



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:42 AM UTC

PDB ID : 7X93 / pdb_00007x93
EMDB ID : EMD-33065
Title : The SARS-CoV-2 receptor binding domain bound with the Fab fragment of a human neutralizing antibody Ab765
Authors : Kamada, K.; Shirouzu, M.
Deposited on : 2022-03-15
Resolution : 3.30 Å(reported)
Based on initial model : 5CCK

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

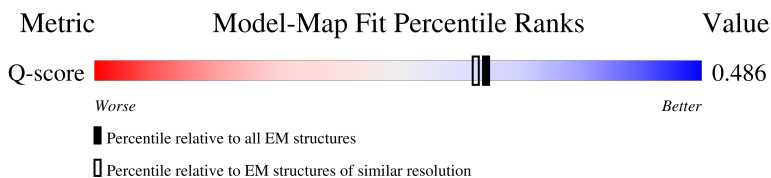
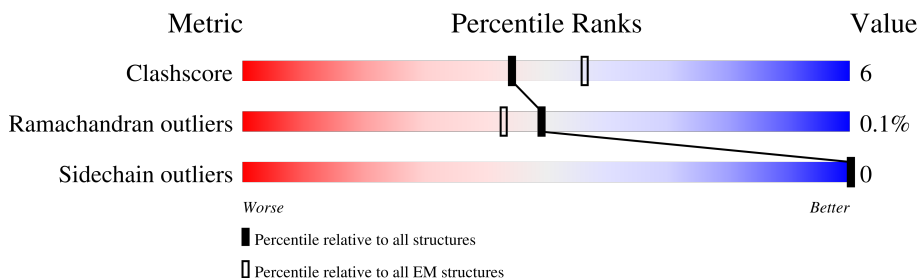
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	A	1278	 13% . 85%
1	D	1278	 14% . 84%
1	G	1278	 13% . 84%
2	E	261	 38% 8% 54%

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Mol	Chain	Length	Quality of chain
3	F	240	 38% 8% 54%
4	B	2	 50% 50%
5	C	5	 60% 80% 20%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12832 atoms, of which 6252 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	198	Total	C	H	N	O	S	0	0
			3057	1005	1489	262	293	8		
1	D	201	Total	C	H	N	O	S	0	0
			3113	1025	1518	266	296	8		
1	G	200	Total	C	H	N	O	S	0	0
			3091	1019	1505	264	295	8		

There are 237 discrepancies between the modelled and reference sequences:

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1266	LYS	-	expression tag	UNP P0DTC2
A	1267	ILE	-	expression tag	UNP P0DTC2
A	1268	GLU	-	expression tag	UNP P0DTC2
A	1269	TRP	-	expression tag	UNP P0DTC2
A	1270	HIS	-	expression tag	UNP P0DTC2
A	1271	GLU	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	HIS	-	expression tag	UNP P0DTC2
A	1274	HIS	-	expression tag	UNP P0DTC2
A	1275	HIS	-	expression tag	UNP P0DTC2
A	1276	HIS	-	expression tag	UNP P0DTC2
A	1277	HIS	-	expression tag	UNP P0DTC2
A	1278	HIS	-	expression tag	UNP P0DTC2
D	682	GLY	ARG	engineered mutation	UNP P0DTC2
D	683	SER	ARG	engineered mutation	UNP P0DTC2
D	685	SER	ARG	engineered mutation	UNP P0DTC2
D	817	PRO	PHE	engineered mutation	UNP P0DTC2
D	892	PRO	ALA	engineered mutation	UNP P0DTC2
D	899	PRO	ALA	engineered mutation	UNP P0DTC2
D	942	PRO	ALA	engineered mutation	UNP P0DTC2
D	986	PRO	LYS	engineered mutation	UNP P0DTC2
D	987	PRO	VAL	engineered mutation	UNP P0DTC2
D	1209	ALA	-	expression tag	UNP P0DTC2
D	1210	ALA	-	expression tag	UNP P0DTC2
D	1211	ALA	-	expression tag	UNP P0DTC2
D	1212	GLY	-	expression tag	UNP P0DTC2
D	1213	SER	-	expression tag	UNP P0DTC2
D	1214	GLY	-	expression tag	UNP P0DTC2
D	1215	TYR	-	expression tag	UNP P0DTC2
D	1216	ILE	-	expression tag	UNP P0DTC2
D	1217	PRO	-	expression tag	UNP P0DTC2
D	1218	GLU	-	expression tag	UNP P0DTC2
D	1219	ALA	-	expression tag	UNP P0DTC2
D	1220	PRO	-	expression tag	UNP P0DTC2
D	1221	ARG	-	expression tag	UNP P0DTC2
D	1222	ASP	-	expression tag	UNP P0DTC2
D	1223	GLY	-	expression tag	UNP P0DTC2
D	1224	GLN	-	expression tag	UNP P0DTC2
D	1225	ALA	-	expression tag	UNP P0DTC2
D	1226	TYR	-	expression tag	UNP P0DTC2
D	1227	VAL	-	expression tag	UNP P0DTC2
D	1228	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1229	LYS	-	expression tag	UNP P0DTC2
D	1230	ASP	-	expression tag	UNP P0DTC2
D	1231	GLY	-	expression tag	UNP P0DTC2
D	1232	GLU	-	expression tag	UNP P0DTC2
D	1233	TRP	-	expression tag	UNP P0DTC2
D	1234	VAL	-	expression tag	UNP P0DTC2
D	1235	LEU	-	expression tag	UNP P0DTC2
D	1236	LEU	-	expression tag	UNP P0DTC2
D	1237	SER	-	expression tag	UNP P0DTC2
D	1238	THR	-	expression tag	UNP P0DTC2
D	1239	PHE	-	expression tag	UNP P0DTC2
D	1240	LEU	-	expression tag	UNP P0DTC2
D	1241	GLY	-	expression tag	UNP P0DTC2
D	1242	SER	-	expression tag	UNP P0DTC2
D	1243	SER	-	expression tag	UNP P0DTC2
D	1244	GLY	-	expression tag	UNP P0DTC2
D	1245	ARG	-	expression tag	UNP P0DTC2
D	1246	GLU	-	expression tag	UNP P0DTC2
D	1247	ASN	-	expression tag	UNP P0DTC2
D	1248	LEU	-	expression tag	UNP P0DTC2
D	1249	TYR	-	expression tag	UNP P0DTC2
D	1250	PHE	-	expression tag	UNP P0DTC2
D	1251	GLN	-	expression tag	UNP P0DTC2
D	1252	GLY	-	expression tag	UNP P0DTC2
D	1253	GLY	-	expression tag	UNP P0DTC2
D	1254	GLY	-	expression tag	UNP P0DTC2
D	1255	GLY	-	expression tag	UNP P0DTC2
D	1256	SER	-	expression tag	UNP P0DTC2
D	1257	GLY	-	expression tag	UNP P0DTC2
D	1258	LEU	-	expression tag	UNP P0DTC2
D	1259	ASN	-	expression tag	UNP P0DTC2
D	1260	ASP	-	expression tag	UNP P0DTC2
D	1261	ILE	-	expression tag	UNP P0DTC2
D	1262	PHE	-	expression tag	UNP P0DTC2
D	1263	GLU	-	expression tag	UNP P0DTC2
D	1264	ALA	-	expression tag	UNP P0DTC2
D	1265	GLN	-	expression tag	UNP P0DTC2
D	1266	LYS	-	expression tag	UNP P0DTC2
D	1267	ILE	-	expression tag	UNP P0DTC2
D	1268	GLU	-	expression tag	UNP P0DTC2
D	1269	TRP	-	expression tag	UNP P0DTC2
D	1270	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1271	GLU	-	expression tag	UNP P0DTC2
D	1272	GLY	-	expression tag	UNP P0DTC2
D	1273	HIS	-	expression tag	UNP P0DTC2
D	1274	HIS	-	expression tag	UNP P0DTC2
D	1275	HIS	-	expression tag	UNP P0DTC2
D	1276	HIS	-	expression tag	UNP P0DTC2
D	1277	HIS	-	expression tag	UNP P0DTC2
D	1278	HIS	-	expression tag	UNP P0DTC2
G	682	GLY	ARG	engineered mutation	UNP P0DTC2
G	683	SER	ARG	engineered mutation	UNP P0DTC2
G	685	SER	ARG	engineered mutation	UNP P0DTC2
G	817	PRO	PHE	engineered mutation	UNP P0DTC2
G	892	PRO	ALA	engineered mutation	UNP P0DTC2
G	899	PRO	ALA	engineered mutation	UNP P0DTC2
G	942	PRO	ALA	engineered mutation	UNP P0DTC2
G	986	PRO	LYS	engineered mutation	UNP P0DTC2
G	987	PRO	VAL	engineered mutation	UNP P0DTC2
G	1209	ALA	-	expression tag	UNP P0DTC2
G	1210	ALA	-	expression tag	UNP P0DTC2
G	1211	ALA	-	expression tag	UNP P0DTC2
G	1212	GLY	-	expression tag	UNP P0DTC2
G	1213	SER	-	expression tag	UNP P0DTC2
G	1214	GLY	-	expression tag	UNP P0DTC2
G	1215	TYR	-	expression tag	UNP P0DTC2
G	1216	ILE	-	expression tag	UNP P0DTC2
G	1217	PRO	-	expression tag	UNP P0DTC2
G	1218	GLU	-	expression tag	UNP P0DTC2
G	1219	ALA	-	expression tag	UNP P0DTC2
G	1220	PRO	-	expression tag	UNP P0DTC2
G	1221	ARG	-	expression tag	UNP P0DTC2
G	1222	ASP	-	expression tag	UNP P0DTC2
G	1223	GLY	-	expression tag	UNP P0DTC2
G	1224	GLN	-	expression tag	UNP P0DTC2
G	1225	ALA	-	expression tag	UNP P0DTC2
G	1226	TYR	-	expression tag	UNP P0DTC2
G	1227	VAL	-	expression tag	UNP P0DTC2
G	1228	ARG	-	expression tag	UNP P0DTC2
G	1229	LYS	-	expression tag	UNP P0DTC2
G	1230	ASP	-	expression tag	UNP P0DTC2
G	1231	GLY	-	expression tag	UNP P0DTC2
G	1232	GLU	-	expression tag	UNP P0DTC2
G	1233	TRP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1234	VAL	-	expression tag	UNP P0DTC2
G	1235	LEU	-	expression tag	UNP P0DTC2
G	1236	LEU	-	expression tag	UNP P0DTC2
G	1237	SER	-	expression tag	UNP P0DTC2
G	1238	THR	-	expression tag	UNP P0DTC2
G	1239	PHE	-	expression tag	UNP P0DTC2
G	1240	LEU	-	expression tag	UNP P0DTC2
G	1241	GLY	-	expression tag	UNP P0DTC2
G	1242	SER	-	expression tag	UNP P0DTC2
G	1243	SER	-	expression tag	UNP P0DTC2
G	1244	GLY	-	expression tag	UNP P0DTC2
G	1245	ARG	-	expression tag	UNP P0DTC2
G	1246	GLU	-	expression tag	UNP P0DTC2
G	1247	ASN	-	expression tag	UNP P0DTC2
G	1248	LEU	-	expression tag	UNP P0DTC2
G	1249	TYR	-	expression tag	UNP P0DTC2
G	1250	PHE	-	expression tag	UNP P0DTC2
G	1251	GLN	-	expression tag	UNP P0DTC2
G	1252	GLY	-	expression tag	UNP P0DTC2
G	1253	GLY	-	expression tag	UNP P0DTC2
G	1254	GLY	-	expression tag	UNP P0DTC2
G	1255	GLY	-	expression tag	UNP P0DTC2
G	1256	SER	-	expression tag	UNP P0DTC2
G	1257	GLY	-	expression tag	UNP P0DTC2
G	1258	LEU	-	expression tag	UNP P0DTC2
G	1259	ASN	-	expression tag	UNP P0DTC2
G	1260	ASP	-	expression tag	UNP P0DTC2
G	1261	ILE	-	expression tag	UNP P0DTC2
G	1262	PHE	-	expression tag	UNP P0DTC2
G	1263	GLU	-	expression tag	UNP P0DTC2
G	1264	ALA	-	expression tag	UNP P0DTC2
G	1265	GLN	-	expression tag	UNP P0DTC2
G	1266	LYS	-	expression tag	UNP P0DTC2
G	1267	ILE	-	expression tag	UNP P0DTC2
G	1268	GLU	-	expression tag	UNP P0DTC2
G	1269	TRP	-	expression tag	UNP P0DTC2
G	1270	HIS	-	expression tag	UNP P0DTC2
G	1271	GLU	-	expression tag	UNP P0DTC2
G	1272	GLY	-	expression tag	UNP P0DTC2
G	1273	HIS	-	expression tag	UNP P0DTC2
G	1274	HIS	-	expression tag	UNP P0DTC2
G	1275	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1276	HIS	-	expression tag	UNP P0DTC2
G	1277	HIS	-	expression tag	UNP P0DTC2
G	1278	HIS	-	expression tag	UNP P0DTC2

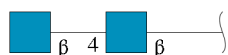
- Molecule 2 is a protein called Ab765 heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	119	Total	C	H	N	O	S	0	0
			1797	577	880	162	175	3		

- Molecule 3 is a protein called Ab765 light chain.

