



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 03:37 PM UTC

PDB ID : 6X6P / pdb_00006x6p
EMDB ID : EMD-22078
Title : Characterization of the SARS-CoV-2 S Protein: Biophysical, Biochemical, Structural, and Antigenic Analysis
Authors : Herrera, N.G.; Morano, N.C.; Celikgil, A.; Georgiev, G.I.; Malonis, R.; Lee, J.H.; Tong, K.; Vergnolle, O.; Massimi, A.; Yen, L.Y.; Noble, A.J.; Kopylov, M.; Bonanno, J.B.; Garrett-Thompson, S.C.; Hayes, D.B.; Brenowitz, M.; Garforth, S.J.; Eng, E.T.; Lai, J.R.; Almo, S.C.
Deposited on : 2020-05-28
Resolution : 3.22 Å (reported)
Based on initial model : 6VXX

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 ⓘ 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)

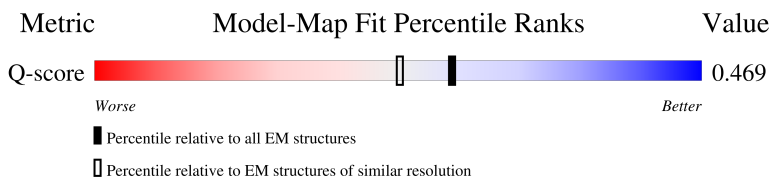
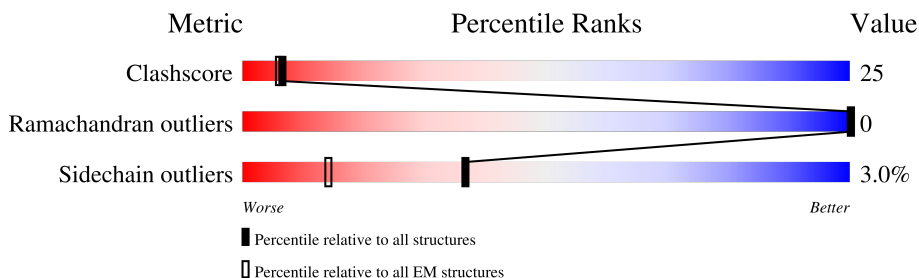
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.22 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	14612 (2.72 - 3.72)

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	

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Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
2	D	2	100%
2	E	2	50%
2	F	2	50%
2	G	2	100%
2	H	2	100%
2	I	2	50%
2	J	2	50%
2	K	2	100%
2	L	2	100%
2	M	2	50%
2	N	2	50%
2	O	2	100%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24615 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1017	Total	C	N	O	S	0	0
			7939	5069	1319	1516	35		
1	B	1017	Total	C	N	O	S	0	0
			7939	5069	1319	1516	35		
1	C	1017	Total	C	N	O	S	0	0
			7939	5069	1319	1516	35		

There are 255 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	GLY	-	expression tag	UNP P0DTC2
A	1239	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	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	ALA	-	expression tag	UNP P0DTC2
A	1260	TRP	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
A	1263	PRO	-	expression tag	UNP P0DTC2
A	1264	GLN	-	expression tag	UNP P0DTC2
A	1265	PHE	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	LYS	-	expression tag	UNP P0DTC2
A	1268	GLY	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	GLY	-	expression tag	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	ALA	-	expression tag	UNP P0DTC2
A	1281	TRP	-	expression tag	UNP P0DTC2
A	1282	SER	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	PRO	-	expression tag	UNP P0DTC2
A	1285	GLN	-	expression tag	UNP P0DTC2
A	1286	PHE	-	expression tag	UNP P0DTC2
A	1287	GLU	-	expression tag	UNP P0DTC2
A	1288	LYS	-	expression tag	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	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	SER	-	expression tag	UNP P0DTC2
B	1259	ALA	-	expression tag	UNP P0DTC2
B	1260	TRP	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
B	1263	PRO	-	expression tag	UNP P0DTC2
B	1264	GLN	-	expression tag	UNP P0DTC2
B	1265	PHE	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	LYS	-	expression tag	UNP P0DTC2
B	1268	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	GLY	-	expression tag	UNP P0DTC2
B	1274	GLY	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	SER	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	SER	-	expression tag	UNP P0DTC2
B	1280	ALA	-	expression tag	UNP P0DTC2
B	1281	TRP	-	expression tag	UNP P0DTC2
B	1282	SER	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	PRO	-	expression tag	UNP P0DTC2
B	1285	GLN	-	expression tag	UNP P0DTC2
B	1286	PHE	-	expression tag	UNP P0DTC2
B	1287	GLU	-	expression tag	UNP P0DTC2
B	1288	LYS	-	expression tag	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	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
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

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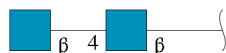
Chain	Residue	Modelled	Actual	Comment	Reference
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression 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	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2
C	1259	ALA	-	expression tag	UNP P0DTC2
C	1260	TRP	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	HIS	-	expression tag	UNP P0DTC2
C	1263	PRO	-	expression tag	UNP P0DTC2
C	1264	GLN	-	expression tag	UNP P0DTC2
C	1265	PHE	-	expression tag	UNP P0DTC2
C	1266	GLU	-	expression tag	UNP P0DTC2
C	1267	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1268	GLY	-	expression tag	UNP P0DTC2
C	1269	GLY	-	expression tag	UNP P0DTC2
C	1270	GLY	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	GLY	-	expression tag	UNP P0DTC2
C	1273	GLY	-	expression tag	UNP P0DTC2
C	1274	GLY	-	expression tag	UNP P0DTC2
C	1275	GLY	-	expression tag	UNP P0DTC2
C	1276	SER	-	expression tag	UNP P0DTC2
C	1277	GLY	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	SER	-	expression tag	UNP P0DTC2
C	1280	ALA	-	expression tag	UNP P0DTC2
C	1281	TRP	-	expression tag	UNP P0DTC2
C	1282	SER	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	PRO	-	expression tag	UNP P0DTC2
C	1285	GLN	-	expression tag	UNP P0DTC2
C	1286	PHE	-	expression tag	UNP P0DTC2
C	1287	GLU	-	expression tag	UNP P0DTC2
C	1288	LYS	-	expression tag	UNP P0DTC2

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



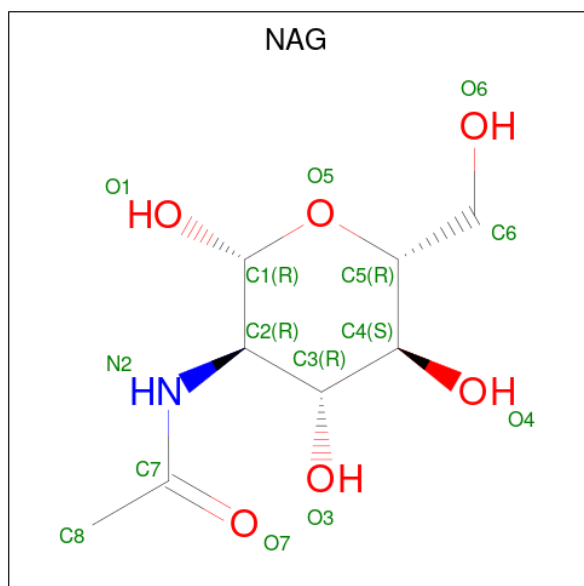
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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

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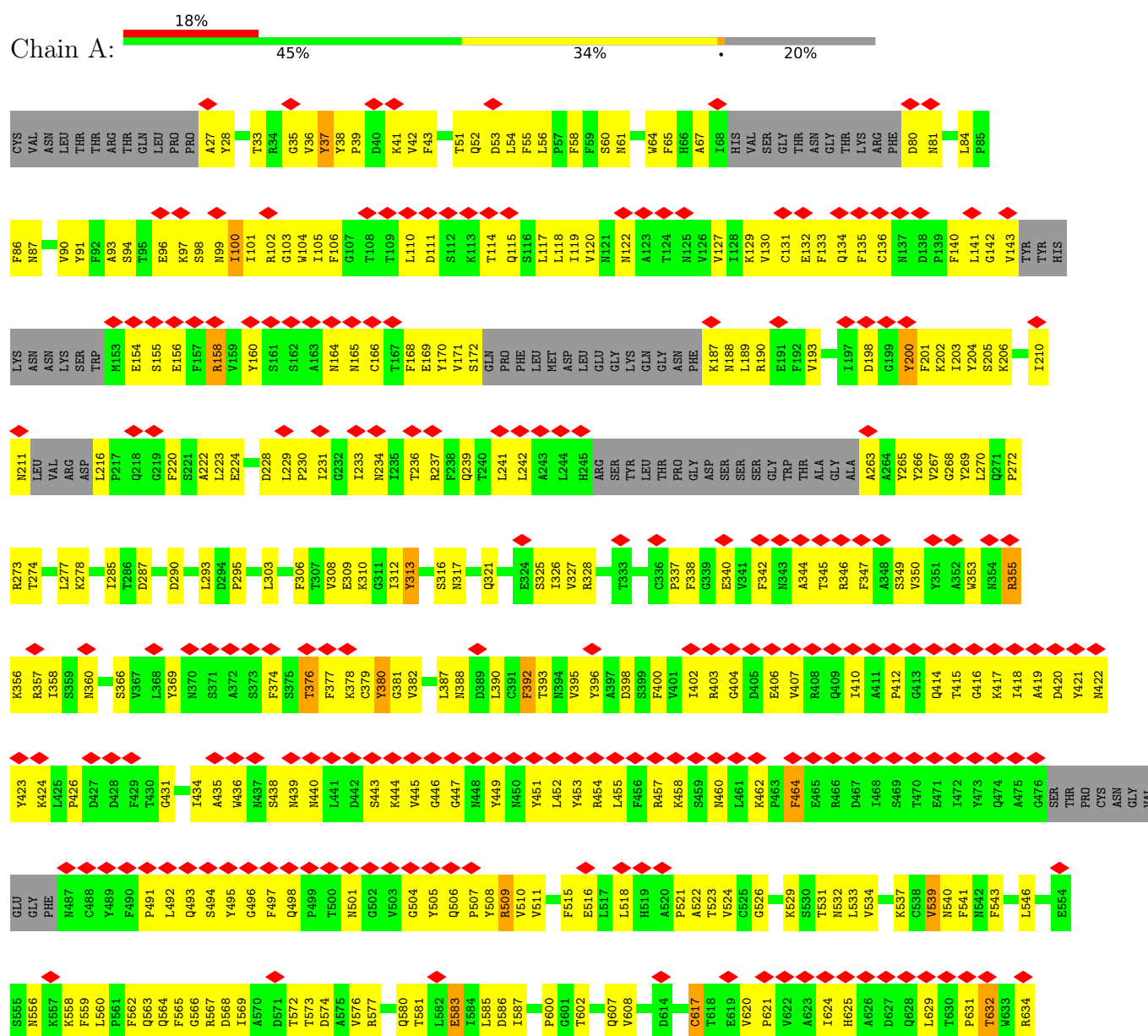
Continued from previous page...

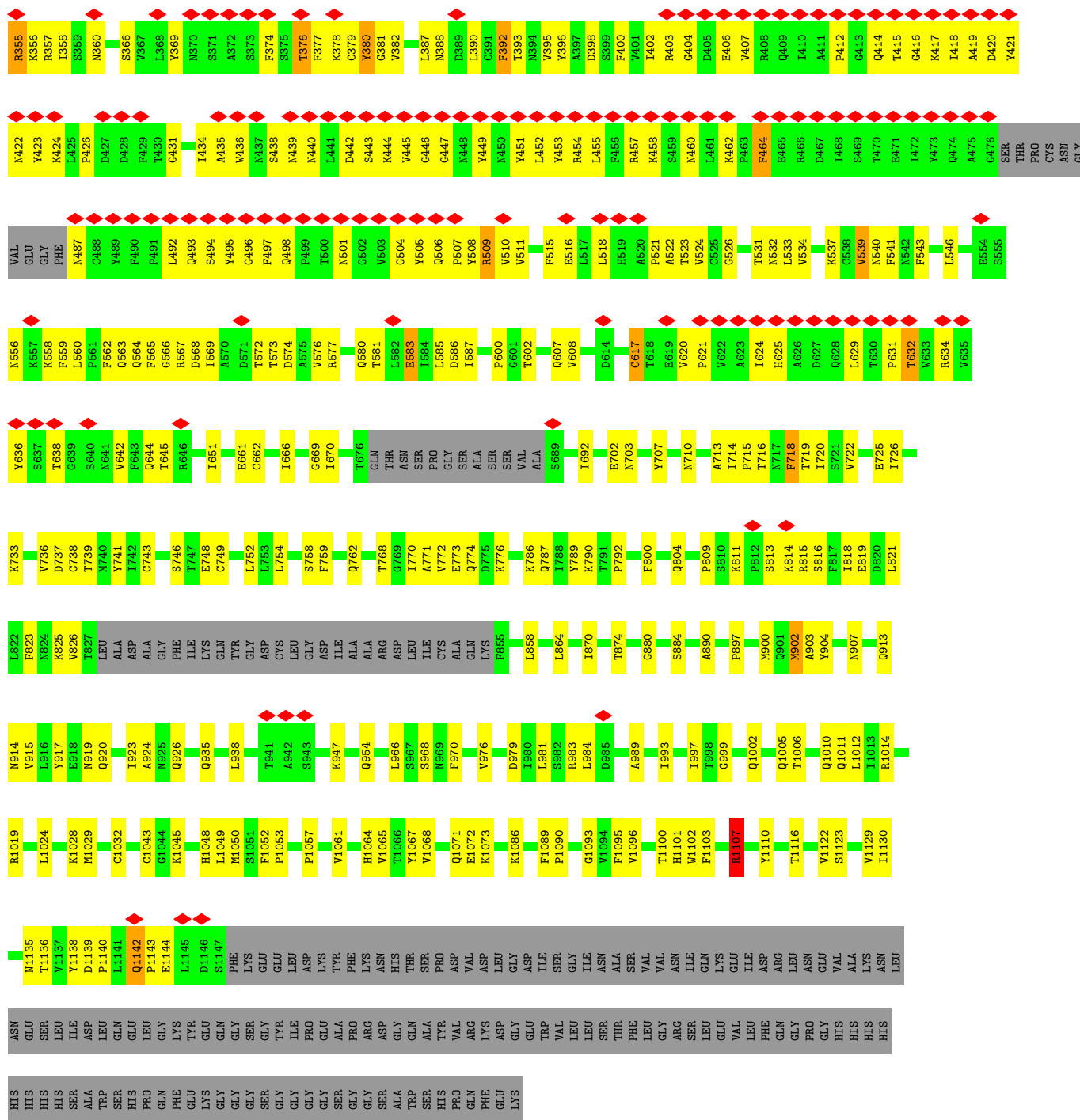
Mol	Chain	Residues	Atoms				AltConf
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots

