



Full wwPDB EM Validation Report ⓘ

Nov 2, 2024 – 11:16 PM EDT

PDB ID : 7SBX
EMDB ID : EMD-24991
Title : Structure of OC43 spike in complex with polyclonal Fab6 (Donor 1051)
Authors : Bangaru, S.; Antanasijevic, A.; Ward, A.
Deposited on : 2021-09-26
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

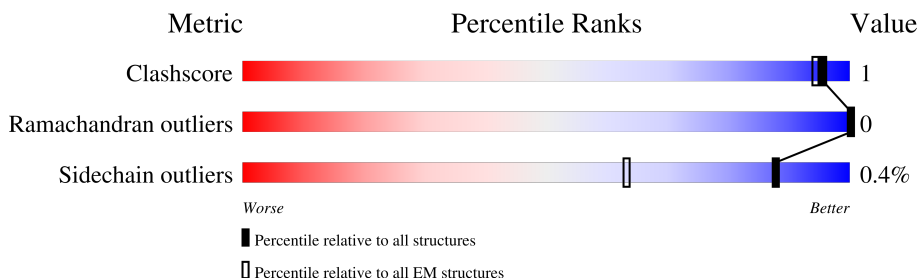
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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.



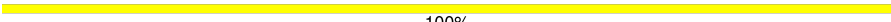
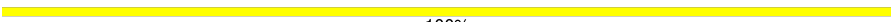

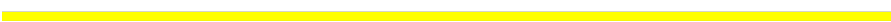






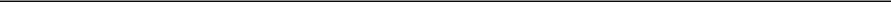

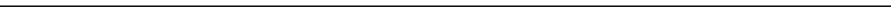


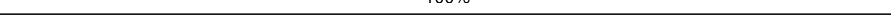
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1367	83% 13%
1	B	1367	82% 13%
1	J	1367	82% 14%
2	H	123	97% ..
2	L	123	82% 15%
3	C	2	100%
3	D	2	100%
3	E	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	2	 100%
3	I	2	 100%
3	K	2	 100%
3	M	2	 100%
3	N	2	 100%
3	P	2	 100%
3	Q	2	 100%
3	R	2	 100%
3	S	2	 100%
3	T	2	 50% 50%
3	U	2	 100%
3	V	2	 100%
3	W	2	 100%
3	X	2	 100%
4	G	3	 100%
4	O	3	 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 29599 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 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	1176	Total	C	N	O	S	0	0
			9152	5835	1504	1750	63		
1	A	1184	Total	C	N	O	S	0	0
			9204	5865	1513	1763	63		
1	B	1183	Total	C	N	O	S	0	0
			9197	5862	1513	1759	63		