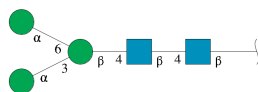
Mol	Chain	Residues	Atoms						AltConf	Trace
3	F	110	Total	C	H	N	O	S	0	0
			1581	507	770	134	166	4		

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	2	Total	C	H	N	O	0	0
			53	16	25	2	10		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	5	Total	C	H	N	O	0	0
			113	34	52	2	25		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
6	G	1	27	8	13	1	5	0

[illegible]

- Molecule 1: Spike glycoprotein

Chain D: 14% . 84%

ARG	GLN	TTR	VAL	ALA	GLY	THR	CYS	LEU	GLY	ASN	ASN	MET
SER	TYR	THR	TYR	VAL	GLY	THR	THR	LEU	LEU	VAL	ASN	THR
PRO	GLY	MET	SER	ARG	THR	LYS	THR	ALA	ALA	THR	ASN	VAL
ILE	SER	SER	THR	ASP	PRO	LYS	LYS	LEU	LEU	THR	THR	THR
GLU	PHE	LEU	GLY	PRO	ASP	SER	SER	HIS	HIS	ASN	ASN	PHE
ASP	CYS	GLY	SER	GLN	THR	PHE	THR	ARG	ARG	VAL	VAL	VAL
LEU	TYR	ALA	ASN	THR	THR	THR	THR	SER	SER	LYS	ALA	LEU
LEU	GLN	GLU	VAL	LEU	LEU	VAL	VAL	TYR	TYR	ASN	ILE	LEU
PHE	ASN	ASN	PHE	ILE	GLU	GLU	GLU	LEU	LEU	VAL	HIS	PRO
ASN	ARG	VAL	THR	LEU	THR	LYS	LYS	THR	THR	VAL	VAL	VAL
LYS	ALA	ALA	ARG	ASP	THR	ILE	ILE	PRO	PRO	CYS	SER	VAL
VAL	ALA	VAL	THR	ASP	ASP	TYR	TYR	ASP	ASP	GLY	THR	SER
THR	LEU	TTR	ALA	ILE	THR	THR	THR	THR	THR	PHE	THR	SER
LEU	THR	ASN	GLY	THR	GLY	GLN	GLN	SER	SER	GLN	ASN	GLN
ALA	GLY	ASN	CYS	PRO	LEU	THR	THR	SER	PHE	THR	ASN	CYS
ASP	ILE	ASN	LEU	CYS	SER	SER	SER	SER	SER	ASN	VAL	ASN
ALA	ALA	ALA	ILE	SER	THR	ASN	ASN	GLY	ILE	ASN	LYS	ASN
GLY	VAL	ILE	GLY	PHE	GLY	THR	PHE	THR	THR	ASP	ASP	LEU
PHE	GLU	ALA	ALA	GLY	LEU	VAL	ARG	ARG	THR	PRO	ARG	THR
ILE	GLN	ILE	GLU	GLY	VAL	VAL	VAL	ALA	ALA	PHE	THR	THR
LYS	ASP	PRO	HIS	VAL	VAL	GLN	GLN	GLY	GLY	ASN	ASN	ARG
GLN	LYS	THR	VAL	SER	SER	PRO	THR	ALA	ALA	VAL	VAL	GLN
TYR	ASN	ASN	ASN	VAL	LYS	THR	THR	ALA	ILE	TYR	THR	LEU
GLY	THR	PHE	ASN	ILE	CYS	VAL	GLU	ALA	ALA	LEU	LEU	LEU
ASP	GLN	THR	SER	THR	VAL	THR	THR	TYR	TYR	TTR	PRO	PRO
CYS	ASN	ILE	TYR	PRO	GLY	ILE	ILE	VAL	VAL	HIS	PHE	PRO
LEU	VAL	SER	GLU	GLY	PHE	ASN	VAL	VAL	VAL	ASN	ASN	ALA
ASP	ALA	VAL	CYS	THR	ASN	ARG	ARG	THR	THR	GLY	ASN	THR
ILE	GLN	THR	ILE	THR	PHE	ASN	F329	TYR	TYR	ASN	GLY	THR
ALA	VAL	GLU	PRO	SER	GLY	ASN	N334	GLN	GLN	LYS	VAL	ASN
ARG	GLN	ILE	ILE	ASN	LEU	LEU	L335	PRO	PRO	SER	THR	PHE
ASP	ILE	PRO	GLY	GLN	THR	THR	V350	ARG	ARG	ALA	THR	THR
LEU	TYR	VAL	ALA	VAL	GLY	GLY		THR	PHE	GLU	SER	ARG
ILE	LYS	SER	ILE	VAL	THR	THR	D364	LEU	LEU	GLU	THR	VAL
CYS	THR	MET	CYS	LEU	GLY	GLY		LEU	LEU	PHE	GLU	VAL
ALA	PRO	ALA	ALA	TYR	VAL	VAL		LEU	LEU	TYR	LYS	TYR
GLN	PRO	LYS	SER	GLN	LEU	LEU	V367	LYS	GLN	ARG	SER	SER
ILE	LYS	THR	THR	ASP	THR	THR		ASN	ASN	VAL	ILE	ASN
PHE	LYS	SER	GLN	VAL	GLU	GLU	T393	GLU	PHE	TTR	ILE	LYS
ASN	ASP	VAL	THR	ASN	SER	SER	N394	ASN	SER	SER	ARG	VAL
GLY	PHE	ASP	GLN	CYS	ASN	LYS	V395	ASN	ALA	SER	ARG	VAL
LEU	THR	CYS	GLN	THR	THR	THR		GLY	LEU	PHE	GLY	THR
THR	GLY	CYS	THR	GLU	GLY	GLY	1402	THR	GLU	ALA	GLY	ARG
VAL	PHE	MET	SER	GLU	PHE	PHE	R403	ILE	PRO	ASN	ILE	THR
LEU	ASN	TYR	PRO	VAL	LEU	LEU		THR	LEU	CYS	PHE	SER
PRO	PHE	ILE	GLY	VAL	PRO	PRO	E406	ASP	VAL	THR	GLY	VAL
PRO	SER	CYS	SER	ALA	PHE	PHE		ALA	ASP	PHE	GLU	THR
LEU	GLN	GLY	ILE	GLN	GLN	GLN	T418	VAL	VAL	THR	THR	HIS
THR	LEU	ASP	SER	ILE	PHE	PHE	N422	CYS	ILE	VAL	ASP	THR
THR	LEU	THR	SER	ALA	GLY	GLY		ALA	GLY	SER	GLN	GLN
ASP	PRO	THR	VAL	ASP	ARG	ARG	N440	LEU	ILE	LYS	LYS	THR
GLU	ASP	GLU	ALA	GLN	ASP	ASP	L441	ASP	ASN	PRO	THR	LEU
MET	PRO	CYS	SER	LEU	ILE	ILE		PRO	ILE	GLN	GLN	PHE
ILE	ALA	SER	THR	THR	ALA	ALA	R454	SER	THR	LEU	LEU	THR
ALA	LYS	ASN	PRO	PRO	ASP	ASP		THR	ARG	MET	LEU	PRO
GLN	PRO	LEU	ILE	THR	THR	THR	R457	GLU	PHE	ASP	LEU	THR
TYR	LYS	LEU	ILE	TTR	THR	THR		THR	GLN	THR	ILE	SER
							N467	LYS	THR	THR	VAL	SER

LEU	LEU	SER	ILE	SER	ARG	GLN	SER
LEU	SER	VAL	THR	ALA	LEU	ASP	ALA
SER	VAL	VAL	THR	PRO	ILE	SER	LEU
THR	ASN	ASN	ASP	HIS	THR	LEU	LEU
PHE	ILE	ILE	ASN	GLY	GLY	SER	GLY
LEU	GLN	GLN	THR	VAL	ARG	SER	THR
GLY	LYS	PHE	VAL	VAL	LEU	THR	ILE
SER	GLU	VAL	THR	PHE	GLN	PRO	GLY
SER	GLU	VAL	THR	HIS	LEU	ALA	SER
GLY	ASP	ILE	GLY	HIS	SER	ALA	THR
ARG	GLU	ASN	ASN	VAL	GLN	LEU	GLY
LEU	LEU	THR	CYS	THR	THR	GLY	THR
ASN	ASN	ASP	ASP	TYR	TYR	LYS	THR
LEU	GLU	VAL	VAL	VAL	VAL	LEU	PHE
TYR	VAL	THR	VAL	PRO	THR	GLN	GLY
PHE	ALA	ILE	ILE	GLN	ALA	ASP	ALA
GLN	LYS	GLY	GLY	GLN	GLN	VAL	GLY
ASN	ASN	ILE	ILE	GLU	LEU	VAL	PRO
GLY	GLY	LEU	VAL	LYS	ILE	ASN	ALA
GLY	GLY	ASN	ASN	ASN	ARG	GLN	LEU
GLY	GLU	GLU	ASN	PHE	ALA	ASN	GLN
SER	SER	SER	THR	THR	ALA	ALA	ILE
GLY	LEU	ILE	VAL	THR	GLU	GLN	PRO
LEU	LEU	TYR	TYR	ALA	ILE	ALA	PHE
ASN	ASN	ASP	ASP	PRO	ARG	LEU	PRO
ASP	ILE	GLN	LEU	ILE	ALA	ASN	GLN
PHE	PHE	GLU	GLN	CYS	ALA	LEU	MET
GLU	GLU	LEU	PRO	HIS	ASN	VAL	ALA
ALA	ALA	GLY	GLU	ASP	LEU	LYS	TYR
GLN	LYS	LYS	LEU	GLY	ALA	GLN	ARG
LYS	ILE	GLU	SER	LYS	ALA	LEU	PHE
ILE	GLU	GLN	PHE	HIS	THR	SER	GLY
GLU	GLU	GLN	GLN	PHE	LYS	SER	ASN
TRP	ALA	ALA	LYS	PHE	MET	ASN	ILE
HIS	HIS	ALA	GLU	PRO	SER	PHE	GLY
GLU	GLU	ALA	GLU	ARG	GLU	GLY	VAL
HIS	HIS	SER	LEU	GLY	VAL	ILE	THR
HIS	HIS	GLY	TYR	VAL	GLY	SER	ASN
HIS	ILE	ILE	PHE	VAL	GLN	VAL	LEU
		PRO	LYS	SER	SER	LEU	TYR
		GLU	ASN	ASN	LYS	LEU	GLU
		ALA	HIS	GLY	ARG	ASP	ASN
		PRO	THR	THR	VAL	ILE	GLN
		ARG	SER	HIS	ASP	LEU	LYS
		ASP	PRO	TRP	PHE	SER	LEU
		GLY	ASP	PHE	CYS	ARG	ILE
		GLN	VAL	VAL	GLY	LEU	ALA
		ALA	ASP	THR	LYS	ASP	ASN
		TYR	GLN	GLN	GLY	PRO	PHE
		VAL	GLY	ARG	TYR	GLU	ASN
		ARG	ASP	ASN	HIS	ALA	SER
		LYS	ILE	LYS	MET	GLU	ILE
		ASP	SER	TYR	GLY	VAL	GLY
		GLY	ILE	PHE	PHE	GLN	ILE
		GLU	ASN	GLN	GLN	ILE	LYS
		TRP	VAL	THR	ASN	ASP	THR