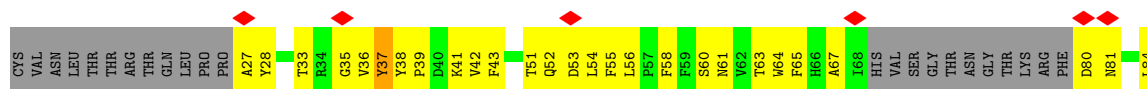
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Spike glycoprotein





• Molecule 1: Spike glycoprotein



V1129	I1013	N907	P812	T719	T630	E554	GLY	N422	K356	P272	T210	HIS	P85
I1130	R1014	Q913	S813	I720	P631	E555	VAL	Y423	R357	R273	N211	LYS	F86
N1135	R1019	Q914	K814	S721	T632	S556	GLY	K424	S359	T274	LEU	ASN	N87
V1136	L1024	N915	R815	W722	W633	N557	PHE	L425	N360	L277	ARG	LYS	V90
V1137	L1136	L916	S816	E725	R634	K558	N487	P426	C361	K278	L216	ASP	F92
Y1138	K1028	E917	R817	I726	W635	F559	C488	D427	S366	E281	P217	TRP	A93
D1139	M1029	E918	E819	W733	W636	F560	Y489	D428	L368	L285	Q218	ASP	S94
P1140	C1032	N919	R820	K733	W637	F561	F490	F429	L369	T286	Q219	LYS	T95
L1141	L1141	Q920	L821	W736	W638	F562	P491	T430	N370	D287	E220	LYS	E96
P1142	C1043	I923	L822	D737	W639	Q563	L492	C432	N371	D290	S221	LYS	K97
P1143	C1043	A924	R823	C738	W640	Q564	Q493	V433	S371	P295	E223	LYS	S98
E1144	G1044	K825	N824	W739	W641	F565	Q493	I434	A372	Y160	E224	LYS	N99
L1145	K1045	N925	W826	W740	W642	R567	S494	A435	S373	L303	D228	LYS	I100
D1146	H1048	Q926	W827	W741	W643	D568	Y495	W436	F374	F306	L229	LYS	R102
S1147	L1049	Q935	LEU	W742	W644	D569	Q496	W437	S375	F307	L230	LYS	G103
PHE	M1050	L938	ALA	C743	W645	A570	F497	N438	T376	E309	P230	LYS	W104
LYS	S1051	A942	ALA	S746	T651	T572	Q498	N439	F377	K378	G232	LYS	F106
GLU	P1052	S943	GLY	T747	T651	D574	T500	N440	C379	K310	G233	LYS	G107
GLU	P1053	K947	PHE	E748	E661	A575	N501	L441	G381	G311	I234	LYS	T108
LEU	P1057	K947	ILE	C749	E662	W576	G502	D442	G382	Y313	I235	LYS	T109
ASP	P1057	K947	LYS	L752	T666	B577	G504	S443	V382	S316	T236	LYS	L110
LYS	V1061	Q954	GLN	L753	T666	Q580	G504	K444	V382	N317	R237	LYS	D111
PHE	V1061	Q954	GLY	L754	T666	T581	G505	V445	L387	Q321	L241	LYS	L112
LYS	H1064	L956	ASP	S758	T666	L582	G506	W446	N388	S325	L242	LYS	Q115
ASN	V1065	L956	CYS	F759	T666	D586	G507	G447	C391	S326	A243	LYS	L117
HIS	T1066	S967	THR	W768	T666	E583	R509	N448	F392	V327	L244	LYS	L118
THR	Y1067	S967	GLY	G769	T666	L584	V510	Y449	T393	R328	H245	LYS	L119
GLY	V1068	N969	ASP	Q762	T666	D586	V511	Y451	N394	Q321	ARG	LYS	W120
PRO	Q1071	F970	ILE	W768	T666	L584	V511	Y452	N394	Q321	ARG	LYS	N121
ASP	E1072	F970	ALA	G769	T666	L584	V511	Y453	N394	Q321	ARG	LYS	N122
LEU	K1073	V976	ALA	G769	T666	L584	V511	Y454	N394	Q321	ARG	LYS	A123
GLY	K1086	D979	ARG	W768	T666	L584	V511	Y455	N394	Q321	ARG	LYS	T124
ASP	I980	L981	ASP	W768	T666	L584	V511	Y456	N394	Q321	ARG	LYS	N125
ILE	L981	S982	ILE	W768	T666	L584	V511	Y457	N394	Q321	ARG	LYS	V126
SER	P1090	R983	CYS	W768	T666	L584	V511	Y458	N394	Q321	ARG	LYS	I127
GLY	L984	L984	GLN	W768	T666	L584	V511	Y459	N394	Q321	ARG	LYS	I128
ILE	G1093	D985	LYS	W768	T666	L584	V511	Y460	N394	Q321	ARG	LYS	K129
ASN	W1094	F855	LYS	W768	T666	L584	V511	Y461	N394	Q321	ARG	LYS	V130
ALA	F1095	F855	LYS	W768	T666	L584	V511	Y462	N394	Q321	ARG	LYS	C131
SER	V1096	F855	LYS	W768	T666	L584	V511	Y463	N394	Q321	ARG	LYS	E132
VAL	T1100	F855	LYS	W768	T666	L584	V511	Y464	N394	Q321	ARG	LYS	Q134
VAL	H1101	F855	LYS	W768	T666	L584	V511	Y465	N394	Q321	ARG	LYS	F135
ASN	W1102	F855	LYS	W768	T666	L584	V511	Y466	N394	Q321	ARG	LYS	F136
ILE	F1103	F855	LYS	W768	T666	L584	V511	Y467	N394	Q321	ARG	LYS	C137
GLN	F1103	F855	LYS	W768	T666	L584	V511	Y468	N394	Q321	ARG	LYS	N137
LYS	R1107	F855	LYS	W768	T666	L584	V511	Y469	N394	Q321	ARG	LYS	N138
GLU	Y1110	F855	LYS	W768	T666	L584	V511	Y470	N394	Q321	ARG	LYS	D138
ASP	T1116	F855	LYS	W768	T666	L584	V511	Y471	N394	Q321	ARG	LYS	P139
ARG	Q1005	F855	LYS	W768	T666	L584	V511	Y472	N394	Q321	ARG	LYS	F140
LEU	T1106	F855	LYS	W768	T666	L584	V511	Y473	N394	Q321	ARG	LYS	L141
ASN	Q1010	F855	LYS	W768	T666	L584	V511	Y474	N394	Q321	ARG	LYS	G142
GLU	Q1011	F855	LYS	W768	T666	L584	V511	Y475	N394	Q321	ARG	LYS	V143
VAL	S1123	F855	LYS	W768	T666	L584	V511	Y476	N394	Q321	ARG	LYS	TYR
ALA		F855	LYS	W768	T666	L584	V511	Y477	N394	Q321	ARG	LYS	TYR

HIS	HIS	HIS	HIS	HIS	HIS	HIS	SER	ALA	TRP	SER	HIS	PRO	GLN	PHE	GLU	LYS	GLY	GLY	GLY	SER	GLY	GLY	GLY	GLY	SER	GLY	GLY	GLY	GLY	SER	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

NAG1
NAG2

NAG1
NAG2

NAG1
NAG2

NAG1

NAG1
NAG2



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



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



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



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



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



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





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	54395	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 ($e^-/\text{\AA}^2$)	66.5	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.126	Depositor
Minimum map value	-0.478	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	406.27197, 406.27197, 406.27197	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	Depositor

5 Model quality

5.1 Standard geometry

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	0.52	0/8118	0.61	3/11050 (0.0%)
1	B	0.52	0/8118	0.61	3/11050 (0.0%)
1	C	0.52	0/8118	0.61	3/11050 (0.0%)
All	All	0.52	0/24354	0.61	9/33150 (0.0%)

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

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	100	ILE	N-CA-C	-7.00	105.96	112.96
1	A	100	ILE	N-CA-C	-6.97	105.99	112.96
1	B	100	ILE	N-CA-C	-6.96	106.00	112.96
1	A	355	ARG	CG-CD-NE	-6.94	96.74	112.00
1	B	355	ARG	CG-CD-NE	-6.92	96.77	112.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	617	CYS	Peptide
1	B	617	CYS	Peptide
1	C	617	CYS	Peptide

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	7939	0	7732	441	0
1	B	7939	0	7732	421	0
1	C	7939	0	7732	440	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	1	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	1	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	0	0
2	N	28	0	25	1	0
2	O	28	0	25	0	0
3	A	154	0	143	3	0
3	B	154	0	143	3	0
3	C	154	0	143	3	0
All	All	24615	0	23925	1220	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 25.

The worst 5 of 1220 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:B:158:ARG:HG3	1:B:158:ARG:HH11	1.20	1.05
1:A:158:ARG:HG3	1:A:158:ARG:HH11	1.20	1.04
1:C:158:ARG:HG3	1:C:158:ARG:HH11	1.20	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:ARG:HE	1:C:533:LEU:HB2	1.25	1.00
1:A:328:ARG:HE	1:A:533:LEU:HB2	1.25	0.98

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	999/1274 (78%)	928 (93%)	71 (7%)	0	100	100
1	B	999/1274 (78%)	928 (93%)	71 (7%)	0	100	100
1	C	999/1274 (78%)	929 (93%)	70 (7%)	0	100	100
All	All	2997/3822 (78%)	2785 (93%)	212 (7%)	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	888/1099 (81%)	861 (97%)	27 (3%)	36	64
1	B	888/1099 (81%)	861 (97%)	27 (3%)	36	64
1	C	888/1099 (81%)	861 (97%)	27 (3%)	36	64
All	All	2664/3297 (81%)	2583 (97%)	81 (3%)	37	64

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	155	SER
1	C	546	LEU
1	C	198	ASP
1	C	392	PHE
1	C	718	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	66	HIS
1	C	926	GLN
1	C	245	HIS
1	C	644	GLN
1	C	957	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

24 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	1,2	14,14,15	0.36	0	17,19,21	0.57	0
2	NAG	D	2	2	14,14,15	0.32	0	17,19,21	0.39	0
2	NAG	E	1	1,2	14,14,15	0.27	0	17,19,21	0.65	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	E	2	2	14,14,15	0.19	0	17,19,21	0.49	0
2	NAG	F	1	1,2	14,14,15	0.54	0	17,19,21	0.47	0
2	NAG	F	2	2	14,14,15	0.21	0	17,19,21	0.37	0
2	NAG	G	1	1,2	14,14,15	0.36	0	17,19,21	0.50	0
2	NAG	G	2	2	14,14,15	0.21	0	17,19,21	0.56	0
2	NAG	H	1	1,2	14,14,15	0.36	0	17,19,21	0.57	0
2	NAG	H	2	2	14,14,15	0.31	0	17,19,21	0.38	0
2	NAG	I	1	1,2	14,14,15	0.28	0	17,19,21	0.65	1 (5%)
2	NAG	I	2	2	14,14,15	0.19	0	17,19,21	0.48	0
2	NAG	J	1	1,2	14,14,15	0.53	0	17,19,21	0.47	0
2	NAG	J	2	2	14,14,15	0.20	0	17,19,21	0.37	0
2	NAG	K	1	1,2	14,14,15	0.36	0	17,19,21	0.49	0
2	NAG	K	2	2	14,14,15	0.19	0	17,19,21	0.56	0
2	NAG	L	1	1,2	14,14,15	0.36	0	17,19,21	0.57	0
2	NAG	L	2	2	14,14,15	0.30	0	17,19,21	0.38	0
2	NAG	M	1	1,2	14,14,15	0.27	0	17,19,21	0.66	1 (5%)
2	NAG	M	2	2	14,14,15	0.18	0	17,19,21	0.49	0
2	NAG	N	1	1,2	14,14,15	0.53	0	17,19,21	0.47	0
2	NAG	N	2	2	14,14,15	0.20	0	17,19,21	0.37	0
2	NAG	O	1	1,2	14,14,15	0.37	0	17,19,21	0.49	0
2	NAG	O	2	2	14,14,15	0.20	0	17,19,21	0.56	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	C1-O5-C5	2.07	114.96	112.19
2	M	1	NAG	C1-O5-C5	2.07	114.95	112.19
2	I	1	NAG	C1-O5-C5	2.06	114.94	112.19

