



## wwPDB EM Validation Summary Report ⓘ

Sep 2, 2025 – 03:58 PM EDT

PDB ID : 9MI3 / pdb\_00009mi3  
EMDB ID : EMD-48284  
Title : Cryo-EM structure of SARS-CoV-2 spike protein in complex with neutralizing human antibody WRAIR-2008  
Authors : Jensen, J.L.; Thomas, P.V.; Joyce, M.G.  
Deposited on : 2024-12-12  
Resolution : 3.23 Å(reported)  
Based on initial model : 6gze

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev126  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : **FAILED**  
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) : 2.45.1

# 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 3.23 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 60821 atoms, of which 29815 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	1065	Total	C	H	N	O	S	0	0
			16466	5322	8129	1394	1584	37		
1	C	1064	Total	C	H	N	O	S	0	0
			16479	5326	8140	1394	1583	36		
1	K	1061	Total	C	H	N	O	S	0	0
			16404	5306	8096	1388	1578	36		

There are 261 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	GLY	-	expression tag	UNP P0DTC2
A	1239	LEU	-	expression tag	UNP P0DTC2
A	1240	GLU	-	expression tag	UNP P0DTC2
A	1241	VAL	-	expression tag	UNP P0DTC2
A	1242	LEU	-	expression tag	UNP P0DTC2
A	1243	PHE	-	expression tag	UNP P0DTC2
A	1244	GLN	-	expression tag	UNP P0DTC2
A	1245	GLY	-	expression tag	UNP P0DTC2
A	1246	PRO	-	expression tag	UNP P0DTC2
A	1247	SER	-	expression tag	UNP P0DTC2
A	1248	ALA	-	expression tag	UNP P0DTC2
A	1249	TRP	-	expression tag	UNP P0DTC2
A	1250	SER	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	PRO	-	expression tag	UNP P0DTC2
A	1253	GLN	-	expression tag	UNP P0DTC2
A	1254	PHE	-	expression tag	UNP P0DTC2
A	1255	GLU	-	expression tag	UNP P0DTC2
A	1256	LYS	-	expression tag	UNP P0DTC2
A	1257	GLY	-	expression tag	UNP P0DTC2
A	1258	GLY	-	expression tag	UNP P0DTC2
A	1259	GLY	-	expression tag	UNP P0DTC2
A	1260	SER	-	expression tag	UNP P0DTC2
A	1261	GLY	-	expression tag	UNP P0DTC2
A	1262	GLY	-	expression tag	UNP P0DTC2
A	1263	GLY	-	expression tag	UNP P0DTC2
A	1264	SER	-	expression tag	UNP P0DTC2
A	1265	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1266	GLY	-	expression tag	UNP P0DTC2
A	1267	SER	-	expression tag	UNP P0DTC2
A	1268	ALA	-	expression tag	UNP P0DTC2
A	1269	TRP	-	expression tag	UNP P0DTC2
A	1270	SER	-	expression tag	UNP P0DTC2
A	1271	HIS	-	expression tag	UNP P0DTC2
A	1272	PRO	-	expression tag	UNP P0DTC2
A	1273	GLN	-	expression tag	UNP P0DTC2
A	1274	PHE	-	expression tag	UNP P0DTC2
A	1275	GLU	-	expression tag	UNP P0DTC2
A	1276	LYS	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	SER	-	expression tag	UNP P0DTC2
A	1279	HIS	-	expression tag	UNP P0DTC2
A	1280	HIS	-	expression tag	UNP P0DTC2
A	1281	HIS	-	expression tag	UNP P0DTC2
A	1282	HIS	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	HIS	-	expression tag	UNP P0DTC2
A	1285	HIS	-	expression tag	UNP P0DTC2
A	1286	HIS	-	expression tag	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	GLY	-	expression tag	UNP P0DTC2
C	1239	LEU	-	expression tag	UNP P0DTC2
C	1240	GLU	-	expression tag	UNP P0DTC2
C	1241	VAL	-	expression tag	UNP P0DTC2
C	1242	LEU	-	expression tag	UNP P0DTC2
C	1243	PHE	-	expression tag	UNP P0DTC2
C	1244	GLN	-	expression tag	UNP P0DTC2
C	1245	GLY	-	expression tag	UNP P0DTC2
C	1246	PRO	-	expression tag	UNP P0DTC2
C	1247	SER	-	expression tag	UNP P0DTC2
C	1248	ALA	-	expression tag	UNP P0DTC2
C	1249	TRP	-	expression tag	UNP P0DTC2
C	1250	SER	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	PRO	-	expression tag	UNP P0DTC2
C	1253	GLN	-	expression tag	UNP P0DTC2
C	1254	PHE	-	expression tag	UNP P0DTC2
C	1255	GLU	-	expression tag	UNP P0DTC2
C	1256	LYS	-	expression tag	UNP P0DTC2
C	1257	GLY	-	expression tag	UNP P0DTC2
C	1258	GLY	-	expression tag	UNP P0DTC2
C	1259	GLY	-	expression tag	UNP P0DTC2
C	1260	SER	-	expression tag	UNP P0DTC2
C	1261	GLY	-	expression tag	UNP P0DTC2
C	1262	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1263	GLY	-	expression tag	UNP P0DTC2
C	1264	SER	-	expression tag	UNP P0DTC2
C	1265	GLY	-	expression tag	UNP P0DTC2
C	1266	GLY	-	expression tag	UNP P0DTC2
C	1267	SER	-	expression tag	UNP P0DTC2
C	1268	ALA	-	expression tag	UNP P0DTC2
C	1269	TRP	-	expression tag	UNP P0DTC2
C	1270	SER	-	expression tag	UNP P0DTC2
C	1271	HIS	-	expression tag	UNP P0DTC2
C	1272	PRO	-	expression tag	UNP P0DTC2
C	1273	GLN	-	expression tag	UNP P0DTC2
C	1274	PHE	-	expression tag	UNP P0DTC2
C	1275	GLU	-	expression tag	UNP P0DTC2
C	1276	LYS	-	expression tag	UNP P0DTC2
C	1277	GLY	-	expression tag	UNP P0DTC2
C	1278	SER	-	expression tag	UNP P0DTC2
C	1279	HIS	-	expression tag	UNP P0DTC2
C	1280	HIS	-	expression tag	UNP P0DTC2
C	1281	HIS	-	expression tag	UNP P0DTC2
C	1282	HIS	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	HIS	-	expression tag	UNP P0DTC2
C	1285	HIS	-	expression tag	UNP P0DTC2
C	1286	HIS	-	expression tag	UNP P0DTC2
K	682	GLY	ARG	conflict	UNP P0DTC2
K	683	SER	ARG	conflict	UNP P0DTC2
K	685	SER	ARG	conflict	UNP P0DTC2
K	817	PRO	PHE	conflict	UNP P0DTC2
K	892	PRO	ALA	conflict	UNP P0DTC2
K	899	PRO	ALA	conflict	UNP P0DTC2
K	942	PRO	ALA	conflict	UNP P0DTC2
K	986	PRO	LYS	conflict	UNP P0DTC2
K	987	PRO	VAL	conflict	UNP P0DTC2
K	1209	GLY	-	expression tag	UNP P0DTC2
K	1210	SER	-	expression tag	UNP P0DTC2
K	1211	GLY	-	expression tag	UNP P0DTC2
K	1212	TYR	-	expression tag	UNP P0DTC2
K	1213	ILE	-	expression tag	UNP P0DTC2
K	1214	PRO	-	expression tag	UNP P0DTC2
K	1215	GLU	-	expression tag	UNP P0DTC2
K	1216	ALA	-	expression tag	UNP P0DTC2
K	1217	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1218	ARG	-	expression tag	UNP P0DTC2
K	1219	ASP	-	expression tag	UNP P0DTC2
K	1220	GLY	-	expression tag	UNP P0DTC2
K	1221	GLN	-	expression tag	UNP P0DTC2
K	1222	ALA	-	expression tag	UNP P0DTC2
K	1223	TYR	-	expression tag	UNP P0DTC2
K	1224	VAL	-	expression tag	UNP P0DTC2
K	1225	ARG	-	expression tag	UNP P0DTC2
K	1226	LYS	-	expression tag	UNP P0DTC2
K	1227	ASP	-	expression tag	UNP P0DTC2
K	1228	GLY	-	expression tag	UNP P0DTC2
K	1229	GLU	-	expression tag	UNP P0DTC2
K	1230	TRP	-	expression tag	UNP P0DTC2
K	1231	VAL	-	expression tag	UNP P0DTC2
K	1232	LEU	-	expression tag	UNP P0DTC2
K	1233	LEU	-	expression tag	UNP P0DTC2
K	1234	SER	-	expression tag	UNP P0DTC2
K	1235	THR	-	expression tag	UNP P0DTC2
K	1236	PHE	-	expression tag	UNP P0DTC2
K	1237	LEU	-	expression tag	UNP P0DTC2
K	1238	GLY	-	expression tag	UNP P0DTC2
K	1239	LEU	-	expression tag	UNP P0DTC2
K	1240	GLU	-	expression tag	UNP P0DTC2
K	1241	VAL	-	expression tag	UNP P0DTC2
K	1242	LEU	-	expression tag	UNP P0DTC2
K	1243	PHE	-	expression tag	UNP P0DTC2
K	1244	GLN	-	expression tag	UNP P0DTC2
K	1245	GLY	-	expression tag	UNP P0DTC2
K	1246	PRO	-	expression tag	UNP P0DTC2
K	1247	SER	-	expression tag	UNP P0DTC2
K	1248	ALA	-	expression tag	UNP P0DTC2
K	1249	TRP	-	expression tag	UNP P0DTC2
K	1250	SER	-	expression tag	UNP P0DTC2
K	1251	HIS	-	expression tag	UNP P0DTC2
K	1252	PRO	-	expression tag	UNP P0DTC2
K	1253	GLN	-	expression tag	UNP P0DTC2
K	1254	PHE	-	expression tag	UNP P0DTC2
K	1255	GLU	-	expression tag	UNP P0DTC2
K	1256	LYS	-	expression tag	UNP P0DTC2
K	1257	GLY	-	expression tag	UNP P0DTC2
K	1258	GLY	-	expression tag	UNP P0DTC2
K	1259	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1260	SER	-	expression tag	UNP P0DTC2
K	1261	GLY	-	expression tag	UNP P0DTC2
K	1262	GLY	-	expression tag	UNP P0DTC2
K	1263	GLY	-	expression tag	UNP P0DTC2
K	1264	SER	-	expression tag	UNP P0DTC2
K	1265	GLY	-	expression tag	UNP P0DTC2
K	1266	GLY	-	expression tag	UNP P0DTC2
K	1267	SER	-	expression tag	UNP P0DTC2
K	1268	ALA	-	expression tag	UNP P0DTC2
K	1269	TRP	-	expression tag	UNP P0DTC2
K	1270	SER	-	expression tag	UNP P0DTC2
K	1271	HIS	-	expression tag	UNP P0DTC2
K	1272	PRO	-	expression tag	UNP P0DTC2
K	1273	GLN	-	expression tag	UNP P0DTC2
K	1274	PHE	-	expression tag	UNP P0DTC2
K	1275	GLU	-	expression tag	UNP P0DTC2
K	1276	LYS	-	expression tag	UNP P0DTC2
K	1277	GLY	-	expression tag	UNP P0DTC2
K	1278	SER	-	expression tag	UNP P0DTC2
K	1279	HIS	-	expression tag	UNP P0DTC2
K	1280	HIS	-	expression tag	UNP P0DTC2
K	1281	HIS	-	expression tag	UNP P0DTC2
K	1282	HIS	-	expression tag	UNP P0DTC2
K	1283	HIS	-	expression tag	UNP P0DTC2
K	1284	HIS	-	expression tag	UNP P0DTC2
K	1285	HIS	-	expression tag	UNP P0DTC2
K	1286	HIS	-	expression tag	UNP P0DTC2

