



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:52 AM UTC

PDB ID : 8ERR / pdb_00008err
EMDB ID : EMD-28559
Title : SARS-CoV-2 Omicron BA.1 spike ectodomain trimer in complex with the S2X324 neutralizing antibody Fab fragment
Authors : Park, Y.J.; Seattle Structural Genomics Center for Infectious Disease (SSG-CID); Veesler, D.
Deposited on : 2022-10-12
Resolution : 3.10 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:

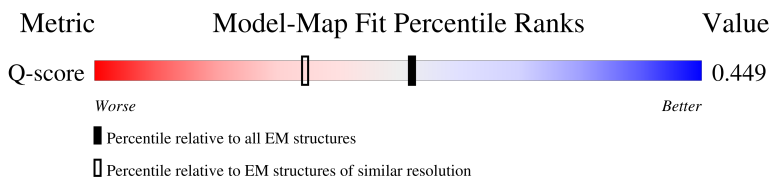
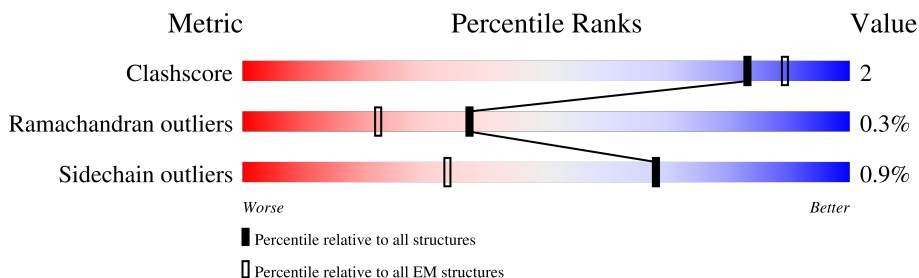
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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.



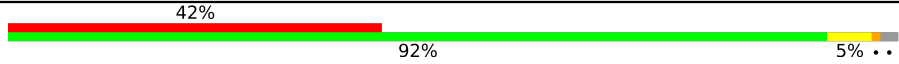
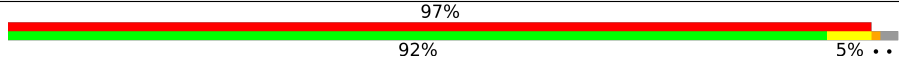
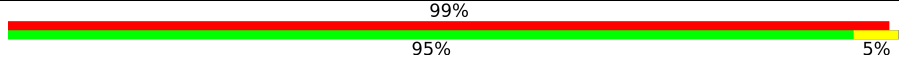
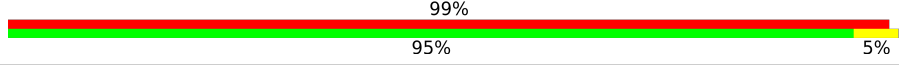
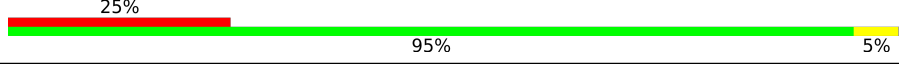
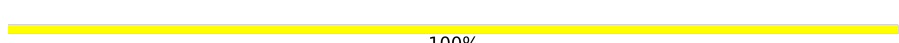
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	1274	
1	B	1274	
1	C	1274	
2	E	119	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	119	 <p>42% 92% 5% ..</p>
2	I	119	 <p>97% 92% 5% ..</p>
3	F	110	 <p>99% 95% 5% .</p>
3	J	110	 <p>99% 95% 5% .</p>
3	L	110	 <p>25% 95% 5% .</p>
4	D	2	 <p>100%</p>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 25780 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1018	7537	4885	1281	1335	36	0	0
1	B	1009	6965	4479	1206	1244	36	0	0
1	C	1037	7164	4585	1250	1291	38	0	0

There are 345 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	210A	ILE	LEU	variant	UNP P0DTC2
A	210D	GLU	-	insertion	UNP P0DTC2
A	210E	PRO	-	insertion	UNP P0DTC2
A	210F	GLU	-	insertion	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	LEU	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	493	ARG	GLN	variant	UNP P0DTC2
A	496	SER	GLY	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	547	LYS	THR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	707	CYS	TYR	variant	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	variant	UNP P0DTC2
A	856	LYS	ASN	variant	UNP P0DTC2
A	883	CYS	THR	variant	UNP P0DTC2
A	892	PRO	ALA	variant	UNP P0DTC2
A	899	PRO	ALA	variant	UNP P0DTC2
A	942	PRO	ALA	variant	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	981	PHE	LEU	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1208	GLN	-	expression tag	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
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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	ARG	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	PHE	-	expression tag	UNP P0DTC2
A	1246	GLN	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	PRO	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	SER	-	expression tag	UNP P0DTC2
A	1251	GLY	-	expression tag	UNP P0DTC2
A	1252	GLY	-	expression tag	UNP P0DTC2
A	1253	LEU	-	expression tag	UNP P0DTC2
A	1254	ASN	-	expression tag	UNP P0DTC2
A	1255	ASP	-	expression tag	UNP P0DTC2
A	1256	ILE	-	expression tag	UNP P0DTC2
A	1257	PHE	-	expression tag	UNP P0DTC2
A	1258	GLU	-	expression tag	UNP P0DTC2
A	1259	ALA	-	expression tag	UNP P0DTC2
A	1260	GLN	-	expression tag	UNP P0DTC2
A	1261	LYS	-	expression tag	UNP P0DTC2
A	1262	ILE	-	expression tag	UNP P0DTC2
A	1263	GLU	-	expression tag	UNP P0DTC2
A	1264	TRP	-	expression tag	UNP P0DTC2
A	1265	HIS	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	GLY	-	expression tag	UNP P0DTC2
A	1268	SER	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	HIS	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1271	HIS	-	expression tag	UNP P0DTC2
A	1272	HIS	-	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
B	67	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	variant	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	210A	ILE	LEU	variant	UNP P0DTC2
B	210D	GLU	-	insertion	UNP P0DTC2
B	210E	PRO	-	insertion	UNP P0DTC2
B	210F	GLU	-	insertion	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	LEU	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2
B	496	SER	GLY	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	547	LYS	THR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	707	CYS	TYR	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	817	PRO	PHE	variant	UNP P0DTC2
B	856	LYS	ASN	variant	UNP P0DTC2
B	883	CYS	THR	variant	UNP P0DTC2
B	892	PRO	ALA	variant	UNP P0DTC2
B	899	PRO	ALA	variant	UNP P0DTC2
B	942	PRO	ALA	variant	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	981	PHE	LEU	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1208	GLN	-	expression tag	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	GLY	-	expression tag	UNP P0DTC2
B	1239	ARG	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1240	SER	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	GLU	-	expression tag	UNP P0DTC2
B	1243	VAL	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	PHE	-	expression tag	UNP P0DTC2
B	1246	GLN	-	expression tag	UNP P0DTC2
B	1247	GLY	-	expression tag	UNP P0DTC2
B	1248	PRO	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	SER	-	expression tag	UNP P0DTC2
B	1251	GLY	-	expression tag	UNP P0DTC2
B	1252	GLY	-	expression tag	UNP P0DTC2
B	1253	LEU	-	expression tag	UNP P0DTC2
B	1254	ASN	-	expression tag	UNP P0DTC2
B	1255	ASP	-	expression tag	UNP P0DTC2
B	1256	ILE	-	expression tag	UNP P0DTC2
B	1257	PHE	-	expression tag	UNP P0DTC2
B	1258	GLU	-	expression tag	UNP P0DTC2
B	1259	ALA	-	expression tag	UNP P0DTC2
B	1260	GLN	-	expression tag	UNP P0DTC2
B	1261	LYS	-	expression tag	UNP P0DTC2
B	1262	ILE	-	expression tag	UNP P0DTC2
B	1263	GLU	-	expression tag	UNP P0DTC2
B	1264	TRP	-	expression tag	UNP P0DTC2
B	1265	HIS	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	GLY	-	expression tag	UNP P0DTC2
B	1268	SER	-	expression tag	UNP P0DTC2
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	HIS	-	expression tag	UNP P0DTC2
B	1271	HIS	-	expression tag	UNP P0DTC2
B	1272	HIS	-	expression tag	UNP P0DTC2
B	1273	HIS	-	expression tag	UNP P0DTC2
B	1274	HIS	-	expression tag	UNP P0DTC2
B	1275	HIS	-	expression tag	UNP P0DTC2
B	1276	HIS	-	expression tag	UNP P0DTC2
B	1277	HIS	-	expression tag	UNP P0DTC2
C	67	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	142	ASP	GLY	variant	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	210A	ILE	LEU	variant	UNP P0DTC2
C	210D	GLU	-	insertion	UNP P0DTC2
C	210E	PRO	-	insertion	UNP P0DTC2
C	210F	GLU	-	insertion	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	LEU	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2
C	496	SER	GLY	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	547	LYS	THR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	707	CYS	TYR	variant	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	variant	UNP P0DTC2
C	856	LYS	ASN	variant	UNP P0DTC2
C	883	CYS	THR	variant	UNP P0DTC2
C	892	PRO	ALA	variant	UNP P0DTC2
C	899	PRO	ALA	variant	UNP P0DTC2
C	942	PRO	ALA	variant	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	981	PHE	LEU	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1208	GLN	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
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	ARG	-	expression tag	UNP P0DTC2
C	1240	SER	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	GLU	-	expression tag	UNP P0DTC2
C	1243	VAL	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	PHE	-	expression tag	UNP P0DTC2
C	1246	GLN	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2
C	1248	PRO	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	SER	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1251	GLY	-	expression tag	UNP P0DTC2
C	1252	GLY	-	expression tag	UNP P0DTC2
C	1253	LEU	-	expression tag	UNP P0DTC2
C	1254	ASN	-	expression tag	UNP P0DTC2
C	1255	ASP	-	expression tag	UNP P0DTC2
C	1256	ILE	-	expression tag	UNP P0DTC2
C	1257	PHE	-	expression tag	UNP P0DTC2
C	1258	GLU	-	expression tag	UNP P0DTC2
C	1259	ALA	-	expression tag	UNP P0DTC2
C	1260	GLN	-	expression tag	UNP P0DTC2
C	1261	LYS	-	expression tag	UNP P0DTC2
C	1262	ILE	-	expression tag	UNP P0DTC2
C	1263	GLU	-	expression tag	UNP P0DTC2
C	1264	TRP	-	expression tag	UNP P0DTC2
C	1265	HIS	-	expression tag	UNP P0DTC2
C	1266	GLU	-	expression tag	UNP P0DTC2
C	1267	GLY	-	expression tag	UNP P0DTC2
C	1268	SER	-	expression tag	UNP P0DTC2
C	1269	GLY	-	expression tag	UNP P0DTC2
C	1270	HIS	-	expression tag	UNP P0DTC2
C	1271	HIS	-	expression tag	UNP P0DTC2
C	1272	HIS	-	expression tag	UNP P0DTC2
C	1273	HIS	-	expression tag	UNP P0DTC2
C	1274	HIS	-	expression tag	UNP P0DTC2
C	1275	HIS	-	expression tag	UNP P0DTC2
C	1276	HIS	-	expression tag	UNP P0DTC2
C	1277	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called S2X324 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	117	Total	C	N	O	S	0	0
			591	355	117	117	2		
2	E	117	Total	C	N	O	S	0	0
			591	355	117	117	2		
2	I	117	Total	C	N	O	S	0	0
			591	355	117	117	2		

- Molecule 3 is a protein called S2X324 light chain.

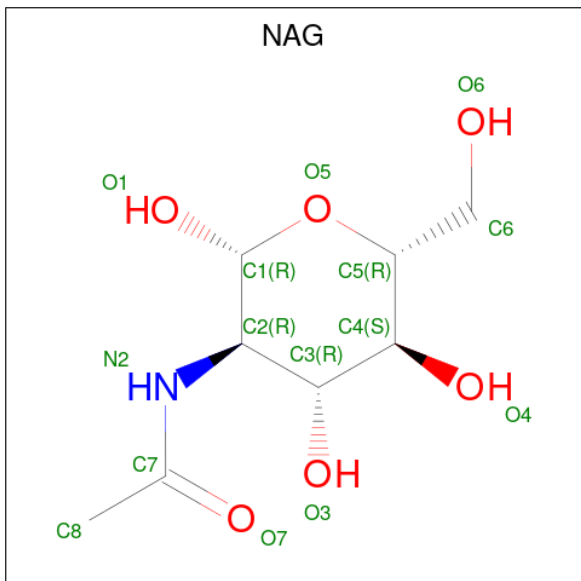
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	L	109	Total 547	C 327	N 109	O 109	S 2	0	0
3	F	109	Total 547	C 327	N 109	O 109	S 2	0	0
3	J	109	Total 547	C 327	N 109	O 109	S 2	0	0

- 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
			Total	C	N	O		
4	D	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

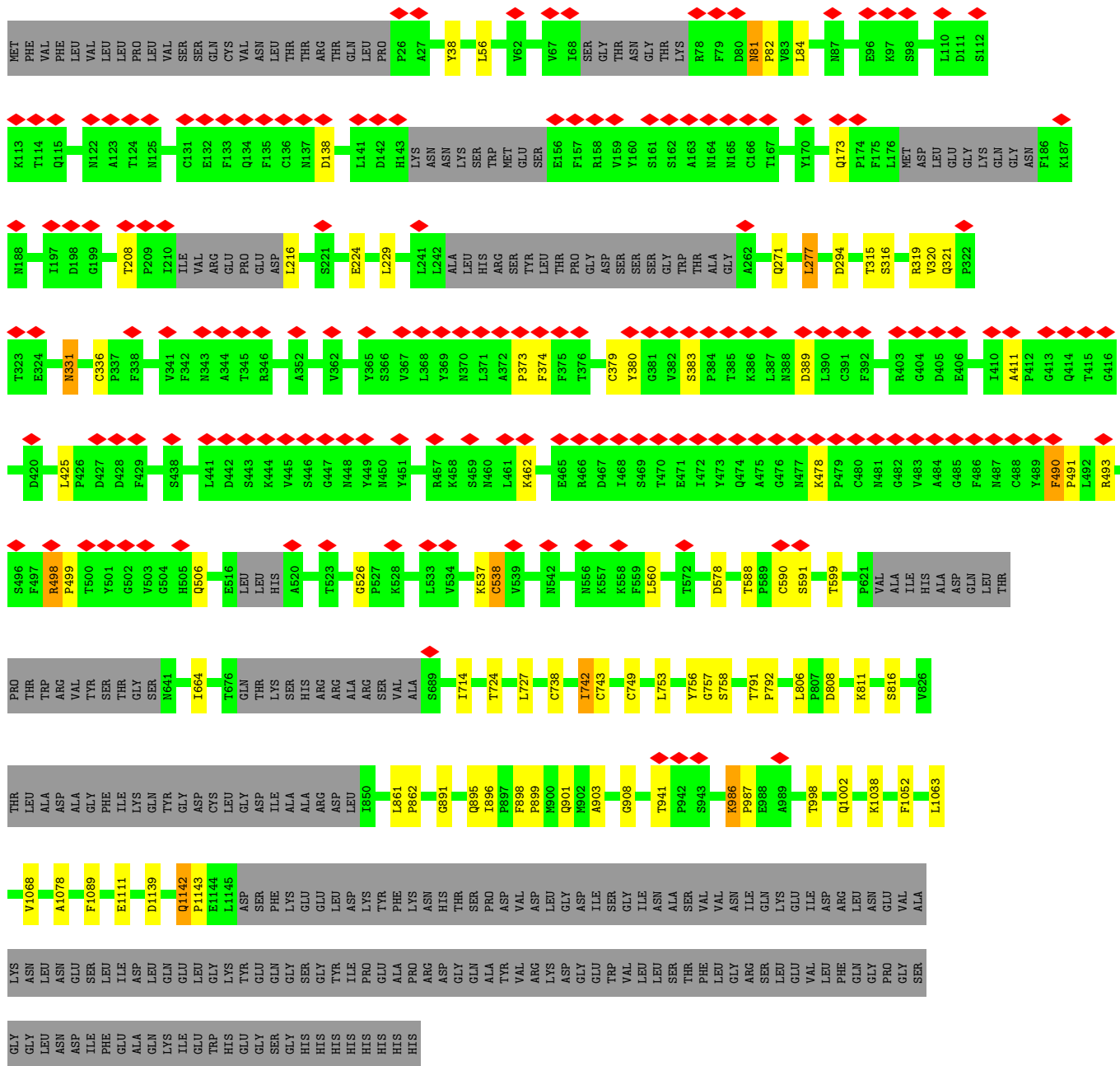


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	A	1	Total 14	C 8	N 1	O 5	0
5	A	1	Total 14	C 8	N 1	O 5	0

