2.19	0.42
2:D:70:THR:OG1	2:D:79:HIS:HB2	2.19	0.42
1:A:97:ILE:O	1:A:239:ALA:N	2.53	0.42
1:B:128:CYS:CA	1:B:162:CYS:HB3	2.47	0.42
1:B:477:ASN:OD1	1:B:477:ASN:N	2.51	0.42
2:D:61:LEU:HD23	2:D:61:LEU:HA	1.86	0.42
2:E:38:ARG:HG3	2:E:46:GLU:OE1	2.20	0.42
2:L:94:TYR:HD1	2:L:108:GLY:HA2	1.84	0.42
1:A:337:VAL:HG23	1:A:338:PHE:CD2	2.55	0.41
1:B:136:PRO:HB3	1:B:155:VAL:HA	2.02	0.41
2:D:36:TRP:HE1	2:D:78:VAL:CG1	2.33	0.41
1:A:481:GLY:HA2	2:D:61:LEU:HD21	2.01	0.41
1:C:387:CYS:HB3	1:C:518:ALA:HB3	2.01	0.41
1:A:140:VAL:HA	1:A:150:GLU:HG3	2.01	0.41
2:L:8:GLY:O	2:L:18:LEU:HD12	2.20	0.41
1:A:417:TYR:CE1	1:A:453:ARG:HB3	2.55	0.41
1:B:26:THR:OG1	1:B:211:ASP:OD2	2.33	0.41
1:B:346:VAL:HG21	1:B:398:ILE:HD11	2.02	0.41
1:C:139:ASP:OD2	1:C:151:SER:OG	2.31	0.41
1:C:227:ILE:HD12	1:C:229:ILE:HG12	2.01	0.41
1:B:516:ALA:HB1	1:B:517:PRO:HD3	2.02	0.41
1:A:97:ILE:HA	1:A:239:ALA:HB3	2.02	0.41
2:L:29:PHE:HD2	2:L:100:LYS:HE2	1.85	0.41
1:A:97:ILE:H	1:A:97:ILE:HG13	1.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LEU:HD23	1:A:138:LEU:HA	1.93	0.41
1:B:324:ARG:HA	1:B:324:ARG:HD2	1.84	0.41
1:A:153:PHE:HA	1:A:156:TYR:O	2.20	0.41
1:A:413:ASN:O	1:A:417:TYR:HB2	2.21	0.41
1:B:427:GLY:HA2	1:B:511:PHE:HD2	1.85	0.41
1:C:462:ARG:NH1	2:E:100:LYS:O	2.44	0.41
1:B:424:ASP:OD1	1:B:424:ASP:N	2.37	0.41
1:A:283:ASP:OD1	1:A:284:ALA:N	2.53	0.40
1:C:81:LEU:O	1:C:233:ARG:HG2	2.21	0.40
2:L:63:VAL:HG22	2:L:63:VAL:O	2.20	0.40
1:A:390:ASN:HB2	1:A:512:GLU:OE2	2.21	0.40
1:A:494:ARG:NE	1:A:497:TYR:HE2	2.19	0.40
1:A:31:ARG:NH1	1:A:213:PRO:HG2	2.35	0.40
1:C:349:TRP:HZ3	1:C:351:ARG:HB2	1.86	0.40
2:L:80:LEU:HD12	2:L:80:LEU:HA	1.83	0.40
1:B:457:LEU:HD23	1:B:457:LEU:HA	1.83	0.40
1:C:207:ASN:OD1	1:C:207:ASN:C	2.59	0.40
1:C:424:ASP:OD1	1:C:424:ASP:N	2.50	0.40
1:C:431:ALA:HB2	1:C:506:VAL:HG22	2.03	0.40
2:D:38:ARG:HH11	2:D:89:ASP:HA	1.87	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	426/1230 (35%)	400 (94%)	26 (6%)	0	100 100
1	B	424/1230 (34%)	389 (92%)	33 (8%)	2 (0%)	25 59
1	C	403/1230 (33%)	386 (96%)	17 (4%)	0	100 100
2	D	113/136 (83%)	107 (95%)	5 (4%)	1 (1%)	14 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	113/136 (83%)	101 (89%)	11 (10%)	1 (1%)	14	49
2	L	113/136 (83%)	105 (93%)	7 (6%)	1 (1%)	14	49
All	All	1592/4098 (39%)	1488 (94%)	99 (6%)	5 (0%)	38	68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	446	ASN
1	B	482	PRO
2	D	28	ILE
2	L	28	ILE
2	E	28	ILE

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	390/1070 (36%)	381 (98%)	9 (2%)	45	69
1	B	388/1070 (36%)	379 (98%)	9 (2%)	45	69
1	C	374/1070 (35%)	367 (98%)	7 (2%)	52	73
2	D	95/111 (86%)	92 (97%)	3 (3%)	34	62
2	E	95/111 (86%)	93 (98%)	2 (2%)	48	71
2	L	95/111 (86%)	93 (98%)	2 (2%)	48	71
All	All	1437/3543 (41%)	1405 (98%)	32 (2%)	47	70

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	SER
1	A	132	PHE
1	A	173	MET
1	A	210	ARG
1	A	216	PHE

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Mol	Chain	Res	Type
1	A	325	PHE
1	A	388	PHE
1	A	493	PHE
1	A	524	LYS
1	B	173	MET
1	B	210	ARG
1	B	213	PRO
1	B	216	PHE
1	B	373	PHE
1	B	390	ASN
1	B	455	SER
1	B	467	GLU
1	B	474	LYS
1	C	53	LEU
1	C	201	SER
1	C	216	PHE
1	C	347	TYR
1	C	371	PHE
1	C	410	GLN
1	C	432	TRP
2	D	5	GLN
2	D	19	ARG
2	D	95	CYS
2	E	76	ASN
2	E	82	MET
2	L	25	SER
2	L	76	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	B	169	GLN
1	B	230	ASN
1	B	235	GLN
2	D	32	ASN
2	D	81	GLN

5.3.3 RNA

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](#)

There are no ligands in this entry.

