wwPDB EM Validation Summary Report (i)

Oct 15, 2026 – 07:22 pm BST

PDB ID	:	9TMF / pdb_00009tmf
EMDB ID	:	EMD-56069
Title	:	Structure of the SARS-CoV-2 BA.2.87.1 spike protein ectodomain
Authors	:	Eray, E.; Antanasijevic, A.
Deposited on	:	2025-12-12
Resolution	:	3.90 Å(reported)
Based on initial model	:	.

This is a wwPDB EM Validation Summary 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 (i) 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 (1)) were used in the production of this report:

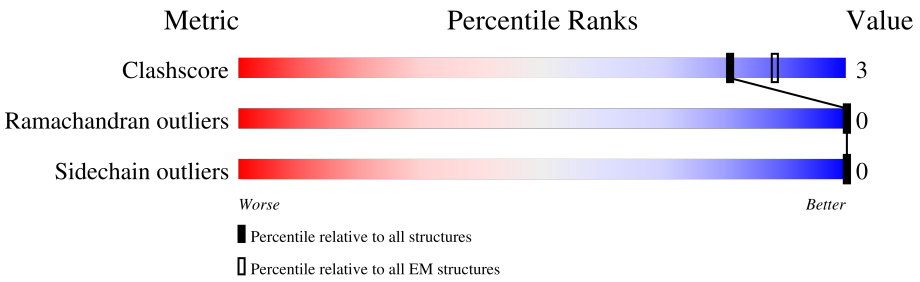
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

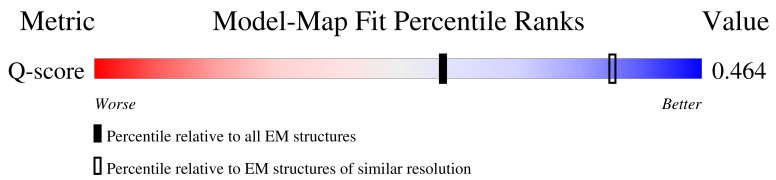
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.90 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	8855 (3.40 - 4.40)

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 <=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	1263	67% 6% • 26%
1	B	1263	67% 6% • 26%
1	C	1263	67% 6% • 26%
2	D	2	50% 100%

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Mol	Chain	Length	Quality of chain
2	F	2	50% 100%
2	G	2	50% 100%
2	I	2	50% 100%
2	J	2	50% 100%
2	L	2	50% 100%
3	E	3	33% 100%
3	H	3	33% 100%
3	K	3	33% 100%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 22572 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,Fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	931	7261	4662	1200	1366	33	0	0
1	B	931	7261	4662	1200	1366	33	0	0
1	C	931	7261	4662	1200	1366	33	0	0

There are 405 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	CYS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	THR	deletion	UNP P0DTC2
A	?	-	THR	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	THR	deletion	UNP P0DTC2
A	?	-	GLN	deletion	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	40	SER	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	86	ASP	GLY	variant	UNP P0DTC2
A	109	PHE	SER	conflict	UNP P0DTC2
A	137	ALA	VAL	conflict	UNP P0DTC2
A	?	-	CYS	deletion	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	?	-	ASP	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PHE	deletion	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLY	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	152	LEU	TRP	variant	UNP P0DTC2
A	190	SER	ARG	variant	UNP P0DTC2
A	213	GLY	VAL	variant	UNP P0DTC2
A	215	GLY	ASP	variant	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	THR	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	444	ASN	LYS	conflict	UNP P0DTC2
A	445	GLY	VAL	conflict	UNP P0DTC2
A	452	MET	LEU	variant	UNP P0DTC2
A	460	LYS	ASN	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	481	LYS	ASN	conflict	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	621	SER	PRO	conflict	UNP P0DTC2
A	642	GLY	VAL	conflict	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	ARG	ASN	engineered mutation	UNP P0DTC2
A	681	HIS	PRO	engineered mutation	UNP P0DTC2
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	691	PRO	SER	conflict	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	791	ILE	THR	conflict	UNP P0DTC2
A	796	HIS	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	936	GLY	ASP	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1202	GLU	-	linker	UNP P0DTC2
A	1203	LEU	-	linker	UNP P0DTC2
A	1204	GLY	-	linker	UNP P0DTC2
A	1205	LYS	-	linker	UNP P0DTC2
A	1206	TYR	-	linker	UNP P0DTC2
A	1207	GLU	-	linker	UNP P0DTC2
A	1208	GLN	-	linker	UNP P0DTC2
A	1209	GLY	-	linker	UNP P0DTC2
A	1210	SER	-	linker	UNP P0DTC2
A	1232	LEU	PHE	engineered mutation	UNP P10104
A	1238	GLY	-	expression tag	UNP P10104
A	1239	ARG	-	expression tag	UNP P10104
A	1240	SER	-	expression tag	UNP P10104
A	1241	LEU	-	expression tag	UNP P10104
A	1242	GLU	-	expression tag	UNP P10104
A	1243	VAL	-	expression tag	UNP P10104
A	1244	LEU	-	expression tag	UNP P10104
A	1245	PHE	-	expression tag	UNP P10104
A	1246	GLN	-	expression tag	UNP P10104
A	1247	GLY	-	expression tag	UNP P10104
A	1248	PRO	-	expression tag	UNP P10104
A	1249	GLY	-	expression tag	UNP P10104
A	1250	HIS	-	expression tag	UNP P10104
A	1251	HIS	-	expression tag	UNP P10104
A	1252	HIS	-	expression tag	UNP P10104
A	1253	HIS	-	expression tag	UNP P10104
A	1254	HIS	-	expression tag	UNP P10104
A	1255	HIS	-	expression tag	UNP P10104
A	1256	HIS	-	expression tag	UNP P10104
A	1257	HIS	-	expression tag	UNP P10104
A	1258	SER	-	expression tag	UNP P10104
A	1259	ALA	-	expression tag	UNP P10104
A	1260	TRP	-	expression tag	UNP P10104
A	1261	SER	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1262	HIS	-	expression tag	UNP P10104
A	1263	PRO	-	expression tag	UNP P10104
A	1264	GLN	-	expression tag	UNP P10104
A	1265	PHE	-	expression tag	UNP P10104
A	1266	GLU	-	expression tag	UNP P10104
A	1267	LYS	-	expression tag	UNP P10104
A	1268	GLY	-	expression tag	UNP P10104
A	1269	GLY	-	expression tag	UNP P10104
A	1270	GLY	-	expression tag	UNP P10104
A	1271	SER	-	expression tag	UNP P10104
A	1272	GLY	-	expression tag	UNP P10104
A	1273	GLY	-	expression tag	UNP P10104
A	1274	GLY	-	expression tag	UNP P10104
A	1275	GLY	-	expression tag	UNP P10104
A	1276	SER	-	expression tag	UNP P10104
A	1277	GLY	-	expression tag	UNP P10104
A	1278	GLY	-	expression tag	UNP P10104
A	1279	SER	-	expression tag	UNP P10104
A	1280	ALA	-	expression tag	UNP P10104
A	1281	TRP	-	expression tag	UNP P10104
A	1282	SER	-	expression tag	UNP P10104
A	1283	HIS	-	expression tag	UNP P10104
A	1284	PRO	-	expression tag	UNP P10104
A	1285	GLN	-	expression tag	UNP P10104
A	1286	PHE	-	expression tag	UNP P10104
A	1287	GLU	-	expression tag	UNP P10104
A	1288	LYS	-	expression tag	UNP P10104
B	?	-	CYS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	THR	deletion	UNP P0DTC2
B	?	-	THR	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	THR	deletion	UNP P0DTC2
B	?	-	GLN	deletion	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	40	SER	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	86	ASP	GLY	variant	UNP P0DTC2
B	109	PHE	SER	conflict	UNP P0DTC2
B	137	ALA	VAL	conflict	UNP P0DTC2
B	?	-	CYS	deletion	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	?	-	ASP	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PHE	deletion	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	GLY	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	152	LEU	TRP	variant	UNP P0DTC2
B	190	SER	ARG	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	215	GLY	ASP	variant	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	THR	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	444	ASN	LYS	conflict	UNP P0DTC2
B	445	GLY	VAL	conflict	UNP P0DTC2
B	452	MET	LEU	variant	UNP P0DTC2
B	460	LYS	ASN	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	481	LYS	ASN	conflict	UNP P0DTC2
B	484	ALA	GLU	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	614	GLY	ASP	variant	UNP P0DTC2
B	621	SER	PRO	conflict	UNP P0DTC2
B	642	GLY	VAL	conflict	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	ARG	ASN	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	681	HIS	PRO	engineered mutation	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	691	PRO	SER	conflict	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	791	ILE	THR	conflict	UNP P0DTC2
B	796	HIS	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	936	GLY	ASP	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1202	GLU	-	linker	UNP P0DTC2
B	1203	LEU	-	linker	UNP P0DTC2
B	1204	GLY	-	linker	UNP P0DTC2
B	1205	LYS	-	linker	UNP P0DTC2
B	1206	TYR	-	linker	UNP P0DTC2
B	1207	GLU	-	linker	UNP P0DTC2
B	1208	GLN	-	linker	UNP P0DTC2
B	1209	GLY	-	linker	UNP P0DTC2
B	1210	SER	-	linker	UNP P0DTC2
B	1232	LEU	PHE	engineered mutation	UNP P10104
B	1238	GLY	-	expression tag	UNP P10104
B	1239	ARG	-	expression tag	UNP P10104
B	1240	SER	-	expression tag	UNP P10104
B	1241	LEU	-	expression tag	UNP P10104
B	1242	GLU	-	expression tag	UNP P10104
B	1243	VAL	-	expression tag	UNP P10104
B	1244	LEU	-	expression tag	UNP P10104
B	1245	PHE	-	expression tag	UNP P10104
B	1246	GLN	-	expression tag	UNP P10104
B	1247	GLY	-	expression tag	UNP P10104
B	1248	PRO	-	expression tag	UNP P10104
B	1249	GLY	-	expression tag	UNP P10104
B	1250	HIS	-	expression tag	UNP P10104
B	1251	HIS	-	expression tag	UNP P10104
B	1252	HIS	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1253	HIS	-	expression tag	UNP P10104
B	1254	HIS	-	expression tag	UNP P10104
B	1255	HIS	-	expression tag	UNP P10104
B	1256	HIS	-	expression tag	UNP P10104
B	1257	HIS	-	expression tag	UNP P10104
B	1258	SER	-	expression tag	UNP P10104
B	1259	ALA	-	expression tag	UNP P10104
B	1260	TRP	-	expression tag	UNP P10104
B	1261	SER	-	expression tag	UNP P10104
B	1262	HIS	-	expression tag	UNP P10104
B	1263	PRO	-	expression tag	UNP P10104
B	1264	GLN	-	expression tag	UNP P10104
B	1265	PHE	-	expression tag	UNP P10104
B	1266	GLU	-	expression tag	UNP P10104
B	1267	LYS	-	expression tag	UNP P10104
B	1268	GLY	-	expression tag	UNP P10104
B	1269	GLY	-	expression tag	UNP P10104
B	1270	GLY	-	expression tag	UNP P10104
B	1271	SER	-	expression tag	UNP P10104
B	1272	GLY	-	expression tag	UNP P10104
B	1273	GLY	-	expression tag	UNP P10104
B	1274	GLY	-	expression tag	UNP P10104
B	1275	GLY	-	expression tag	UNP P10104
B	1276	SER	-	expression tag	UNP P10104
B	1277	GLY	-	expression tag	UNP P10104
B	1278	GLY	-	expression tag	UNP P10104
B	1279	SER	-	expression tag	UNP P10104
B	1280	ALA	-	expression tag	UNP P10104
B	1281	TRP	-	expression tag	UNP P10104
B	1282	SER	-	expression tag	UNP P10104
B	1283	HIS	-	expression tag	UNP P10104
B	1284	PRO	-	expression tag	UNP P10104
B	1285	GLN	-	expression tag	UNP P10104
B	1286	PHE	-	expression tag	UNP P10104
B	1287	GLU	-	expression tag	UNP P10104
B	1288	LYS	-	expression tag	UNP P10104
C	?	-	CYS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	THR	deletion	UNP P0DTC2
C	?	-	THR	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	THR	deletion	UNP P0DTC2
C	?	-	GLN	deletion	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	40	SER	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	86	ASP	GLY	variant	UNP P0DTC2
C	109	PHE	SER	conflict	UNP P0DTC2
C	137	ALA	VAL	conflict	UNP P0DTC2
C	?	-	CYS	deletion	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	?	-	ASP	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PHE	deletion	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	152	LEU	TRP	variant	UNP P0DTC2
C	190	SER	ARG	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	215	GLY	ASP	variant	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	THR	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	444	ASN	LYS	conflict	UNP P0DTC2
C	445	GLY	VAL	conflict	UNP P0DTC2
C	452	MET	LEU	variant	UNP P0DTC2
C	460	LYS	ASN	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	481	LYS	ASN	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	484	ALA	GLU	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	614	GLY	ASP	variant	UNP P0DTC2
C	621	SER	PRO	conflict	UNP P0DTC2
C	642	GLY	VAL	conflict	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	ARG	ASN	engineered mutation	UNP P0DTC2
C	681	HIS	PRO	engineered mutation	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	691	PRO	SER	conflict	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	791	ILE	THR	conflict	UNP P0DTC2
C	796	HIS	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	936	GLY	ASP	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1202	GLU	-	linker	UNP P0DTC2
C	1203	LEU	-	linker	UNP P0DTC2
C	1204	GLY	-	linker	UNP P0DTC2
C	1205	LYS	-	linker	UNP P0DTC2
C	1206	TYR	-	linker	UNP P0DTC2
C	1207	GLU	-	linker	UNP P0DTC2
C	1208	GLN	-	linker	UNP P0DTC2
C	1209	GLY	-	linker	UNP P0DTC2
C	1210	SER	-	linker	UNP P0DTC2
C	1232	LEU	PHE	engineered mutation	UNP P10104
C	1238	GLY	-	expression tag	UNP P10104
C	1239	ARG	-	expression tag	UNP P10104
C	1240	SER	-	expression tag	UNP P10104
C	1241	LEU	-	expression tag	UNP P10104
C	1242	GLU	-	expression tag	UNP P10104
C	1243	VAL	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1244	LEU	-	expression tag	UNP P10104
C	1245	PHE	-	expression tag	UNP P10104
C	1246	GLN	-	expression tag	UNP P10104
C	1247	GLY	-	expression tag	UNP P10104
C	1248	PRO	-	expression tag	UNP P10104
C	1249	GLY	-	expression tag	UNP P10104
C	1250	HIS	-	expression tag	UNP P10104
C	1251	HIS	-	expression tag	UNP P10104
C	1252	HIS	-	expression tag	UNP P10104
C	1253	HIS	-	expression tag	UNP P10104
C	1254	HIS	-	expression tag	UNP P10104
C	1255	HIS	-	expression tag	UNP P10104
C	1256	HIS	-	expression tag	UNP P10104
C	1257	HIS	-	expression tag	UNP P10104
C	1258	SER	-	expression tag	UNP P10104
C	1259	ALA	-	expression tag	UNP P10104
C	1260	TRP	-	expression tag	UNP P10104
C	1261	SER	-	expression tag	UNP P10104
C	1262	HIS	-	expression tag	UNP P10104
C	1263	PRO	-	expression tag	UNP P10104
C	1264	GLN	-	expression tag	UNP P10104
C	1265	PHE	-	expression tag	UNP P10104
C	1266	GLU	-	expression tag	UNP P10104
C	1267	LYS	-	expression tag	UNP P10104
C	1268	GLY	-	expression tag	UNP P10104
C	1269	GLY	-	expression tag	UNP P10104
C	1270	GLY	-	expression tag	UNP P10104
C	1271	SER	-	expression tag	UNP P10104
C	1272	GLY	-	expression tag	UNP P10104
C	1273	GLY	-	expression tag	UNP P10104
C	1274	GLY	-	expression tag	UNP P10104
C	1275	GLY	-	expression tag	UNP P10104
C	1276	SER	-	expression tag	UNP P10104
C	1277	GLY	-	expression tag	UNP P10104
C	1278	GLY	-	expression tag	UNP P10104
C	1279	SER	-	expression tag	UNP P10104
C	1280	ALA	-	expression tag	UNP P10104
C	1281	TRP	-	expression tag	UNP P10104
C	1282	SER	-	expression tag	UNP P10104
C	1283	HIS	-	expression tag	UNP P10104
C	1284	PRO	-	expression tag	UNP P10104
C	1285	GLN	-	expression tag	UNP P10104

