



Full wwPDB EM Validation Report ⓘ

Sep 2, 2026 – 12:59 PM EDT

PDB ID : 9Y54 / pdb_00009y54
EMDB ID : EMD-72507
Title : The spike protein of HCoV-OC43 obtained from data collected on 100 kV
Tundra with Ceta detector
Authors : Pathirage, R.; Acharya, P.
Deposited on : 2025-09-04
Resolution : 4.55 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
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

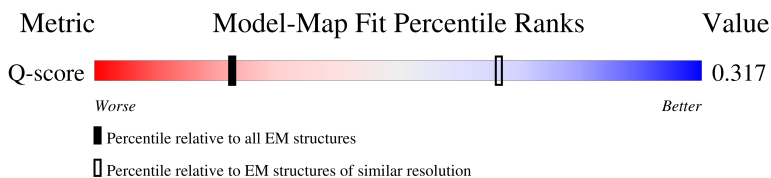
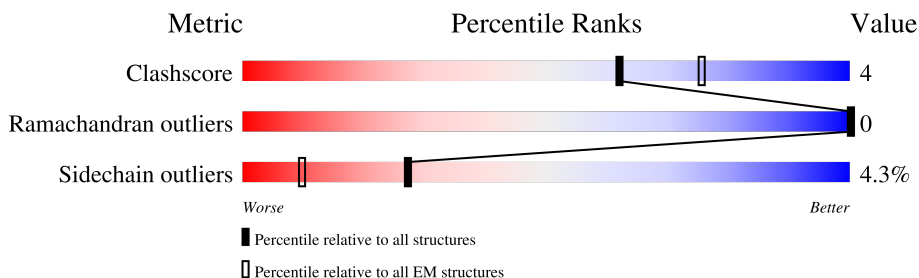
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.55 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	2458 (4.05 - 5.04)

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	1353	
1	B	1353	
1	C	1353	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 27450 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
1	A	1175	Total	C	N	O	S	0	0
			9150	5832	1506	1751	61		
1	B	1175	Total	C	N	O	S	0	0
			9150	5832	1506	1751	61		
1	C	1175	Total	C	N	O	S	0	0
			9150	5832	1506	1751	61		

There are 318 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP Q696P8
A	-8	PRO	-	expression tag	UNP Q696P8
A	-7	MET	-	expression tag	UNP Q696P8
A	-6	GLY	-	expression tag	UNP Q696P8
A	-5	SER	-	expression tag	UNP Q696P8
A	-4	LEU	-	expression tag	UNP Q696P8
A	-3	GLN	-	expression tag	UNP Q696P8
A	-2	PRO	-	expression tag	UNP Q696P8
A	-1	LEU	-	expression tag	UNP Q696P8
A	0	ALA	-	expression tag	UNP Q696P8
A	1	THR	-	expression tag	UNP Q696P8
A	2	LEU	-	expression tag	UNP Q696P8
A	3	TYR	-	expression tag	UNP Q696P8
A	4	LEU	-	expression tag	UNP Q696P8
A	5	LEU	-	expression tag	UNP Q696P8
A	6	GLY	-	expression tag	UNP Q696P8
A	7	MET	-	expression tag	UNP Q696P8
A	8	LEU	-	expression tag	UNP Q696P8
A	9	VAL	-	expression tag	UNP Q696P8
A	10	ALA	-	expression tag	UNP Q696P8
A	11	SER	-	expression tag	UNP Q696P8
A	12	VAL	-	expression tag	UNP Q696P8
A	13	LEU	-	expression tag	UNP Q696P8
A	764	GLY	ARG	conflict	UNP Q696P8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	765	GLY	ARG	conflict	UNP Q696P8
A	767	GLY	ARG	conflict	UNP Q696P8
A	1274	GLY	-	expression tag	UNP Q696P8
A	1275	SER	-	expression tag	UNP Q696P8
A	1276	GLY	-	expression tag	UNP Q696P8
A	1277	TYR	-	expression tag	UNP Q696P8
A	1278	ILE	-	expression tag	UNP Q696P8
A	1279	PRO	-	expression tag	UNP Q696P8
A	1280	GLU	-	expression tag	UNP Q696P8
A	1281	ALA	-	expression tag	UNP Q696P8
A	1282	PRO	-	expression tag	UNP Q696P8
A	1283	ARG	-	expression tag	UNP Q696P8
A	1284	ASP	-	expression tag	UNP Q696P8
A	1285	GLY	-	expression tag	UNP Q696P8
A	1286	GLN	-	expression tag	UNP Q696P8
A	1287	ALA	-	expression tag	UNP Q696P8
A	1288	TYR	-	expression tag	UNP Q696P8
A	1289	VAL	-	expression tag	UNP Q696P8
A	1290	ARG	-	expression tag	UNP Q696P8
A	1291	LYS	-	expression tag	UNP Q696P8
A	1292	ASP	-	expression tag	UNP Q696P8
A	1293	GLY	-	expression tag	UNP Q696P8
A	1294	GLU	-	expression tag	UNP Q696P8
A	1295	TRP	-	expression tag	UNP Q696P8
A	1296	VAL	-	expression tag	UNP Q696P8
A	1297	LEU	-	expression tag	UNP Q696P8
A	1298	LEU	-	expression tag	UNP Q696P8
A	1299	SER	-	expression tag	UNP Q696P8
A	1300	THR	-	expression tag	UNP Q696P8
A	1301	PHE	-	expression tag	UNP Q696P8
A	1302	LEU	-	expression tag	UNP Q696P8
A	1303	GLY	-	expression tag	UNP Q696P8
A	1304	ARG	-	expression tag	UNP Q696P8
A	1305	SER	-	expression tag	UNP Q696P8
A	1306	LEU	-	expression tag	UNP Q696P8
A	1307	GLU	-	expression tag	UNP Q696P8
A	1308	VAL	-	expression tag	UNP Q696P8
A	1309	LEU	-	expression tag	UNP Q696P8
A	1310	PHE	-	expression tag	UNP Q696P8
A	1311	GLN	-	expression tag	UNP Q696P8
A	1312	GLY	-	expression tag	UNP Q696P8
A	1313	PRO	-	expression tag	UNP Q696P8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1314	GLY	-	expression tag	UNP Q696P8
A	1315	HIS	-	expression tag	UNP Q696P8
A	1316	HIS	-	expression tag	UNP Q696P8
A	1317	HIS	-	expression tag	UNP Q696P8
A	1318	HIS	-	expression tag	UNP Q696P8
A	1319	HIS	-	expression tag	UNP Q696P8
A	1320	HIS	-	expression tag	UNP Q696P8
A	1321	HIS	-	expression tag	UNP Q696P8
A	1322	HIS	-	expression tag	UNP Q696P8
A	1323	SER	-	expression tag	UNP Q696P8
A	1324	ALA	-	expression tag	UNP Q696P8
A	1325	TRP	-	expression tag	UNP Q696P8
A	1326	SER	-	expression tag	UNP Q696P8
A	1327	HIS	-	expression tag	UNP Q696P8
A	1328	PRO	-	expression tag	UNP Q696P8
A	1329	GLN	-	expression tag	UNP Q696P8
A	1330	PHE	-	expression tag	UNP Q696P8
A	1331	GLU	-	expression tag	UNP Q696P8
A	1332	LYS	-	expression tag	UNP Q696P8
A	1333	GLY	-	expression tag	UNP Q696P8
A	1334	GLY	-	expression tag	UNP Q696P8
A	1335	GLY	-	expression tag	UNP Q696P8
A	1336	SER	-	expression tag	UNP Q696P8
A	1337	GLY	-	expression tag	UNP Q696P8
A	1338	GLY	-	expression tag	UNP Q696P8
A	1339	GLY	-	expression tag	UNP Q696P8
A	1340	GLY	-	expression tag	UNP Q696P8
A	1341	SER	-	expression tag	UNP Q696P8
A	1342	GLY	-	expression tag	UNP Q696P8
A	1343	GLY	-	expression tag	UNP Q696P8
A	1344	SER	-	expression tag	UNP Q696P8
A	1345	ALA	-	expression tag	UNP Q696P8
A	1346	TRP	-	expression tag	UNP Q696P8
A	1347	SER	-	expression tag	UNP Q696P8
A	1348	HIS	-	expression tag	UNP Q696P8
A	1349	PRO	-	expression tag	UNP Q696P8
A	1350	GLN	-	expression tag	UNP Q696P8
A	1351	PHE	-	expression tag	UNP Q696P8
A	1352	GLU	-	expression tag	UNP Q696P8
A	1353	LYS	-	expression tag	UNP Q696P8
B	-9	MET	-	initiating methionine	UNP Q696P8
B	-8	PRO	-	expression tag	UNP Q696P8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	MET	-	expression tag	UNP Q696P8
B	-6	GLY	-	expression tag	UNP Q696P8
B	-5	SER	-	expression tag	UNP Q696P8
B	-4	LEU	-	expression tag	UNP Q696P8
B	-3	GLN	-	expression tag	UNP Q696P8
B	-2	PRO	-	expression tag	UNP Q696P8
B	-1	LEU	-	expression tag	UNP Q696P8
B	0	ALA	-	expression tag	UNP Q696P8
B	1	THR	-	expression tag	UNP Q696P8
B	2	LEU	-	expression tag	UNP Q696P8
B	3	TYR	-	expression tag	UNP Q696P8
B	4	LEU	-	expression tag	UNP Q696P8
B	5	LEU	-	expression tag	UNP Q696P8
B	6	GLY	-	expression tag	UNP Q696P8
B	7	MET	-	expression tag	UNP Q696P8
B	8	LEU	-	expression tag	UNP Q696P8
B	9	VAL	-	expression tag	UNP Q696P8
B	10	ALA	-	expression tag	UNP Q696P8
B	11	SER	-	expression tag	UNP Q696P8
B	12	VAL	-	expression tag	UNP Q696P8
B	13	LEU	-	expression tag	UNP Q696P8
B	764	GLY	ARG	conflict	UNP Q696P8
B	765	GLY	ARG	conflict	UNP Q696P8
B	767	GLY	ARG	conflict	UNP Q696P8
B	1274	GLY	-	expression tag	UNP Q696P8
B	1275	SER	-	expression tag	UNP Q696P8
B	1276	GLY	-	expression tag	UNP Q696P8
B	1277	TYR	-	expression tag	UNP Q696P8
B	1278	ILE	-	expression tag	UNP Q696P8
B	1279	PRO	-	expression tag	UNP Q696P8
B	1280	GLU	-	expression tag	UNP Q696P8
B	1281	ALA	-	expression tag	UNP Q696P8
B	1282	PRO	-	expression tag	UNP Q696P8
B	1283	ARG	-	expression tag	UNP Q696P8
B	1284	ASP	-	expression tag	UNP Q696P8
B	1285	GLY	-	expression tag	UNP Q696P8
B	1286	GLN	-	expression tag	UNP Q696P8
B	1287	ALA	-	expression tag	UNP Q696P8
B	1288	TYR	-	expression tag	UNP Q696P8
B	1289	VAL	-	expression tag	UNP Q696P8
B	1290	ARG	-	expression tag	UNP Q696P8
B	1291	LYS	-	expression tag	UNP Q696P8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1292	ASP	-	expression tag	UNP Q696P8
B	1293	GLY	-	expression tag	UNP Q696P8
B	1294	GLU	-	expression tag	UNP Q696P8
B	1295	TRP	-	expression tag	UNP Q696P8
B	1296	VAL	-	expression tag	UNP Q696P8
B	1297	LEU	-	expression tag	UNP Q696P8
B	1298	LEU	-	expression tag	UNP Q696P8
B	1299	SER	-	expression tag	UNP Q696P8
B	1300	THR	-	expression tag	UNP Q696P8
B	1301	PHE	-	expression tag	UNP Q696P8
B	1302	LEU	-	expression tag	UNP Q696P8
B	1303	GLY	-	expression tag	UNP Q696P8
B	1304	ARG	-	expression tag	UNP Q696P8
B	1305	SER	-	expression tag	UNP Q696P8
B	1306	LEU	-	expression tag	UNP Q696P8
B	1307	GLU	-	expression tag	UNP Q696P8
B	1308	VAL	-	expression tag	UNP Q696P8
B	1309	LEU	-	expression tag	UNP Q696P8
B	1310	PHE	-	expression tag	UNP Q696P8
B	1311	GLN	-	expression tag	UNP Q696P8
B	1312	GLY	-	expression tag	UNP Q696P8
B	1313	PRO	-	expression tag	UNP Q696P8
B	1314	GLY	-	expression tag	UNP Q696P8
B	1315	HIS	-	expression tag	UNP Q696P8
B	1316	HIS	-	expression tag	UNP Q696P8
B	1317	HIS	-	expression tag	UNP Q696P8
B	1318	HIS	-	expression tag	UNP Q696P8
B	1319	HIS	-	expression tag	UNP Q696P8
B	1320	HIS	-	expression tag	UNP Q696P8
B	1321	HIS	-	expression tag	UNP Q696P8
B	1322	HIS	-	expression tag	UNP Q696P8
B	1323	SER	-	expression tag	UNP Q696P8
B	1324	ALA	-	expression tag	UNP Q696P8
B	1325	TRP	-	expression tag	UNP Q696P8
B	1326	SER	-	expression tag	UNP Q696P8
B	1327	HIS	-	expression tag	UNP Q696P8
B	1328	PRO	-	expression tag	UNP Q696P8
B	1329	GLN	-	expression tag	UNP Q696P8
B	1330	PHE	-	expression tag	UNP Q696P8
B	1331	GLU	-	expression tag	UNP Q696P8
B	1332	LYS	-	expression tag	UNP Q696P8
B	1333	GLY	-	expression tag	UNP Q696P8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1334	GLY	-	expression tag	UNP Q696P8
B	1335	GLY	-	expression tag	UNP Q696P8
B	1336	SER	-	expression tag	UNP Q696P8
B	1337	GLY	-	expression tag	UNP Q696P8
B	1338	GLY	-	expression tag	UNP Q696P8
B	1339	GLY	-	expression tag	UNP Q696P8
B	1340	GLY	-	expression tag	UNP Q696P8
B	1341	SER	-	expression tag	UNP Q696P8
B	1342	GLY	-	expression tag	UNP Q696P8
B	1343	GLY	-	expression tag	UNP Q696P8
B	1344	SER	-	expression tag	UNP Q696P8
B	1345	ALA	-	expression tag	UNP Q696P8
B	1346	TRP	-	expression tag	UNP Q696P8
B	1347	SER	-	expression tag	UNP Q696P8
B	1348	HIS	-	expression tag	UNP Q696P8
B	1349	PRO	-	expression tag	UNP Q696P8
B	1350	GLN	-	expression tag	UNP Q696P8
B	1351	PHE	-	expression tag	UNP Q696P8
B	1352	GLU	-	expression tag	UNP Q696P8
B	1353	LYS	-	expression tag	UNP Q696P8
C	-9	MET	-	initiating methionine	UNP Q696P8
C	-8	PRO	-	expression tag	UNP Q696P8
C	-7	MET	-	expression tag	UNP Q696P8
C	-6	GLY	-	expression tag	UNP Q696P8
C	-5	SER	-	expression tag	UNP Q696P8
C	-4	LEU	-	expression tag	UNP Q696P8
C	-3	GLN	-	expression tag	UNP Q696P8
C	-2	PRO	-	expression tag	UNP Q696P8
C	-1	LEU	-	expression tag	UNP Q696P8
C	0	ALA	-	expression tag	UNP Q696P8
C	1	THR	-	expression tag	UNP Q696P8
C	2	LEU	-	expression tag	UNP Q696P8
C	3	TYR	-	expression tag	UNP Q696P8
C	4	LEU	-	expression tag	UNP Q696P8
C	5	LEU	-	expression tag	UNP Q696P8
C	6	GLY	-	expression tag	UNP Q696P8
C	7	MET	-	expression tag	UNP Q696P8
C	8	LEU	-	expression tag	UNP Q696P8
C	9	VAL	-	expression tag	UNP Q696P8
C	10	ALA	-	expression tag	UNP Q696P8
C	11	SER	-	expression tag	UNP Q696P8
C	12	VAL	-	expression tag	UNP Q696P8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	13	LEU	-	expression tag	UNP Q696P8
C	764	GLY	ARG	conflict	UNP Q696P8
C	765	GLY	ARG	conflict	UNP Q696P8
C	767	GLY	ARG	conflict	UNP Q696P8
C	1274	GLY	-	expression tag	UNP Q696P8
C	1275	SER	-	expression tag	UNP Q696P8
C	1276	GLY	-	expression tag	UNP Q696P8
C	1277	TYR	-	expression tag	UNP Q696P8
C	1278	ILE	-	expression tag	UNP Q696P8
C	1279	PRO	-	expression tag	UNP Q696P8
C	1280	GLU	-	expression tag	UNP Q696P8
C	1281	ALA	-	expression tag	UNP Q696P8
C	1282	PRO	-	expression tag	UNP Q696P8
C	1283	ARG	-	expression tag	UNP Q696P8
C	1284	ASP	-	expression tag	UNP Q696P8
C	1285	GLY	-	expression tag	UNP Q696P8
C	1286	GLN	-	expression tag	UNP Q696P8
C	1287	ALA	-	expression tag	UNP Q696P8
C	1288	TYR	-	expression tag	UNP Q696P8
C	1289	VAL	-	expression tag	UNP Q696P8
C	1290	ARG	-	expression tag	UNP Q696P8
C	1291	LYS	-	expression tag	UNP Q696P8
C	1292	ASP	-	expression tag	UNP Q696P8
C	1293	GLY	-	expression tag	UNP Q696P8
C	1294	GLU	-	expression tag	UNP Q696P8
C	1295	TRP	-	expression tag	UNP Q696P8
C	1296	VAL	-	expression tag	UNP Q696P8
C	1297	LEU	-	expression tag	UNP Q696P8
C	1298	LEU	-	expression tag	UNP Q696P8
C	1299	SER	-	expression tag	UNP Q696P8
C	1300	THR	-	expression tag	UNP Q696P8
C	1301	PHE	-	expression tag	UNP Q696P8
C	1302	LEU	-	expression tag	UNP Q696P8
C	1303	GLY	-	expression tag	UNP Q696P8
C	1304	ARG	-	expression tag	UNP Q696P8
C	1305	SER	-	expression tag	UNP Q696P8
C	1306	LEU	-	expression tag	UNP Q696P8
C	1307	GLU	-	expression tag	UNP Q696P8
C	1308	VAL	-	expression tag	UNP Q696P8
C	1309	LEU	-	expression tag	UNP Q696P8
C	1310	PHE	-	expression tag	UNP Q696P8
C	1311	GLN	-	expression tag	UNP Q696P8