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.

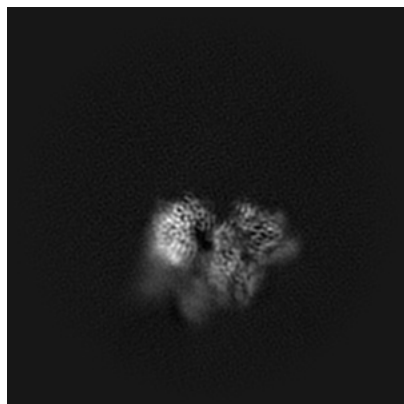
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43832. These allow visual inspection of the internal detail of the map and identification of artifacts.

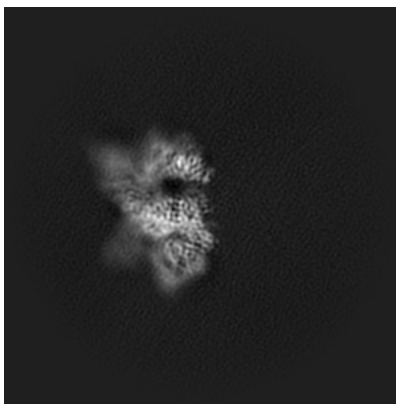
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

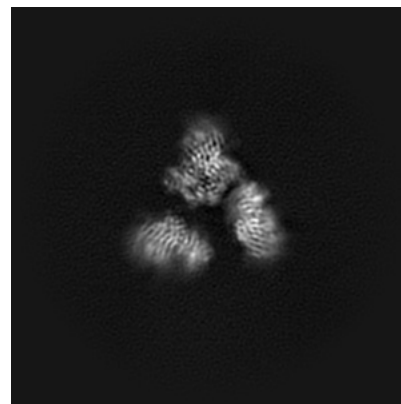
6.1.1 Primary map



X

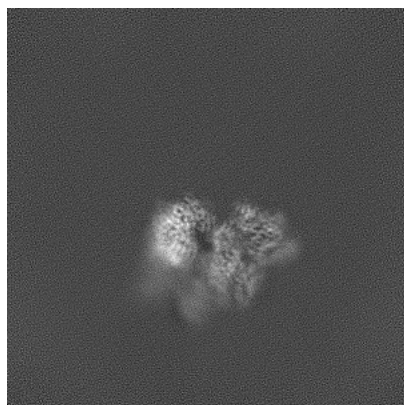


Y

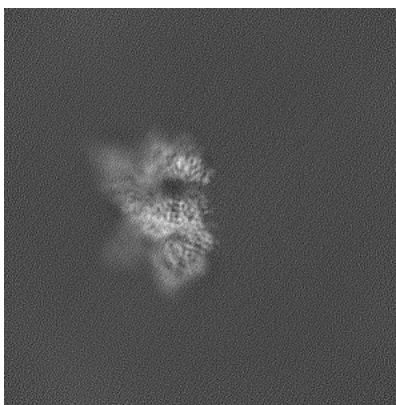


Z

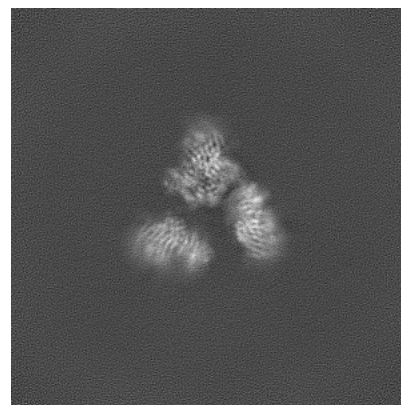
6.1.2 Raw map



X



Y

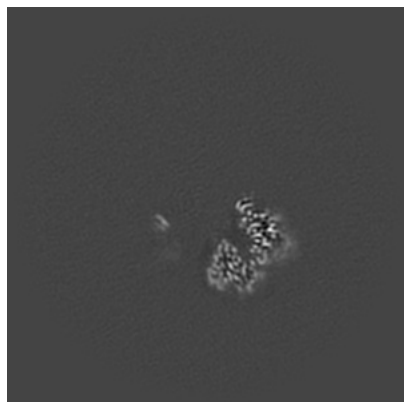


Z

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

6.2 Central slices [i](#)

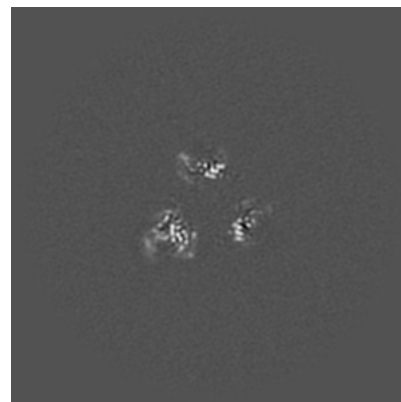
6.2.1 Primary map



X Index: 192

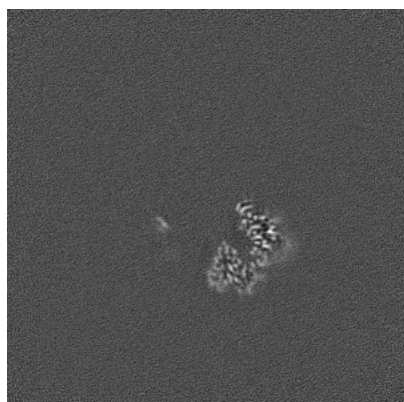


Y Index: 192



Z Index: 192

6.2.2 Raw map



X Index: 192



Y Index: 192

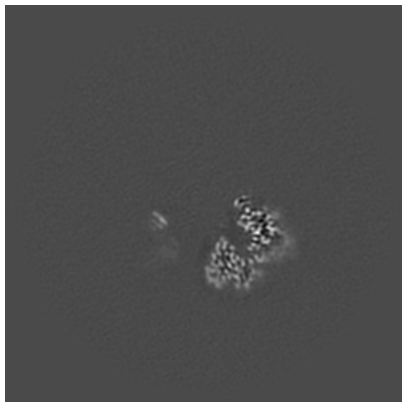


Z Index: 192

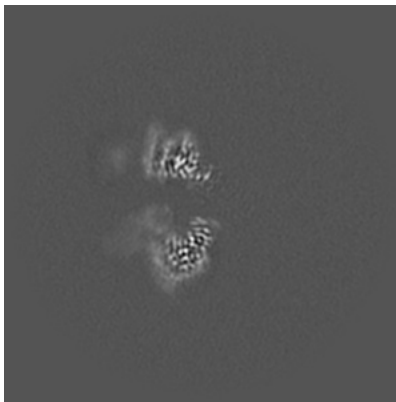
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