There are 264 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	177	HIS	LEU	conflict	UNP A0A7U1BGV5
J	261	ILE	VAL	conflict	UNP A0A7U1BGV5
J	545	PRO	SER	conflict	UNP A0A7U1BGV5
J	762	ASN	THR	conflict	UNP A0A7U1BGV5
J	1079	PRO	ALA	conflict	UNP A0A7U1BGV5
J	1080	PRO	LEU	conflict	UNP A0A7U1BGV5
J	1217	MET	ILE	conflict	UNP A0A7U1BGV5
J	1269	PHE	LEU	conflict	UNP A0A7U1BGV5
J	1288	GLY	-	expression tag	UNP A0A7U1BGV5
J	1289	SER	-	expression tag	UNP A0A7U1BGV5
J	1290	GLY	-	expression tag	UNP A0A7U1BGV5
J	1291	TYR	-	expression tag	UNP A0A7U1BGV5
J	1292	ILE	-	expression tag	UNP A0A7U1BGV5
J	1293	PRO	-	expression tag	UNP A0A7U1BGV5
J	1294	GLU	-	expression tag	UNP A0A7U1BGV5
J	1295	ALA	-	expression tag	UNP A0A7U1BGV5
J	1296	PRO	-	expression tag	UNP A0A7U1BGV5
J	1297	ARG	-	expression tag	UNP A0A7U1BGV5
J	1298	ASP	-	expression tag	UNP A0A7U1BGV5
J	1299	GLY	-	expression tag	UNP A0A7U1BGV5
J	1300	GLN	-	expression tag	UNP A0A7U1BGV5
J	1301	ALA	-	expression tag	UNP A0A7U1BGV5
J	1302	TYR	-	expression tag	UNP A0A7U1BGV5
J	1303	VAL	-	expression tag	UNP A0A7U1BGV5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	1304	ARG	-	expression tag	UNP A0A7U1BGV5
J	1305	LYS	-	expression tag	UNP A0A7U1BGV5
J	1306	ASP	-	expression tag	UNP A0A7U1BGV5
J	1307	GLY	-	expression tag	UNP A0A7U1BGV5
J	1308	GLU	-	expression tag	UNP A0A7U1BGV5
J	1309	TRP	-	expression tag	UNP A0A7U1BGV5
J	1310	VAL	-	expression tag	UNP A0A7U1BGV5
J	1311	LEU	-	expression tag	UNP A0A7U1BGV5
J	1312	LEU	-	expression tag	UNP A0A7U1BGV5
J	1313	SER	-	expression tag	UNP A0A7U1BGV5
J	1314	THR	-	expression tag	UNP A0A7U1BGV5
J	1315	PHE	-	expression tag	UNP A0A7U1BGV5
J	1316	LEU	-	expression tag	UNP A0A7U1BGV5
J	1317	GLY	-	expression tag	UNP A0A7U1BGV5
J	1318	ARG	-	expression tag	UNP A0A7U1BGV5
J	1319	SER	-	expression tag	UNP A0A7U1BGV5
J	1320	LEU	-	expression tag	UNP A0A7U1BGV5
J	1321	GLU	-	expression tag	UNP A0A7U1BGV5
J	1322	VAL	-	expression tag	UNP A0A7U1BGV5
J	1323	LEU	-	expression tag	UNP A0A7U1BGV5
J	1324	PHE	-	expression tag	UNP A0A7U1BGV5
J	1325	GLN	-	expression tag	UNP A0A7U1BGV5
J	1326	GLY	-	expression tag	UNP A0A7U1BGV5
J	1327	PRO	-	expression tag	UNP A0A7U1BGV5
J	1328	GLY	-	expression tag	UNP A0A7U1BGV5
J	1329	HIS	-	expression tag	UNP A0A7U1BGV5
J	1330	HIS	-	expression tag	UNP A0A7U1BGV5
J	1331	HIS	-	expression tag	UNP A0A7U1BGV5
J	1332	HIS	-	expression tag	UNP A0A7U1BGV5
J	1333	HIS	-	expression tag	UNP A0A7U1BGV5
J	1334	HIS	-	expression tag	UNP A0A7U1BGV5
J	1335	HIS	-	expression tag	UNP A0A7U1BGV5
J	1336	HIS	-	expression tag	UNP A0A7U1BGV5
J	1337	SER	-	expression tag	UNP A0A7U1BGV5
J	1338	ALA	-	expression tag	UNP A0A7U1BGV5
J	1339	TRP	-	expression tag	UNP A0A7U1BGV5
J	1340	SER	-	expression tag	UNP A0A7U1BGV5
J	1341	HIS	-	expression tag	UNP A0A7U1BGV5
J	1342	PRO	-	expression tag	UNP A0A7U1BGV5
J	1343	GLN	-	expression tag	UNP A0A7U1BGV5
J	1344	PHE	-	expression tag	UNP A0A7U1BGV5
J	1345	GLU	-	expression tag	UNP A0A7U1BGV5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	1346	LYS	-	expression tag	UNP A0A7U1BGV5
J	1347	GLY	-	expression tag	UNP A0A7U1BGV5
J	1348	GLY	-	expression tag	UNP A0A7U1BGV5
J	1349	GLY	-	expression tag	UNP A0A7U1BGV5
J	1350	SER	-	expression tag	UNP A0A7U1BGV5
J	1351	GLY	-	expression tag	UNP A0A7U1BGV5
J	1352	GLY	-	expression tag	UNP A0A7U1BGV5
J	1353	GLY	-	expression tag	UNP A0A7U1BGV5
J	1354	GLY	-	expression tag	UNP A0A7U1BGV5
J	1355	SER	-	expression tag	UNP A0A7U1BGV5
J	1356	GLY	-	expression tag	UNP A0A7U1BGV5
J	1357	GLY	-	expression tag	UNP A0A7U1BGV5
J	1358	SER	-	expression tag	UNP A0A7U1BGV5
J	1359	ALA	-	expression tag	UNP A0A7U1BGV5
J	1360	TRP	-	expression tag	UNP A0A7U1BGV5
J	1361	SER	-	expression tag	UNP A0A7U1BGV5
J	1362	HIS	-	expression tag	UNP A0A7U1BGV5
J	1363	PRO	-	expression tag	UNP A0A7U1BGV5
J	1364	GLN	-	expression tag	UNP A0A7U1BGV5
J	1365	PHE	-	expression tag	UNP A0A7U1BGV5
J	1366	GLU	-	expression tag	UNP A0A7U1BGV5
J	1367	LYS	-	expression tag	UNP A0A7U1BGV5
A	177	HIS	LEU	conflict	UNP A0A7U1BGV5
A	261	ILE	VAL	conflict	UNP A0A7U1BGV5
A	545	PRO	SER	conflict	UNP A0A7U1BGV5
A	762	ASN	THR	conflict	UNP A0A7U1BGV5
A	1079	PRO	ALA	conflict	UNP A0A7U1BGV5
A	1080	PRO	LEU	conflict	UNP A0A7U1BGV5
A	1217	MET	ILE	conflict	UNP A0A7U1BGV5
A	1269	PHE	LEU	conflict	UNP A0A7U1BGV5
A	1288	GLY	-	expression tag	UNP A0A7U1BGV5
A	1289	SER	-	expression tag	UNP A0A7U1BGV5
A	1290	GLY	-	expression tag	UNP A0A7U1BGV5
A	1291	TYR	-	expression tag	UNP A0A7U1BGV5
A	1292	ILE	-	expression tag	UNP A0A7U1BGV5
A	1293	PRO	-	expression tag	UNP A0A7U1BGV5
A	1294	GLU	-	expression tag	UNP A0A7U1BGV5
A	1295	ALA	-	expression tag	UNP A0A7U1BGV5
A	1296	PRO	-	expression tag	UNP A0A7U1BGV5
A	1297	ARG	-	expression tag	UNP A0A7U1BGV5
A	1298	ASP	-	expression tag	UNP A0A7U1BGV5
A	1299	GLY	-	expression tag	UNP A0A7U1BGV5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1300	GLN	-	expression tag	UNP A0A7U1BGV5
A	1301	ALA	-	expression tag	UNP A0A7U1BGV5
A	1302	TYR	-	expression tag	UNP A0A7U1BGV5
A	1303	VAL	-	expression tag	UNP A0A7U1BGV5
A	1304	ARG	-	expression tag	UNP A0A7U1BGV5
A	1305	LYS	-	expression tag	UNP A0A7U1BGV5
A	1306	ASP	-	expression tag	UNP A0A7U1BGV5
A	1307	GLY	-	expression tag	UNP A0A7U1BGV5
A	1308	GLU	-	expression tag	UNP A0A7U1BGV5
A	1309	TRP	-	expression tag	UNP A0A7U1BGV5
A	1310	VAL	-	expression tag	UNP A0A7U1BGV5
A	1311	LEU	-	expression tag	UNP A0A7U1BGV5
A	1312	LEU	-	expression tag	UNP A0A7U1BGV5
A	1313	SER	-	expression tag	UNP A0A7U1BGV5
A	1314	THR	-	expression tag	UNP A0A7U1BGV5
A	1315	PHE	-	expression tag	UNP A0A7U1BGV5
A	1316	LEU	-	expression tag	UNP A0A7U1BGV5
A	1317	GLY	-	expression tag	UNP A0A7U1BGV5
A	1318	ARG	-	expression tag	UNP A0A7U1BGV5
A	1319	SER	-	expression tag	UNP A0A7U1BGV5
A	1320	LEU	-	expression tag	UNP A0A7U1BGV5
A	1321	GLU	-	expression tag	UNP A0A7U1BGV5
A	1322	VAL	-	expression tag	UNP A0A7U1BGV5
A	1323	LEU	-	expression tag	UNP A0A7U1BGV5
A	1324	PHE	-	expression tag	UNP A0A7U1BGV5
A	1325	GLN	-	expression tag	UNP A0A7U1BGV5
A	1326	GLY	-	expression tag	UNP A0A7U1BGV5
A	1327	PRO	-	expression tag	UNP A0A7U1BGV5
A	1328	GLY	-	expression tag	UNP A0A7U1BGV5
A	1329	HIS	-	expression tag	UNP A0A7U1BGV5
A	1330	HIS	-	expression tag	UNP A0A7U1BGV5
A	1331	HIS	-	expression tag	UNP A0A7U1BGV5
A	1332	HIS	-	expression tag	UNP A0A7U1BGV5
A	1333	HIS	-	expression tag	UNP A0A7U1BGV5
A	1334	HIS	-	expression tag	UNP A0A7U1BGV5
A	1335	HIS	-	expression tag	UNP A0A7U1BGV5
A	1336	HIS	-	expression tag	UNP A0A7U1BGV5
A	1337	SER	-	expression tag	UNP A0A7U1BGV5
A	1338	ALA	-	expression tag	UNP A0A7U1BGV5
A	1339	TRP	-	expression tag	UNP A0A7U1BGV5
A	1340	SER	-	expression tag	UNP A0A7U1BGV5
A	1341	HIS	-	expression tag	UNP A0A7U1BGV5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1342	PRO	-	expression tag	UNP A0A7U1BGV5
A	1343	GLN	-	expression tag	UNP A0A7U1BGV5
A	1344	PHE	-	expression tag	UNP A0A7U1BGV5
A	1345	GLU	-	expression tag	UNP A0A7U1BGV5
A	1346	LYS	-	expression tag	UNP A0A7U1BGV5
A	1347	GLY	-	expression tag	UNP A0A7U1BGV5
A	1348	GLY	-	expression tag	UNP A0A7U1BGV5
A	1349	GLY	-	expression tag	UNP A0A7U1BGV5
A	1350	SER	-	expression tag	UNP A0A7U1BGV5
A	1351	GLY	-	expression tag	UNP A0A7U1BGV5
A	1352	GLY	-	expression tag	UNP A0A7U1BGV5
A	1353	GLY	-	expression tag	UNP A0A7U1BGV5
A	1354	GLY	-	expression tag	UNP A0A7U1BGV5
A	1355	SER	-	expression tag	UNP A0A7U1BGV5
A	1356	GLY	-	expression tag	UNP A0A7U1BGV5
A	1357	GLY	-	expression tag	UNP A0A7U1BGV5
A	1358	SER	-	expression tag	UNP A0A7U1BGV5
A	1359	ALA	-	expression tag	UNP A0A7U1BGV5
A	1360	TRP	-	expression tag	UNP A0A7U1BGV5
A	1361	SER	-	expression tag	UNP A0A7U1BGV5
A	1362	HIS	-	expression tag	UNP A0A7U1BGV5
A	1363	PRO	-	expression tag	UNP A0A7U1BGV5
A	1364	GLN	-	expression tag	UNP A0A7U1BGV5
A	1365	PHE	-	expression tag	UNP A0A7U1BGV5
A	1366	GLU	-	expression tag	UNP A0A7U1BGV5
A	1367	LYS	-	expression tag	UNP A0A7U1BGV5
B	177	HIS	LEU	conflict	UNP A0A7U1BGV5
B	261	ILE	VAL	conflict	UNP A0A7U1BGV5
B	545	PRO	SER	conflict	UNP A0A7U1BGV5
B	762	ASN	THR	conflict	UNP A0A7U1BGV5
B	1079	PRO	ALA	conflict	UNP A0A7U1BGV5
B	1080	PRO	LEU	conflict	UNP A0A7U1BGV5
B	1217	MET	ILE	conflict	UNP A0A7U1BGV5
B	1269	PHE	LEU	conflict	UNP A0A7U1BGV5
B	1288	GLY	-	expression tag	UNP A0A7U1BGV5
B	1289	SER	-	expression tag	UNP A0A7U1BGV5
B	1290	GLY	-	expression tag	UNP A0A7U1BGV5
B	1291	TYR	-	expression tag	UNP A0A7U1BGV5
B	1292	ILE	-	expression tag	UNP A0A7U1BGV5
B	1293	PRO	-	expression tag	UNP A0A7U1BGV5
B	1294	GLU	-	expression tag	UNP A0A7U1BGV5
B	1295	ALA	-	expression tag	UNP A0A7U1BGV5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1296	PRO	-	expression tag	UNP A0A7U1BGV5
B	1297	ARG	-	expression tag	UNP A0A7U1BGV5
B	1298	ASP	-	expression tag	UNP A0A7U1BGV5
B	1299	GLY	-	expression tag	UNP A0A7U1BGV5
B	1300	GLN	-	expression tag	UNP A0A7U1BGV5
B	1301	ALA	-	expression tag	UNP A0A7U1BGV5
B	1302	TYR	-	expression tag	UNP A0A7U1BGV5
B	1303	VAL	-	expression tag	UNP A0A7U1BGV5
B	1304	ARG	-	expression tag	UNP A0A7U1BGV5
B	1305	LYS	-	expression tag	UNP A0A7U1BGV5
B	1306	ASP	-	expression tag	UNP A0A7U1BGV5
B	1307	GLY	-	expression tag	UNP A0A7U1BGV5
B	1308	GLU	-	expression tag	UNP A0A7U1BGV5
B	1309	TRP	-	expression tag	UNP A0A7U1BGV5
B	1310	VAL	-	expression tag	UNP A0A7U1BGV5
B	1311	LEU	-	expression tag	UNP A0A7U1BGV5
B	1312	LEU	-	expression tag	UNP A0A7U1BGV5
B	1313	SER	-	expression tag	UNP A0A7U1BGV5
B	1314	THR	-	expression tag	UNP A0A7U1BGV5
B	1315	PHE	-	expression tag	UNP A0A7U1BGV5
B	1316	LEU	-	expression tag	UNP A0A7U1BGV5
B	1317	GLY	-	expression tag	UNP A0A7U1BGV5
B	1318	ARG	-	expression tag	UNP A0A7U1BGV5
B	1319	SER	-	expression tag	UNP A0A7U1BGV5
B	1320	LEU	-	expression tag	UNP A0A7U1BGV5
B	1321	GLU	-	expression tag	UNP A0A7U1BGV5
B	1322	VAL	-	expression tag	UNP A0A7U1BGV5
B	1323	LEU	-	expression tag	UNP A0A7U1BGV5
B	1324	PHE	-	expression tag	UNP A0A7U1BGV5
B	1325	GLN	-	expression tag	UNP A0A7U1BGV5
B	1326	GLY	-	expression tag	UNP A0A7U1BGV5
B	1327	PRO	-	expression tag	UNP A0A7U1BGV5
B	1328	GLY	-	expression tag	UNP A0A7U1BGV5
B	1329	HIS	-	expression tag	UNP A0A7U1BGV5
B	1330	HIS	-	expression tag	UNP A0A7U1BGV5
B	1331	HIS	-	expression tag	UNP A0A7U1BGV5
B	1332	HIS	-	expression tag	UNP A0A7U1BGV5
B	1333	HIS	-	expression tag	UNP A0A7U1BGV5
B	1334	HIS	-	expression tag	UNP A0A7U1BGV5
B	1335	HIS	-	expression tag	UNP A0A7U1BGV5
B	1336	HIS	-	expression tag	UNP A0A7U1BGV5
B	1337	SER	-	expression tag	UNP A0A7U1BGV5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1338	ALA	-	expression tag	UNP A0A7U1BGV5
B	1339	TRP	-	expression tag	UNP A0A7U1BGV5
B	1340	SER	-	expression tag	UNP A0A7U1BGV5
B	1341	HIS	-	expression tag	UNP A0A7U1BGV5
B	1342	PRO	-	expression tag	UNP A0A7U1BGV5
B	1343	GLN	-	expression tag	UNP A0A7U1BGV5
B	1344	PHE	-	expression tag	UNP A0A7U1BGV5
B	1345	GLU	-	expression tag	UNP A0A7U1BGV5
B	1346	LYS	-	expression tag	UNP A0A7U1BGV5
B	1347	GLY	-	expression tag	UNP A0A7U1BGV5
B	1348	GLY	-	expression tag	UNP A0A7U1BGV5
B	1349	GLY	-	expression tag	UNP A0A7U1BGV5
B	1350	SER	-	expression tag	UNP A0A7U1BGV5
B	1351	GLY	-	expression tag	UNP A0A7U1BGV5
B	1352	GLY	-	expression tag	UNP A0A7U1BGV5
B	1353	GLY	-	expression tag	UNP A0A7U1BGV5
B	1354	GLY	-	expression tag	UNP A0A7U1BGV5
B	1355	SER	-	expression tag	UNP A0A7U1BGV5
B	1356	GLY	-	expression tag	UNP A0A7U1BGV5
B	1357	GLY	-	expression tag	UNP A0A7U1BGV5
B	1358	SER	-	expression tag	UNP A0A7U1BGV5
B	1359	ALA	-	expression tag	UNP A0A7U1BGV5
B	1360	TRP	-	expression tag	UNP A0A7U1BGV5
B	1361	SER	-	expression tag	UNP A0A7U1BGV5
B	1362	HIS	-	expression tag	UNP A0A7U1BGV5
B	1363	PRO	-	expression tag	UNP A0A7U1BGV5
B	1364	GLN	-	expression tag	UNP A0A7U1BGV5
B	1365	PHE	-	expression tag	UNP A0A7U1BGV5
B	1366	GLU	-	expression tag	UNP A0A7U1BGV5
B	1367	LYS	-	expression tag	UNP A0A7U1BGV5