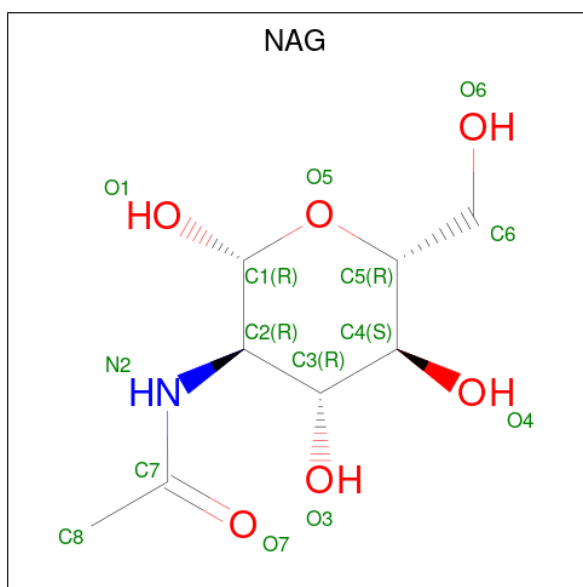
- Molecule 2 is a protein called WRAIR-2008 antibody Fab heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	128	Total	C	H	N	O	S	0	0
			1904	613	924	161	200	6		
2	E	128	Total	C	H	N	O	S	0	0
			1904	613	924	161	200	6		
2	H	128	Total	C	H	N	O	S	0	0
			1904	613	924	161	200	6		

- Molecule 3 is a protein called WRAIR-2008 antibody Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	113	Total	C	H	N	O	S	
			1749	554	871	152	168	4	0
3	F	113	Total	C	H	N	O	S	
			1749	554	871	152	168	4	0
3	L	113	Total	C	H	N	O	S	
			1749	554	871	152	168	4	0

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



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	H	N	O	
			27	8	13	1	5	0
4	A	1	Total	C	H	N	O	
			27	8	13	1	5	0
4	A	1	Total	C	N	O		
			14	8	1	5		0
4	A	1	Total	C	N	O		
			14	8	1	5		0
4	A	1	Total	C	N	O		
			14	8	1	5		0
4	A	1	Total	C	N	O		
			14	8	1	5		0
4	A	1	Total	C	N	O		
			14	8	1	5		0

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Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 14	C 8	N 1	O 5	0	
4	A	1	Total 14	C 8	N 1	O 5	0	
4	A	1	Total 14	C 8	N 1	O 5	0	
4	C	1	Total 27	C 8	H 13	N 1	O 5	0
4	C	1	Total 27	C 8	H 13	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0	
4	C	1	Total 14	C 8	N 1	O 5	0	
4	C	1	Total 14	C 8	N 1	O 5	0	
4	C	1	Total 14	C 8	N 1	O 5	0	
4	C	1	Total 14	C 8	N 1	O 5	0	
4	C	1	Total 14	C 8	N 1	O 5	0	
4	C	1	Total 14	C 8	N 1	O 5	0	
4	C	1	Total 14	C 8	N 1	O 5	0	
4	C	1	Total 14	C 8	N 1	O 5	0	
4	C	1	Total 14	C 8	N 1	O 5	0	
4	K	1	Total 27	C 8	H 13	N 1	O 5	0
4	K	1	Total 14	C 8	N 1	O 5	0	
4	K	1	Total 14	C 8	N 1	O 5	0	
4	K	1	Total 14	C 8	N 1	O 5	0	
4	K	1	Total 14	C 8	N 1	O 5	0	
4	K	1	Total 14	C 8	N 1	O 5	0	
4	K	1	Total 14	C 8	N 1	O 5	0	
4	K	1	Total 14	C 8	N 1	O 5	0	
4	K	1	Total 14	C 8	N 1	O 5	0	

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

MolProbity failed to run properly - this section is therefore empty.