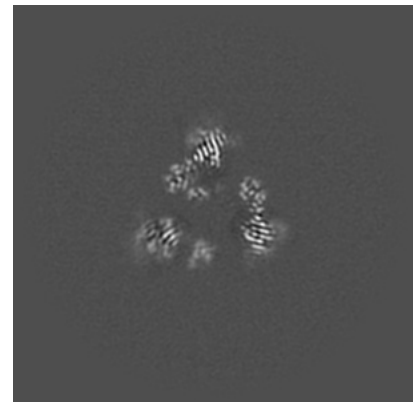
6.3.1 Primary map



X Index: 191

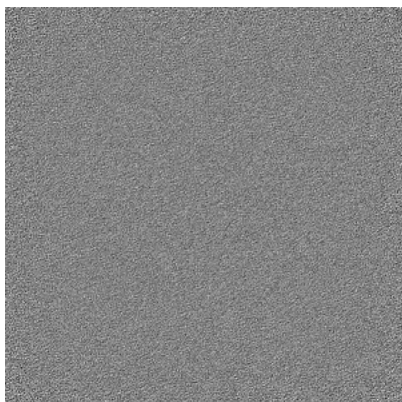


Y Index: 163

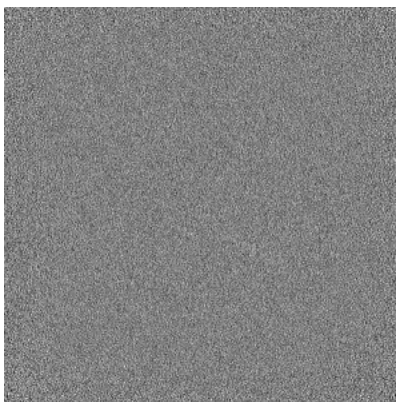


Z Index: 169

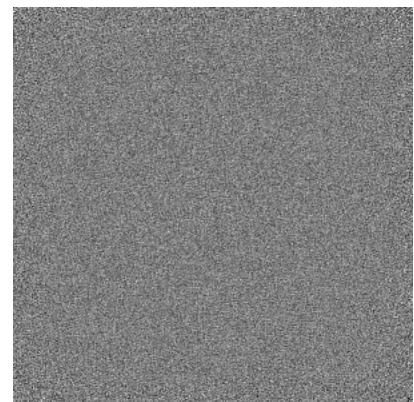
6.3.2 Raw map



X Index: 0



Y Index: 0

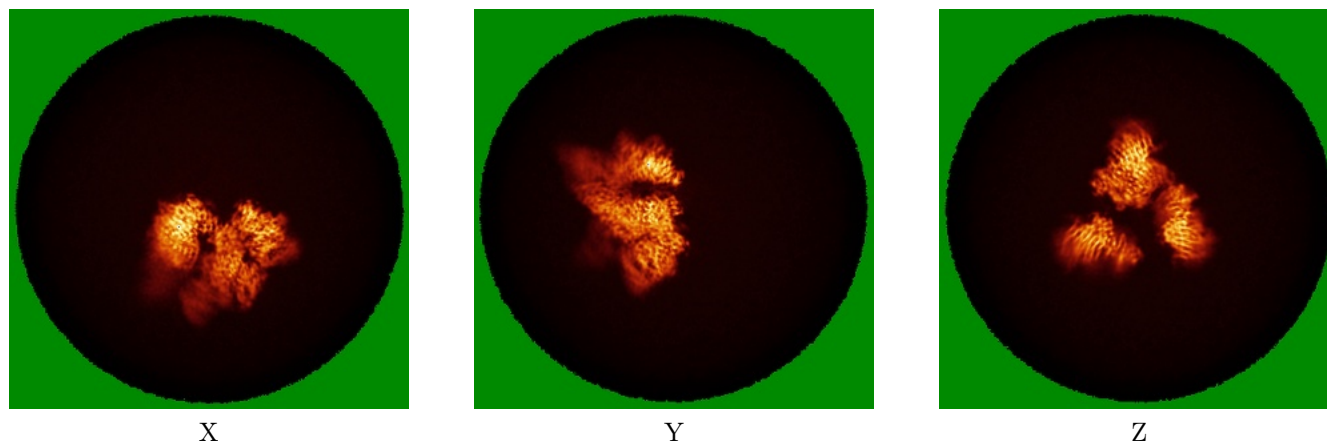


Z Index: 383

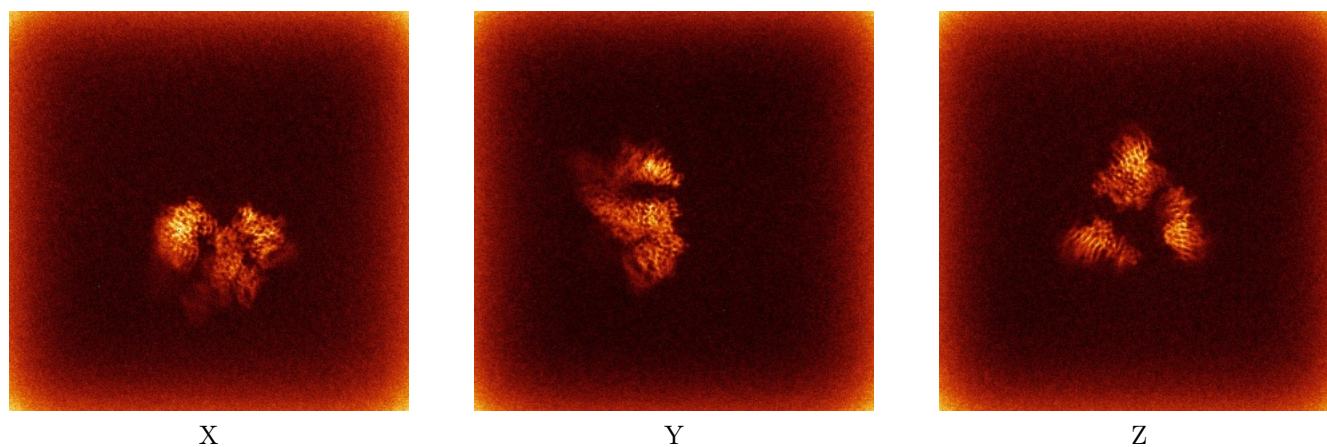
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



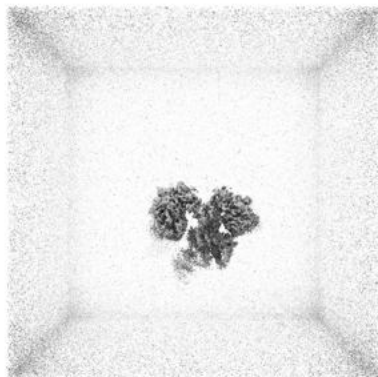
Y



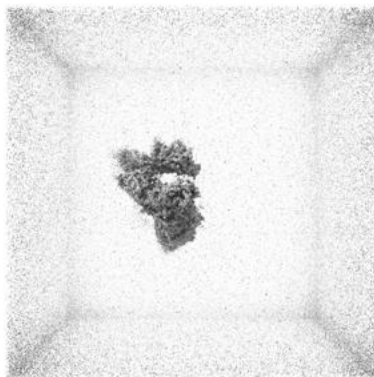
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0311. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