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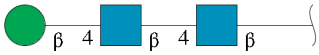
Chain	Residue	Modelled	Actual	Comment	Reference
C	1286	PHE	-	expression tag	UNP P10104
C	1287	GLU	-	expression tag	UNP P10104
C	1288	LYS	-	expression tag	UNP P10104

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

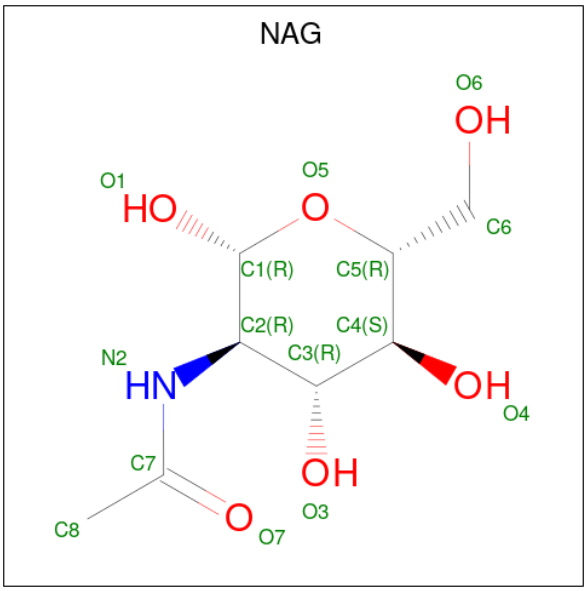
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	D	2	28	16	2	10	0	0
2	F	2	28	16	2	10	0	0
2	G	2	28	16	2	10	0	0
2	I	2	28	16	2	10	0	0
2	J	2	28	16	2	10	0	0
2	L	2	28	16	2	10	0	0

- Molecule 3 is an oligosaccharide called 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
			Total	C	N	O		
3	E	3	39	22	2	15	0	0
3	H	3	39	22	2	15	0	0
3	K	3	39	22	2	15	0	0

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



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

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

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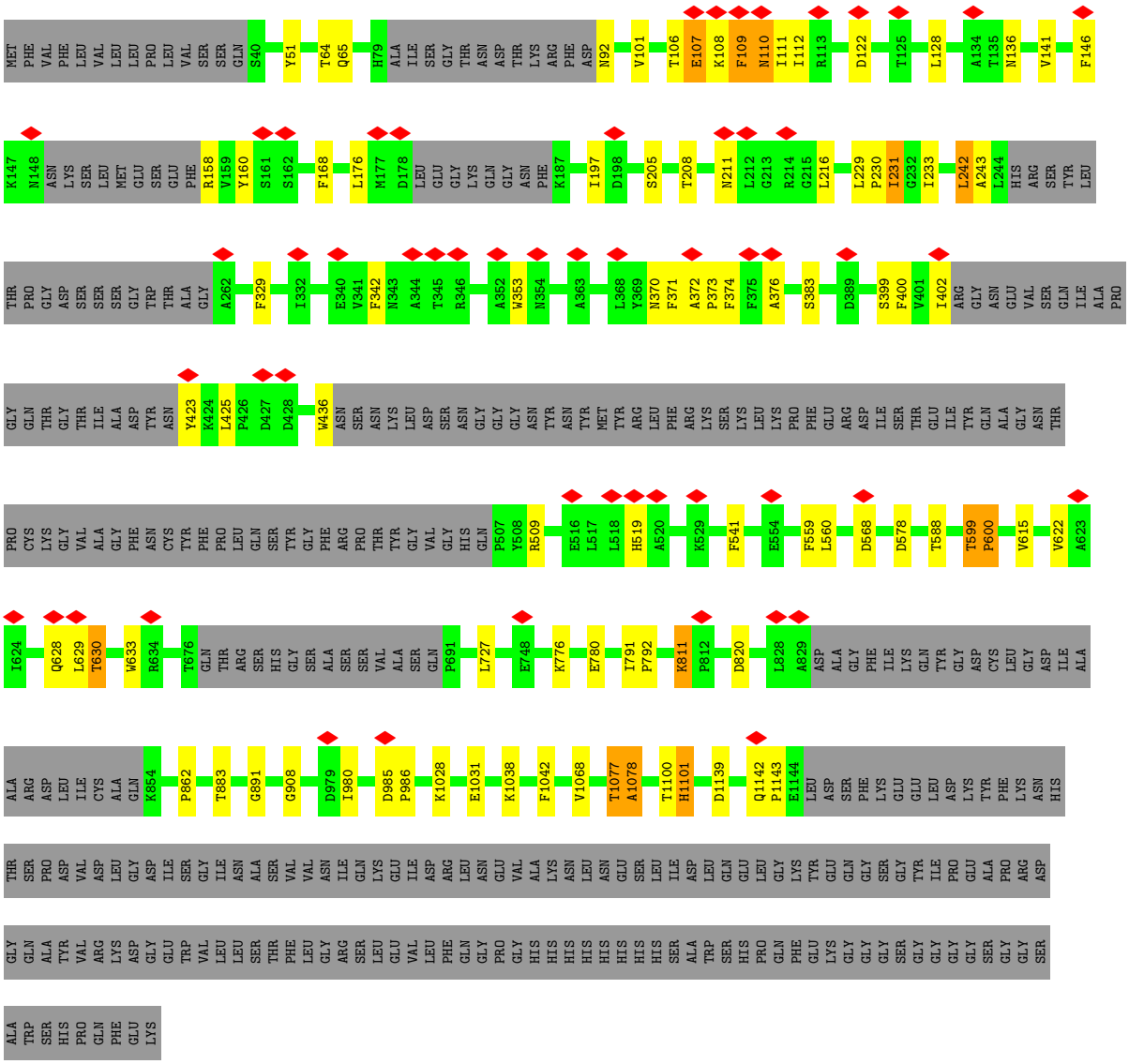
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	C	1	14	8	1	5	0

3 Residue-property plots (i)

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

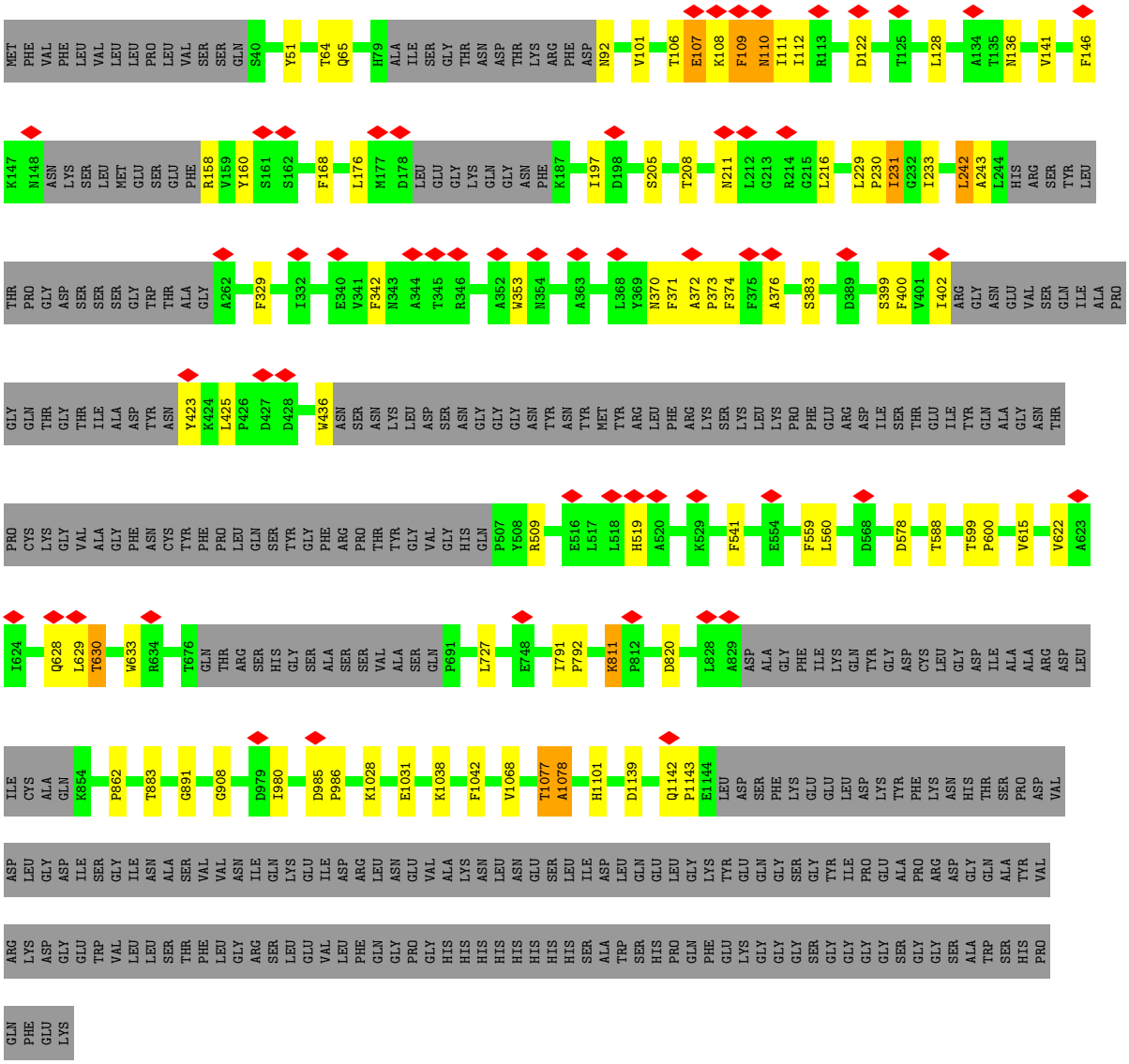
- Molecule 1: Spike glycoprotein,Fibritin

Chain A: 67% 6% 26%



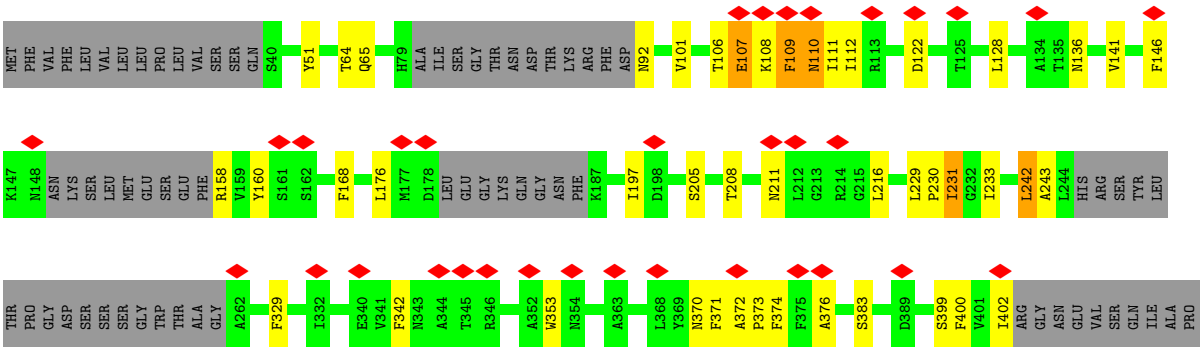
- Molecule 1: Spike glycoprotein,Fibritin

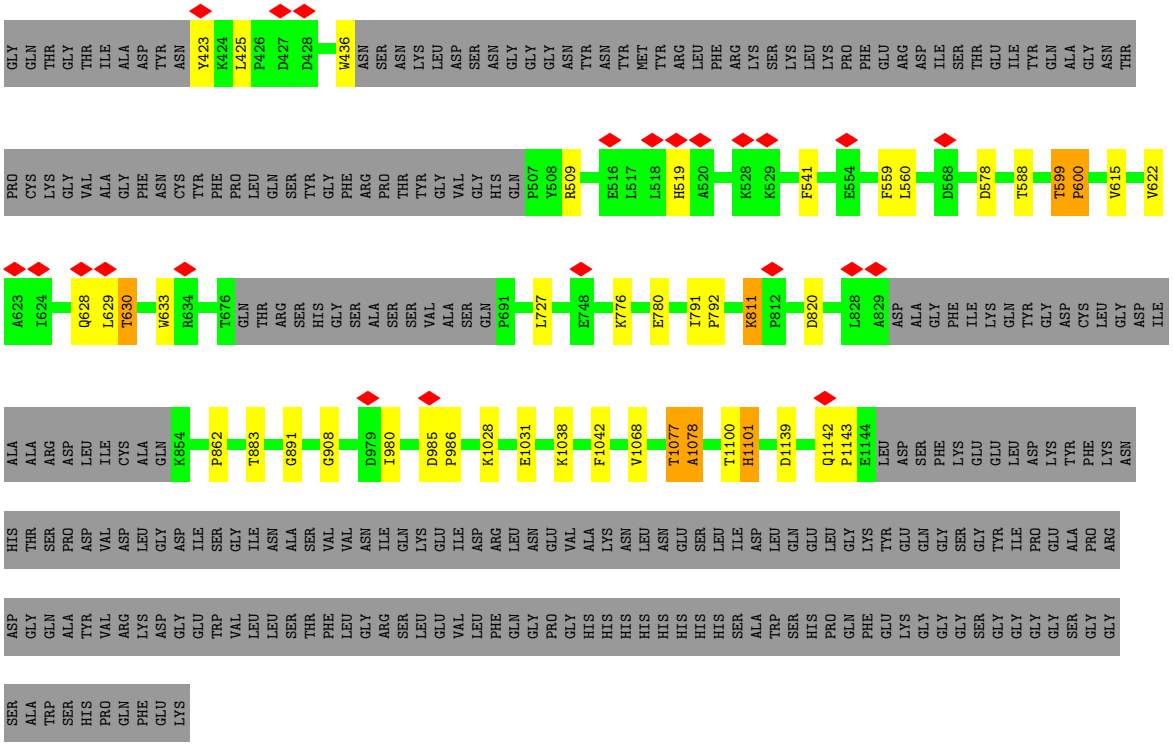
Chain B:



- Molecule 1: Spike glycoprotein,Fibritin

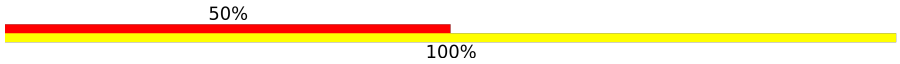
Chain C:





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

Chain D:

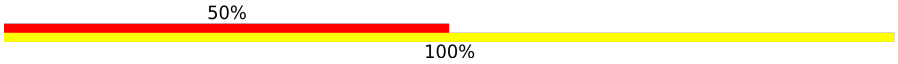


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

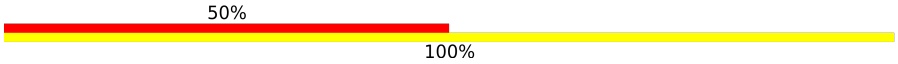
Chain F:

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

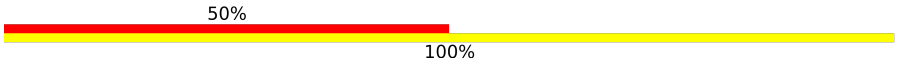
Chain G:



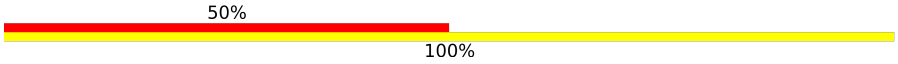
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 

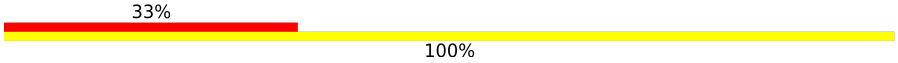
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 

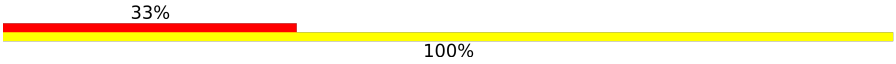
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L: 

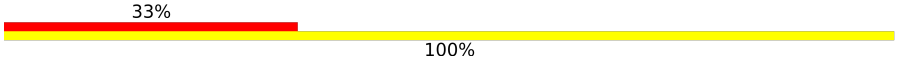
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 

• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 

• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	37658	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	150000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.022	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	333.36, 333.36, 333.36	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.92599994, 0.92599994, 0.92599994	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

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	1.05	6/7431 (0.1%)	1.28	72/10116 (0.7%)
1	B	1.05	6/7431 (0.1%)	1.28	72/10116 (0.7%)
1	C	1.05	6/7431 (0.1%)	1.28	72/10116 (0.7%)
All	All	1.05	18/22293 (0.1%)	1.28	216/30348 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	158	ARG	NE-CZ	6.85	1.40	1.33
1	B	158	ARG	NE-CZ	6.80	1.40	1.33
1	A	158	ARG	NE-CZ	6.80	1.40	1.33
1	B	436	TRP	CD2-CE3	6.35	1.50	1.40
1	A	436	TRP	CD2-CE3	6.35	1.50	1.40

The worst 5 of 216 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	107	GLU	CB-CG-CD	8.81	127.57	112.60
1	A	107	GLU	CB-CG-CD	8.80	127.56	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	107	GLU	CB-CG-CD	8.80	127.56	112.60
1	C	862	PRO	CA-C-N	7.97	127.92	120.03
1	C	862	PRO	C-N-CA	7.97	127.92	120.03

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	509	ARG	Sidechain
1	B	509	ARG	Sidechain
1	C	509	ARG	Sidechain

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	7261	0	7131	40	0
1	B	7261	0	7131	36	0
1	C	7261	0	7131	39	0
2	D	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	L	28	0	25	0	0
3	E	39	0	34	0	0
3	H	39	0	34	0	0
3	K	39	0	34	0	0
4	A	168	0	156	1	0
4	B	168	0	156	1	0
4	C	168	0	156	1	0
All	All	22572	0	22113	115	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 3.

The worst 5 of 115 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:C:111:ILE:O	1:C:242:LEU:HA	1.94	0.67
1:A:111:ILE:O	1:A:242:LEU:HA	1.94	0.67
1:B:111:ILE:O	1:B:242:LEU:HA	1.95	0.67
1:C:141:VAL:HG21	1:C:231:ILE:HG21	1.81	0.63
1:A:141:VAL:HG21	1:A:231:ILE:HG21	1.81	0.62

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	913/1263 (72%)	886 (97%)	27 (3%)	0	100	100
1	B	913/1263 (72%)	886 (97%)	27 (3%)	0	100	100
1	C	913/1263 (72%)	886 (97%)	27 (3%)	0	100	100
All	All	2739/3789 (72%)	2658 (97%)	81 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	813/1086 (75%)	813 (100%)	0	100	100
1	B	813/1086 (75%)	813 (100%)	0	100	100
1	C	813/1086 (75%)	813 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2439/3258 (75%)	2439 (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 (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	519	HIS
1	B	65	GLN
1	C	65	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)

21 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	$\#\|Z\| > 2$
2	NAG	D	1	2,1	14,14,15	2.00	6 (42%)	17,19,21	0.99	0
2	NAG	D	2	2	14,14,15	1.86	4 (28%)	17,19,21	0.89	1 (5%)
3	NAG	E	1	3,1	14,14,15	1.83	4 (28%)	17,19,21	0.99	1 (5%)
3	NAG	E	2	3	14,14,15	1.90	6 (42%)	17,19,21	0.89	1 (5%)
3	BMA	E	3	3	11,11,12	1.81	4 (36%)	15,15,17	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	F	1	2,1	14,14,15	2.09	4 (28%)	17,19,21	0.90	0
2	NAG	F	2	2	14,14,15	1.86	5 (35%)	17,19,21	0.92	1 (5%)
2	NAG	G	1	2,1	14,14,15	2.00	6 (42%)	17,19,21	0.99	0
2	NAG	G	2	2	14,14,15	1.85	4 (28%)	17,19,21	0.89	1 (5%)
3	NAG	H	1	3,1	14,14,15	1.83	4 (28%)	17,19,21	0.99	1 (5%)
3	NAG	H	2	3	14,14,15	1.90	6 (42%)	17,19,21	0.90	1 (5%)
3	BMA	H	3	3	11,11,12	1.81	4 (36%)	15,15,17	0.74	0
2	NAG	I	1	2,1	14,14,15	2.08	4 (28%)	17,19,21	0.90	0
2	NAG	I	2	2	14,14,15	1.85	5 (35%)	17,19,21	0.92	1 (5%)
2	NAG	J	1	2,1	14,14,15	1.99	6 (42%)	17,19,21	0.99	0
2	NAG	J	2	2	14,14,15	1.86	4 (28%)	17,19,21	0.89	1 (5%)
3	NAG	K	1	3,1	14,14,15	1.83	4 (28%)	17,19,21	0.99	1 (5%)
3	NAG	K	2	3	14,14,15	1.90	6 (42%)	17,19,21	0.90	1 (5%)
3	BMA	K	3	3	11,11,12	1.81	4 (36%)	15,15,17	0.74	0
2	NAG	L	1	2,1	14,14,15	2.09	4 (28%)	17,19,21	0.90	0
2	NAG	L	2	2	14,14,15	1.85	5 (35%)	17,19,21	0.92	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
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
3	NAG	E	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	1/2/19/22	0/1/1/1
2	NAG	F	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	F	2	2	-	1/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	1/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	BMA	H	3	3	-	1/2/19/22	0/1/1/1
2	NAG	I	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	I	2	2	-	1/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	J	2	2	-	1/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	BMA	K	3	3	-	1/2/19/22	0/1/1/1
2	NAG	L	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	L	2	2	-	1/6/23/26	0/1/1/1

The worst 5 of 99 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	1	NAG	C1-C2	5.50	1.60	1.52
2	F	1	NAG	C1-C2	5.49	1.60	1.52
2	I	1	NAG	C1-C2	5.49	1.60	1.52
2	D	1	NAG	C1-C2	4.94	1.59	1.52
2	G	1	NAG	C1-C2	4.93	1.59	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	2	NAG	C8-C7-N2	2.39	120.15	116.10
2	L	2	NAG	C8-C7-N2	2.39	120.15	116.10
2	F	2	NAG	C8-C7-N2	2.39	120.15	116.10
3	K	1	NAG	C8-C7-N2	2.34	120.05	116.10
3	E	1	NAG	C8-C7-N2	2.32	120.03	116.10

There are no chirality outliers.

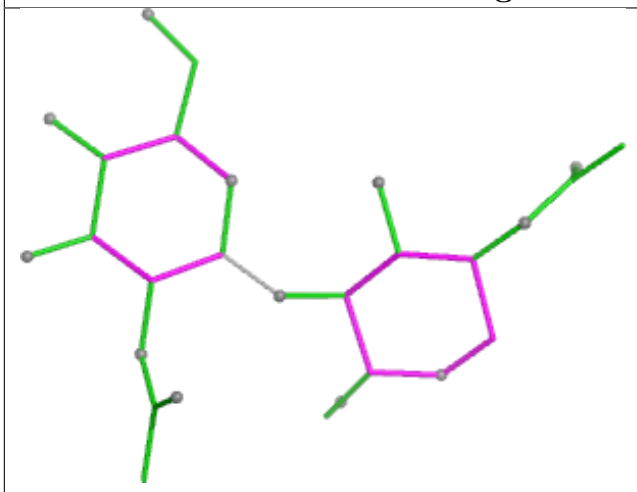
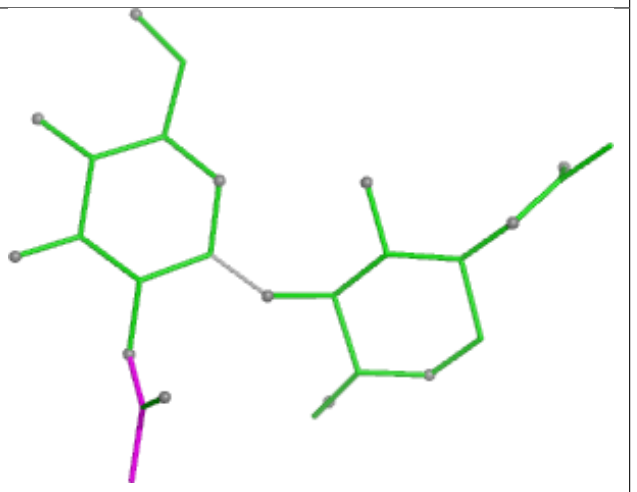
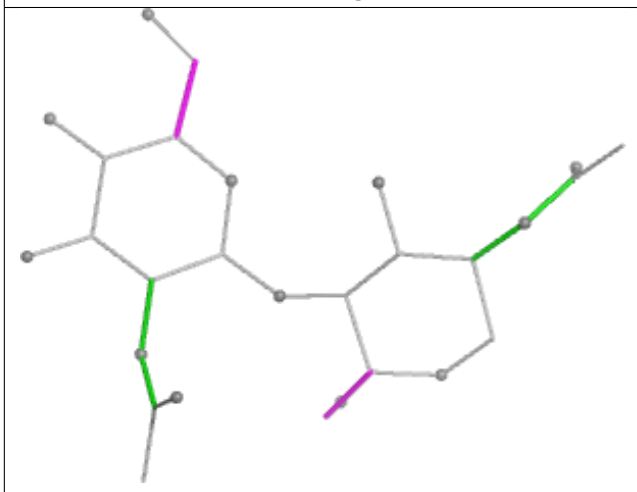
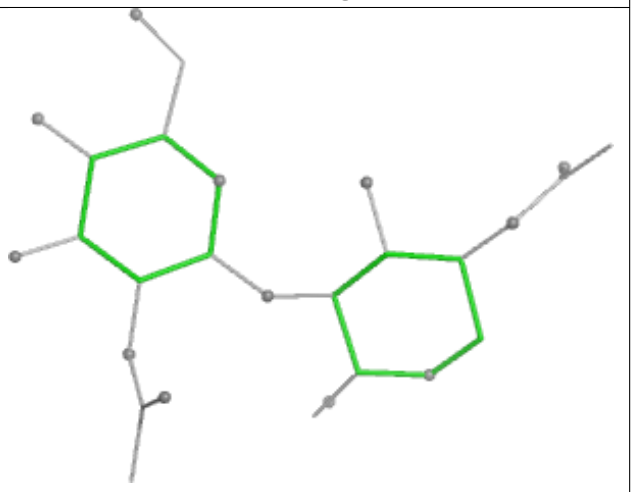
5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	3	BMA	O5-C5-C6-O6
3	H	3	BMA	O5-C5-C6-O6
3	K	3	BMA	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6

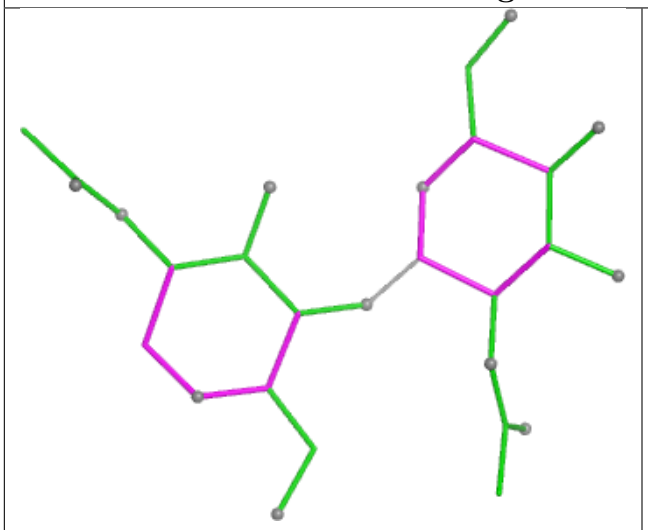
There are no ring outliers.

No monomer is involved in short contacts.