- Molecule 2 is a protein called Human polyclonal Fab model with polyalanine backbone - Heavy chain.

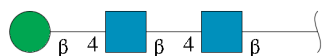
Mol	Chain	Residues	Atoms				AltConf	Trace
2	H	121	Total	C	N	O	0	0
			605	363	121	121		
2	L	105	Total	C	N	O	0	0
			525	315	105	105		

- 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	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
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	K	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	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	R	2	Total	C	N	O	0	0
			28	16	2	10		
3	S	2	Total	C	N	O	0	0
			28	16	2	10		
3	T	2	Total	C	N	O	0	0
			28	16	2	10		
3	U	2	Total	C	N	O	0	0
			28	16	2	10		
3	V	2	Total	C	N	O	0	0
			28	16	2	10		
3	W	2	Total	C	N	O	0	0
			28	16	2	10		
3	X	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	O	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



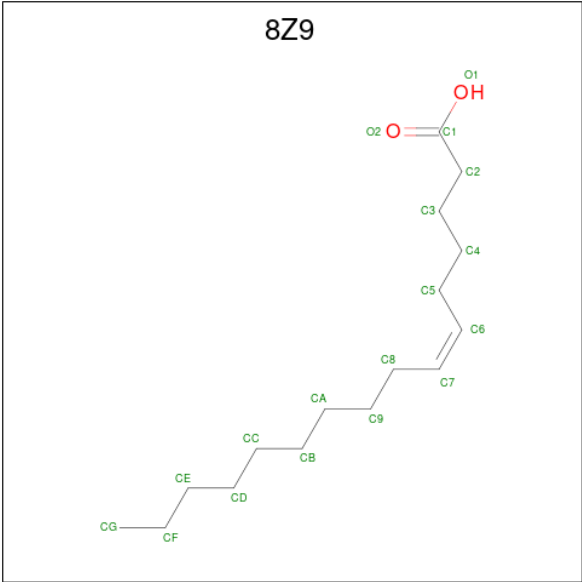
Mol	Chain	Residues	Atoms				AltConf
5	J	1	Total	C	N	O	0
			14	8	1	5	
5	J	1	Total	C	N	O	0
			14	8	1	5	
5	J	1	Total	C	N	O	0
			14	8	1	5	
5	J	1	Total	C	N	O	0
			14	8	1	5	
5	J	1	Total	C	N	O	0
			14	8	1	5	
5	J	1	Total	C	N	O	0
			14	8	1	5	

Continued on next page...