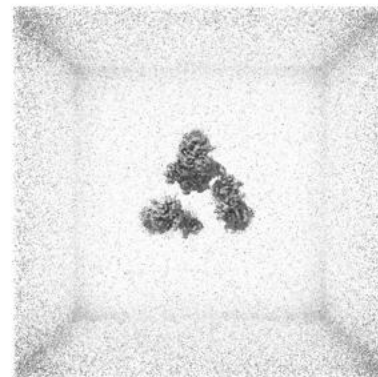
6.5.2 Raw map



X



Y



Z

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

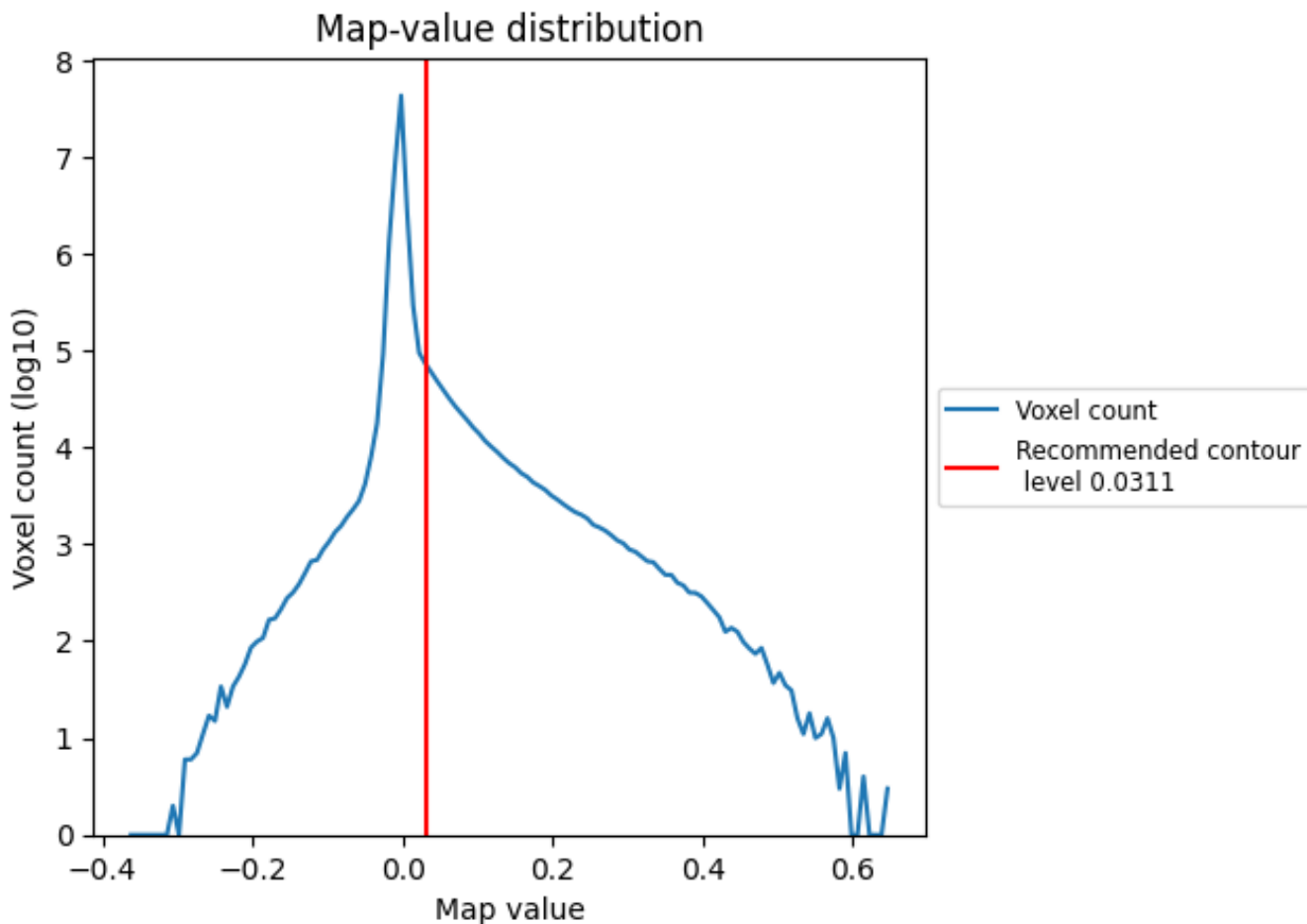