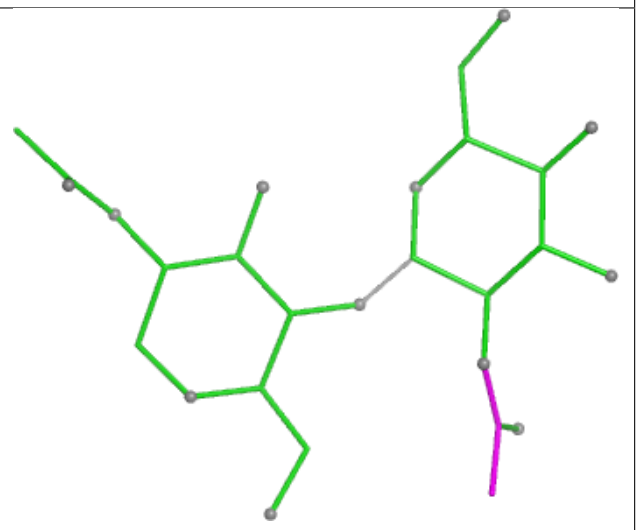
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain D	
 Bond lengths	 Bond angles
 Torsions	 Rings

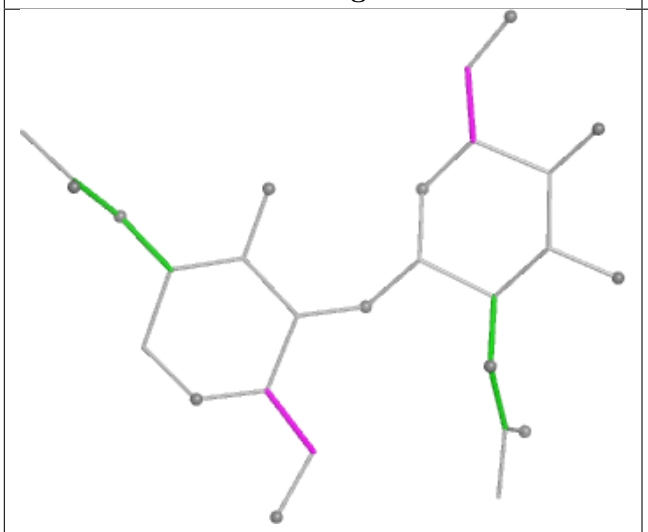
Oligosaccharide Chain F



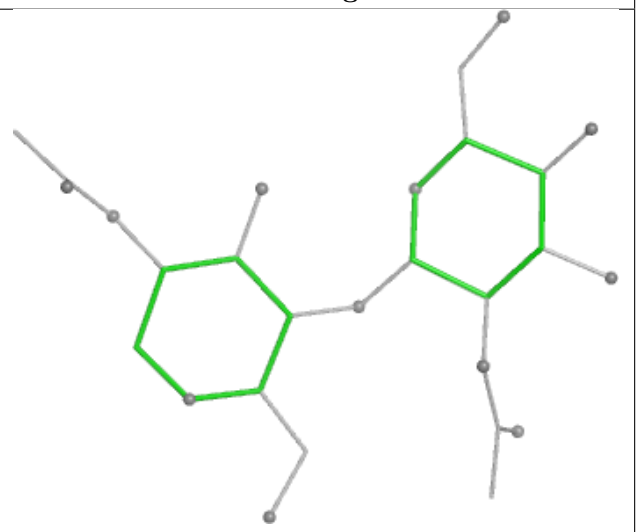
Bond lengths



Bond angles

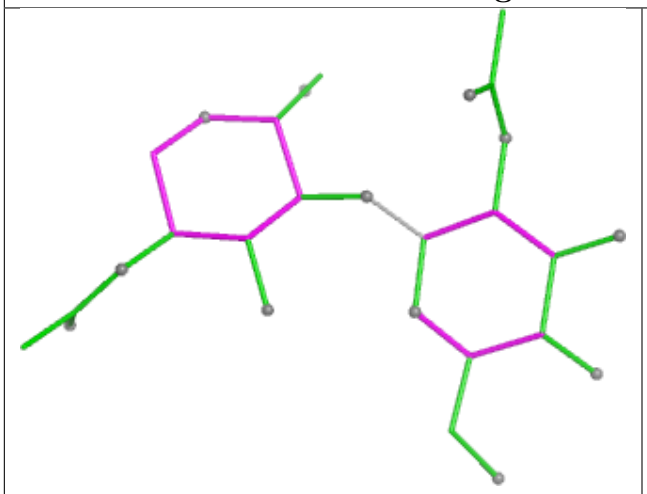


Torsions

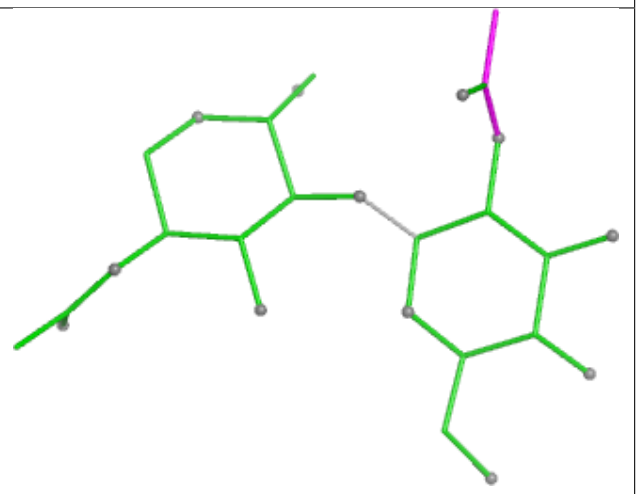


Rings

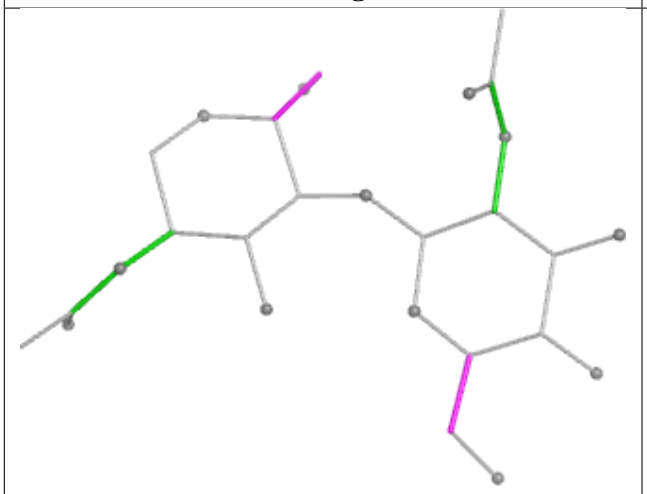
Oligosaccharide Chain G



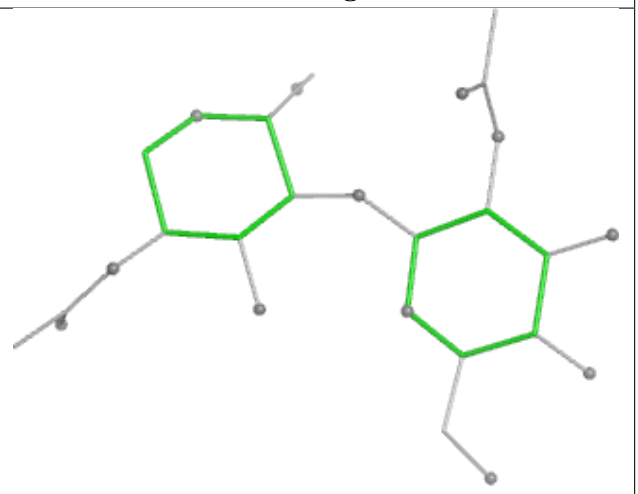
Bond lengths



Bond angles

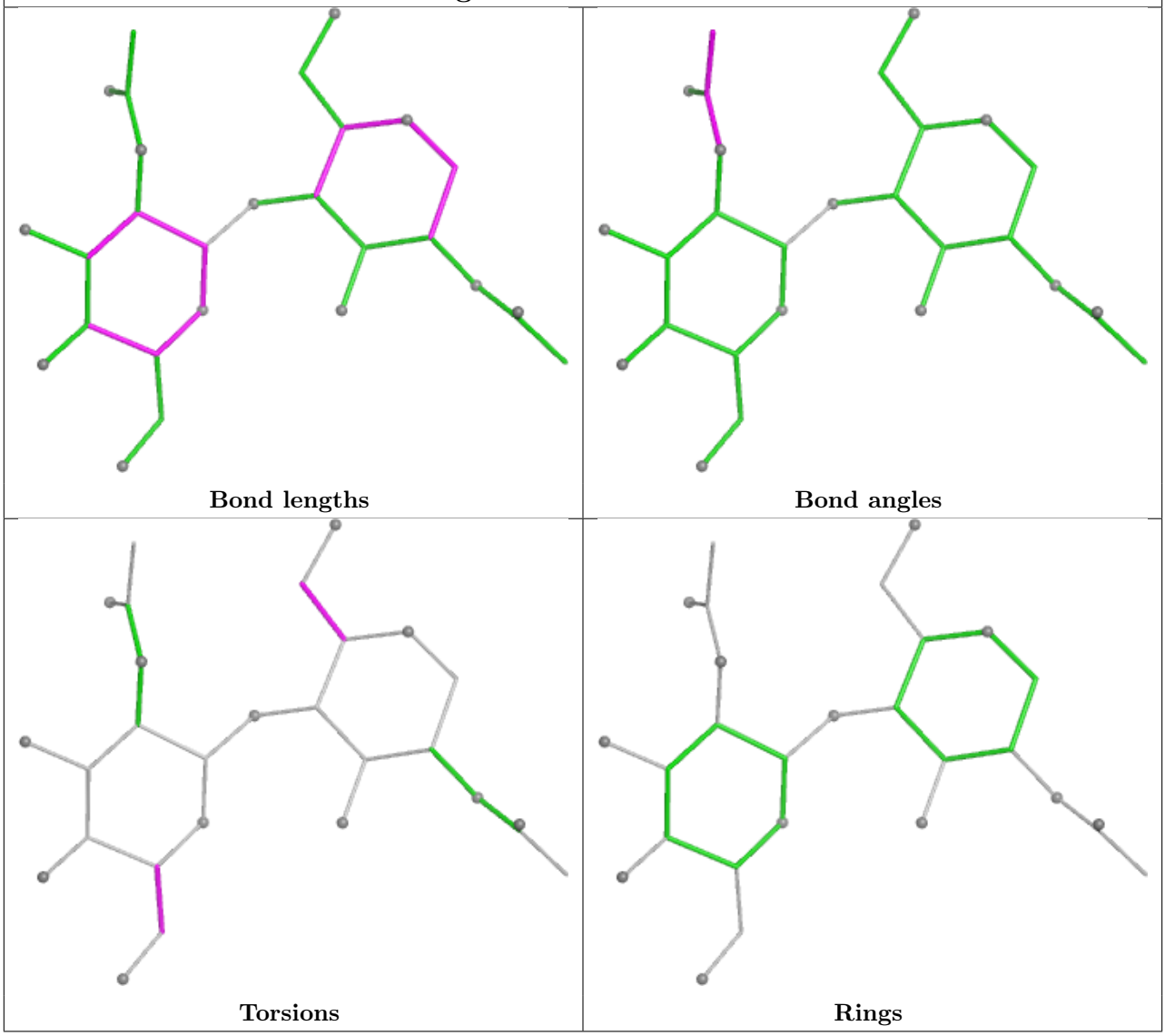


Torsions

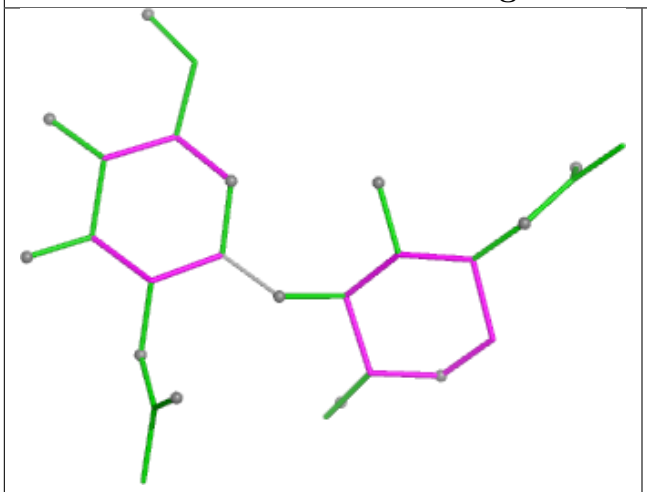


Rings

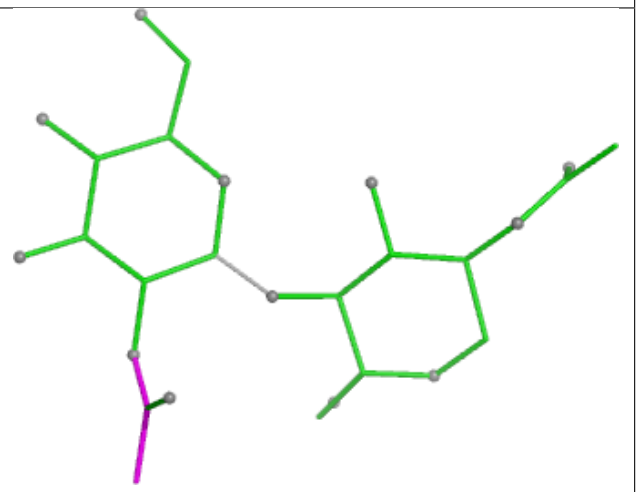
Oligosaccharide Chain I



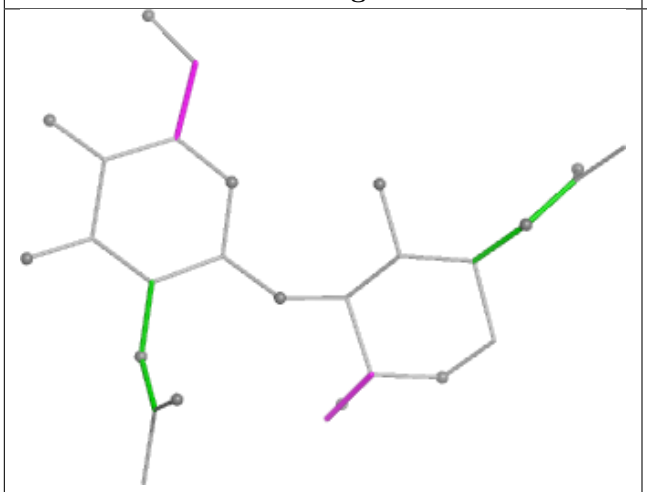
Oligosaccharide Chain J



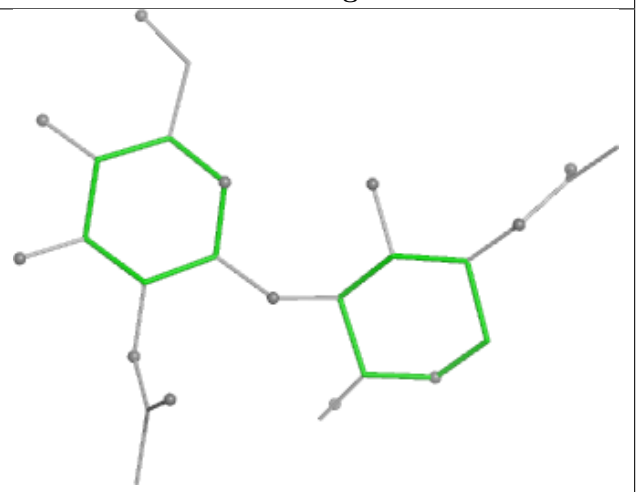
Bond lengths