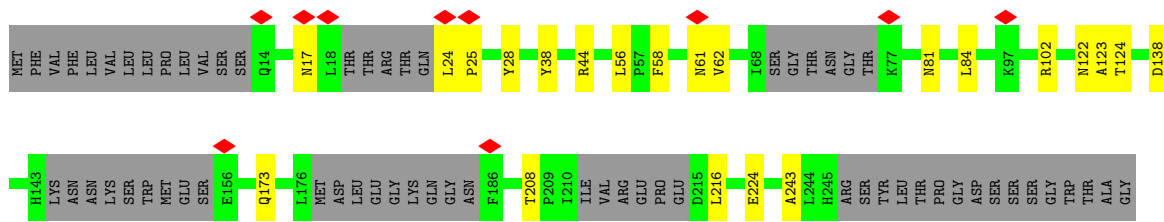
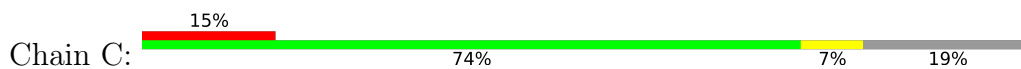
Continued on next page...

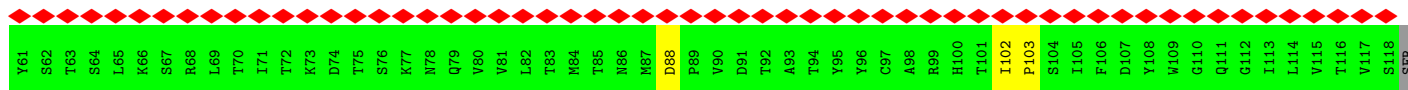
Continued from previous page...

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

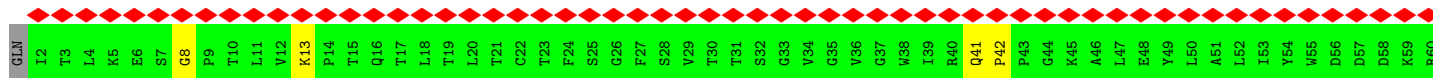
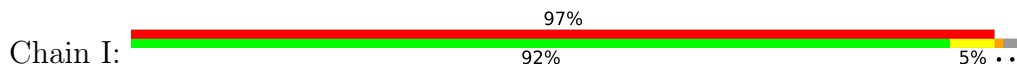


● Molecule 1: Spike glycoprotein

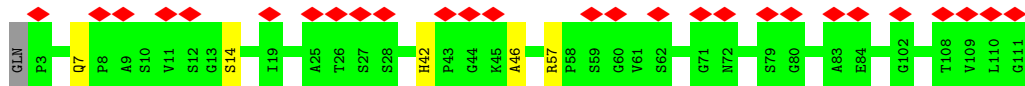




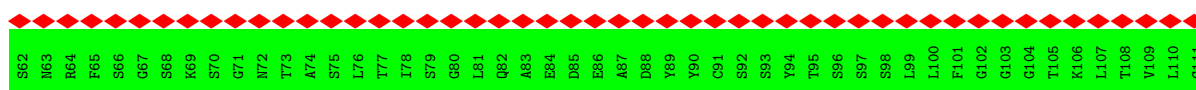
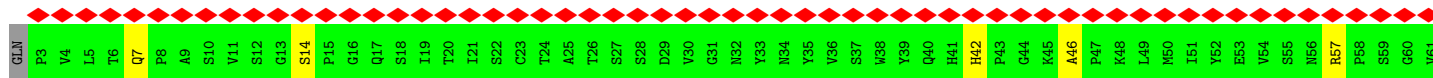
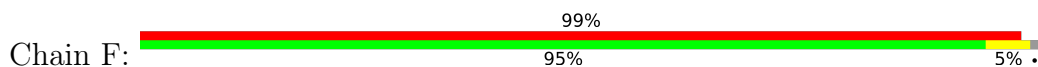
• Molecule 2: S2X324 heavy chain



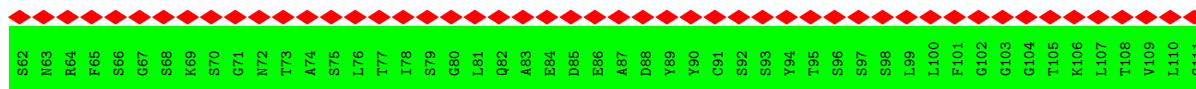
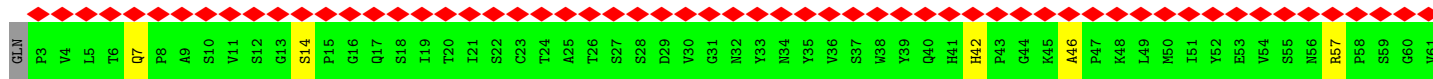
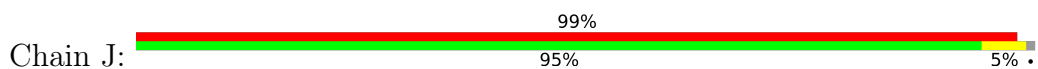
• Molecule 3: S2X324 light chain



• Molecule 3: S2X324 light chain



• Molecule 3: S2X324 light chain



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



MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	537649	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	7.116	Depositor
Minimum map value	-4.431	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.079	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	512.0, 512.0, 512.0	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	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: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.58	1/7719 (0.0%)	1.01	99/10541 (0.9%)
1	B	0.54	0/7129	1.02	101/9768 (1.0%)
1	C	0.55	0/7318	1.04	111/10033 (1.1%)
2	E	0.45	0/596	1.13	10/832 (1.2%)
2	H	0.45	0/596	1.16	12/832 (1.4%)
2	I	0.46	0/596	1.15	12/832 (1.4%)
3	F	0.45	0/552	1.08	10/767 (1.3%)
3	J	0.46	0/552	1.08	10/767 (1.3%)
3	L	0.45	0/552	1.06	10/767 (1.3%)
All	All	0.55	1/25610 (0.0%)	1.04	375/35139 (1.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	616	ASN	C-O	-5.53	1.17	1.24