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

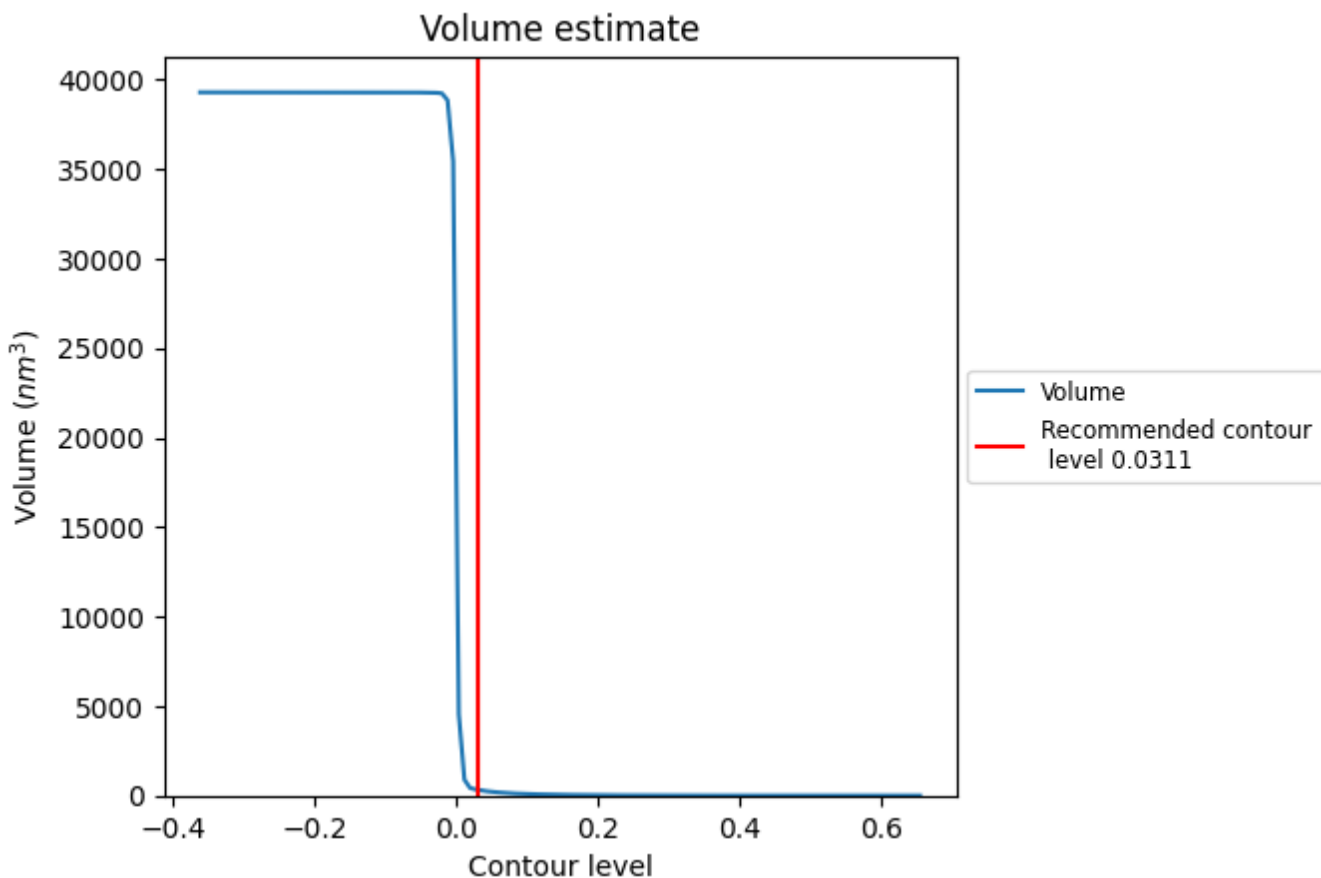
This section contains the results of statistical analysis of the map.