Bond angles

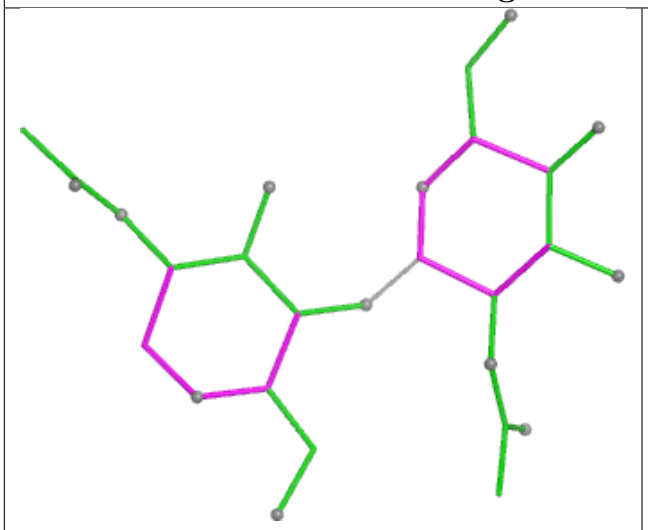


Torsions

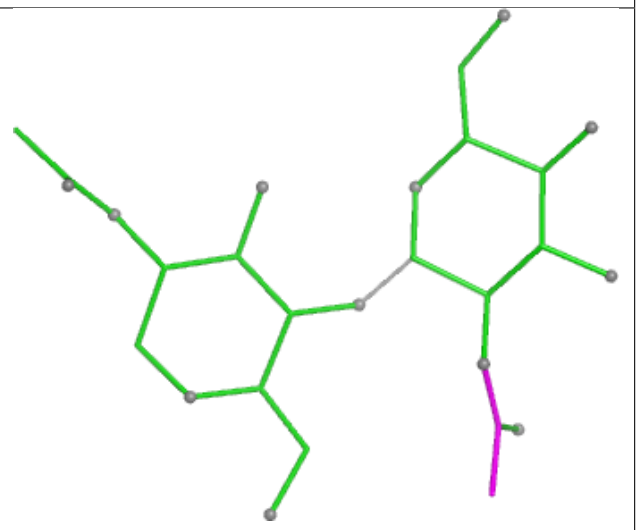


Rings

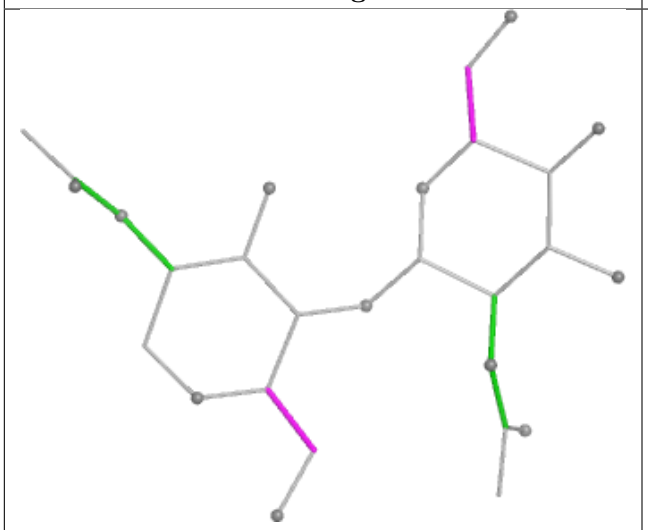
Oligosaccharide Chain L



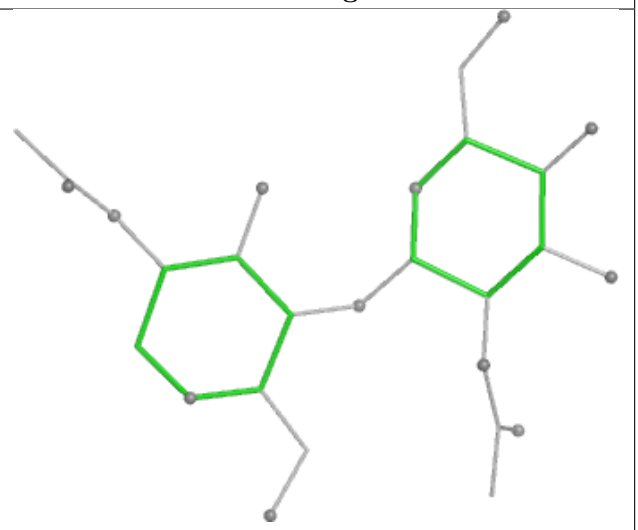
Bond lengths



Bond angles

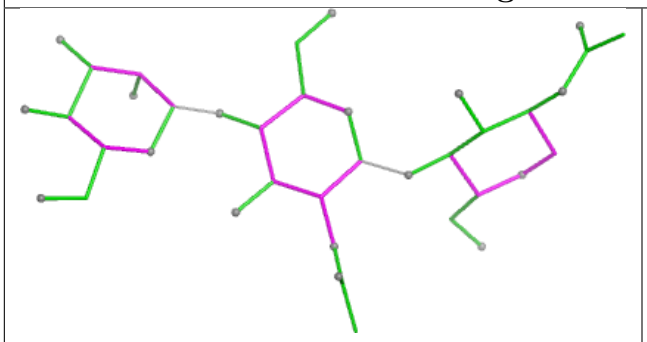


Torsions

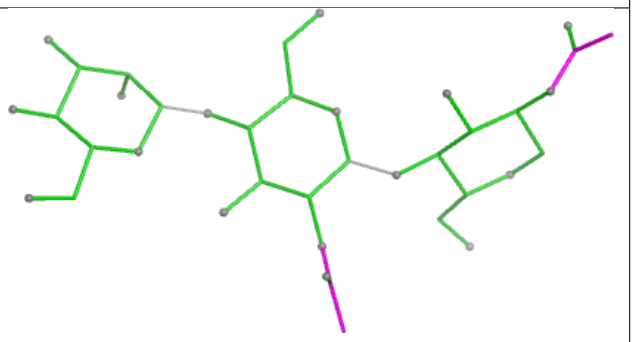


Rings

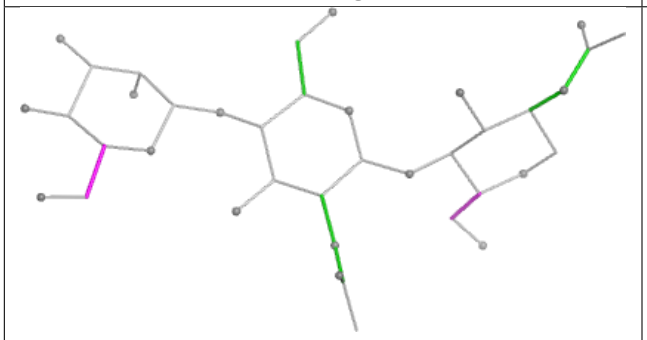
Oligosaccharide Chain E



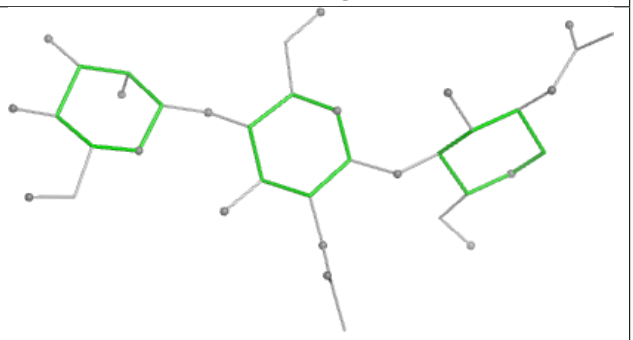
Bond lengths



Bond angles

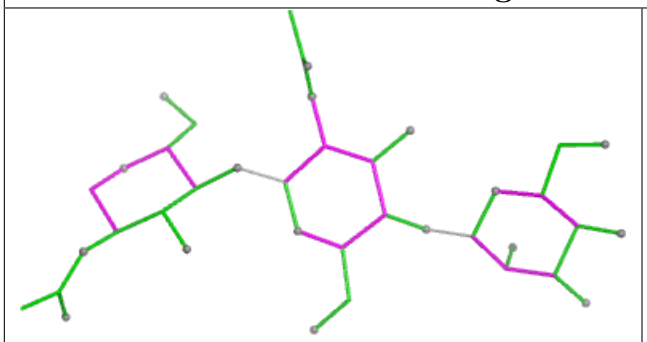


Torsions

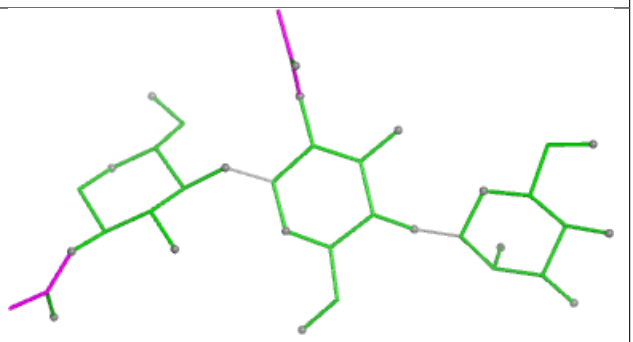


Rings

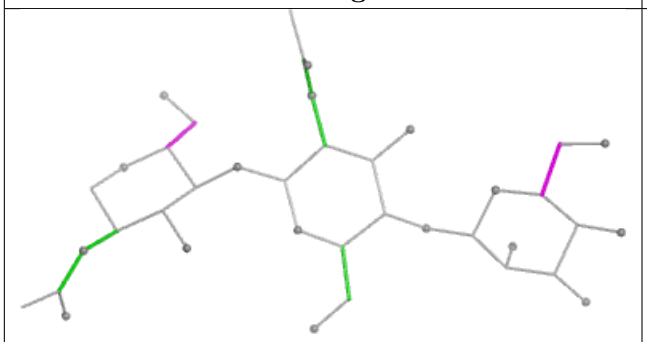
Oligosaccharide Chain H



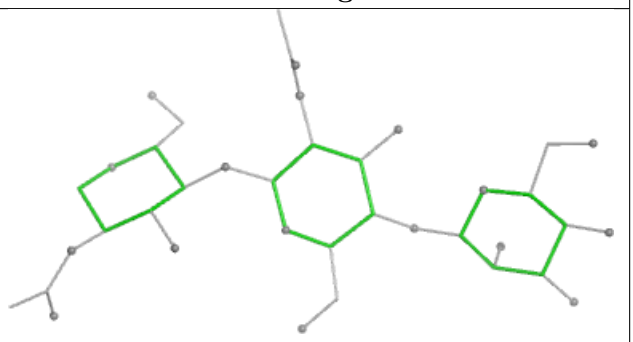
Bond lengths



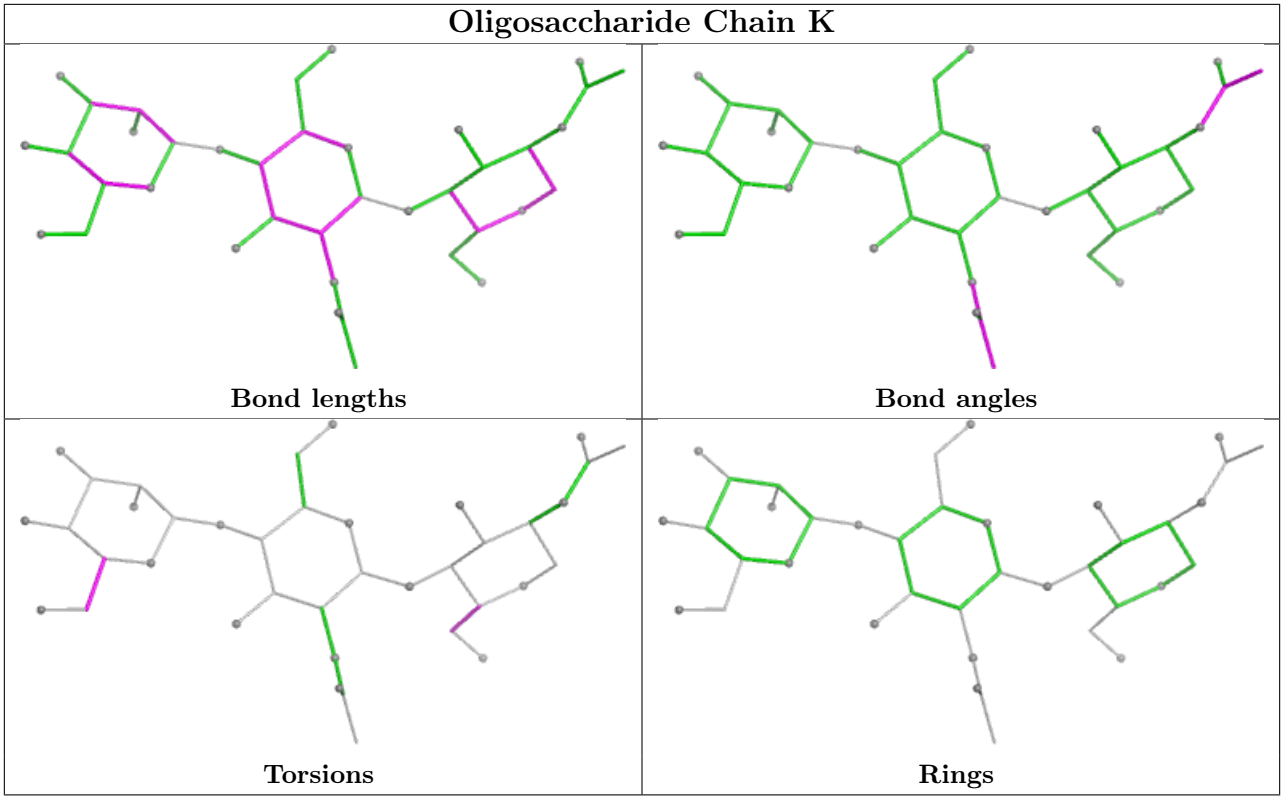
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