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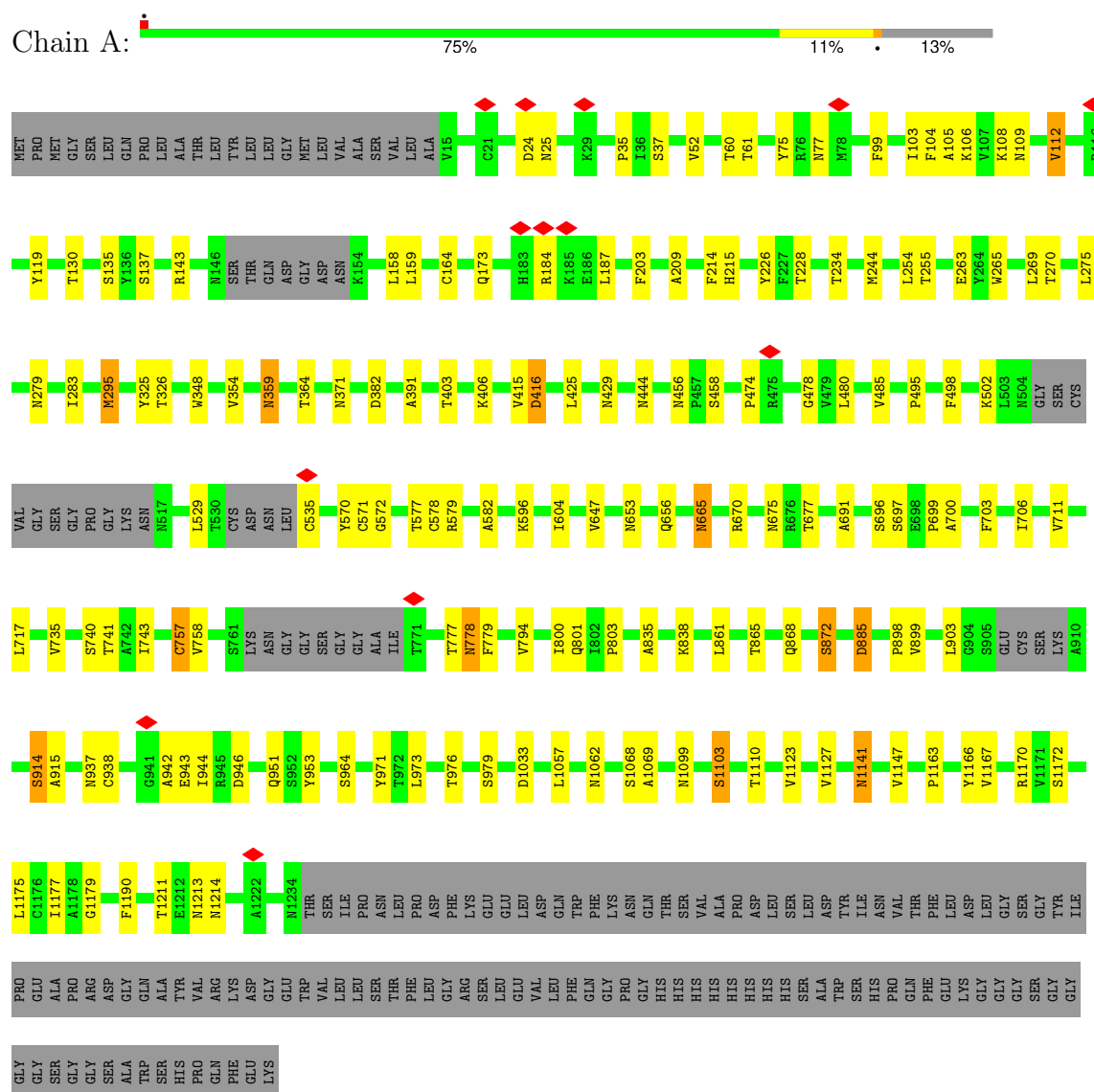
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1312	GLY	-	expression tag	UNP Q696P8
C	1313	PRO	-	expression tag	UNP Q696P8
C	1314	GLY	-	expression tag	UNP Q696P8
C	1315	HIS	-	expression tag	UNP Q696P8
C	1316	HIS	-	expression tag	UNP Q696P8
C	1317	HIS	-	expression tag	UNP Q696P8
C	1318	HIS	-	expression tag	UNP Q696P8
C	1319	HIS	-	expression tag	UNP Q696P8
C	1320	HIS	-	expression tag	UNP Q696P8
C	1321	HIS	-	expression tag	UNP Q696P8
C	1322	HIS	-	expression tag	UNP Q696P8
C	1323	SER	-	expression tag	UNP Q696P8
C	1324	ALA	-	expression tag	UNP Q696P8
C	1325	TRP	-	expression tag	UNP Q696P8
C	1326	SER	-	expression tag	UNP Q696P8
C	1327	HIS	-	expression tag	UNP Q696P8
C	1328	PRO	-	expression tag	UNP Q696P8
C	1329	GLN	-	expression tag	UNP Q696P8
C	1330	PHE	-	expression tag	UNP Q696P8
C	1331	GLU	-	expression tag	UNP Q696P8
C	1332	LYS	-	expression tag	UNP Q696P8
C	1333	GLY	-	expression tag	UNP Q696P8
C	1334	GLY	-	expression tag	UNP Q696P8
C	1335	GLY	-	expression tag	UNP Q696P8
C	1336	SER	-	expression tag	UNP Q696P8
C	1337	GLY	-	expression tag	UNP Q696P8
C	1338	GLY	-	expression tag	UNP Q696P8
C	1339	GLY	-	expression tag	UNP Q696P8
C	1340	GLY	-	expression tag	UNP Q696P8
C	1341	SER	-	expression tag	UNP Q696P8
C	1342	GLY	-	expression tag	UNP Q696P8
C	1343	GLY	-	expression tag	UNP Q696P8
C	1344	SER	-	expression tag	UNP Q696P8
C	1345	ALA	-	expression tag	UNP Q696P8
C	1346	TRP	-	expression tag	UNP Q696P8
C	1347	SER	-	expression tag	UNP Q696P8
C	1348	HIS	-	expression tag	UNP Q696P8
C	1349	PRO	-	expression tag	UNP Q696P8
C	1350	GLN	-	expression tag	UNP Q696P8
C	1351	PHE	-	expression tag	UNP Q696P8
C	1352	GLU	-	expression tag	UNP Q696P8
C	1353	LYS	-	expression tag	UNP Q696P8