### 3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	296457	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 200	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	100	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.658	Depositor
Minimum map value	-1.034	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.12	Depositor
Map size ( $\text{\AA}$ )	522.24, 522.24, 522.24	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.02, 1.02, 1.02	Depositor

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

### 4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 4.6 Ligand geometry [i](#)

32 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	A	1310	1	14,14,15	0.75	0	17,19,21	0.86	0
4	NAG	A	1309	1	14,14,15	0.69	0	17,19,21	1.47	2 (11%)
4	NAG	K	1301	1	14,14,15	0.73	0	17,19,21	0.88	0
4	NAG	C	1302	1	14,14,15	0.72	0	17,19,21	0.83	0
4	NAG	A	1308	1	14,14,15	0.71	0	17,19,21	1.19	1 (5%)
4	NAG	K	1302	1	14,14,15	0.71	0	17,19,21	0.76	0
4	NAG	C	1304	1	14,14,15	0.66	0	17,19,21	1.39	2 (11%)
4	NAG	C	1308	1	14,14,15	0.71	0	17,19,21	1.32	1 (5%)
4	NAG	A	1306	1	14,14,15	0.72	0	17,19,21	0.78	0
4	NAG	A	1304	1	14,14,15	0.71	0	17,19,21	0.79	0
4	NAG	K	1307	1	14,14,15	0.71	0	17,19,21	0.78	0
4	NAG	K	1306	1	14,14,15	0.76	0	17,19,21	1.25	1 (5%)
4	NAG	K	1311	1	14,14,15	0.70	0	17,19,21	0.83	0
4	NAG	C	1310	1	14,14,15	0.76	0	17,19,21	0.84	0
4	NAG	K	1303	1	14,14,15	0.69	0	17,19,21	0.78	0
4	NAG	K	1304	1	14,14,15	0.77	0	17,19,21	0.83	0
4	NAG	C	1309	1	14,14,15	0.80	0	17,19,21	0.83	0
4	NAG	K	1308	1	14,14,15	0.73	0	17,19,21	1.28	1 (5%)
4	NAG	A	1305	1	14,14,15	0.71	0	17,19,21	0.77	0
4	NAG	C	1303	1	14,14,15	0.71	0	17,19,21	0.74	0
4	NAG	A	1301	1	14,14,15	0.68	0	17,19,21	0.87	1 (5%)
4	NAG	A	1307	1	14,14,15	0.73	0	17,19,21	0.90	1 (5%)
4	NAG	K	1305	1	14,14,15	0.74	0	17,19,21	1.24	1 (5%)
4	NAG	C	1306	1	14,14,15	0.72	0	17,19,21	1.44	1 (5%)
4	NAG	K	1310	1	14,14,15	0.71	0	17,19,21	1.57	1 (5%)
4	NAG	C	1307	1	14,14,15	0.77	0	17,19,21	0.80	0
4	NAG	K	1309	1	14,14,15	0.72	0	17,19,21	0.79	0
4	NAG	A	1303	1	14,14,15	0.73	0	17,19,21	0.75	0
4	NAG	A	1311	1	14,14,15	0.75	0	17,19,21	0.96	0
4	NAG	C	1305	1	14,14,15	0.72	0	17,19,21	0.89	0
4	NAG	A	1302	1	14,14,15	0.74	0	17,19,21	0.83	0
4	NAG	C	1301	1	14,14,15	0.70	0	17,19,21	0.82	0

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



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	4/6/23/26	0/1/1/1
4	NAG	K	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	4/6/23/26	0/1/1/1
4	NAG	K	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	3/6/23/26	0/1/1/1
4	NAG	K	1307	1	-	1/6/23/26	0/1/1/1
4	NAG	K	1306	1	-	1/6/23/26	0/1/1/1
4	NAG	K	1311	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1310	1	-	0/6/23/26	0/1/1/1
4	NAG	K	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	K	1304	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	K	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	K	1305	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	3/6/23/26	0/1/1/1
4	NAG	K	1310	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	1/6/23/26	0/1/1/1
4	NAG	K	1309	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1311	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	1310	NAG	C2-N2-C7	5.49	130.26	122.90
4	C	1304	NAG	C2-N2-C7	4.32	128.69	122.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1306	NAG	C2-N2-C7	4.17	128.49	122.90
4	A	1308	NAG	C2-N2-C7	3.86	128.07	122.90
4	K	1308	NAG	C2-N2-C7	3.78	127.96	122.90

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1311	NAG	C3-C2-N2-C7
4	C	1302	NAG	C1-C2-N2-C7
4	C	1306	NAG	C1-C2-N2-C7
4	K	1305	NAG	C1-C2-N2-C7
4	K	1306	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

## 4.7 Other polymers [i](#)

There are no such residues in this entry.

## 4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

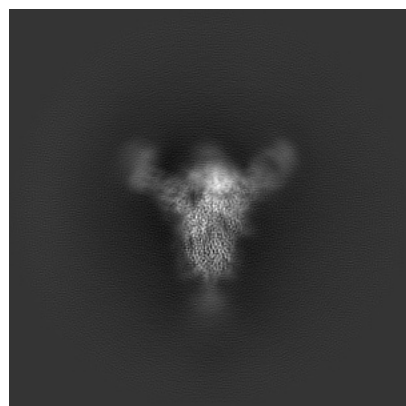
## 5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48284. These allow visual inspection of the internal detail of the map and identification of artifacts.

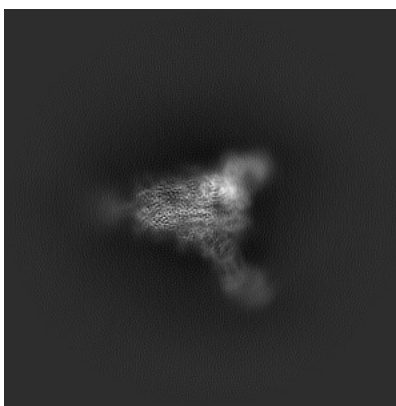
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 5.1 Orthogonal projections [i](#)