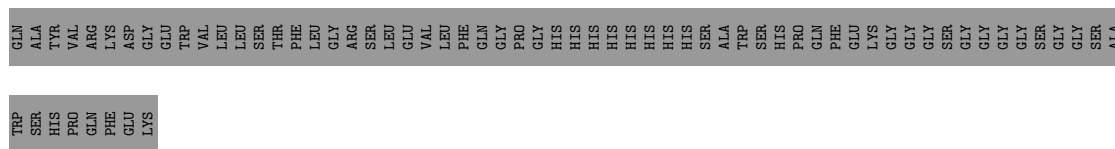
Continued from previous page...

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

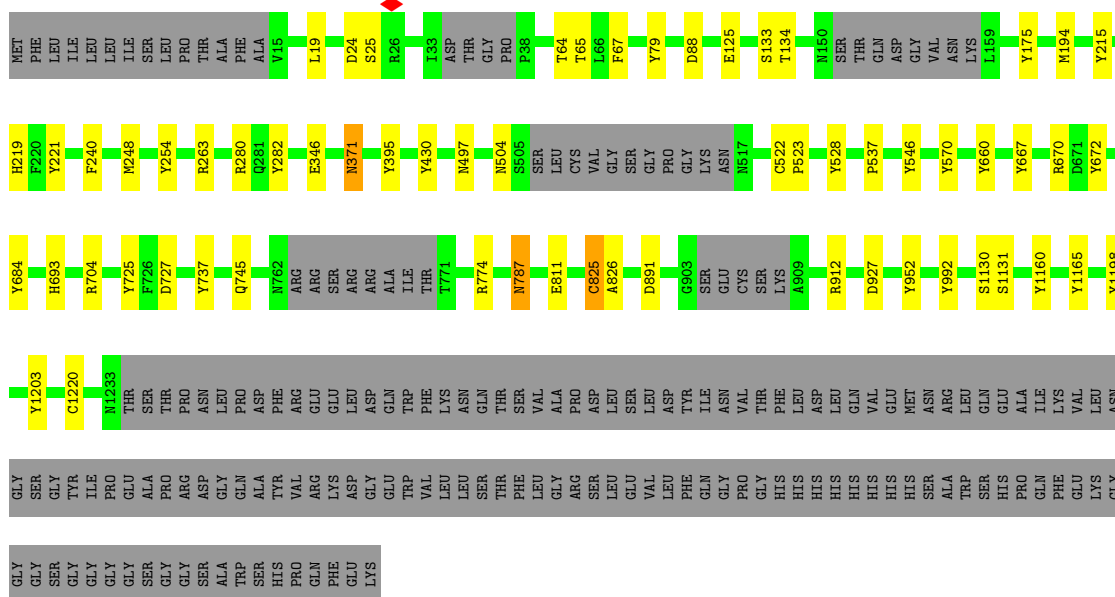
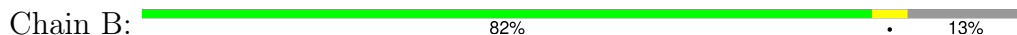
- Molecule 6 is Sapientic acid (three-letter code: 8Z9) (formula: C₁₆H₃₀O₂).



Mol	Chain	Residues	Atoms			AltConf
6	J	1	Total	C	O	0
			18	16	2	
6	A	1	Total	C	O	0
			18	16	2	
6	A	1	Total	C	O	0
			18	16	2	



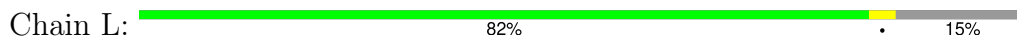
- Molecule 1: Spike protein



- Molecule 2: Human polyclonal Fab model with polyalanine backbone - Heavy chain



- Molecule 2: Human polyclonal Fab model with polyalanine backbone - Heavy chain



- 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 D:  100%

MAG1
MAG2

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

Chain E:  100%

MAG1
MAG2

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

Chain F:  100%

MAG1
MAG2

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

Chain I:  100%

MAG1
MAG2

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

Chain K:  100%

MAG1
MAG2

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

Chain M:  100%

MAG1
MAG2

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

Chain N:  100%

MAG1
MAG2

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

Chain P:  100%MAG1
MAG2


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

Chain Q:  100%MAG1
MAG2


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

Chain R:  100%MAG1
MAG2

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

Chain S:  100%MAG1
MAG2

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

Chain T:  50% 50%MAG1
MAG2

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

Chain U:  100%MAG1
MAG2

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

Chain V:  100%

MAG1
MAG2

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

Chain W:  100%

MAG1
MAG2

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

Chain X:  100%

MAG1
MAG2

- 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%

MAG1
MAG2
BMA3

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

Chain O:  100%

MAG1
MAG2
BMA3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	54733	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.106	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	350.19998, 350.19998, 350.19998	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	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, 8Z9, 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	A	1.23	30/9417 (0.3%)	0.91	18/12821 (0.1%)
1	B	1.24	22/9410 (0.2%)	0.90	17/12810 (0.1%)
1	J	1.23	21/9363 (0.2%)	0.90	16/12743 (0.1%)
All	All	1.23	73/28190 (0.3%)	0.90	51/38374 (0.1%)

