



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 04:23 PM UTC

PDB ID : 7MY2 / pdb_00007my2
EMDB ID : EMD-24077
Title : CryoEM structure of neutralizing nanobody Nb30 in complex with SARS-CoV2 spike
Authors : Xu, K.; Kwong, P.D.
Deposited on : 2021-05-20
Resolution : 2.65 Å(reported)
Based on initial model : 6XKL

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:

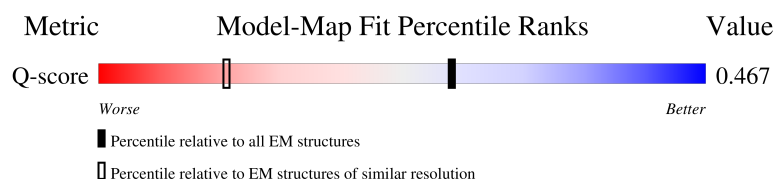
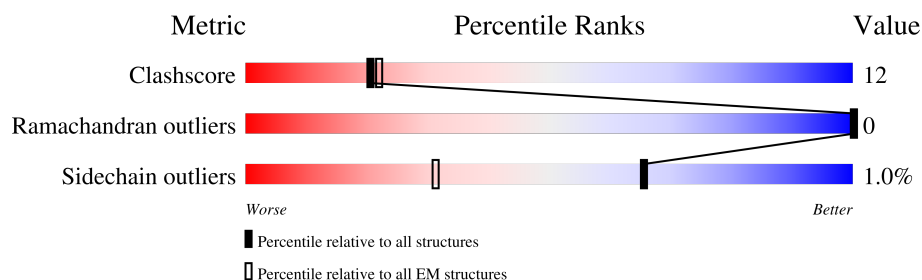
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.65 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	9050 (2.15 - 3.15)

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	B	1288	5% 62% 18% 20%
1	C	1288	9% 60% 20% 19%
1	E	1288	62% 18% 19%
2	A	131	22% 51% 40% 8%

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Mol	Chain	Length	Quality of chain
2	D	131	
2	H	131	
3	F	2	
3	I	2	
3	J	2	
3	K	2	
3	L	2	
3	M	2	
3	N	2	
3	O	2	
3	P	2	
3	Q	2	
3	T	2	
4	G	3	
4	S	3	
4	U	3	
4	V	3	
5	R	2	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 27884 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	B	1036	Total	C	N	O	S	0	0
			8062	5154	1339	1533	36		
1	C	1038	Total	C	N	O	S	0	0
			8083	5168	1344	1535	36		
1	E	1042	Total	C	N	O	S	0	0
			8114	5190	1348	1539	37		

There are 267 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	GLY	-	expression tag	UNP P0DTC2
B	1239	ARG	-	expression tag	UNP P0DTC2
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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	LYS	-	expression tag	UNP P0DTC2
B	1268	GLY	-	expression tag	UNP P0DTC2
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	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
E	682	GLY	ARG	engineered mutation	UNP P0DTC2
E	683	SER	ARG	engineered mutation	UNP P0DTC2
E	685	SER	ARG	engineered mutation	UNP P0DTC2
E	817	PRO	PHE	engineered mutation	UNP P0DTC2
E	892	PRO	ALA	engineered mutation	UNP P0DTC2
E	899	PRO	ALA	engineered mutation	UNP P0DTC2
E	942	PRO	ALA	engineered mutation	UNP P0DTC2
E	986	PRO	LYS	engineered mutation	UNP P0DTC2
E	987	PRO	VAL	engineered mutation	UNP P0DTC2
E	1209	GLY	-	expression tag	UNP P0DTC2
E	1210	SER	-	expression tag	UNP P0DTC2
E	1211	GLY	-	expression tag	UNP P0DTC2
E	1212	TYR	-	expression tag	UNP P0DTC2
E	1213	ILE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1214	PRO	-	expression tag	UNP P0DTC2
E	1215	GLU	-	expression tag	UNP P0DTC2
E	1216	ALA	-	expression tag	UNP P0DTC2
E	1217	PRO	-	expression tag	UNP P0DTC2
E	1218	ARG	-	expression tag	UNP P0DTC2
E	1219	ASP	-	expression tag	UNP P0DTC2
E	1220	GLY	-	expression tag	UNP P0DTC2
E	1221	GLN	-	expression tag	UNP P0DTC2
E	1222	ALA	-	expression tag	UNP P0DTC2
E	1223	TYR	-	expression tag	UNP P0DTC2
E	1224	VAL	-	expression tag	UNP P0DTC2
E	1225	ARG	-	expression tag	UNP P0DTC2
E	1226	LYS	-	expression tag	UNP P0DTC2
E	1227	ASP	-	expression tag	UNP P0DTC2
E	1228	GLY	-	expression tag	UNP P0DTC2
E	1229	GLU	-	expression tag	UNP P0DTC2
E	1230	TRP	-	expression tag	UNP P0DTC2
E	1231	VAL	-	expression tag	UNP P0DTC2
E	1232	LEU	-	expression tag	UNP P0DTC2
E	1233	LEU	-	expression tag	UNP P0DTC2
E	1234	SER	-	expression tag	UNP P0DTC2
E	1235	THR	-	expression tag	UNP P0DTC2
E	1236	PHE	-	expression tag	UNP P0DTC2
E	1237	LEU	-	expression tag	UNP P0DTC2
E	1238	GLY	-	expression tag	UNP P0DTC2
E	1239	ARG	-	expression tag	UNP P0DTC2
E	1240	SER	-	expression tag	UNP P0DTC2
E	1241	LEU	-	expression tag	UNP P0DTC2
E	1242	GLU	-	expression tag	UNP P0DTC2
E	1243	VAL	-	expression tag	UNP P0DTC2
E	1244	LEU	-	expression tag	UNP P0DTC2
E	1245	PHE	-	expression tag	UNP P0DTC2
E	1246	GLN	-	expression tag	UNP P0DTC2
E	1247	GLY	-	expression tag	UNP P0DTC2
E	1248	PRO	-	expression tag	UNP P0DTC2
E	1249	GLY	-	expression tag	UNP P0DTC2
E	1250	HIS	-	expression tag	UNP P0DTC2
E	1251	HIS	-	expression tag	UNP P0DTC2
E	1252	HIS	-	expression tag	UNP P0DTC2
E	1253	HIS	-	expression tag	UNP P0DTC2
E	1254	HIS	-	expression tag	UNP P0DTC2
E	1255	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1256	HIS	-	expression tag	UNP P0DTC2
E	1257	HIS	-	expression tag	UNP P0DTC2
E	1258	SER	-	expression tag	UNP P0DTC2
E	1259	ALA	-	expression tag	UNP P0DTC2
E	1260	TRP	-	expression tag	UNP P0DTC2
E	1261	SER	-	expression tag	UNP P0DTC2
E	1262	HIS	-	expression tag	UNP P0DTC2
E	1263	PRO	-	expression tag	UNP P0DTC2
E	1264	GLN	-	expression tag	UNP P0DTC2
E	1265	PHE	-	expression tag	UNP P0DTC2
E	1266	GLU	-	expression tag	UNP P0DTC2
E	1267	LYS	-	expression tag	UNP P0DTC2
E	1268	GLY	-	expression tag	UNP P0DTC2
E	1269	GLY	-	expression tag	UNP P0DTC2
E	1270	GLY	-	expression tag	UNP P0DTC2
E	1271	SER	-	expression tag	UNP P0DTC2
E	1272	GLY	-	expression tag	UNP P0DTC2
E	1273	GLY	-	expression tag	UNP P0DTC2
E	1274	GLY	-	expression tag	UNP P0DTC2
E	1275	GLY	-	expression tag	UNP P0DTC2
E	1276	SER	-	expression tag	UNP P0DTC2
E	1277	GLY	-	expression tag	UNP P0DTC2
E	1278	GLY	-	expression tag	UNP P0DTC2
E	1279	SER	-	expression tag	UNP P0DTC2
E	1280	ALA	-	expression tag	UNP P0DTC2
E	1281	TRP	-	expression tag	UNP P0DTC2
E	1282	SER	-	expression tag	UNP P0DTC2
E	1283	HIS	-	expression tag	UNP P0DTC2
E	1284	PRO	-	expression tag	UNP P0DTC2
E	1285	GLN	-	expression tag	UNP P0DTC2
E	1286	PHE	-	expression tag	UNP P0DTC2
E	1287	GLU	-	expression tag	UNP P0DTC2
E	1288	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Nanobody Nb30.

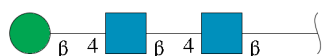
Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	120	Total	C	N	O	S	0	0
			910	571	157	176	6		
2	A	120	Total	C	N	O	S	0	0
			910	571	157	176	6		
2	D	120	Total	C	N	O	S	0	0
			910	571	157	176	6		

- Molecule 3 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
3	F	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	K	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	N	2	Total	C	N	O	0	0
			28	16	2	10		
3	O	2	Total	C	N	O	0	0
			28	16	2	10		
3	P	2	Total	C	N	O	0	0
			28	16	2	10		
3	Q	2	Total	C	N	O	0	0
			28	16	2	10		
3	T	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 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
4	G	3	Total	C	N	O	0	0
			39	22	2	15		
4	S	3	Total	C	N	O	0	0
			39	22	2	15		

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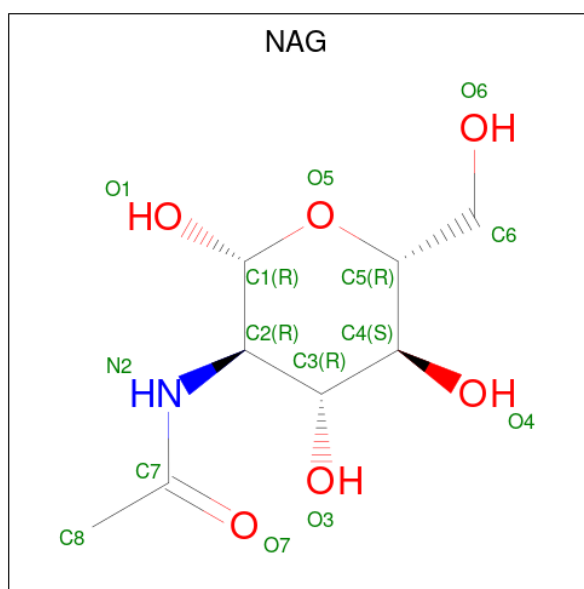
Mol	Chain	Residues	Atoms				AltConf	Trace
4	U	3	Total	C	N	O	0	0
			39	22	2	15		
4	V	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	R	2	Total	C	N	O	0	0
			25	14	1	10		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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

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

[illegible]

- Molecule 1: Spike glycoprotein



N87	PHE	VAL	VAL	VAL	LEU	LEU	PRO	VAL	SER	SER	GLN	CYS	VAL	ASN	LEU	THR	THR	THR	GLN	LEU	PRO	P26	P27	Y28	T29	T33	R34	D53	L54	F55	L56	P57	F58	M61	F65	H66	ALA	ILE	HIS	VAL	SER	GLY	THR	LYS	ARG	F79	V83	T84
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PHE	LEU	MET	ASP	LEU	GLU	GLY	LYS	GLN	GLY	ASN	F186	K187	M188	L189	R190	E191	I201	I203	Y204	S205		T208		L212	V213		Y227	D228	L229	P230	I231	G232	I233	N234	L235	Q239	T240	L241	L242	A243	L244	H245	R246	SER	TYR	LEU	THR	PRO	GLY	ASP	SER	SER	SER	GLY	THR	ALA	GLY
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A262	Y265	Y269	L270	Q271	R273	L276	V289	L293	D294	E295	E298	T299	T302	L303	K304	T315	F318	R319	P322	S325	L326	V327	R328	F329	P330	N331	T332	L333	F338	G339	E340	V341	F342	N343	A344	T345	A348	S349	V350	F351	A352	N353	R354	R355	L356
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[illegible]

A419	D420	Y421	N422	Y423	K424	L425	P426	D427	F428	F429	T430	V431	V433	L434	A435	V436	M437	S438	M439	M440	L441	D442	S443	K444	V445	C446	C447	Y449	M450	Y451	L452	Y453	R454	L455	F456	R457	K458	S459	M460	L461	K462	P463	F464	S465	R466	D467	L468	S469	T470	S471	L472	Y473	Q474	A475	C476	S477	T478	S479	S480	S481	S482	S483	S484	S485	S486	S487	S488	S489	S490	S491	S492	S493	S494	S495	S496	S497	S498	S499	S500	S501	S502	S503	S504	S505	S506	S507	S508	S509	S510	S511	S512	S513	S514	S515	S516	S517	S518	S519	S520	S521	S522	S523	S524	S525	S526	S527	S528	S529	S530	S531	S532	S533	S534	S535	S536	S537	S538	S539	S540	S541	S542	S543	S544	S545	S546	S547	S548	S549	S550	S551	S552	S553	S554	S555	S556	S557	S558	S559	S560	S561	S562	S563	S564	S565	S566	S567	S568	S569	S570	S571	S572	S573	S574	S575	S576	S577	S578	S579	S580	S581	S582	S583	S584	S585	S586	S587	S588	S589	S590	S591	S592	S593	S594	S595	S596	S597	S598	S599	S600	S601	S602	S603	S604	S605	S606	S607	S608	S609	S610	S611	S612	S613	S614	S615	S616	S617	S618	S619	S620	S621	S622	S623	S624	S625	S626	S627	S628	S629	S630	S631	S632	S633	S634	S635	S636	S637	S638	S639	S640	S641	S642	S643	S644	S645	S646	S647	S648	S649	S650	S651	S652	S653	S654	S655	S656	S657	S658	S659	S660	S661	S662	S663	S664	S665	S666	S667	S668	S669	S670	S671	S672	S673	S674	S675	S676	S677	S678	S679	S680	S681	S682	S683	S684	S685	S686	S687	S688	S689	S690	S691	S692	S693	S694	S695	S696	S697	S698	S699	S700	S701	S702	S703	S704	S705	S706	S707	S708	S709	S710	S711	S712	S713	S714	S715	S716	S717	S718	S719	S720	S721	S722	S723	S724	S725	S726	S727	S728	S729	S730	S731	S732	S733	S734	S735	S736	S737	S738	S739	S740	S741	S742	S743	S744	S745	S746	S747	S748	S749	S750	S751	S752	S753	S754	S755	S756	S757	S758	S759	S760	S761	S762	S763	S764	S765	S766	S767	S768	S769	S770	S771	S772	S773	S774	S775	S776	S777	S778	S779	S780	S781	S782	S783	S784	S785	S786	S787	S788	S789	S790	S791	S792	S793	S794	S795	S796	S797	S798	S799	S800	S801	S802	S803	S804	S805	S806	S807	S808	S809	S810	S811	S812	S813	S814	S815	S816	S817	S818	S819	S820	S821	S822	S823	S824	S825	S826	S827	S828	S829	S830	S831	S832	S833	S834	S835	S836	S837	S838	S839	S840	S841	S842	S843	S844	S845	S846	S847	S848	S849	S850	S851	S852	S853	S854	S855	S856	S857	S858	S859	S860	S861	S862	S863	S864	S865	S866	S867	S868	S869	S870	S871	S872	S873	S874	S875	S876	S877	S878	S879	S880	S881	S882	S883	S884	S885	S886	S887	S888	S889	S890	S891	S892	S893	S894	S895	S896	S897	S898	S899	S900	S901	S902	S903	S904	S905	S906	S907	S908	S909	S910	S911	S912	S913	S914	S915	S916	S917	S918	S919	S920	S921	S922	S923	S924	S925	S926	S927	S928	S929	S930	S931	S932	S933	S934	S935	S936	S937	S938	S939	S940	S941	S942	S943	S944	S945	S946	S947	S948	S949	S950	S951	S952	S953	S954	S955	S956	S957	S958	S959	S960	S961	S962	S963	S964	S965	S966	S967	S968	S969	S970	S971	S972	S973	S974	S975	S976	S977	S978	S979	S980	S981	S982	S983	S984	S985	S986	S987	S988	S989	S990	S991	S992	S993	S994	S995	S996	S997	S998	S999	S1000
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C480	M481	G482	V483	E484	G485	F486	M487	C488	F489	F490	P491	L492	Q493	S494	Y495	Q496	F497		Q498	P499	T500	N501	G502	V503	V503	G504	Y505	Q506	P507		Y508	R509	V510	V511	V512		L513	S514	F515	F516	L517	L518	H519	A520	P521	A522		T523	V524	C525	G526	P527	K528		C538	Y539		N542	F543	N544	G545	L546		S555
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I560	P561	F562	D578	P579	Q580	I584	S605	N606	C617	A623	D627	T632	V633	V642	I651	Q675	THR	GLN	THR	ASN	SER	PRO	PRO	GLY	SER	ALA	SER	SER	VAL	ALA	SER	Q690	V729	M740	L752	Q755	L767	K776	E780	S803
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P807	K314	R815	S816	P817	D820	L821	L828	A830	ASP	ALA	GLY	GLY	PHE	ILE	ILE	LYS	GLN	TYR	ASP	GLY	ASP	CYS	LEU	GLY	A852	Q853	G857	I870	Y873	T874		T883	F888	P892		Q895	T896	P897	F898	P899	M900	Q901		Y904	P905
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V915	L916	K921	T934	G935	D936	S937	L938	S939	S940	S943	A944	L945	L984	D985	P986	E988	A989	T993	D994	T998	C1043	G1059	H1064	P1069	K1073	H1088	R1091	T1100	H1101	V1104	T1115	D1118	K1119	T1120	K1149	GLU	GLU	LEU	LEU
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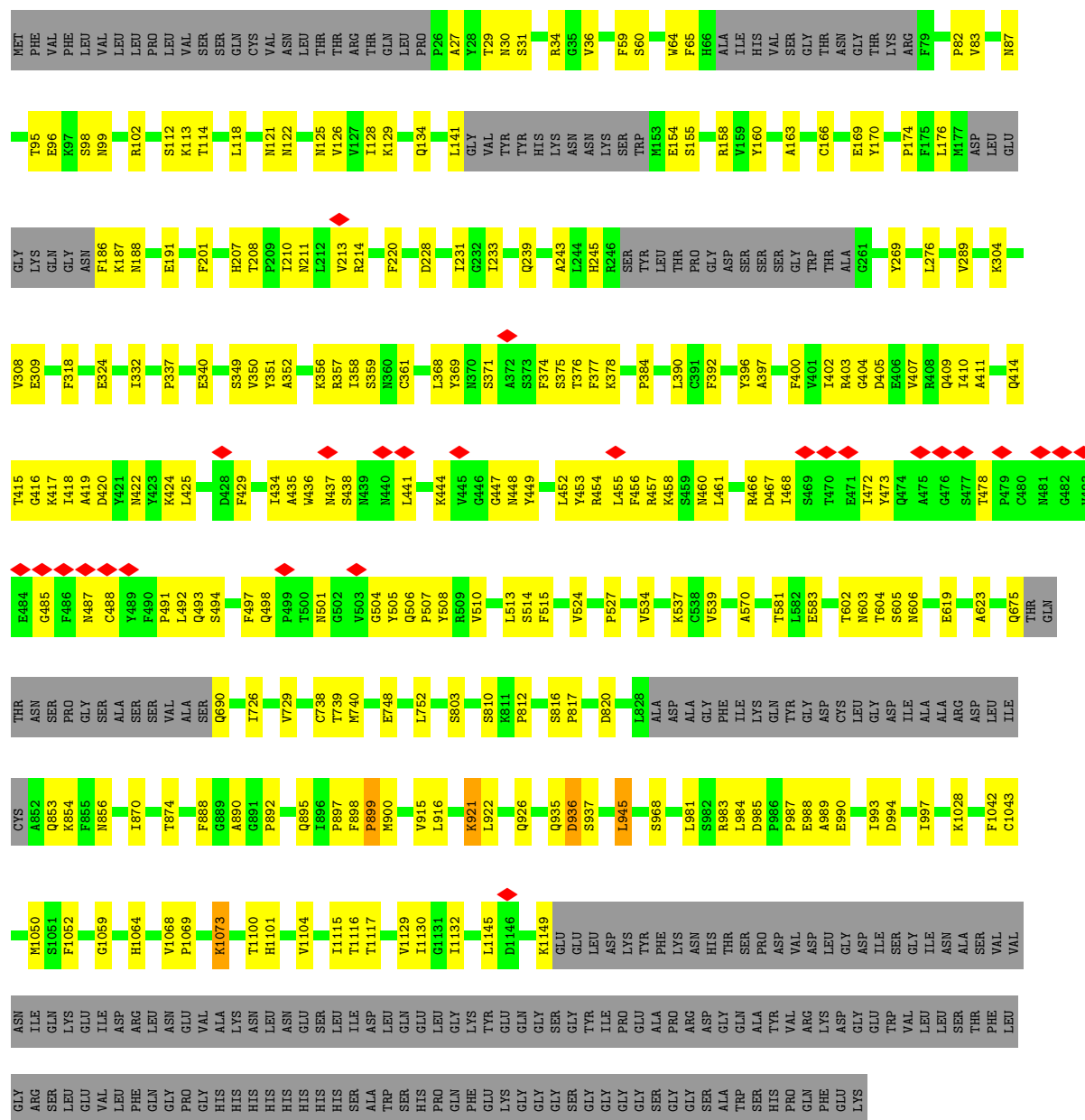
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PRO GLU ALA PRO ARG ASP GLY GLN TYR ALA VAL ARG LYS ASP GLY GLU TRP VAL LEU LEU SER SER THR PHE PHE LEU LEU GLY ARG SER LEU LEU VAL LEU PHE GLN GLY PRO PRO GLY HIS HIS HIS HIS HIS HIS HIS SER ALA TRP TRP SER HIS PRO GLN PHE PHE GLU GLY LYS GLY GLY GLY GLY