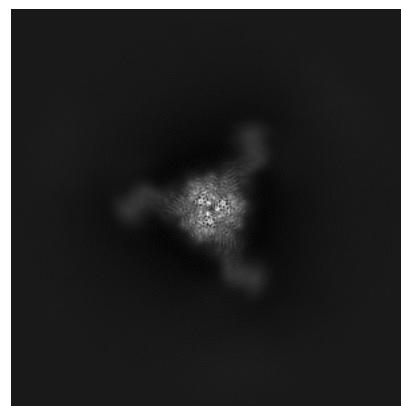
#### 5.1.1 Primary map



X

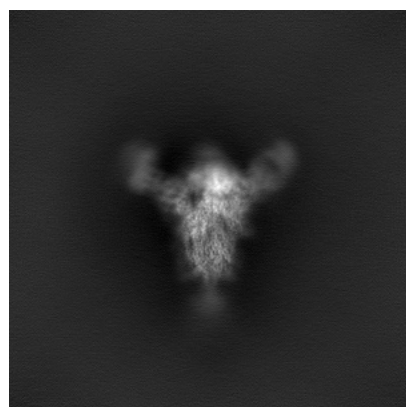


Y

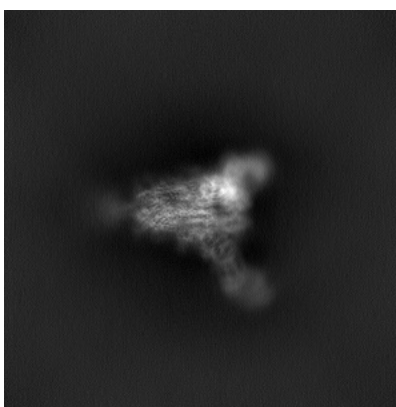


Z

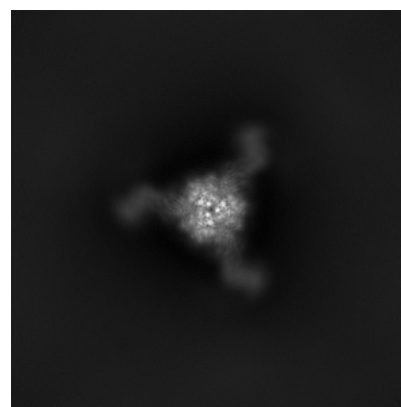
#### 5.1.2 Raw map



X



Y

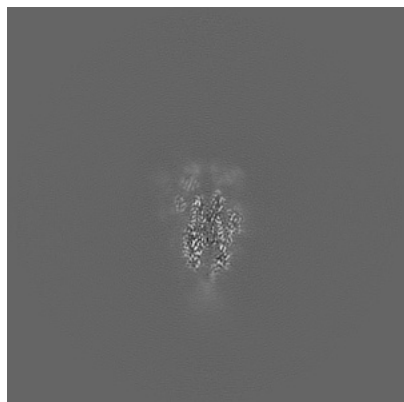


Z

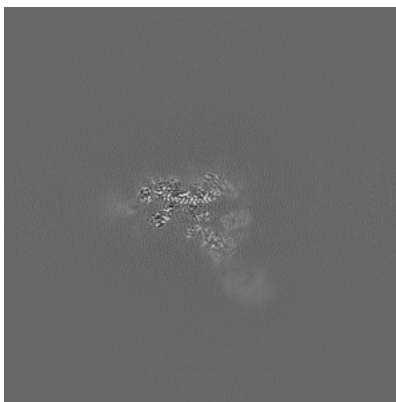
The images above show the map projected in three orthogonal directions.

## 5.2 Central slices [i](#)

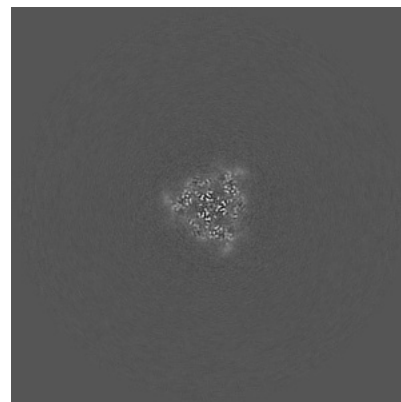
### 5.2.1 Primary map



X Index: 256

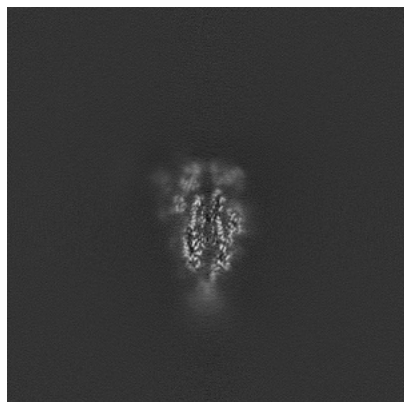


Y Index: 256

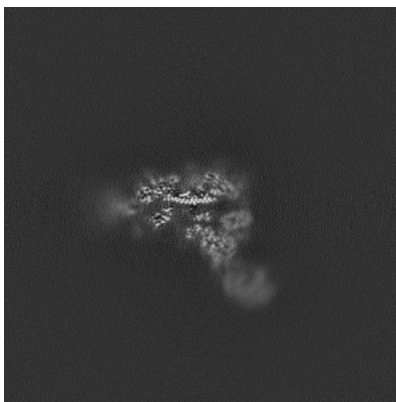


Z Index: 256

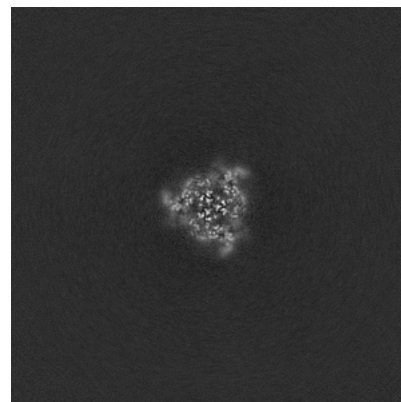
### 5.2.2 Raw map



X Index: 256



Y Index: 256

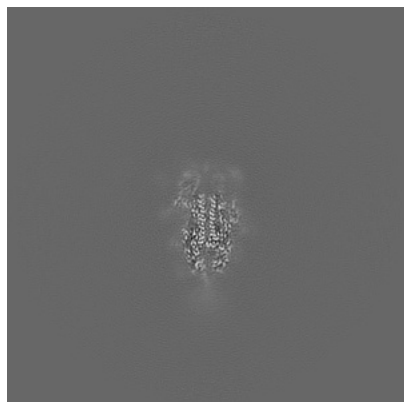


Z Index: 256

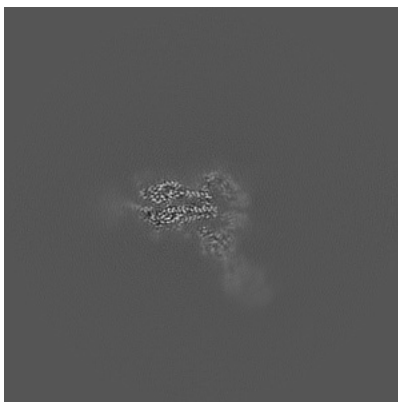
The images above show central slices of the map in three orthogonal directions.

## 5.3 Largest variance slices [i](#)

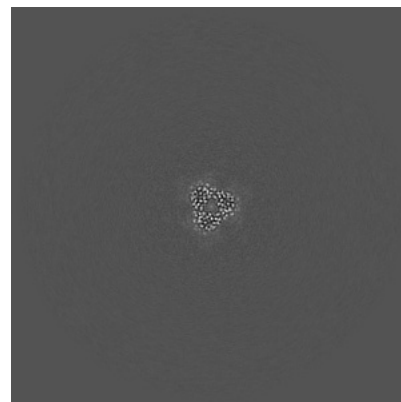
### 5.3.1 Primary map



X Index: 251

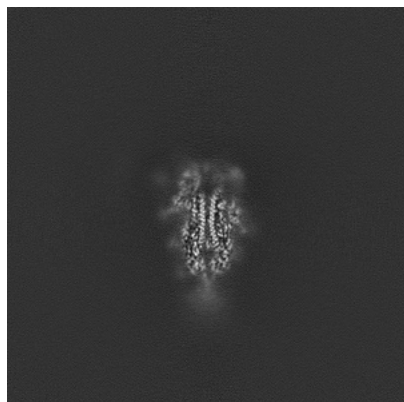


Y Index: 264

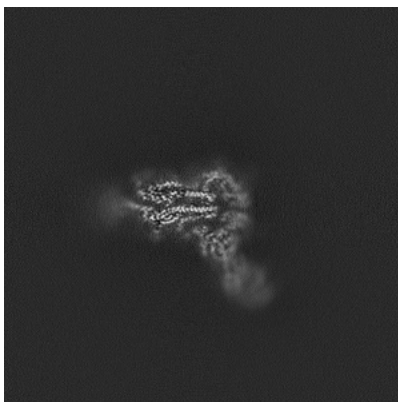


Z Index: 202

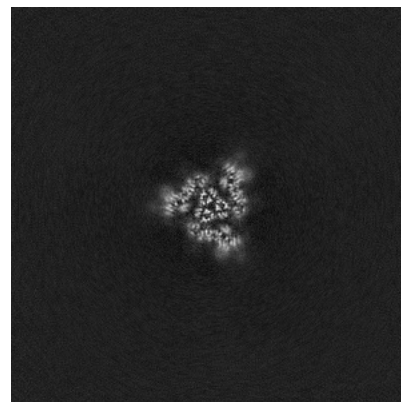
### 5.3.2 Raw map



X Index: 252



Y Index: 263



Z Index: 265

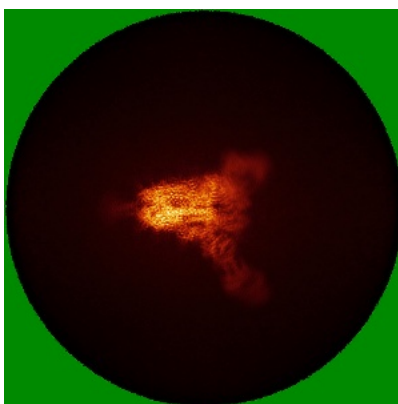
The images above show the largest variance slices of the map in three orthogonal directions.