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.

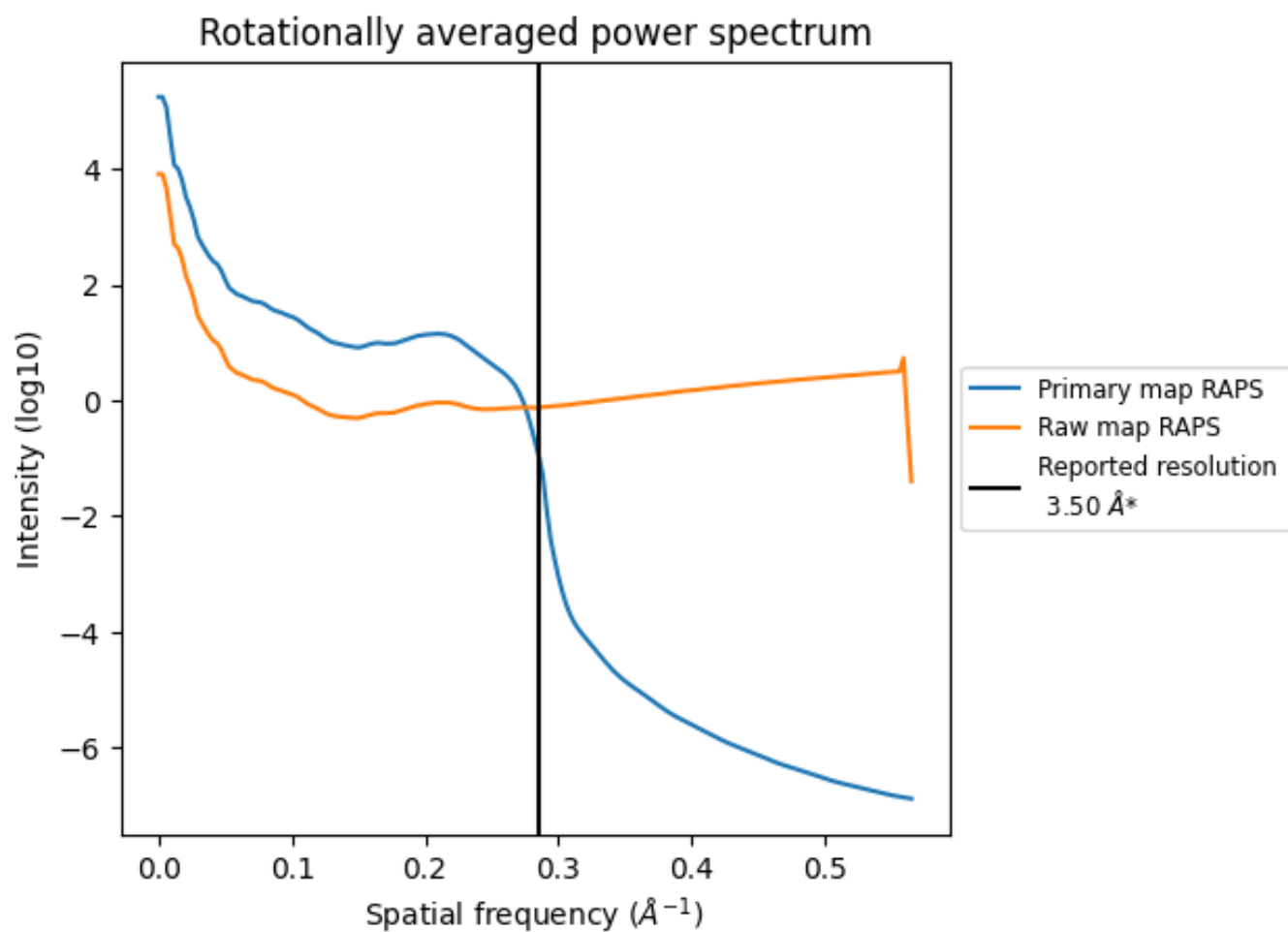
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 316 nm³; this corresponds to an approximate mass of 285 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 [i](#)