- Molecule 1: Spike glycoprotein

Chain G: 13% 84%

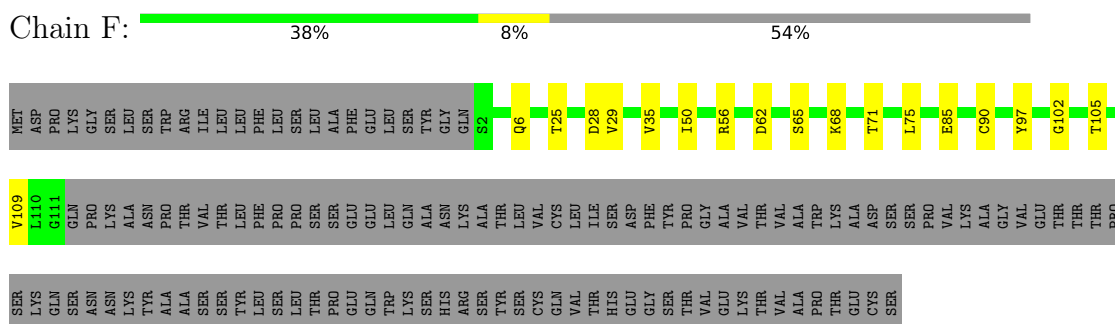
ALA	ILE	GLN	N448	CYS	LEU	GLY	ASN	ASN	ASN	MET
SER	HIS	PHE	N449	THR	LEU	LYS	ASN	PHE	THR	PHE
VAL	ALA	GLY	N450	LEU	ALA	GLN	ALA	VAL	THR	VAL
ASP	GLN	ARG	R454	LYS	LEU	GLY	THR	THR	TRP	THR
SER	LEU	ASP	R454	SER	HIS	ASN	ASN	PHE	HIS	VAL
GLN	LEU	ILE	R457	PHE	ARG	PHE	VAL	VAL	ALA	LEU
THR	PRO	ALA	R457	THR	SER	LYS	ASN	THR	ALA	LEU
ILE	THR	THR	D467	VAL	TYR	ASN	THR	THR	HIS	PRO
ALA	ARG	ASP	I468	GLN	THR	PHE	GLN	VAL	VAL	LEU
THR	VAL	ALA	S469	ILE	GLY	GLY	CYS	GLY	SER	VAL
THR	TYR	VAL	T470	TYR	ASP	VAL	PHE	GLY	GLY	SER
TYR	SER	ARG	E471	THR	THR	THR	ASN	THR	THR	SER
GLY	SER	ASP	Q498	THR	SER	LYS	ASN	GLY	GLY	SER
PHE	GLY	PRO	V512	SER	GLY	ILE	ASN	THR	THR	SER
THR	ASN	THR	V512	PHE	TRP	ASP	ASP	ARG	THR	THR
GLN	VAL	LEU	F515	ARG	THR	GLY	PRO	PHE	THR	THR
ASN	PHE	GLU	F515	VAL	ALA	TYR	PHE	ASP	THR	THR
SER	GLN	ILE	I518	GLN	GLY	PHE	GLY	GLN	ASN	THR
ARG	THR	LEU	I518	PRO	ALA	THR	GLY	THR	PRO	THR
VAL	THR	VAL	C525	THR	ALA	ILE	VAL	VAL	VAL	GLN
ALA	ALA	ASP	C525	THR	ALA	THR	VAL	VAL	VAL	LEU
LEU	ALA	ILE	R528	SER	TYR	THR	THR	THR	LEU	LEU
THR	GLY	THR	R528	ASN	SER	SER	PRO	PRO	PRO	PRO
ILE	CYS	PRO	LYS	ILE	TYR	THR	HIS	PHE	PHE	ASN
ASN	ILE	CYS	SER	ARG	GLY	THR	LYS	ASN	ASN	TYR
SER	ILE	PHE	THR	THR	THR	ASN	ASN	GLY	GLY	THR
VAL	GLY	THR	ASN	F329	LEU	ILE	LYS	VAL	VAL	ASN
ALA	ALA	GLY	LEU	N334	GLN	ASN	THR	THR	THR	SER
GLN	GLU	VAL	N334	ASN	PRO	ASN	SER	THR	THR	SER
ASN	HIS	VAL	LYS	N343	ARG	VAL	THR	ALA	ALA	THR
ASN	ASN	VAL	ASN	N343	THR	ARG	GLY	SER	THR	ARG
THR	ASN	ILE	LYS	V350	PHE	ASP	THR	GLY	GLY	GLY
SER	SER	THR	CYS	Y351	LEU	LEU	SER	GLU	GLU	VAL
THR	THR	THR	VAL	Y351	LEU	PRO	THR	LYS	LYS	THR
ILE	TYR	PRO	ASN	I358	LEU	GLY	ARG	THR	THR	THR
ALA	CYS	PHE	ASN	I358	LYS	GLN	THR	ASN	ASN	PRO
THR	THR	THR	PHE	C391	ASN	PHE	TYR	ILE	ILE	LYS
GLN	ILE	THR	ASN	C391	GLU	SER	SER	THR	THR	LYS
VAL	PRO	SER	GLY	V395	ASN	ALA	SER	ARG	VAL	VAL
ILE	ILE	ASN	LEU	V395	GLY	ALA	THR	THR	THR	THR
GLN	GLY	GLN	THR	R403	THR	LEU	ALA	GLY	GLY	PHE
VAL	ALA	VAL	GLY	G404	ILE	PRO	ASN	THR	THR	THR
VAL	GLY	ALA	THR	D405	THR	LEU	CYS	PHE	GLY	SER
SER	ILE	VAL	GLY	E406	ASP	VAL	THR	THR	GLY	LEU
THR	CYS	LEU	VAL	I418	ALA	ASP	PHE	THR	THR	LEU
PRO	ALA	TYR	LEU	I418	VAL	LEU	THR	GLU	THR	HIS
THR	SER	GLN	THR	T430	ASP	PRO	THR	THR	THR	THR
VAL	TYR	THR	GLU	T430	CYS	ILE	SER	GLN	ASP	THR
ASN	GLN	VAL	SER	V433	ALA	GLY	THR	GLN	GLY	THR
CYS	THR	ASN	ASN	V433	LEU	THR	LYS	LYS	LYS	ASP
THR	GLN	CYS	LYS	N439	ASP	ASN	PRO	PRO	THR	LEU
GLY	THR	THR	LYS	N439	PRO	ILE	PHE	PHE	GLN	THR
THR	ASN	GLU	PHE	S443	LEU	ARG	THR	LEU	GLN	PHE
PHE	SER	VAL	VAL	S443	SER	THR	THR	LEU	SER	THR
ASN	PRO	PRO	PRO	K444	GLU	PHE	ASN	MET	LEU	PRO
THR	GLY	VAL	PHE	V445	THR	GLN	THR	THR	THR	THR
CYS	SER	ALA	THR	V445	LYS	THR	THR	THR	VAL	SER

[illegible]

- Molecule 2: Ab765 heavy chain



- Molecule 3: Ab765 light chain

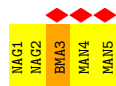
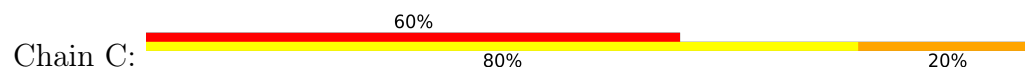


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	167456	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)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.041	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00703	Depositor
Map size (Å)	180.722, 180.722, 180.722	wwPDB
Map dimensions	218, 218, 218	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.829, 0.829, 0.829	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

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	0.11	0/1612	0.31	1/2194 (0.0%)
1	D	0.11	0/1641	0.24	0/2233
1	G	0.10	0/1632	0.23	0/2222
2	E	0.11	0/937	0.23	0/1273
3	F	0.10	0/832	0.23	0/1133
All	All	0.11	0/6654	0.25	1/9055 (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	478	THR	OG1-CB-CG2	5.74	120.78	109.30

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	1568	1489	1489	15	0
1	D	1595	1518	1518	15	0
1	G	1586	1505	1505	22	0
2	E	917	880	882	15	0
3	F	811	770	770	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	28	25	25	1	0
5	C	61	52	52	4	0
6	G	14	13	13	3	0
All	All	6580	6252	6254	82	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 6.