## 5.4 Orthogonal standard-deviation projections (False-color) ⓘ

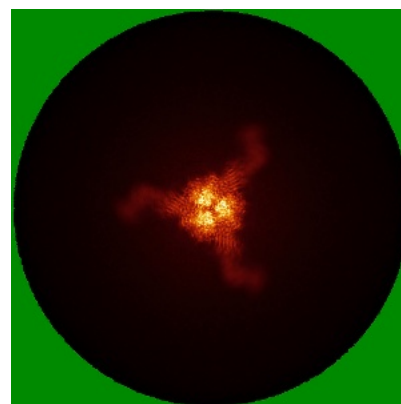
### 5.4.1 Primary map



X



Y

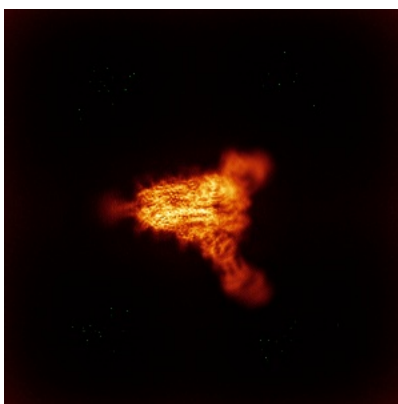


Z

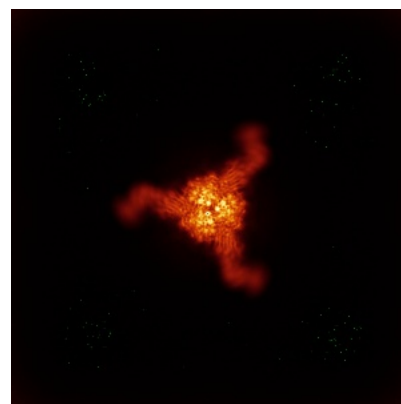
### 5.4.2 Raw map



X



Y



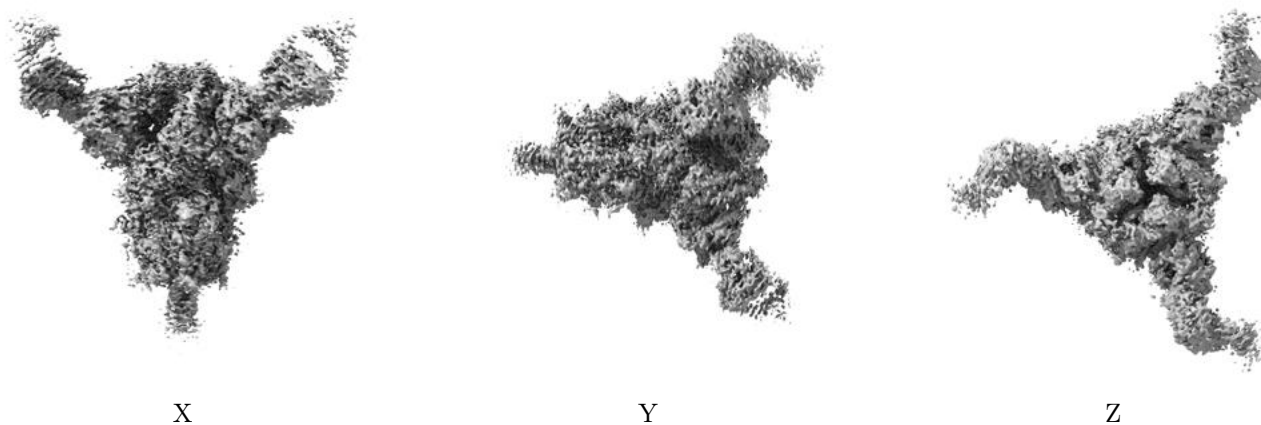
Z

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.



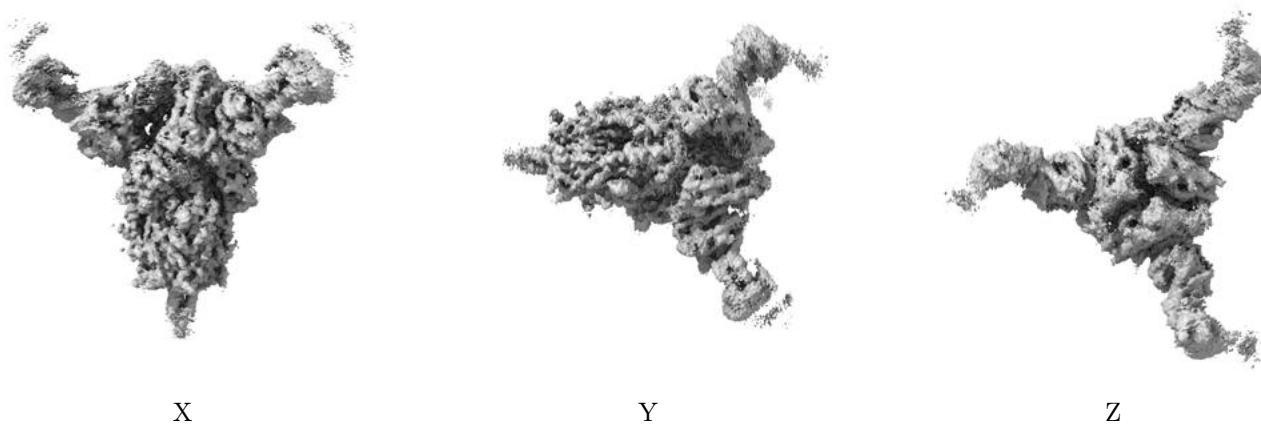
## 5.5 Orthogonal surface views [i](#)

### 5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 5.5.2 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.

## 5.6 Mask visualisation [i](#)

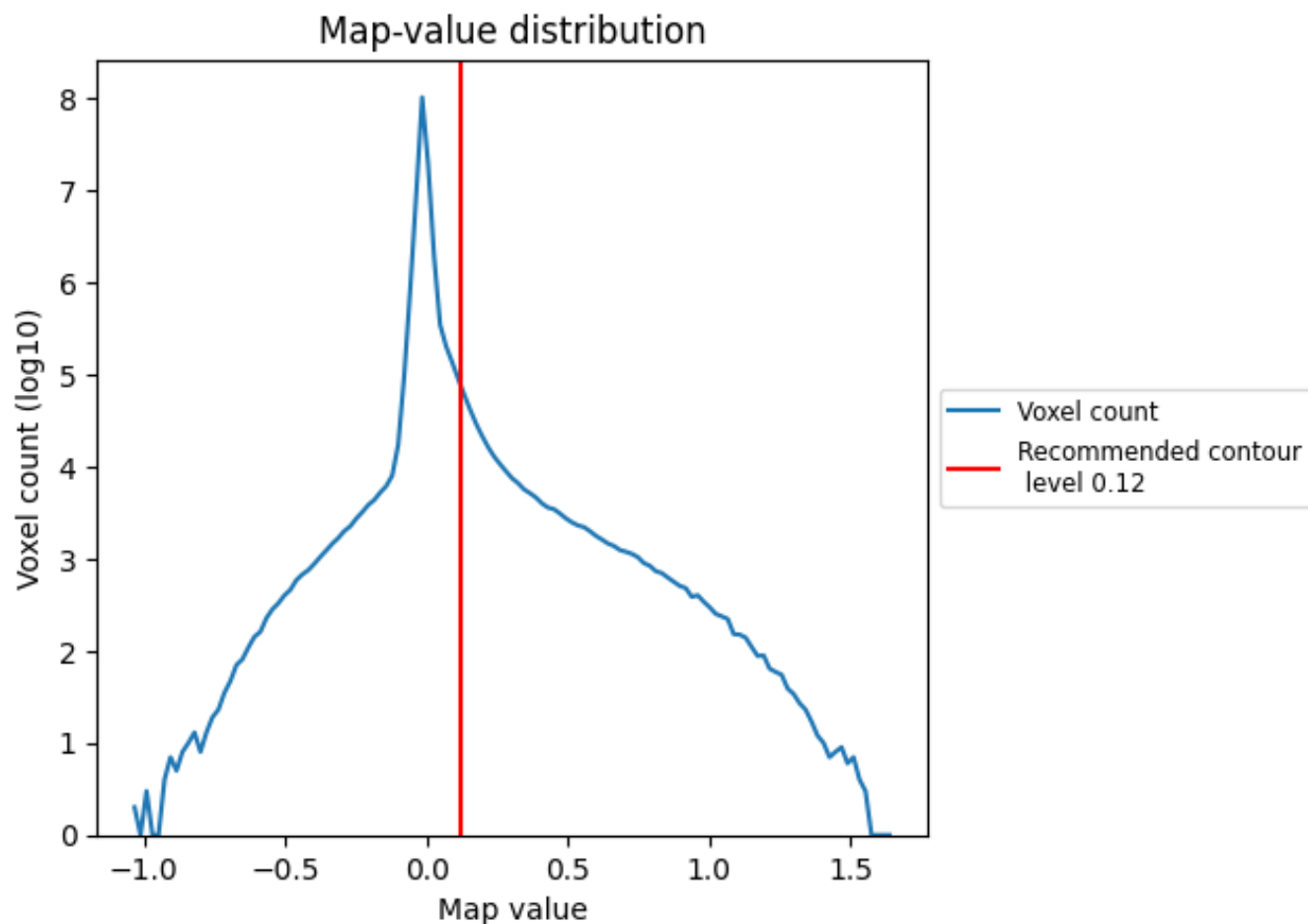
This section was not generated. No masks/segmentation were deposited.