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

- Molecule 1: Spike glycoprotein

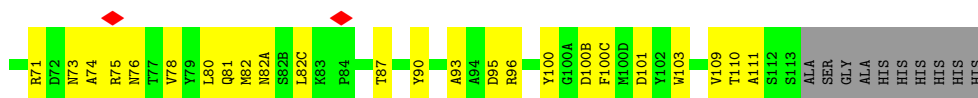
Chain E:  62% 18% 19%



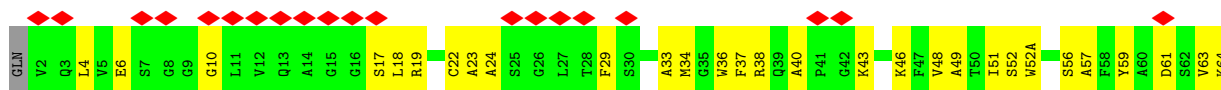
- Molecule 2: Nanobody Nb30

Chain H:  8% 47% 44% 8%

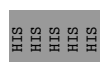
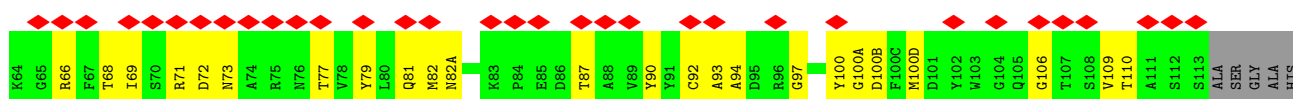




• Molecule 2: Nanobody Nb30



• Molecule 2: Nanobody Nb30



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



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



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





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

Chain K:  100%



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

Chain L:  100%



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

Chain M:  100%



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

Chain N:  100%



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

Chain O:  100%



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

Chain P:  100%



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

Chain Q:  100%



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

Chain T:  50% 50%



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

Chain G:  100%



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

Chain S:  100%



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

Chain U:  100%



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

Chain V:  100%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  100%

MOL
EMD

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	333232	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 ($e^-/\text{\AA}^2$)	40.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.098	Depositor
Minimum map value	-0.807	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	513.0, 513.0, 513.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.855, 0.855, 0.855	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	B	0.43	8/8251 (0.1%)	0.53	2/11238 (0.0%)
1	C	0.47	10/8273 (0.1%)	0.57	3/11268 (0.0%)
1	E	0.46	9/8305 (0.1%)	0.54	4/11310 (0.0%)
2	A	0.15	0/930	0.41	0/1254
2	D	0.14	0/930	0.40	0/1254
2	H	0.15	0/930	0.46	0/1254
All	All	0.43	27/27619 (0.1%)	0.54	9/37578 (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	B	0	1
1	C	0	1
All	All	0	2

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	899	PRO	C-O	-7.52	1.14	1.24
1	E	897	PRO	C-O	-7.39	1.15	1.23
1	C	897	PRO	C-O	-7.36	1.15	1.23
1	C	899	PRO	C-O	-7.30	1.15	1.24
1	E	899	PRO	C-O	-7.16	1.15	1.24

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	941	THR	CB-CA-C	9.16	121.78	109.42
1	C	897	PRO	N-CA-CB	-7.75	96.41	103.31
1	C	904	TYR	CB-CA-C	-6.67	96.78	110.38
1	E	897	PRO	N-CA-CB	-6.04	97.93	103.31
1	C	888	PHE	CA-CB-CG	5.81	119.61	113.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	122	ASN	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	B	8062	0	7839	190	0
1	C	8083	0	7857	184	0
1	E	8114	0	7889	167	0
2	A	910	0	864	47	0
2	D	910	0	864	45	0
2	H	910	0	864	49	0
3	F	28	0	25	0	0
3	I	28	0	25	0	0
3	J	28	0	25	1	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	0	0
3	N	28	0	25	0	0
3	O	28	0	25	0	0
3	P	28	0	25	0	0
3	Q	28	0	25	0	0
3	T	28	0	25	1	0
4	G	39	0	34	0	0
4	S	39	0	34	0	0
4	U	39	0	34	0	0
4	V	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	R	25	0	22	0	0
6	B	140	0	130	1	0
6	C	140	0	130	3	0
6	E	126	0	117	0	0
All	All	27884	0	26987	665	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 12.

The worst 5 of 665 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:E:402:ILE:O	1:E:507:PRO:HA	1.49	1.11
2:D:90:TYR:O	2:D:106:GLY:HA2	1.58	1.01
1:B:434:ILE:O	1:B:510:VAL:HA	1.64	0.98
1:E:411:ALA:HB3	1:E:414:GLN:HB3	1.55	0.88
1:B:318:PHE:HZ	1:B:615:VAL:HG21	1.41	0.86

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	B	1022/1288 (79%)	951 (93%)	71 (7%)	0	100	100
1	C	1024/1288 (80%)	947 (92%)	77 (8%)	0	100	100
1	E	1028/1288 (80%)	966 (94%)	62 (6%)	0	100	100
2	A	118/131 (90%)	106 (90%)	12 (10%)	0	100	100
2	D	118/131 (90%)	106 (90%)	12 (10%)	0	100	100
2	H	118/131 (90%)	112 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3428/4257 (80%)	3188 (93%)	240 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	B	898/1116 (80%)	893 (99%)	5 (1%)	78	88
1	C	900/1116 (81%)	884 (98%)	16 (2%)	51	72
1	E	903/1116 (81%)	893 (99%)	10 (1%)	65	80
2	A	92/100 (92%)	92 (100%)	0	100	100
2	D	92/100 (92%)	92 (100%)	0	100	100
2	H	92/100 (92%)	92 (100%)	0	100	100
All	All	2977/3648 (82%)	2946 (99%)	31 (1%)	65	81

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	936	ASP
1	E	935	GLN
1	C	940	SER
1	E	945	LEU
1	E	915	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	901	GLN
1	E	1011	GLN
1	E	207	HIS
1	E	751	ASN
1	E	188	ASN

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 ⓘ

36 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	$\# Z > 2$
3	NAG	F	1	3,1	14,14,15	0.21	0	17,19,21	0.53	0
3	NAG	F	2	3	14,14,15	0.20	0	17,19,21	0.45	0
4	NAG	G	1	4,1	14,14,15	0.23	0	17,19,21	0.51	0
4	NAG	G	2	4	14,14,15	0.24	0	17,19,21	0.48	0
4	BMA	G	3	4	11,11,12	0.56	0	15,15,17	0.64	0
3	NAG	I	1	3,1	14,14,15	0.24	0	17,19,21	0.47	0
3	NAG	I	2	3	14,14,15	0.20	0	17,19,21	0.47	0
3	NAG	J	1	3,1	14,14,15	0.43	0	17,19,21	0.46	0
3	NAG	J	2	3	14,14,15	0.30	0	17,19,21	0.53	0
3	NAG	K	1	3,1	14,14,15	0.17	0	17,19,21	0.45	0
3	NAG	K	2	3	14,14,15	0.19	0	17,19,21	0.48	0
3	NAG	L	1	3,1	14,14,15	0.25	0	17,19,21	0.54	0
3	NAG	L	2	3	14,14,15	0.19	0	17,19,21	0.43	0
3	NAG	M	1	3,1	14,14,15	0.21	0	17,19,21	0.51	0
3	NAG	M	2	3	14,14,15	0.20	0	17,19,21	0.45	0
3	NAG	N	1	3,1	14,14,15	0.24	0	17,19,21	0.50	0
3	NAG	N	2	3	14,14,15	0.19	0	17,19,21	0.51	0
3	NAG	O	1	3,1	14,14,15	0.16	0	17,19,21	0.48	0
3	NAG	O	2	3	14,14,15	0.22	0	17,19,21	0.46	0
3	NAG	P	1	3,1	14,14,15	0.33	0	17,19,21	0.61	0
3	NAG	P	2	3	14,14,15	0.29	0	17,19,21	0.53	0
3	NAG	Q	1	3,1	14,14,15	0.16	0	17,19,21	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	Q	2	3	14,14,15	0.20	0	17,19,21	0.44	0
5	NAG	R	1	5,1	14,14,15	0.29	0	17,19,21	0.49	0
5	BMA	R	2	5	11,11,12	0.58	0	15,15,17	0.62	0
4	NAG	S	1	4,1	14,14,15	0.26	0	17,19,21	0.50	0
4	NAG	S	2	4	14,14,15	0.26	0	17,19,21	0.46	0
4	BMA	S	3	4	11,11,12	0.54	0	15,15,17	0.69	0
3	NAG	T	1	3,1	14,14,15	0.28	0	17,19,21	0.53	0
3	NAG	T	2	3	14,14,15	0.45	0	17,19,21	1.34	2 (11%)
4	NAG	U	1	4,1	14,14,15	0.22	0	17,19,21	0.52	0
4	NAG	U	2	4	14,14,15	0.18	0	17,19,21	0.47	0
4	BMA	U	3	4	11,11,12	0.56	0	15,15,17	0.73	0
4	NAG	V	1	4,1	14,14,15	0.35	0	17,19,21	0.51	0
4	NAG	V	2	4	14,14,15	0.22	0	17,19,21	0.45	0
4	BMA	V	3	4	11,11,12	0.65	0	15,15,17	0.97	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	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	NAG	L	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	NAG	M	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
3	NAG	N	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1
3	NAG	O	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	P	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	P	2	3	-	3/6/23/26	0/1/1/1
3	NAG	Q	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	0/6/23/26	0/1/1/1
5	NAG	R	1	5,1	-	2/6/23/26	0/1/1/1
5	BMA	R	2	5	-	0/2/19/22	0/1/1/1
4	NAG	S	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	2/6/23/26	0/1/1/1
4	BMA	S	3	4	-	2/2/19/22	0/1/1/1
3	NAG	T	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	T	2	3	-	6/6/23/26	0/1/1/1
4	NAG	U	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	U	2	4	-	0/6/23/26	0/1/1/1
4	BMA	U	3	4	-	2/2/19/22	0/1/1/1
4	NAG	V	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	V	2	4	-	1/6/23/26	0/1/1/1
4	BMA	V	3	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	2	NAG	C2-N2-C7	4.60	129.07	122.90
3	T	2	NAG	C1-C2-N2	2.11	113.77	110.43