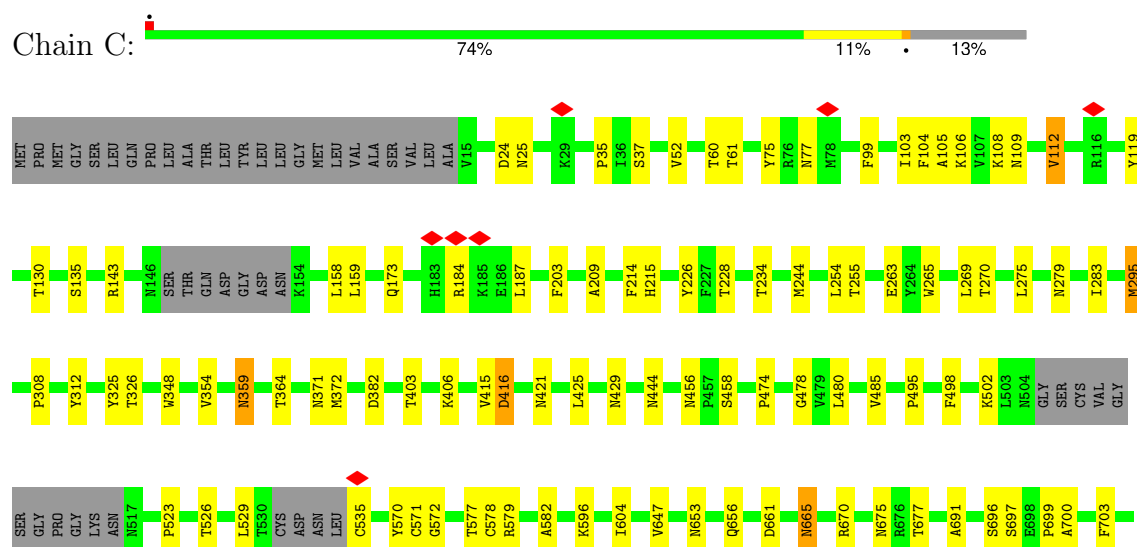
3 Residue-property plots

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: Spike glycoprotein



• Molecule 1: Spike glycoprotein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	195202	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS TUNDRA	Depositor
Voltage (kV)	100	Depositor
Electron dose ($e^-/\text{\AA}^2$)	26.75	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI CETA (4k x 4k)	Depositor
Maximum map value	1.036	Depositor
Minimum map value	-0.586	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.221	Depositor
Map size (Å)	304.0, 304.0, 304.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.76, 0.76, 0.76	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	0.13	0/9359	0.34	0/12744
1	B	0.13	0/9359	0.34	0/12744
1	C	0.13	0/9359	0.34	0/12744
All	All	0.13	0/28077	0.34	0/38232