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

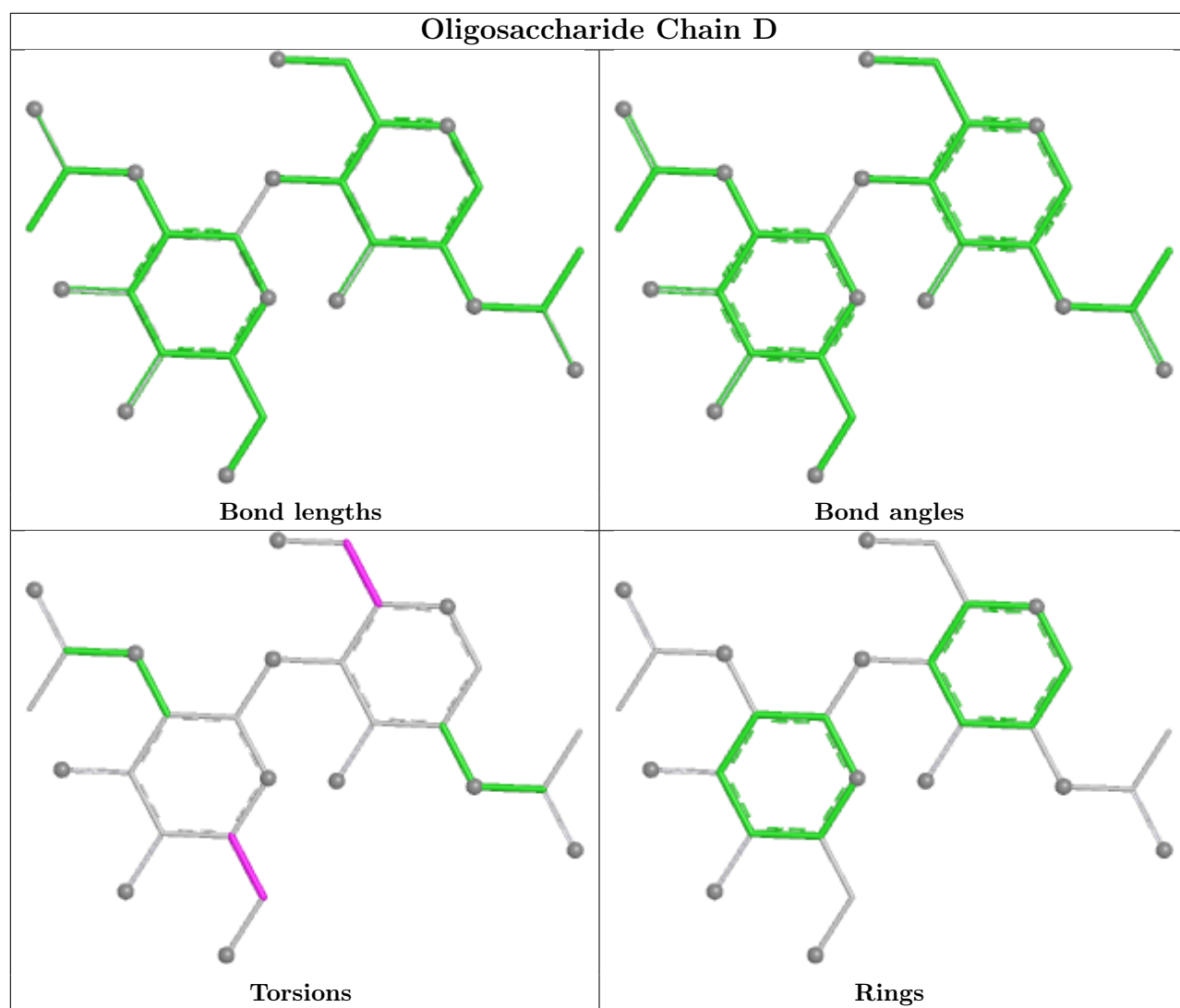
Mol	Chain	Res	Type	Atoms
2	G	1	NAG	O5-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6

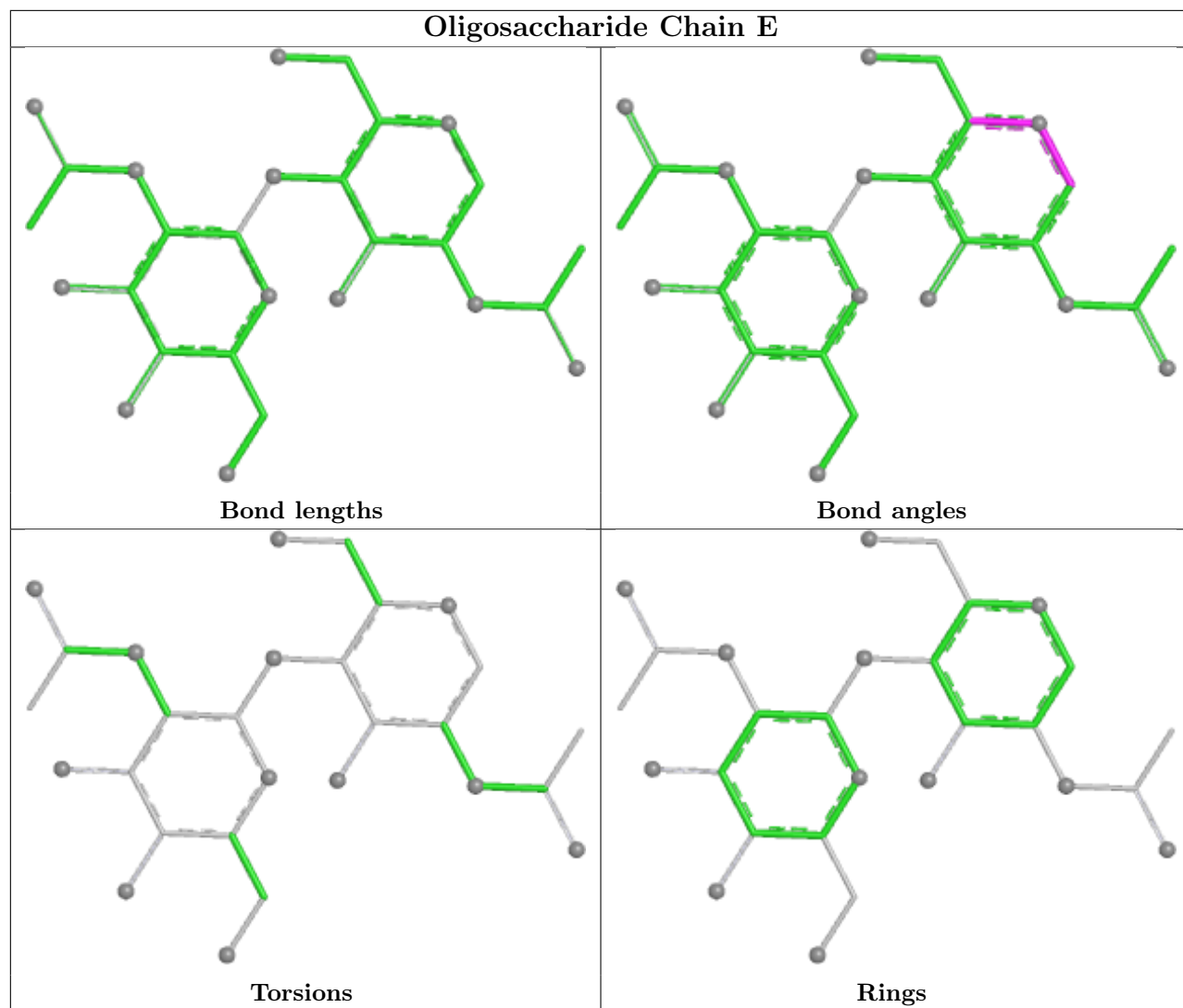
There are no ring outliers.

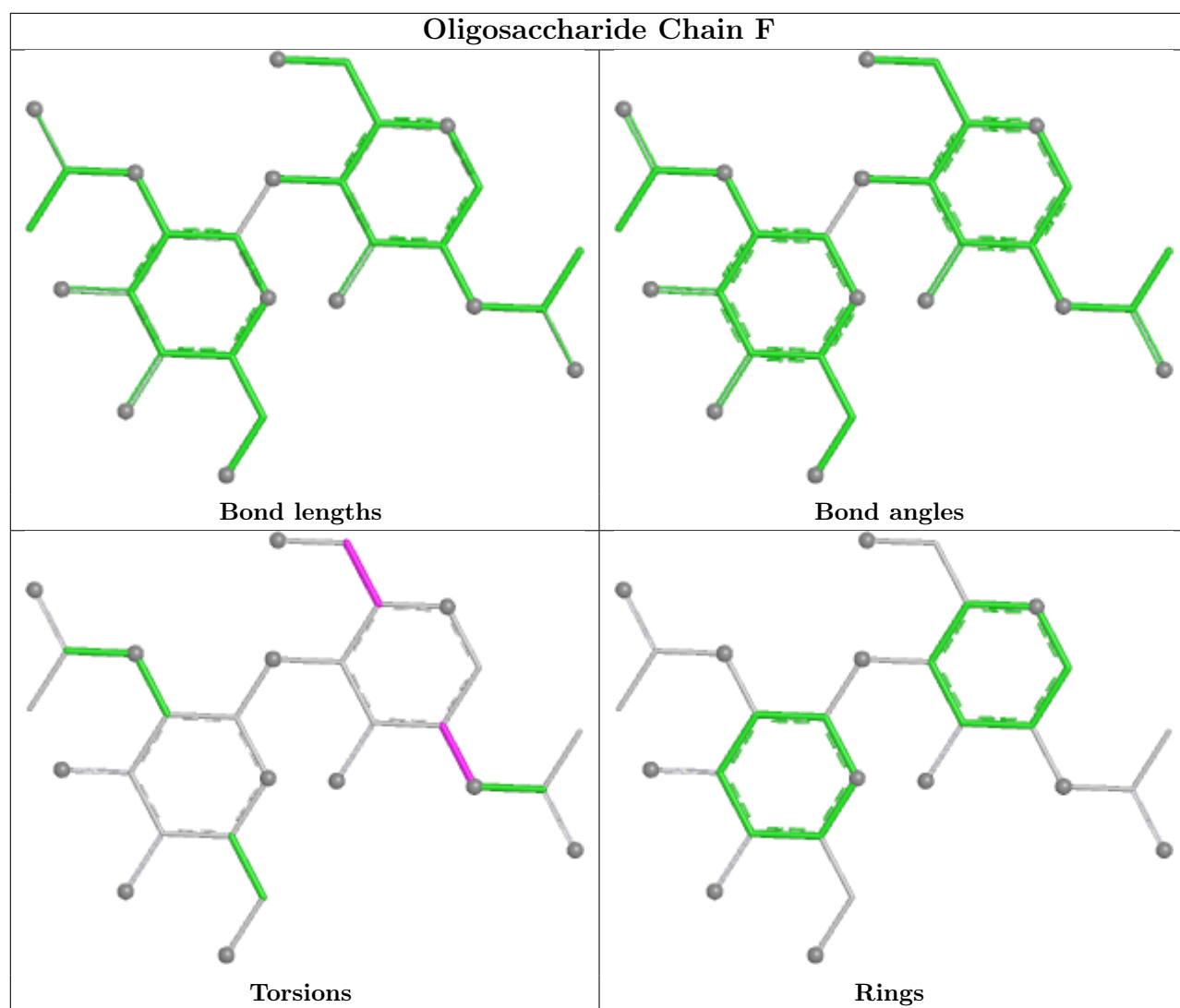
3 monomers are involved in 3 short contacts:

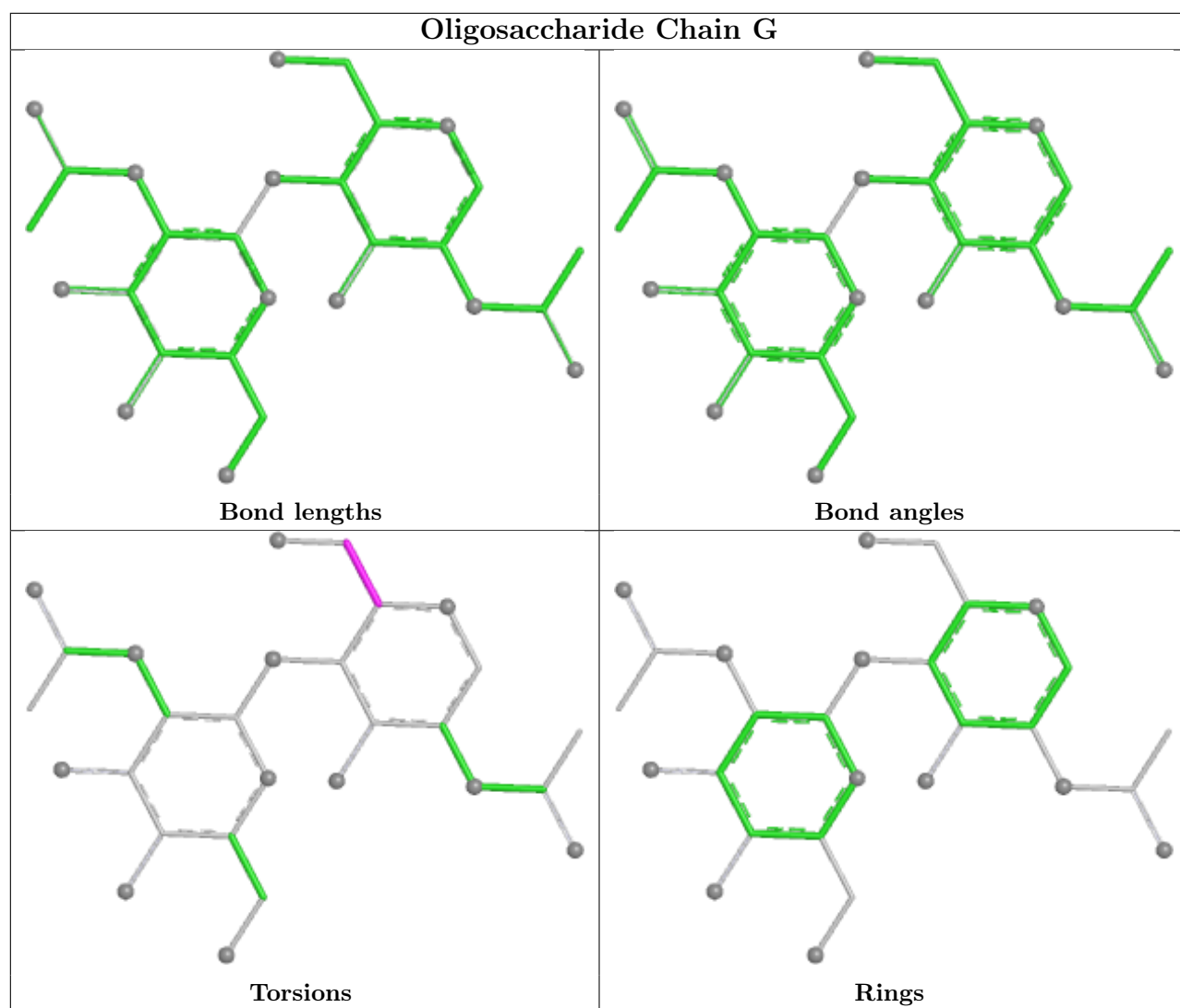
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	NAG	1	0
2	N	1	NAG	1	0
2	J	1	NAG	1	0