All (375) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	861	LEU	CA-C-N	9.24	126.31	119.66
1	B	861	LEU	C-N-CA	9.24	126.31	119.66
1	A	861	LEU	CA-C-N	8.84	126.03	119.66
1	A	861	LEU	C-N-CA	8.84	126.03	119.66
2	I	41	GLN	CA-C-N	8.23	125.58	119.66
2	I	41	GLN	C-N-CA	8.23	125.58	119.66
2	H	41	GLN	CA-C-N	8.09	125.49	119.66
2	H	41	GLN	C-N-CA	8.09	125.49	119.66
1	A	801	ASN	N-CA-C	-7.94	95.34	108.76
1	C	862	PRO	CA-C-N	7.88	127.83	120.03
1	C	862	PRO	C-N-CA	7.88	127.83	120.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	498	ARG	CA-C-N	7.81	127.53	119.56
1	C	498	ARG	C-N-CA	7.81	127.53	119.56
2	E	41	GLN	CA-C-N	7.80	125.27	119.66
2	E	41	GLN	C-N-CA	7.80	125.27	119.66
1	B	498	ARG	CA-C-N	7.78	127.50	119.56
1	B	498	ARG	C-N-CA	7.78	127.50	119.56
1	A	714	ILE	CA-C-N	7.73	127.72	119.76
1	A	714	ILE	C-N-CA	7.73	127.72	119.76
1	B	1111	GLU	CA-C-N	7.66	127.42	119.76
1	B	1111	GLU	C-N-CA	7.66	127.42	119.76
1	B	862	PRO	CA-C-N	7.61	127.53	119.85
1	B	862	PRO	C-N-CA	7.61	127.53	119.85
1	A	862	PRO	CA-C-N	7.59	127.52	119.85
1	A	862	PRO	C-N-CA	7.59	127.52	119.85
1	A	891	GLY	CA-C-N	7.59	127.60	119.78
1	A	891	GLY	C-N-CA	7.59	127.60	119.78
1	A	498	ARG	CA-C-N	7.59	127.30	119.56
1	A	498	ARG	C-N-CA	7.59	127.30	119.56
1	B	792	PRO	CA-C-N	7.56	127.20	119.56
1	B	792	PRO	C-N-CA	7.56	127.20	119.56
1	C	25	PRO	CA-C-N	7.52	127.48	120.03
1	C	25	PRO	C-N-CA	7.52	127.48	120.03
1	A	1078	ALA	CA-C-N	7.50	127.87	119.32
1	A	1078	ALA	C-N-CA	7.50	127.87	119.32
1	B	891	GLY	CA-C-N	7.43	127.43	119.78
1	B	891	GLY	C-N-CA	7.43	127.43	119.78
1	B	1078	ALA	CA-C-N	7.42	127.78	119.32
1	B	1078	ALA	C-N-CA	7.42	127.78	119.32
1	C	891	GLY	CA-C-N	7.42	127.42	119.78
1	C	891	GLY	C-N-CA	7.42	127.42	119.78
1	C	808	ASP	CA-C-N	7.41	127.12	119.56
1	C	808	ASP	C-N-CA	7.41	127.12	119.56
3	F	57	ARG	CA-C-N	7.40	127.36	120.03
3	F	57	ARG	C-N-CA	7.40	127.36	120.03
1	C	372	ALA	CA-C-N	7.38	127.08	119.56
1	C	372	ALA	C-N-CA	7.38	127.08	119.56
3	J	57	ARG	CA-C-N	7.37	127.32	120.03
3	J	57	ARG	C-N-CA	7.37	127.32	120.03
2	H	8	GLY	CA-C-N	7.36	127.34	119.76
2	H	8	GLY	C-N-CA	7.36	127.34	119.76
2	I	8	GLY	CA-C-N	7.33	127.31	119.76
2	I	8	GLY	C-N-CA	7.33	127.31	119.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1078	ALA	CA-C-N	7.32	126.95	119.56
1	C	1078	ALA	C-N-CA	7.32	126.95	119.56
3	L	57	ARG	CA-C-N	7.30	127.25	120.03
3	L	57	ARG	C-N-CA	7.30	127.25	120.03
1	A	801	ASN	N-CA-CB	-7.27	98.22	110.80
1	C	792	PRO	CA-C-N	7.27	126.97	119.56
1	C	792	PRO	C-N-CA	7.27	126.97	119.56
1	B	526	GLY	CA-C-N	7.23	127.19	120.03
1	B	526	GLY	C-N-CA	7.23	127.19	120.03
1	C	321	GLN	CA-C-N	7.23	126.86	119.19
1	C	321	GLN	C-N-CA	7.23	126.86	119.19
1	C	816	SER	CA-C-N	7.23	126.76	119.24
1	C	816	SER	C-N-CA	7.23	126.76	119.24
1	A	1111	GLU	CA-C-N	7.20	126.96	119.76
1	A	1111	GLU	C-N-CA	7.20	126.96	119.76
1	A	806	LEU	CA-C-N	7.17	127.21	119.90
1	A	806	LEU	C-N-CA	7.17	127.21	119.90
2	E	8	GLY	CA-C-N	7.16	127.15	119.78
2	E	8	GLY	C-N-CA	7.16	127.15	119.78
1	C	208	THR	CA-C-N	7.14	127.06	119.85
1	C	208	THR	C-N-CA	7.14	127.06	119.85
1	A	321	GLN	CA-C-N	7.13	127.05	119.85
1	A	321	GLN	C-N-CA	7.13	127.05	119.85
1	C	941	THR	CA-C-N	7.10	126.80	119.56
1	C	941	THR	C-N-CA	7.10	126.80	119.56
1	A	752	LEU	N-CA-C	-7.09	104.26	113.12
1	C	411	ALA	CA-C-N	7.05	127.09	119.90
1	C	411	ALA	C-N-CA	7.05	127.09	119.90
1	C	526	GLY	CA-C-N	7.04	126.96	119.85
1	C	526	GLY	C-N-CA	7.04	126.96	119.85
1	B	1139	ASP	CA-C-N	7.01	127.16	119.87
1	B	1139	ASP	C-N-CA	7.01	127.16	119.87
1	B	138	ASP	CA-C-N	7.00	126.76	119.76
1	B	138	ASP	C-N-CA	7.00	126.76	119.76
1	A	216	LEU	CA-C-N	6.99	126.95	120.03
1	A	216	LEU	C-N-CA	6.99	126.95	120.03
1	A	808	ASP	CA-C-N	6.98	127.13	119.87
1	A	808	ASP	C-N-CA	6.98	127.13	119.87
1	C	173	GLN	CA-C-N	6.98	126.90	119.85
1	C	173	GLN	C-N-CA	6.98	126.90	119.85
1	C	490	PHE	CA-C-N	6.95	127.24	119.32
1	C	490	PHE	C-N-CA	6.95	127.24	119.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	216	LEU	CA-C-N	6.95	126.91	120.03
1	B	216	LEU	C-N-CA	6.95	126.91	120.03
1	B	81	ASN	CA-C-N	6.94	126.90	120.03
1	B	81	ASN	C-N-CA	6.94	126.90	120.03
1	B	811	LYS	CA-C-N	6.93	126.63	119.56
1	B	811	LYS	C-N-CA	6.93	126.63	119.56
1	C	81	ASN	CA-C-N	6.91	127.36	120.52
1	C	81	ASN	C-N-CA	6.91	127.36	120.52
1	A	138	ASP	CA-C-N	6.87	126.63	119.76
1	A	138	ASP	C-N-CA	6.87	126.63	119.76
1	B	941	THR	CA-C-N	6.87	126.56	119.56
1	B	941	THR	C-N-CA	6.87	126.56	119.56
1	B	808	ASP	CA-C-N	6.86	127.00	119.87
1	B	808	ASP	C-N-CA	6.86	127.00	119.87
1	B	321	GLN	CA-C-N	6.83	126.59	119.76
1	B	321	GLN	C-N-CA	6.83	126.59	119.76
1	A	81	ASN	CA-C-N	6.83	127.00	120.31
1	A	81	ASN	C-N-CA	6.83	127.00	120.31
1	A	490	PHE	CA-C-N	6.83	127.10	119.32
1	A	490	PHE	C-N-CA	6.83	127.10	119.32
1	C	216	LEU	CA-C-N	6.82	126.81	119.78
1	C	216	LEU	C-N-CA	6.82	126.81	119.78
1	C	278	LYS	N-CA-C	6.81	119.83	108.73
1	B	901	GLN	N-CA-C	-6.81	103.79	111.07
1	B	578	ASP	CA-C-N	6.76	126.39	119.56
1	B	578	ASP	C-N-CA	6.76	126.39	119.56
1	A	941	THR	CA-C-N	6.72	126.98	119.32
1	A	941	THR	C-N-CA	6.72	126.98	119.32
1	B	806	LEU	CA-C-N	6.71	126.68	119.76
1	B	806	LEU	C-N-CA	6.71	126.68	119.76
1	C	714	ILE	CA-C-N	6.71	126.67	119.76
1	C	714	ILE	C-N-CA	6.71	126.67	119.76
1	C	329	PHE	CA-C-N	6.69	126.66	120.03
1	C	329	PHE	C-N-CA	6.69	126.66	120.03
1	C	294	ASP	CA-C-N	6.68	126.37	119.56
1	C	294	ASP	C-N-CA	6.68	126.37	119.56
1	B	727	LEU	CA-C-N	6.67	126.63	119.76
1	B	727	LEU	C-N-CA	6.67	126.63	119.76
1	C	1068	VAL	CA-C-N	6.67	126.64	119.78
1	C	1068	VAL	C-N-CA	6.67	126.64	119.78
1	C	1111	GLU	CA-C-N	6.66	126.42	119.76
1	C	1111	GLU	C-N-CA	6.66	126.42	119.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	224	GLU	CA-C-N	6.62	126.38	119.76
1	B	224	GLU	C-N-CA	6.62	126.38	119.76
1	B	490	PHE	CA-C-N	6.62	126.86	119.32
1	B	490	PHE	C-N-CA	6.62	126.86	119.32
1	C	806	LEU	CA-C-N	6.59	126.62	119.90
1	C	806	LEU	C-N-CA	6.59	126.62	119.90
1	B	38	TYR	CA-C-N	6.59	126.22	119.56
1	B	38	TYR	C-N-CA	6.59	126.22	119.56
1	A	506	GLN	CA-C-N	6.57	126.33	119.76
1	A	506	GLN	C-N-CA	6.57	126.33	119.76
1	C	38	TYR	CA-C-N	6.57	126.19	119.56
1	C	38	TYR	C-N-CA	6.57	126.19	119.56
1	B	599	THR	CA-C-N	6.56	126.51	120.21
1	B	599	THR	C-N-CA	6.56	126.51	120.21
1	C	578	ASP	CA-C-N	6.56	126.25	119.56
1	C	578	ASP	C-N-CA	6.56	126.25	119.56
1	A	411	ALA	CA-C-N	6.55	126.51	119.76
1	A	411	ALA	C-N-CA	6.55	126.51	119.76
1	A	811	LYS	CA-C-N	6.55	126.24	119.56
1	A	811	LYS	C-N-CA	6.55	126.24	119.56
1	A	383	SER	CA-C-N	6.53	127.04	119.47
1	A	383	SER	C-N-CA	6.53	127.04	119.47
3	L	7	GLN	CA-C-N	6.53	126.44	119.85
3	L	7	GLN	C-N-CA	6.53	126.44	119.85
1	C	506	GLN	CA-C-N	6.53	126.29	119.76
1	C	506	GLN	C-N-CA	6.53	126.29	119.76
1	A	620	VAL	N-CA-C	-6.52	104.53	112.35
1	A	1068	VAL	CA-C-N	6.50	126.41	119.85
1	A	1068	VAL	C-N-CA	6.50	126.41	119.85
3	J	7	GLN	CA-C-N	6.49	126.41	119.85
3	J	7	GLN	C-N-CA	6.49	126.41	119.85
1	C	425	LEU	CA-C-N	6.49	126.40	119.85
1	C	425	LEU	C-N-CA	6.49	126.40	119.85
1	B	425	LEU	CA-C-N	6.48	126.40	119.85
1	B	425	LEU	C-N-CA	6.48	126.40	119.85
1	A	294	ASP	CA-C-N	6.47	126.40	119.28
1	A	294	ASP	C-N-CA	6.47	126.40	119.28
1	B	383	SER	CA-C-N	6.47	126.97	119.47
1	B	383	SER	C-N-CA	6.47	126.97	119.47
1	C	84	LEU	CA-C-N	6.46	126.44	119.78
1	C	84	LEU	C-N-CA	6.46	126.44	119.78
1	A	224	GLU	CA-C-N	6.46	126.43	119.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	GLU	C-N-CA	6.46	126.43	119.78
1	B	714	ILE	CA-C-N	6.46	126.80	119.83
1	B	714	ILE	C-N-CA	6.46	126.80	119.83
1	B	896	ILE	CA-C-N	6.46	126.41	119.76
1	B	896	ILE	C-N-CA	6.46	126.41	119.76
1	B	506	GLN	CA-C-N	6.44	126.20	119.76
1	B	506	GLN	C-N-CA	6.44	126.20	119.76
1	A	208	THR	CA-C-N	6.42	126.34	119.85
1	A	208	THR	C-N-CA	6.42	126.34	119.85
1	C	138	ASP	CA-C-N	6.41	126.75	119.83
1	C	138	ASP	C-N-CA	6.41	126.75	119.83
3	F	7	GLN	CA-C-N	6.40	126.31	119.85
3	F	7	GLN	C-N-CA	6.40	126.31	119.85
1	B	208	THR	CA-C-N	6.39	126.30	119.85
1	B	208	THR	C-N-CA	6.39	126.30	119.85
1	C	224	GLU	CA-C-N	6.37	126.39	119.90
1	C	224	GLU	C-N-CA	6.37	126.39	119.90
1	A	173	GLN	CA-C-N	6.36	126.31	119.76
1	A	173	GLN	C-N-CA	6.36	126.31	119.76
1	A	425	LEU	CA-C-N	6.35	126.27	119.85
1	A	425	LEU	C-N-CA	6.35	126.27	119.85
1	C	1139	ASP	CA-C-N	6.34	127.77	119.84
1	C	1139	ASP	C-N-CA	6.34	127.77	119.84
3	F	46	ALA	CA-C-N	6.32	126.27	119.76
3	F	46	ALA	C-N-CA	6.32	126.27	119.76
1	B	478	LYS	CA-C-N	6.30	126.51	119.90
1	B	478	LYS	C-N-CA	6.30	126.51	119.90
3	J	46	ALA	CA-C-N	6.28	126.23	119.76
3	J	46	ALA	C-N-CA	6.28	126.23	119.76
1	B	411	ALA	CA-C-N	6.26	126.63	119.93
1	B	411	ALA	C-N-CA	6.26	126.63	119.93
1	C	727	LEU	CA-C-N	6.25	126.16	119.85
1	C	727	LEU	C-N-CA	6.25	126.16	119.85
1	A	816	SER	CA-C-N	6.22	126.68	119.47
1	A	816	SER	C-N-CA	6.22	126.68	119.47
1	B	294	ASP	CA-C-N	6.20	126.39	119.32
1	B	294	ASP	C-N-CA	6.20	126.39	119.32
1	B	84	LEU	CA-C-N	6.18	126.09	119.85
1	B	84	LEU	C-N-CA	6.18	126.09	119.85
1	C	986	LYS	CA-C-N	6.13	125.82	119.56
1	C	986	LYS	C-N-CA	6.13	125.82	119.56
1	B	664	ILE	CA-C-N	6.13	125.89	119.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	664	ILE	C-N-CA	6.13	125.89	119.76
1	A	727	LEU	CA-C-N	6.12	126.03	119.85
1	A	727	LEU	C-N-CA	6.12	126.03	119.85
1	B	173	GLN	CA-C-N	6.12	126.14	119.90
1	B	173	GLN	C-N-CA	6.12	126.14	119.90
1	A	1139	ASP	CA-C-N	6.11	125.81	119.82
1	A	1139	ASP	C-N-CA	6.11	125.81	119.82
3	L	46	ALA	CA-C-N	6.11	126.05	119.76
3	L	46	ALA	C-N-CA	6.11	126.05	119.76
1	B	229	LEU	CA-C-N	6.10	126.01	119.85
1	B	229	LEU	C-N-CA	6.10	126.01	119.85
1	C	620	VAL	CA-C-N	6.09	125.78	119.56
1	C	620	VAL	C-N-CA	6.09	125.78	119.56
3	F	14	SER	CA-C-N	6.09	125.85	119.76
3	F	14	SER	C-N-CA	6.09	125.85	119.76
1	A	981	PHE	N-CA-C	-6.09	105.68	113.23
1	A	84	LEU	CA-C-N	6.09	126.00	119.85
1	A	84	LEU	C-N-CA	6.09	126.00	119.85
1	B	1068	VAL	CA-C-N	6.08	125.99	119.85
1	B	1068	VAL	C-N-CA	6.08	125.99	119.85
1	A	588	THR	CA-C-N	6.07	126.09	119.89
1	A	588	THR	C-N-CA	6.07	126.09	119.89
1	B	56	LEU	CA-C-N	6.04	126.00	119.78
1	B	56	LEU	C-N-CA	6.04	126.00	119.78
1	C	630	THR	CA-C-N	6.02	126.45	119.47
1	C	630	THR	C-N-CA	6.02	126.45	119.47
1	C	1052	PHE	CA-C-N	6.02	126.52	120.14
1	C	1052	PHE	C-N-CA	6.02	126.52	120.14
1	B	903	ALA	N-CA-C	6.00	118.58	111.33
1	C	383	SER	CA-C-N	5.99	127.33	119.84
1	C	383	SER	C-N-CA	5.99	127.33	119.84
1	C	24	LEU	CA-C-N	5.97	126.53	120.38
1	C	24	LEU	C-N-CA	5.97	126.53	120.38
1	B	816	SER	CA-C-N	5.97	126.40	119.47
1	B	816	SER	C-N-CA	5.97	126.40	119.47
1	A	578	ASP	CA-C-N	5.96	127.29	119.84
1	A	578	ASP	C-N-CA	5.96	127.29	119.84
1	A	1052	PHE	CA-C-N	5.93	126.43	120.14
1	A	1052	PHE	C-N-CA	5.93	126.43	120.14
1	C	791	THR	CA-C-N	5.90	126.45	120.38
1	C	791	THR	C-N-CA	5.90	126.45	120.38
1	B	1052	PHE	CA-C-N	5.89	126.39	120.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1052	PHE	C-N-CA	5.89	126.39	120.14
1	C	56	LEU	CA-C-N	5.89	125.83	119.76
1	C	56	LEU	C-N-CA	5.89	125.83	119.76
1	A	38	TYR	CA-C-N	5.86	126.37	120.04
1	A	38	TYR	C-N-CA	5.86	126.37	120.04
1	A	896	ILE	CA-C-N	5.82	125.75	119.76
1	A	896	ILE	C-N-CA	5.82	125.75	119.76
1	B	1142	GLN	CA-C-N	5.81	125.49	119.56
1	B	1142	GLN	C-N-CA	5.81	125.49	119.56
1	C	588	THR	CA-C-N	5.79	125.80	119.89
1	C	588	THR	C-N-CA	5.79	125.80	119.89
1	C	1142	GLN	CA-C-N	5.77	125.44	119.56
1	C	1142	GLN	C-N-CA	5.77	125.44	119.56
1	B	791	THR	CA-C-N	5.76	126.32	120.38
1	B	791	THR	C-N-CA	5.76	126.32	120.38
1	C	664	ILE	CA-C-N	5.76	125.52	119.76
1	C	664	ILE	C-N-CA	5.76	125.52	119.76
1	A	56	LEU	CA-C-N	5.75	125.70	119.78
1	A	56	LEU	C-N-CA	5.75	125.70	119.78
1	C	896	ILE	CA-C-N	5.74	125.67	119.76
1	C	896	ILE	C-N-CA	5.74	125.67	119.76
2	E	42	PRO	CA-C-N	5.71	125.99	119.83
2	E	42	PRO	C-N-CA	5.71	125.99	119.83
2	H	42	PRO	CA-C-N	5.70	125.98	119.83
2	H	42	PRO	C-N-CA	5.70	125.98	119.83
1	A	478	LYS	CA-C-N	5.68	126.94	119.84
1	A	478	LYS	C-N-CA	5.68	126.94	119.84
1	B	336	CYS	CA-C-N	5.67	126.93	119.84
1	B	336	CYS	C-N-CA	5.67	126.93	119.84
2	E	13	LYS	CA-C-N	5.66	125.68	119.90
2	E	13	LYS	C-N-CA	5.66	125.68	119.90
2	I	42	PRO	CA-C-N	5.66	125.94	119.83
2	I	42	PRO	C-N-CA	5.66	125.94	119.83
3	J	14	SER	CA-C-N	5.63	125.56	119.76
3	J	14	SER	C-N-CA	5.63	125.56	119.76
1	A	664	ILE	CA-C-N	5.63	125.39	119.76
1	A	664	ILE	C-N-CA	5.63	125.39	119.76
1	C	861	LEU	CA-C-N	5.62	126.17	120.38
1	C	861	LEU	C-N-CA	5.62	126.17	120.38
1	A	271	GLN	CA-C-N	5.61	126.85	119.84
1	A	271	GLN	C-N-CA	5.61	126.85	119.84
1	B	986	LYS	CA-C-N	5.60	125.27	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	986	LYS	C-N-CA	5.60	125.27	119.56
1	A	520	ALA	CA-C-N	5.59	125.92	119.93
1	A	520	ALA	C-N-CA	5.59	125.92	119.93
2	I	13	LYS	CA-C-N	5.59	125.60	119.90
2	I	13	LYS	C-N-CA	5.59	125.60	119.90
1	C	478	LYS	CA-C-N	5.59	126.82	119.84
1	C	478	LYS	C-N-CA	5.59	126.82	119.84
1	A	754	LEU	N-CA-C	5.58	119.18	112.38
2	H	88	ASP	CA-C-N	5.57	125.94	119.47
2	H	88	ASP	C-N-CA	5.57	125.94	119.47
1	A	753	LEU	CA-C-O	5.57	126.23	119.49
1	B	588	THR	CA-C-N	5.56	125.51	119.78
1	B	588	THR	C-N-CA	5.56	125.51	119.78
1	B	560	LEU	CA-C-N	5.55	126.78	119.84
1	B	560	LEU	C-N-CA	5.55	126.78	119.84
1	B	462	LYS	CA-C-N	5.53	125.84	119.93
1	B	462	LYS	C-N-CA	5.53	125.84	119.93
1	C	599	THR	CA-C-N	5.52	126.00	120.04
1	C	599	THR	C-N-CA	5.52	126.00	120.04
2	H	13	LYS	CA-C-N	5.51	125.53	119.90
2	H	13	LYS	C-N-CA	5.51	125.53	119.90
1	C	1089	PHE	CA-C-N	5.49	125.25	119.76
1	C	1089	PHE	C-N-CA	5.49	125.25	119.76
1	B	1089	PHE	CA-C-N	5.45	125.21	119.76
1	B	1089	PHE	C-N-CA	5.45	125.21	119.76
2	I	88	ASP	CA-C-N	5.44	126.64	119.84
2	I	88	ASP	C-N-CA	5.44	126.64	119.84
1	C	560	LEU	CA-C-N	5.43	126.62	119.84
1	C	560	LEU	C-N-CA	5.43	126.62	119.84
2	E	88	ASP	CA-C-N	5.40	126.59	119.84
2	E	88	ASP	C-N-CA	5.40	126.59	119.84
1	A	1089	PHE	CA-C-N	5.39	125.15	119.76
1	A	1089	PHE	C-N-CA	5.39	125.15	119.76
1	C	898	PHE	CA-C-N	5.39	125.21	119.28
1	C	898	PHE	C-N-CA	5.39	125.21	119.28
1	C	811	LYS	CA-C-N	5.38	126.56	119.84
1	C	811	LYS	C-N-CA	5.38	126.56	119.84
1	A	599	THR	CA-C-N	5.36	125.83	120.04
1	A	599	THR	C-N-CA	5.36	125.83	120.04
1	A	560	LEU	CA-C-N	5.36	126.54	119.84
1	A	560	LEU	C-N-CA	5.36	126.54	119.84
1	A	799	GLY	N-CA-C	-5.32	108.36	114.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	271	GLN	CA-C-N	5.31	126.48	119.84
1	B	271	GLN	C-N-CA	5.31	126.48	119.84
3	F	42	HIS	CA-C-N	5.28	125.58	119.93
3	F	42	HIS	C-N-CA	5.28	125.58	119.93
1	A	1142	GLN	CA-C-N	5.28	125.59	119.47
1	A	1142	GLN	C-N-CA	5.28	125.59	119.47
1	C	462	LYS	CA-C-N	5.27	125.57	119.93
1	C	462	LYS	C-N-CA	5.27	125.57	119.93
3	J	42	HIS	CA-C-N	5.19	125.48	119.93
3	J	42	HIS	C-N-CA	5.19	125.48	119.93
1	B	320	VAL	N-CA-C	5.14	115.91	110.72
1	C	271	GLN	CA-C-N	5.12	126.23	119.84
1	C	271	GLN	C-N-CA	5.12	126.23	119.84
1	A	330	PRO	CA-C-N	-5.10	115.64	122.42
1	A	330	PRO	C-N-CA	-5.10	115.64	122.42
3	L	14	SER	CA-C-N	5.08	124.99	119.76
3	L	14	SER	C-N-CA	5.08	124.99	119.76
1	A	462	LYS	CA-C-N	5.07	125.35	119.93
1	A	462	LYS	C-N-CA	5.07	125.35	119.93
1	C	336	CYS	CA-C-N	5.06	126.17	119.84
1	C	336	CYS	C-N-CA	5.06	126.17	119.84
2	I	102	ILE	CA-C-N	5.05	124.66	119.56
2	I	102	ILE	C-N-CA	5.05	124.66	119.56
2	H	102	ILE	CA-C-N	5.03	124.69	119.56
2	H	102	ILE	C-N-CA	5.03	124.69	119.56
3	L	42	HIS	CA-C-N	5.01	125.30	119.93
3	L	42	HIS	C-N-CA	5.01	125.30	119.93
1	A	619	GLU	CB-CA-C	-5.00	102.91	111.46