## 6 Map analysis [i](#)

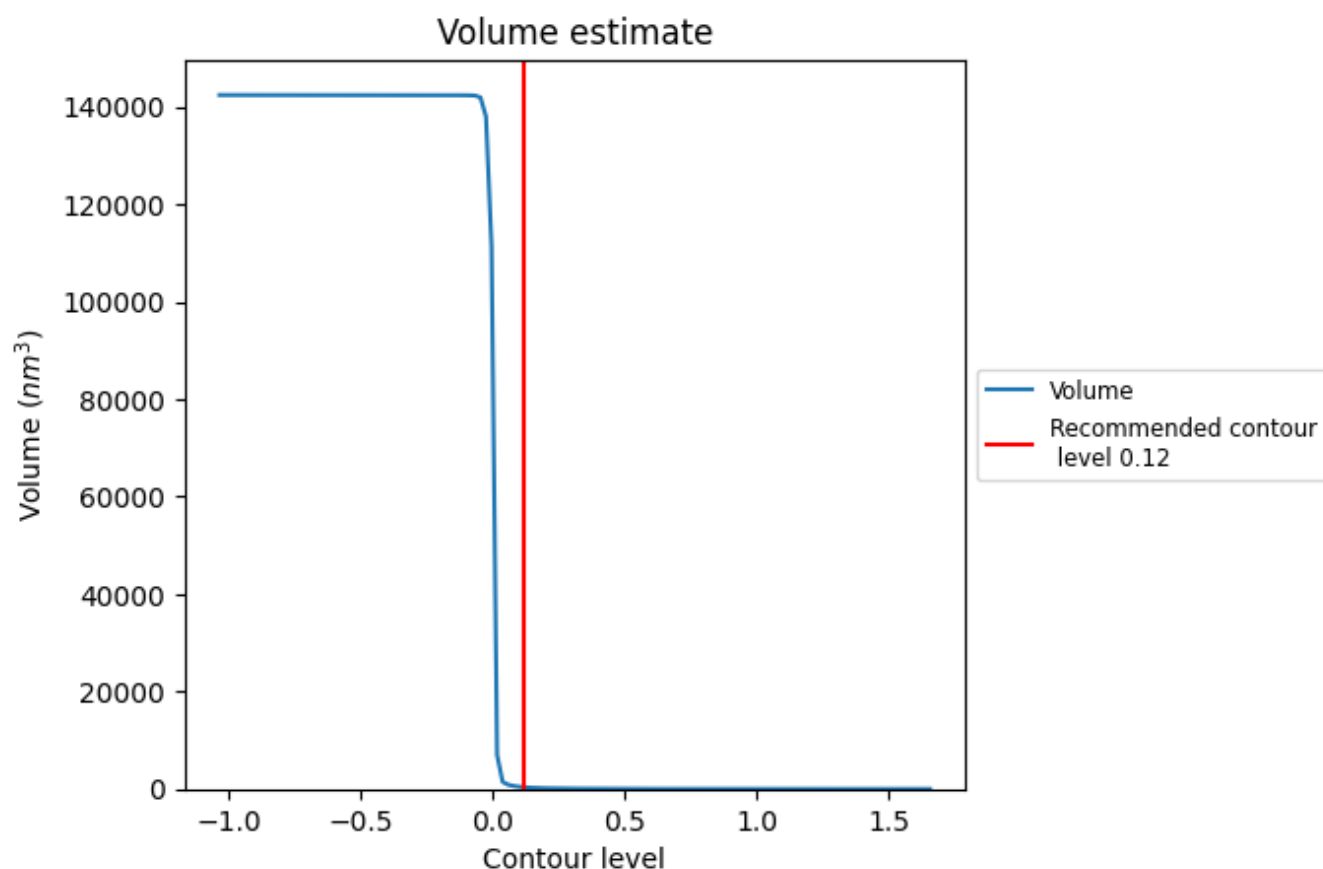
This section contains the results of statistical analysis of the map.

### 6.1 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.

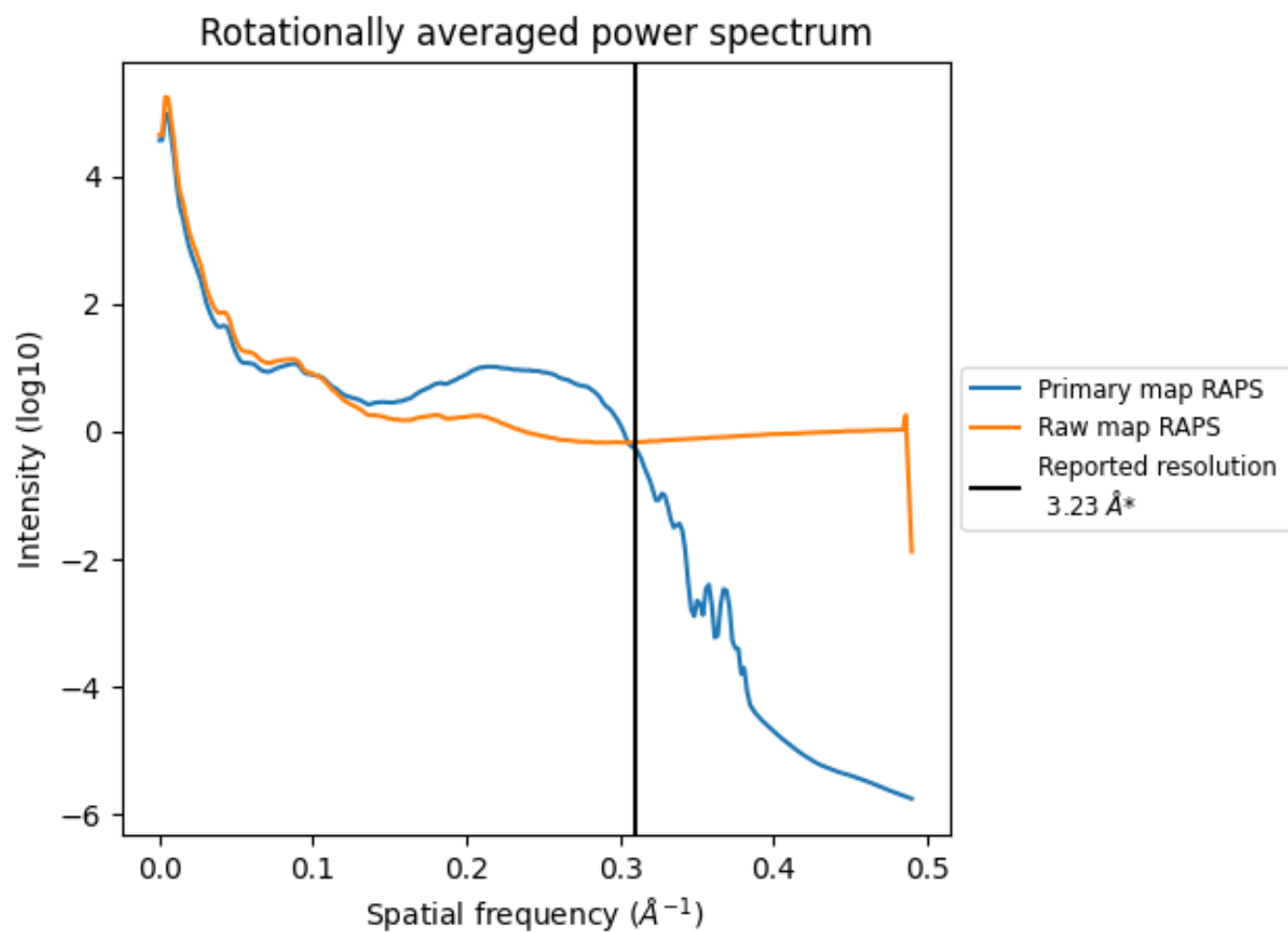
## 6.2 Volume estimate [i](#)