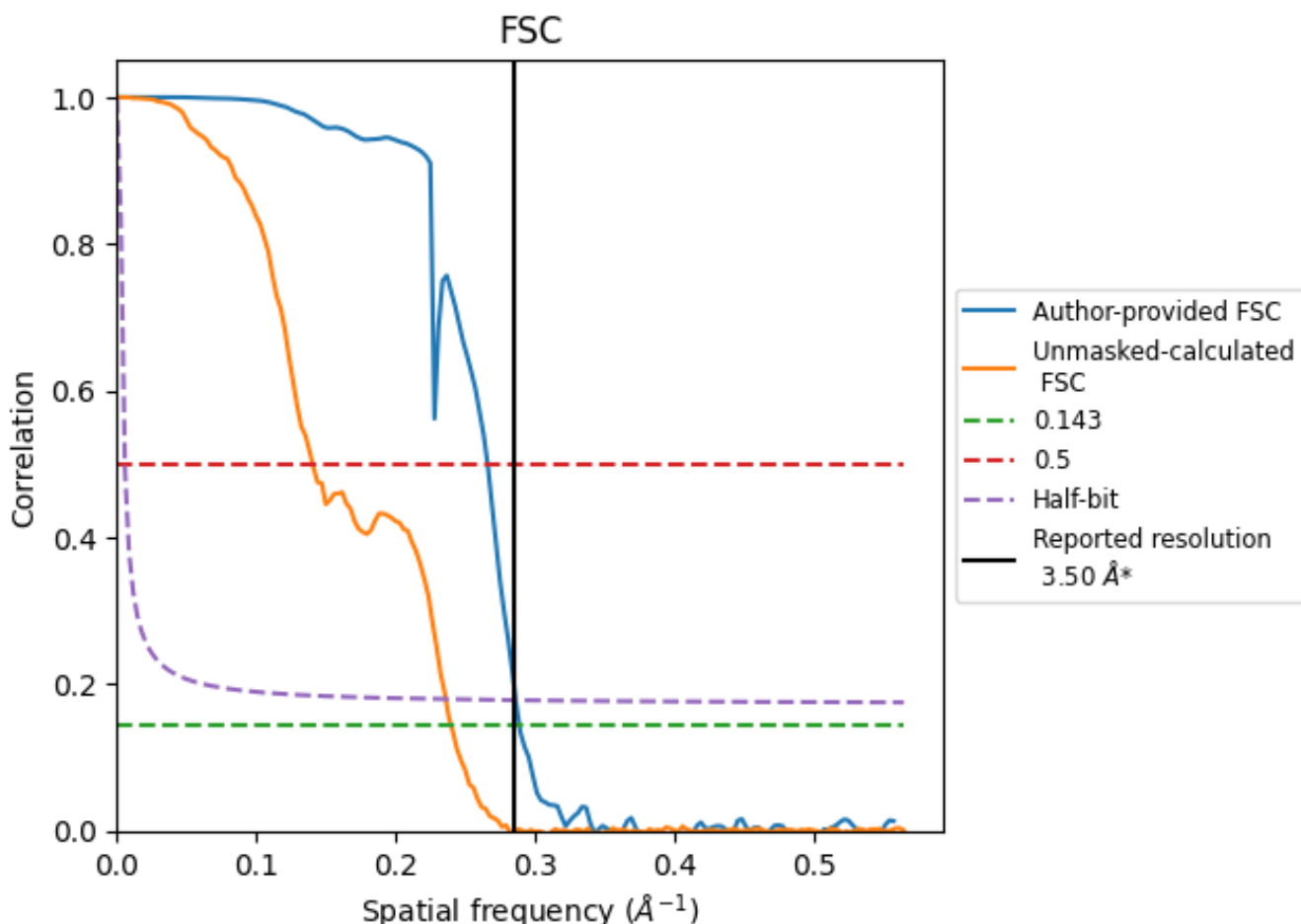


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286\AA^{-1}

8.2 Resolution estimates [i](#)

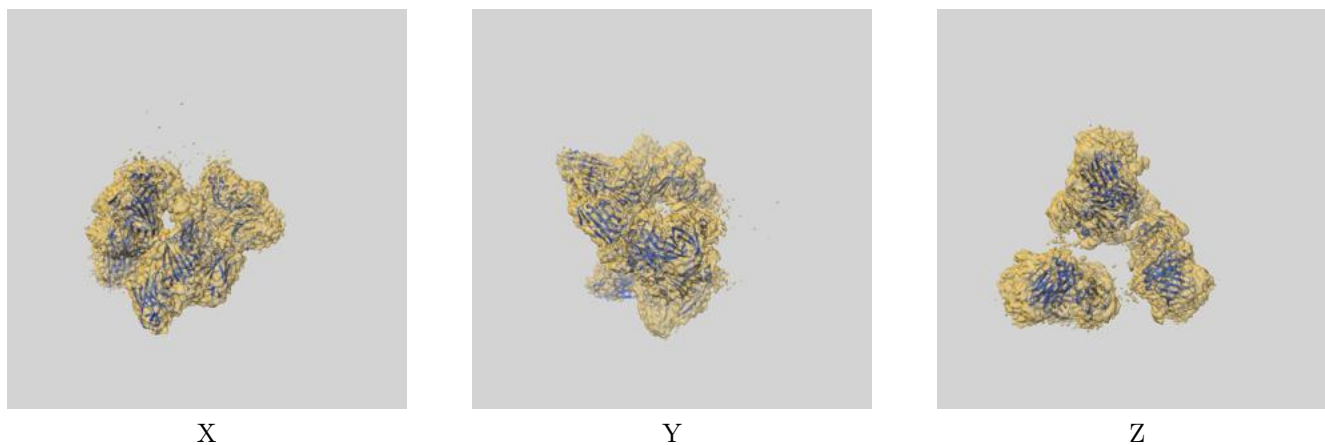
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.46	3.76	3.49
Unmasked-calculated*	4.17	7.12	4.24

*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 4.17 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-43832 and PDB model 9ATP. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0311 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 [\(i\)](#)