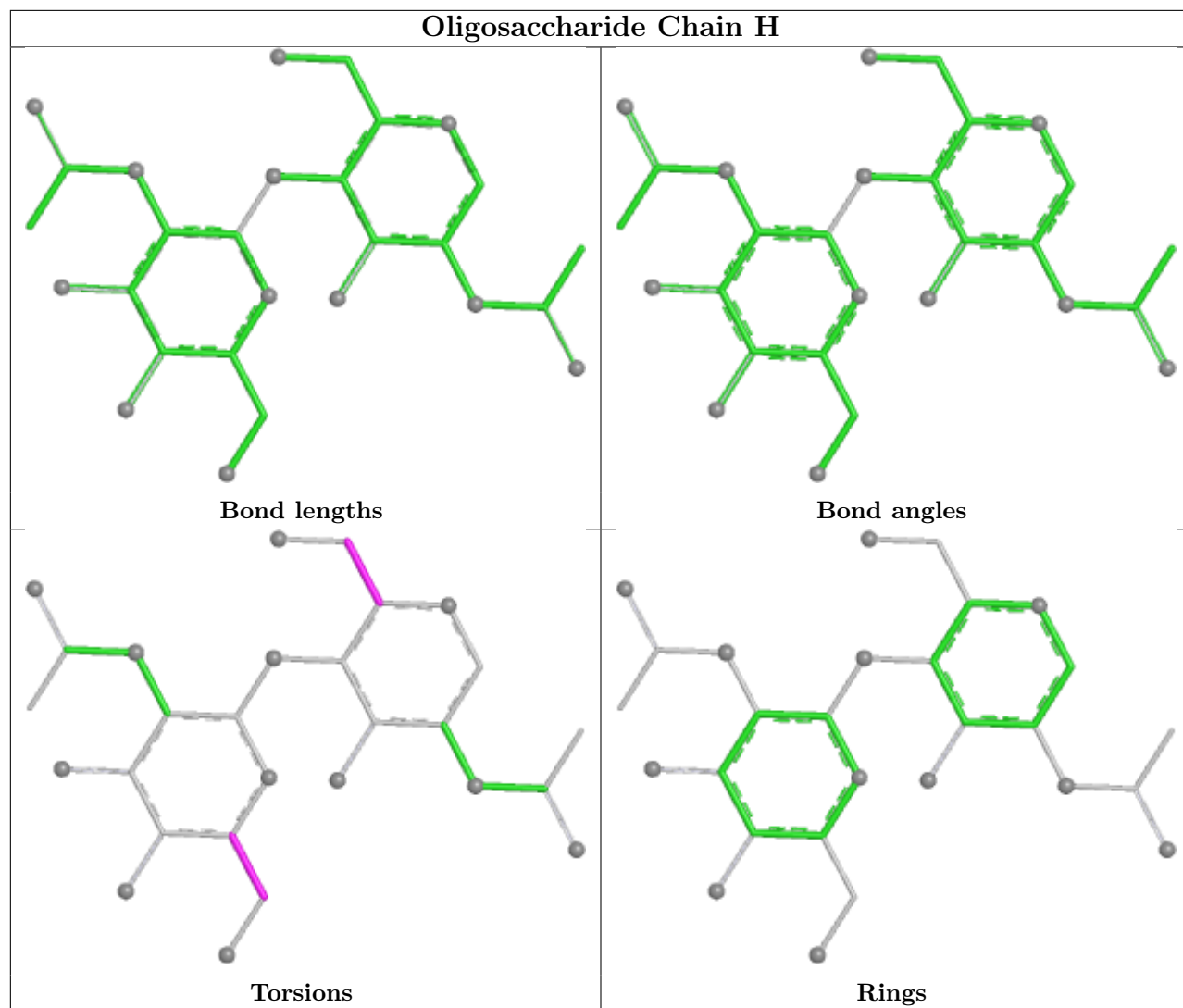
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