The volume at the recommended contour level is 345  $\text{nm}^3$ ; this corresponds to an approximate mass of 312 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.

### 6.3 Rotationally averaged power spectrum ⓘ

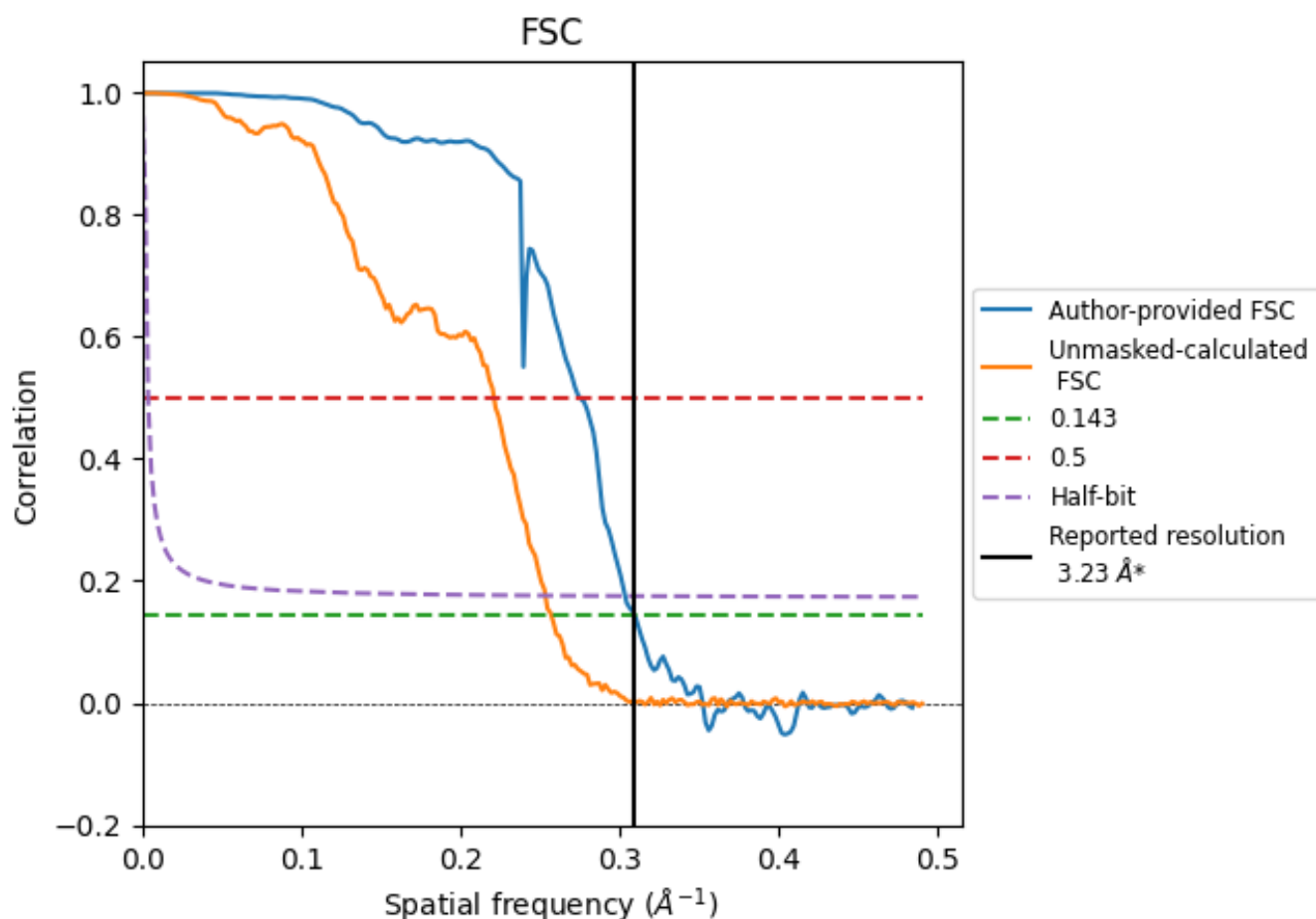


\*Reported resolution corresponds to spatial frequency of 0.310 Å<sup>-1</sup>

## 7 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.

### 7.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.310 \text{ \AA}^{-1}$

## 7.2 Resolution estimates [i](#)

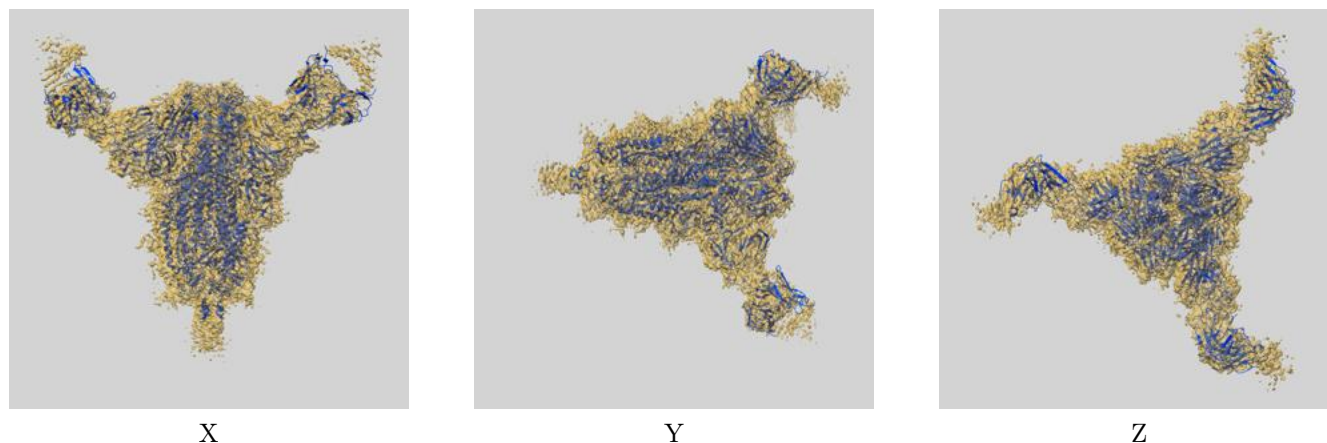
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.23	-	-
Author-provided FSC curve	3.23	3.63	3.29
Unmasked-calculated*	3.89	4.52	3.95

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.89 differs from the reported value 3.23 by more than 10 %