36 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	B	1302	1	14,14,15	2.05	5 (35%)	17,19,21	1.20	3 (17%)
4	NAG	C	1312	1	14,14,15	2.13	5 (35%)	17,19,21	1.09	3 (17%)
4	NAG	A	1303	1	14,14,15	2.06	5 (35%)	17,19,21	1.05	1 (5%)
4	NAG	A	1312	1	14,14,15	2.12	5 (35%)	17,19,21	1.08	3 (17%)
4	NAG	C	1308	1	14,14,15	2.22	5 (35%)	17,19,21	0.99	0
4	NAG	B	1306	1	14,14,15	2.02	5 (35%)	17,19,21	0.95	0
4	NAG	B	1310	1	14,14,15	2.03	5 (35%)	17,19,21	1.04	2 (11%)
4	NAG	C	1306	1	14,14,15	2.02	5 (35%)	17,19,21	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	B	1304	1	14,14,15	2.12	5 (35%)	17,19,21	0.97	1 (5%)
4	NAG	C	1305	1	14,14,15	2.05	5 (35%)	17,19,21	1.08	2 (11%)
4	NAG	B	1308	1	14,14,15	2.21	5 (35%)	17,19,21	0.99	0
4	NAG	C	1302	1	14,14,15	2.05	5 (35%)	17,19,21	1.20	3 (17%)
4	NAG	B	1312	1	14,14,15	2.13	5 (35%)	17,19,21	1.09	3 (17%)
4	NAG	C	1304	1	14,14,15	2.12	5 (35%)	17,19,21	0.97	2 (11%)
4	NAG	A	1307	1	14,14,15	0.42	0	17,19,21	0.50	0
4	NAG	B	1311	1	14,14,15	0.39	0	17,19,21	0.39	0
4	NAG	A	1302	1	14,14,15	2.05	5 (35%)	17,19,21	1.20	3 (17%)
4	NAG	A	1310	1	14,14,15	2.03	5 (35%)	17,19,21	1.03	2 (11%)
4	NAG	A	1308	1	14,14,15	2.21	5 (35%)	17,19,21	0.99	0
4	NAG	C	1307	1	14,14,15	0.42	0	17,19,21	0.50	0
4	NAG	A	1309	1	14,14,15	2.19	6 (42%)	17,19,21	0.94	1 (5%)
4	NAG	C	1311	1	14,14,15	0.41	0	17,19,21	0.40	0
4	NAG	C	1301	1	14,14,15	2.14	5 (35%)	17,19,21	1.00	1 (5%)
4	NAG	A	1311	1	14,14,15	0.40	0	17,19,21	0.40	0
4	NAG	B	1307	1	14,14,15	0.42	0	17,19,21	0.50	0
4	NAG	A	1306	1	14,14,15	2.02	4 (28%)	17,19,21	0.95	0
4	NAG	A	1301	1	14,14,15	2.13	5 (35%)	17,19,21	1.00	1 (5%)
4	NAG	B	1305	1	14,14,15	2.05	5 (35%)	17,19,21	1.08	2 (11%)
4	NAG	B	1309	1	14,14,15	2.20	6 (42%)	17,19,21	0.94	1 (5%)
4	NAG	A	1304	1	14,14,15	2.12	5 (35%)	17,19,21	0.98	2 (11%)
4	NAG	B	1303	1	14,14,15	2.06	5 (35%)	17,19,21	1.05	1 (5%)
4	NAG	C	1303	1	14,14,15	2.06	5 (35%)	17,19,21	1.05	1 (5%)
4	NAG	C	1309	1	14,14,15	2.20	6 (42%)	17,19,21	0.94	1 (5%)
4	NAG	C	1310	1	14,14,15	2.03	5 (35%)	17,19,21	1.03	2 (11%)
4	NAG	B	1301	1	14,14,15	2.13	5 (35%)	17,19,21	1.00	1 (5%)
4	NAG	A	1305	1	14,14,15	2.05	5 (35%)	17,19,21	1.08	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	B	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1312	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1303	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1312	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1310	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1312	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1311	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1310	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1311	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1310	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	0/6/23/26	0/1/1/1

The worst 5 of 152 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1308	NAG	C1-C2	6.01	1.61	1.52
4	A	1308	NAG	C1-C2	5.98	1.61	1.52
4	B	1308	NAG	C1-C2	5.97	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1309	NAG	C1-C2	5.80	1.61	1.52
4	B	1309	NAG	C1-C2	5.78	1.61	1.52

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1302	NAG	C8-C7-N2	2.97	121.13	116.10
4	A	1302	NAG	C8-C7-N2	2.95	121.10	116.10
4	B	1302	NAG	C8-C7-N2	2.95	121.10	116.10
4	A	1305	NAG	C8-C7-N2	2.67	120.61	116.10
4	B	1305	NAG	C8-C7-N2	2.66	120.61	116.10

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1311	NAG	C8-C7-N2-C2
4	A	1311	NAG	O7-C7-N2-C2
4	B	1311	NAG	C8-C7-N2-C2
4	B	1311	NAG	O7-C7-N2-C2
4	C	1311	NAG	C8-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1309	NAG	1	0
4	B	1309	NAG	1	0
4	C	1309	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.

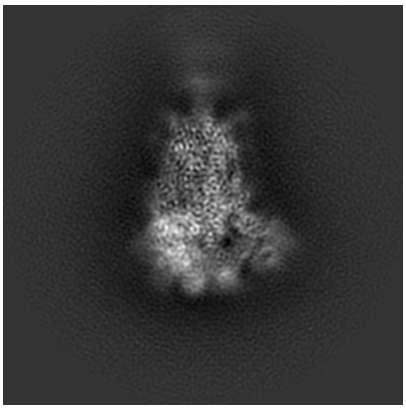
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-56069. These allow visual inspection of the internal detail of the map and identification of artifacts.

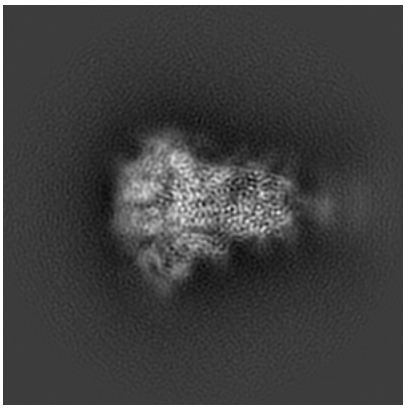
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

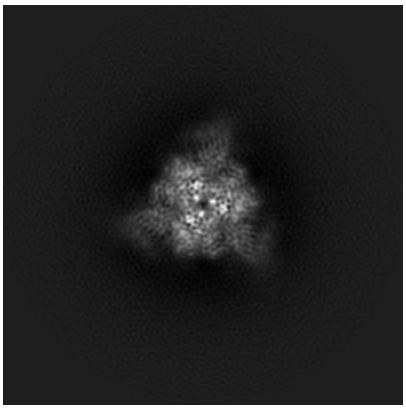
6.1.1 Primary map



X

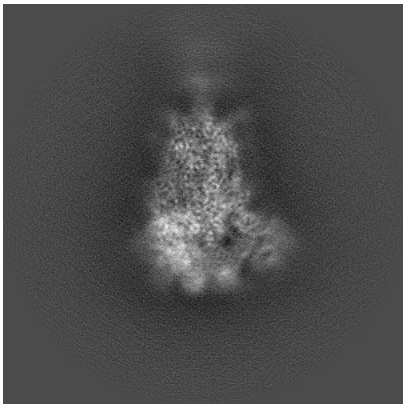


Y

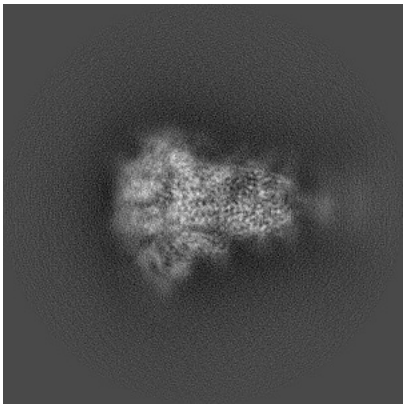


Z

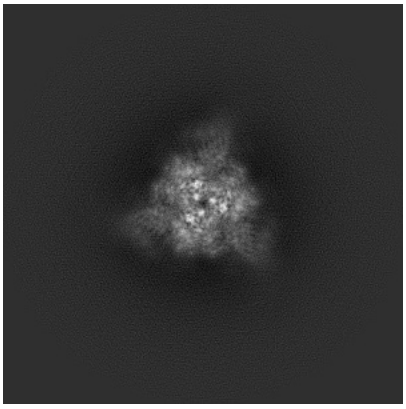
6.1.2 Raw map



X



Y

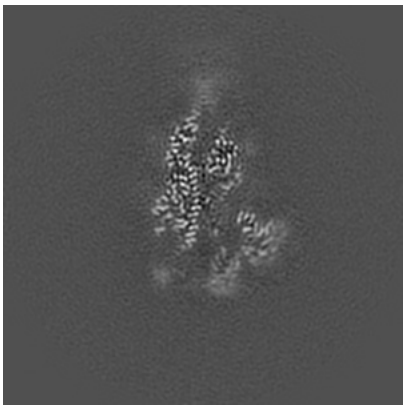


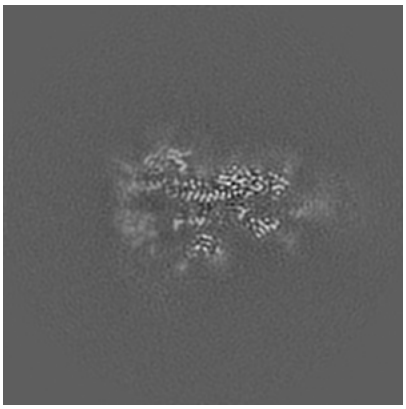
Z

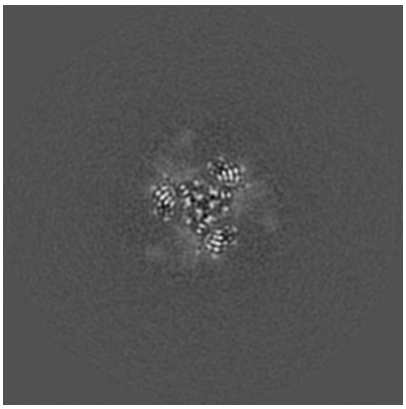
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

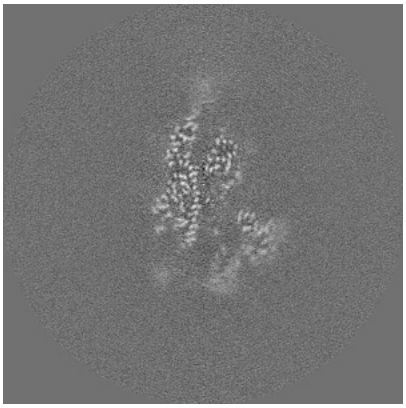
6.2.1 Primary map

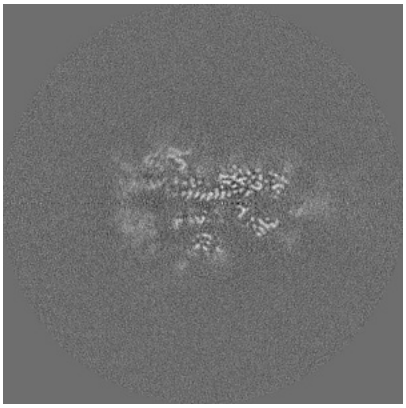

X Index: 180

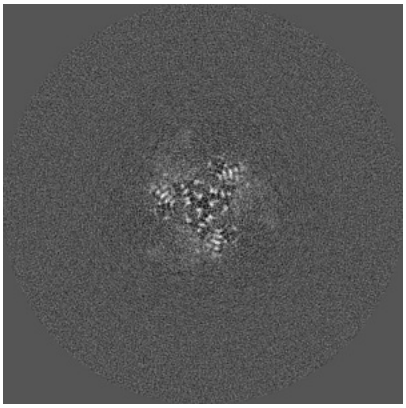

Y Index: 180


Z Index: 180

6.2.2 Raw map


X Index: 180

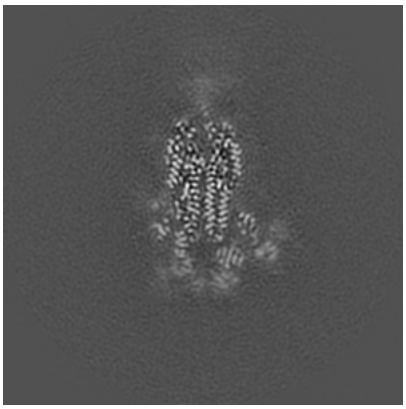

Y Index: 180

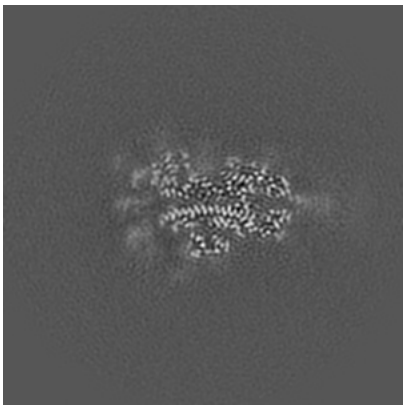

Z Index: 180

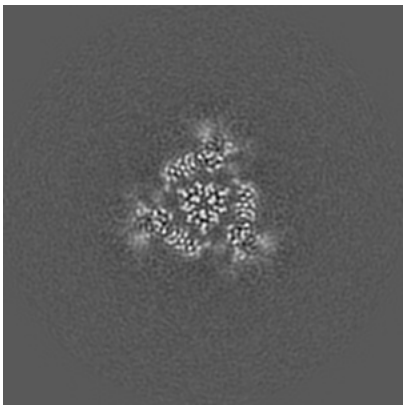
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