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

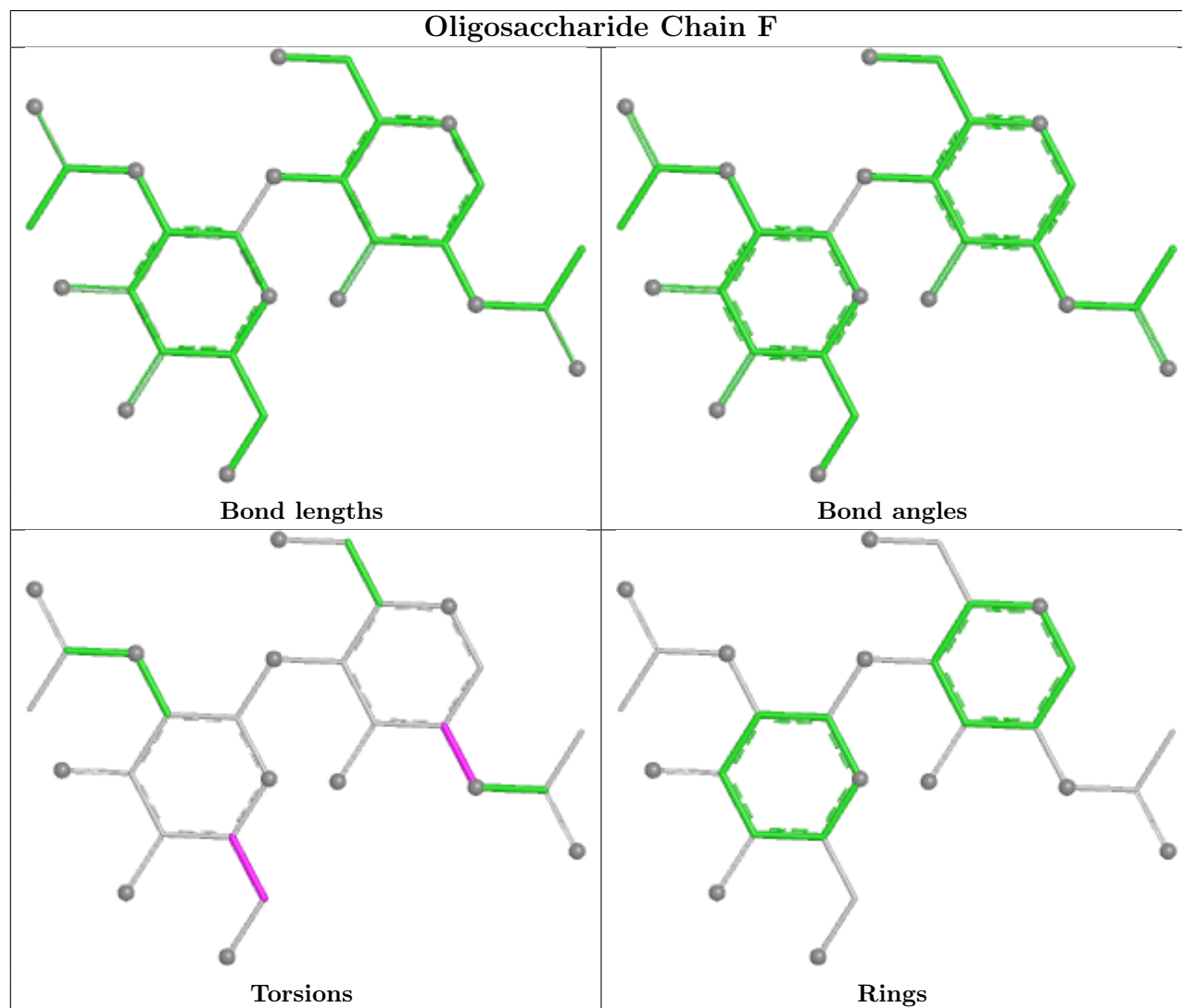
Mol	Chain	Res	Type	Atoms
3	J	1	NAG	C4-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
4	U	3	BMA	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6

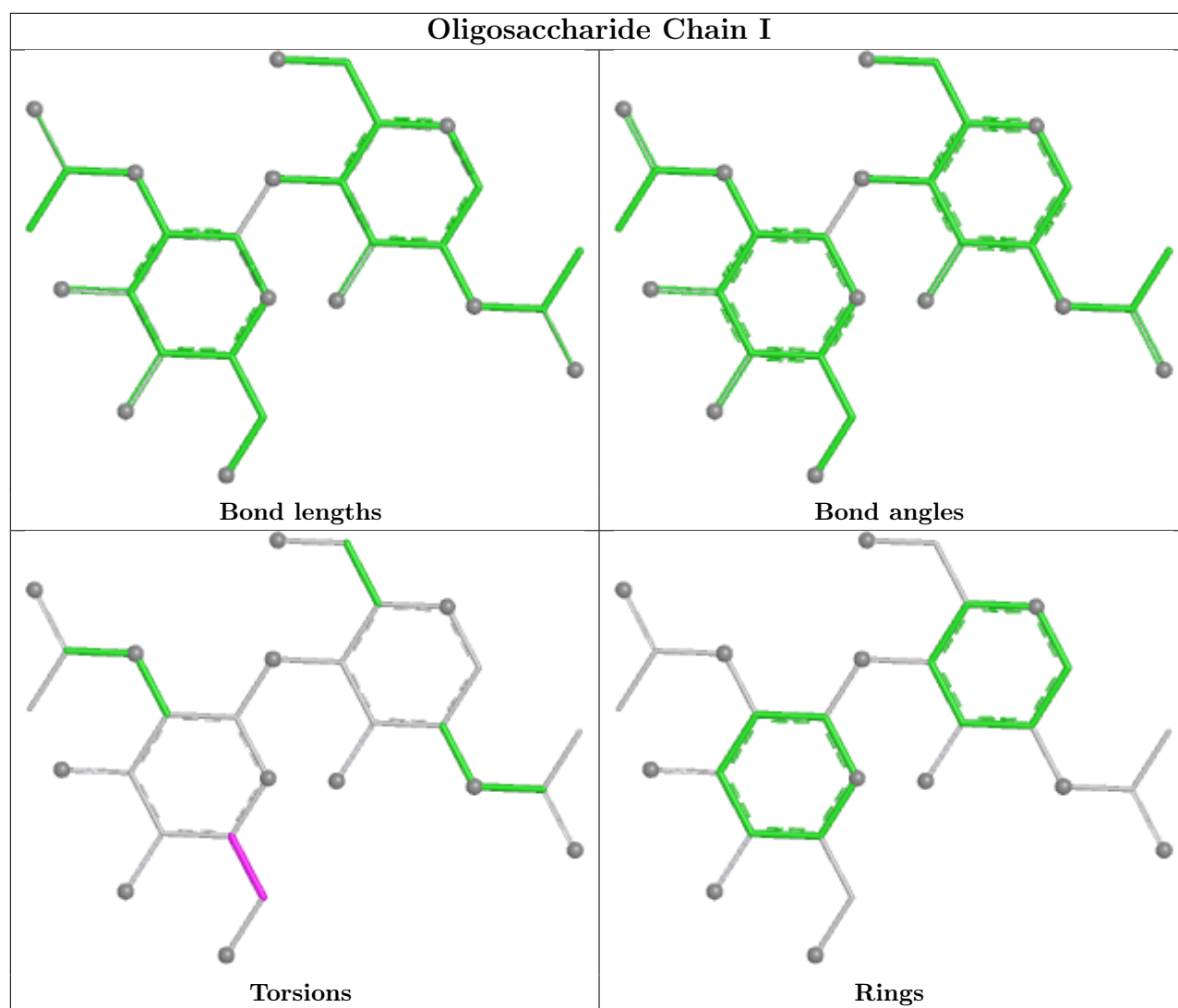
There are no ring outliers.

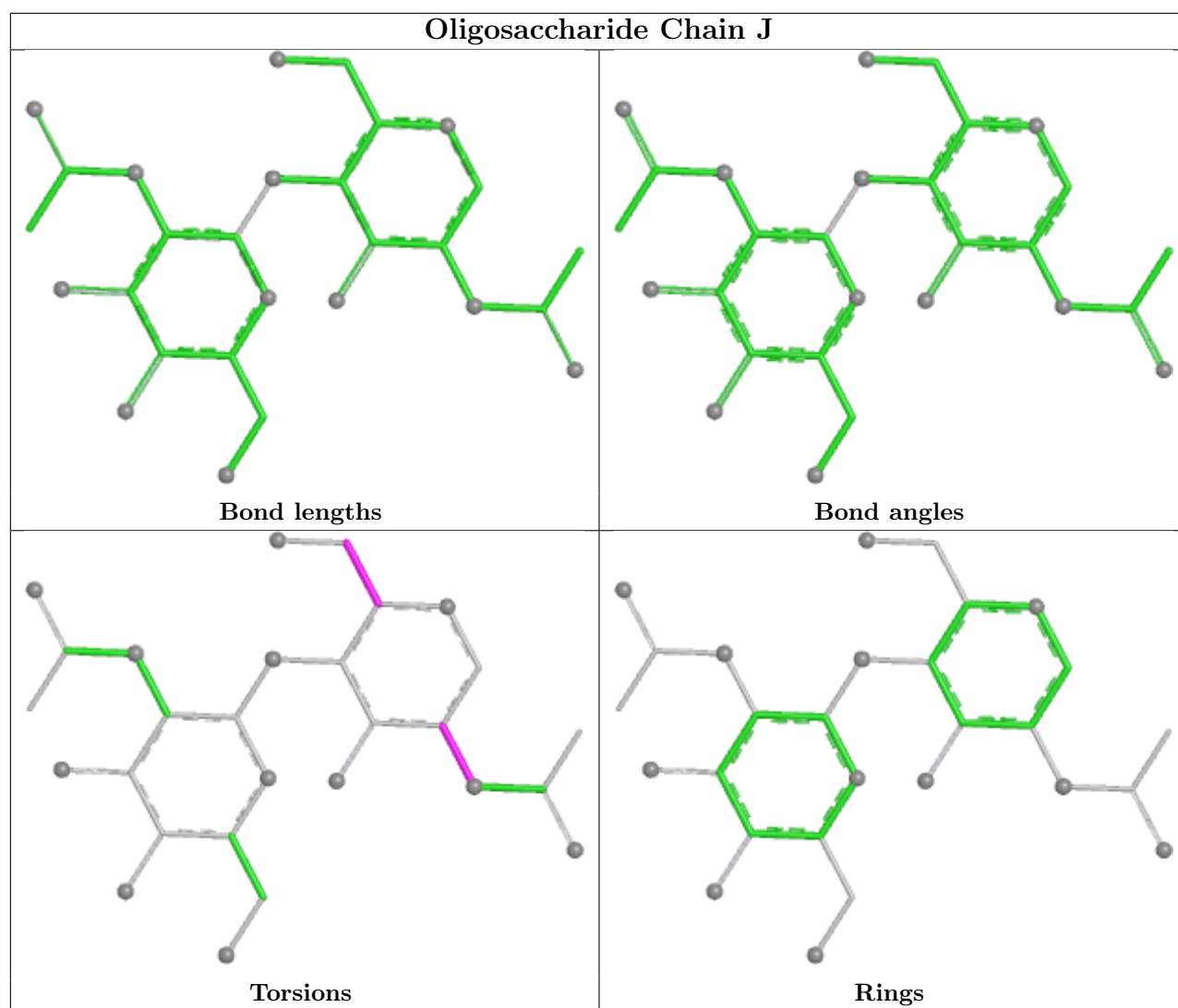
2 monomers are involved in 2 short contacts:

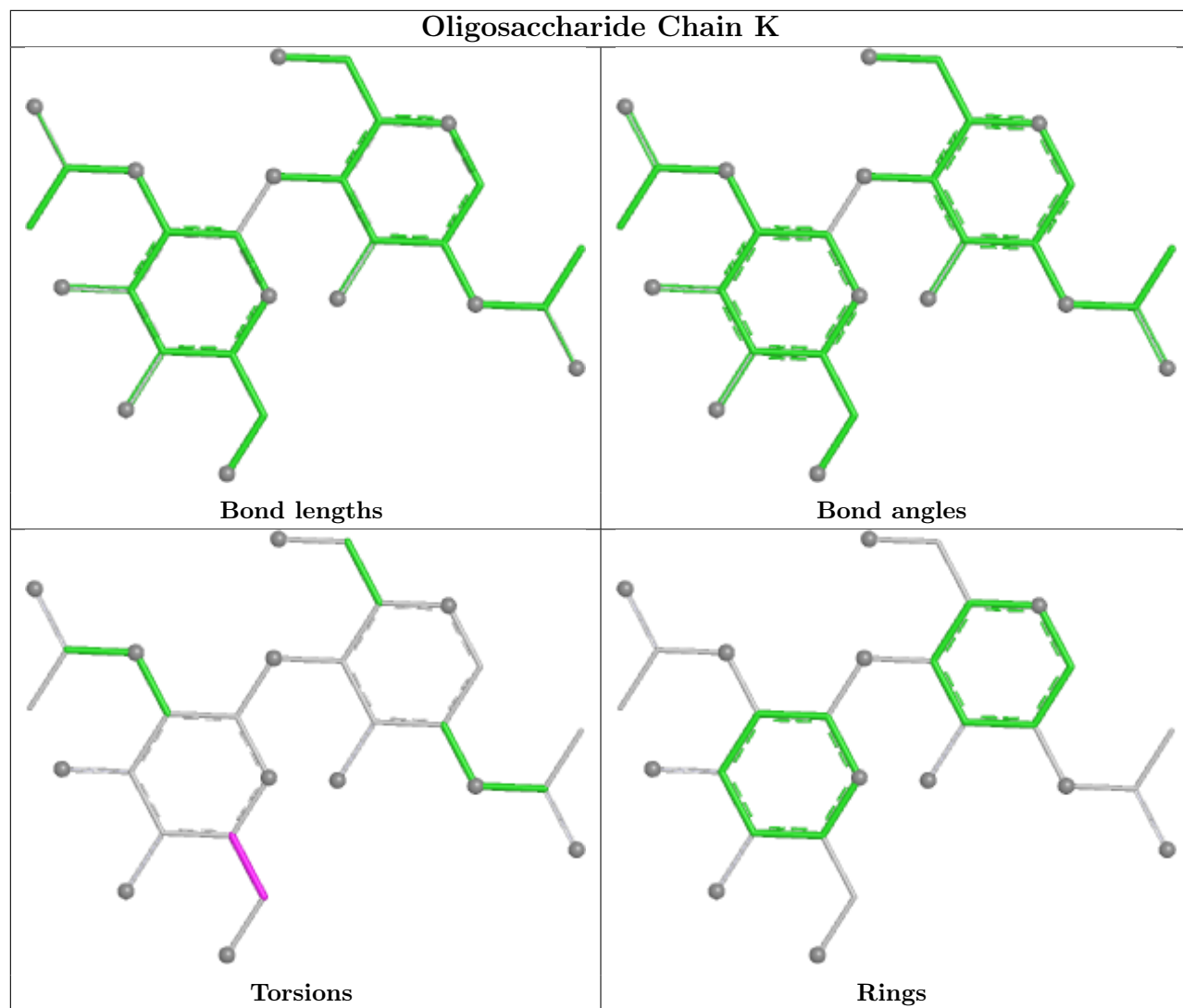
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	T	2	NAG	1	0
3	J	1	NAG	1	0

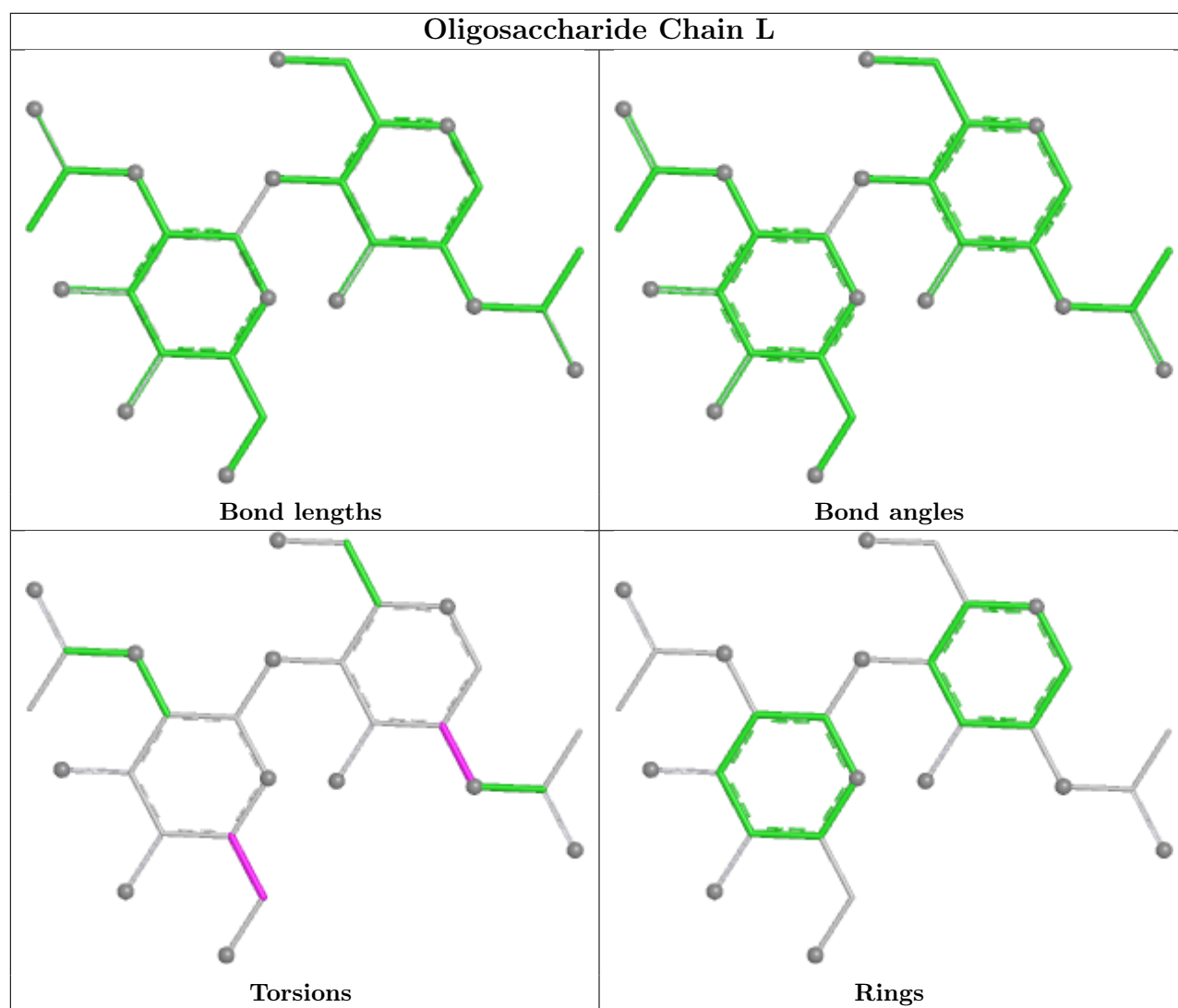
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