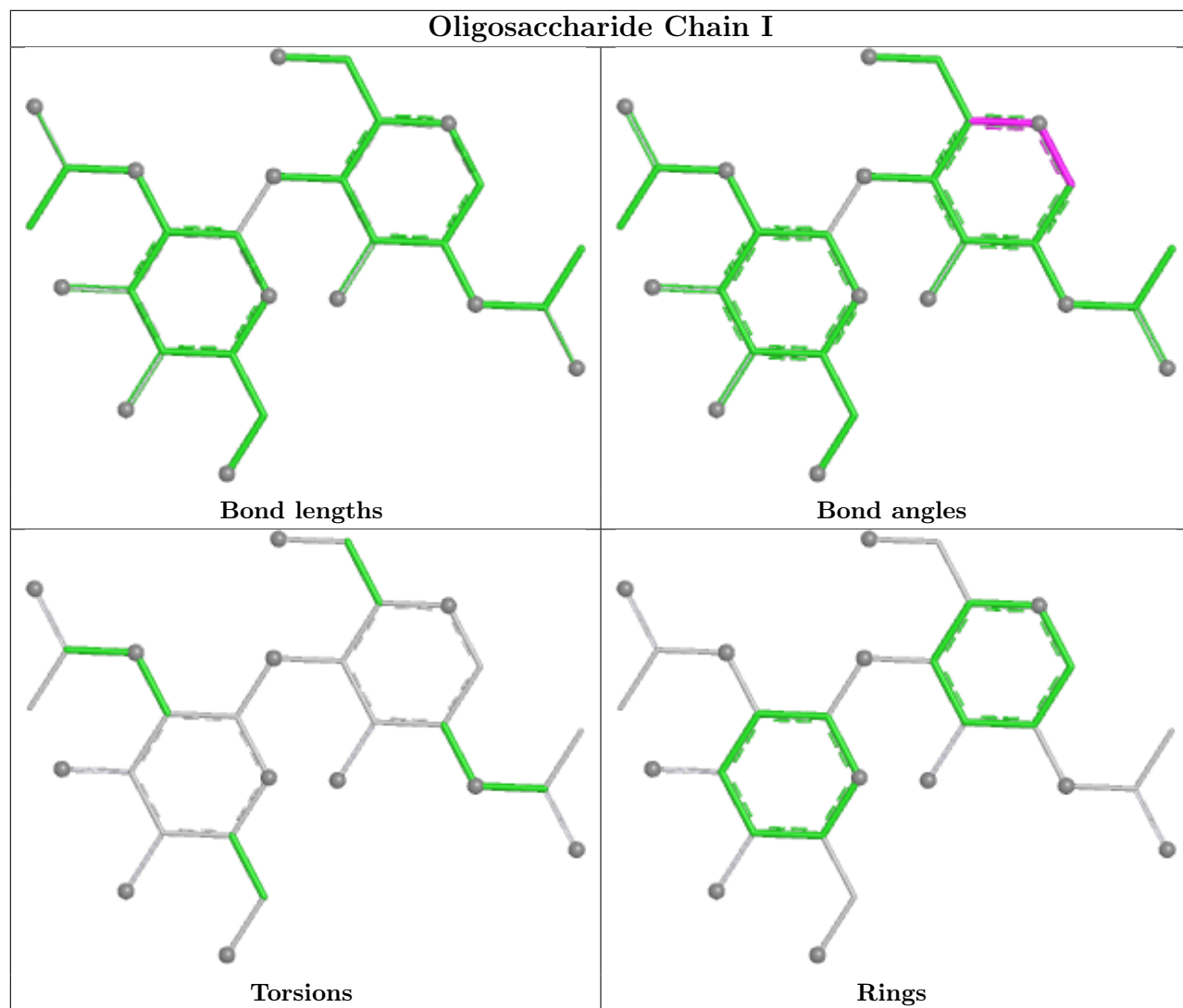


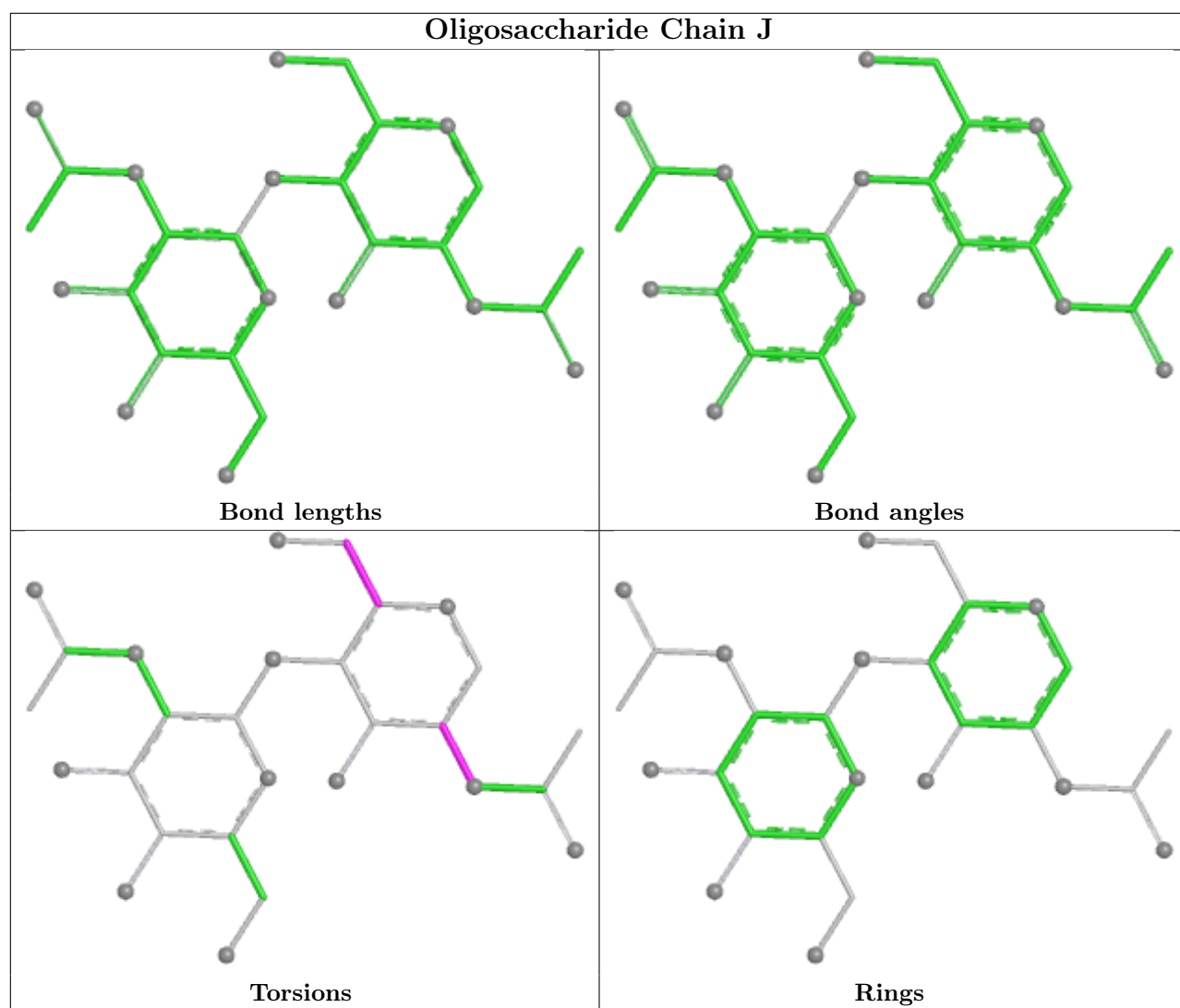


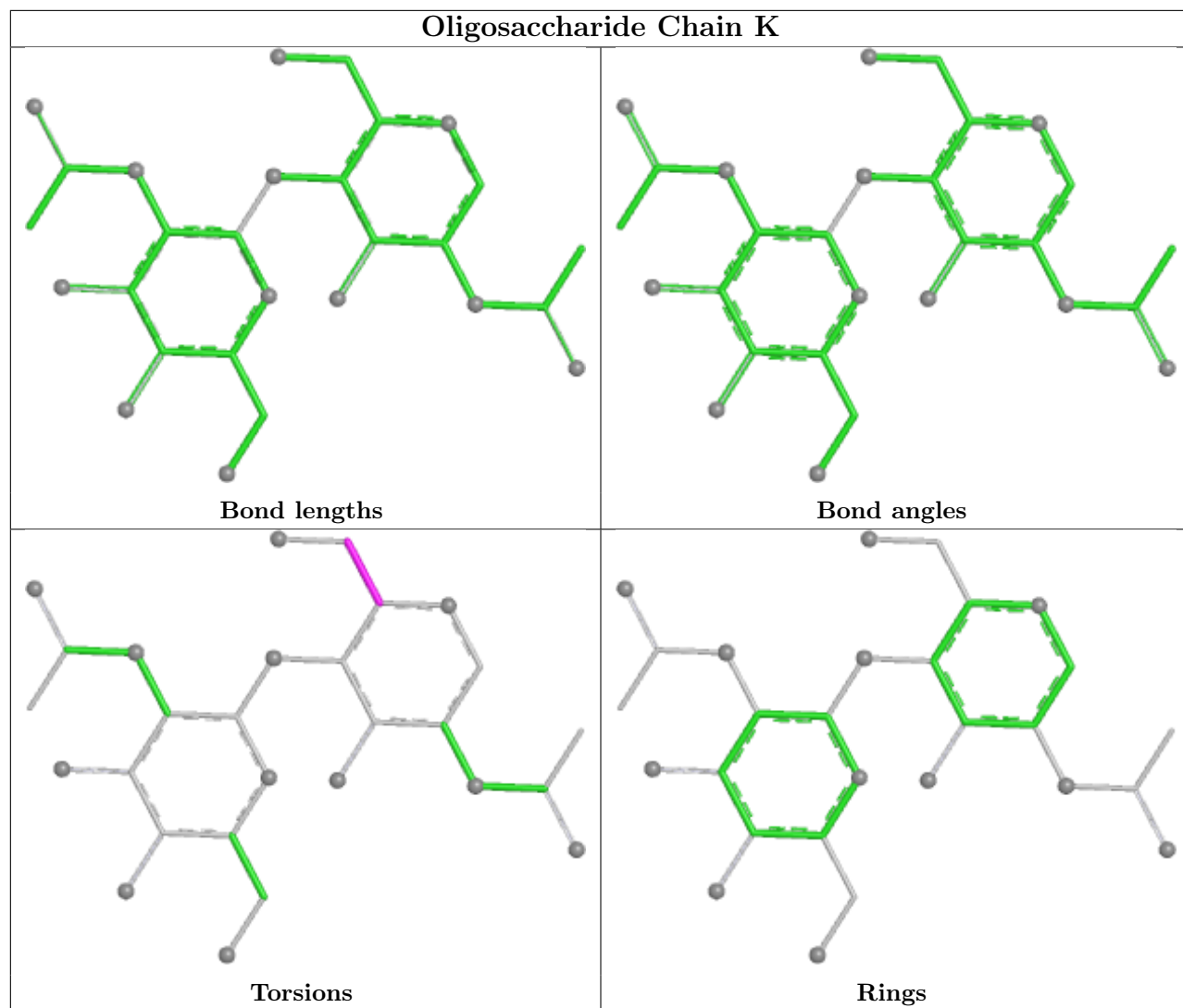


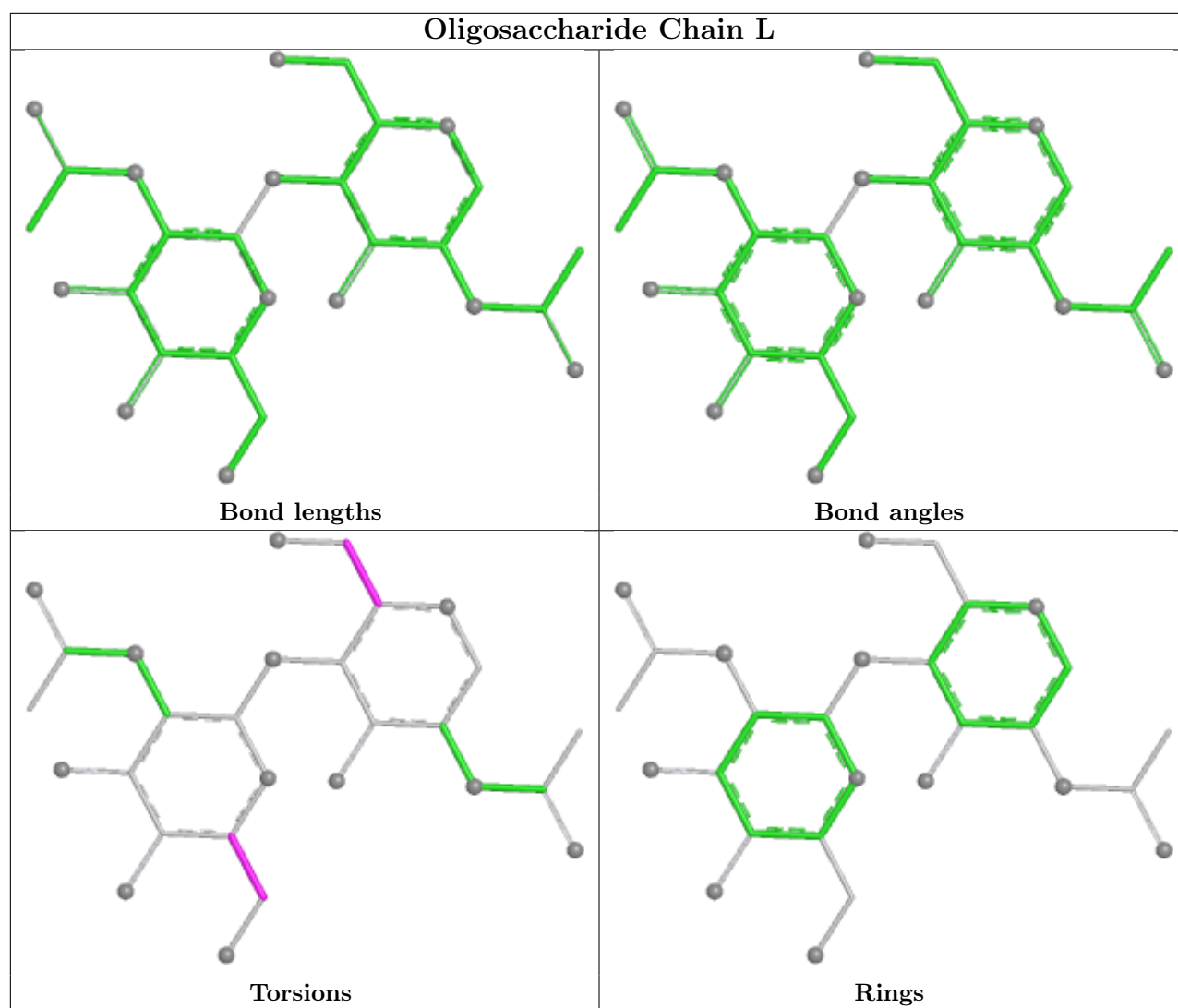


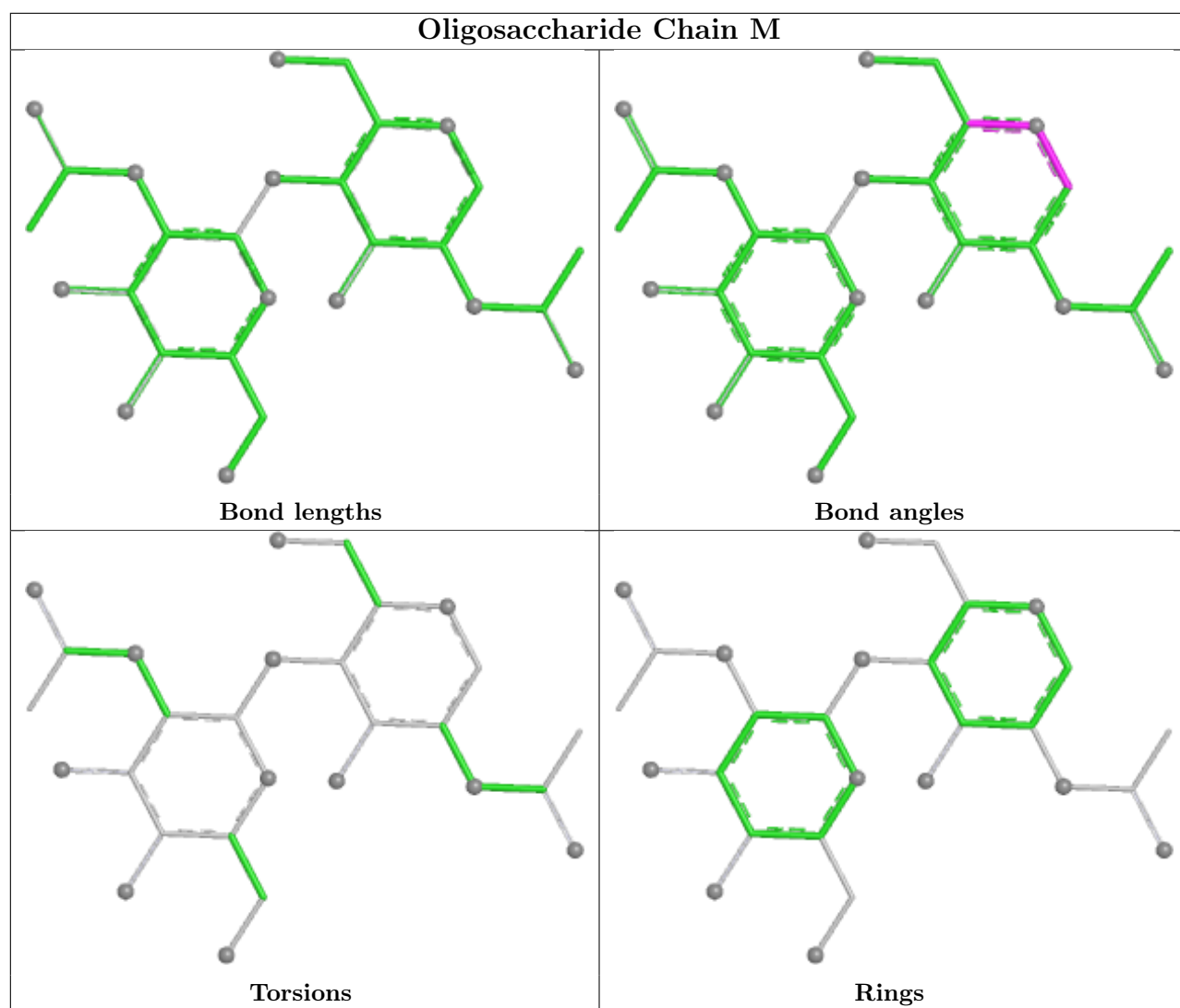


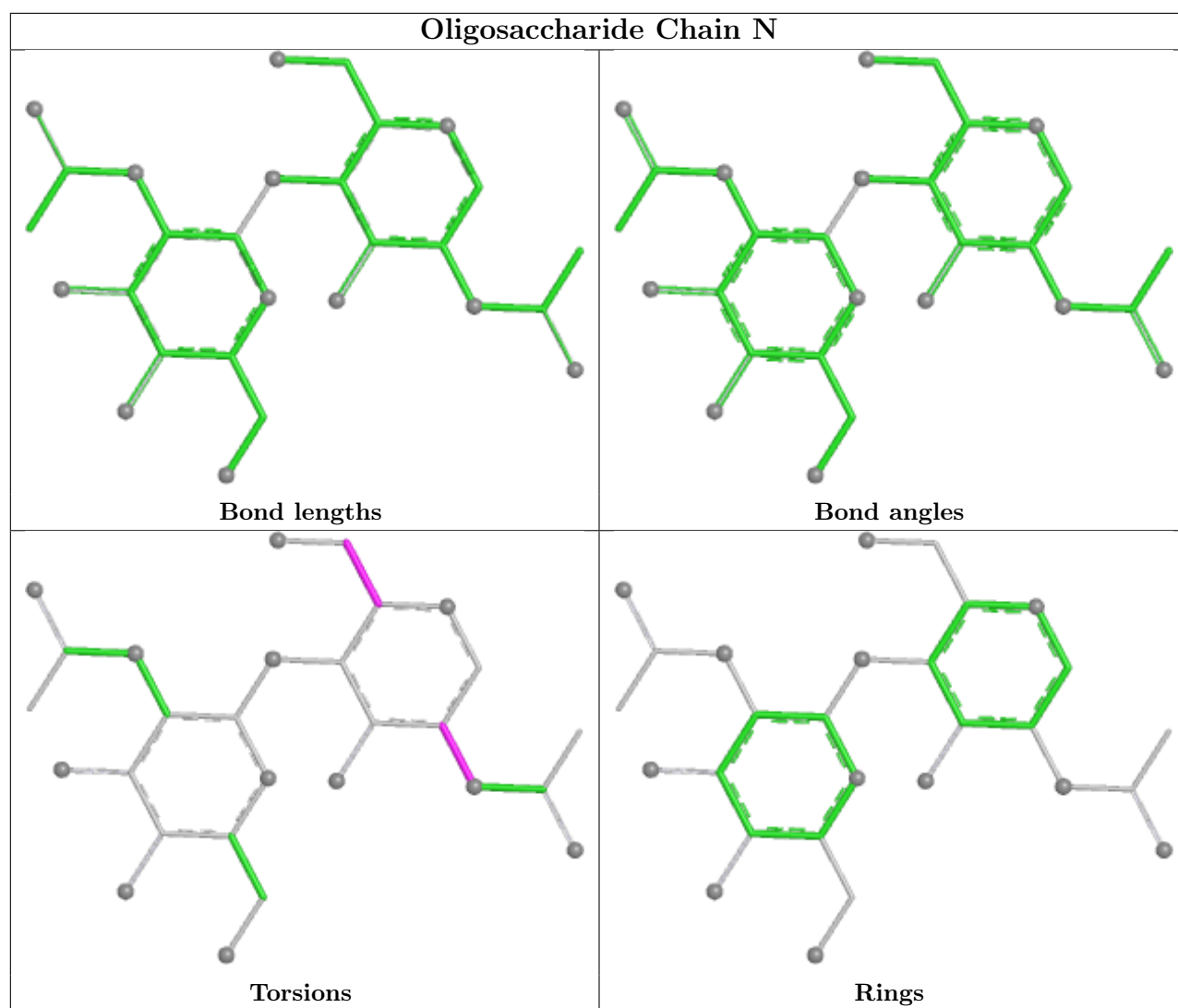


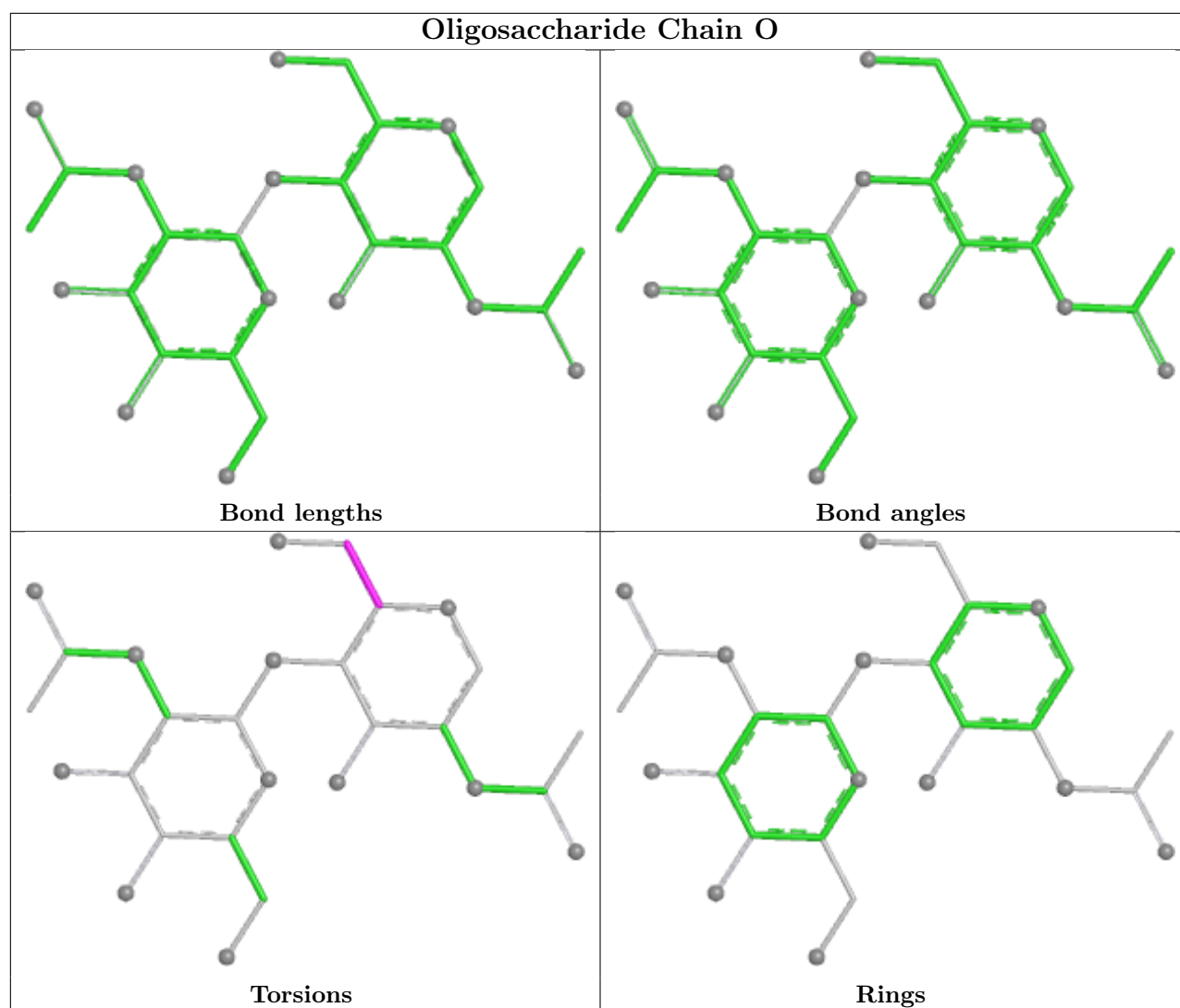












5.6 Ligand geometry [i](#)

33 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	$\# Z > 2$
3	NAG	B	1301	1	14,14,15	0.51	0	17,19,21	0.45	0
3	NAG	C	1301	1	14,14,15	0.51	0	17,19,21	0.45	0
3	NAG	C	1306	1	14,14,15	0.43	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	1309	1	14,14,15	0.34	0	17,19,21	0.46	0
3	NAG	A	1314	1	14,14,15	0.19	0	17,19,21	0.52	0
3	NAG	B	1306	1	14,14,15	0.43	0	17,19,21	0.55	0
3	NAG	C	1308	1	14,14,15	0.40	0	17,19,21	0.46	0
3	NAG	A	1303	1	14,14,15	0.19	0	17,19,21	0.50	0
3	NAG	A	1304	1	14,14,15	0.27	0	17,19,21	0.44	0
3	NAG	B	1303	1	14,14,15	0.20	0	17,19,21	0.50	0
3	NAG	A	1307	1	14,14,15	0.19	0	17,19,21	0.51	0
3	NAG	A	1309	1	14,14,15	0.34	0	17,19,21	0.46	0
3	NAG	A	1306	1	14,14,15	0.44	0	17,19,21	0.55	0
3	NAG	A	1308	1	14,14,15	0.39	0	17,19,21	0.45	0
3	NAG	C	1314	1	14,14,15	0.20	0	17,19,21	0.52	0
3	NAG	C	1309	1	14,14,15	0.34	0	17,19,21	0.46	0
3	NAG	B	1302	1	14,14,15	0.35	0	17,19,21	0.63	1 (5%)
3	NAG	A	1302	1	14,14,15	0.35	0	17,19,21	0.62	1 (5%)
3	NAG	C	1305	1	14,14,15	0.29	0	17,19,21	0.65	1 (5%)
3	NAG	C	1303	1	14,14,15	0.20	0	17,19,21	0.50	0
3	NAG	C	1307	1	14,14,15	0.19	0	17,19,21	0.50	0
3	NAG	C	1319	1	14,14,15	0.41	0	17,19,21	0.44	0
3	NAG	B	1307	1	14,14,15	0.19	0	17,19,21	0.51	0
3	NAG	A	1319	1	14,14,15	0.40	0	17,19,21	0.44	0
3	NAG	B	1305	1	14,14,15	0.28	0	17,19,21	0.66	1 (5%)
3	NAG	B	1304	1	14,14,15	0.27	0	17,19,21	0.44	0
3	NAG	B	1314	1	14,14,15	0.20	0	17,19,21	0.52	0
3	NAG	A	1301	1	14,14,15	0.51	0	17,19,21	0.46	0
3	NAG	A	1305	1	14,14,15	0.28	0	17,19,21	0.65	1 (5%)
3	NAG	C	1302	1	14,14,15	0.34	0	17,19,21	0.63	1 (5%)
3	NAG	B	1308	1	14,14,15	0.40	0	17,19,21	0.46	0
3	NAG	B	1319	1	14,14,15	0.41	0	17,19,21	0.44	0