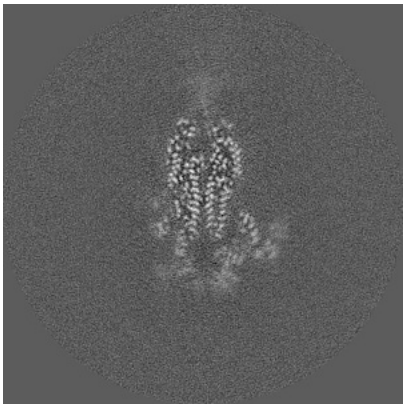
6.3.1 Primary map

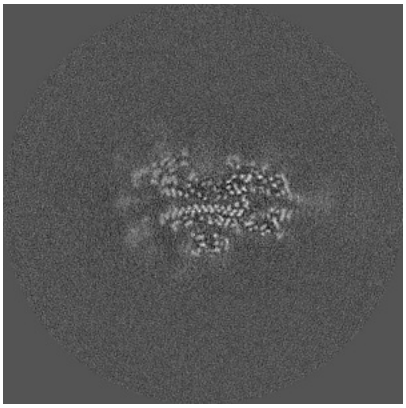

X Index: 175

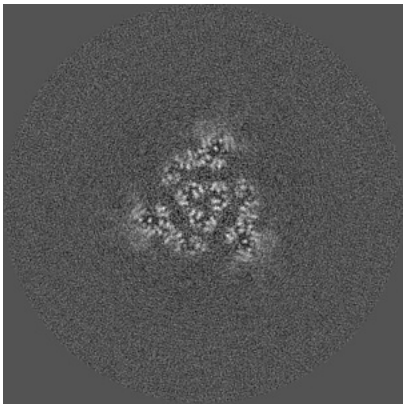

Y Index: 187


Z Index: 160

6.3.2 Raw map


X Index: 176

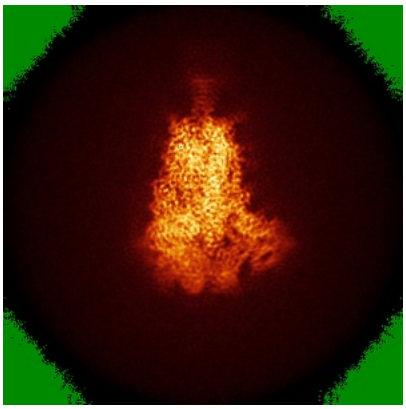

Y Index: 186

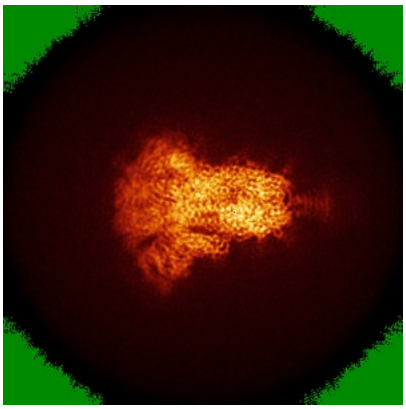

Z Index: 156

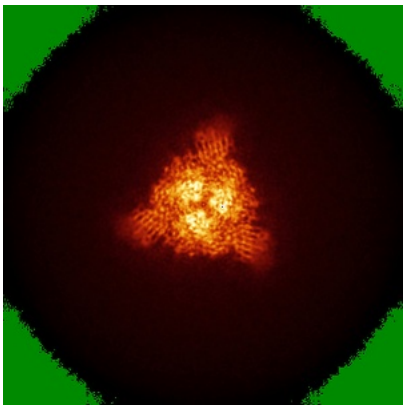
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

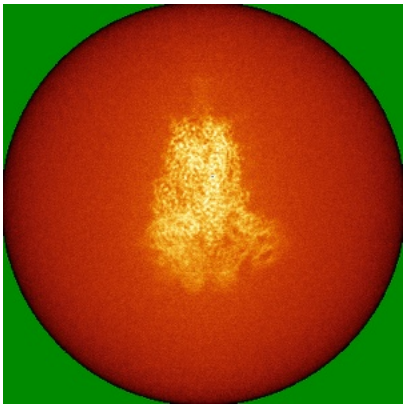
6.4.1 Primary map

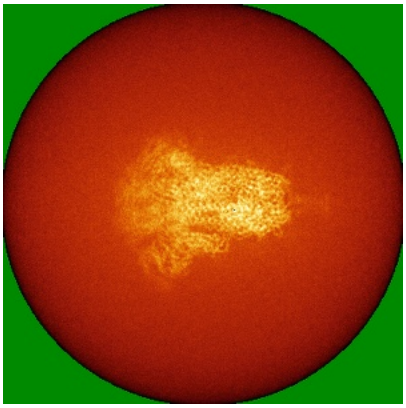

X

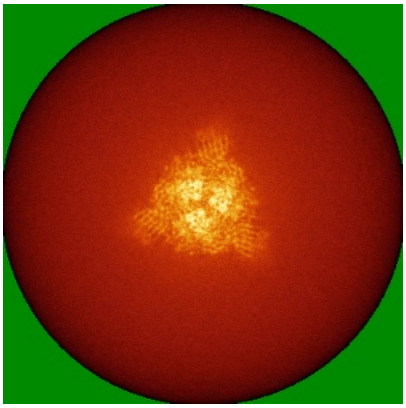

Y


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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

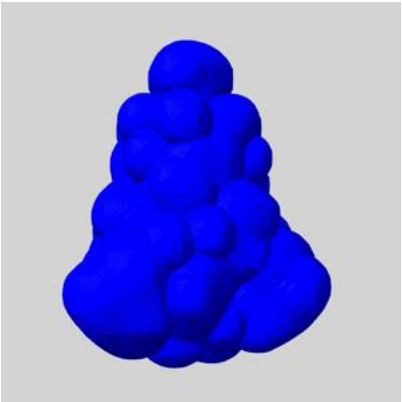
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

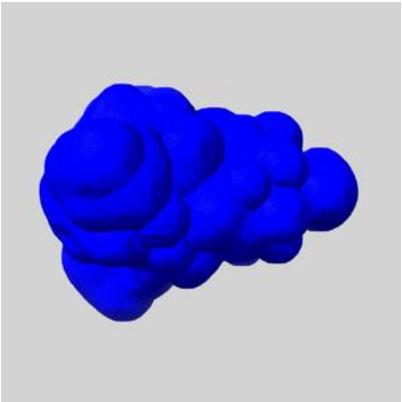
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

6.6.1 emd_56069_msk_1.map (i)



X



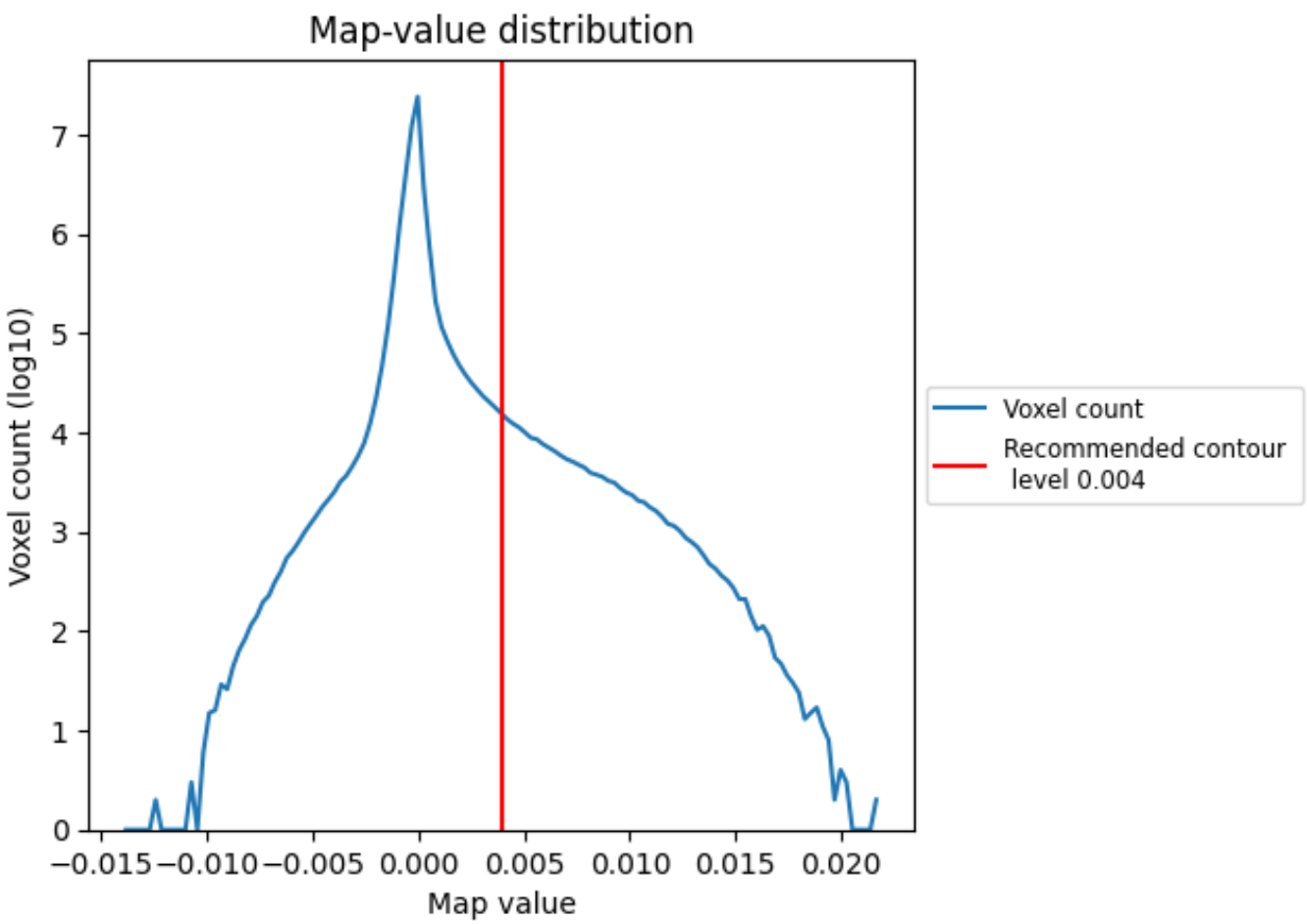
Y

Z

7 Map analysis (i)

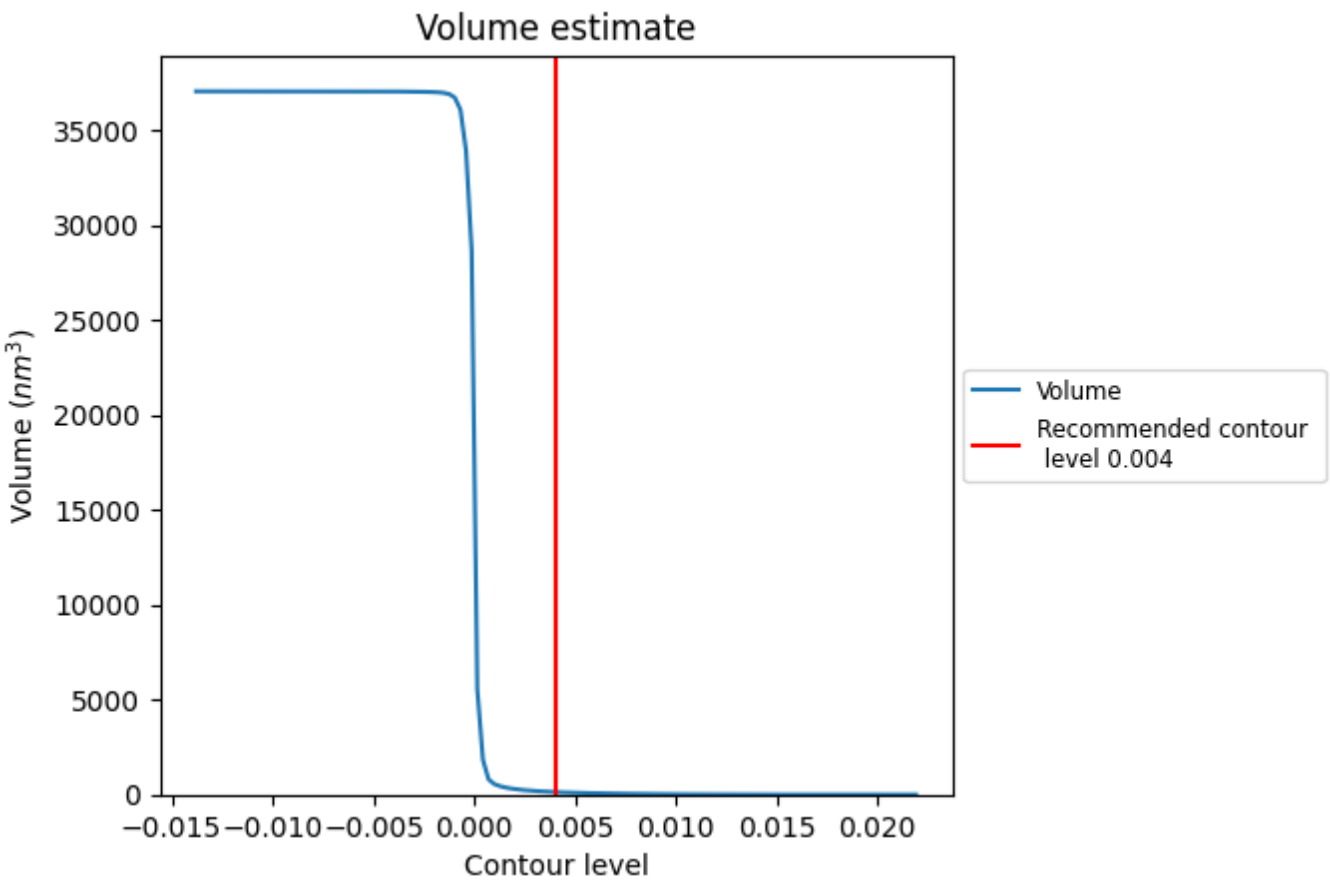
This section contains the results of statistical analysis of the map.

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.