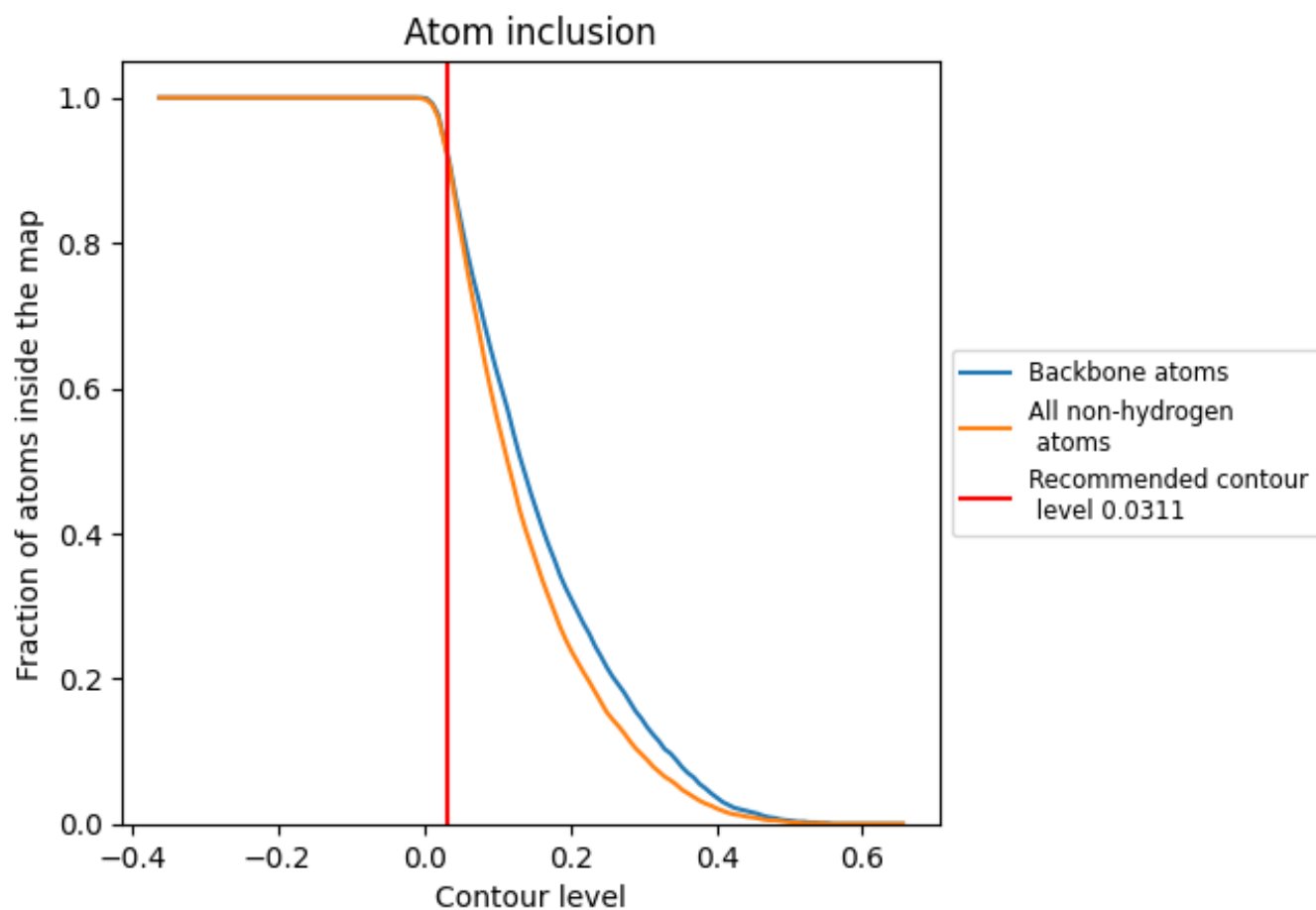
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0311).















9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 92% 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 (0.0311) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9240	 0.3160
A	 0.9630	 0.3390
B	 0.9920	 0.4400
C	 0.9240	 0.2590
D	 0.9070	 0.1030
E	 0.4470	 0.0520
L	 0.9950	 0.4220