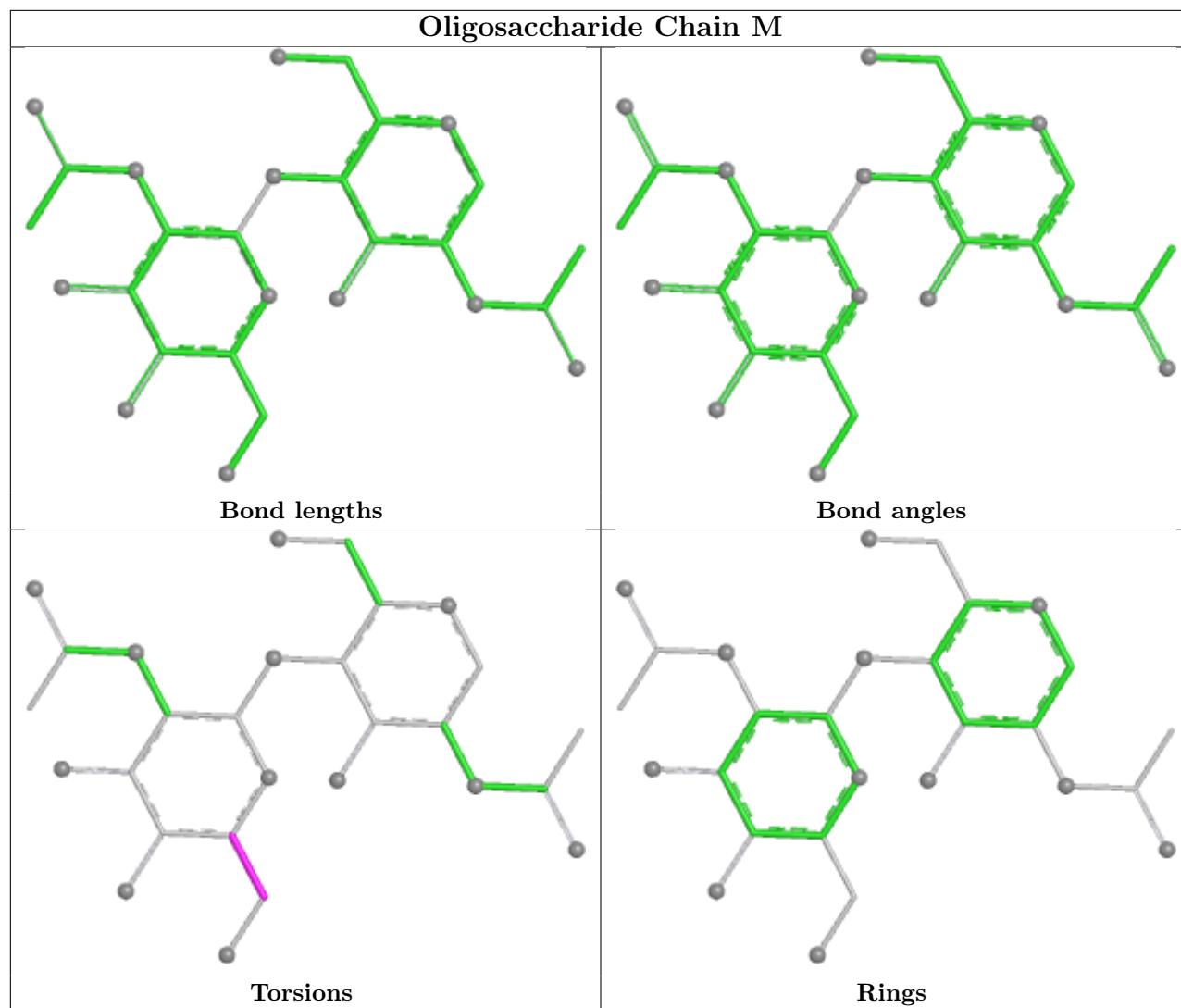


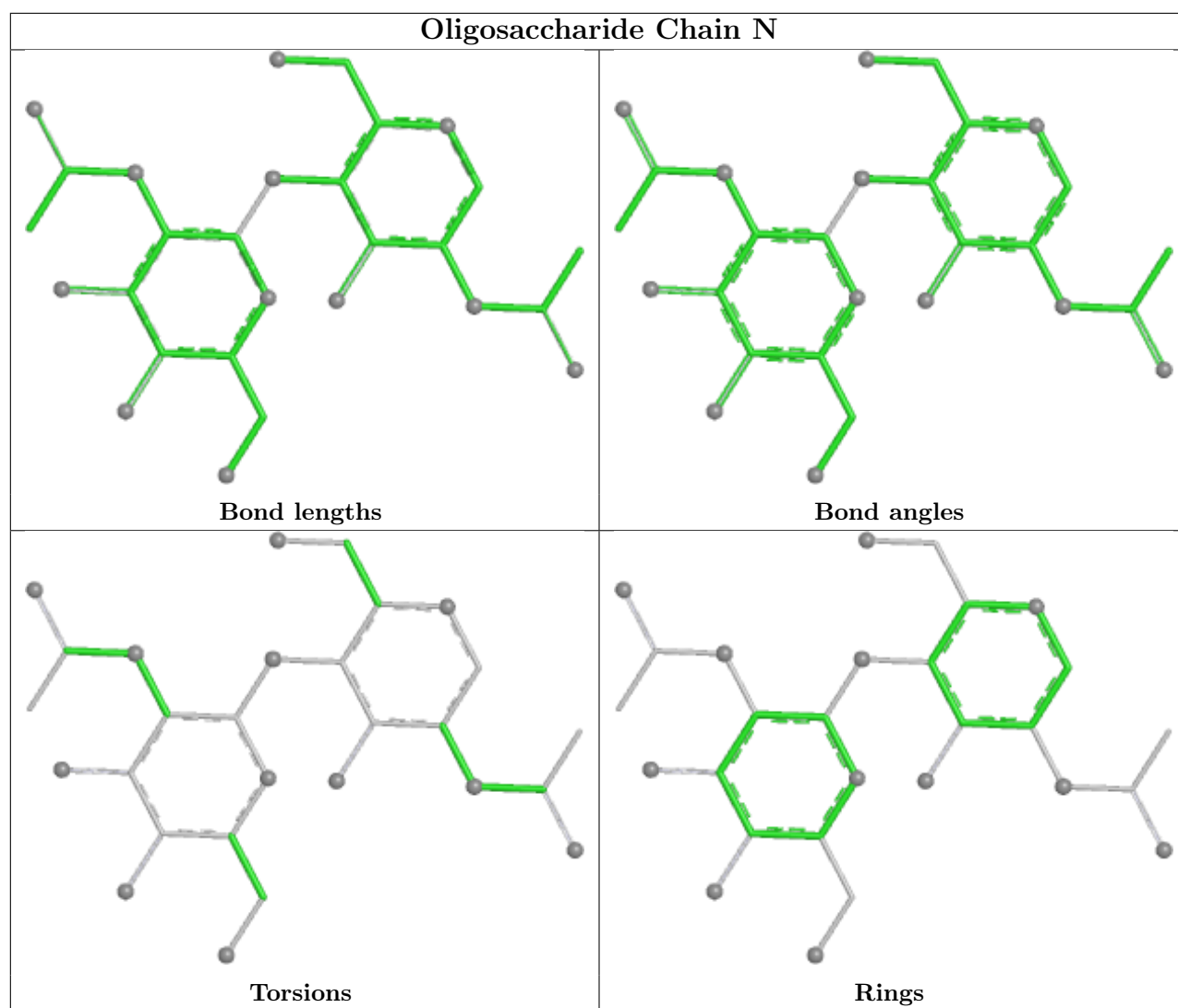


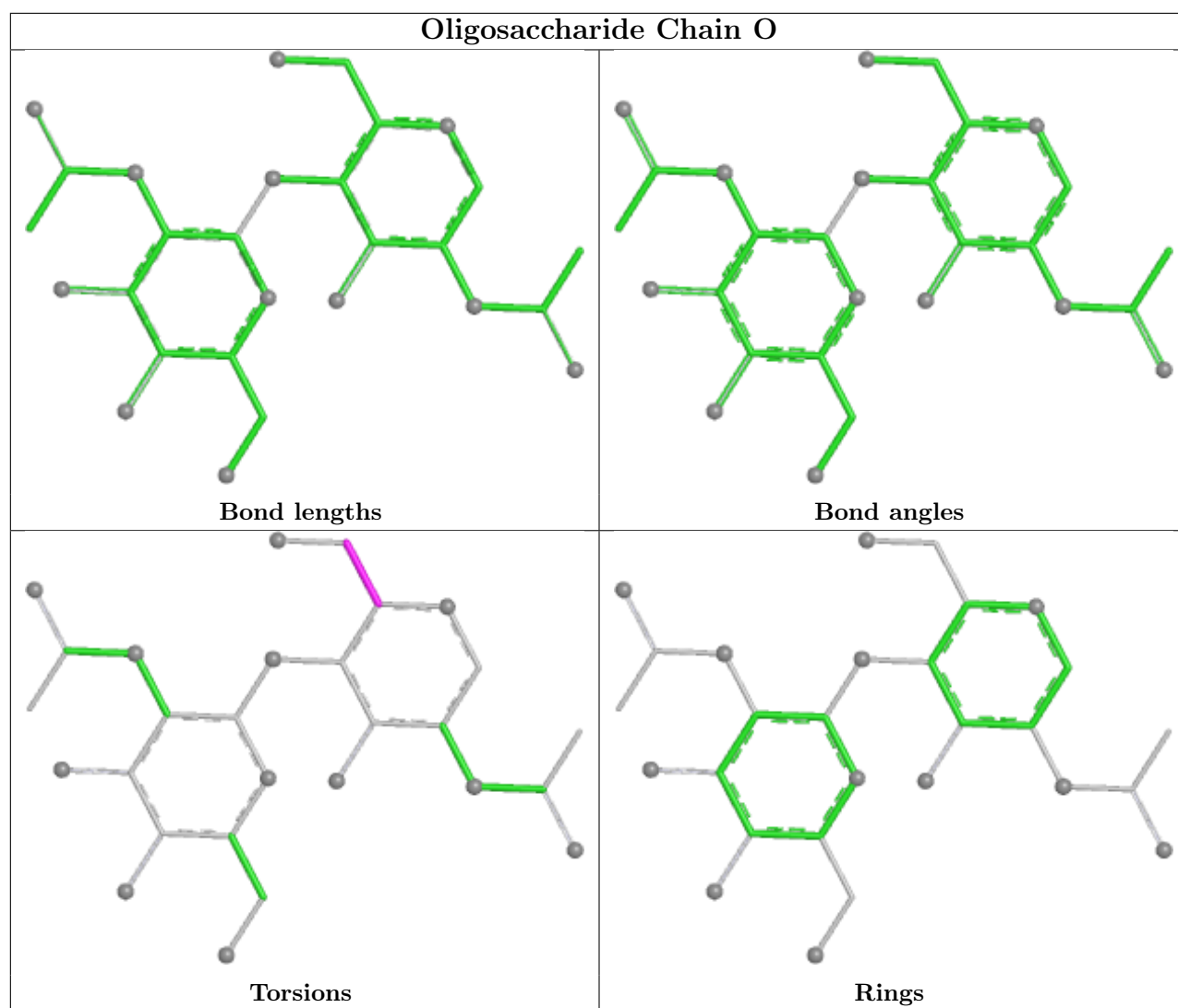


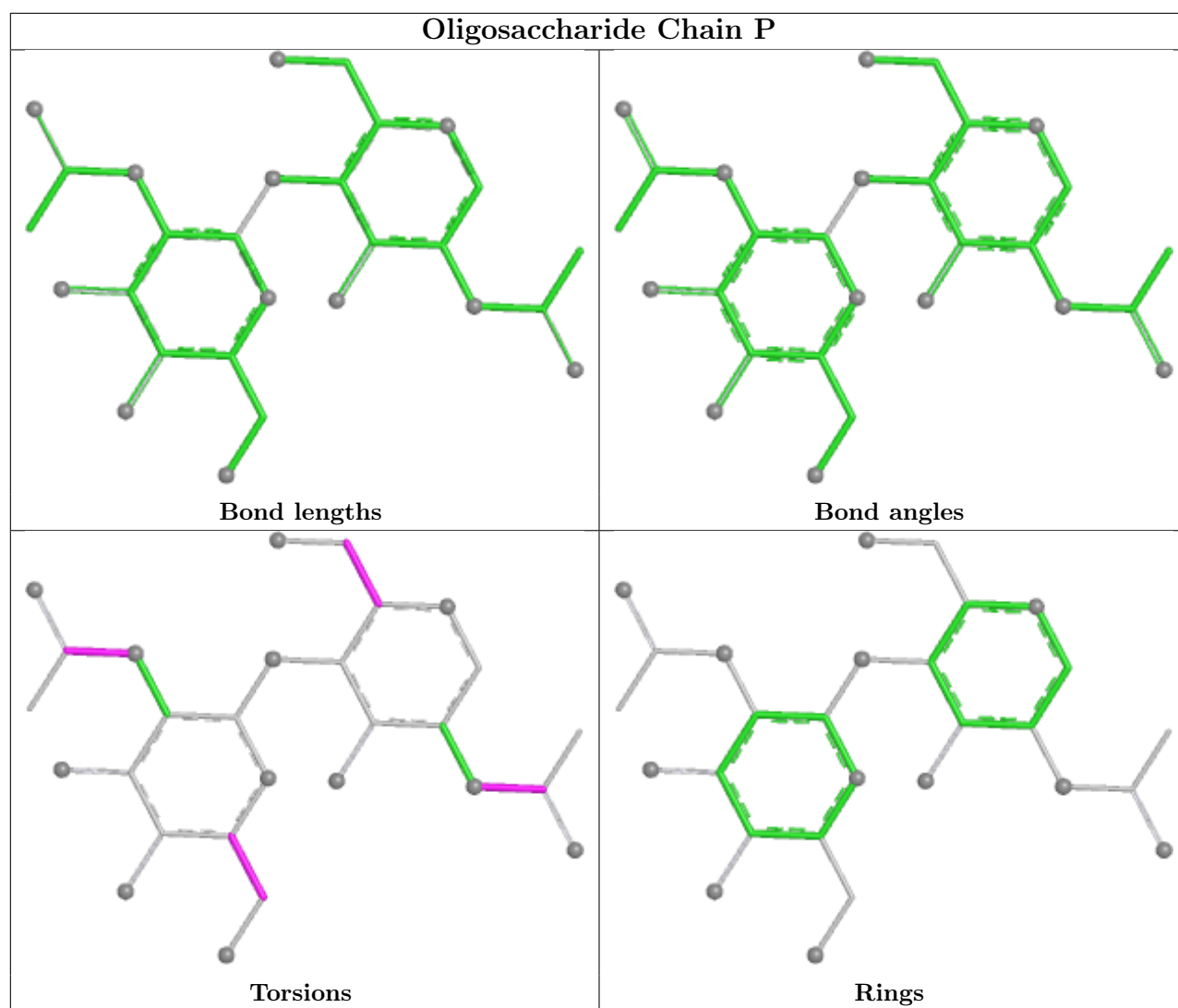


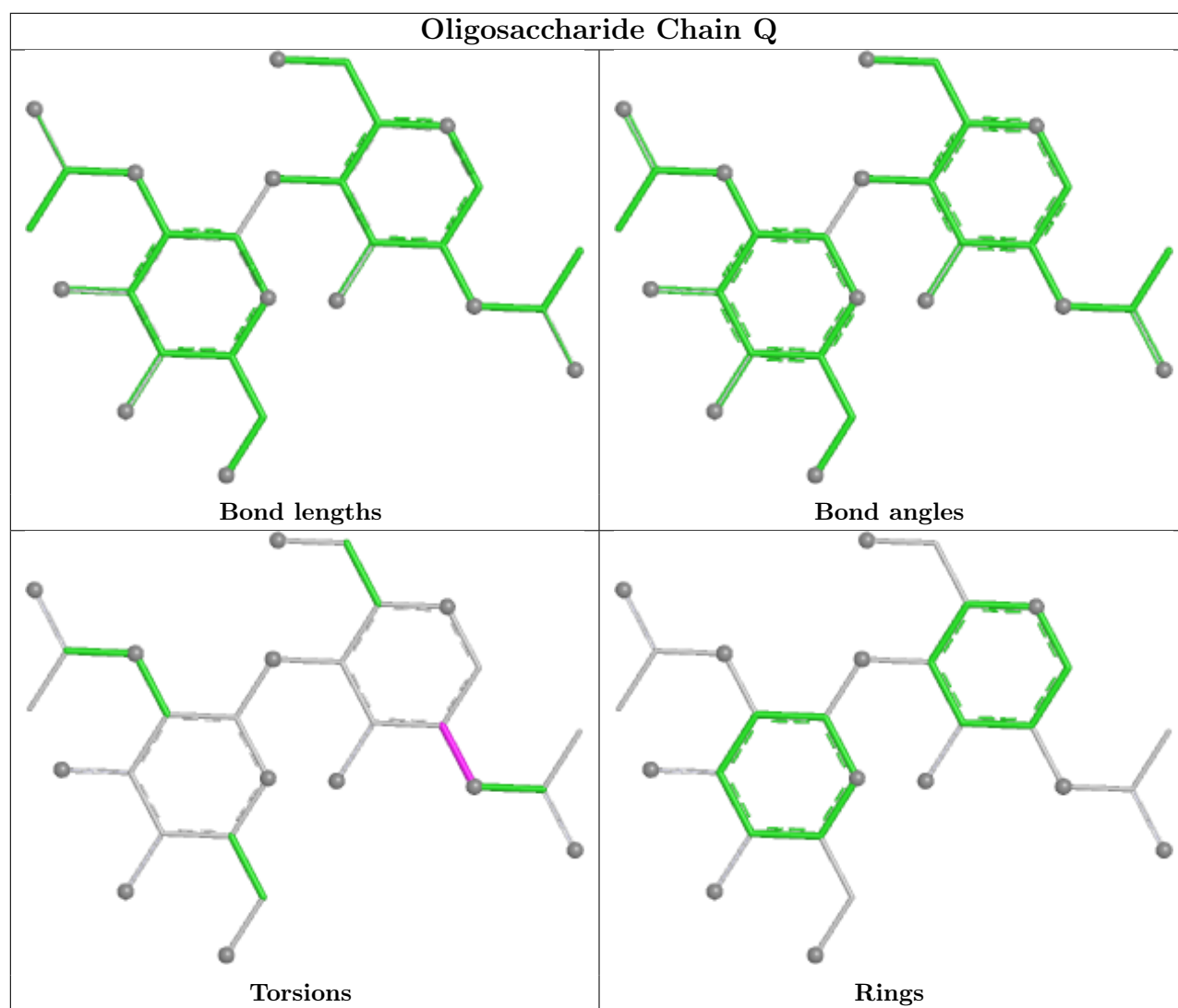