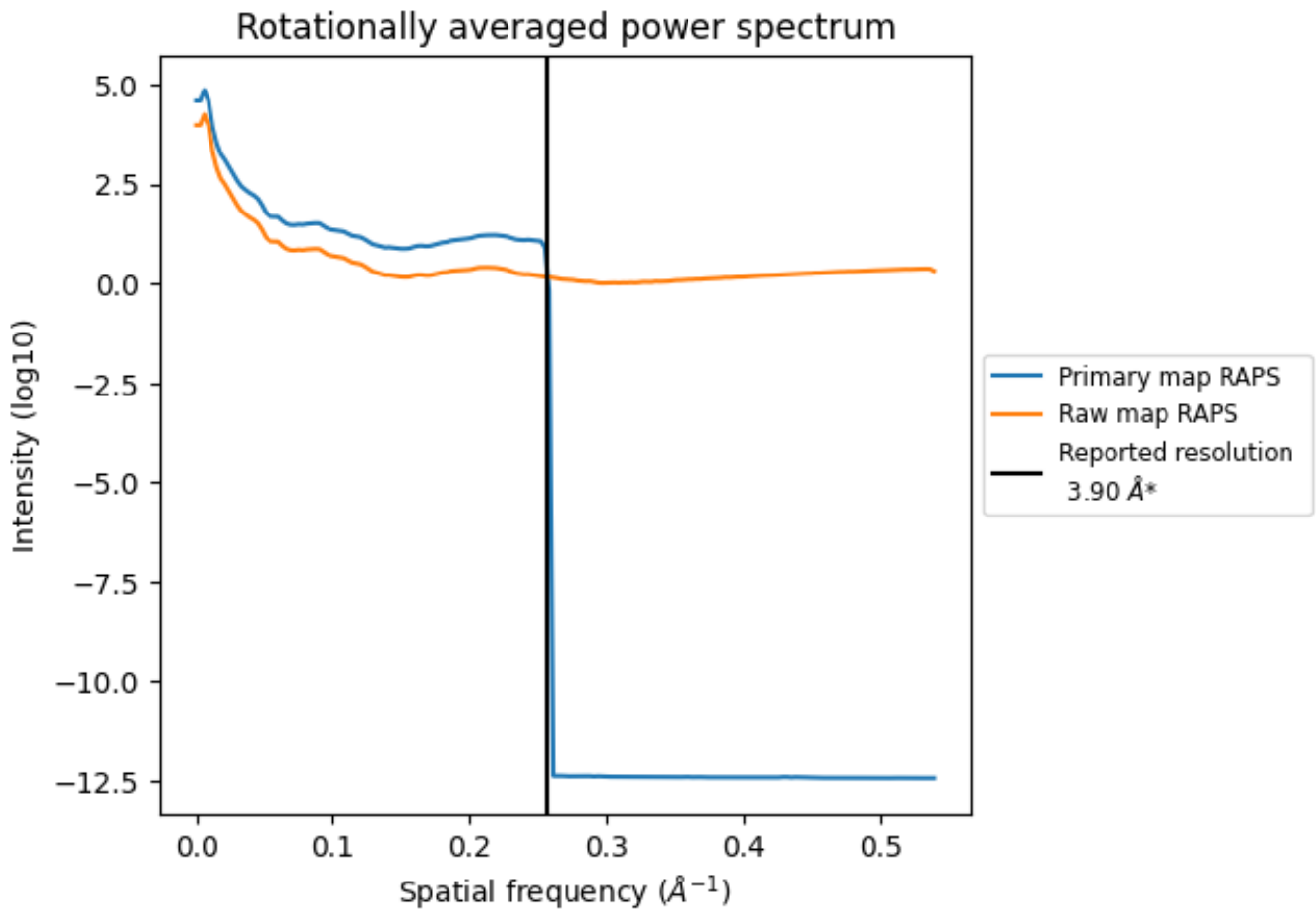
7.2 Volume estimate (i)



The volume at the recommended contour level is 132 nm^3; this corresponds to an approximate mass of 119 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)

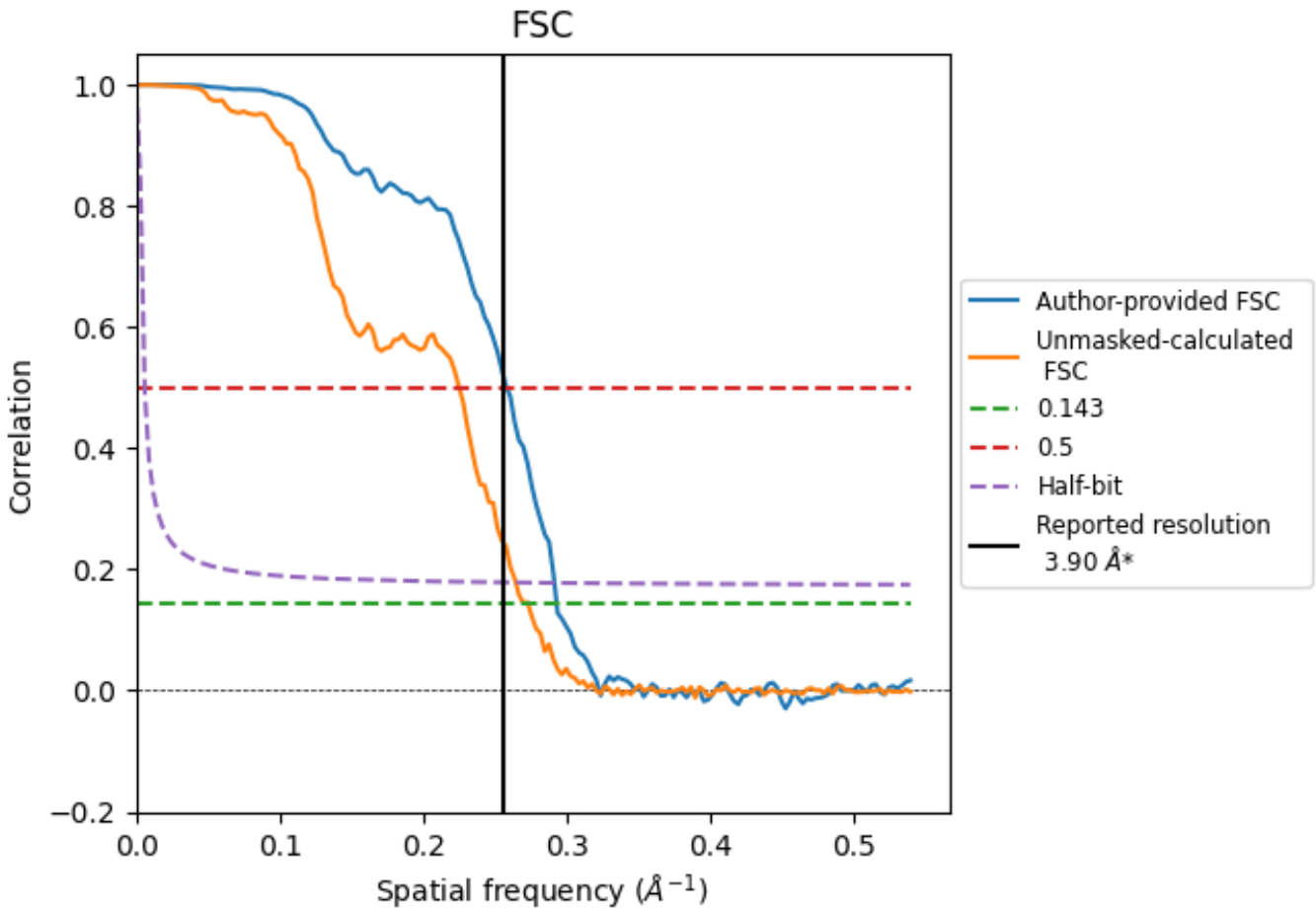


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

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 0.256 Å^{-1}

8.2 Resolution estimates (i)

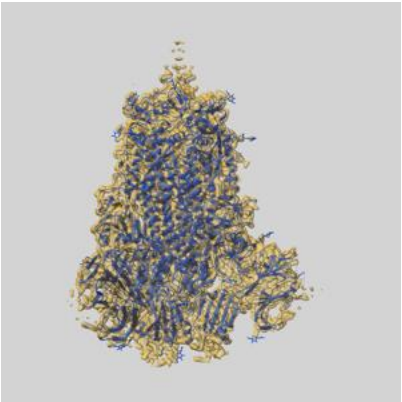
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.41	3.87	3.43
Unmasked-calculated*	3.66	4.44	3.78

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.41 differs from the reported value 3.9 by more than 10 %

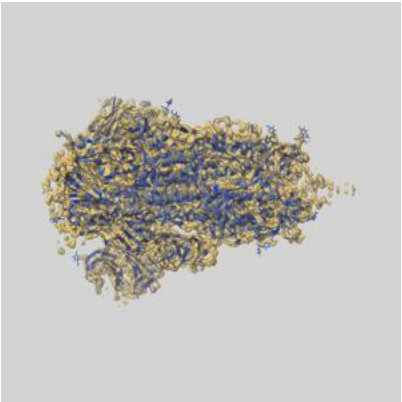
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-56069 and PDB model 9TMF. Per-residue inclusion information can be found in section 3 on page 18.

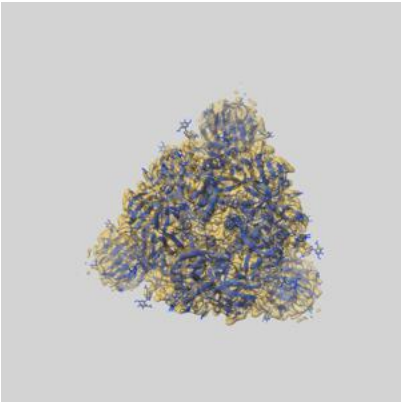
9.1 Map-model overlay (i)



X



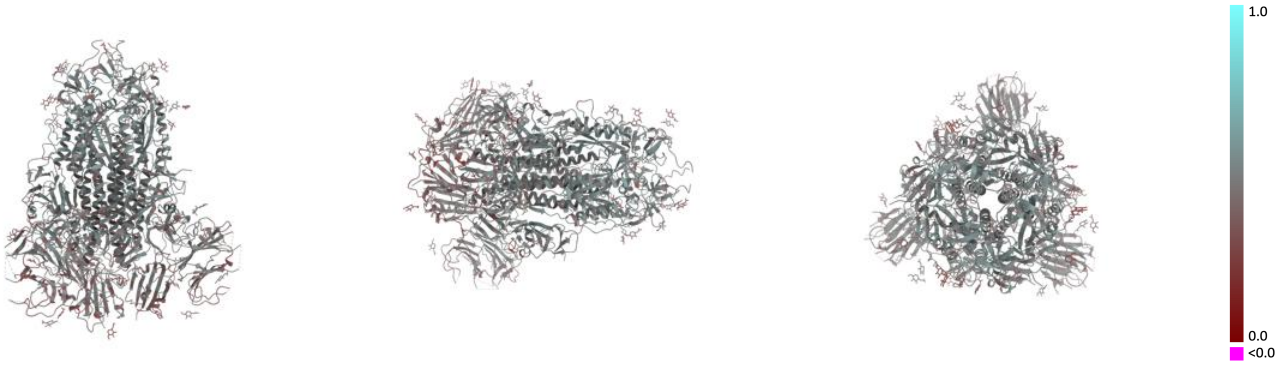
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.004 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.

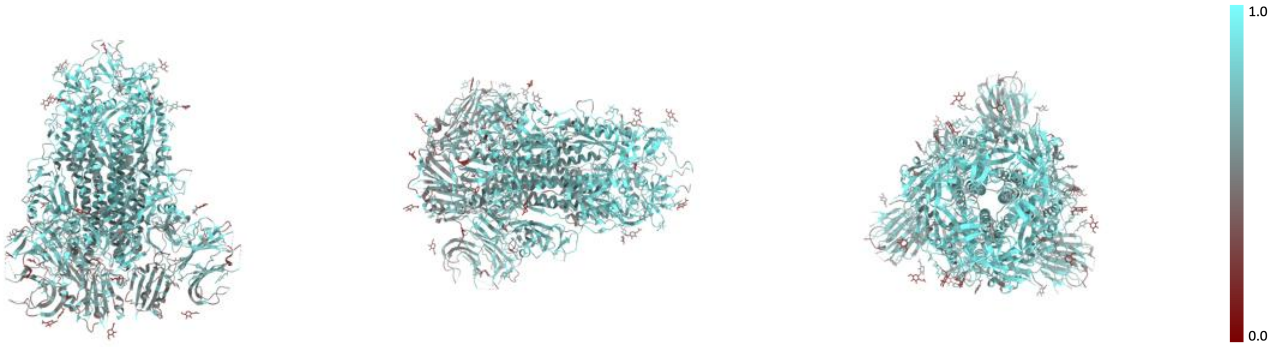
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

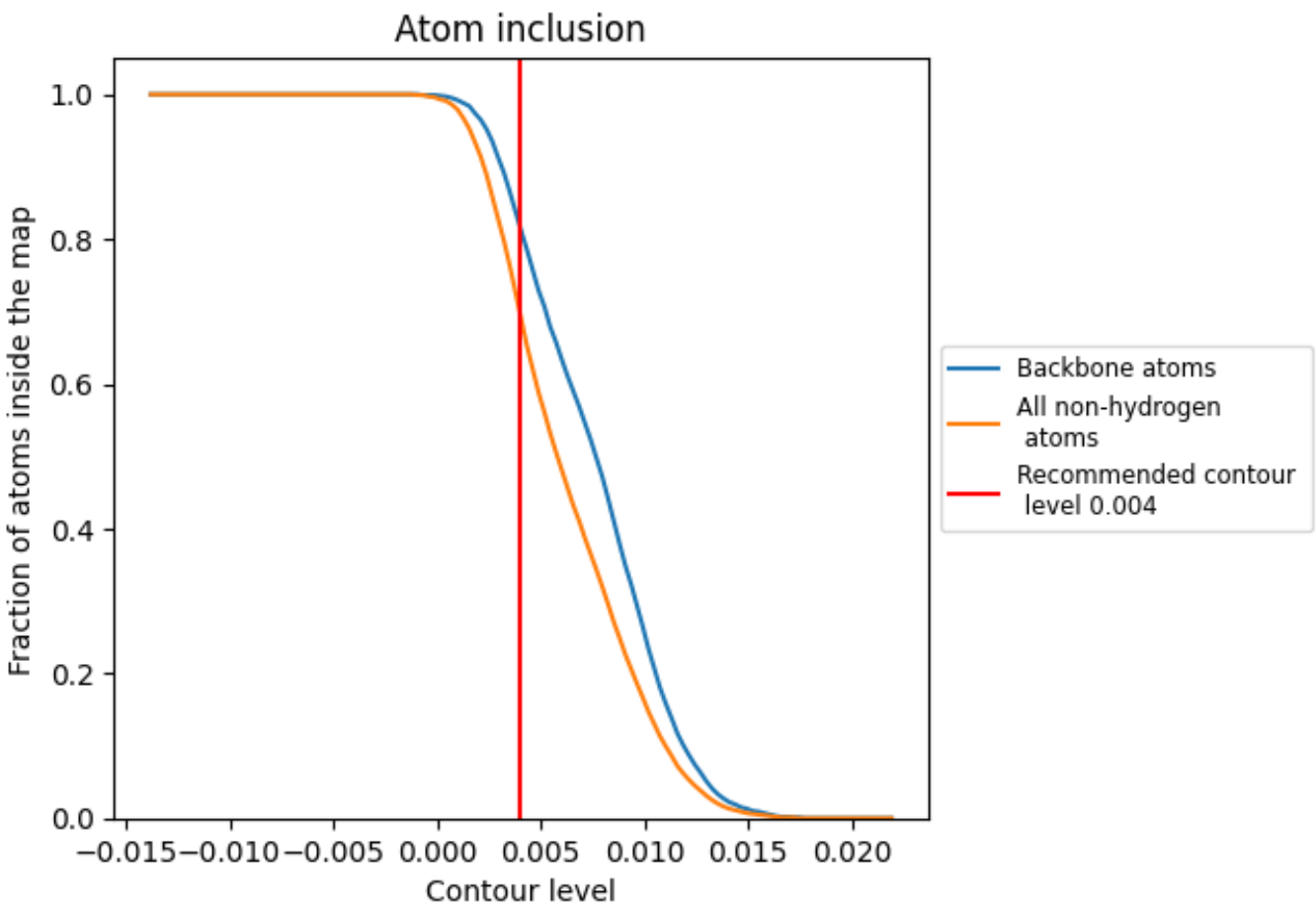
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.004).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6970	0.4640
A	0.7010	0.4650
B	0.7000	0.4640
C	0.7020	0.4650
D	0.2860	0.4230
E	0.5380	0.4380
F	0.4290	0.3450
G	0.2860	0.4090
H	0.5130	0.4120
I	0.4290	0.3620
J	0.2860	0.4180
K	0.5130	0.4100
L	0.4290	0.3520