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	7537	0	6964	59	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	6965	0	5854	27	0
1	C	7164	0	6166	26	0
2	E	591	0	287	2	0
2	H	591	0	287	1	0
2	I	591	0	287	1	0
3	F	547	0	282	0	0
3	J	547	0	282	0	0
3	L	547	0	282	0	0
4	D	28	0	25	0	0
5	A	224	0	208	0	0
5	B	210	0	195	0	0
5	C	238	0	221	2	0
All	All	25780	0	21340	111	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 2.

All (111) 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:368:LEU:H	1:A:368:LEU:HD23	1.34	0.90
1:A:620:VAL:HB	1:A:621:PRO:HD3	1.59	0.82
1:A:619:GLU:O	1:A:619:GLU:HG3	1.77	0.82
1:A:330:PRO:HD3	1:A:544:ASN:OD1	1.85	0.77
1:A:368:LEU:H	1:A:368:LEU:CD2	1.99	0.75
1:A:988:GLU:O	1:A:991:VAL:HG12	1.89	0.71
1:C:864:LEU:HD23	1:C:864:LEU:O	1.93	0.68
1:C:62:VAL:HG12	1:C:266:TYR:HB3	1.78	0.66
1:B:277:LEU:HD22	1:B:277:LEU:N	2.12	0.65
1:A:620:VAL:HG21	1:A:651:ILE:HD11	1.78	0.65
1:A:620:VAL:CB	1:A:621:PRO:HD3	2.28	0.64
1:A:825:LYS:HE3	1:A:939:SER:HA	1.80	0.63
1:C:864:LEU:HD23	1:C:864:LEU:C	2.23	0.63
1:A:368:LEU:HD23	1:A:368:LEU:N	2.10	0.62
1:A:986:LYS:N	1:A:987:PRO:HD2	2.15	0.62
1:C:102:ARG:HD2	1:C:243:ALA:HB2	1.82	0.61
1:A:330:PRO:HD2	1:A:525:CYS:SG	2.41	0.60
1:A:389:ASP:OD1	1:A:528:LYS:NZ	2.35	0.59
1:B:895:GLN:HE21	1:C:708:SER:H	1.49	0.59
1:A:31:SER:HB3	1:A:62:VAL:CG2	2.32	0.58
1:A:336:CYS:SG	1:A:358:ILE:HG23	2.45	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1099:GLY:HA3	5:C:1316:NAG:H82	1.86	0.57
1:A:335:LEU:HA	1:A:362:VAL:HG13	1.87	0.56
1:A:745:ASP:HA	1:B:319:ARG:NH1	2.21	0.56
1:A:745:ASP:HA	1:B:319:ARG:HH12	1.71	0.55
1:A:111:ASP:C	1:A:113:LYS:H	2.15	0.54
1:A:794:ILE:HD11	1:A:796:TYR:O	2.07	0.54
1:A:853:GLN:NE2	1:A:959:LEU:HD23	2.23	0.54
1:C:277:LEU:N	1:C:277:LEU:HD12	2.23	0.53
1:B:724:THR:HG22	1:B:1063:LEU:CD2	2.39	0.53
1:B:1142:GLN:N	1:B:1143:PRO:CD	2.72	0.53
1:C:620:VAL:N	1:C:621:PRO:CD	2.72	0.52
1:A:112:SER:N	1:A:133:PHE:O	2.43	0.51
1:B:998:THR:O	1:B:1002:GLN:HG3	2.12	0.50
1:A:335:LEU:HA	1:A:362:VAL:CG1	2.42	0.50
2:E:102:ILE:N	2:E:103:PRO:HD2	2.27	0.50
1:A:825:LYS:HB2	1:A:945:LEU:HD12	1.94	0.50
1:A:1072:GLU:H	1:A:1072:GLU:CD	2.19	0.50
1:C:44:ARG:O	1:C:283:GLY:HA2	2.12	0.50
1:A:984:LEU:CB	1:A:989:ALA:HB2	2.43	0.49
1:C:898:PHE:N	1:C:899:PRO:CD	2.76	0.49
1:C:864:LEU:C	1:C:864:LEU:CD2	2.85	0.49
1:C:124:THR:CB	5:C:1303:NAG:H82	2.43	0.48
1:C:1142:GLN:N	1:C:1143:PRO:CD	2.76	0.48
1:A:898:PHE:N	1:A:899:PRO:CD	2.76	0.48
2:I:102:ILE:N	2:I:103:PRO:HD2	2.28	0.48
1:A:794:ILE:HG23	1:A:797:PHE:CZ	2.49	0.48
1:C:28:TYR:HD2	1:C:61:ASN:HB3	1.78	0.48
1:A:454:ARG:NH2	1:A:469:SER:O	2.47	0.47
2:H:102:ILE:N	2:H:103:PRO:HD2	2.30	0.47
1:B:742:ILE:HD12	1:B:753:LEU:HD21	1.97	0.47
1:A:336:CYS:SG	1:A:358:ILE:CG2	3.03	0.46
1:A:353:TRP:H	1:A:353:TRP:CD1	2.32	0.46
1:A:794:ILE:HG12	1:A:796:TYR:H	1.80	0.46
1:A:314:GLN:HG2	1:C:764:LYS:HD2	1.98	0.46
1:A:959:LEU:O	1:A:962:LEU:HB3	2.15	0.46
1:B:277:LEU:N	1:B:277:LEU:CD2	2.79	0.46
1:A:988:GLU:O	1:A:989:ALA:C	2.59	0.45
1:C:986:LYS:N	1:C:987:PRO:CD	2.78	0.45
1:A:709:ASN:N	1:A:709:ASN:OD1	2.49	0.45
1:B:81:ASN:N	1:B:82:PRO:CD	2.80	0.45
1:A:81:ASN:N	1:A:82:PRO:CD	2.79	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:853:GLN:CD	1:A:959:LEU:HD23	2.42	0.45
1:B:898:PHE:N	1:B:899:PRO:CD	2.80	0.45
1:A:333:THR:O	1:A:334:ASN:C	2.60	0.45
1:C:58:PHE:CD2	1:C:290:ASP:HB2	2.52	0.45
1:A:703:ASN:ND2	1:C:787:GLN:OE1	2.50	0.44
1:C:742:ILE:O	1:C:743:CYS:HB2	2.17	0.44
1:B:331:ASN:OD1	1:B:331:ASN:N	2.48	0.44
1:A:982:SER:C	1:A:984:LEU:H	2.25	0.44
1:A:336:CYS:SG	1:A:337:PRO:HD2	2.57	0.44
1:A:468:ILE:O	1:A:468:ILE:HG22	2.18	0.44
1:A:111:ASP:C	1:A:133:PHE:O	2.62	0.43
1:A:616:ASN:O	1:A:618:THR:N	2.52	0.43
1:C:28:TYR:CD2	1:C:61:ASN:HB3	2.53	0.43
1:C:102:ARG:CD	1:C:243:ALA:HB2	2.49	0.43
1:A:988:GLU:O	1:A:991:VAL:N	2.47	0.42
1:A:620:VAL:HB	1:A:621:PRO:CD	2.39	0.42
1:B:908:GLY:O	1:B:1038:LYS:NZ	2.53	0.42
1:A:81:ASN:N	1:A:82:PRO:HD3	2.34	0.42
1:A:365:TYR:O	1:A:368:LEU:HD21	2.20	0.42
1:A:981:PHE:CE1	1:A:993:ILE:HD12	2.55	0.42
1:A:1141:LEU:C	1:A:1143:PRO:HD2	2.45	0.42
1:B:81:ASN:N	1:B:82:PRO:HD3	2.35	0.42
1:C:62:VAL:CG1	1:C:266:TYR:HB3	2.48	0.42
1:A:808:ASP:OD1	1:A:808:ASP:C	2.63	0.42
1:B:315:THR:OG1	1:B:316:SER:N	2.53	0.41
1:B:590:CYS:O	1:B:591:SER:C	2.62	0.41
1:B:756:TYR:O	1:B:758:SER:N	2.53	0.41
1:A:821:LEU:O	1:A:825:LYS:HG2	2.21	0.41
1:B:738:CYS:O	1:B:742:ILE:HG13	2.20	0.41
1:C:122:ASN:OD1	1:C:123:ALA:N	2.52	0.41
1:A:986:LYS:N	1:A:987:PRO:CD	2.83	0.41
1:B:537:LYS:O	1:B:538:CYS:HB2	2.21	0.41
1:B:743:CYS:HB3	1:B:749:CYS:HB3	1.93	0.41
1:B:986:LYS:N	1:B:987:PRO:CD	2.83	0.41
1:A:616:ASN:C	1:A:618:THR:N	2.78	0.41
1:A:990:GLU:O	1:A:993:ILE:HG22	2.20	0.41
1:C:277:LEU:HD23	1:C:285:ILE:HG21	2.03	0.41
1:B:379:CYS:O	1:B:380:TYR:CG	2.74	0.41
1:B:498:ARG:HA	1:B:499:PRO:HD3	1.93	0.41
1:C:1001:LEU:O	1:C:1005:GLN:HG3	2.21	0.41
1:B:490:PHE:O	1:B:493:ARG:NH1	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:616:ASN:O	1:C:617:CYS:HB2	2.21	0.41
1:A:111:ASP:C	1:A:113:LYS:N	2.79	0.40
1:A:1078:ALA:HA	1:A:1079:PRO:HD3	1.96	0.40
1:B:898:PHE:HB3	1:B:899:PRO:HD3	2.04	0.40
2:E:41:GLN:HA	2:E:42:PRO:HD2	1.93	0.40
1:A:578:ASP:HA	1:A:579:PRO:HD3	1.89	0.40
1:B:490:PHE:HA	1:B:491:PRO:HD3	1.92	0.40
1:B:986:LYS:HB3	1:B:987:PRO:HD3	2.03	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	1000/1274 (78%)	972 (97%)	25 (2%)	3 (0%)	36	67
1	B	989/1274 (78%)	954 (96%)	29 (3%)	6 (1%)	21	52
1	C	1017/1274 (80%)	970 (95%)	44 (4%)	3 (0%)	36	67
2	E	115/119 (97%)	113 (98%)	2 (2%)	0	100	100
2	H	115/119 (97%)	112 (97%)	3 (3%)	0	100	100
2	I	115/119 (97%)	112 (97%)	3 (3%)	0	100	100
3	F	107/110 (97%)	106 (99%)	1 (1%)	0	100	100
3	J	107/110 (97%)	106 (99%)	1 (1%)	0	100	100
3	L	107/110 (97%)	105 (98%)	2 (2%)	0	100	100
All	All	3672/4509 (81%)	3550 (97%)	110 (3%)	12 (0%)	37	67

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	538	CYS
1	B	374	PHE
1	B	742	ILE
1	B	757	GLY
1	C	743	CYS
1	B	373	PRO
1	C	323	THR
1	A	112	SER
1	A	334	ASN
1	B	389	ASP
1	C	389	ASP
1	A	983	ARG