3	NAG	C	1304	1	14,14,15	0.25	0	17,19,21	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1314	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1314	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1319	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1319	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1314	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1319	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1305	NAG	C1-O5-C5	2.30	115.27	112.19
3	C	1305	NAG	C1-O5-C5	2.27	115.23	112.19
3	A	1305	NAG	C1-O5-C5	2.27	115.23	112.19
3	B	1302	NAG	C1-O5-C5	2.05	114.94	112.19
3	C	1302	NAG	C1-O5-C5	2.05	114.93	112.19

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1303	NAG	O5-C5-C6-O6
3	B	1303	NAG	O5-C5-C6-O6
3	C	1303	NAG	O5-C5-C6-O6
3	A	1301	NAG	C4-C5-C6-O6
3	B	1301	NAG	C4-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1301	NAG	1	0
3	C	1301	NAG	1	0
3	B	1302	NAG	1	0
3	A	1302	NAG	1	0
3	C	1319	NAG	1	0
3	A	1319	NAG	1	0
3	A	1301	NAG	1	0
3	C	1302	NAG	1	0
3	B	1319	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.

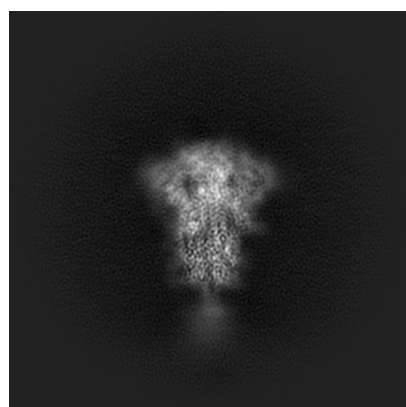
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22078. These allow visual inspection of the internal detail of the map and identification of artifacts.

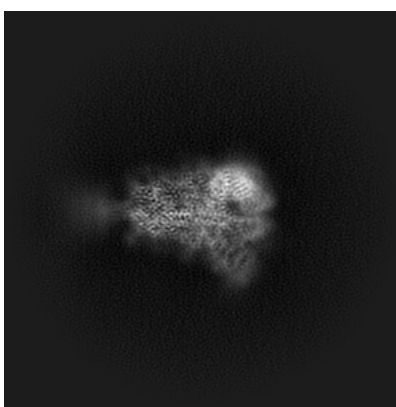
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

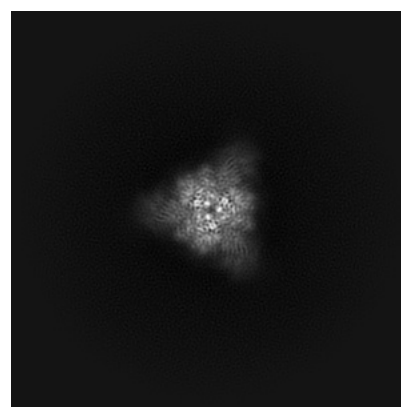
6.1.1 Primary map



X



Y

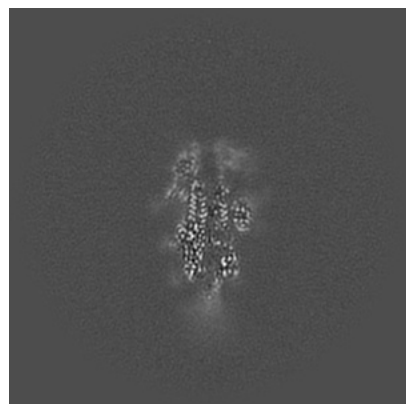


Z

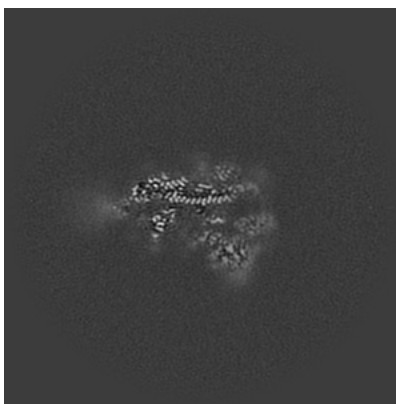
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

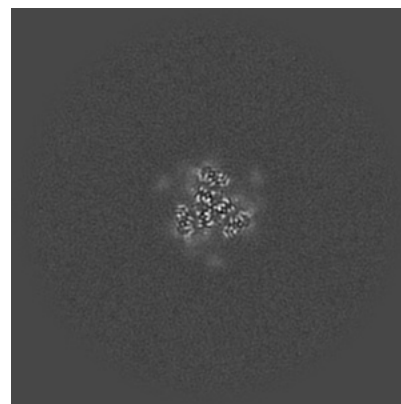
6.2.1 Primary map



X Index: 192



Y Index: 192

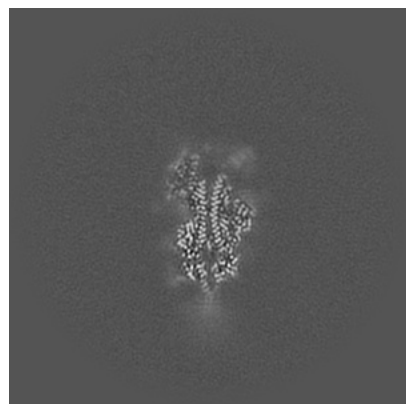


Z Index: 192

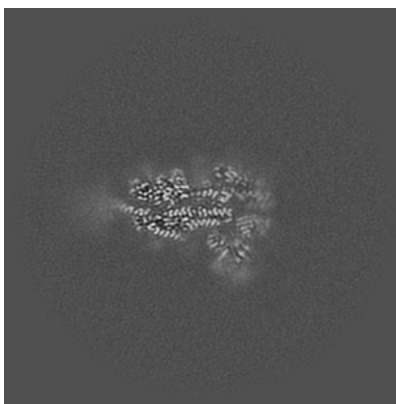
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

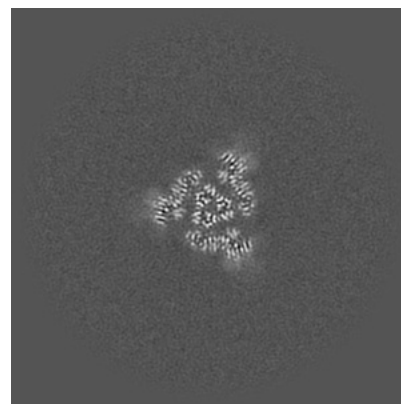
6.3.1 Primary map



X Index: 188



Y Index: 199

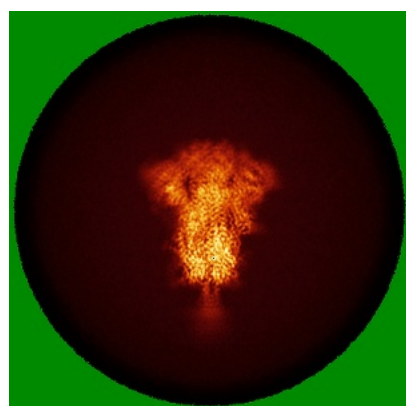


Z Index: 210

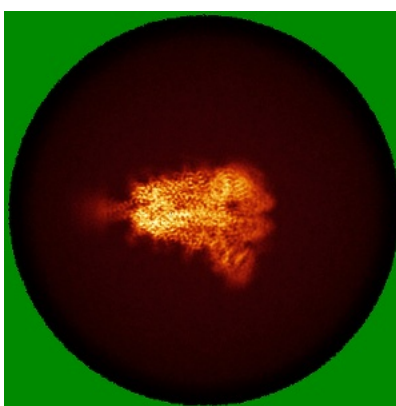
The images above show the largest variance slices of the map in three orthogonal directions.