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1220	CYS	CB-SG	-7.32	1.69	1.82
1	B	79	TYR	CB-CG	-6.95	1.41	1.51
1	B	67	PHE	CB-CG	-6.95	1.39	1.51
1	B	125	GLU	CG-CD	-6.86	1.41	1.51
1	B	1203	TYR	CB-CG	-6.77	1.41	1.51
1	A	1203	TYR	CB-CG	-6.77	1.41	1.51
1	J	528	TYR	CB-CG	-6.72	1.41	1.51
1	B	240	PHE	CB-CG	-6.67	1.40	1.51
1	A	430	TYR	CG-CD1	-6.63	1.30	1.39
1	J	756	CYS	CB-SG	-6.62	1.71	1.82
1	J	79	TYR	CB-CG	-6.54	1.41	1.51
1	J	1124	GLU	CG-CD	-6.44	1.42	1.51
1	B	737	TYR	CB-CG	-6.38	1.42	1.51
1	J	170	TYR	CG-CD2	-6.36	1.30	1.39
1	A	79	TYR	CB-CG	-6.35	1.42	1.51
1	J	67	PHE	CB-CG	-6.31	1.40	1.51
1	A	1136	CYS	CB-SG	-6.29	1.71	1.82
1	A	125	GLU	CG-CD	-6.27	1.42	1.51
1	B	528	TYR	CB-CG	-6.25	1.42	1.51
1	A	215	TYR	CB-CG	-6.12	1.42	1.51
1	B	430	TYR	CG-CD1	-6.11	1.31	1.39
1	A	667	TYR	CB-CG	-6.05	1.42	1.51
1	J	1203	TYR	CB-CG	-6.02	1.42	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	1146	VAL	CB-CG2	-6.01	1.40	1.52
1	A	67	PHE	CB-CG	-5.99	1.41	1.51
1	A	305	GLU	CD-OE1	-5.99	1.19	1.25
1	A	254	TYR	CB-CG	-5.98	1.42	1.51
1	J	430	TYR	CG-CD1	-5.98	1.31	1.39
1	J	305	GLU	CD-OE1	-5.91	1.19	1.25
1	A	756	CYS	CB-SG	-5.89	1.72	1.81
1	J	667	TYR	CB-CG	-5.88	1.42	1.51
1	A	528	TYR	CB-CG	-5.82	1.43	1.51
1	J	725	TYR	CB-CG	-5.81	1.43	1.51
1	A	843	TYR	CB-CG	-5.76	1.43	1.51
1	A	570	TYR	CB-CG	-5.74	1.43	1.51
1	A	725	TYR	CB-CG	-5.71	1.43	1.51
1	B	125	GLU	CD-OE1	-5.65	1.19	1.25
1	B	1160	TYR	CB-CG	-5.55	1.43	1.51
1	B	725	TYR	CB-CG	-5.53	1.43	1.51
1	B	1220	CYS	CB-SG	-5.42	1.73	1.81
1	J	215	TYR	CB-CG	-5.40	1.43	1.51
1	J	570	TYR	CB-CG	-5.38	1.43	1.51
1	J	228	TYR	CB-CG	-5.37	1.43	1.51
1	A	221	TYR	CB-CG	-5.34	1.43	1.51
1	A	737	TYR	CB-CG	-5.34	1.43	1.51
1	A	1203	TYR	CG-CD2	-5.32	1.32	1.39
1	B	1165	TYR	CB-CG	-5.31	1.43	1.51
1	A	125	GLU	CD-OE1	-5.30	1.19	1.25
1	A	546	TYR	CB-CG	-5.30	1.43	1.51
1	J	797	TYR	CB-CG	-5.29	1.43	1.51
1	B	221	TYR	CB-CG	-5.28	1.43	1.51
1	B	570	TYR	CB-CG	-5.27	1.43	1.51
1	B	672	TYR	CG-CD1	-5.26	1.32	1.39
1	J	485	VAL	CB-CG1	-5.23	1.41	1.52
1	J	811	GLU	CG-CD	-5.22	1.44	1.51
1	A	346	GLU	CD-OE2	-5.19	1.20	1.25
1	A	219	HIS	CB-CG	-5.19	1.40	1.50
1	J	240	PHE	CB-CG	-5.17	1.42	1.51
1	A	485	VAL	CB-CG1	-5.15	1.42	1.52
1	J	346	GLU	CD-OE2	-5.14	1.20	1.25
1	B	346	GLU	CD-OE2	-5.13	1.20	1.25
1	A	286	PHE	CB-CG	-5.12	1.42	1.51
1	B	1203	TYR	CG-CD2	-5.12	1.32	1.39
1	A	282	TYR	CB-CG	-5.09	1.44	1.51
1	A	672	TYR	CG-CD1	-5.09	1.32	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	PHE	CB-CG	-5.08	1.42	1.51
1	B	811	GLU	CG-CD	-5.07	1.44	1.51
1	J	1220	CYS	CB-SG	-5.07	1.73	1.81
1	B	254	TYR	CB-CG	-5.06	1.44	1.51
1	B	175	TYR	CG-CD2	-5.05	1.32	1.39
1	A	240	PHE	CB-CG	-5.04	1.42	1.51
1	A	646	GLU	CD-OE1	-5.02	1.20	1.25
1	B	219	HIS	CB-CG	-5.01	1.41	1.50

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	ARG	NE-CZ-NH2	-8.77	115.92	120.30
1	A	282	TYR	CB-CG-CD2	-8.69	115.79	121.00
1	J	282	TYR	CB-CG-CD2	-8.63	115.82	121.00
1	A	912	ARG	NE-CZ-NH2	-8.31	116.14	120.30
1	B	282	TYR	CB-CG-CD2	-8.17	116.10	121.00
1	B	912	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	J	774	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	B	704	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	B	263	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	B	395	TYR	CB-CG-CD1	-6.54	117.08	121.00
1	B	280	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	A	704	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	B	774	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	J	395	TYR	CB-CG-CD1	-6.30	117.22	121.00
1	J	670	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	A	147	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	B	737	TYR	CB-CG-CD1	-6.22	117.27	121.00
1	B	1198	TYR	CB-CG-CD2	-6.20	117.28	121.00
1	J	660	TYR	CB-CG-CD2	-6.16	117.31	121.00
1	J	528	TYR	CB-CG-CD2	-6.14	117.32	121.00
1	A	263	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	B	952	TYR	CB-CG-CD1	-6.12	117.33	121.00
1	B	660	TYR	CB-CG-CD2	-6.10	117.34	121.00
1	J	254	TYR	CB-CG-CD1	-6.04	117.38	121.00
1	A	660	TYR	CB-CG-CD2	-6.03	117.39	121.00
1	B	546	TYR	CB-CG-CD1	-6.01	117.39	121.00
1	A	774	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	A	575	PRO	N-CA-C	-5.86	96.87	112.10
1	J	1132	ARG	NE-CZ-NH2	5.82	123.21	120.30
1	J	704	ARG	NE-CZ-NH1	5.80	123.20	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	670	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	J	684	TYR	CB-CG-CD1	-5.52	117.69	121.00
1	J	280	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	528	TYR	CB-CG-CD2	-5.49	117.70	121.00
1	B	670	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	J	1198	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	A	395	TYR	CB-CG-CD1	-5.40	117.76	121.00
1	B	684	TYR	CB-CG-CD1	-5.34	117.80	121.00
1	J	944	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	B	667	TYR	CB-CG-CD1	-5.27	117.84	121.00
1	A	684	TYR	CB-CG-CD1	-5.21	117.87	121.00
1	J	282	TYR	CB-CG-CD1	5.21	124.13	121.00
1	J	681	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	215	TYR	CB-CG-CD2	-5.19	117.89	121.00
1	A	1224	TYR	CB-CG-CD2	-5.14	117.91	121.00
1	J	952	TYR	CB-CG-CD2	-5.14	117.91	121.00
1	A	667	TYR	CB-CG-CD1	-5.13	117.92	121.00
1	A	26	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	A	215	TYR	CB-CG-CD2	-5.11	117.93	121.00
1	B	537	PRO	N-CA-C	-5.10	98.84	112.10
1	A	282	TYR	CB-CG-CD1	5.02	124.01	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	9204	0	8891	12	0
1	B	9197	0	8890	19	0
1	J	9152	0	8845	15	0
2	H	605	0	155	1	0
2	L	525	0	127	2	0
3	C	28	0	25	0	0
3	D	28	0	25	0	0
3	E	28	0	25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	28	0	25	0	0
3	I	28	0	25	0	0
3	K	28	0	25	0	0
3	M	28	0	25	0	0
3	N	28	0	25	0	0
3	P	28	0	25	0	0
3	Q	28	0	25	0	0
3	R	28	0	25	0	0
3	S	28	0	25	0	0
3	T	28	0	25	1	0
3	U	28	0	25	0	0
3	V	28	0	25	0	0
3	W	28	0	25	0	0
3	X	28	0	25	0	0
4	G	39	0	33	0	0
4	O	39	0	33	0	0
5	A	112	0	104	1	0
5	B	70	0	65	2	0
5	J	126	0	117	1	0
6	A	36	0	0	0	0
6	J	18	0	0	0	0
All	All	29599	0	27685	49	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 1.