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	720/1112 (65%)	710 (99%)	10 (1%)	59	76
1	B	559/1112 (50%)	557 (100%)	2 (0%)	84	86
1	C	605/1112 (54%)	600 (99%)	5 (1%)	73	81
2	E	8/107 (8%)	8 (100%)	0	100	100
2	H	8/107 (8%)	8 (100%)	0	100	100
2	I	8/107 (8%)	8 (100%)	0	100	100
3	F	8/92 (9%)	8 (100%)	0	100	100
3	J	8/92 (9%)	8 (100%)	0	100	100
3	L	8/92 (9%)	8 (100%)	0	100	100
All	All	1932/3933 (49%)	1915 (99%)	17 (1%)	68	80

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	332	ILE
1	A	336	CYS
1	A	368	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	537	LYS
1	A	709	ASN
1	A	794	ILE
1	A	825	LYS
1	A	918	GLU
1	A	1073	LYS
1	A	1134	ASN
1	B	277	LEU
1	B	331	ASN
1	C	17	ASN
1	C	633	TRP
1	C	641	ASN
1	C	821	LEU
1	C	1098	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	314	GLN
1	A	414	GLN
1	A	564	GLN
1	A	703	ASN
1	A	762	GLN
1	A	901	GLN
1	A	949	GLN
1	A	1010	GLN
1	A	1101	HIS
1	B	564	GLN
1	B	703	ASN
1	B	804	GLN
1	B	895	GLN
1	B	949	GLN
1	B	965	GLN
1	B	1002	GLN
1	B	1023	ASN
1	B	1101	HIS
1	C	115	GLN
1	C	271	GLN
1	C	641	ASN
1	C	690	GLN
1	C	703	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1101	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

2 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	D	1	1,4	14,14,15	1.32	1 (7%)	17,19,21	1.16	1 (5%)
4	NAG	D	2	4	14,14,15	1.10	2 (14%)	17,19,21	1.20	2 (11%)

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	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	NAG	C1-C2	3.53	1.57	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2	NAG	C1-C2	2.68	1.56	1.52
4	D	2	NAG	O5-C5	2.16	1.47	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2	NAG	C8-C7-N2	2.65	120.51	116.12
4	D	1	NAG	C8-C7-N2	2.40	120.09	116.12
4	D	2	NAG	C2-N2-C7	-2.30	119.82	122.90

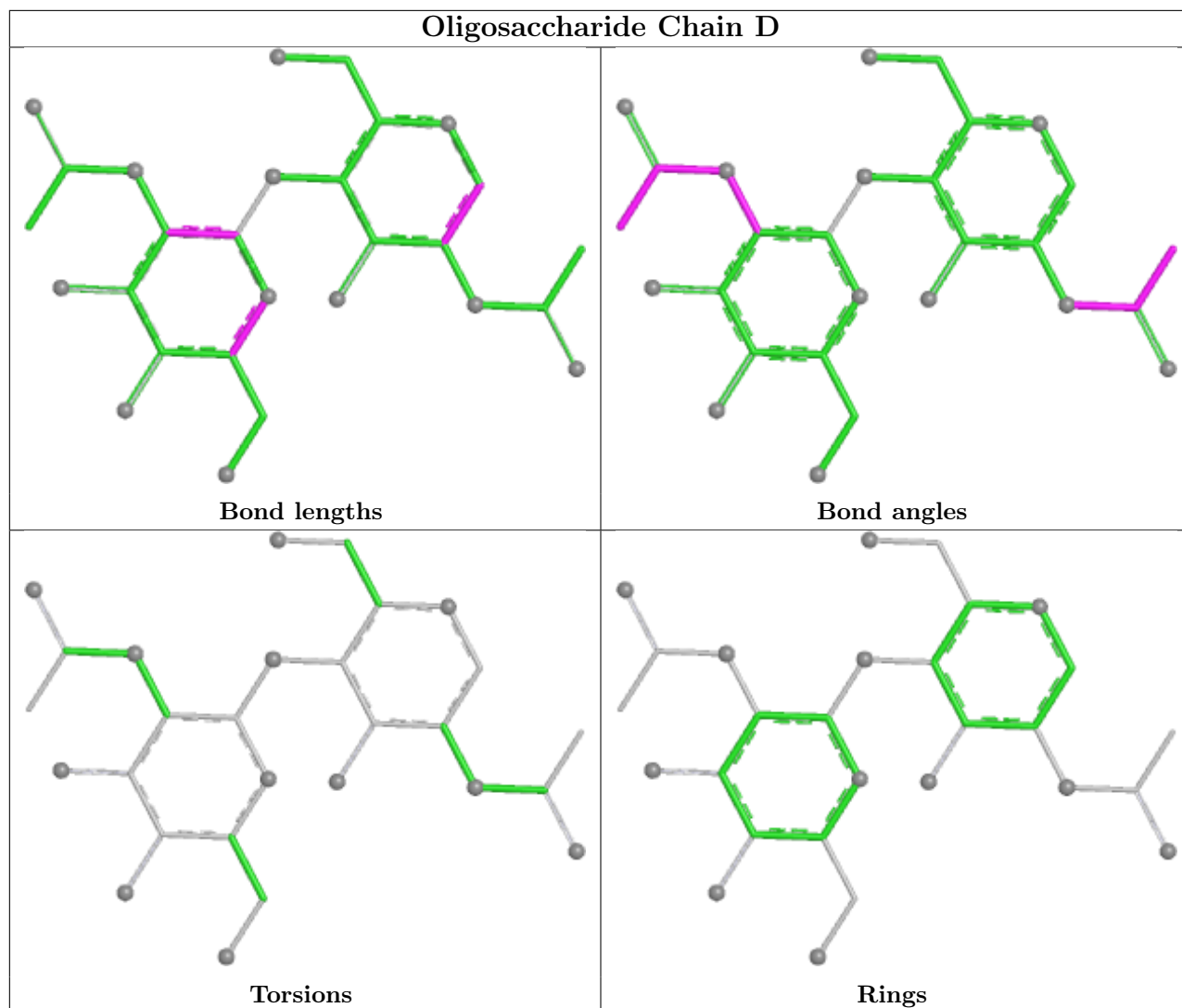
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

48 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
5	NAG	B	1308	1	14,14,15	1.21	1 (7%)	17,19,21	1.06	1 (5%)
5	NAG	A	1305	1	14,14,15	1.28	1 (7%)	17,19,21	1.05	1 (5%)
5	NAG	C	1304	1	14,14,15	1.17	1 (7%)	17,19,21	1.07	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	1302	1	14,14,15	1.24	1 (7%)	17,19,21	1.06	1 (5%)
5	NAG	B	1306	1	14,14,15	1.25	1 (7%)	17,19,21	1.12	2 (11%)
5	NAG	A	1316	1	14,14,15	1.12	1 (7%)	17,19,21	1.03	1 (5%)
5	NAG	C	1307	1	14,14,15	1.18	1 (7%)	17,19,21	0.85	1 (5%)
5	NAG	C	1312	1	14,14,15	0.30	0	17,19,21	0.51	0
5	NAG	B	1309	1	14,14,15	1.28	1 (7%)	17,19,21	1.01	0
5	NAG	C	1311	1	14,14,15	1.15	1 (7%)	17,19,21	1.05	1 (5%)
5	NAG	C	1303	1	14,14,15	1.18	1 (7%)	17,19,21	1.06	1 (5%)
5	NAG	B	1307	1	14,14,15	1.26	1 (7%)	17,19,21	1.07	1 (5%)
5	NAG	A	1307	1	14,14,15	1.17	1 (7%)	17,19,21	1.08	1 (5%)
5	NAG	A	1314	1	14,14,15	1.13	1 (7%)	17,19,21	0.95	1 (5%)
5	NAG	C	1309	1	14,14,15	1.25	1 (7%)	17,19,21	1.00	1 (5%)
5	NAG	B	1312	1	14,14,15	1.13	1 (7%)	17,19,21	1.02	1 (5%)
5	NAG	B	1310	1	14,14,15	1.32	2 (14%)	17,19,21	0.84	0
5	NAG	A	1306	1	14,14,15	1.33	1 (7%)	17,19,21	1.08	1 (5%)
5	NAG	A	1308	1	14,14,15	1.16	1 (7%)	17,19,21	0.97	1 (5%)
5	NAG	A	1311	1	14,14,15	1.18	1 (7%)	17,19,21	1.11	1 (5%)
5	NAG	B	1303	1	14,14,15	1.26	1 (7%)	17,19,21	0.99	2 (11%)
5	NAG	A	1315	1	14,14,15	1.24	1 (7%)	17,19,21	1.01	1 (5%)
5	NAG	A	1304	1	14,14,15	1.21	1 (7%)	17,19,21	1.01	1 (5%)
5	NAG	B	1301	1	14,14,15	1.25	1 (7%)	17,19,21	1.11	2 (11%)
5	NAG	B	1311	1	14,14,15	1.21	1 (7%)	17,19,21	1.01	1 (5%)
5	NAG	C	1301	1	14,14,15	1.33	1 (7%)	17,19,21	1.08	1 (5%)
5	NAG	C	1314	1	14,14,15	1.27	1 (7%)	17,19,21	1.05	1 (5%)
5	NAG	A	1313	1	14,14,15	1.15	1 (7%)	17,19,21	1.04	1 (5%)
5	NAG	C	1302	1	14,14,15	1.20	1 (7%)	17,19,21	1.16	2 (11%)
5	NAG	A	1310	1	14,14,15	1.14	1 (7%)	17,19,21	0.99	1 (5%)
5	NAG	C	1306	1	14,14,15	1.20	1 (7%)	17,19,21	0.97	1 (5%)
5	NAG	C	1316	1	14,14,15	1.39	1 (7%)	17,19,21	1.15	1 (5%)
5	NAG	A	1309	1	14,14,15	1.18	1 (7%)	17,19,21	1.01	1 (5%)
5	NAG	B	1302	1	14,14,15	1.19	1 (7%)	17,19,21	1.14	1 (5%)
5	NAG	C	1305	1	14,14,15	1.28	1 (7%)	17,19,21	1.03	1 (5%)
5	NAG	C	1315	1	14,14,15	1.30	2 (14%)	17,19,21	1.46	3 (17%)
5	NAG	B	1314	1	14,14,15	1.23	1 (7%)	17,19,21	0.99	1 (5%)
5	NAG	A	1303	1	14,14,15	1.20	1 (7%)	17,19,21	1.07	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	1301	1	14,14,15	1.22	1 (7%)	17,19,21	1.05	1 (5%)
5	NAG	C	1310	1	14,14,15	1.15	1 (7%)	17,19,21	1.23	2 (11%)
5	NAG	C	1317	1	14,14,15	1.18	1 (7%)	17,19,21	0.96	1 (5%)
5	NAG	B	1315	1	14,14,15	1.17	1 (7%)	17,19,21	0.94	1 (5%)
5	NAG	B	1304	1	14,14,15	1.21	1 (7%)	17,19,21	0.98	1 (5%)
5	NAG	C	1313	1	14,14,15	1.10	1 (7%)	17,19,21	1.05	1 (5%)
5	NAG	C	1308	1	14,14,15	1.25	1 (7%)	17,19,21	1.01	1 (5%)
5	NAG	B	1313	1	14,14,15	1.16	1 (7%)	17,19,21	0.96	1 (5%)
5	NAG	B	1305	1	14,14,15	1.12	1 (7%)	17,19,21	0.94	1 (5%)
5	NAG	A	1312	1	14,14,15	1.10	1 (7%)	17,19,21	0.96	1 (5%)

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
5	NAG	B	1308	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1316	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1312	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1309	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1311	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1314	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1312	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1310	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1311	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1315	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1304	1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1311	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1314	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1313	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1310	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1306	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1316	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1315	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1314	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1310	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1317	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1315	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1313	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1313	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1312	1	-	0/6/23/26	0/1/1/1

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1316	NAG	C1-C2	4.41	1.58	1.52
5	A	1306	NAG	C1-C2	4.27	1.58	1.52
5	C	1314	NAG	C1-C2	4.08	1.57	1.52
5	B	1310	NAG	C1-C2	4.02	1.57	1.52
5	C	1305	NAG	C1-C2	4.00	1.57	1.52
5	B	1309	NAG	C1-C2	3.96	1.57	1.52
5	C	1301	NAG	C1-C2	3.96	1.57	1.52
5	A	1305	NAG	C1-C2	3.84	1.57	1.52
5	C	1309	NAG	C1-C2	3.82	1.57	1.52
5	A	1315	NAG	C1-C2	3.76	1.57	1.52
5	B	1314	NAG	C1-C2	3.76	1.57	1.52
5	B	1311	NAG	C1-C2	3.73	1.57	1.52
5	B	1307	NAG	C1-C2	3.72	1.57	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1306	NAG	C1-C2	3.71	1.57	1.52
5	A	1302	NAG	C1-C2	3.70	1.57	1.52
5	C	1308	NAG	C1-C2	3.70	1.57	1.52
5	A	1311	NAG	C1-C2	3.68	1.57	1.52
5	B	1301	NAG	C1-C2	3.68	1.57	1.52
5	A	1304	NAG	C1-C2	3.67	1.57	1.52
5	B	1308	NAG	C1-C2	3.64	1.57	1.52
5	C	1317	NAG	C1-C2	3.63	1.57	1.52
5	A	1301	NAG	C1-C2	3.62	1.57	1.52
5	A	1303	NAG	C1-C2	3.62	1.57	1.52
5	B	1303	NAG	C1-C2	3.61	1.57	1.52
5	C	1306	NAG	C1-C2	3.58	1.57	1.52
5	B	1302	NAG	C1-C2	3.58	1.57	1.52
5	A	1309	NAG	C1-C2	3.57	1.57	1.52
5	C	1307	NAG	C1-C2	3.55	1.57	1.52
5	C	1315	NAG	C1-C2	3.55	1.57	1.52
5	C	1304	NAG	C1-C2	3.54	1.57	1.52
5	C	1302	NAG	C1-C2	3.52	1.57	1.52
5	A	1308	NAG	C1-C2	3.49	1.57	1.52
5	C	1303	NAG	C1-C2	3.48	1.57	1.52
5	B	1313	NAG	C1-C2	3.47	1.57	1.52
5	C	1311	NAG	C1-C2	3.47	1.57	1.52
5	B	1304	NAG	C1-C2	3.46	1.57	1.52
5	A	1310	NAG	C1-C2	3.46	1.57	1.52
5	B	1315	NAG	C1-C2	3.46	1.57	1.52
5	A	1313	NAG	C1-C2	3.39	1.57	1.52
5	A	1307	NAG	C1-C2	3.39	1.57	1.52
5	A	1314	NAG	C1-C2	3.34	1.56	1.52
5	B	1312	NAG	C1-C2	3.33	1.56	1.52
5	B	1305	NAG	C1-C2	3.32	1.56	1.52
5	A	1316	NAG	C1-C2	3.25	1.56	1.52
5	C	1313	NAG	C1-C2	3.24	1.56	1.52
5	A	1312	NAG	C1-C2	3.20	1.56	1.52
5	C	1310	NAG	C1-C2	3.10	1.56	1.52
5	C	1315	NAG	O5-C5	2.40	1.48	1.43
5	B	1310	NAG	O5-C5	2.16	1.47	1.43