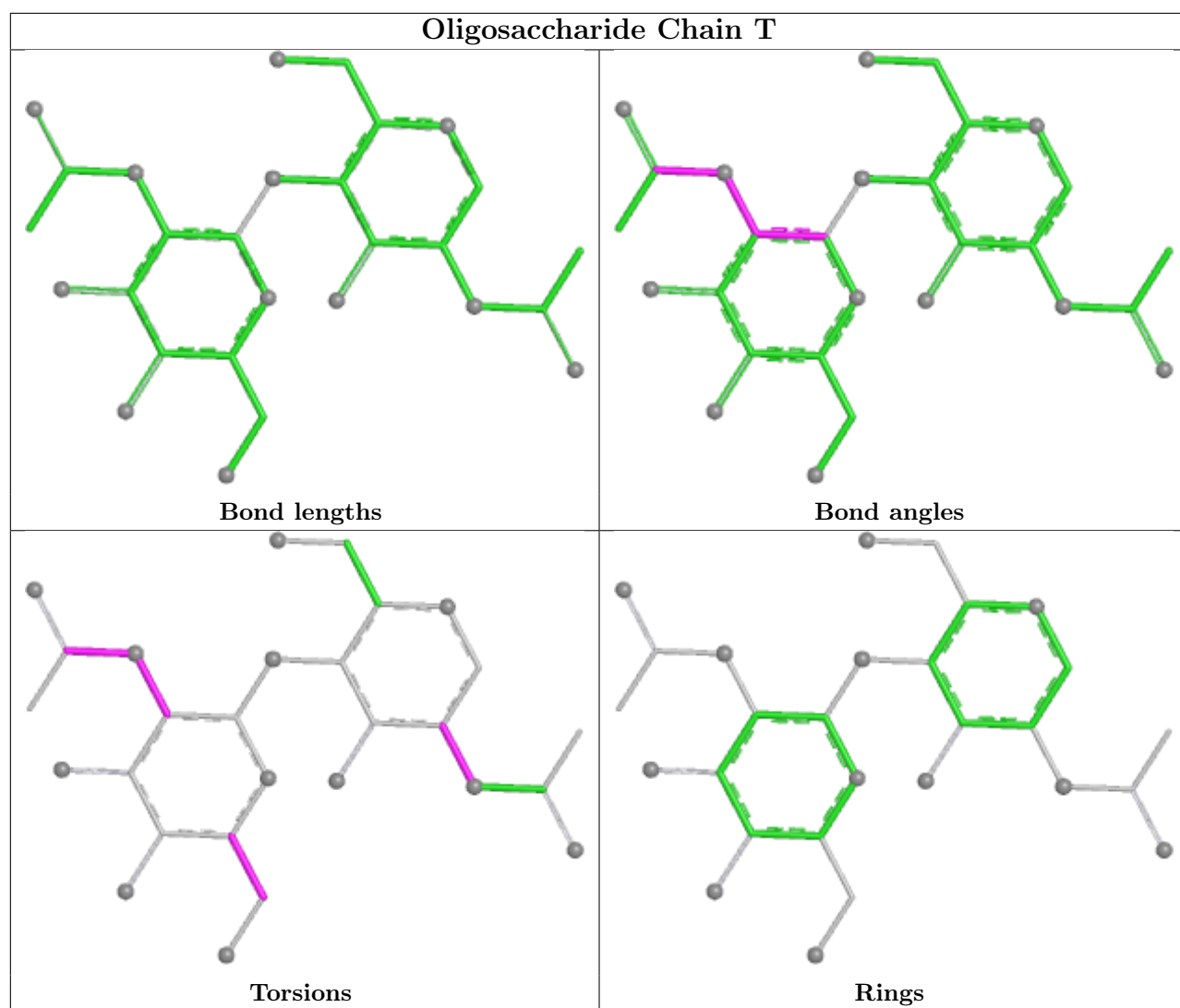


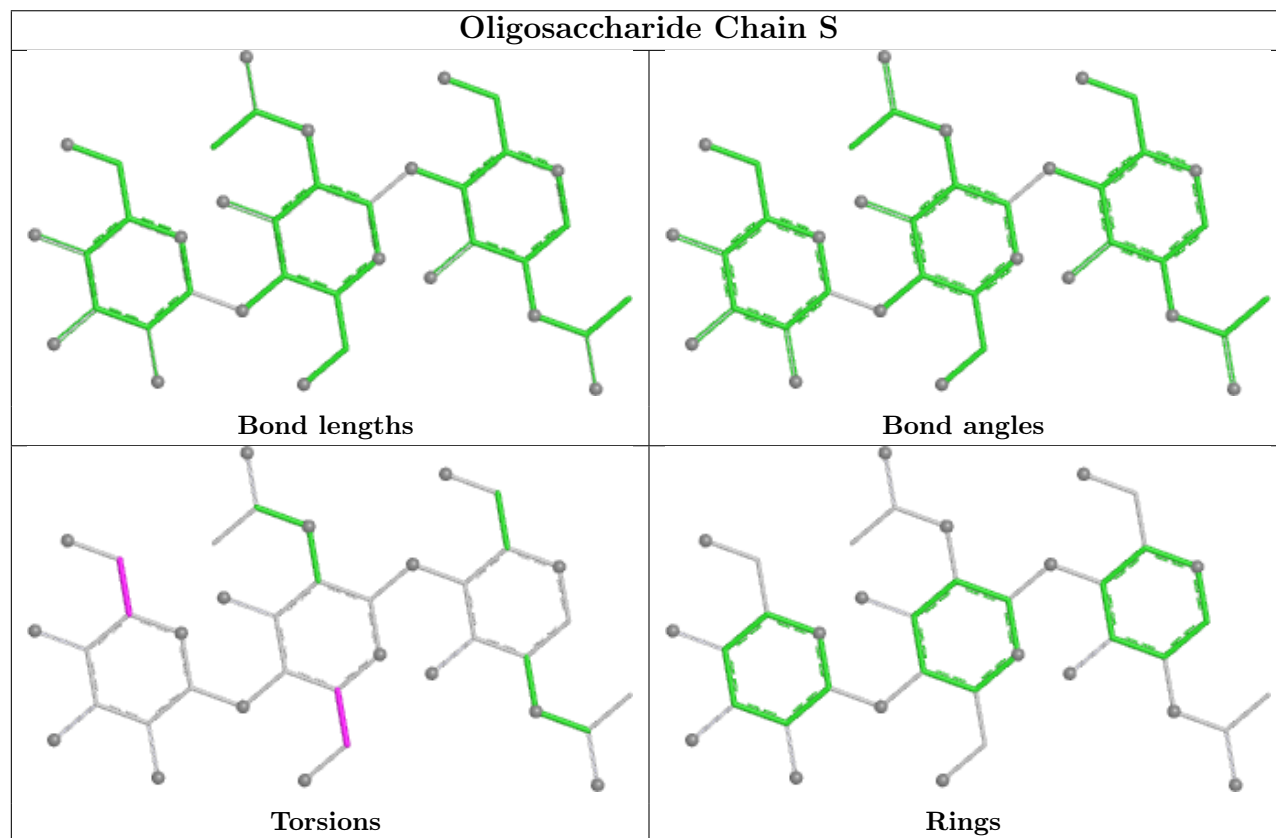
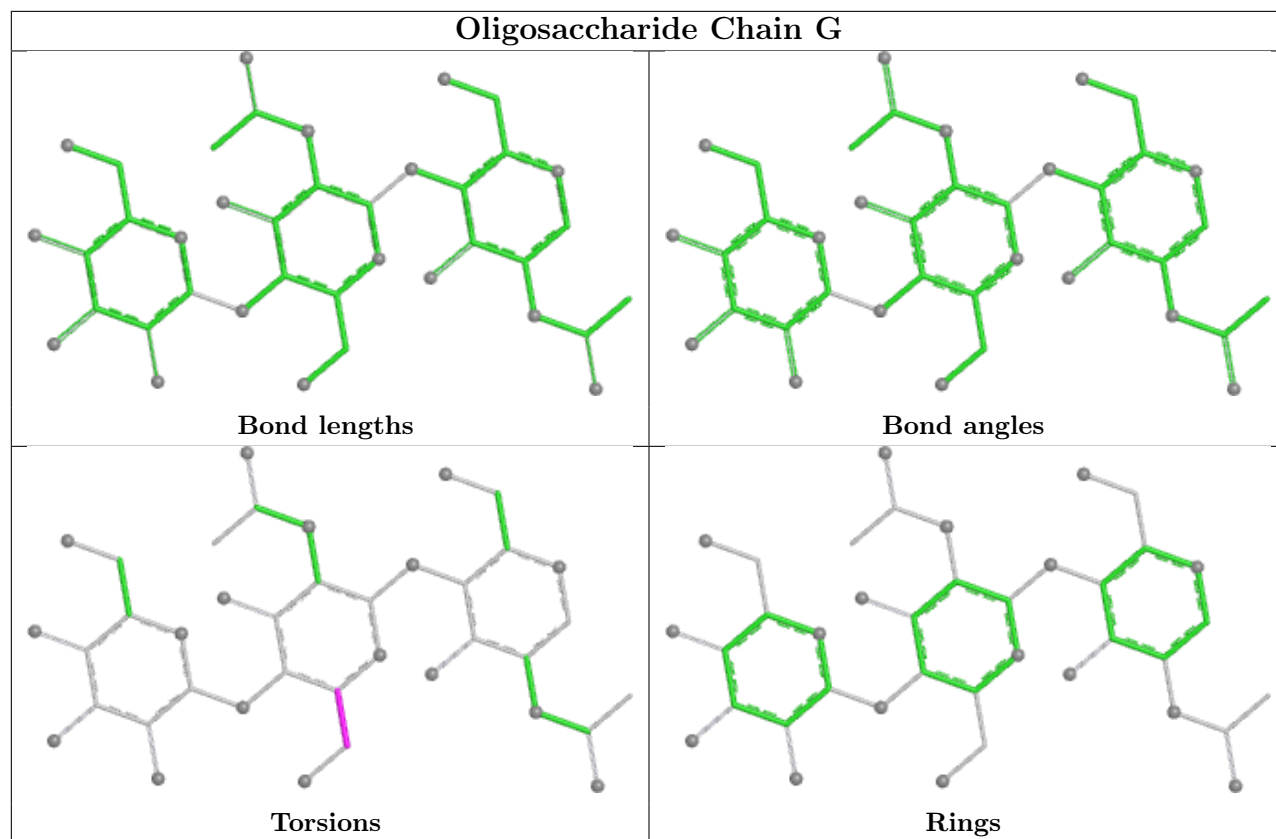


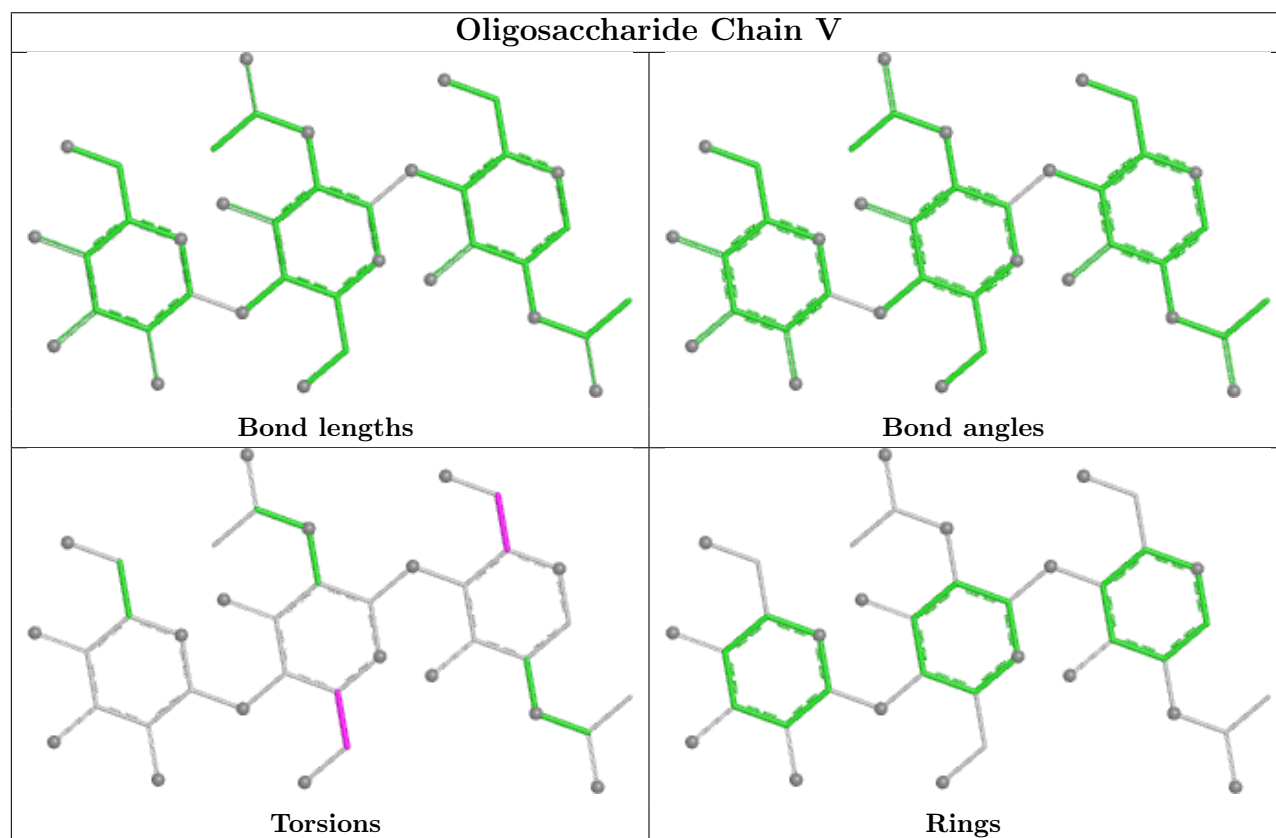
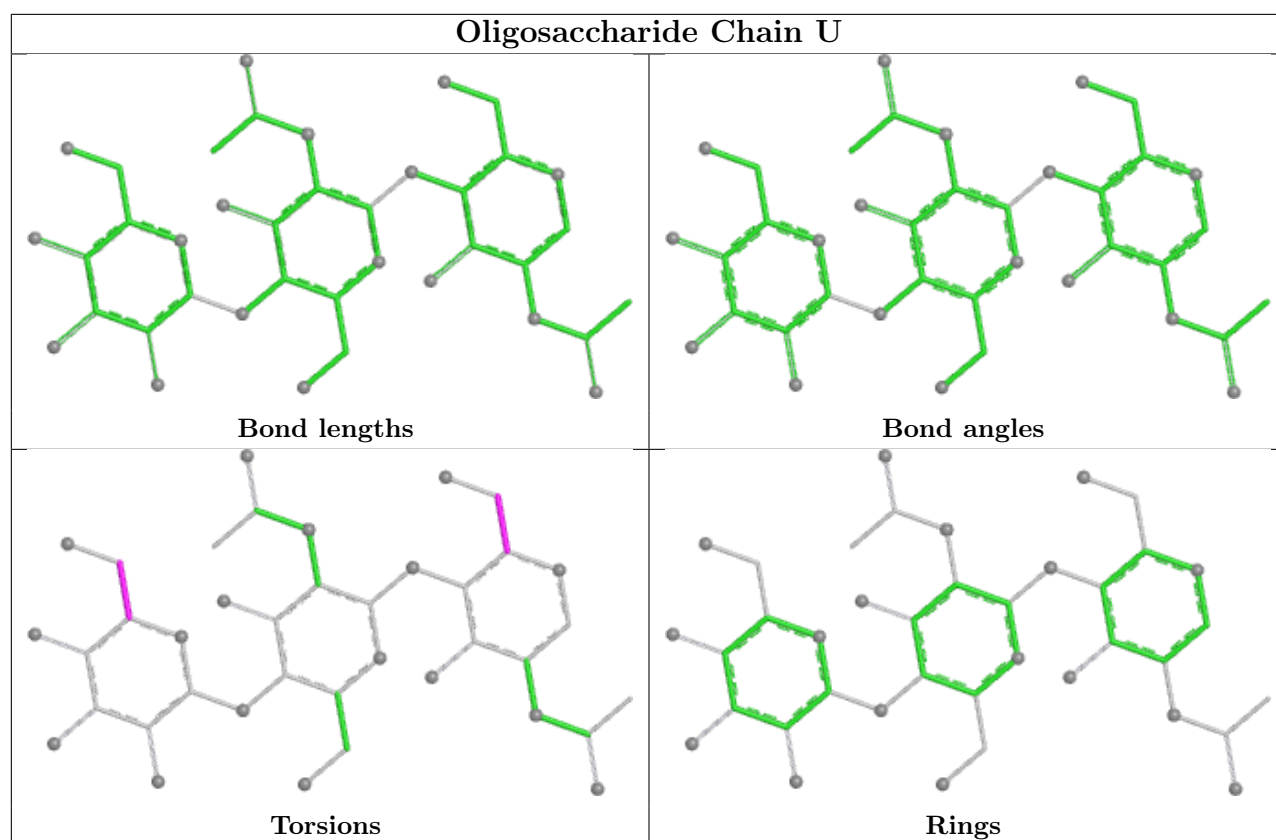