All (49) 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:371:ASN:N	1:B:371:ASN:OD1	2.28	0.66
1:J:371:ASN:N	1:J:371:ASN:OD1	2.31	0.62
1:A:371:ASN:N	1:A:371:ASN:OD1	2.31	0.62
1:B:24:ASP:N	1:B:24:ASP:OD1	2.35	0.58
1:B:693:HIS:NE2	5:B:1404:NAG:H82	2.20	0.57
1:J:713:ASN:O	5:J:1403:NAG:H82	2.05	0.55
1:A:713:ASN:O	5:A:1402:NAG:H82	2.08	0.54
1:A:24:ASP:OD1	1:A:24:ASP:N	2.44	0.51
2:H:74:UNK:O	2:H:75:UNK:C	2.59	0.51
1:B:727:ASP:O	3:T:1:NAG:H81	2.12	0.49
1:B:787:ASN:OD1	1:B:787:ASN:N	2.46	0.48
1:J:927:ASP:N	1:J:927:ASP:OD1	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:927:ASP:N	1:B:927:ASP:OD1	2.46	0.48
1:J:536:ASN:HB2	1:J:537:PRO:HD3	1.94	0.48
1:J:504:ASN:OD1	1:J:504:ASN:N	2.47	0.48
1:A:927:ASP:N	1:A:927:ASP:OD1	2.46	0.48
1:B:504:ASN:N	1:B:504:ASN:OD1	2.46	0.47
1:B:64:THR:OG1	1:B:65:THR:N	2.48	0.47
1:B:88:ASP:OD1	1:B:88:ASP:N	2.44	0.47
1:A:133:SER:OG	1:A:134:THR:N	2.46	0.46
1:B:1130:SER:OG	1:B:1131:SER:N	2.47	0.46
1:A:504:ASN:OD1	1:A:504:ASN:N	2.48	0.46
1:B:693:HIS:CE1	5:B:1404:NAG:H82	2.51	0.46
2:L:81:UNK:O	2:L:82:UNK:C	2.63	0.46
1:J:133:SER:OG	1:J:134:THR:N	2.48	0.46
1:J:1046:ASN:O	1:J:1047:ALA:HB3	2.16	0.45
1:J:1045:VAL:C	1:J:1046:ASN:O	2.54	0.45
1:A:900:GLY:O	1:A:901:CYS:C	2.55	0.45
1:J:901:CYS:SG	1:J:901:CYS:O	2.75	0.45
1:J:137:ASN:OD1	1:J:137:ASN:C	2.56	0.44
1:B:19:LEU:HD21	1:B:194:MET:HB3	2.00	0.44
1:A:901:CYS:O	1:A:901:CYS:SG	2.75	0.44
1:B:825:CYS:SG	1:B:826:ALA:N	2.90	0.44
1:J:96:LYS:HB3	1:J:97:PRO:HD2	2.00	0.43
1:A:64:THR:OG1	1:A:65:THR:N	2.50	0.43
1:B:522:CYS:HA	1:B:523:PRO:HD3	1.90	0.43
1:A:137:ASN:OD1	1:A:137:ASN:C	2.57	0.43
1:A:787:ASN:OD1	1:A:787:ASN:N	2.52	0.43
1:B:497:ASN:OD1	1:B:497:ASN:N	2.48	0.42
1:J:339:ASP:OD1	1:J:339:ASP:N	2.46	0.42
1:B:24:ASP:CG	1:B:25:SER:N	2.72	0.42
1:J:891:ASP:OD2	1:J:992:TYR:HB3	2.20	0.41
1:J:64:THR:OG1	1:J:65:THR:N	2.53	0.41
1:B:133:SER:OG	1:B:134:THR:N	2.53	0.41
2:L:70:UNK:O	2:L:71:UNK:C	2.68	0.41
1:B:891:ASP:OD2	1:B:992:TYR:HB3	2.22	0.40
1:A:738:ASN:OD1	1:A:738:ASN:C	2.59	0.40
1:J:745:GLN:CD	1:J:745:GLN:N	2.75	0.40
1:B:745:GLN:N	1:B:745:GLN:CD	2.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1172/1367 (86%)	1153 (98%)	19 (2%)	0	100	100
1	B	1171/1367 (86%)	1151 (98%)	20 (2%)	0	100	100
1	J	1162/1367 (85%)	1143 (98%)	19 (2%)	0	100	100
All	All	3505/4101 (86%)	3447 (98%)	58 (2%)	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	A	1030/1182 (87%)	1027 (100%)	3 (0%)	91	96
1	B	1028/1182 (87%)	1024 (100%)	4 (0%)	89	95
1	J	1024/1182 (87%)	1019 (100%)	5 (0%)	86	94
All	All	3082/3546 (87%)	3070 (100%)	12 (0%)	88	95

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	137	ASN
1	J	162	LEU
1	J	371	ASN
1	J	787	ASN
1	J	992	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	137	ASN
1	A	371	ASN
1	A	787	ASN
1	B	248	MET
1	B	371	ASN
1	B	787	ASN
1	B	825	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	219	HIS
1	J	252	HIS
1	J	418	GLN
1	J	1103	GLN
1	A	219	HIS
1	A	252	HIS
1	A	1011	GLN
1	B	219	HIS
1	B	252	HIS
1	B	849	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 ⓘ

40 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	C	1	1,3	14,14,15	2.09	3 (21%)	17,19,21	1.01	1 (5%)
3	NAG	C	2	3	14,14,15	2.10	2 (14%)	17,19,21	0.71	0
3	NAG	D	1	1,3	14,14,15	1.94	3 (21%)	17,19,21	1.32	3 (17%)
3	NAG	D	2	3	14,14,15	1.98	2 (14%)	17,19,21	0.96	0
3	NAG	E	1	1,3	14,14,15	2.10	3 (21%)	17,19,21	1.27	3 (17%)
3	NAG	E	2	3	14,14,15	2.09	3 (21%)	17,19,21	0.76	0
3	NAG	F	1	1,3	14,14,15	2.02	3 (21%)	17,19,21	0.85	1 (5%)
3	NAG	F	2	3	14,14,15	2.08	2 (14%)	17,19,21	0.72	0
4	NAG	G	1	1,4	14,14,15	1.97	2 (14%)	17,19,21	0.97	1 (5%)
4	NAG	G	2	4	14,14,15	2.11	4 (28%)	17,19,21	0.96	0
4	BMA	G	3	4	11,11,12	1.78	2 (18%)	15,15,17	0.69	0
3	NAG	I	1	1,3	14,14,15	2.05	3 (21%)	17,19,21	0.80	0
3	NAG	I	2	3	14,14,15	2.07	2 (14%)	17,19,21	0.72	0
3	NAG	K	1	1,3	14,14,15	1.95	3 (21%)	17,19,21	1.57	4 (23%)
3	NAG	K	2	3	14,14,15	2.06	2 (14%)	17,19,21	0.85	0
3	NAG	M	1	1,3	14,14,15	2.02	3 (21%)	17,19,21	1.23	3 (17%)
3	NAG	M	2	3	14,14,15	2.08	3 (21%)	17,19,21	0.82	1 (5%)
3	NAG	N	1	1,3	14,14,15	2.01	2 (14%)	17,19,21	0.82	1 (5%)
3	NAG	N	2	3	14,14,15	2.12	2 (14%)	17,19,21	0.77	0
4	NAG	O	1	1,4	14,14,15	1.92	2 (14%)	17,19,21	1.06	2 (11%)
4	NAG	O	2	4	14,14,15	2.06	2 (14%)	17,19,21	0.80	0
4	BMA	O	3	4	11,11,12	1.77	2 (18%)	15,15,17	0.81	1 (6%)
3	NAG	P	1	1,3	14,14,15	2.01	4 (28%)	17,19,21	1.06	2 (11%)
3	NAG	P	2	3	14,14,15	2.12	2 (14%)	17,19,21	0.74	0
3	NAG	Q	1	1,3	14,14,15	1.99	3 (21%)	17,19,21	0.84	0
3	NAG	Q	2	3	14,14,15	2.08	2 (14%)	17,19,21	0.73	0
3	NAG	R	1	1,3	14,14,15	0.30	0	17,19,21	1.04	1 (5%)
3	NAG	R	2	3	14,14,15	2.03	3 (21%)	17,19,21	0.96	1 (5%)
3	NAG	S	1	1,3	14,14,15	2.09	3 (21%)	17,19,21	0.74	0
3	NAG	S	2	3	14,14,15	2.11	3 (21%)	17,19,21	0.80	1 (5%)
3	NAG	T	1	1,3	14,14,15	1.90	3 (21%)	17,19,21	1.46	3 (17%)
3	NAG	T	2	3	14,14,15	2.09	3 (21%)	17,19,21	0.72	0
3	NAG	U	1	1,3	14,14,15	1.95	4 (28%)	17,19,21	1.13	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	U	2	3	14,14,15	2.12	2 (14%)	17,19,21	0.79	1 (5%)
3	NAG	V	1	1,3	14,14,15	2.09	2 (14%)	17,19,21	0.70	0
3	NAG	V	2	3	14,14,15	2.15	3 (21%)	17,19,21	0.83	1 (5%)
3	NAG	W	1	1,3	14,14,15	1.96	2 (14%)	17,19,21	0.96	2 (11%)
3	NAG	W	2	3	14,14,15	2.06	2 (14%)	17,19,21	0.82	0
3	NAG	X	1	1,3	14,14,15	1.97	2 (14%)	17,19,21	0.98	2 (11%)
3	NAG	X	2	3	14,14,15	2.11	2 (14%)	17,19,21	0.79	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	1/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	1/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	1/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	NAG	M	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	1/6/23/26	0/1/1/1
4	NAG	O	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	0/1/1/1
4	BMA	O	3	4	-	1/2/19/22	0/1/1/1
3	NAG	P	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	P	2	3	-	1/6/23/26	0/1/1/1
3	NAG	Q	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	1/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	R	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	R	2	3	-	0/6/23/26	0/1/1/1
3	NAG	S	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1
3	NAG	T	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	T	2	3	-	1/6/23/26	0/1/1/1
3	NAG	U	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
3	NAG	V	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	2/6/23/26	0/1/1/1
3	NAG	W	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	W	2	3	-	0/6/23/26	0/1/1/1
3	NAG	X	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	X	2	3	-	2/6/23/26	0/1/1/1