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1315	NAG	C8-C7-N2	3.06	121.19	116.12
5	C	1316	NAG	C8-C7-N2	2.76	120.70	116.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1309	NAG	C8-C7-N2	2.71	120.61	116.12
5	C	1310	NAG	C8-C7-N2	2.67	120.55	116.12
5	A	1305	NAG	C8-C7-N2	2.59	120.42	116.12
5	B	1302	NAG	C8-C7-N2	2.59	120.41	116.12
5	A	1311	NAG	C8-C7-N2	2.58	120.40	116.12
5	A	1307	NAG	C8-C7-N2	2.57	120.39	116.12
5	B	1307	NAG	C8-C7-N2	2.56	120.36	116.12
5	C	1305	NAG	C8-C7-N2	2.55	120.35	116.12
5	B	1308	NAG	C8-C7-N2	2.54	120.33	116.12
5	A	1303	NAG	C8-C7-N2	2.53	120.32	116.12
5	A	1302	NAG	C8-C7-N2	2.53	120.32	116.12
5	C	1302	NAG	C8-C7-N2	2.53	120.31	116.12
5	C	1301	NAG	C8-C7-N2	2.53	120.31	116.12
5	C	1308	NAG	C8-C7-N2	2.52	120.30	116.12
5	A	1313	NAG	C8-C7-N2	2.52	120.30	116.12
5	C	1303	NAG	C8-C7-N2	2.50	120.26	116.12
5	C	1314	NAG	C8-C7-N2	2.49	120.24	116.12
5	A	1306	NAG	C8-C7-N2	2.48	120.24	116.12
5	C	1315	NAG	C2-N2-C7	-2.48	119.58	122.90
5	B	1306	NAG	C8-C7-N2	2.45	120.19	116.12
5	A	1304	NAG	C8-C7-N2	2.45	120.18	116.12
5	A	1315	NAG	C8-C7-N2	2.41	120.11	116.12
5	C	1309	NAG	C8-C7-N2	2.41	120.11	116.12
5	A	1316	NAG	C8-C7-N2	2.40	120.09	116.12
5	B	1301	NAG	C8-C7-N2	2.39	120.09	116.12
5	C	1304	NAG	C8-C7-N2	2.39	120.08	116.12
5	B	1311	NAG	C8-C7-N2	2.39	120.08	116.12
5	B	1314	NAG	C8-C7-N2	2.38	120.07	116.12
5	C	1310	NAG	C4-C3-C2	-2.36	107.56	111.02
5	A	1301	NAG	C8-C7-N2	2.34	119.99	116.12
5	A	1310	NAG	C8-C7-N2	2.33	119.99	116.12
5	A	1312	NAG	C8-C7-N2	2.32	119.97	116.12
5	B	1304	NAG	C8-C7-N2	2.31	119.96	116.12
5	C	1306	NAG	C8-C7-N2	2.30	119.94	116.12
5	C	1313	NAG	C8-C7-N2	2.30	119.94	116.12
5	B	1312	NAG	C8-C7-N2	2.29	119.92	116.12
5	A	1308	NAG	C8-C7-N2	2.29	119.91	116.12
5	B	1301	NAG	C2-N2-C7	-2.28	119.85	122.90
5	C	1311	NAG	C8-C7-N2	2.27	119.89	116.12
5	A	1314	NAG	C8-C7-N2	2.24	119.83	116.12
5	C	1317	NAG	C8-C7-N2	2.21	119.78	116.12
5	B	1313	NAG	C8-C7-N2	2.19	119.75	116.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1306	NAG	C4-C3-C2	-2.18	107.83	111.02
5	B	1303	NAG	C8-C7-N2	2.14	119.67	116.12
5	C	1315	NAG	O5-C1-C2	-2.10	108.05	111.29
5	B	1305	NAG	C8-C7-N2	2.09	119.59	116.12
5	B	1303	NAG	C4-C3-C2	-2.07	107.99	111.02
5	B	1315	NAG	C8-C7-N2	2.07	119.54	116.12
5	C	1307	NAG	C8-C7-N2	2.06	119.53	116.12
5	C	1302	NAG	C4-C3-C2	-2.05	108.02	111.02

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1316	NAG	O5-C5-C6-O6
5	C	1316	NAG	C4-C5-C6-O6
5	C	1314	NAG	O5-C5-C6-O6
5	C	1312	NAG	O5-C5-C6-O6
5	C	1315	NAG	O5-C5-C6-O6
5	B	1303	NAG	C1-C2-N2-C7
5	B	1303	NAG	C3-C2-N2-C7
5	A	1311	NAG	C1-C2-N2-C7
5	A	1316	NAG	C4-C5-C6-O6
5	A	1310	NAG	C4-C5-C6-O6
5	B	1312	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1303	NAG	1	0
5	C	1316	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28559. These allow visual inspection of the internal detail of the map and identification of artifacts.

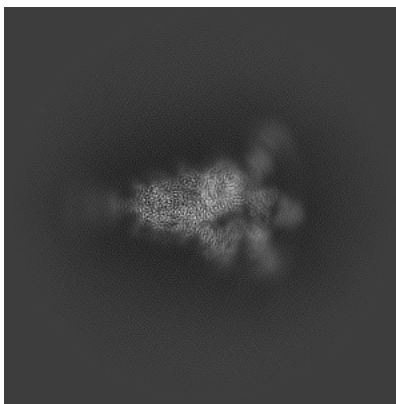
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

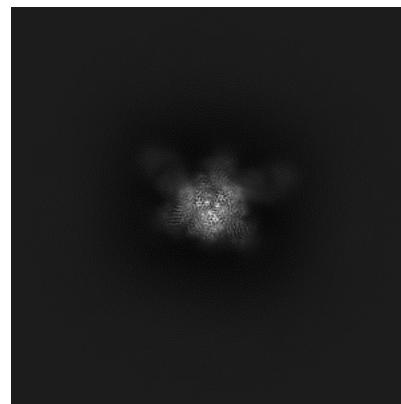
6.1.1 Primary map



X

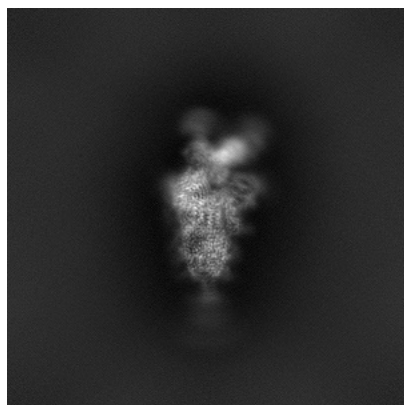


Y

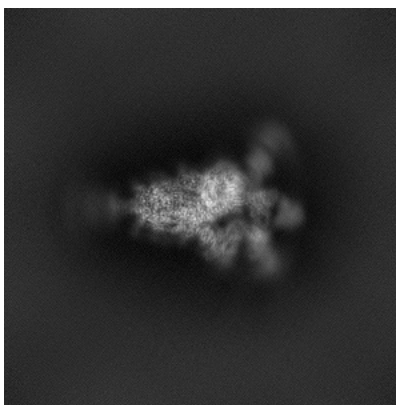


Z

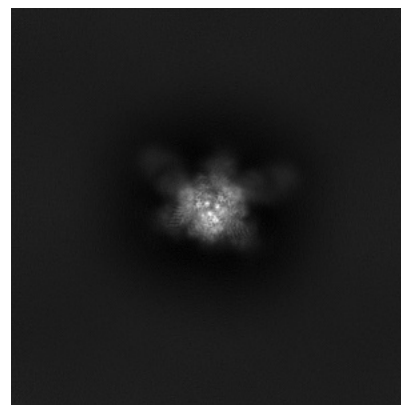
6.1.2 Raw map



X



Y

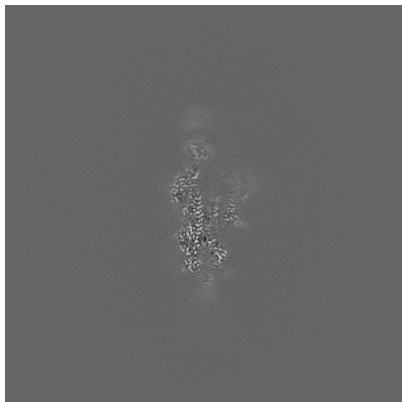


Z

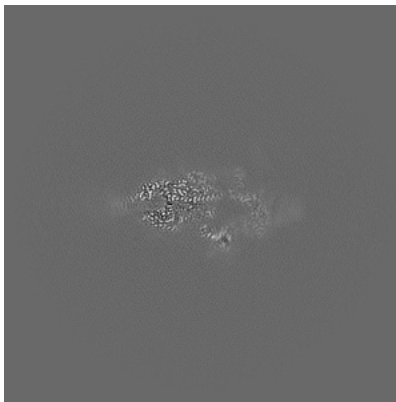
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

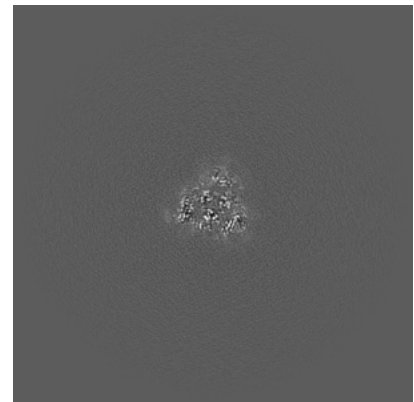
6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

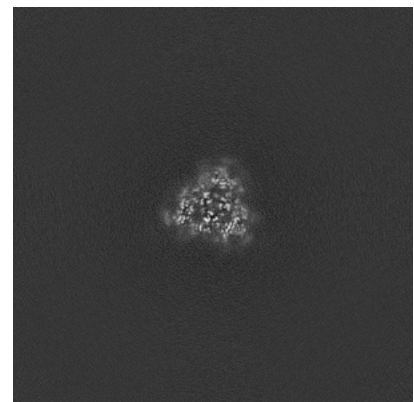
6.2.2 Raw map



X Index: 256



Y Index: 256

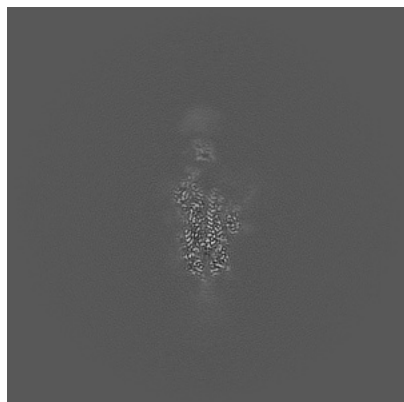


Z Index: 256

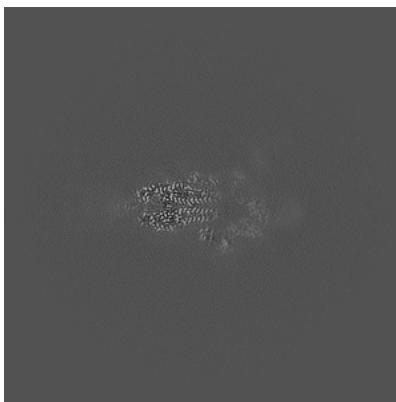
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

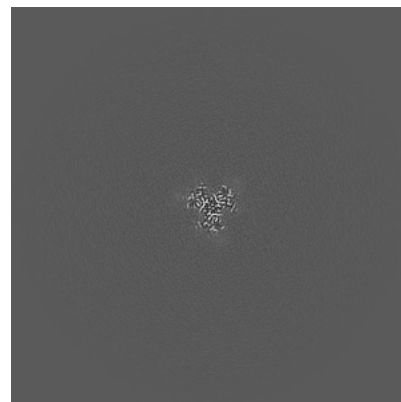
6.3.1 Primary map



X Index: 250



Y Index: 259

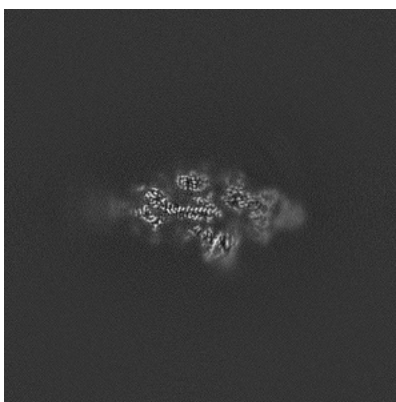


Z Index: 210

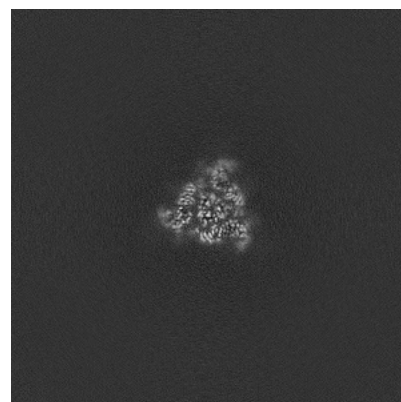
6.3.2 Raw map



X Index: 250



Y Index: 247

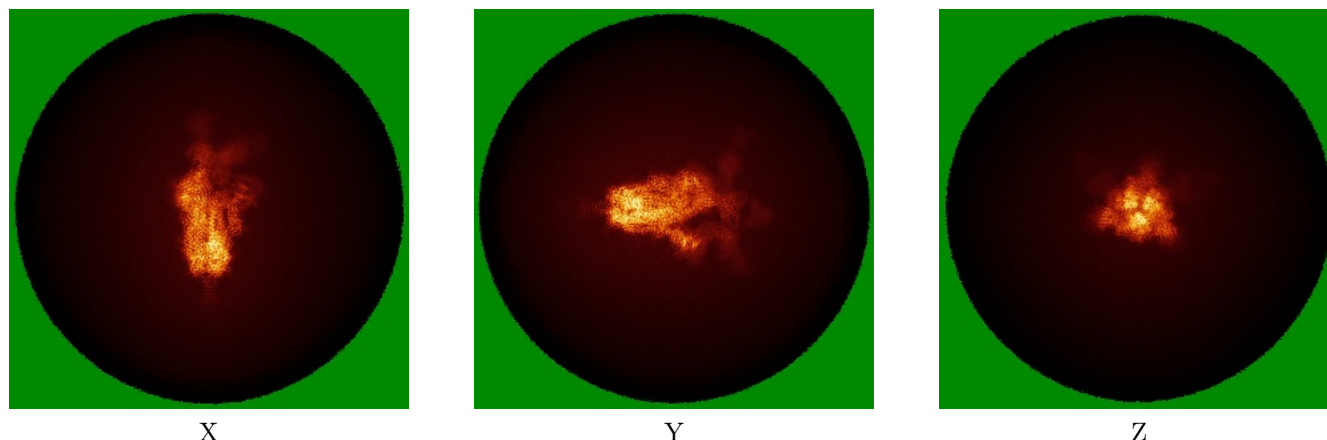


Z Index: 261

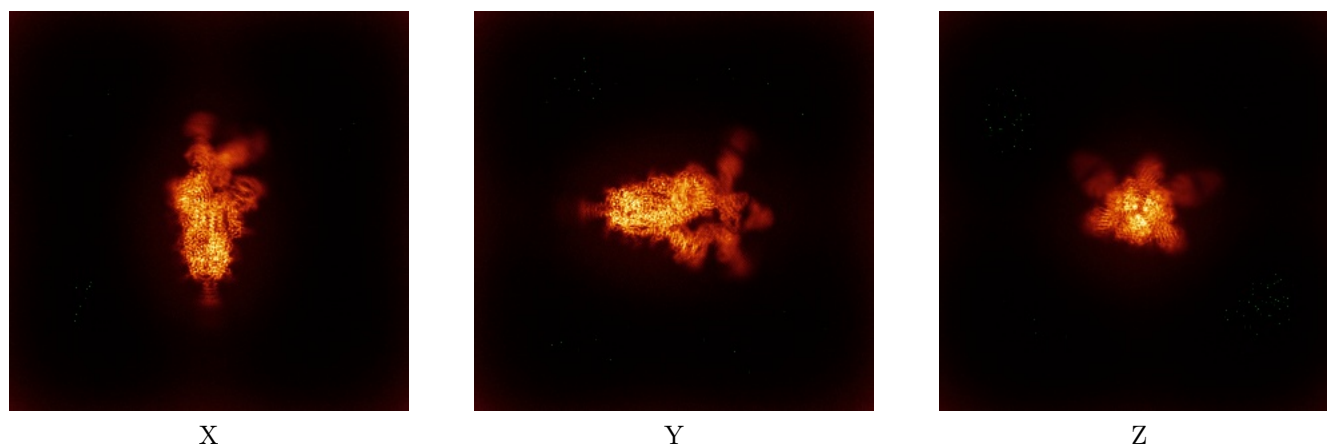
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