All (82) 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)
5:C:1:NAG:O3	5:C:2:NAG:O5	1.89	0.91
1:D:457:ARG:NH1	1:D:467:ASP:OD2	2.20	0.74
5:C:2:NAG:O3	5:C:3:BMA:O5	2.06	0.71
1:A:393:THR:O	1:A:394:ASN:ND2	2.26	0.69
1:D:440:ASN:OD1	1:D:441:LEU:N	2.29	0.66
1:G:439:ASN:O	1:G:443:SER:OG	2.12	0.66
6:G:1301:NAG:O3	6:G:1301:NAG:O7	2.14	0.66
1:D:395:VAL:HG23	1:D:524:VAL:HG11	1.77	0.66
1:G:405:ASP:OD1	1:G:406:GLU:N	2.29	0.65
1:A:353:TRP:O	1:A:466:ARG:NH1	2.30	0.64
1:A:498:GLN:N	1:A:501:ASN:OD1	2.28	0.64
3:F:6:GLN:NE2	3:F:105:THR:OG1	2.30	0.64
3:F:29:VAL:HG12	3:F:35:VAL:HG22	1.79	0.63
1:G:343:ASN:OD1	6:G:1301:NAG:N2	2.32	0.62
1:D:493:GLN:NE2	1:D:494:SER:O	2.33	0.62
2:E:8:GLY:HA2	2:E:115:THR:HG21	1.82	0.61
3:F:29:VAL:O	3:F:68:LYS:NZ	2.33	0.61
3:F:71:THR:O	3:F:71:THR:HG22	2.03	0.58
1:G:457:ARG:NE	1:G:467:ASP:OD2	2.33	0.58
1:G:350:VAL:HG21	1:G:418:ILE:HD11	1.86	0.58
2:E:19:ARG:NE	2:E:82:GLN:OE1	2.36	0.57
1:G:403:ARG:NH1	1:G:405:ASP:OD2	2.38	0.57
2:E:13:GLN:N	2:E:13:GLN:OE1	2.39	0.56
1:A:361:CYS:SG	1:A:362:VAL:N	2.79	0.55
1:G:471:GLU:N	1:G:471:GLU:OE1	2.39	0.54
3:F:85:GLU:OE2	3:F:109:VAL:N	2.40	0.54
1:G:470:THR:HG23	1:G:470:THR:O	2.08	0.54
5:C:2:NAG:C3	5:C:3:BMA:O5	2.56	0.53
1:A:468:ILE:HG22	1:A:468:ILE:O	2.10	0.52
1:A:471:GLU:N	1:A:471:GLU:OE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:364:ASP:O	1:D:367:VAL:HG12	2.10	0.52
3:F:50:ILE:HD12	3:F:75:LEU:HD13	1.92	0.51
1:A:345:THR:HG23	1:A:346:ARG:HG2	1.93	0.50
1:D:393:THR:O	1:D:523:THR:OG1	2.29	0.50
1:G:454:ARG:NH2	1:G:469:SER:O	2.45	0.50
3:F:97:TYR:OH	1:G:498:GLN:NE2	2.44	0.50
1:G:433:VAL:HG23	1:G:512:VAL:HG12	1.93	0.50
5:C:1:NAG:HO3	5:C:2:NAG:C1	2.14	0.50
2:E:78:VAL:HG12	2:E:79:LEU:N	2.27	0.50
1:G:395:VAL:HG23	1:G:515:PHE:HD1	1.76	0.50
2:E:67:ARG:NH2	2:E:90:ASP:OD2	2.40	0.49
3:F:90:CYS:O	3:F:102:GLY:N	2.46	0.49
1:G:391:CYS:HA	1:G:525:CYS:CB	2.42	0.49
2:E:116:LEU:H	2:E:116:LEU:HD23	1.77	0.48
1:A:467:ASP:OD1	1:A:467:ASP:O	2.32	0.48
1:G:391:CYS:HA	1:G:525:CYS:HB3	1.95	0.48
1:G:448:ASN:OD1	1:G:450:ASN:ND2	2.46	0.48
1:A:493:GLN:NE2	1:A:494:SER:O	2.48	0.47
3:F:25:THR:HG22	3:F:28:ASP:OD2	2.14	0.47
1:D:418:ILE:HD11	1:D:495:TYR:OH	2.15	0.47
1:D:395:VAL:CG2	1:D:524:VAL:HG11	2.43	0.47
1:D:402:ILE:HG22	1:D:403:ARG:N	2.31	0.46
1:D:454:ARG:NH2	1:D:467:ASP:O	2.47	0.46
4:B:1:NAG:O7	4:B:1:NAG:O3	2.30	0.46
1:G:430:THR:HG23	1:G:430:THR:O	2.15	0.46
2:E:101:GLU:OE1	1:G:445:VAL:HG23	2.16	0.46
2:E:62:ASP:OD2	2:E:62:ASP:N	2.45	0.46
1:G:343:ASN:OD1	6:G:1301:NAG:C2	2.64	0.45
1:D:470:THR:HG22	1:D:470:THR:O	2.16	0.45
2:E:52:SER:O	2:E:72:ARG:NH1	2.47	0.44
1:A:433:VAL:HG12	1:A:512:VAL:HG23	2.00	0.44
1:D:406:GLU:OE1	1:D:418:ILE:HD12	2.18	0.43
1:D:334:ASN:O	1:D:335:LEU:HD22	2.18	0.43
2:E:52:SER:OG	2:E:53:TYR:N	2.51	0.43
1:D:350:VAL:HG12	1:D:422:ASN:HB3	2.00	0.43
1:G:358:ILE:HB	1:G:395:VAL:HG13	2.00	0.43
1:A:343:ASN:O	1:A:344:ALA:O	2.37	0.42
2:E:50:LEU:HD23	2:E:51:ILE:N	2.33	0.42
1:A:440:ASN:OD1	1:A:441:LEU:N	2.52	0.42
2:E:36:TRP:O	2:E:48:VAL:HG22	2.20	0.42
1:A:454:ARG:NH2	1:A:467:ASP:O	2.47	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:395:VAL:HG23	1:G:515:PHE:CD1	2.55	0.42
2:E:8:GLY:CA	2:E:115:THR:HG21	2.50	0.41
2:E:8:GLY:HA2	2:E:20:LEU:HD22	2.02	0.41
3:F:65:SER:O	3:F:75:LEU:HD12	2.20	0.41
1:A:445:VAL:HG13	1:A:446:GLY:N	2.36	0.41
1:A:428:ASP:O	1:A:428:ASP:OD1	2.38	0.41
3:F:56:ARG:NH2	3:F:62:ASP:OD1	2.54	0.40
1:G:334:ASN:OD1	1:G:334:ASN:N	2.54	0.40
1:D:393:THR:HG22	1:D:516:GLU:O	2.20	0.40
2:E:91:THR:O	2:E:91:THR:HG23	2.20	0.40
1:G:350:VAL:HG13	1:G:351:TYR:N	2.35	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	196/1278 (15%)	182 (93%)	13 (7%)	1 (0%)	24	55
1	D	199/1278 (16%)	192 (96%)	7 (4%)	0	100	100
1	G	198/1278 (16%)	189 (96%)	9 (4%)	0	100	100
2	E	117/261 (45%)	110 (94%)	7 (6%)	0	100	100
3	F	108/240 (45%)	98 (91%)	10 (9%)	0	100	100
All	All	818/4335 (19%)	771 (94%)	46 (6%)	1 (0%)	49	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	344	ALA

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	171/1108 (15%)	171 (100%)	0	100	100
1	D	174/1108 (16%)	174 (100%)	0	100	100
1	G	173/1108 (16%)	173 (100%)	0	100	100
2	E	94/218 (43%)	94 (100%)	0	100	100
3	F	90/204 (44%)	90 (100%)	0	100	100
All	All	702/3746 (19%)	702 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	394	ASN
1	A	519	HIS
3	F	39	GLN
1	G	487	ASN
1	G	498	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](#)

7 monosaccharides are modelled in this entry.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	1	4,1	14,14,15	0.30	0	17,19,21	0.44	0
4	NAG	B	2	4	14,14,15	0.23	0	17,19,21	0.49	0
5	NAG	C	1	1,5	14,14,15	0.22	0	17,19,21	0.52	0
5	NAG	C	2	5	14,14,15	0.31	0	17,19,21	0.73	0
5	BMA	C	3	5	11,11,12	0.89	1 (9%)	15,15,17	0.72	0
5	MAN	C	4	5	11,11,12	0.60	0	15,15,17	1.09	2 (13%)
5	MAN	C	5	5	11,11,12	0.64	0	15,15,17	0.94	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	B	2	4	-	0/6/23/26	0/1/1/1
5	NAG	C	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	C	2	5	-	1/6/23/26	0/1/1/1
5	BMA	C	3	5	-	2/2/19/22	0/1/1/1
5	MAN	C	4	5	-	2/2/19/22	1/1/1/1
5	MAN	C	5	5	-	1/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	3	BMA	C1-C2	2.31	1.57	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	4	MAN	C1-O5-C5	3.12	116.36	112.19
5	C	5	MAN	C1-O5-C5	2.16	115.08	112.19
5	C	5	MAN	O2-C2-C3	-2.15	105.69	110.15
5	C	4	MAN	O2-C2-C3	-2.14	105.72	110.15

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	3	BMA	C4-C5-C6-O6
5	C	3	BMA	O5-C5-C6-O6
5	C	4	MAN	C4-C5-C6-O6
5	C	4	MAN	O5-C5-C6-O6
5	C	1	NAG	C4-C5-C6-O6
5	C	1	NAG	O5-C5-C6-O6
5	C	5	MAN	O5-C5-C6-O6
5	C	2	NAG	O5-C5-C6-O6
4	B	1	NAG	C3-C2-N2-C7
5	C	1	NAG	C3-C2-N2-C7
4	B	1	NAG	C4-C5-C6-O6
5	C	1	NAG	C1-C2-N2-C7

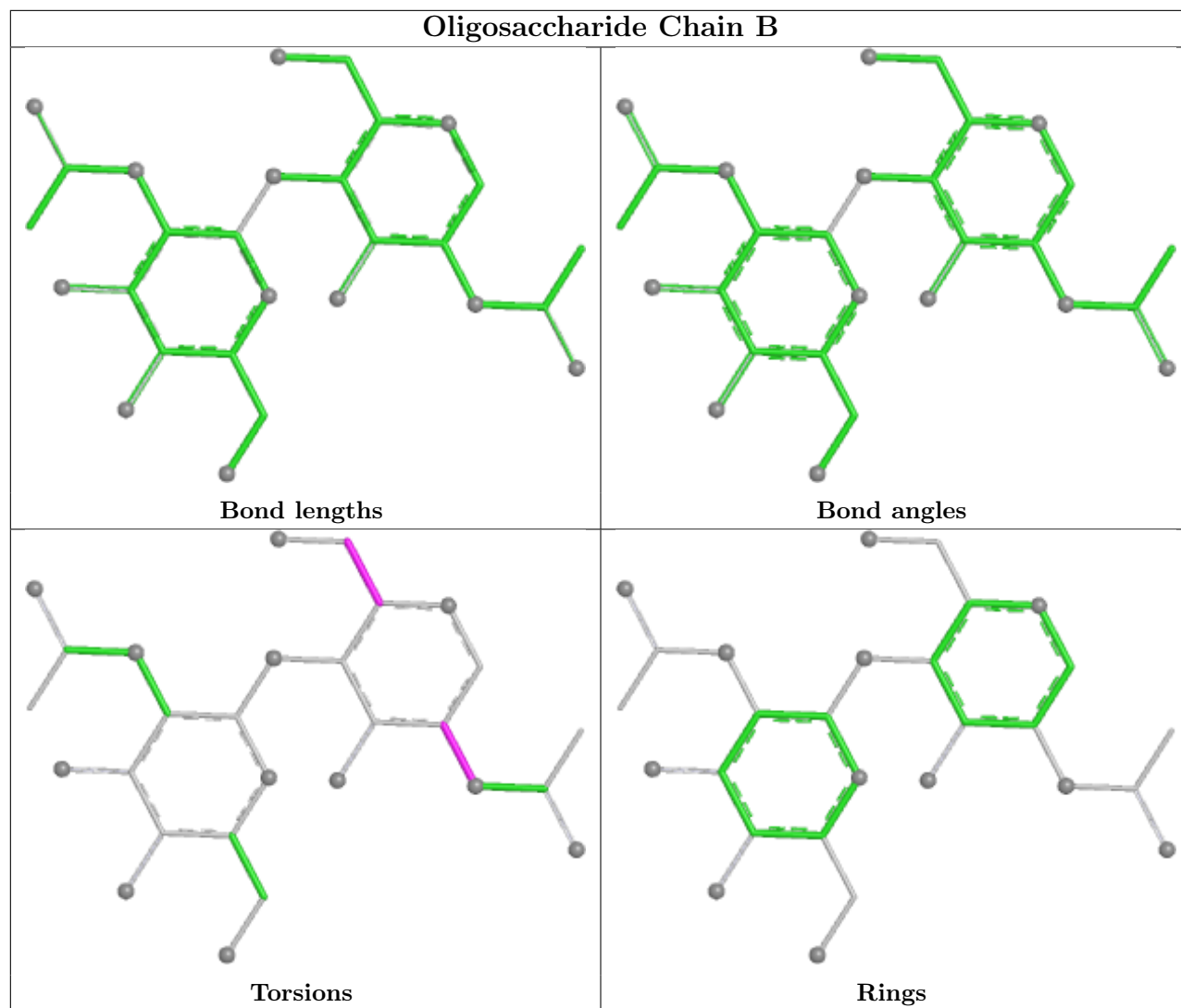
All (1) ring outliers are listed below:

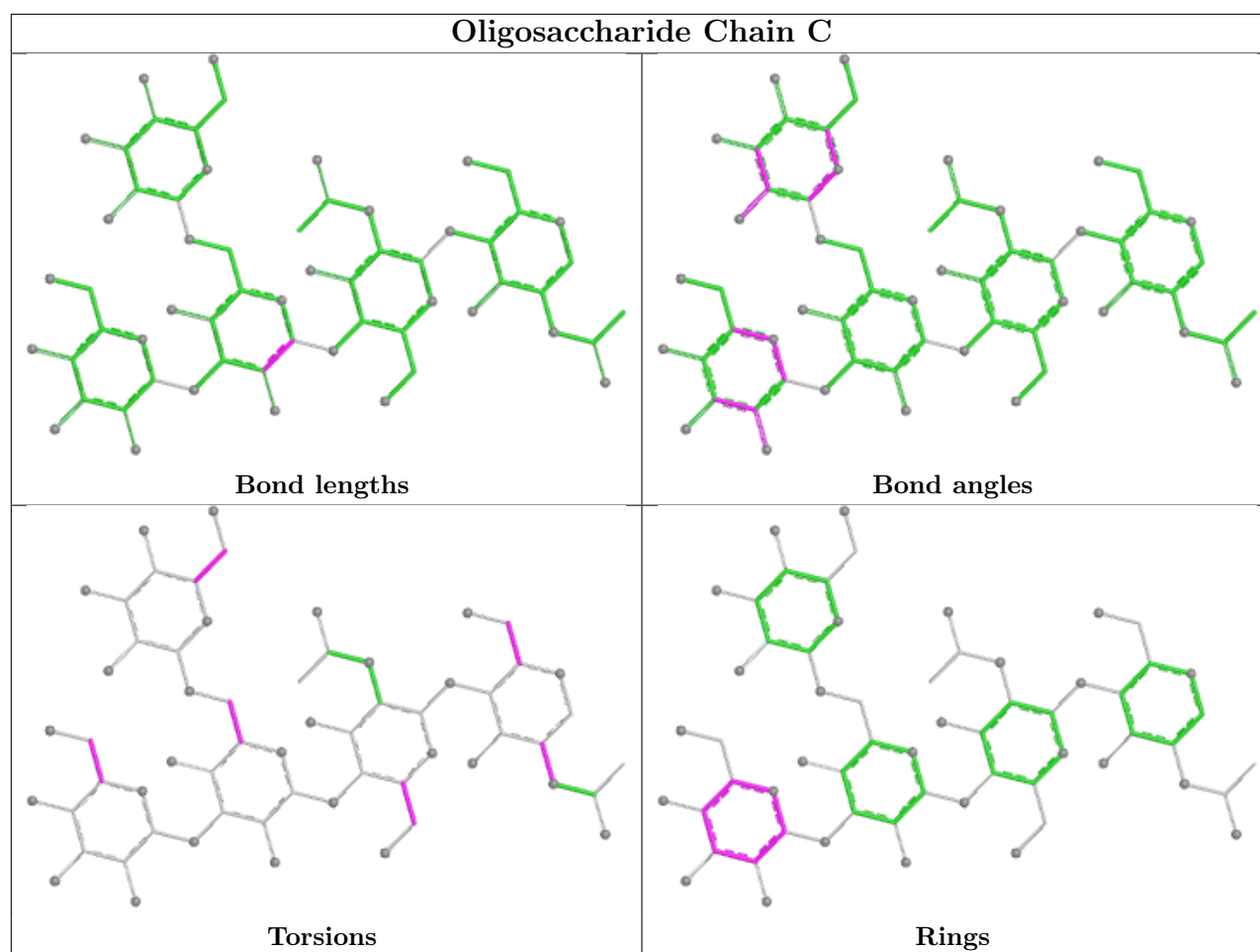
Mol	Chain	Res	Type	Atoms
5	C	4	MAN	C1-C2-C3-C4-C5-O5

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	2	NAG	4	0
5	C	3	BMA	2	0
4	B	1	NAG	1	0
5	C	1	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
6	NAG	G	1301	1	14,14,15	0.41	0	17,19,21	0.49	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
6	NAG	G	1301	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

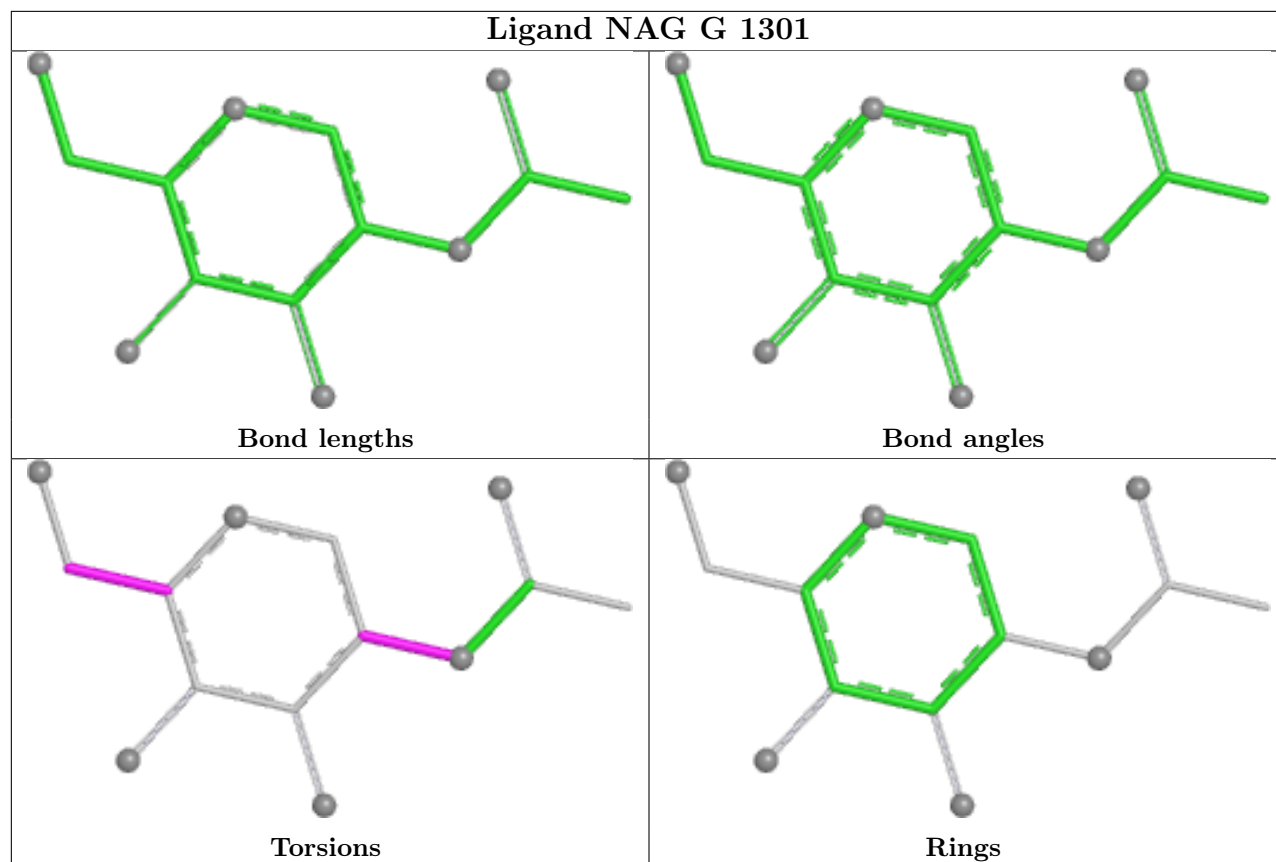
Mol	Chain	Res	Type	Atoms
6	G	1301	NAG	O5-C5-C6-O6
6	G	1301	NAG	C1-C2-N2-C7
6	G	1301	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	1301	NAG	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

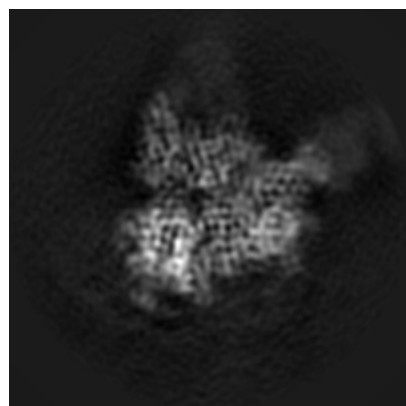
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33065. These allow visual inspection of the internal detail of the map and identification of artifacts.

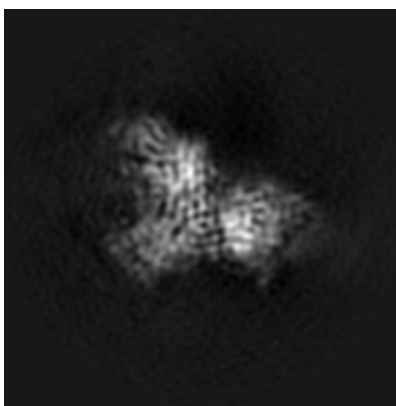
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

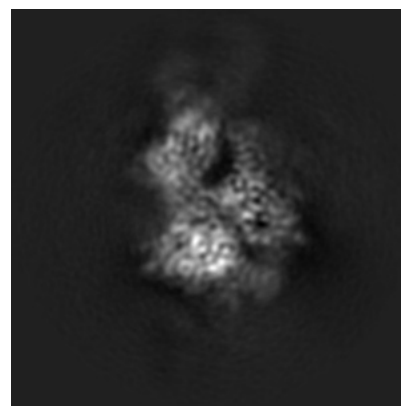
6.1.1 Primary map



X

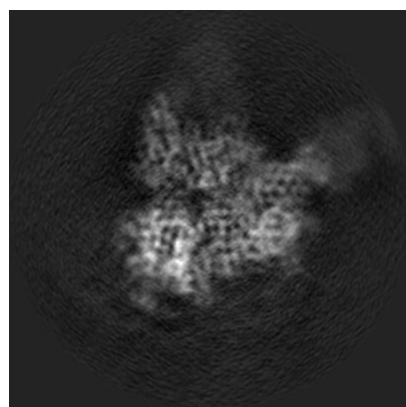


Y

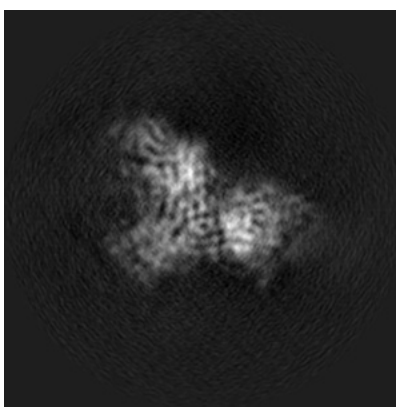


Z

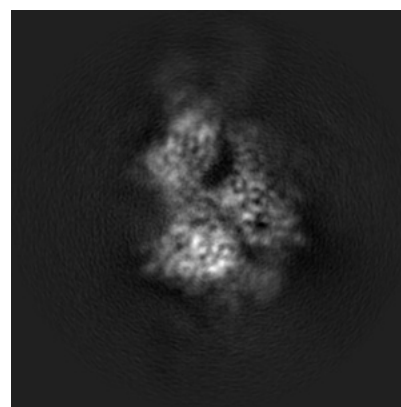
6.1.2 Raw map



X



Y

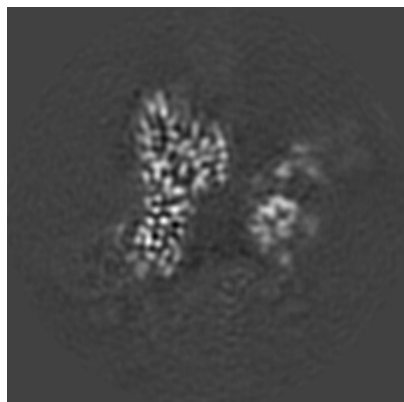


Z

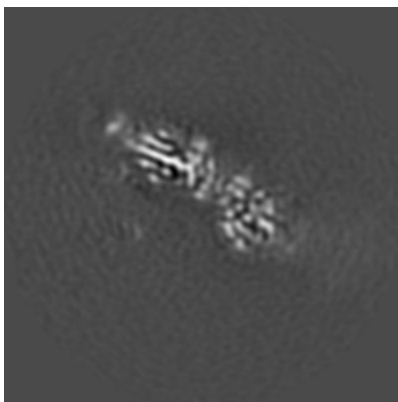
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