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

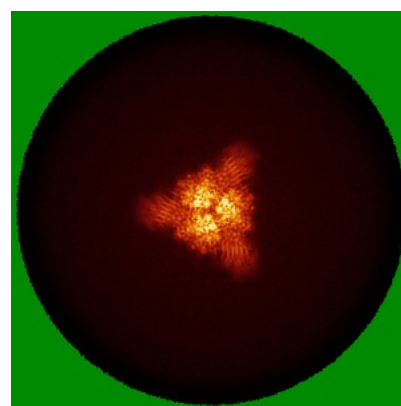
6.4.1 Primary map



X



Y



Z

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

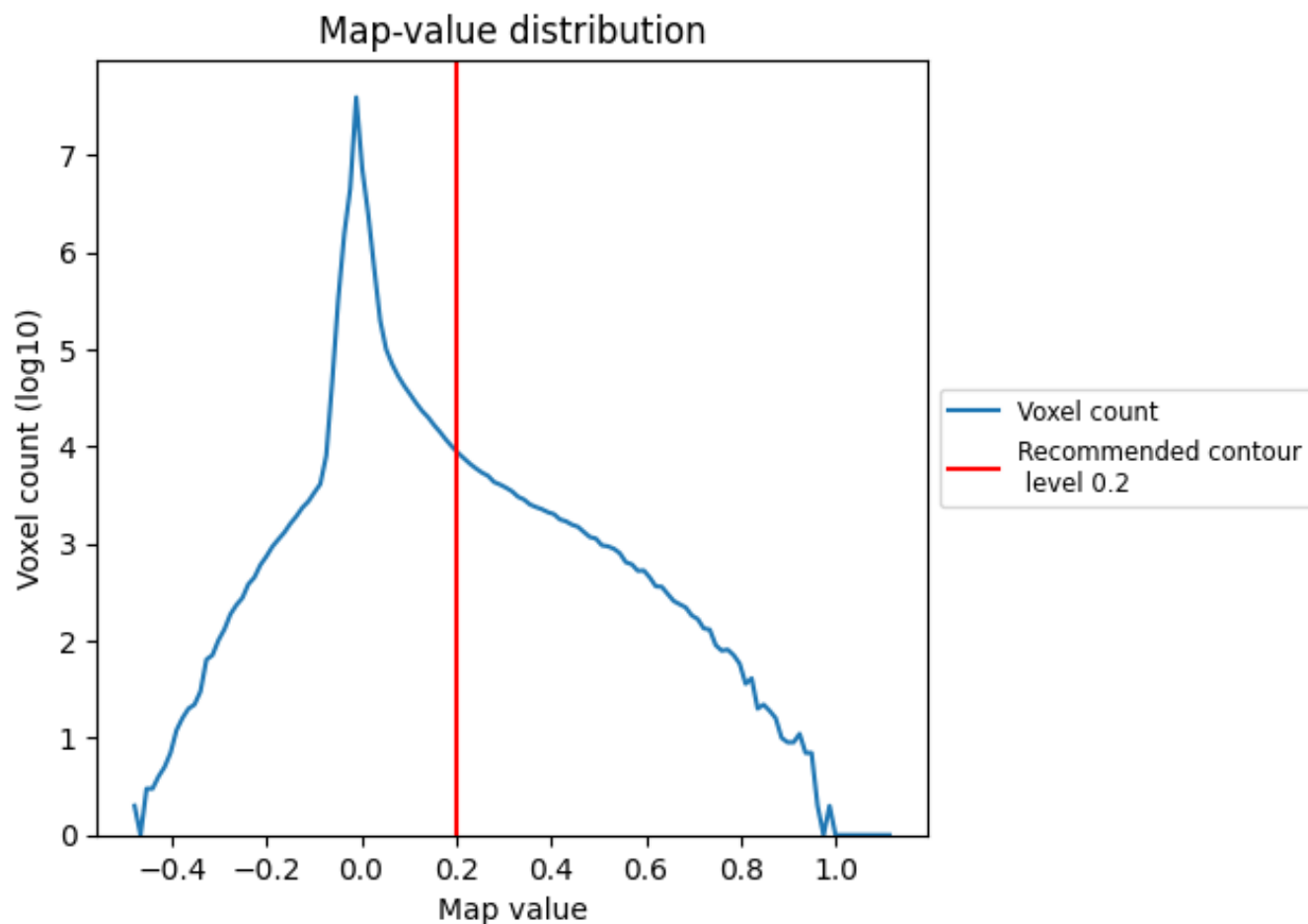
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

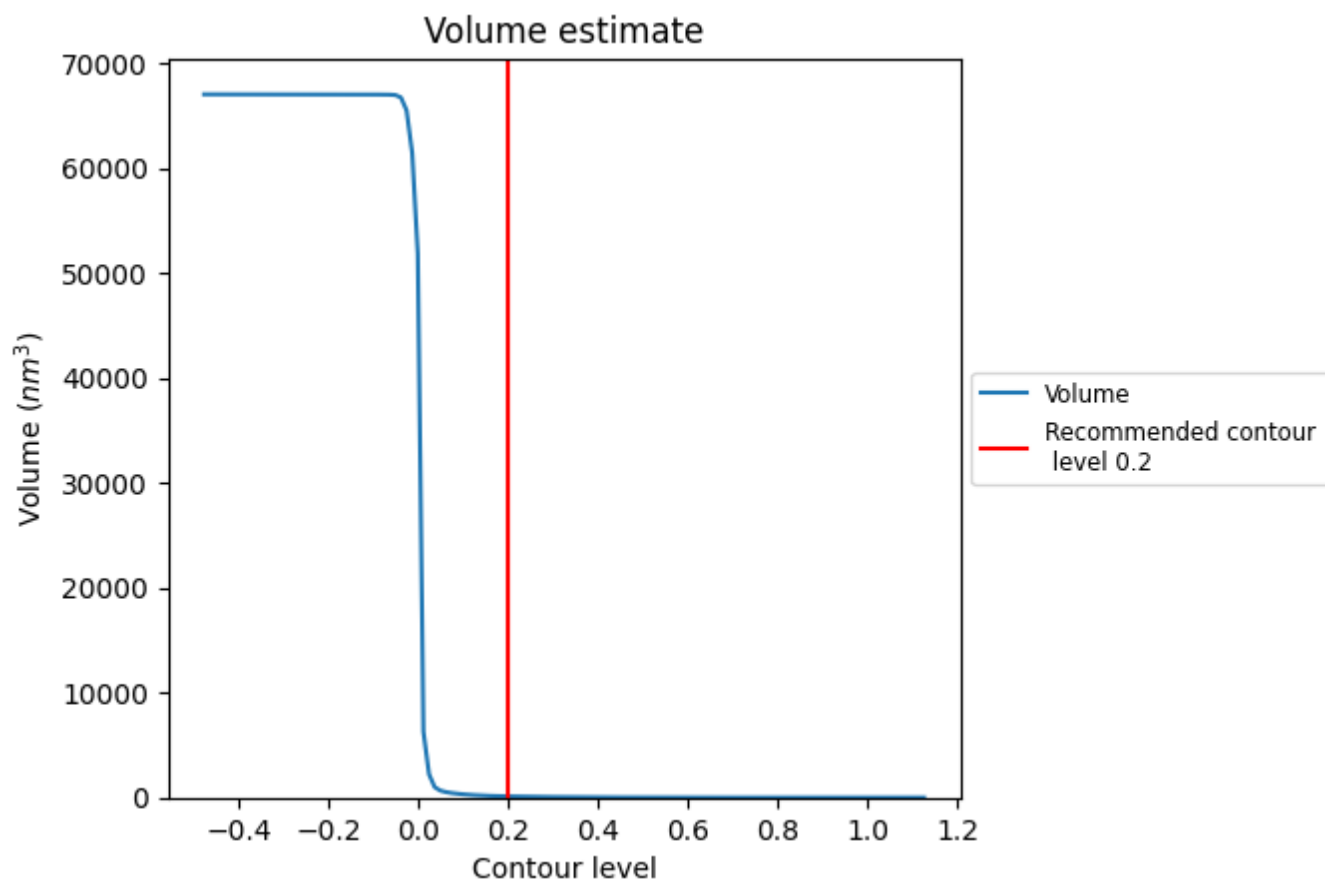
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

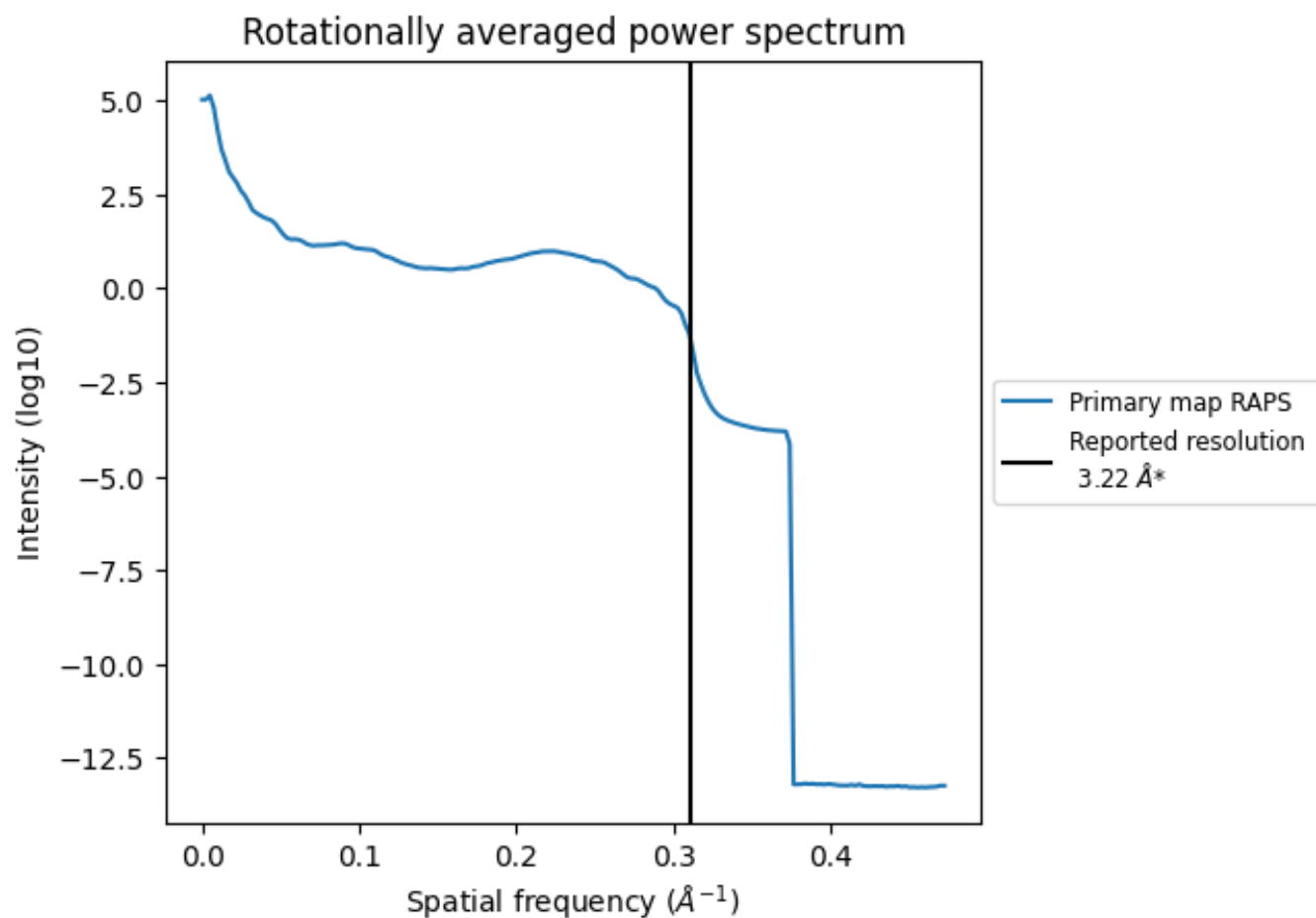
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 111 nm³; this corresponds to an approximate mass of 101 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