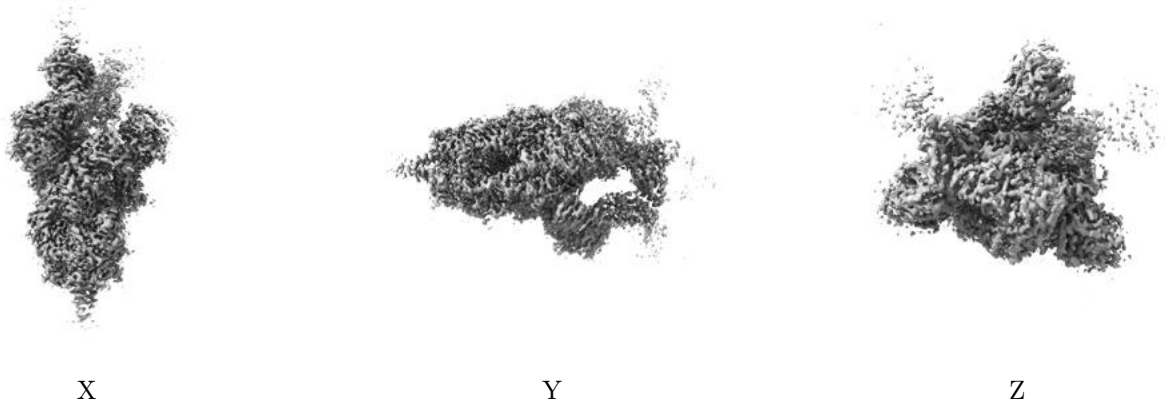
6.4.2 Raw map



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

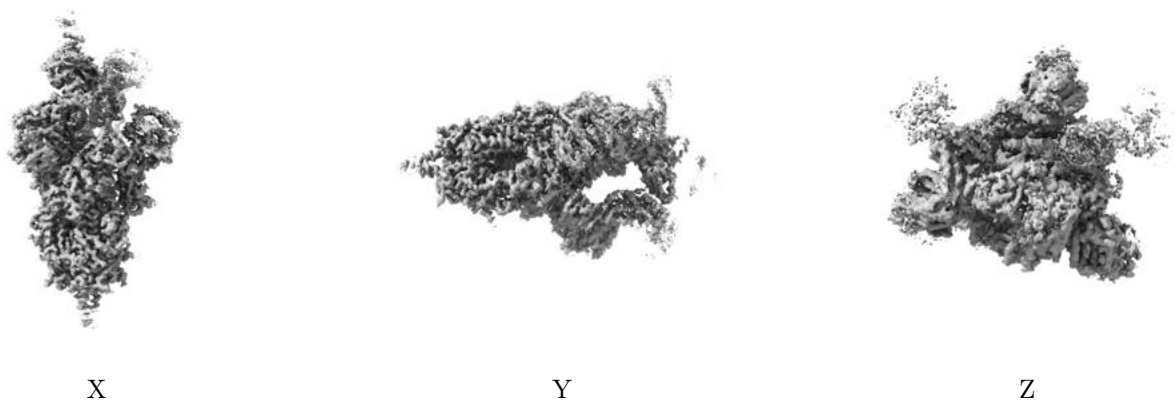
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.6. 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.

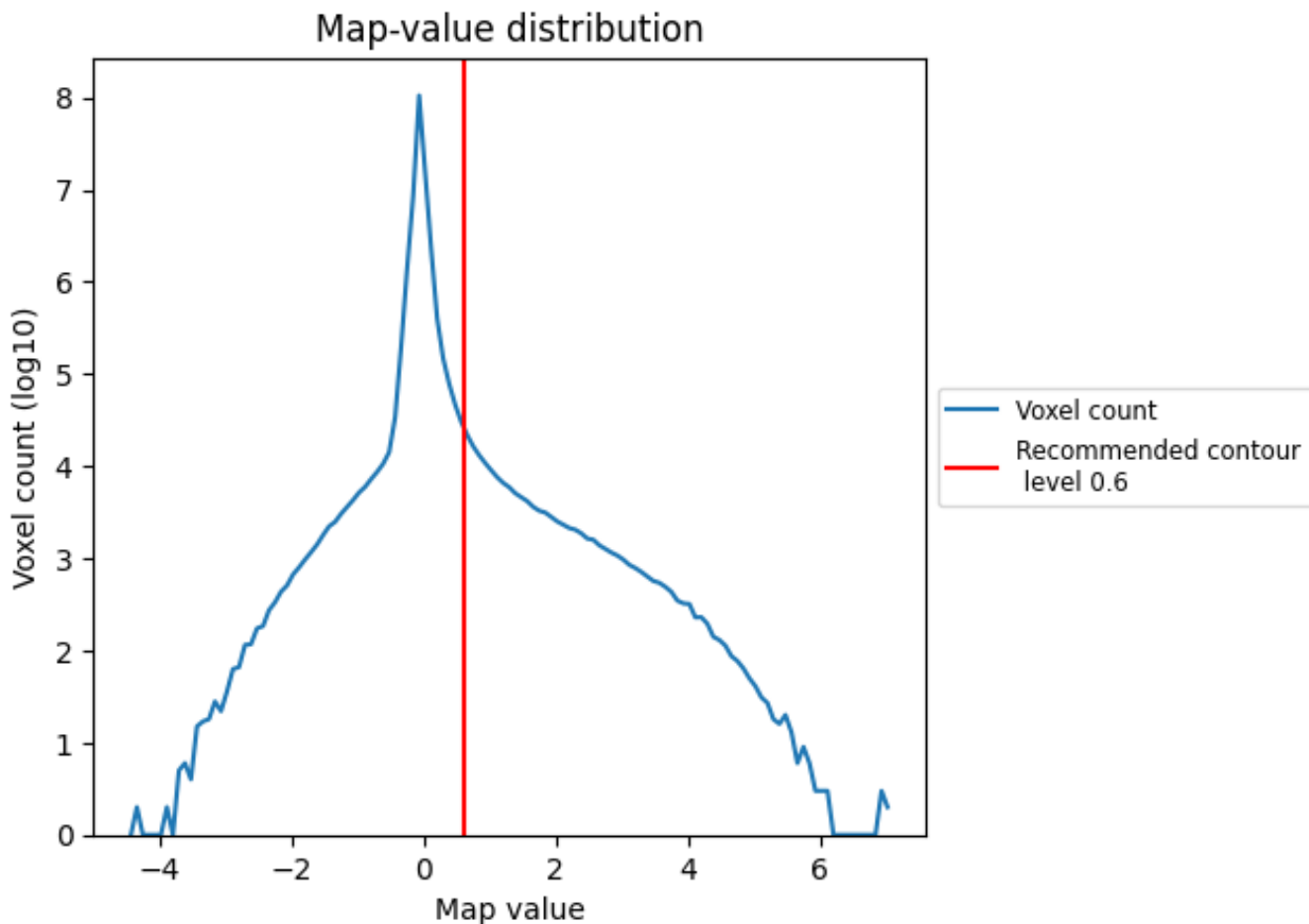
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

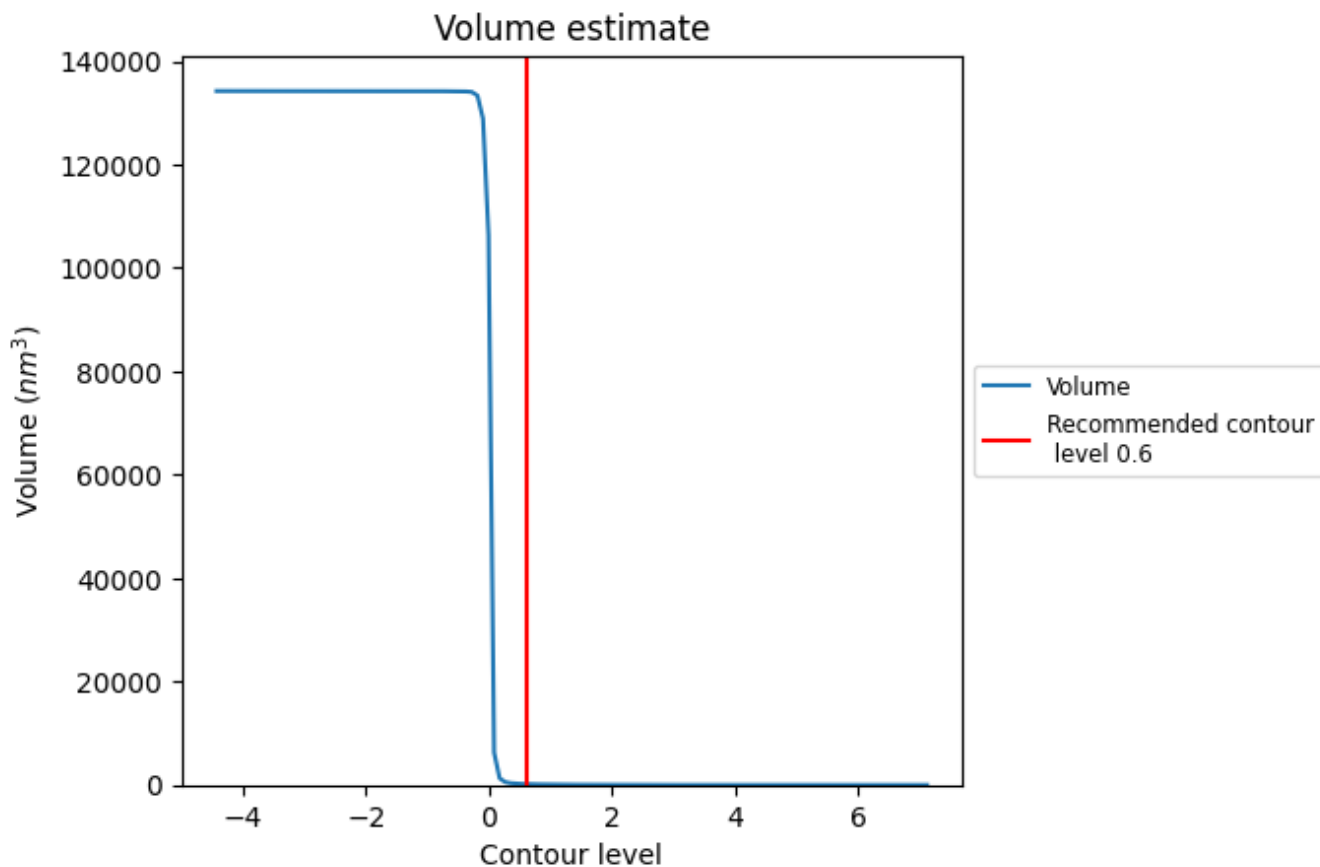
This section contains the results of statistical analysis of the map.

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.

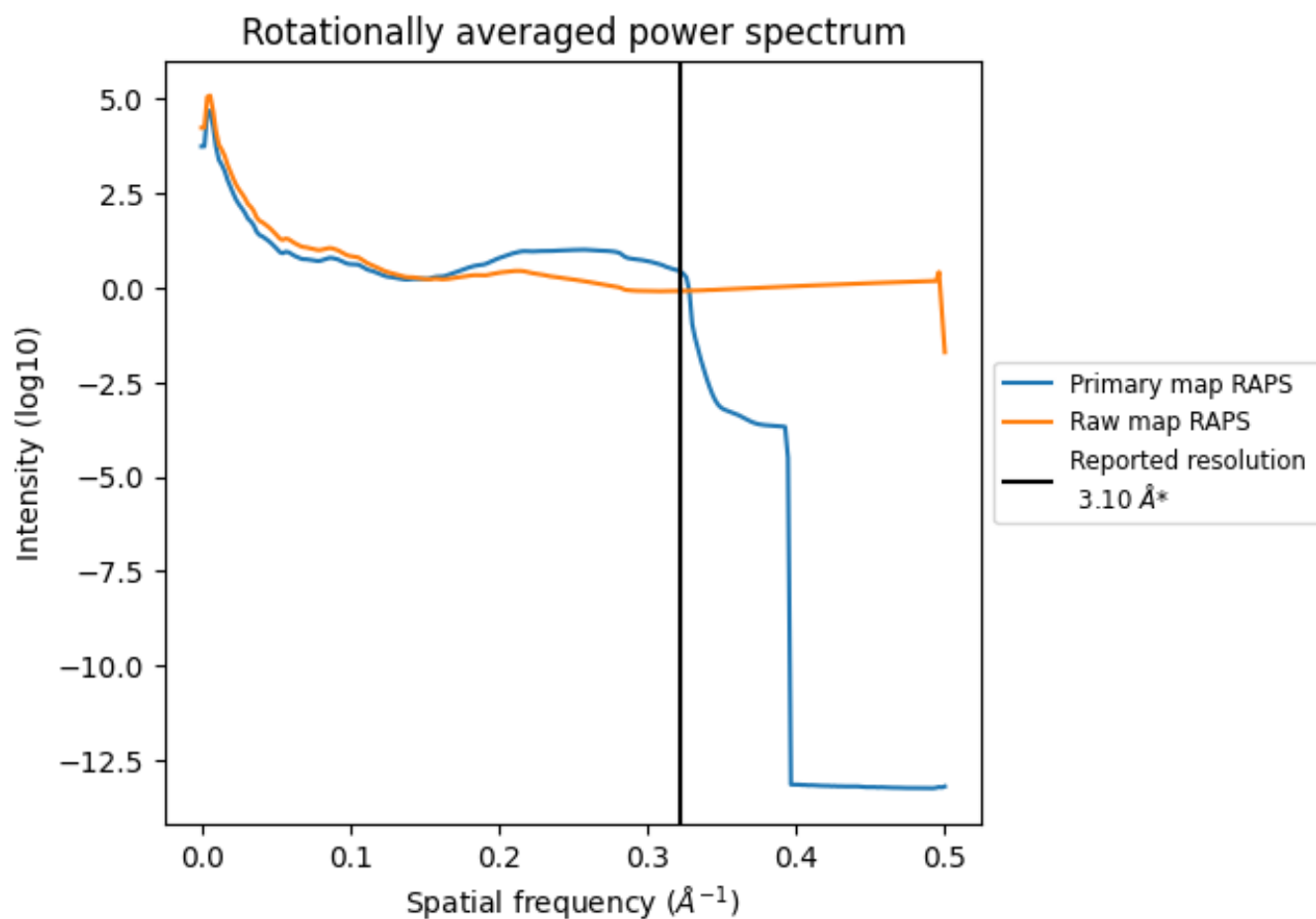
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 166 nm³; this corresponds to an approximate mass of 150 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