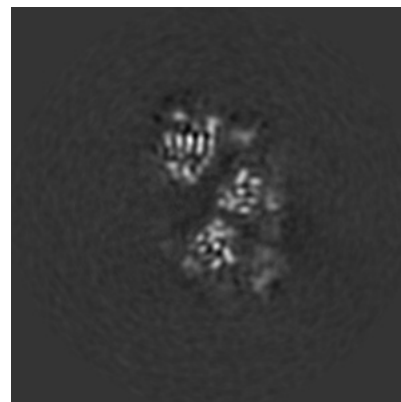
6.2.1 Primary map



X Index: 109

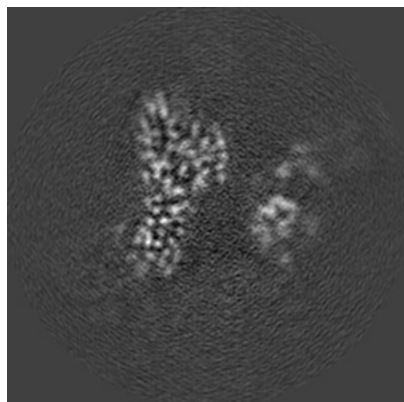


Y Index: 109

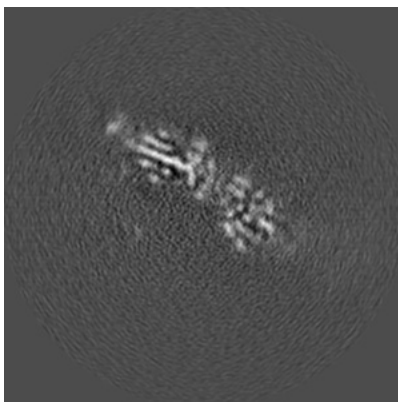


Z Index: 109

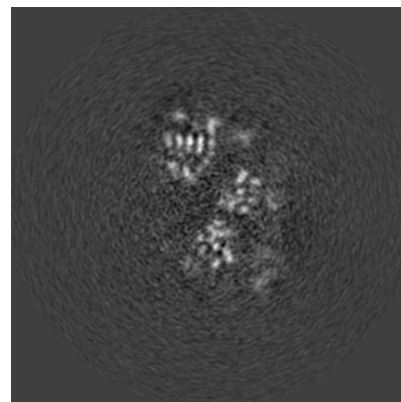
6.2.2 Raw map



X Index: 109



Y Index: 109

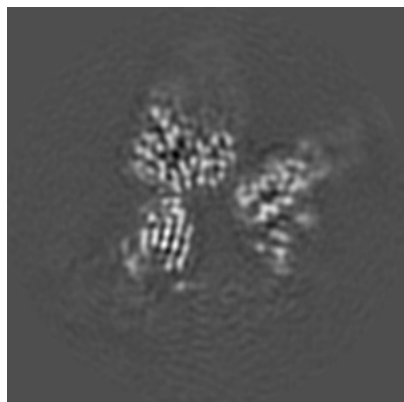


Z Index: 109

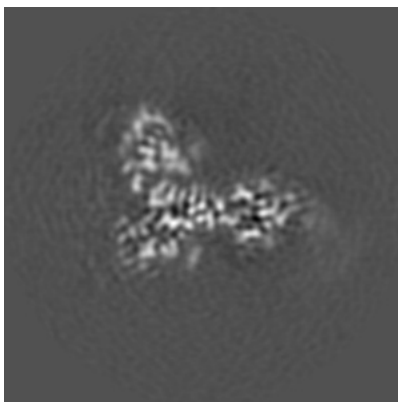
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

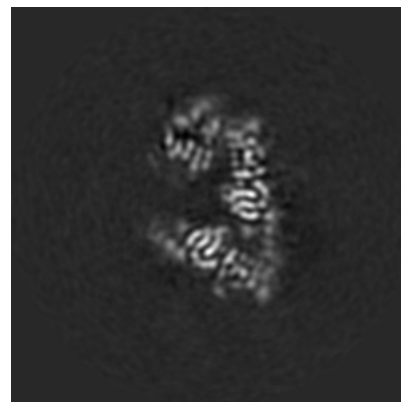
6.3.1 Primary map



X Index: 102

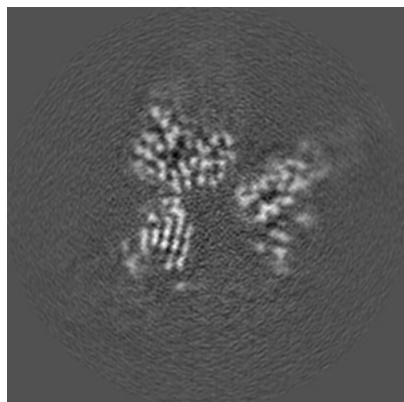


Y Index: 92

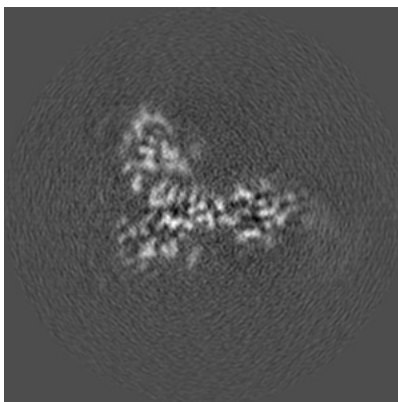


Z Index: 101

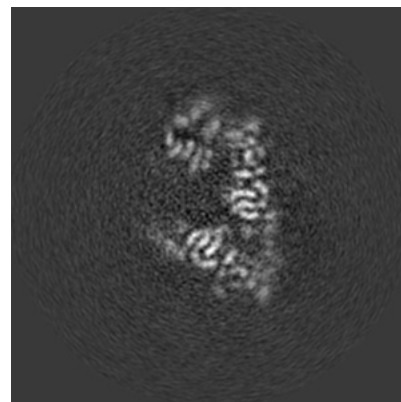
6.3.2 Raw map



X Index: 102



Y Index: 92

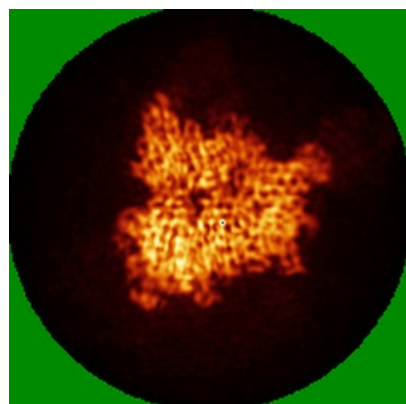


Z Index: 101

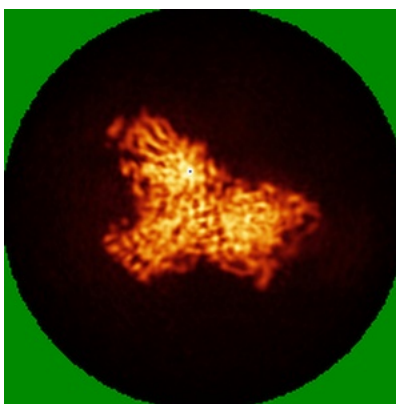
The images above show the largest variance slices of the map in three orthogonal directions.

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

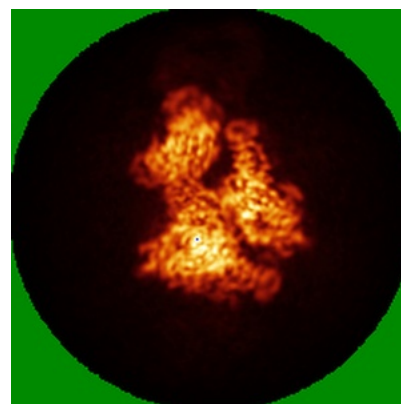
6.4.1 Primary map



X

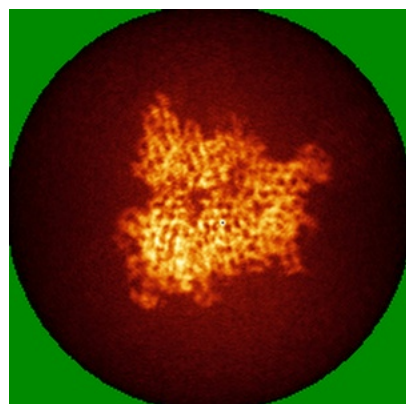


Y

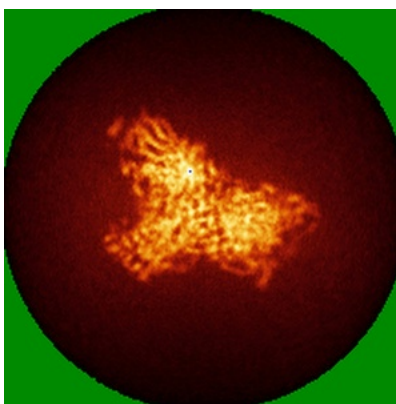


Z

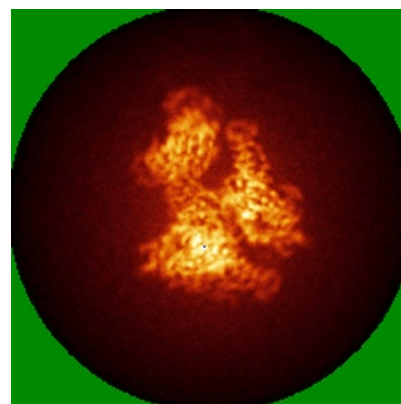
6.4.2 Raw map



X



Y

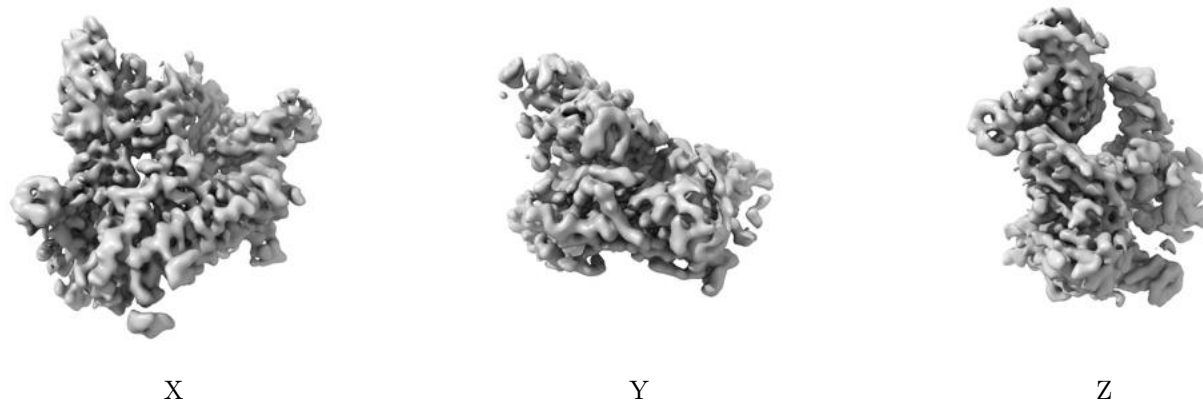


Z

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 0.00703. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