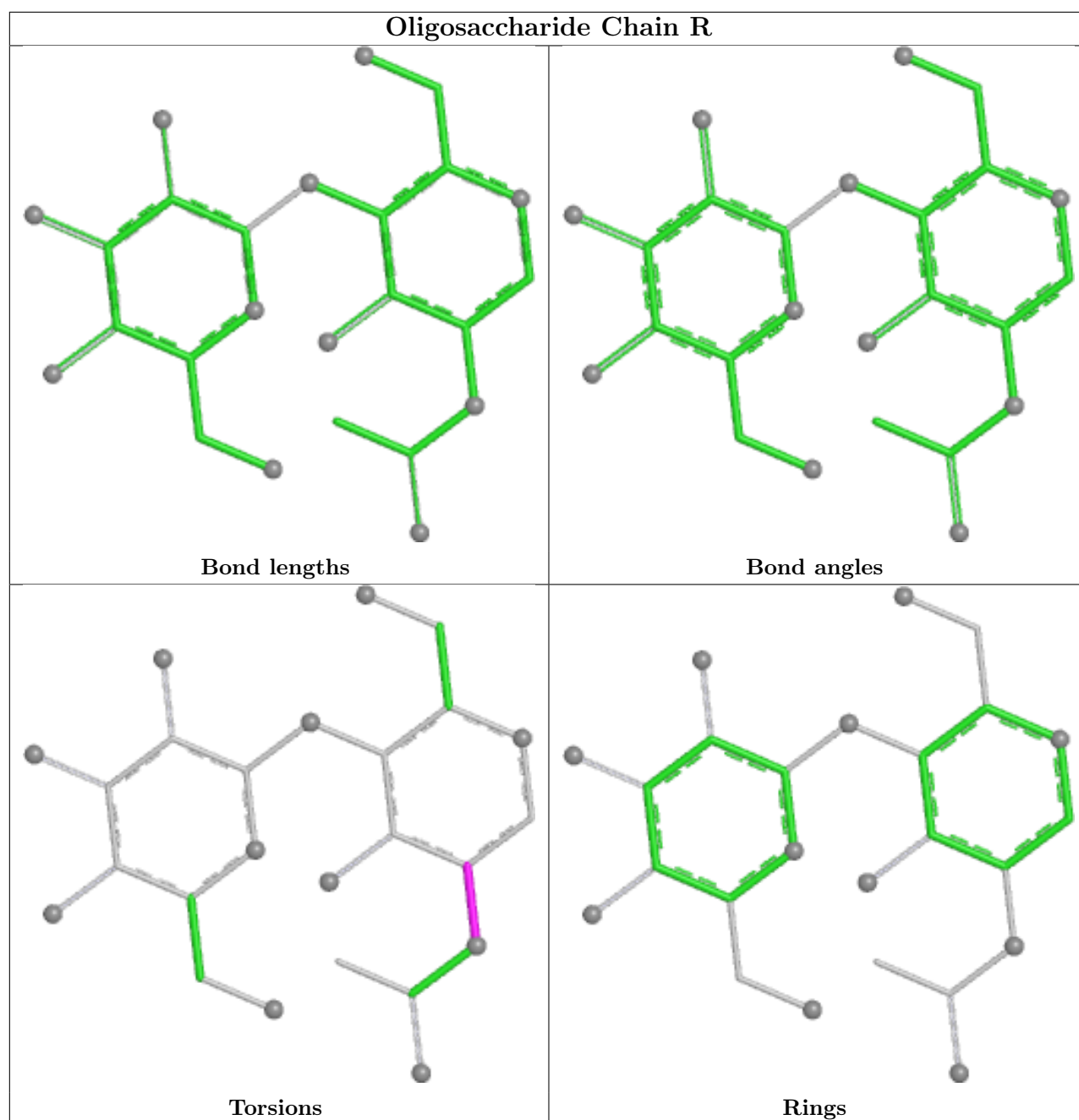












5.6 Ligand geometry [i](#)

29 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
6	NAG	C	1303	1	14,14,15	0.22	0	17,19,21	0.47	0
6	NAG	C	1302	1	14,14,15	0.19	0	17,19,21	0.53	0
6	NAG	C	1309	1	14,14,15	0.20	0	17,19,21	0.47	0
6	NAG	B	1302	1	14,14,15	0.15	0	17,19,21	0.57	0
6	NAG	B	1304	1	14,14,15	0.24	0	17,19,21	0.42	0
6	NAG	B	1305	1	14,14,15	0.20	0	17,19,21	0.47	0
6	NAG	C	1301	1	14,14,15	0.20	0	17,19,21	0.49	0
6	NAG	E	1308	1	14,14,15	0.29	0	17,19,21	1.11	2 (11%)
6	NAG	C	1304	1	14,14,15	0.20	0	17,19,21	0.44	0
6	NAG	E	1307	1	14,14,15	0.30	0	17,19,21	1.04	2 (11%)
6	NAG	C	1305	1	14,14,15	0.27	0	17,19,21	0.39	0
6	NAG	B	1306	1	14,14,15	0.41	0	17,19,21	0.52	0
6	NAG	E	1309	1	14,14,15	0.26	0	17,19,21	0.57	0
6	NAG	B	1310	1	14,14,15	0.28	0	17,19,21	0.54	0
6	NAG	C	1307	1	14,14,15	0.31	0	17,19,21	0.53	0
6	NAG	C	1308	1	14,14,15	0.21	0	17,19,21	0.44	0
6	NAG	B	1301	1	14,14,15	0.23	0	17,19,21	0.43	0
6	NAG	B	1303	1	14,14,15	0.32	0	17,19,21	0.48	0
6	NAG	E	1304	1	14,14,15	0.24	0	17,19,21	0.41	0
6	NAG	E	1306	1	14,14,15	0.38	0	17,19,21	1.13	3 (17%)
6	NAG	E	1302	1	14,14,15	0.21	0	17,19,21	0.57	0
6	NAG	E	1303	1	14,14,15	0.24	0	17,19,21	0.49	0
6	NAG	B	1307	1	14,14,15	0.42	0	17,19,21	0.76	0
6	NAG	E	1305	1	14,14,15	0.25	0	17,19,21	0.41	0
6	NAG	C	1306	1	14,14,15	0.27	0	17,19,21	0.37	0
6	NAG	E	1301	1	14,14,15	0.21	0	17,19,21	0.53	0
6	NAG	C	1310	1	14,14,15	0.26	0	17,19,21	0.48	0
6	NAG	B	1308	1	14,14,15	0.31	0	17,19,21	0.55	0
6	NAG	B	1309	1	14,14,15	0.26	0	17,19,21	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1302	1	-	4/6/23/26	0/1/1/1
6	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1302	1	-	4/6/23/26	0/1/1/1
6	NAG	B	1304	1	-	0/6/23/26	0/1/1/1

Continued on next page...

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
6	NAG	E	1308	1	-	4/6/23/26	0/1/1/1
6	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
6	NAG	E	1307	1	-	3/6/23/26	0/1/1/1
6	NAG	C	1305	1	-	3/6/23/26	0/1/1/1
6	NAG	B	1306	1	-	5/6/23/26	0/1/1/1
6	NAG	E	1309	1	-	4/6/23/26	0/1/1/1
6	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
6	NAG	E	1304	1	-	3/6/23/26	0/1/1/1
6	NAG	E	1306	1	-	0/6/23/26	0/1/1/1
6	NAG	E	1302	1	-	0/6/23/26	0/1/1/1
6	NAG	E	1303	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
6	NAG	E	1305	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
6	NAG	E	1301	1	-	4/6/23/26	0/1/1/1
6	NAG	C	1310	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1308	1	-	4/6/23/26	0/1/1/1
6	NAG	B	1309	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	1307	NAG	C1-O5-C5	-2.78	108.47	112.19
6	E	1308	NAG	O5-C1-C2	-2.33	107.68	111.29
6	E	1306	NAG	C1-O5-C5	-2.33	109.06	112.19
6	E	1308	NAG	C1-O5-C5	-2.28	109.13	112.19
6	E	1306	NAG	C2-N2-C7	-2.28	119.84	122.90

There are no chirality outliers.

5 of 63 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1308	NAG	C8-C7-N2-C2
6	B	1308	NAG	O7-C7-N2-C2
6	C	1306	NAG	C4-C5-C6-O6
6	B	1310	NAG	O5-C5-C6-O6
6	E	1301	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1309	NAG	1	0
6	B	1303	NAG	1	0
6	C	1306	NAG	2	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.

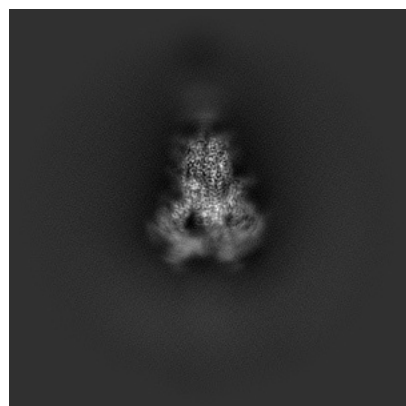
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24077. These allow visual inspection of the internal detail of the map and identification of artifacts.

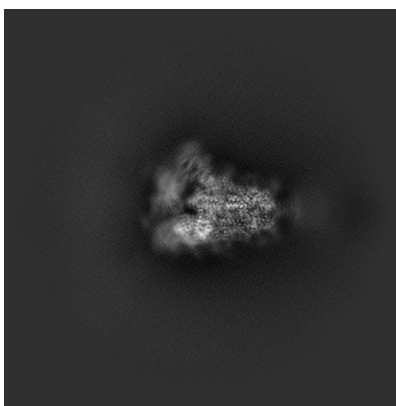
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

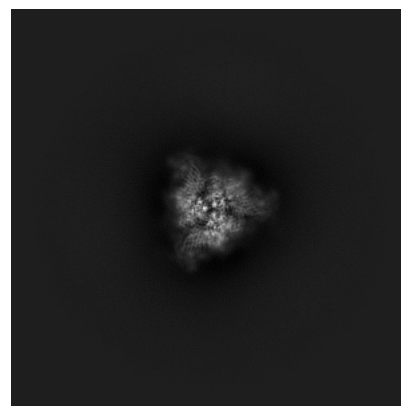
6.1.1 Primary map



X

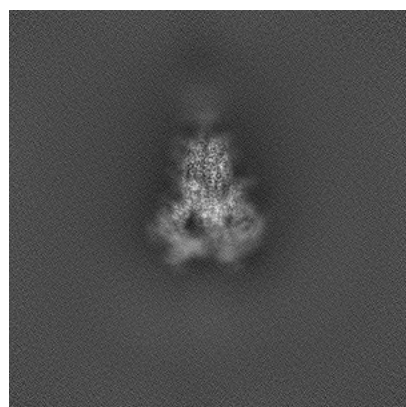


Y

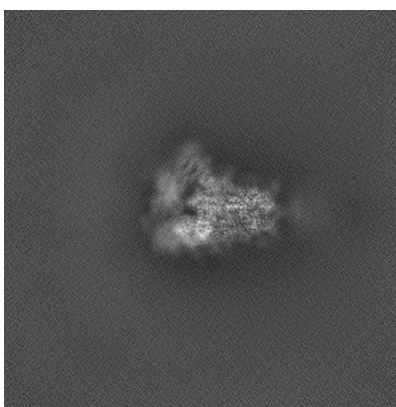


Z

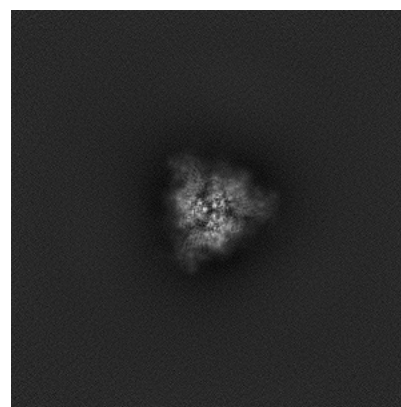
6.1.2 Raw map



X



Y

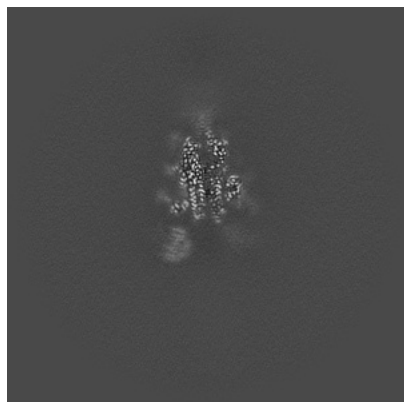


Z

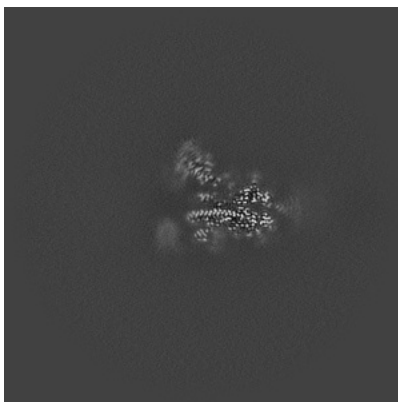
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