## 8 Map-model fit [i](#)

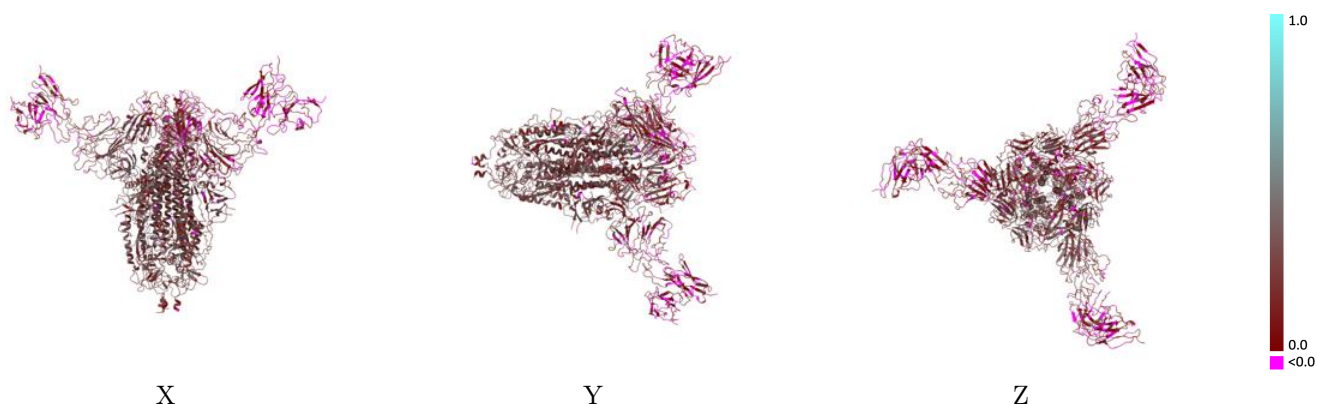
This section contains information regarding the fit between EMDB map EMD-48284 and PDB model 9MI3. Per-residue inclusion information can be found in section ?? on page ??.

### 8.1 Map-model overlay [i](#)



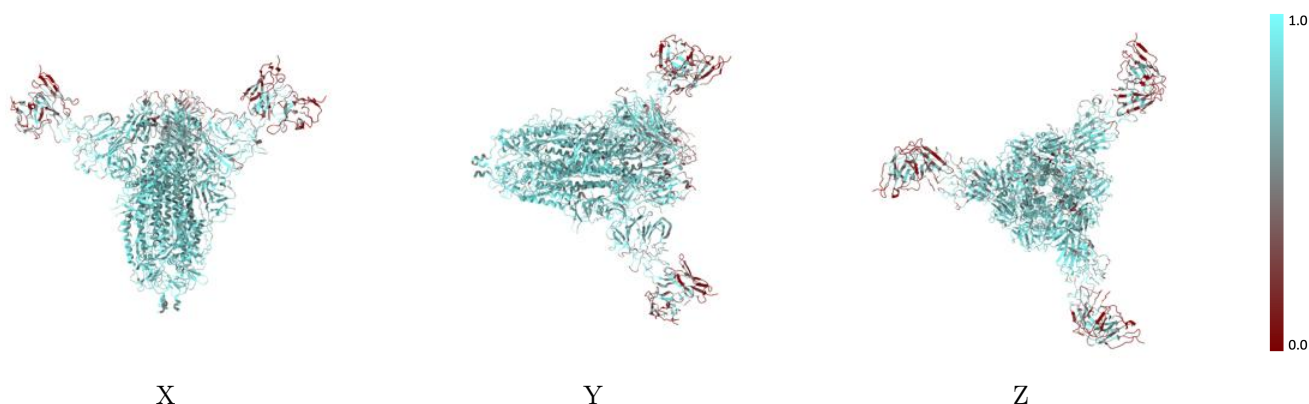
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 8.2 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.

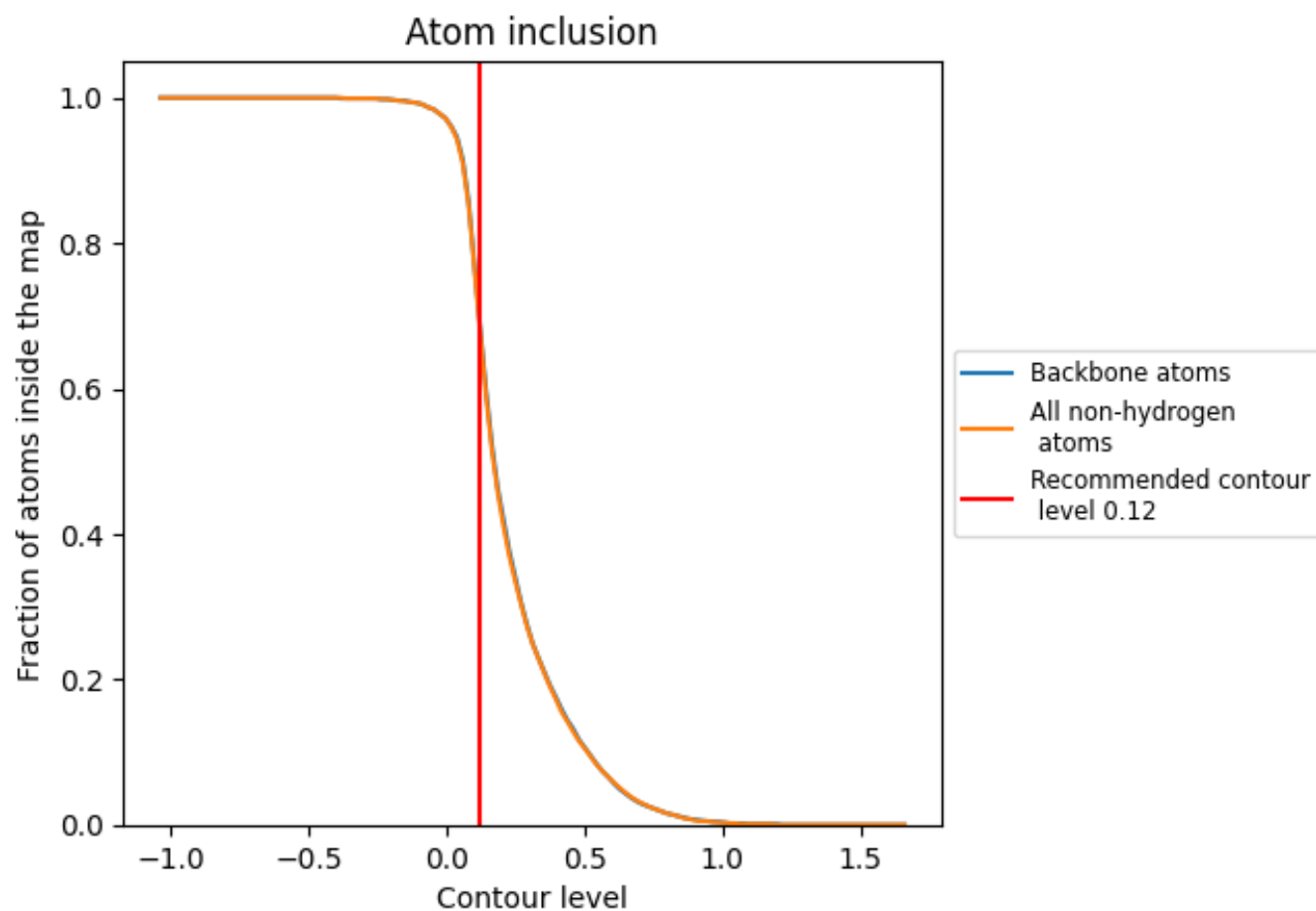
## 8.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.12).



## 8.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6920	<div></div> 0.2080
A	<div></div> 0.7540	<div></div> 0.2200
B	<div></div> 0.4050	<div></div> 0.0470
C	<div></div> 0.7680	<div></div> 0.2410
D	<div></div> 0.3510	<div></div> 0.0480
E	<div></div> 0.4100	<div></div> 0.0880
F	<div></div> 0.4040	<div></div> 0.0740
H	<div></div> 0.3990	<div></div> 0.1000
K	<div></div> 0.7790	<div></div> 0.2510
L	<div></div> 0.4170	<div></div> 0.0790

1.0

0.0

<0.0