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9150	0	8863	76	0
1	B	9150	0	8863	79	0
1	C	9150	0	8863	83	0
All	All	27450	0	26589	234	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 (234) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:HIS:HB2	1:A:226:TYR:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:HIS:HB2	1:C:226:TYR:HB2	1.77	0.66
1:B:215:HIS:HB2	1:B:226:TYR:HB2	1.77	0.66
1:C:570:TYR:HB3	1:C:579:ARG:HB2	1.79	0.64
1:B:570:TYR:HB3	1:B:579:ARG:HB2	1.79	0.63
1:A:570:TYR:HB3	1:A:579:ARG:HB2	1.79	0.62
1:B:937:ASN:HB3	1:B:942:ALA:HB2	1.82	0.62
1:C:570:TYR:HA	1:C:579:ARG:HH21	1.65	0.62
1:A:937:ASN:HB3	1:A:942:ALA:HB2	1.82	0.61
1:C:937:ASN:HB3	1:C:942:ALA:HB2	1.82	0.61
1:B:570:TYR:HA	1:B:579:ARG:HH21	1.65	0.61
1:A:570:TYR:HA	1:A:579:ARG:HH21	1.65	0.61
1:B:130:THR:HG1	1:B:135:SER:HG	1.52	0.56
1:A:130:THR:HG1	1:A:135:SER:HG	1.52	0.56
1:A:159:LEU:HB2	1:A:203:PHE:HB2	1.88	0.56
1:A:778:ASN:OD1	1:A:778:ASN:N	2.39	0.55
1:B:159:LEU:HB2	1:B:203:PHE:HB2	1.88	0.55
1:B:778:ASN:N	1:B:778:ASN:OD1	2.39	0.55
1:C:159:LEU:HB2	1:C:203:PHE:HB2	1.89	0.55
1:A:570:TYR:HB2	1:A:582:ALA:HB2	1.89	0.54
1:B:295:MET:HB2	1:B:699:PRO:HD3	1.89	0.54
1:C:778:ASN:OD1	1:C:778:ASN:N	2.39	0.54
1:A:24:ASP:O	1:A:184:ARG:NH2	2.40	0.54
1:C:24:ASP:O	1:C:184:ARG:NH2	2.40	0.54
1:B:835:ALA:HA	1:B:838:LYS:HD2	1.90	0.54
1:B:943:GLU:HB3	1:B:946:ASP:HB2	1.90	0.54
1:A:835:ALA:HA	1:A:838:LYS:HD2	1.90	0.54
1:B:570:TYR:HB2	1:B:582:ALA:HB2	1.89	0.54
1:C:570:TYR:HB2	1:C:582:ALA:HB2	1.89	0.53
1:C:943:GLU:HB3	1:C:946:ASP:HB2	1.90	0.53
1:C:495:PRO:HG2	1:C:498:PHE:HB2	1.90	0.53
1:A:943:GLU:HB3	1:A:946:ASP:HB2	1.90	0.53
1:C:295:MET:HB2	1:C:699:PRO:HD3	1.89	0.53
1:C:835:ALA:HA	1:C:838:LYS:HD2	1.90	0.53
1:B:24:ASP:O	1:B:184:ARG:NH2	2.40	0.53
1:B:794:VAL:O	1:B:1170:ARG:NH2	2.42	0.53
1:A:35:PRO:HD2	1:A:77:ASN:HB3	1.91	0.53
1:A:295:MET:HB2	1:A:699:PRO:HD3	1.89	0.53
1:A:495:PRO:HG2	1:A:498:PHE:HB2	1.90	0.53
1:B:495:PRO:HG2	1:B:498:PHE:HB2	1.90	0.53
1:C:35:PRO:HD2	1:C:77:ASN:HB3	1.91	0.52
1:A:794:VAL:O	1:A:1170:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:PRO:HD2	1:B:77:ASN:HB3	1.91	0.52
1:A:971:TYR:OH	1:C:780:GLU:OE2	2.26	0.52
1:C:794:VAL:O	1:C:1170:ARG:NH2	2.42	0.52
1:A:106:LYS:HB3	1:A:265:TRP:HB2	1.92	0.52
1:A:757:CYS:SG	1:A:758:VAL:N	2.83	0.52
1:B:757:CYS:SG	1:B:758:VAL:N	2.83	0.52
1:B:416:ASP:OD1	1:B:416:ASP:N	2.42	0.52
1:B:106:LYS:HB3	1:B:265:TRP:HB2	1.92	0.52
1:A:868:GLN:O	1:A:872:SER:OG	2.28	0.51
1:B:359:ASN:OD1	1:B:359:ASN:N	2.43	0.51
1:B:703:PHE:HB3	1:B:706:ILE:HD12	1.92	0.51
1:B:403:THR:HB	1:B:604:ILE:HB	1.92	0.51
1:C:403:THR:HB	1:C:604:ILE:HB	1.92	0.51
1:C:416:ASP:OD1	1:C:416:ASP:N	2.42	0.51
1:C:359:ASN:N	1:C:359:ASN:OD1	2.43	0.51
1:C:703:PHE:HB3	1:C:706:ILE:HD12	1.92	0.51
1:B:868:GLN:O	1:B:872:SER:OG	2.28	0.51
1:C:757:CYS:SG	1:C:758:VAL:N	2.83	0.51
1:A:359:ASN:OD1	1:A:359:ASN:N	2.43	0.51
1:A:703:PHE:HB3	1:A:706:ILE:HD12	1.92	0.51
1:C:868:GLN:O	1:C:872:SER:OG	2.28	0.51
1:B:456:ASN:HD21	1:B:458:SER:HB3	1.77	0.50
1:C:106:LYS:HB3	1:C:265:TRP:HB2	1.92	0.50
1:C:348:TRP:O	1:C:406:LYS:NZ	2.45	0.50
1:A:403:THR:HB	1:A:604:ILE:HB	1.93	0.50
1:A:898:PRO:HA	1:A:915:ALA:HB3	1.94	0.50
1:A:348:TRP:O	1:A:406:LYS:NZ	2.45	0.50
1:C:104:PHE:HB2	1:C:269:LEU:HD21	1.94	0.49
1:A:184:ARG:HB2	1:A:255:THR:HG21	1.95	0.49
1:B:104:PHE:HB2	1:B:269:LEU:HD21	1.94	0.49
1:C:898:PRO:HA	1:C:915:ALA:HB3	1.94	0.49
1:A:104:PHE:HB2	1:A:269:LEU:HD21	1.94	0.49
1:C:571:CYS:HA	1:C:578:CYS:HA	1.95	0.49
1:B:571:CYS:HA	1:B:578:CYS:HA	1.95	0.49
1:C:184:ARG:HB2	1:C:255:THR:HG21	1.94	0.49
1:B:898:PRO:HA	1:B:915:ALA:HB3	1.94	0.49
1:B:173:GLN:HE22	1:B:184:ARG:HB3	1.78	0.49
1:A:456:ASN:HD21	1:A:458:SER:HB3	1.77	0.49
1:A:571:CYS:HA	1:A:578:CYS:HA	1.95	0.48
1:A:416:ASP:N	1:A:416:ASP:OD1	2.42	0.48
1:B:184:ARG:HB2	1:B:255:THR:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:ASN:HB3	1:A:596:LYS:HB3	1.95	0.48
1:C:456:ASN:HD21	1:C:458:SER:HB3	1.77	0.48
1:C:173:GLN:HE22	1:C:184:ARG:HB3	1.78	0.48
1:A:1099:ASN:O	1:A:1103:SER:OG	2.31	0.48
1:A:173:GLN:HE22	1:A:184:ARG:HB3	1.78	0.48
1:B:444:ASN:HB3	1:B:596:LYS:HB3	1.95	0.48
1:B:61:THR:HB	1:B:275:LEU:HD11	1.96	0.48
1:B:348:TRP:O	1:B:406:LYS:NZ	2.45	0.48
1:C:1172:SER:HB3	1:C:1190:PHE:HB2	1.96	0.48
1:A:647:VAL:O	1:A:677:THR:OG1	2.32	0.48
1:B:1099:ASN:O	1:B:1103:SER:OG	2.31	0.48
1:B:938:CYS:O	1:B:953:TYR:OH	2.33	0.47
1:A:1123:VAL:O	1:A:1127:VAL:HB	2.15	0.47
1:A:1172:SER:HB3	1:A:1190:PHE:HB2	1.96	0.47
1:C:803:PRO:HB3	1:C:1163:PRO:HB3	1.97	0.47
1:A:425:LEU:HA	1:A:429:ASN:HD22	1.79	0.47
1:C:61:THR:HB	1:C:275:LEU:HD11	1.96	0.47
1:C:647:VAL:O	1:C:677:THR:OG1	2.32	0.47
1:C:444:ASN:HB3	1:C:596:LYS:HB3	1.95	0.47
1:C:938:CYS:O	1:C:953:TYR:OH	2.33	0.47
1:C:1099:ASN:O	1:C:1103:SER:OG	2.31	0.47
1:A:938:CYS:O	1:A:953:TYR:OH	2.33	0.47
1:A:61:THR:HB	1:A:275:LEU:HD11	1.96	0.47
1:B:109:ASN:ND2	1:B:209:ALA:O	2.43	0.47
1:B:647:VAL:O	1:B:677:THR:OG1	2.32	0.47
1:B:1172:SER:HB3	1:B:1190:PHE:HB2	1.96	0.47
1:B:112:VAL:HG13	1:B:119:TYR:HB2	1.97	0.47
1:B:1177:ILE:HG13	1:B:1179:GLY:H	1.80	0.46
1:C:425:LEU:HA	1:C:429:ASN:HD22	1.79	0.46
1:C:1123:VAL:O	1:C:1127:VAL:HB	2.15	0.46
1:A:60:THR:OG1	1:A:61:THR:N	2.48	0.46
1:B:60:THR:OG1	1:B:61:THR:N	2.48	0.46
1:B:502:LYS:HG2	1:B:529:LEU:HB2	1.98	0.46
1:C:885:ASP:OD1	1:C:885:ASP:N	2.49	0.46
1:B:425:LEU:HA	1:B:429:ASN:HD22	1.79	0.46
1:B:803:PRO:HB3	1:B:1163:PRO:HB3	1.97	0.46
1:C:228:THR:HB	1:C:234:THR:HA	1.97	0.46
1:A:803:PRO:HB3	1:A:1163:PRO:HB3	1.97	0.46
1:B:474:PRO:O	1:B:478:GLY:N	2.42	0.46
1:B:228:THR:HB	1:B:234:THR:HA	1.97	0.46
1:A:228:THR:HB	1:A:234:THR:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:VAL:HG13	1:C:119:TYR:HB2	1.98	0.46
1:A:109:ASN:ND2	1:A:209:ALA:O	2.43	0.46
1:A:1177:ILE:HG13	1:A:1179:GLY:H	1.80	0.46
1:B:108:LYS:HB3	1:B:263:GLU:HB2	1.98	0.46
1:B:1123:VAL:O	1:B:1127:VAL:HB	2.15	0.46
1:A:112:VAL:HG13	1:A:119:TYR:HB2	1.98	0.45
1:B:653:ASN:H	1:B:656:GLN:HB2	1.82	0.45
1:C:1177:ILE:HG13	1:C:1179:GLY:H	1.80	0.45
1:C:108:LYS:HB3	1:C:263:GLU:HB2	1.99	0.45
1:C:502:LYS:HG2	1:C:529:LEU:HB2	1.98	0.45
1:A:108:LYS:HB3	1:A:263:GLU:HB2	1.98	0.45
1:A:665:ASN:OD1	1:A:665:ASN:N	2.50	0.45
1:A:502:LYS:HG2	1:A:529:LEU:HB2	1.98	0.45
1:A:653:ASN:H	1:A:656:GLN:HB2	1.82	0.45
1:A:885:ASP:N	1:A:885:ASP:OD1	2.48	0.45
1:C:60:THR:OG1	1:C:61:THR:N	2.48	0.45
1:C:757:CYS:HB3	1:C:779:PHE:HB2	1.99	0.45
1:A:279:ASN:OD1	1:A:283:ILE:N	2.45	0.45
1:B:665:ASN:N	1:B:665:ASN:OD1	2.50	0.44
1:B:757:CYS:HB3	1:B:779:PHE:HB2	1.99	0.44
1:B:653:ASN:ND2	1:B:656:GLN:OE1	2.50	0.44
1:C:653:ASN:H	1:C:656:GLN:HB2	1.82	0.44
1:B:885:ASP:OD1	1:B:885:ASP:N	2.48	0.44
1:C:572:GLY:O	1:C:577:THR:N	2.51	0.44
1:A:572:GLY:O	1:A:577:THR:N	2.51	0.44
1:C:308:PRO:O	1:C:312:TYR:OH	2.34	0.44
1:C:696:SER:OG	1:C:697:SER:N	2.51	0.44
1:C:740:SER:HB3	1:C:743:ILE:HD12	1.99	0.44
1:A:740:SER:HB3	1:A:743:ILE:HD12	1.99	0.44
1:B:572:GLY:O	1:B:577:THR:N	2.51	0.44
1:B:661:ASP:OD1	1:B:665:ASN:N	2.38	0.44
1:B:691:ALA:HB3	1:B:700:ALA:HB3	2.00	0.44
1:A:696:SER:OG	1:A:697:SER:N	2.51	0.44
1:A:391:ALA:HB3	1:C:421:ASN:HA	2.00	0.44
1:B:653:ASN:O	1:B:670:ARG:NH2	2.42	0.44
1:B:1142:HIS:NE2	1:B:1145:SER:OG	2.46	0.44
1:A:711:VAL:HG13	1:A:717:LEU:HB2	2.00	0.44
1:B:711:VAL:HG13	1:B:717:LEU:HB2	2.00	0.44
1:B:898:PRO:O	1:B:914:SER:OG	2.30	0.44
1:A:800:ILE:HD11	1:B:983:PRO:HB3	2.00	0.43
1:B:696:SER:OG	1:B:697:SER:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:PHE:HE1	1:A:103:ILE:HG12	1.84	0.43
1:A:757:CYS:HB3	1:A:779:PHE:HB2	1.99	0.43
1:A:474:PRO:O	1:A:478:GLY:N	2.42	0.43
1:C:109:ASN:ND2	1:C:209:ALA:O	2.43	0.43
1:C:425:LEU:HA	1:C:429:ASN:ND2	2.34	0.43
1:B:740:SER:HB3	1:B:743:ILE:HD12	1.99	0.43
1:C:711:VAL:HG13	1:C:717:LEU:HB2	2.00	0.43
1:A:425:LEU:HA	1:A:429:ASN:ND2	2.34	0.43
1:B:928:ASP:OD1	1:B:928:ASP:N	2.52	0.43
1:B:37:SER:OG	1:B:75:TYR:N	2.51	0.43
1:A:691:ALA:HB3	1:A:700:ALA:HB3	2.00	0.42
1:C:474:PRO:O	1:C:478:GLY:N	2.42	0.42
1:C:691:ALA:HB3	1:C:700:ALA:HB3	2.00	0.42
1:A:898:PRO:O	1:A:914:SER:OG	2.30	0.42
1:B:99:PHE:HE1	1:B:103:ILE:HG12	1.84	0.42
1:C:928:ASP:OD1	1:C:928:ASP:N	2.52	0.42
1:B:1211:THR:HG23	1:B:1213:ASN:H	1.84	0.42
1:C:665:ASN:OD1	1:C:665:ASN:N	2.50	0.42
1:C:914:SER:O	1:C:918:ASP:N	2.48	0.42
1:C:1142:HIS:NE2	1:C:1145:SER:OG	2.46	0.42
1:A:37:SER:OG	1:A:75:TYR:N	2.51	0.42
1:C:279:ASN:OD1	1:C:283:ILE:N	2.45	0.42
1:C:99:PHE:HE1	1:C:103:ILE:HG12	1.84	0.42
1:A:653:ASN:ND2	1:A:656:GLN:OE1	2.50	0.42
1:B:425:LEU:HA	1:B:429:ASN:ND2	2.34	0.42
1:C:1211:THR:HG23	1:C:1213:ASN:H	1.84	0.42
1:C:898:PRO:O	1:C:914:SER:OG	2.30	0.42
1:C:143:ARG:HB2	1:C:158:LEU:HB2	2.02	0.42
1:A:801:GLN:HB3	1:A:1166:TYR:HB3	2.02	0.42
1:B:1068:SER:OG	1:B:1069:ALA:N	2.53	0.42
1:C:895:ASN:OD1	1:C:897:SER:OG	2.32	0.42
1:B:279:ASN:OD1	1:B:283:ILE:N	2.45	0.41
1:A:1068:SER:OG	1:A:1069:ALA:N	2.53	0.41
1:C:653:ASN:O	1:C:670:ARG:NH2	2.42	0.41
1:C:801:GLN:HB3	1:C:1166:TYR:HB3	2.02	0.41
1:C:951:GLN:HG3	1:C:1057:LEU:HD22	2.02	0.41
1:A:143:ARG:HB2	1:A:158:LEU:HB2	2.02	0.41
1:A:656:GLN:O	1:A:670:ARG:NH2	2.54	0.41
1:A:1211:THR:HG23	1:A:1213:ASN:H	1.84	0.41
1:B:308:PRO:O	1:B:312:TYR:OH	2.34	0.41
1:C:37:SER:OG	1:C:75:TYR:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:661:ASP:OD1	1:C:665:ASN:N	2.38	0.41
1:A:474:PRO:HA	1:A:480:LEU:HB2	2.03	0.41
1:A:1141:ASN:OD1	1:A:1141:ASN:N	2.54	0.41
1:B:656:GLN:O	1:B:670:ARG:NH2	2.54	0.41
1:C:709:ASN:OD1	1:C:709:ASN:N	2.54	0.41
1:C:523:PRO:O	1:C:526:THR:OG1	2.38	0.41
1:C:656:GLN:O	1:C:670:ARG:NH2	2.54	0.41
1:A:861:LEU:O	1:A:865:THR:OG1	2.34	0.41
1:A:951:GLN:HG3	1:A:1057:LEU:HD22	2.02	0.41
1:B:474:PRO:HA	1:B:480:LEU:HB2	2.03	0.41
1:B:705:ASN:HD21	1:C:932:VAL:HG13	1.86	0.41
1:C:105:ALA:HB3	1:C:214:PHE:HB2	2.02	0.41
1:A:25:ASN:HB2	1:A:184:ARG:HH21	1.86	0.41
1:A:105:ALA:HB3	1:A:214:PHE:HB2	2.02	0.41
1:B:1131:SER:OG	1:B:1132:SER:N	2.54	0.41
1:C:130:THR:OG1	1:C:135:SER:OG	2.39	0.41
1:A:137:SER:N	1:A:164:CYS:O	2.55	0.40
1:B:951:GLN:HG3	1:B:1057:LEU:HD22	2.02	0.40
1:C:25:ASN:HB2	1:C:184:ARG:HH21	1.87	0.40
1:B:801:GLN:HB3	1:B:1166:TYR:HB3	2.02	0.40
1:C:372:MET:HE3	1:C:372:MET:HB3	1.98	0.40
1:C:474:PRO:HA	1:C:480:LEU:HB2	2.03	0.40
1:B:105:ALA:HB3	1:B:214:PHE:HB2	2.02	0.40
1:B:143:ARG:HB2	1:B:158:LEU:HB2	2.02	0.40
1:B:1141:ASN:OD1	1:B:1141:ASN:N	2.54	0.40
1:B:25:ASN:HB2	1:B:184:ARG:HH21	1.86	0.40
1:C:1141:ASN:OD1	1:C:1141:ASN:N	2.54	0.40
1:C:1106:LEU:O	1:C:1110:THR:OG1	2.39	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	1163/1353 (86%)	1123 (97%)	40 (3%)	0	100	100
1	B	1163/1353 (86%)	1123 (97%)	40 (3%)	0	100	100
1	C	1163/1353 (86%)	1123 (97%)	40 (3%)	0	100	100
All	All	3489/4059 (86%)	3369 (97%)	120 (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	1022/1164 (88%)	978 (96%)	44 (4%)	26	48
1	B	1022/1164 (88%)	978 (96%)	44 (4%)	26	48
1	C	1022/1164 (88%)	978 (96%)	44 (4%)	26	48
All	All	3066/3492 (88%)	2934 (96%)	132 (4%)	27	48