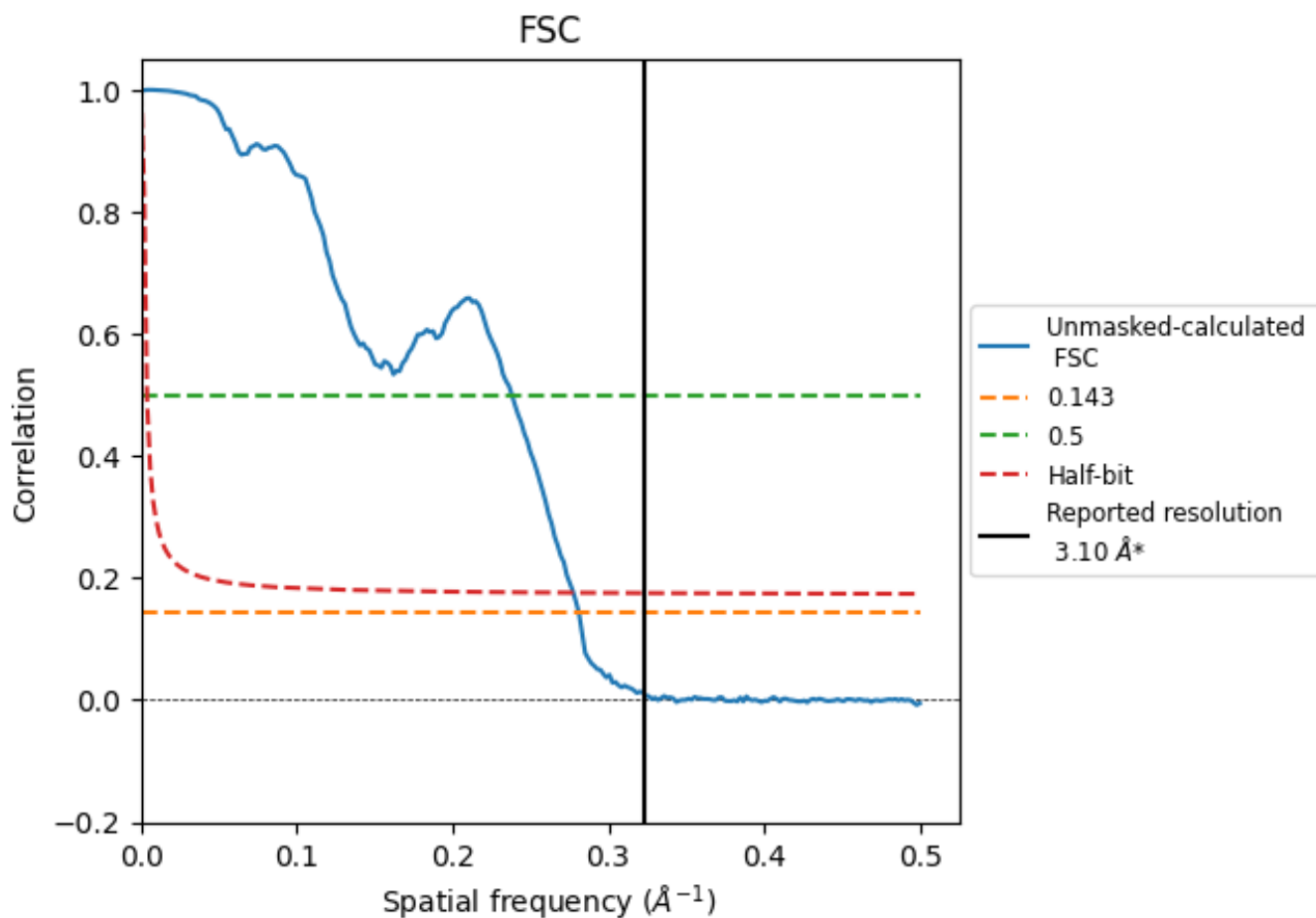


*Reported resolution corresponds to spatial frequency of 0.323 \AA^{-1}

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 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

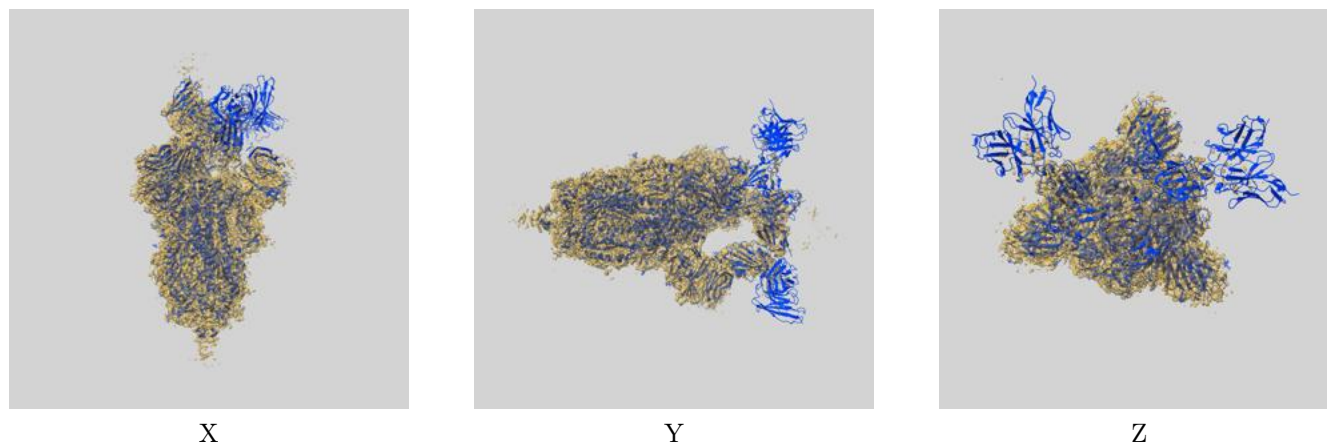
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.56	4.20	3.60

*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 3.56 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

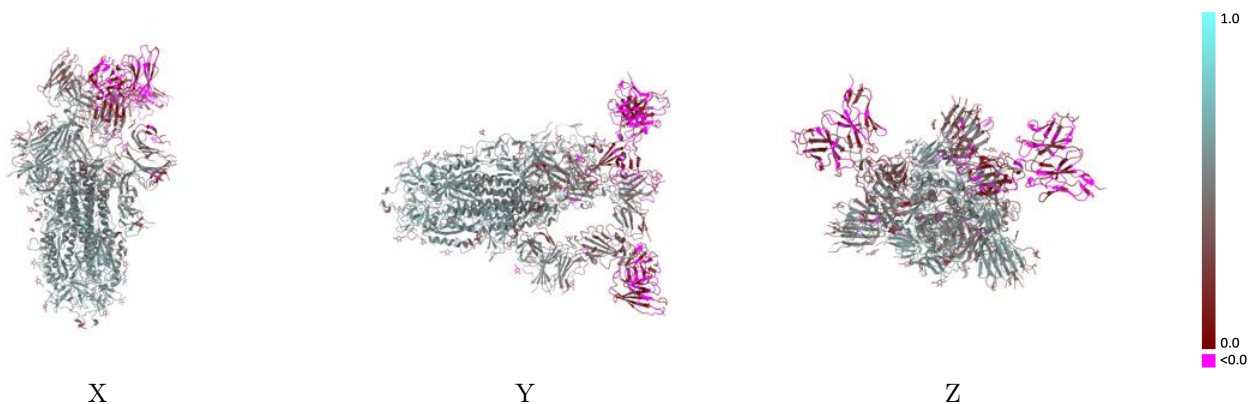
This section contains information regarding the fit between EMDB map EMD-28559 and PDB model 8ERR. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



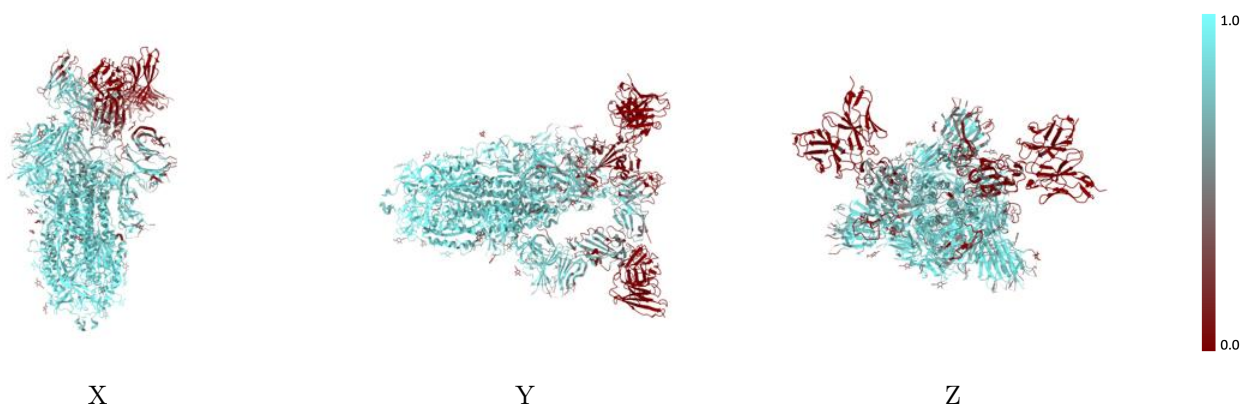
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



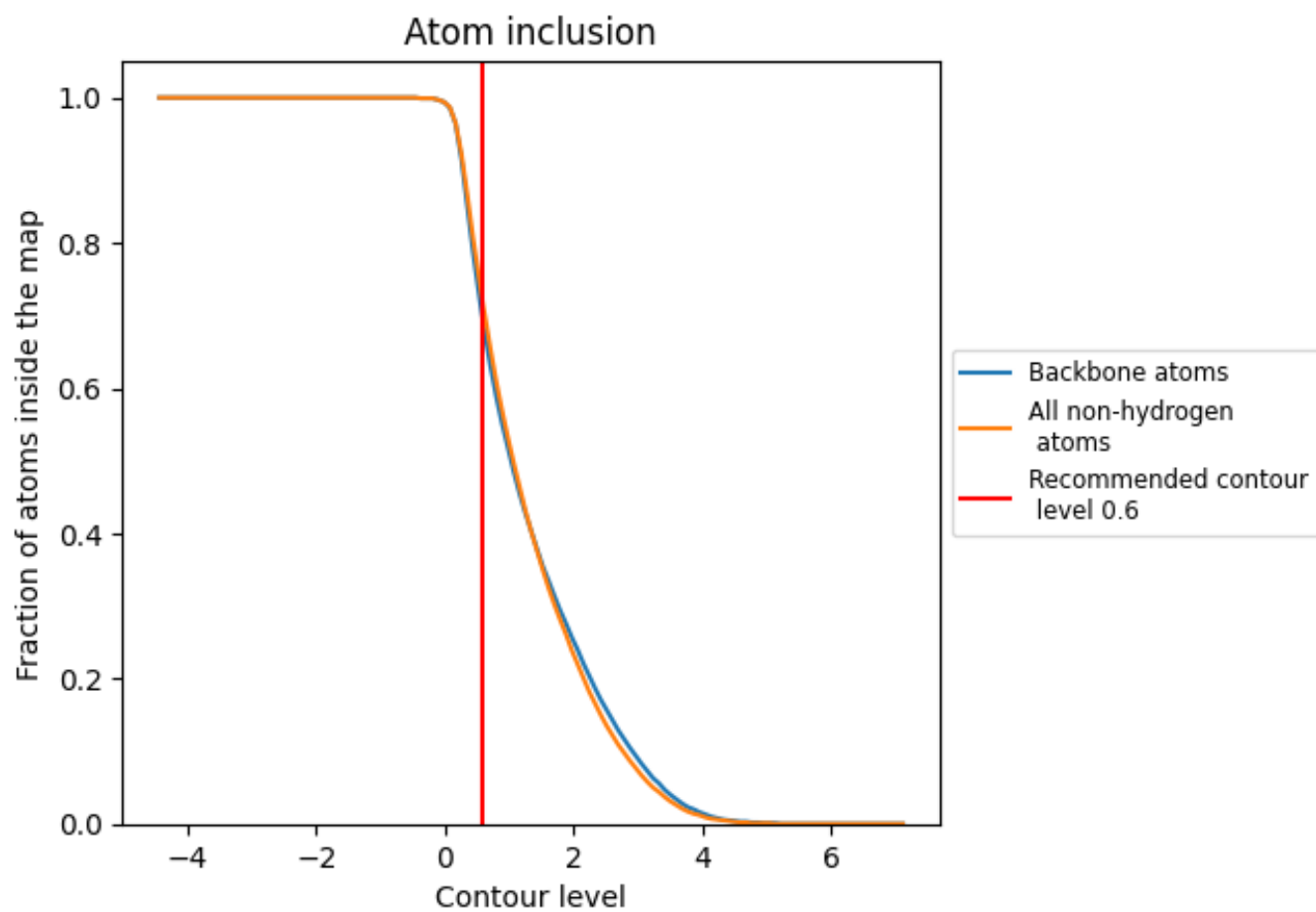
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.6).























9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 71% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7120	 0.4490
A	 0.8550	 0.5260
B	 0.7400	 0.4680
C	 0.7760	 0.4820
D	 0.7140	 0.4070
E	 0.0030	 0.0480
F	 0.0000	 0.0220
H	 0.5210	 0.3710
I	 0.0190	 0.0880
J	 0.0050	 0.0660
L	 0.6290	 0.4000