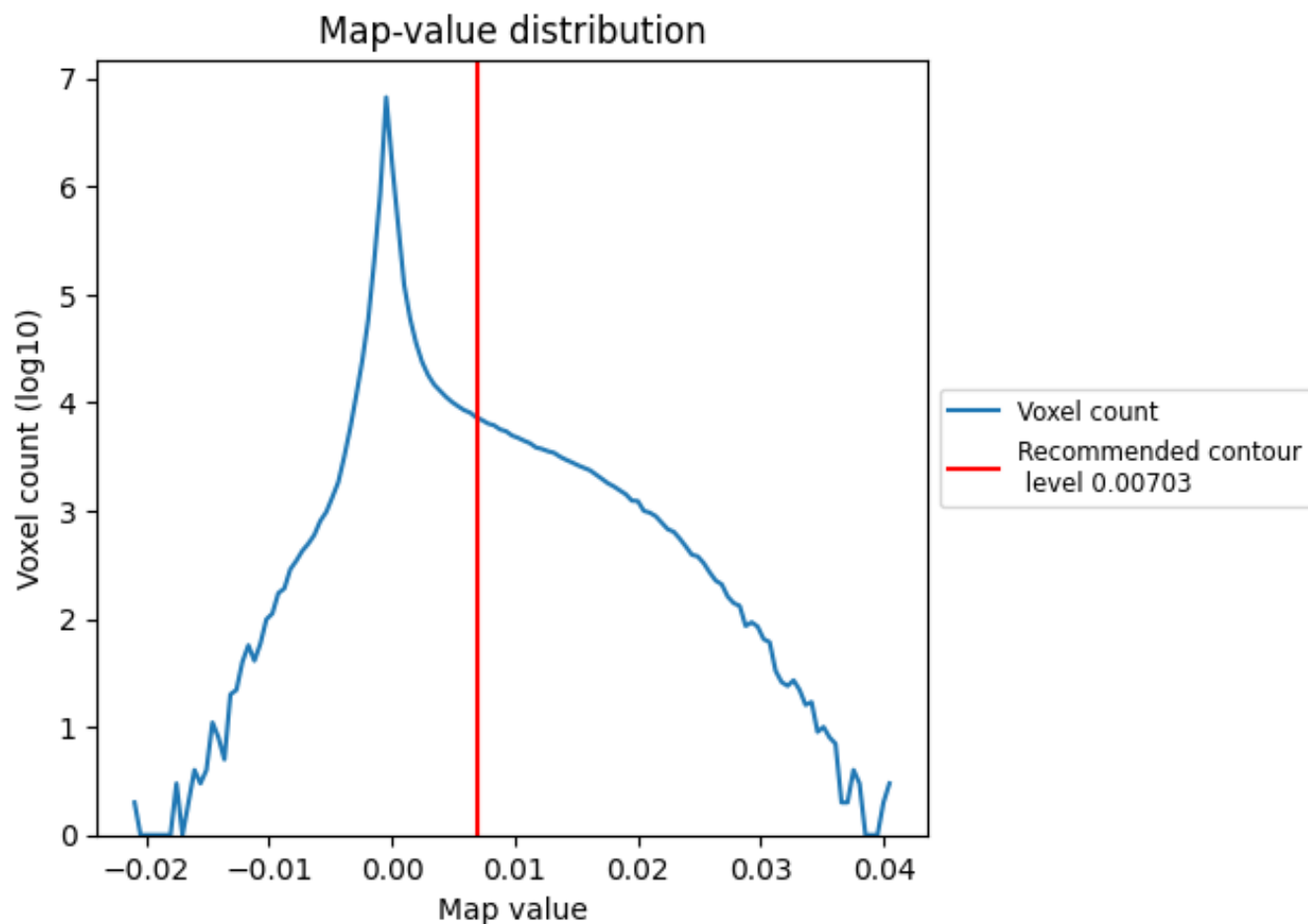
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

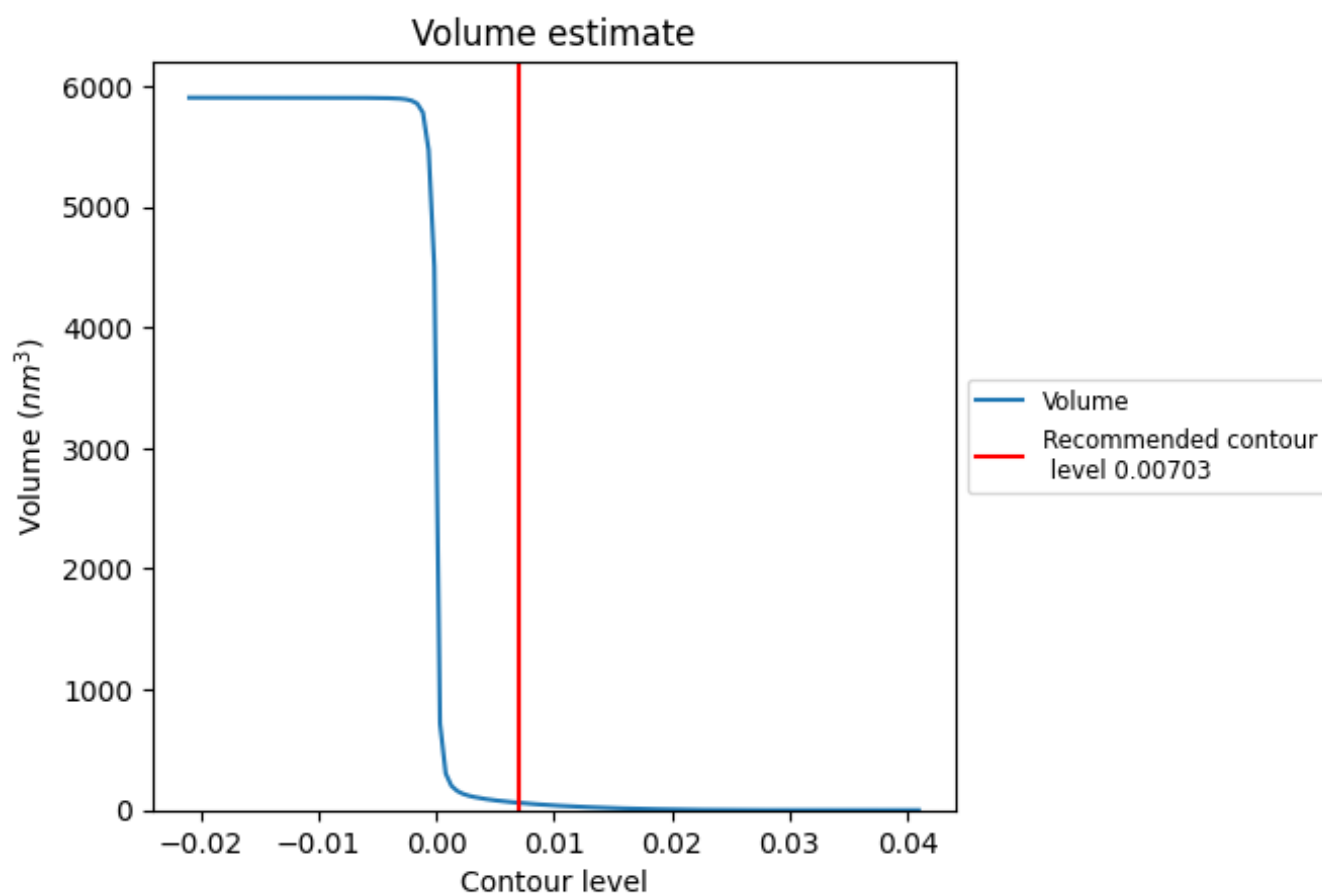
This section contains the results of statistical analysis of the map.

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.

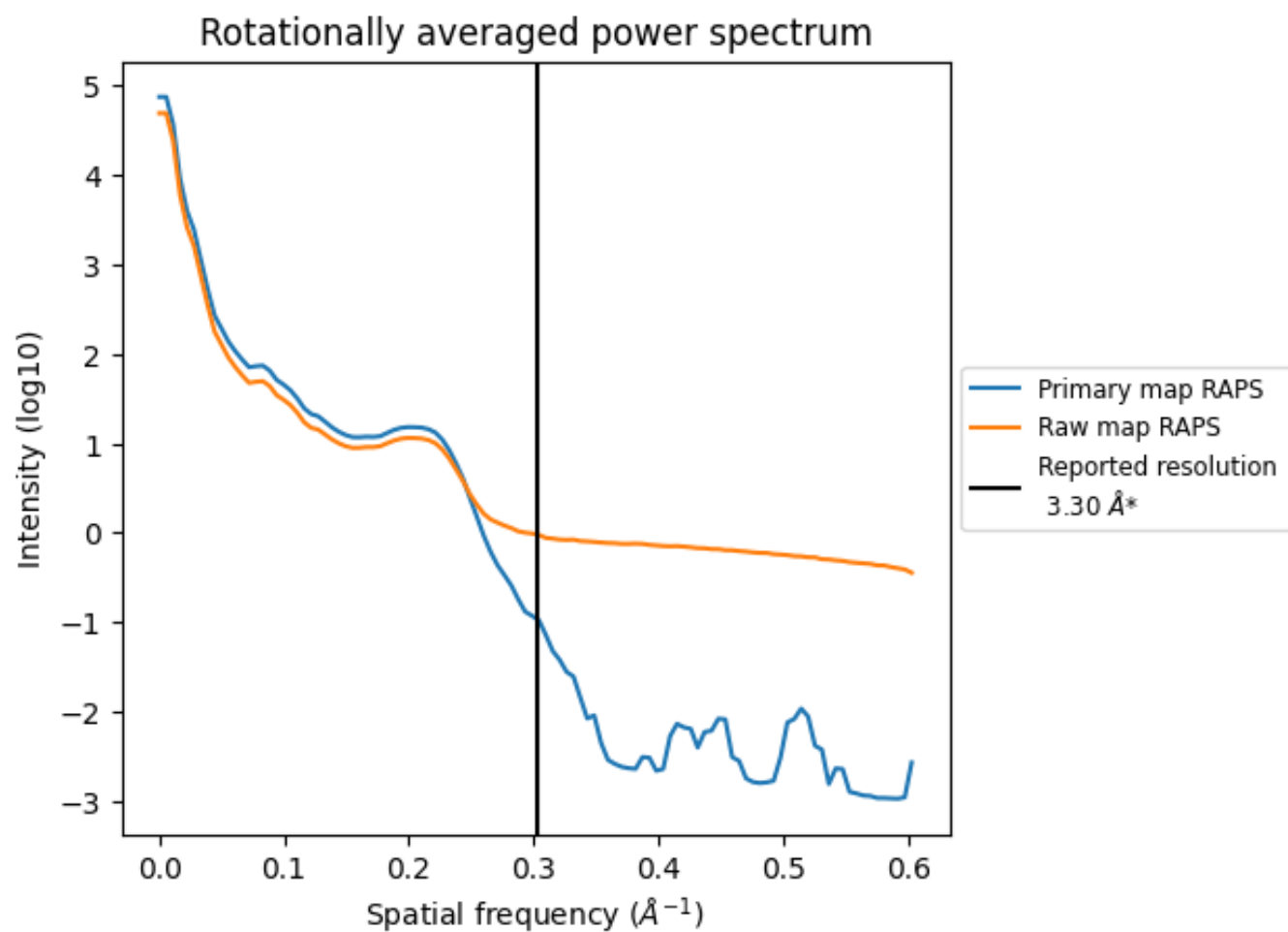
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 61 nm³; this corresponds to an approximate mass of 55 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