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	A	112	VAL
1	A	187	LEU
1	A	244	MET
1	A	254	LEU
1	A	270	THR
1	A	295	MET
1	A	325	TYR
1	A	326	THR
1	A	354	VAL
1	A	359	ASN
1	A	364	THR
1	A	371	ASN
1	A	382	ASP
1	A	415	VAL

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Mol	Chain	Res	Type
1	A	416	ASP
1	A	485	VAL
1	A	535	CYS
1	A	665	ASN
1	A	675	ASN
1	A	735	VAL
1	A	741	THR
1	A	757	CYS
1	A	777	THR
1	A	778	ASN
1	A	872	SER
1	A	885	ASP
1	A	899	VAL
1	A	903	LEU
1	A	914	SER
1	A	944	ILE
1	A	964	SER
1	A	973	LEU
1	A	976	THR
1	A	979	SER
1	A	1033	ASP
1	A	1062	ASN
1	A	1103	SER
1	A	1110	THR
1	A	1141	ASN
1	A	1147	VAL
1	A	1167	VAL
1	A	1175	LEU
1	A	1214	ASN
1	B	52	VAL
1	B	112	VAL
1	B	187	LEU
1	B	244	MET
1	B	254	LEU
1	B	270	THR
1	B	295	MET
1	B	325	TYR
1	B	326	THR
1	B	354	VAL
1	B	359	ASN
1	B	364	THR
1	B	371	ASN

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Mol	Chain	Res	Type
1	B	382	ASP
1	B	415	VAL
1	B	416	ASP
1	B	485	VAL
1	B	535	CYS
1	B	665	ASN
1	B	675	ASN
1	B	735	VAL
1	B	741	THR
1	B	757	CYS
1	B	777	THR
1	B	778	ASN
1	B	872	SER
1	B	885	ASP
1	B	899	VAL
1	B	903	LEU
1	B	914	SER
1	B	944	ILE
1	B	964	SER
1	B	973	LEU
1	B	976	THR
1	B	979	SER
1	B	1033	ASP
1	B	1062	ASN
1	B	1103	SER
1	B	1110	THR
1	B	1141	ASN
1	B	1147	VAL
1	B	1167	VAL
1	B	1175	LEU
1	B	1214	ASN
1	C	52	VAL
1	C	112	VAL
1	C	187	LEU
1	C	244	MET
1	C	254	LEU
1	C	270	THR
1	C	295	MET
1	C	325	TYR
1	C	326	THR
1	C	354	VAL
1	C	359	ASN

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Mol	Chain	Res	Type
1	C	364	THR
1	C	371	ASN
1	C	382	ASP
1	C	415	VAL
1	C	416	ASP
1	C	485	VAL
1	C	535	CYS
1	C	665	ASN
1	C	675	ASN
1	C	735	VAL
1	C	741	THR
1	C	757	CYS
1	C	777	THR
1	C	778	ASN
1	C	872	SER
1	C	885	ASP
1	C	899	VAL
1	C	903	LEU
1	C	914	SER
1	C	944	ILE
1	C	964	SER
1	C	973	LEU
1	C	976	THR
1	C	979	SER
1	C	1033	ASP
1	C	1062	ASN
1	C	1103	SER
1	C	1110	THR
1	C	1141	ASN
1	C	1147	VAL
1	C	1167	VAL
1	C	1175	LEU
1	C	1214	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	344	ASN
1	A	456	ASN
1	A	890	ASN
1	A	1001	ASN
1	A	1086	GLN

Continued on next page...

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Mol	Chain	Res	Type
1	A	1148	GLN
1	B	344	ASN
1	B	456	ASN
1	B	871	ASN
1	B	890	ASN
1	B	1086	GLN
1	B	1148	GLN
1	C	344	ASN
1	C	456	ASN
1	C	705	ASN
1	C	785	ASN
1	C	871	ASN
1	C	875	ASN
1	C	890	ASN
1	C	1001	ASN
1	C	1086	GLN
1	C	1148	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 ⓘ

There are no chain breaks in this entry.

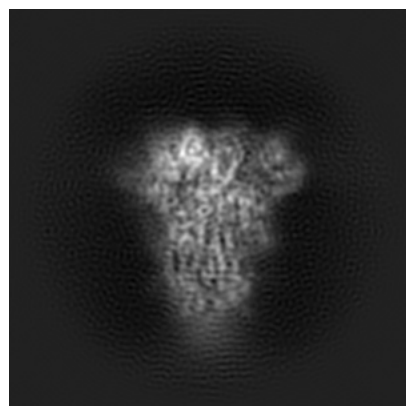
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72507. These allow visual inspection of the internal detail of the map and identification of artifacts.

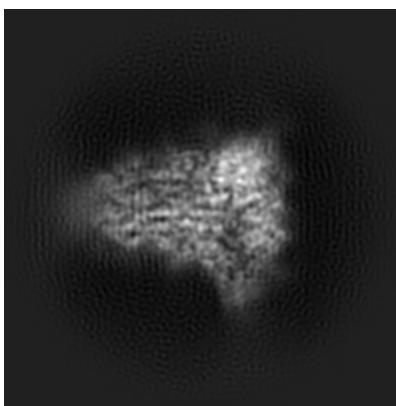
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

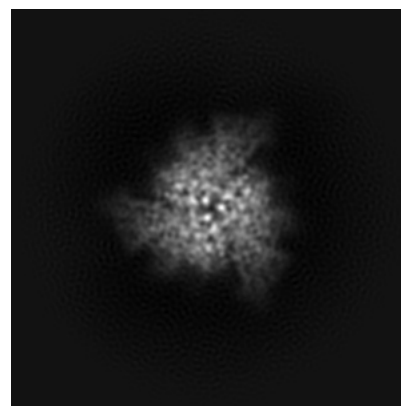
6.1.1 Primary map



X

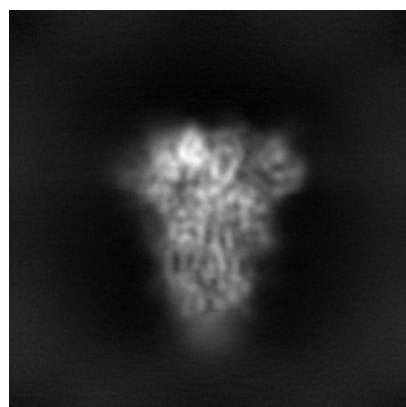


Y

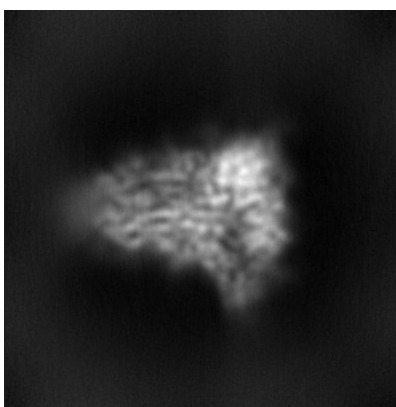


Z

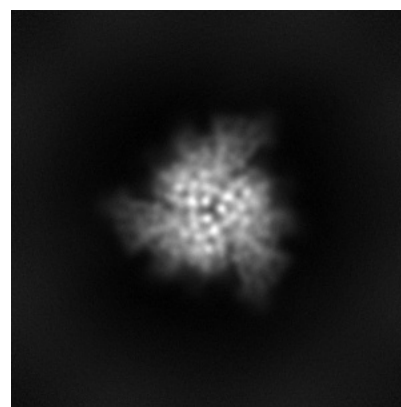
6.1.2 Raw map



X



Y

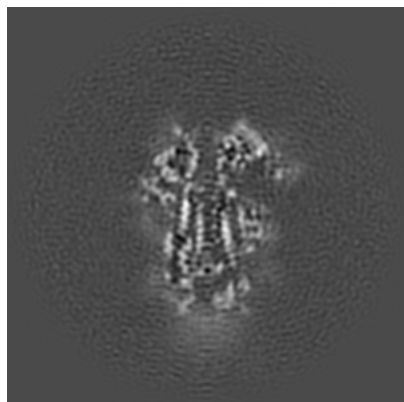


Z

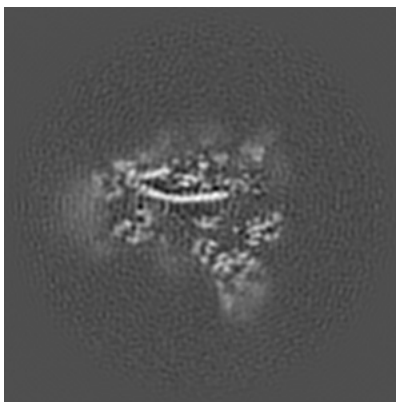
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

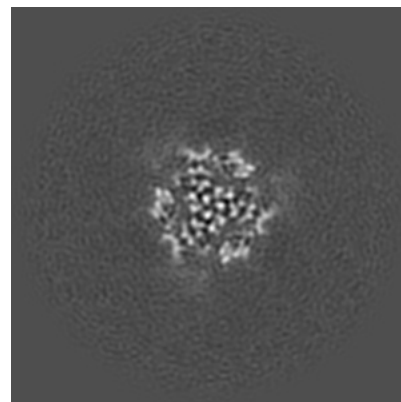
6.2.1 Primary map



X Index: 200

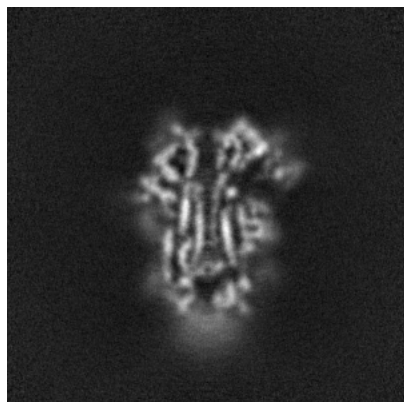


Y Index: 200

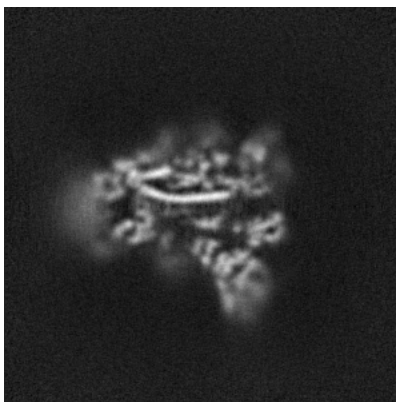


Z Index: 200

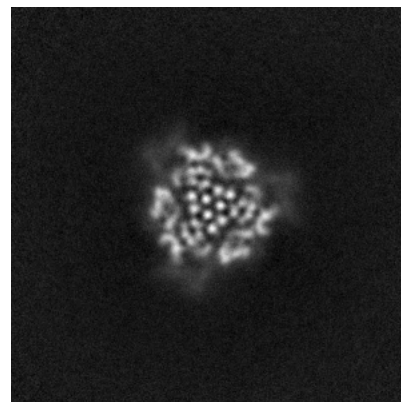
6.2.2 Raw map



X Index: 200



Y Index: 200

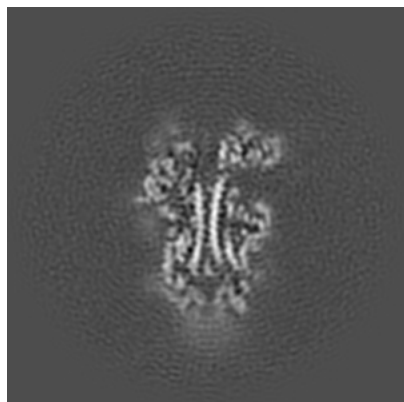


Z Index: 200

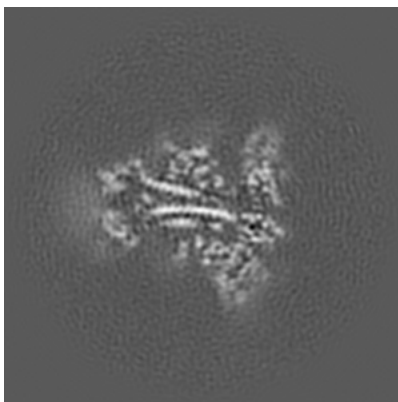
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