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	2	NAG	O5-C1	6.79	1.55	1.43
3	N	2	NAG	O5-C1	6.73	1.55	1.43
3	P	2	NAG	O5-C1	6.70	1.54	1.43
3	F	2	NAG	O5-C1	6.67	1.54	1.43
3	V	2	NAG	O5-C1	6.64	1.54	1.43
3	C	2	NAG	O5-C1	6.63	1.54	1.43
3	S	2	NAG	O5-C1	6.57	1.54	1.43
3	Q	2	NAG	O5-C1	6.54	1.54	1.43
3	T	2	NAG	O5-C1	6.53	1.54	1.43
3	X	2	NAG	O5-C1	6.52	1.54	1.43
3	C	1	NAG	O5-C1	6.51	1.54	1.43
3	E	2	NAG	O5-C1	6.47	1.54	1.43
3	I	2	NAG	O5-C1	6.44	1.54	1.43
3	V	1	NAG	O5-C1	6.43	1.54	1.43
3	W	2	NAG	O5-C1	6.42	1.54	1.43
4	G	2	NAG	O5-C1	6.38	1.54	1.43
3	M	2	NAG	O5-C1	6.36	1.54	1.43
3	F	1	NAG	O5-C1	6.35	1.54	1.43
3	K	2	NAG	O5-C1	6.35	1.54	1.43
4	O	2	NAG	O5-C1	6.34	1.54	1.43
3	I	1	NAG	O5-C1	6.32	1.54	1.43
3	N	1	NAG	O5-C1	6.24	1.54	1.43
3	S	1	NAG	O5-C1	6.23	1.54	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2	NAG	O5-C1	6.19	1.54	1.43
4	G	1	NAG	O5-C1	6.14	1.54	1.43
3	P	1	NAG	O5-C1	6.11	1.54	1.43
3	R	2	NAG	O5-C1	6.10	1.53	1.43
3	X	1	NAG	O5-C1	6.10	1.53	1.43
3	W	1	NAG	O5-C1	6.03	1.53	1.43
3	Q	1	NAG	O5-C1	6.00	1.53	1.43
3	E	1	NAG	O5-C1	5.84	1.53	1.43
3	M	1	NAG	O5-C1	5.82	1.53	1.43
3	K	1	NAG	O5-C1	5.78	1.53	1.43
4	O	1	NAG	O5-C1	5.75	1.53	1.43
3	D	1	NAG	O5-C1	5.71	1.53	1.43
3	U	1	NAG	O5-C1	5.59	1.53	1.43
3	T	1	NAG	O5-C1	5.51	1.53	1.43
4	G	3	BMA	O2-C2	-4.15	1.34	1.43
4	O	3	BMA	O2-C2	-4.15	1.34	1.43
3	E	1	NAG	C1-C2	-2.94	1.48	1.52
3	E	1	NAG	C3-C2	-2.80	1.46	1.52
3	R	2	NAG	C3-C2	-2.68	1.46	1.52
3	M	1	NAG	C3-C2	-2.68	1.46	1.52
3	K	2	NAG	C3-C2	-2.63	1.47	1.52
4	G	2	NAG	C3-C2	-2.61	1.47	1.52
3	S	1	NAG	C3-C2	-2.59	1.47	1.52
4	O	2	NAG	C3-C2	-2.57	1.47	1.52
3	M	2	NAG	C3-C2	-2.56	1.47	1.52
3	W	1	NAG	C3-C2	-2.53	1.47	1.52
3	D	1	NAG	C1-C2	-2.51	1.48	1.52
3	K	1	NAG	C3-C2	-2.51	1.47	1.52
3	S	1	NAG	C1-C2	-2.50	1.48	1.52
3	Q	1	NAG	C3-C2	-2.50	1.47	1.52
4	G	1	NAG	C3-C2	-2.48	1.47	1.52
3	M	1	NAG	C1-C2	-2.46	1.49	1.52
4	O	1	NAG	C3-C2	-2.45	1.47	1.52
3	U	1	NAG	C1-C2	-2.44	1.49	1.52
3	T	1	NAG	C1-C2	-2.42	1.49	1.52
3	V	1	NAG	C3-C2	-2.41	1.47	1.52
3	T	2	NAG	C3-C2	-2.41	1.47	1.52
3	E	2	NAG	C3-C2	-2.40	1.47	1.52
3	W	2	NAG	C3-C2	-2.40	1.47	1.52
3	X	2	NAG	C3-C2	-2.38	1.47	1.52
3	I	1	NAG	C3-C2	-2.38	1.47	1.52
3	C	1	NAG	C3-C2	-2.35	1.47	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	2	NAG	C3-C2	-2.33	1.47	1.52
3	P	2	NAG	C3-C2	-2.32	1.47	1.52
3	N	1	NAG	C3-C2	-2.31	1.47	1.52
3	N	2	NAG	C3-C2	-2.29	1.47	1.52
3	D	2	NAG	C3-C2	-2.29	1.47	1.52
3	K	1	NAG	C1-C2	-2.24	1.49	1.52
3	I	2	NAG	C3-C2	-2.21	1.47	1.52
3	T	1	NAG	C3-C2	-2.21	1.47	1.52
3	S	2	NAG	C3-C2	-2.20	1.47	1.52
3	F	2	NAG	C3-C2	-2.19	1.47	1.52
3	U	2	NAG	C3-C2	-2.19	1.47	1.52
4	O	3	BMA	C2-C3	-2.18	1.49	1.52
4	G	3	BMA	C2-C3	-2.18	1.49	1.52
3	C	2	NAG	C3-C2	-2.18	1.47	1.52
3	P	1	NAG	C1-C2	-2.18	1.49	1.52
3	P	1	NAG	C4-C3	2.16	1.57	1.52
3	V	2	NAG	C1-C2	-2.16	1.49	1.52
3	F	1	NAG	C3-C2	-2.15	1.48	1.52
3	D	1	NAG	C3-C2	-2.14	1.48	1.52
3	C	1	NAG	C1-C2	-2.13	1.49	1.52
3	Q	2	NAG	C3-C2	-2.13	1.48	1.52
3	U	1	NAG	C3-C2	-2.12	1.48	1.52
3	U	1	NAG	C4-C3	2.12	1.57	1.52
3	S	2	NAG	C1-C2	-2.10	1.49	1.52
3	M	2	NAG	C1-C2	-2.10	1.49	1.52
3	R	2	NAG	C1-C2	-2.08	1.49	1.52
4	G	2	NAG	C1-C2	-2.08	1.49	1.52
3	X	1	NAG	C3-C2	-2.06	1.48	1.52
3	P	1	NAG	C3-C2	-2.05	1.48	1.52
3	I	1	NAG	C4-C3	2.04	1.57	1.52
4	G	2	NAG	C4-C3	2.04	1.57	1.52
3	F	1	NAG	C4-C3	2.04	1.57	1.52
3	Q	1	NAG	C1-C2	-2.03	1.49	1.52
3	E	2	NAG	C4-C3	2.01	1.57	1.52
3	T	2	NAG	C4-C3	2.01	1.57	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	1	NAG	O5-C5-C6	-4.46	98.98	107.66
3	T	1	NAG	O5-C5-C6	-3.49	100.86	107.66
3	R	2	NAG	C4-C3-C2	-2.96	106.68	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	NAG	O4-C4-C3	-2.92	103.50	110.38
4	O	1	NAG	C3-C4-C5	-2.85	105.06	110.23
3	M	1	NAG	O5-C5-C6	-2.79	102.23	107.66
3	D	1	NAG	C1-O5-C5	-2.79	108.45	112.19
3	D	1	NAG	O5-C5-C6	-2.78	102.26	107.66
3	M	1	NAG	O4-C4-C3	-2.76	103.88	110.38
3	K	1	NAG	O4-C4-C3	-2.75	103.89	110.38
3	E	1	NAG	O5-C5-C6	-2.67	102.47	107.66
3	F	1	NAG	C3-C4-C5	-2.64	105.45	110.23
3	N	1	NAG	C3-C4-C5	-2.60	105.52	110.23
3	W	1	NAG	C3-C4-C5	-2.49	105.72	110.23
4	G	1	NAG	C3-C4-C5	-2.48	105.74	110.23
3	R	1	NAG	C3-C4-C5	2.42	114.63	110.23
3	E	1	NAG	C3-C4-C5	-2.36	105.95	110.23
3	D	1	NAG	C3-C4-C5	-2.35	105.96	110.23
3	K	1	NAG	C3-C4-C5	-2.27	106.11	110.23
3	M	2	NAG	C4-C3-C2	-2.24	107.73	111.02
3	T	1	NAG	C1-C2-N2	2.19	113.89	110.43
3	M	1	NAG	C3-C4-C5	-2.18	106.28	110.23
3	V	2	NAG	C4-C3-C2	-2.18	107.83	111.02
4	O	1	NAG	O5-C5-C6	-2.17	103.44	107.66
3	P	1	NAG	C1-O5-C5	-2.14	109.31	112.19
3	C	1	NAG	C4-C3-C2	-2.13	107.89	111.02
4	O	3	BMA	C2-C3-C4	-2.13	107.11	110.86
3	W	1	NAG	C1-O5-C5	-2.12	109.34	112.19
3	U	1	NAG	C3-C4-C5	-2.11	106.41	110.23
3	X	2	NAG	C4-C3-C2	-2.11	107.93	111.02
3	P	1	NAG	C4-C3-C2	-2.10	107.94	111.02
3	S	2	NAG	C4-C3-C2	-2.09	107.96	111.02
3	X	1	NAG	C4-C3-C2	-2.08	107.97	111.02
3	T	1	NAG	O5-C1-C2	-2.08	108.07	111.29
3	X	1	NAG	C1-O5-C5	-2.07	109.41	112.19
3	K	1	NAG	C1-O5-C5	-2.05	109.44	112.19
3	U	2	NAG	C4-C3-C2	-2.03	108.04	111.02