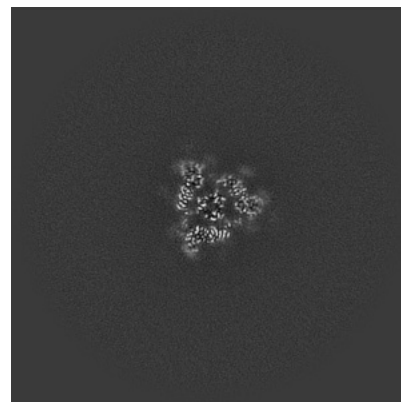
6.2.1 Primary map



X Index: 300

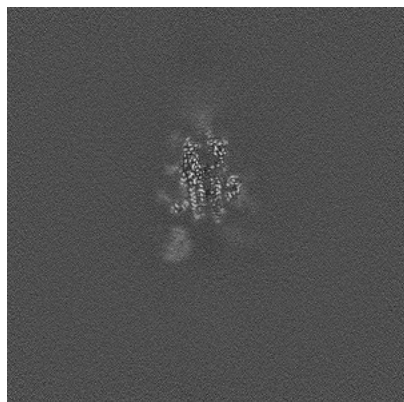


Y Index: 300

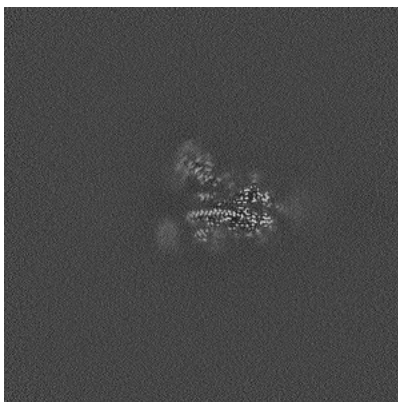


Z Index: 300

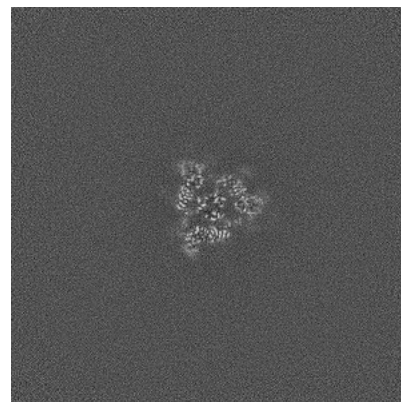
6.2.2 Raw map



X Index: 300



Y Index: 300

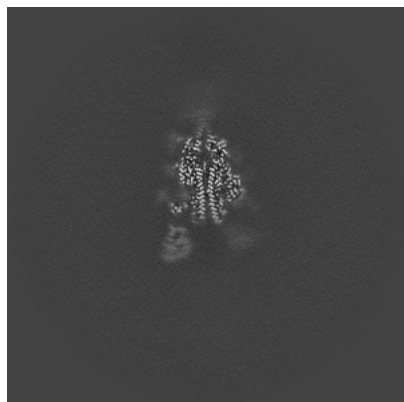


Z Index: 300

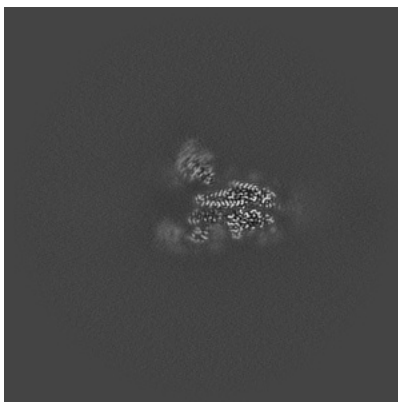
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

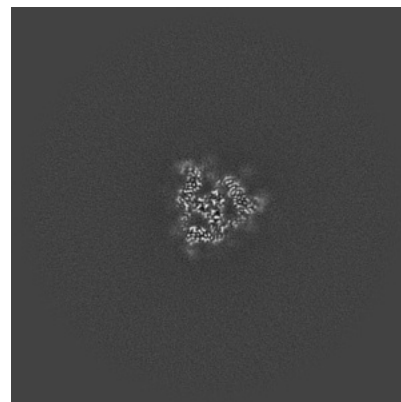
6.3.1 Primary map



X Index: 304

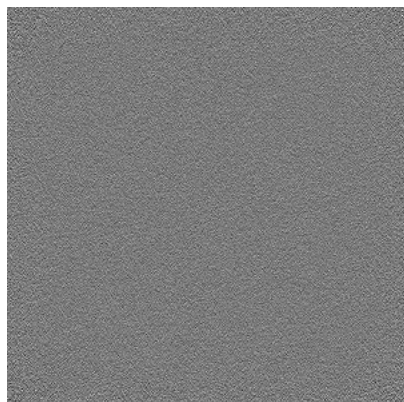


Y Index: 306

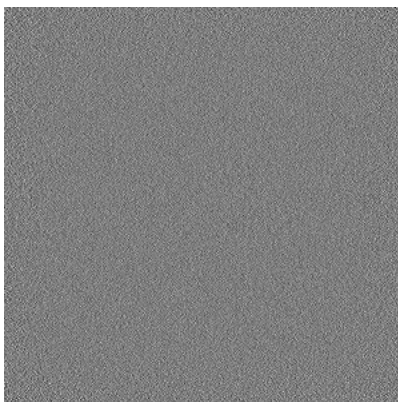


Z Index: 304

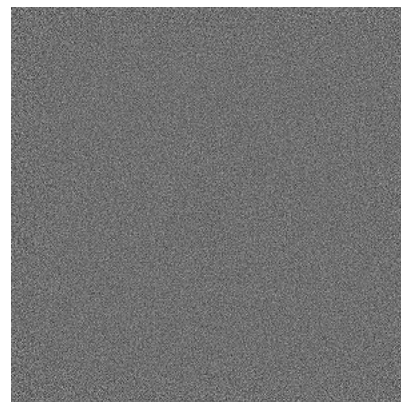
6.3.2 Raw map



X Index: 0



Y Index: 0

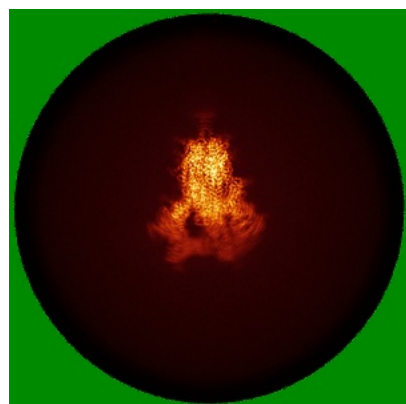


Z Index: 0

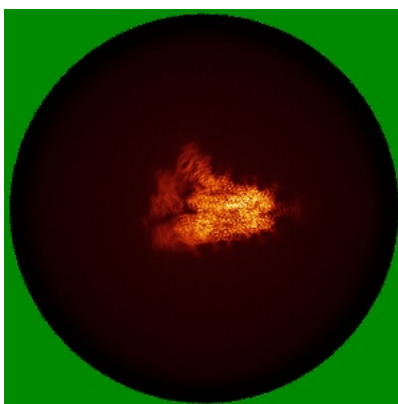
The images above show the largest variance slices of the map in three orthogonal directions.

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

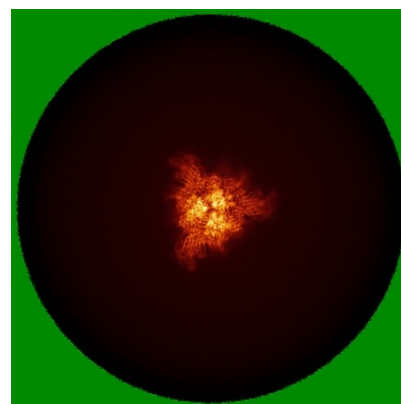
6.4.1 Primary map



X

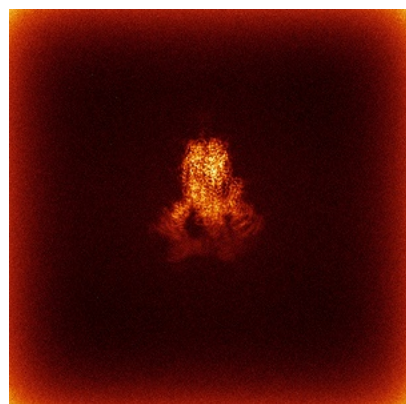


Y

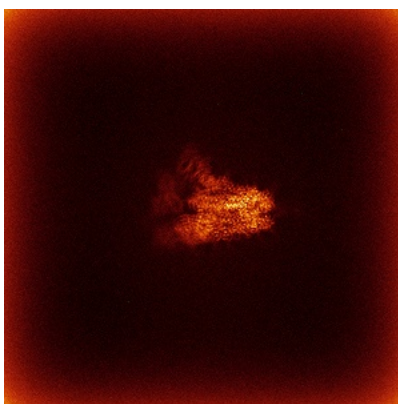


Z

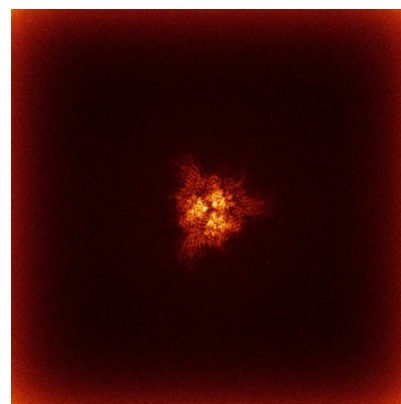
6.4.2 Raw map



X



Y



Z

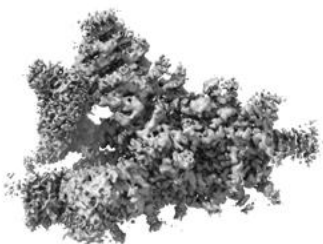
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

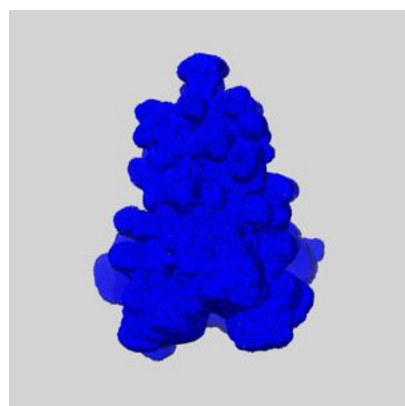
6.6 Mask visualisation [i](#)

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

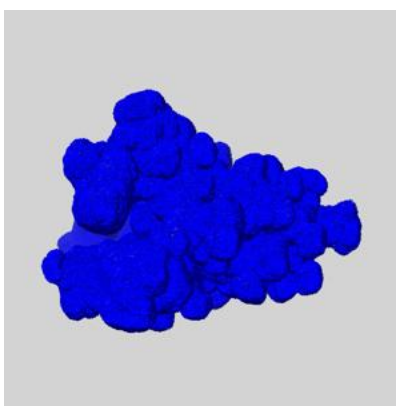
A mask typically either:

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

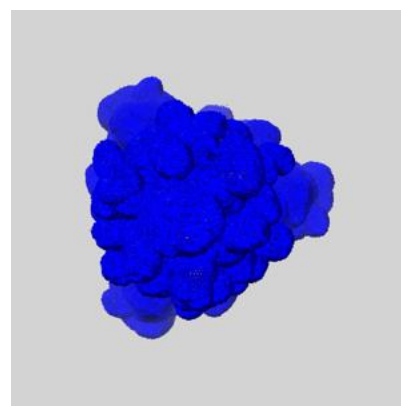
6.6.1 emd_24077_msk_1.map [i](#)



X



Y

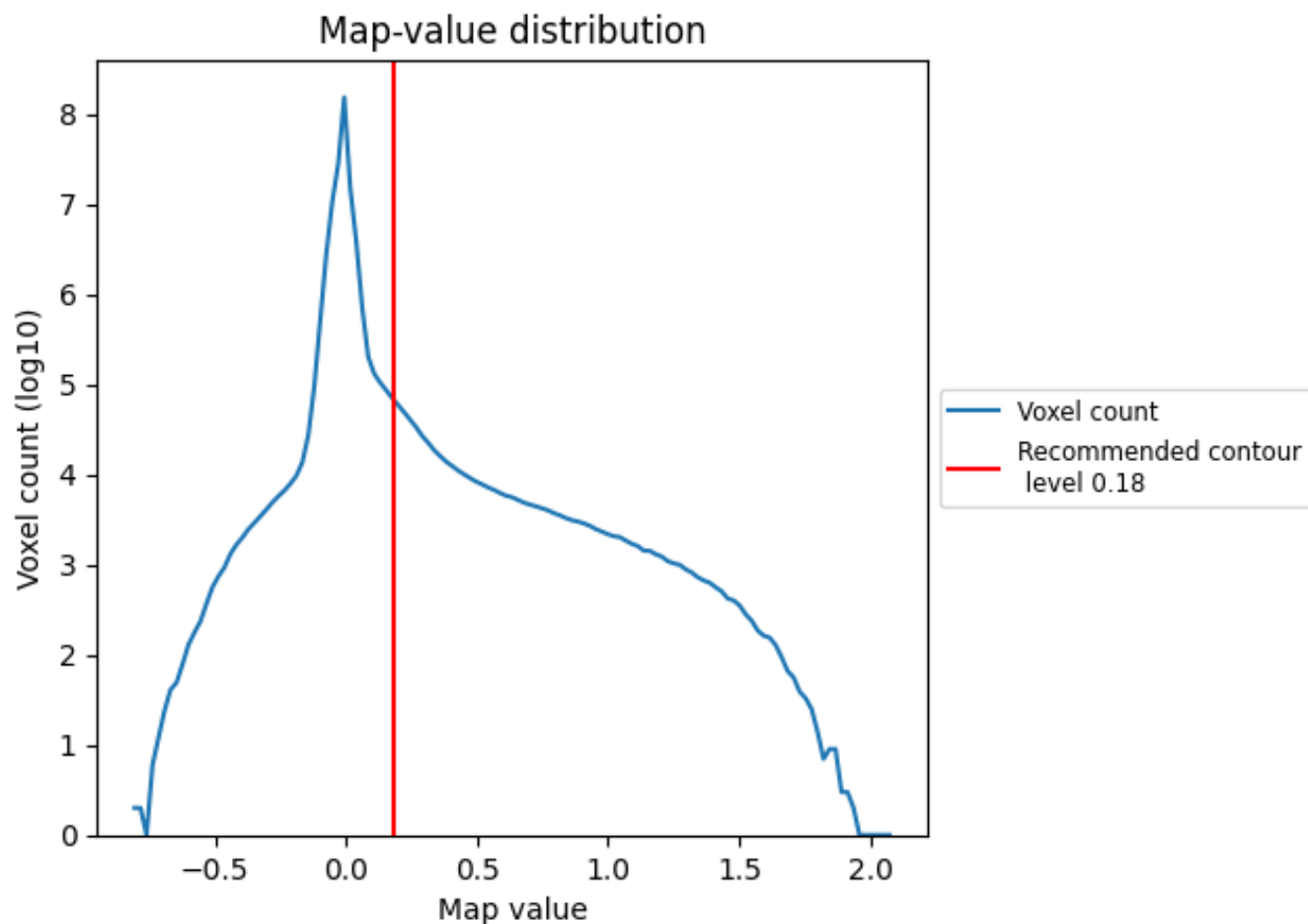


Z

7 Map analysis [i](#)

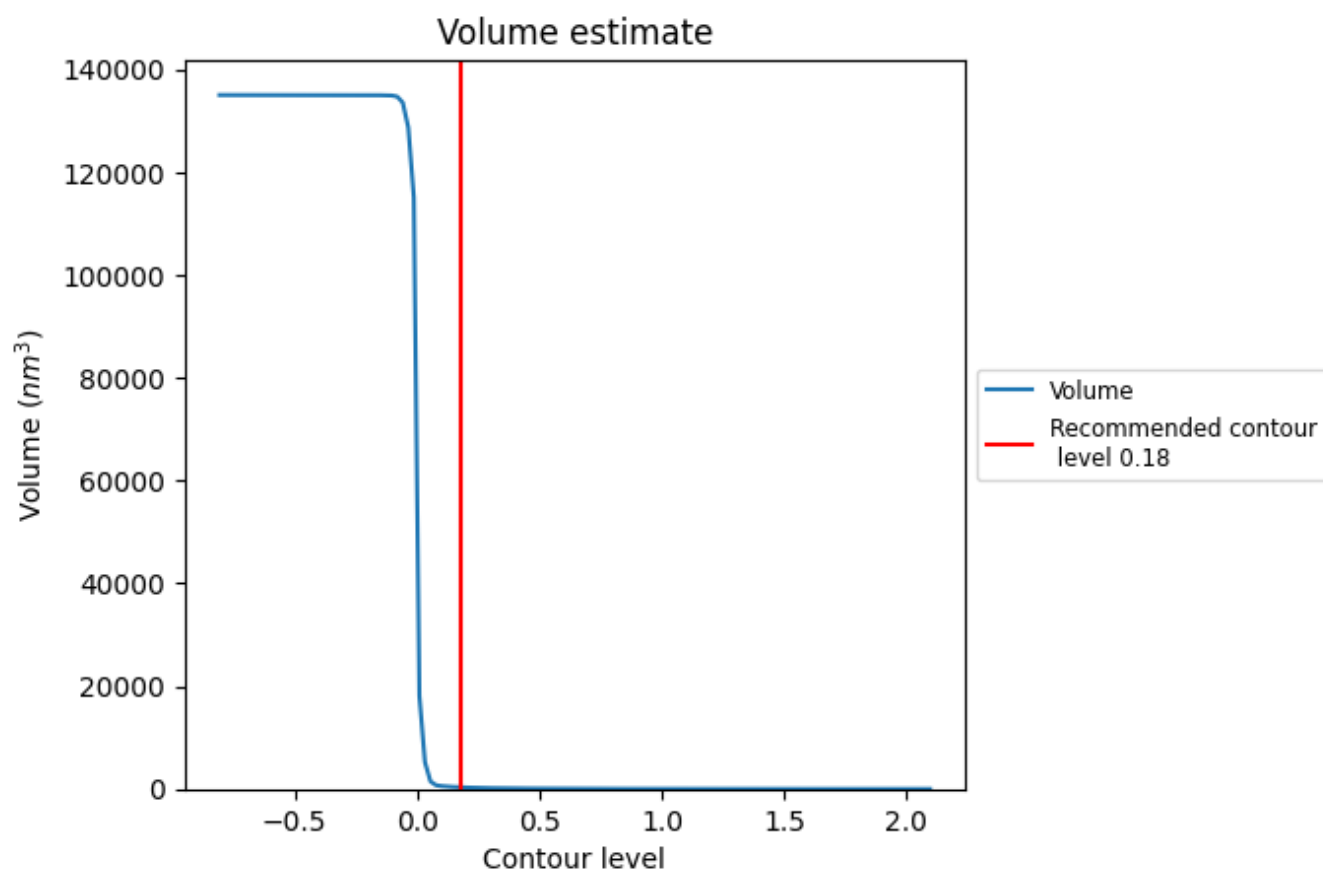
This section contains the results of statistical analysis of the map.