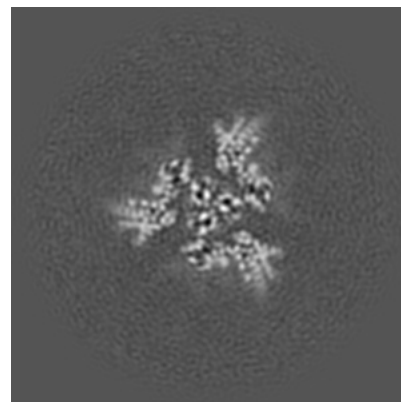
6.3.1 Primary map



X Index: 195

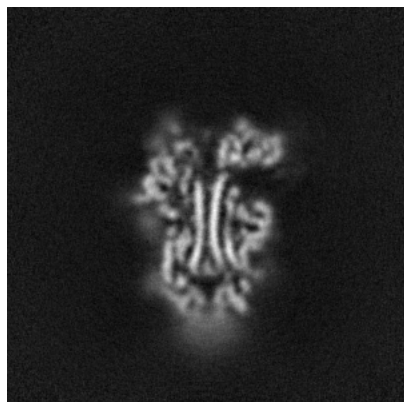


Y Index: 191

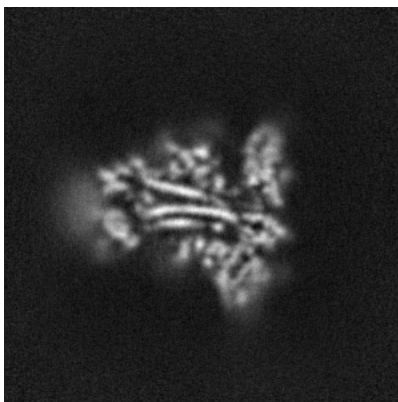


Z Index: 218

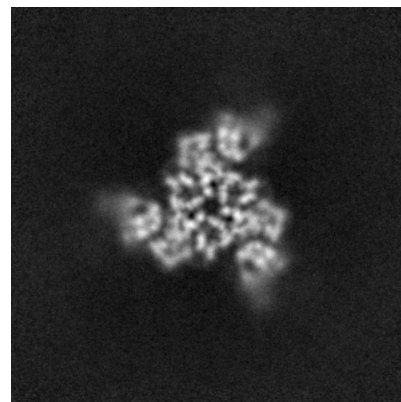
6.3.2 Raw map



X Index: 195



Y Index: 190

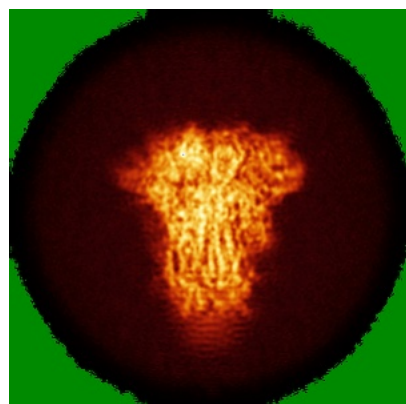


Z Index: 250

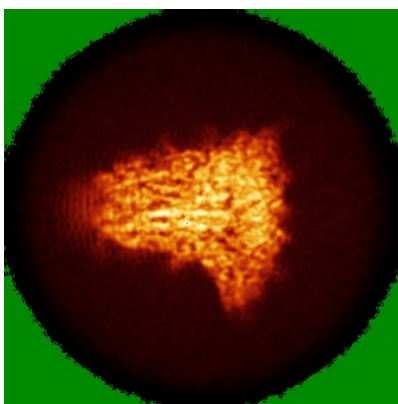
The images above show the largest variance slices of the map in three orthogonal directions.

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

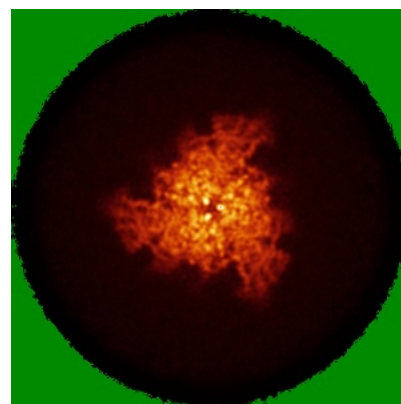
6.4.1 Primary map



X

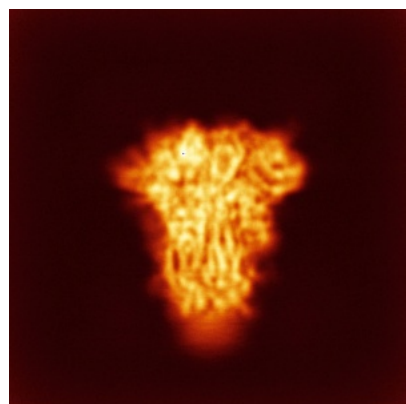


Y

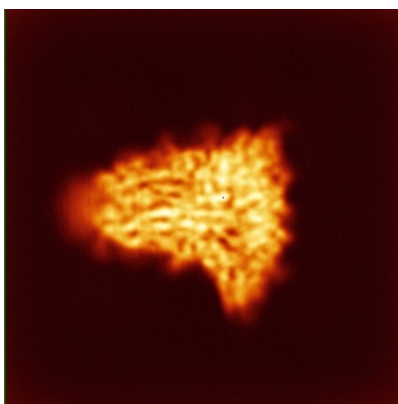


Z

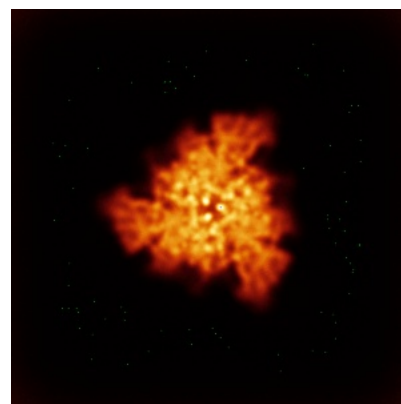
6.4.2 Raw map



X



Y

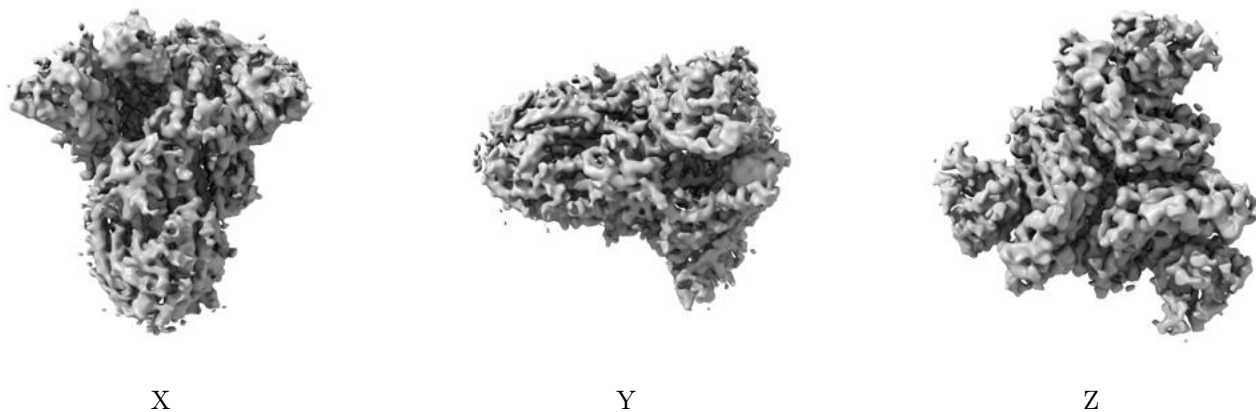


Z

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.

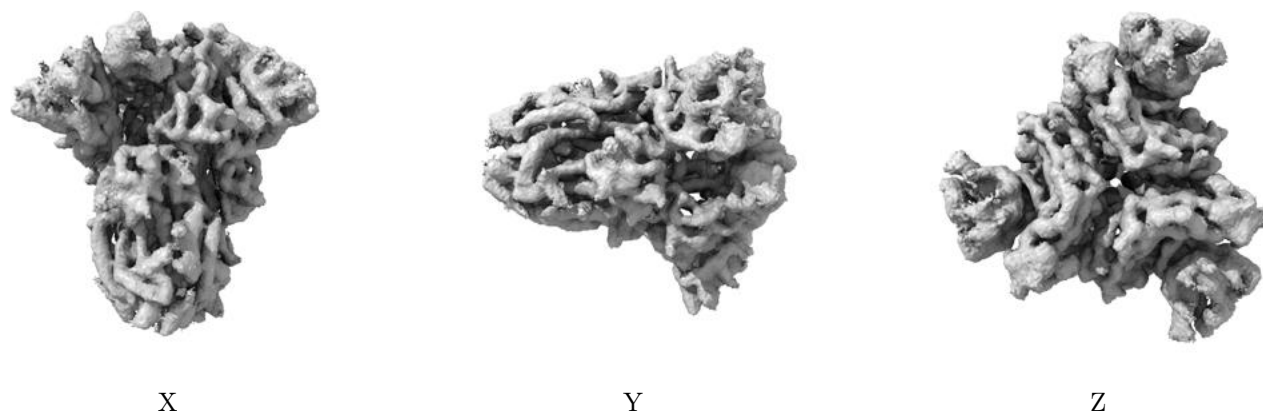
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.221. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