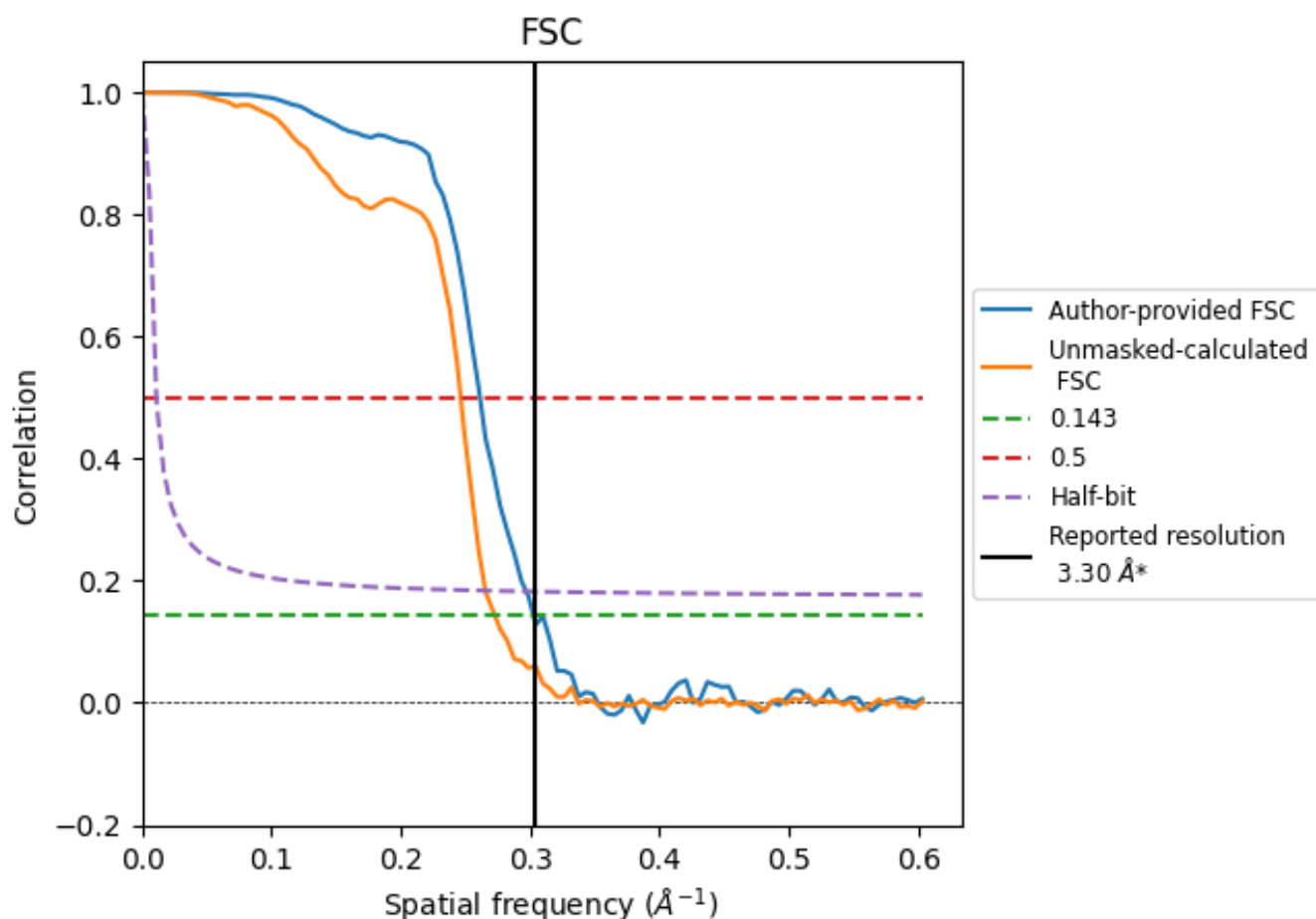


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

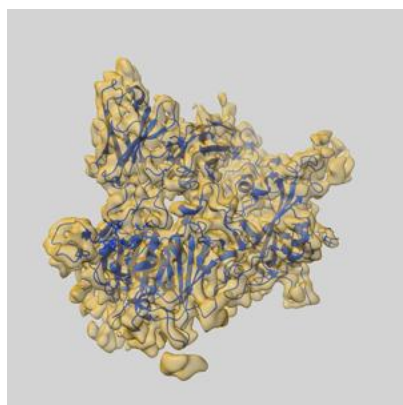
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.31	3.83	3.37
Unmasked-calculated*	3.67	4.06	3.77

*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 3.67 differs from the reported value 3.3 by more than 10 %

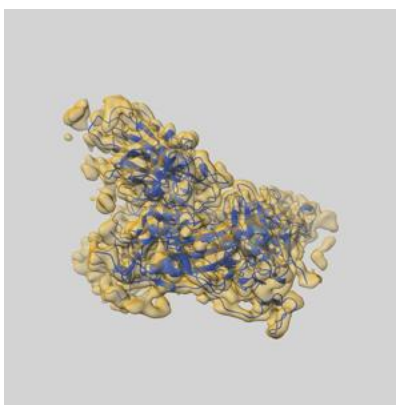
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33065 and PDB model 7X93. Per-residue inclusion information can be found in section [3](#) on page [12](#).

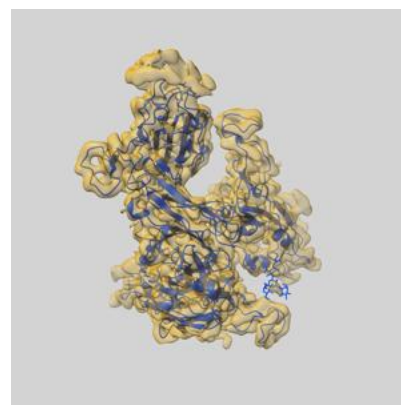
9.1 Map-model overlay [i](#)



X



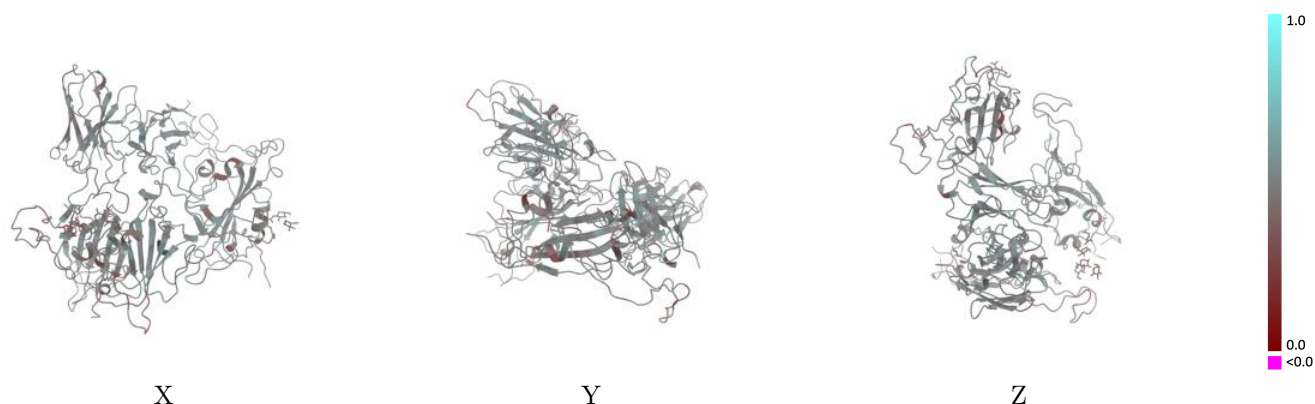
Y



Z

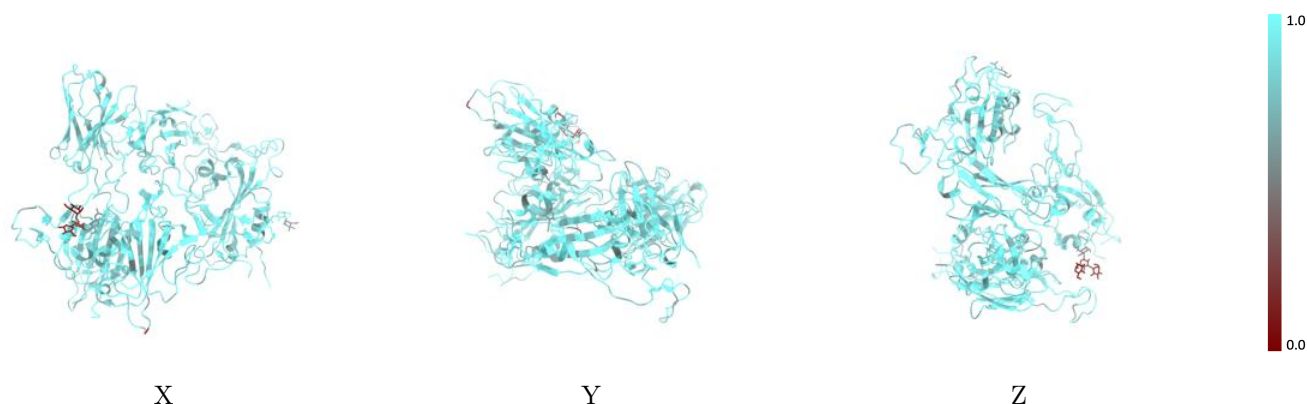
The images above show the 3D surface view of the map at the recommended contour level 0.00703 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



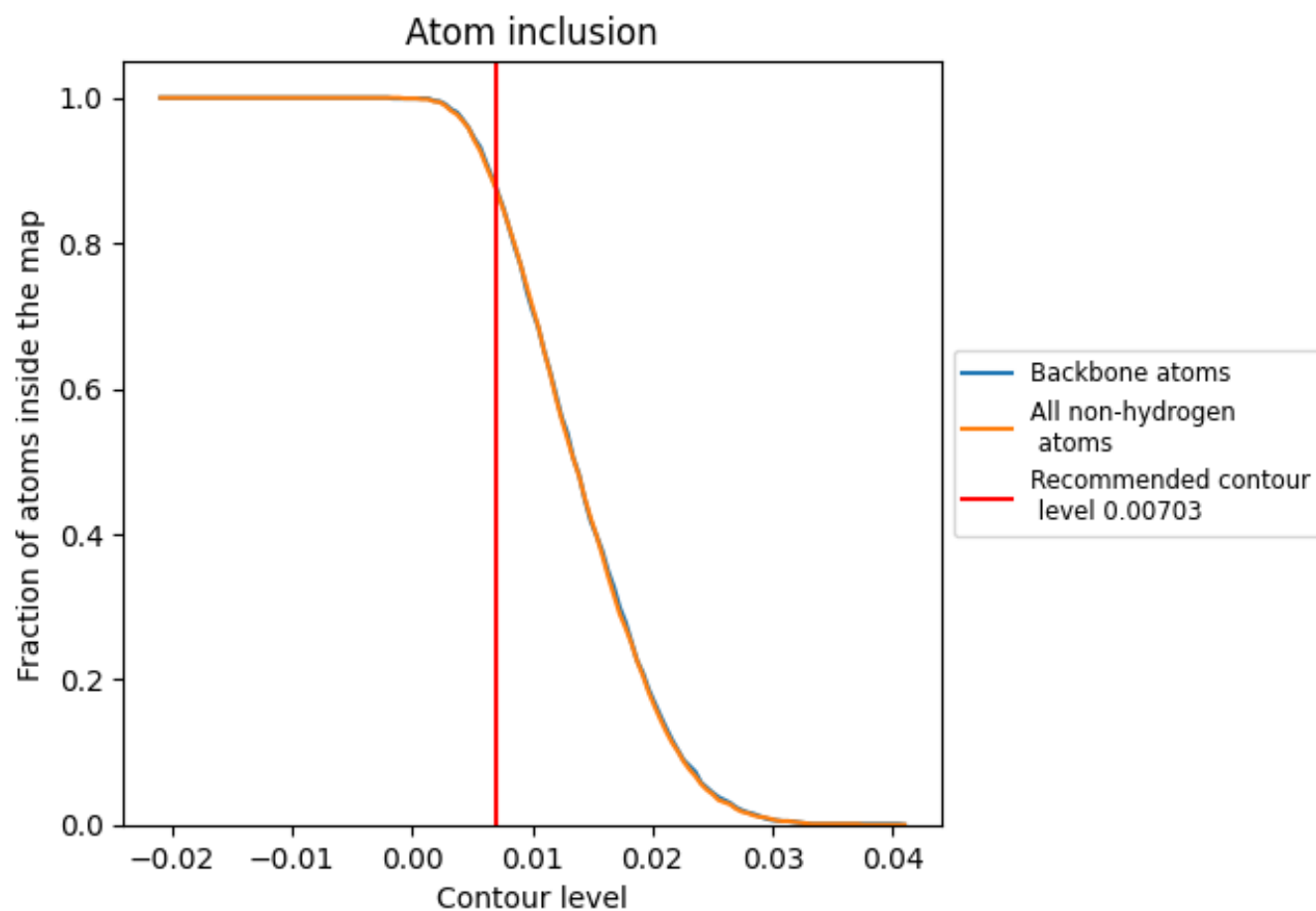
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00703).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 87% 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 (0.00703) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8730	0.4860
A	0.8670	0.4720
B	0.7500	0.4190
C	0.3770	0.3690
D	0.8950	0.4990
E	0.8920	0.4910
F	0.8990	0.5050
G	0.8820	0.4790

1.0

0.0

<0.0