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.

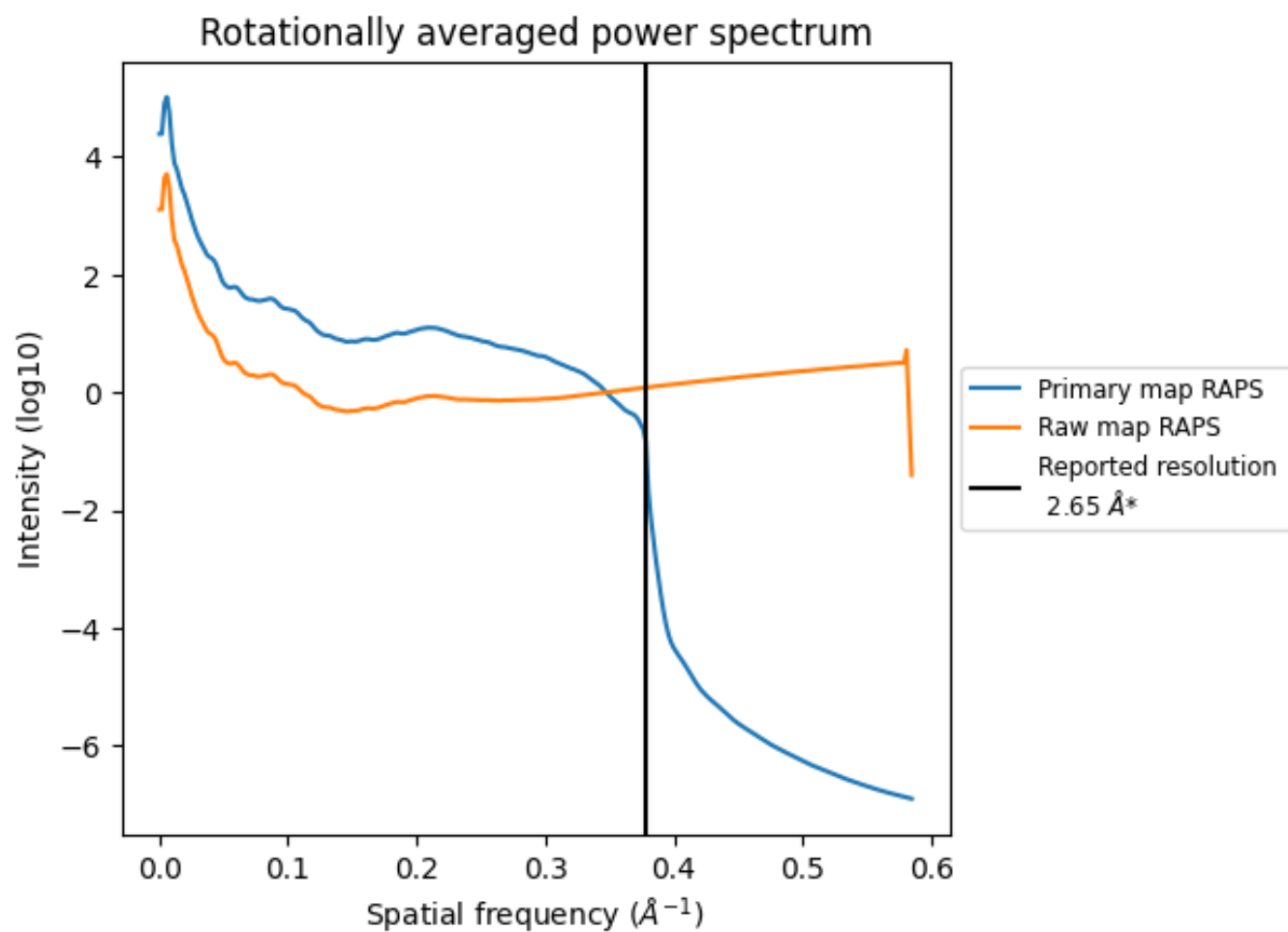
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 320 nm^3 ; this corresponds to an approximate mass of 289 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 ⓘ

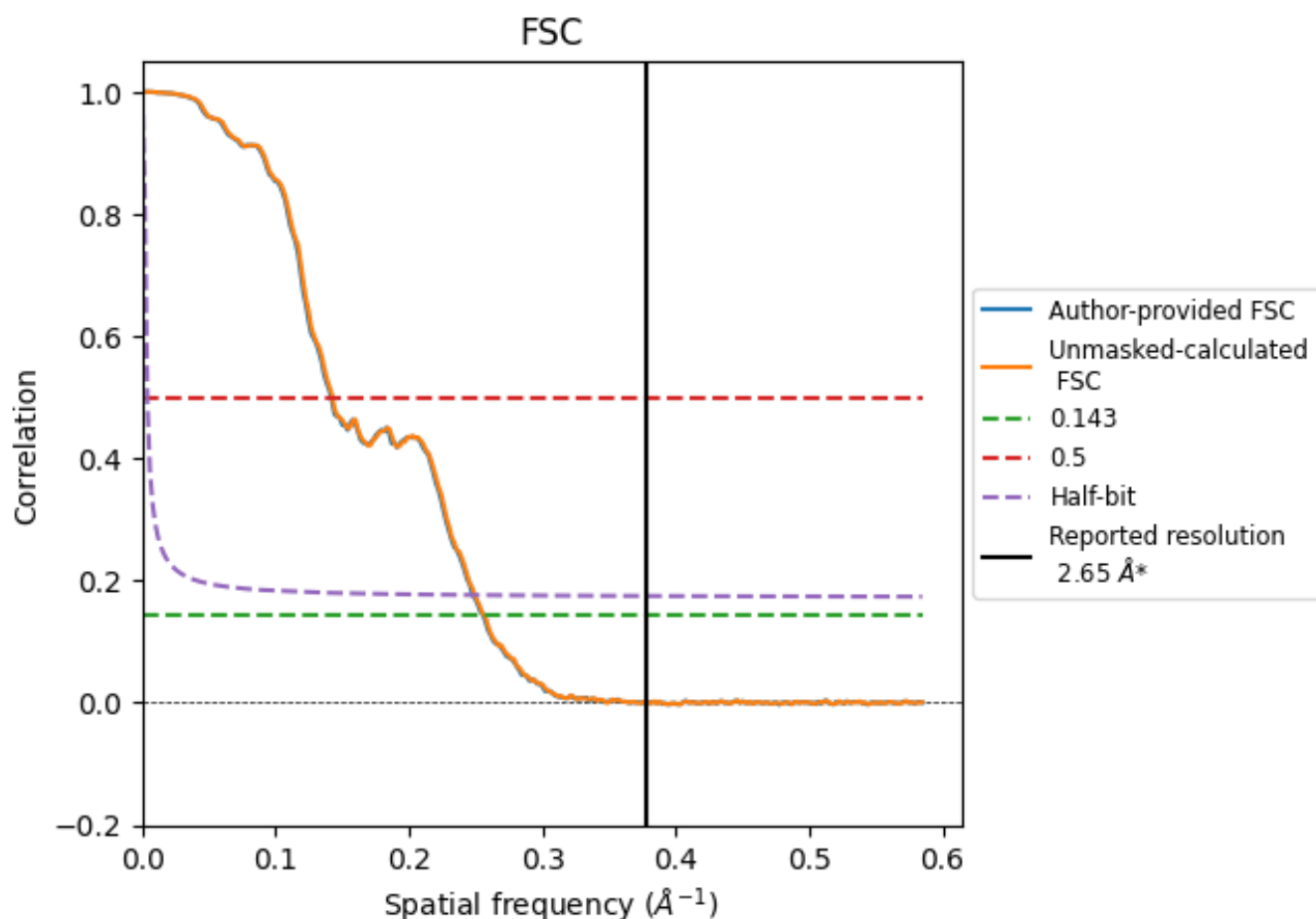


*Reported resolution corresponds to spatial frequency of 0.377 Å⁻¹

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 0.377 $\text{\AA}^{-1}$

8.2 Resolution estimates

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.65	-	-
Author-provided FSC curve	3.91	7.06	4.04
Unmasked-calculated*	3.90	7.01	4.01

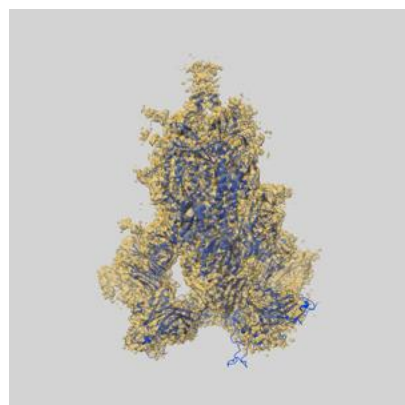
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.91 differs from the reported value 2.65 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.90 differs from the reported value 2.65 by more than 10 %

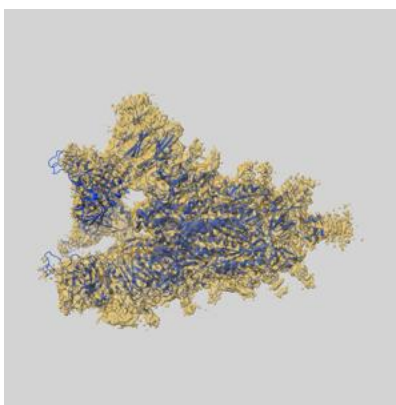
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24077 and PDB model 7MY2. Per-residue inclusion information can be found in section [3](#) on page [15](#).

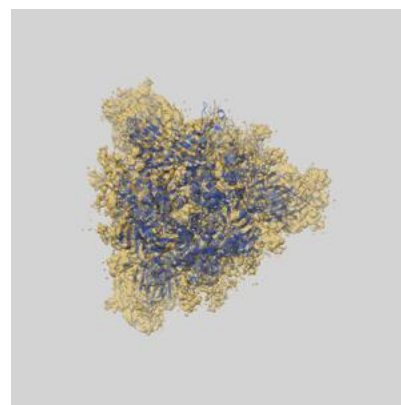
9.1 Map-model overlay [i](#)



X



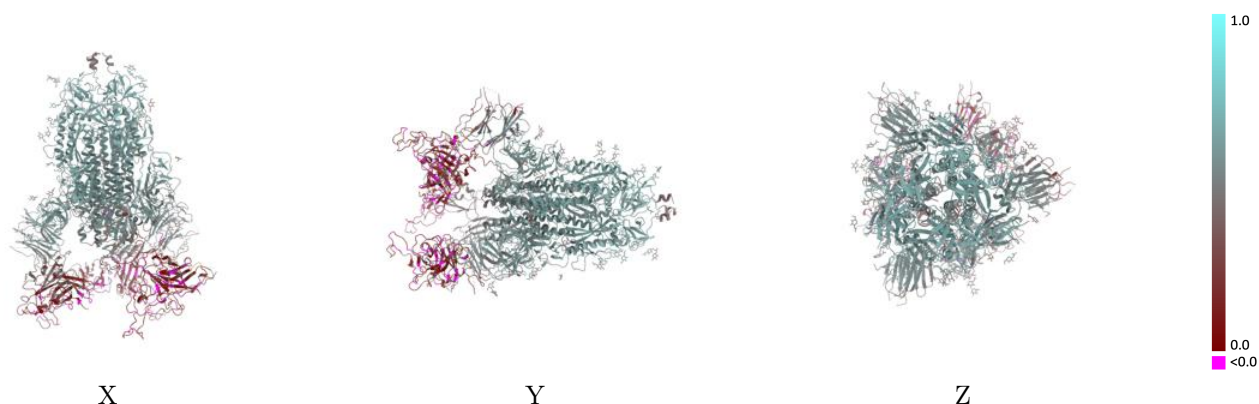
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.18 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](#)

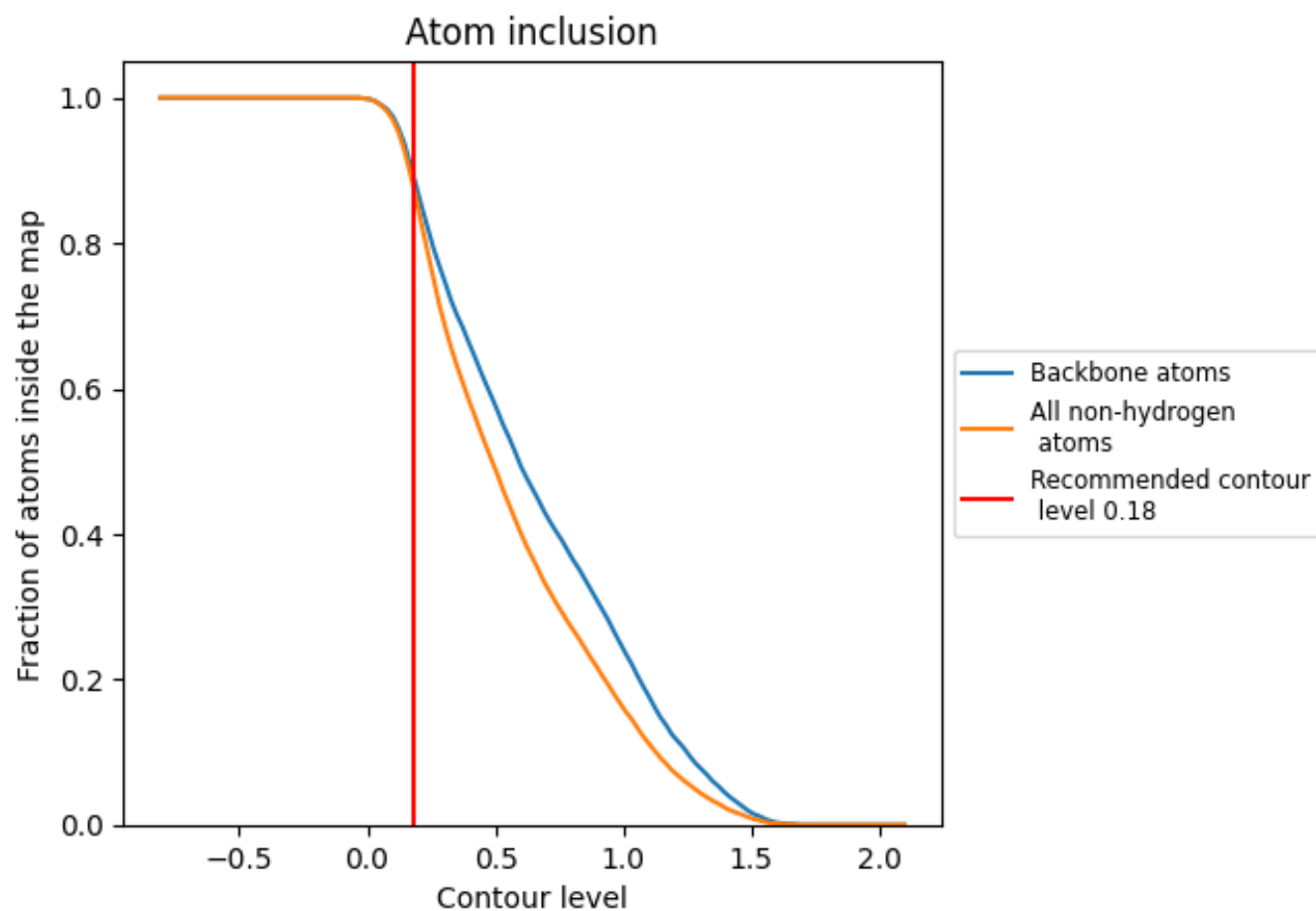


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 88% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8780	 0.4670
A	 0.6680	 0.2040
B	 0.9110	 0.4990
C	 0.8640	 0.4850
D	 0.3090	 0.1880
E	 0.9420	 0.5010
F	 1.0000	 0.5170
G	 1.0000	 0.5430
H	 0.8310	 0.2500
I	 1.0000	 0.5010
J	 0.9290	 0.4720
K	 1.0000	 0.5000
L	 1.0000	 0.5290
M	 1.0000	 0.5250
N	 1.0000	 0.5070
O	 0.9640	 0.5340
P	 0.9290	 0.3920
Q	 0.9640	 0.4880
R	 1.0000	 0.5400
S	 1.0000	 0.5490
T	 0.8930	 0.4630
U	 1.0000	 0.4870
V	 0.9740	 0.4860