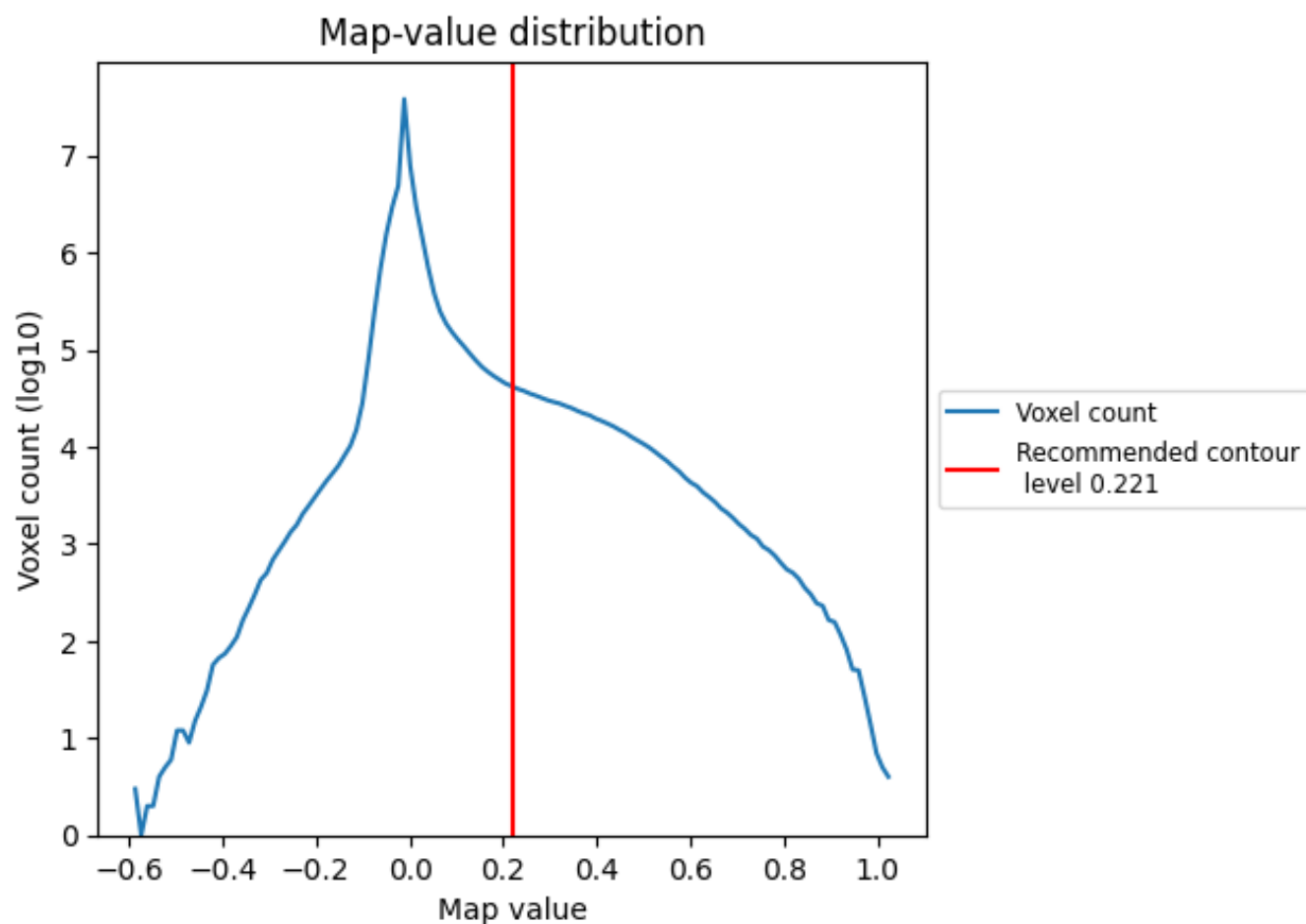
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

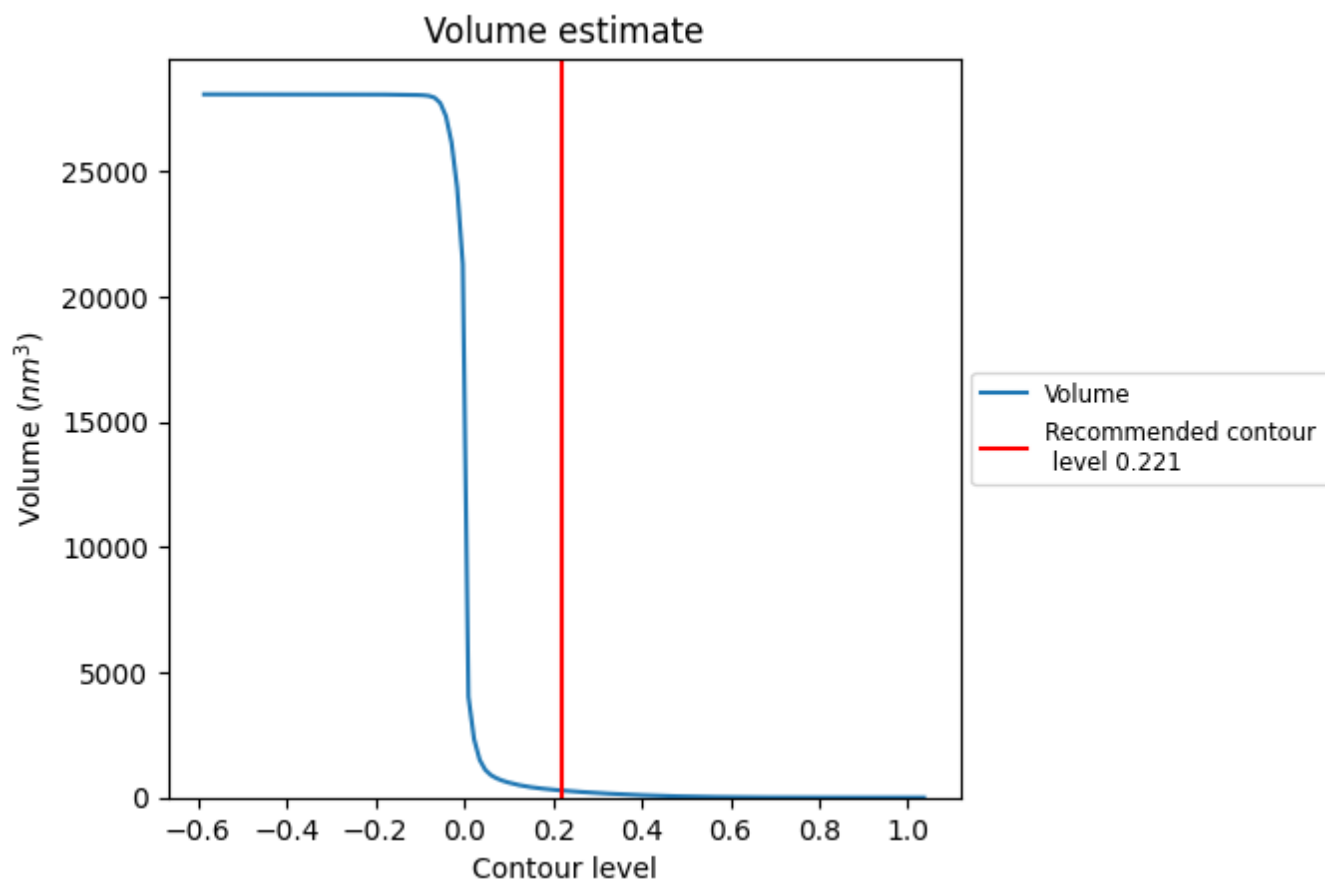
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

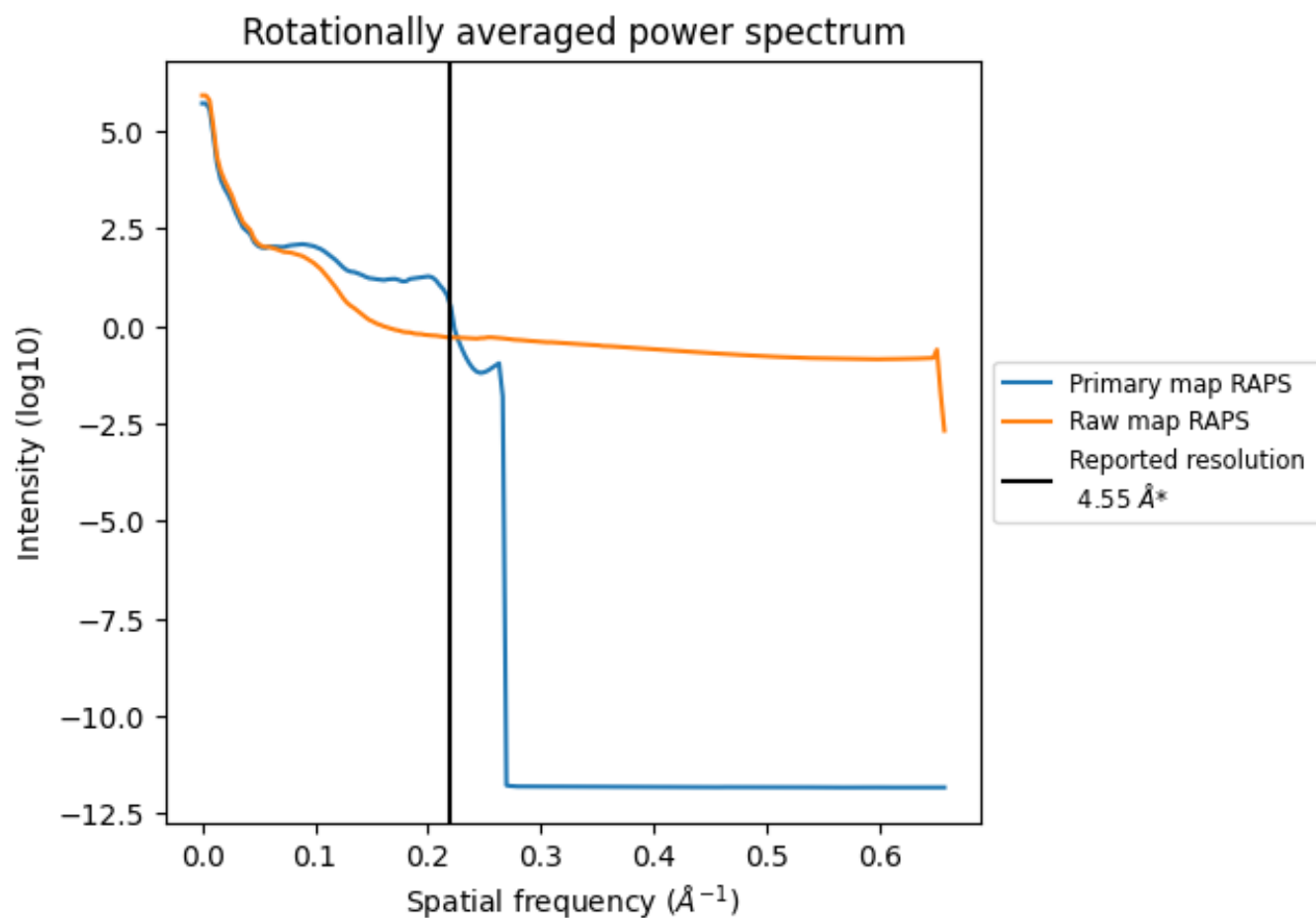
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 281 nm³; this corresponds to an approximate mass of 254 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 ⓘ