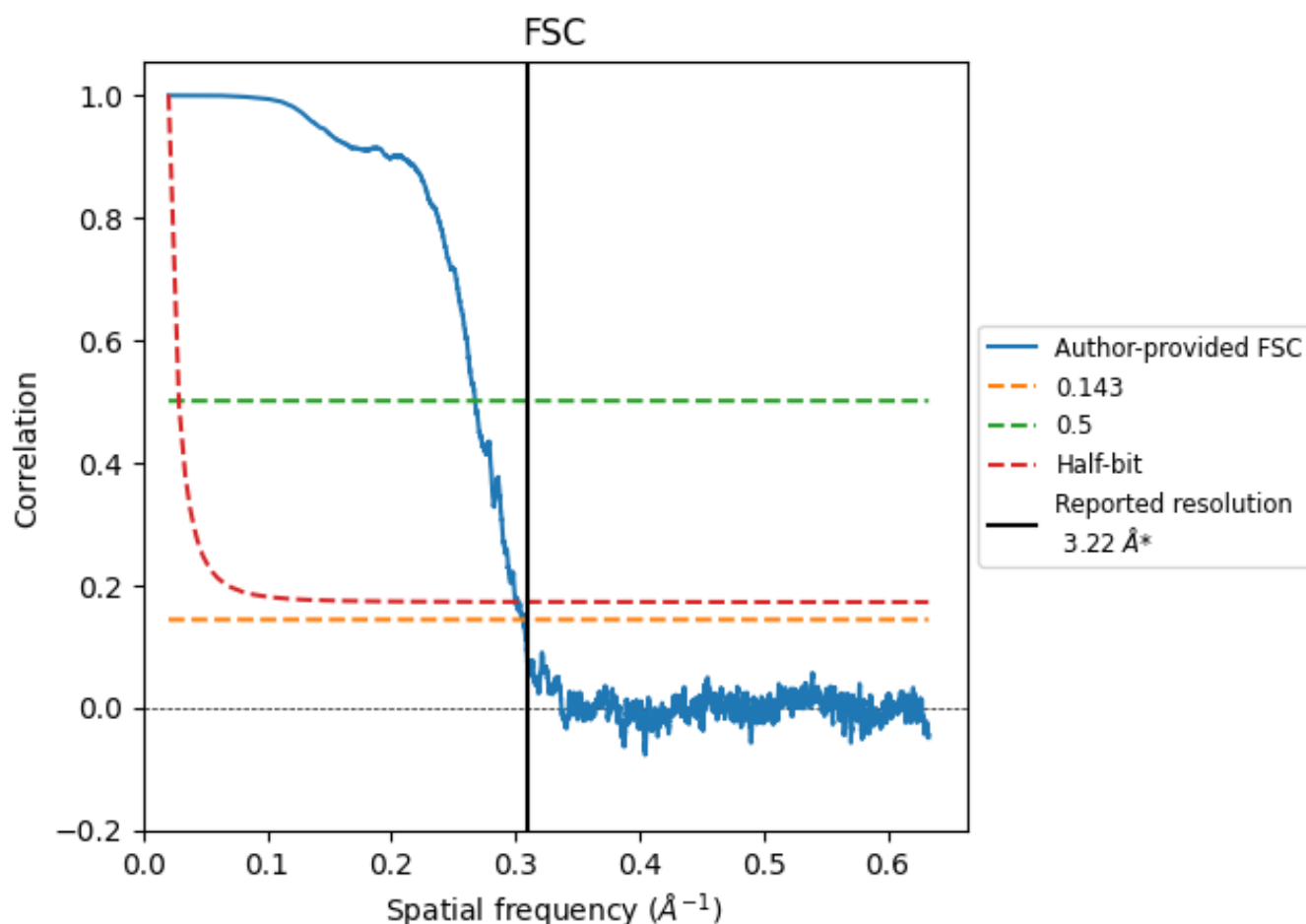


*Reported resolution corresponds to spatial frequency of 0.311 Å⁻¹

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 0.311 Å⁻¹

8.2 Resolution estimates [i](#)

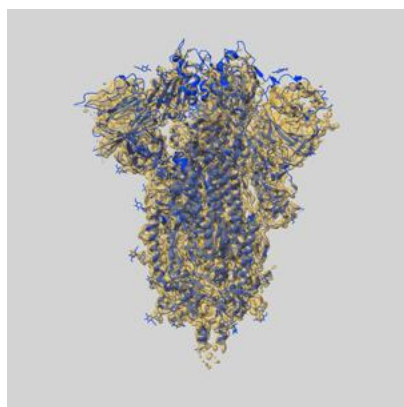
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.22	-	-
Author-provided FSC curve	3.26	3.74	3.33
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

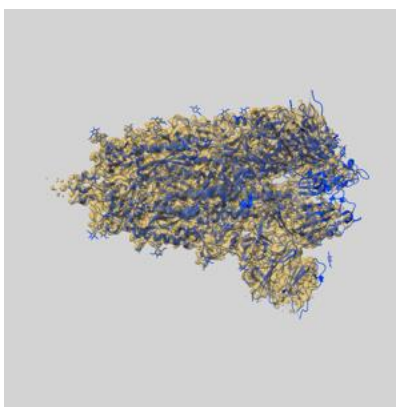
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22078 and PDB model 6X6P. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

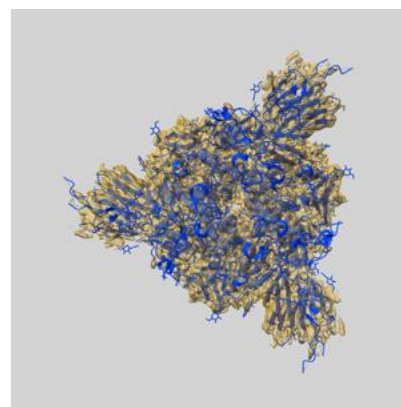
9.1 Map-model overlay [i](#)



X



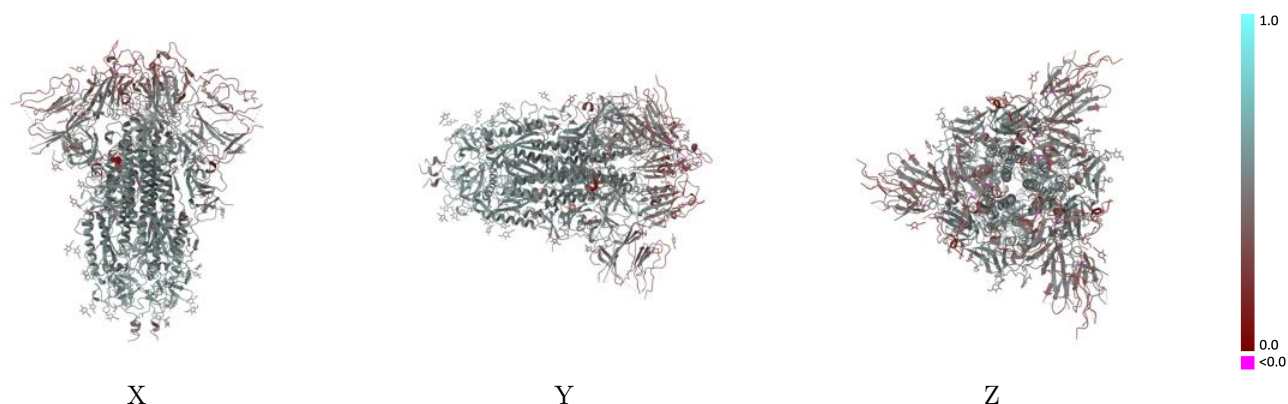
Y



Z

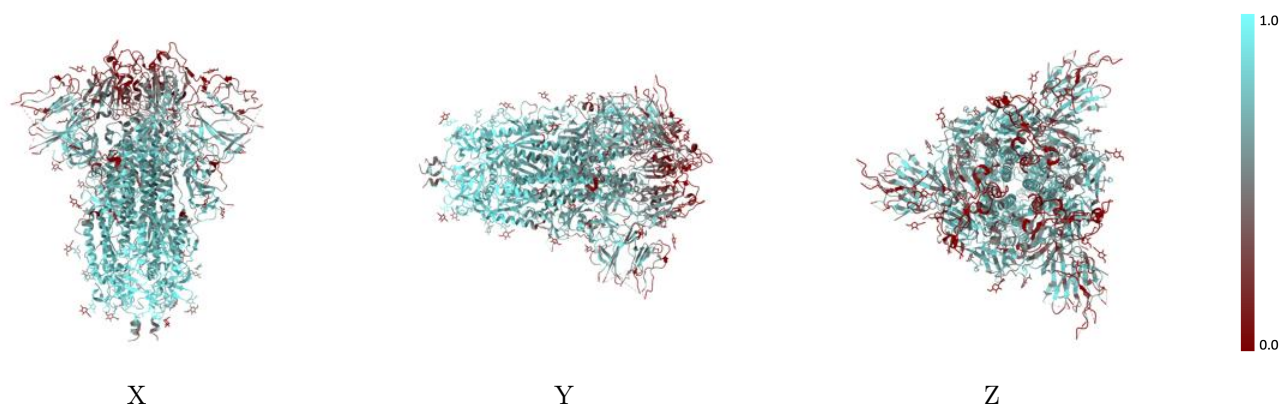
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



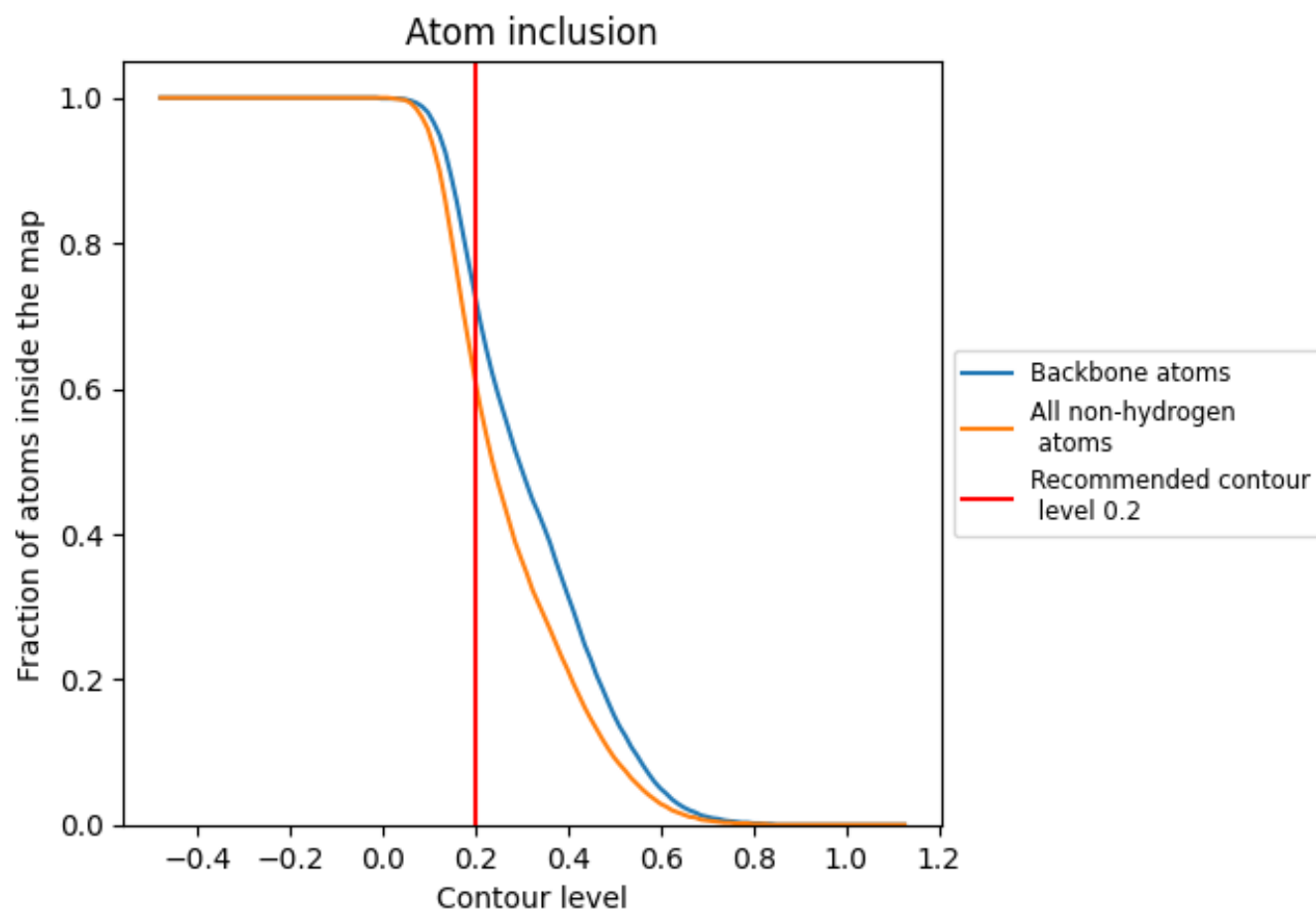
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 61% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6120	0.4690
A	0.6130	0.4690
B	0.6140	0.4690
C	0.6130	0.4690
D	0.6790	0.4900
E	0.4640	0.4690
F	0.5710	0.4940
G	0.5000	0.4600
H	0.6790	0.4810
I	0.4640	0.4760
J	0.4640	0.5030
K	0.5000	0.4420
L	0.6430	0.4980
M	0.4640	0.4830
N	0.5000	0.4910
O	0.5000	0.4590

1.0

0.0

<0.0