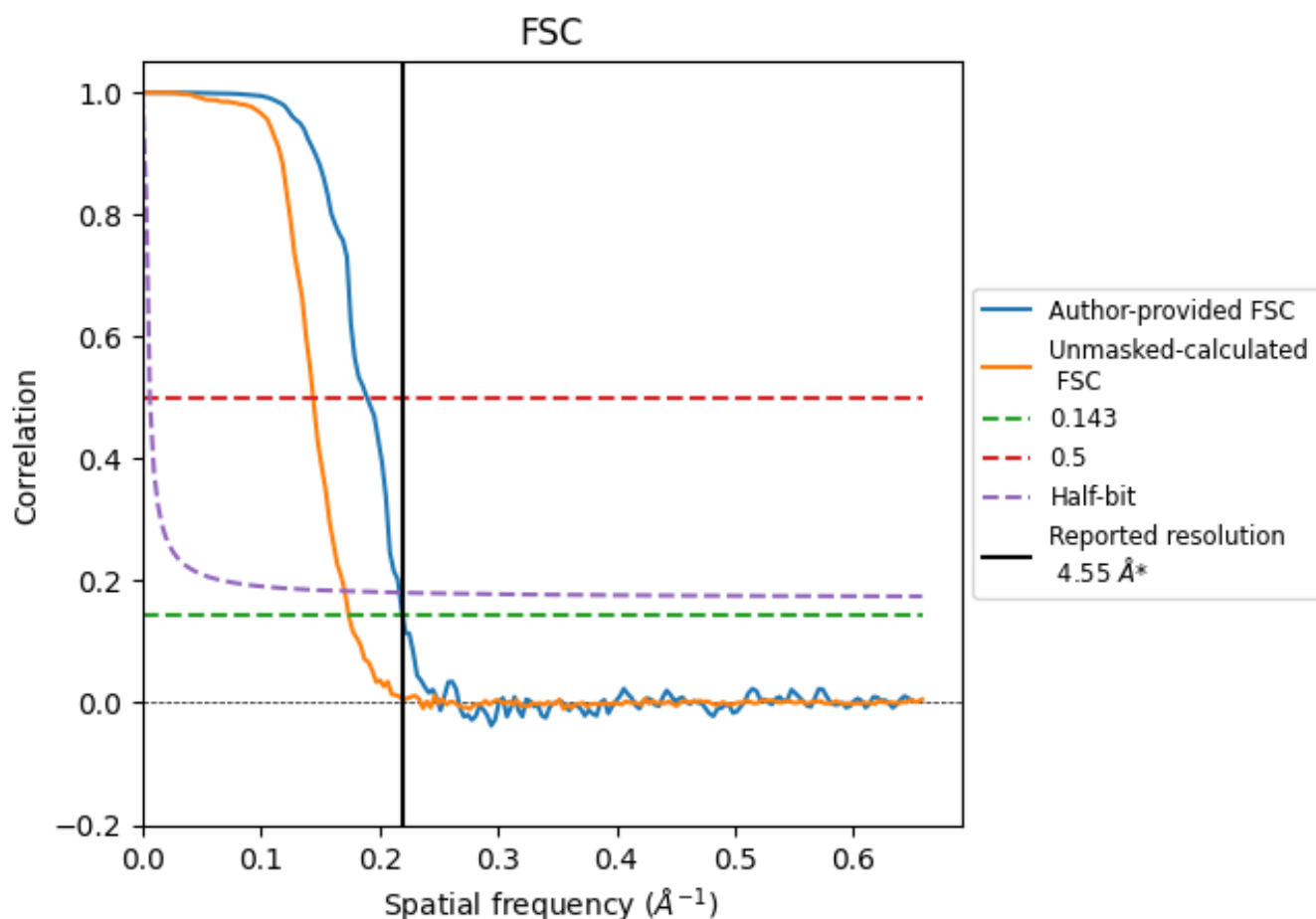


*Reported resolution corresponds to spatial frequency of 0.220 Å⁻¹

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 0.220 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

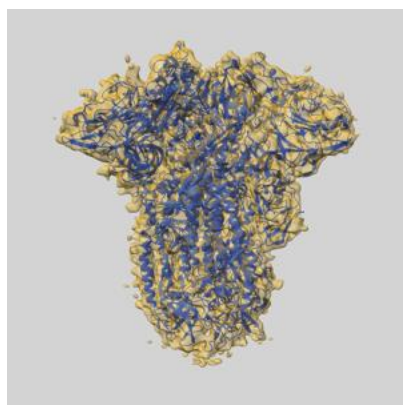
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.55	-	-
Author-provided FSC curve	4.55	5.27	4.61
Unmasked-calculated*	5.74	6.93	5.85

*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 5.74 differs from the reported value 4.55 by more than 10 %

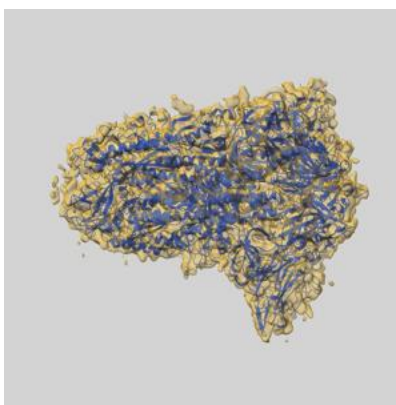
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-72507 and PDB model 9Y54. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

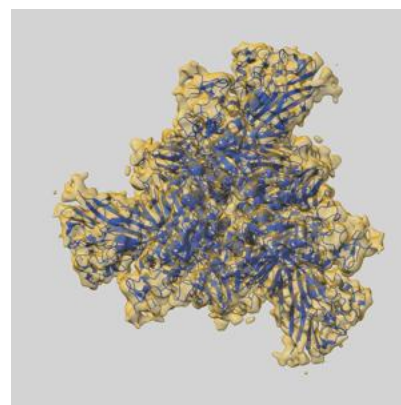
9.1 Map-model overlay [i](#)



X



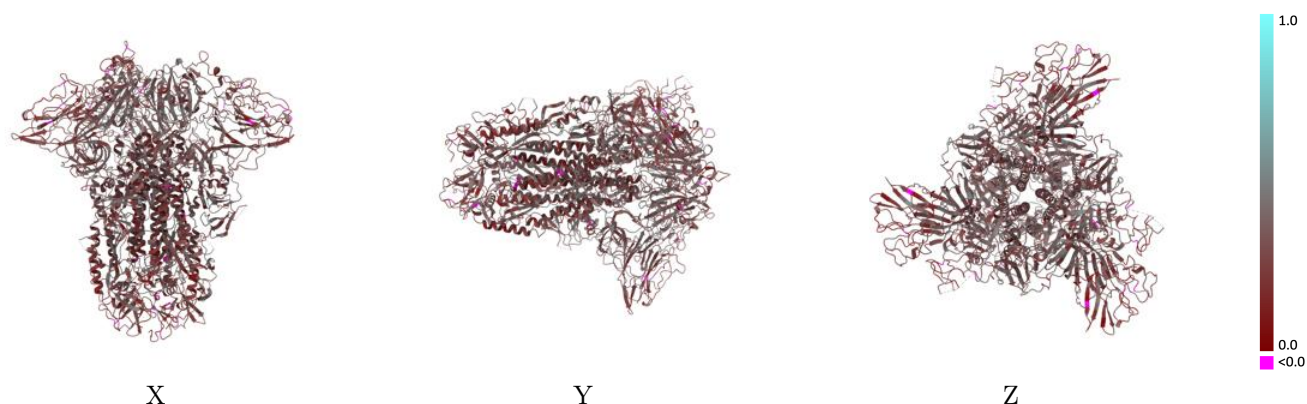
Y



Z

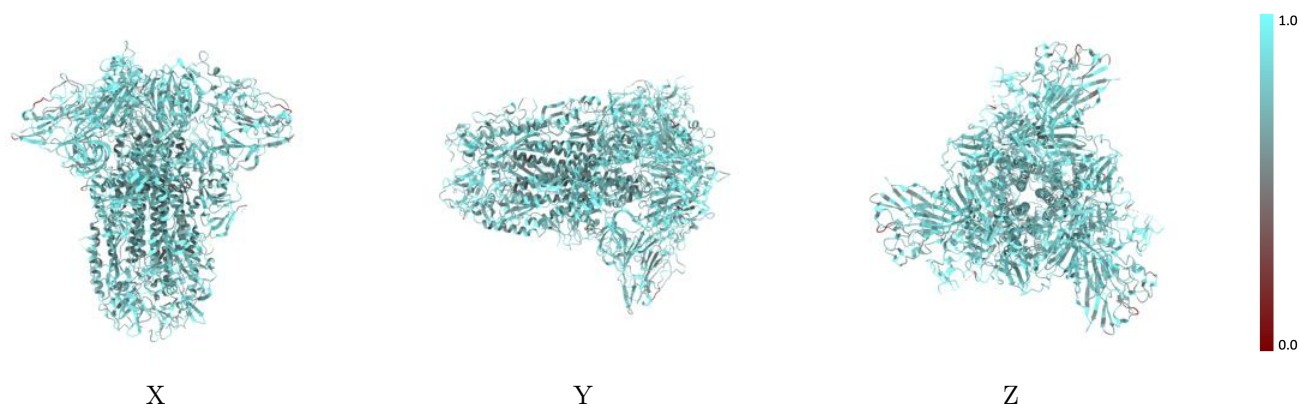
The images above show the 3D surface view of the map at the recommended contour level 0.221 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



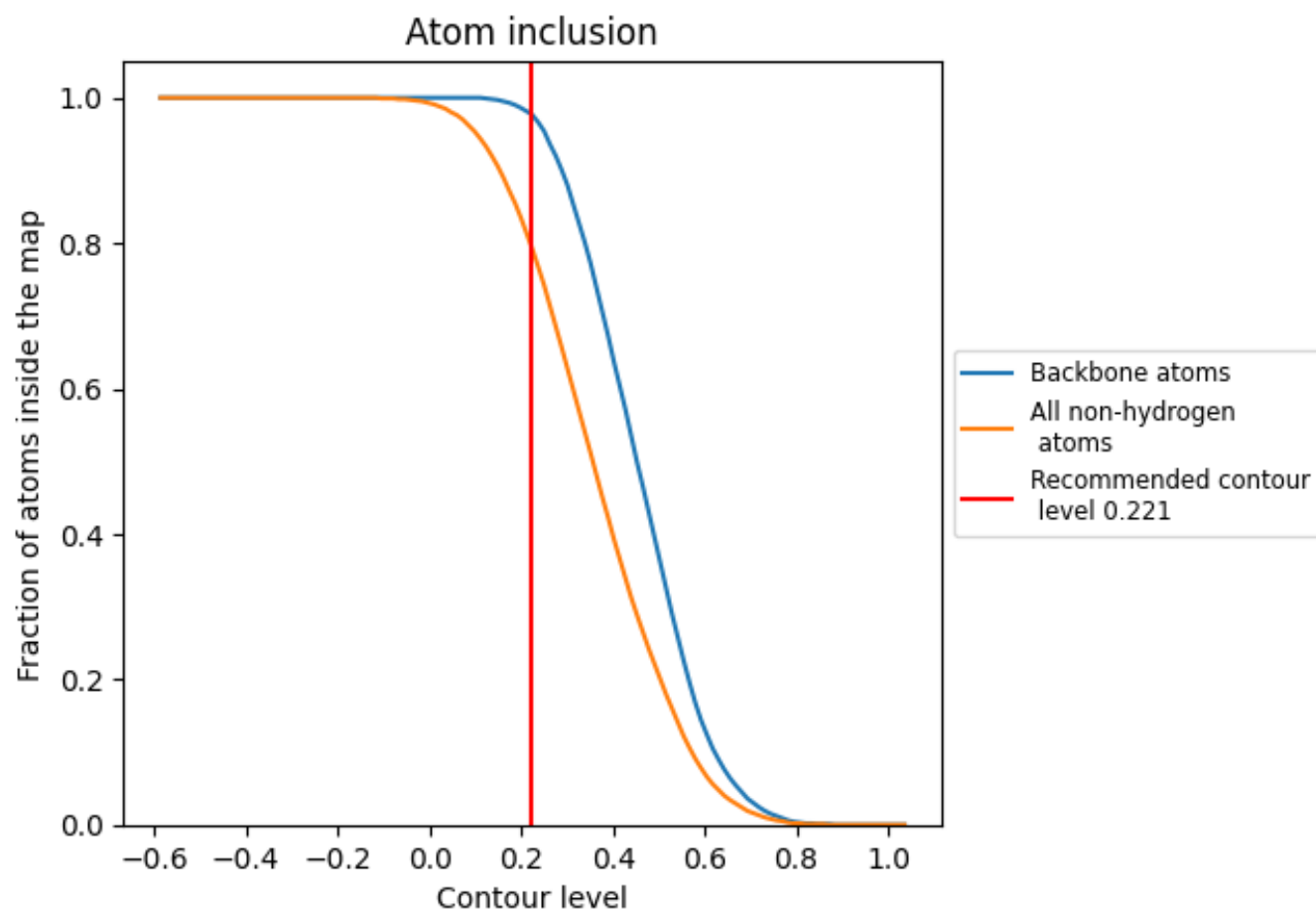
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.221).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 80% 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 (0.221) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7980	0.3170
A	0.7970	0.3150
B	0.7980	0.3170
C	0.7980	0.3170