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	S	2	NAG	O5-C5-C6-O6
3	R	1	NAG	C8-C7-N2-C2
3	U	2	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

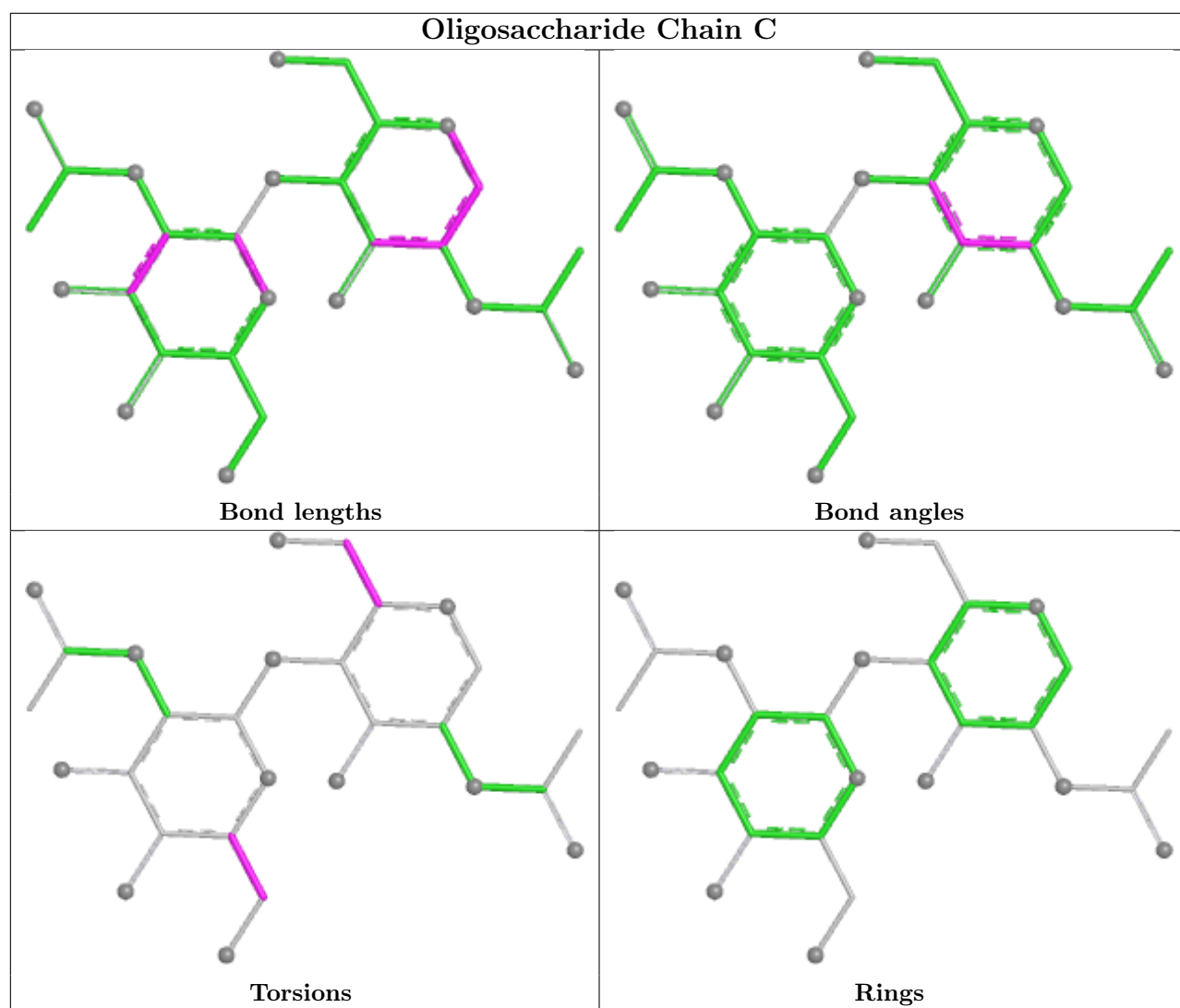
Mol	Chain	Res	Type	Atoms
3	V	2	NAG	O5-C5-C6-O6
3	X	2	NAG	O5-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
3	R	1	NAG	O7-C7-N2-C2
4	G	3	BMA	O5-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
3	S	2	NAG	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
4	O	3	BMA	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	U	2	NAG	C4-C5-C6-O6
3	T	1	NAG	C1-C2-N2-C7
3	P	1	NAG	C3-C2-N2-C7
3	X	1	NAG	C3-C2-N2-C7
3	R	1	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	T	2	NAG	O5-C5-C6-O6
3	P	1	NAG	C1-C2-N2-C7
3	X	1	NAG	C1-C2-N2-C7
3	T	1	NAG	C4-C5-C6-O6
3	T	1	NAG	C3-C2-N2-C7
3	V	2	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	X	2	NAG	C4-C5-C6-O6

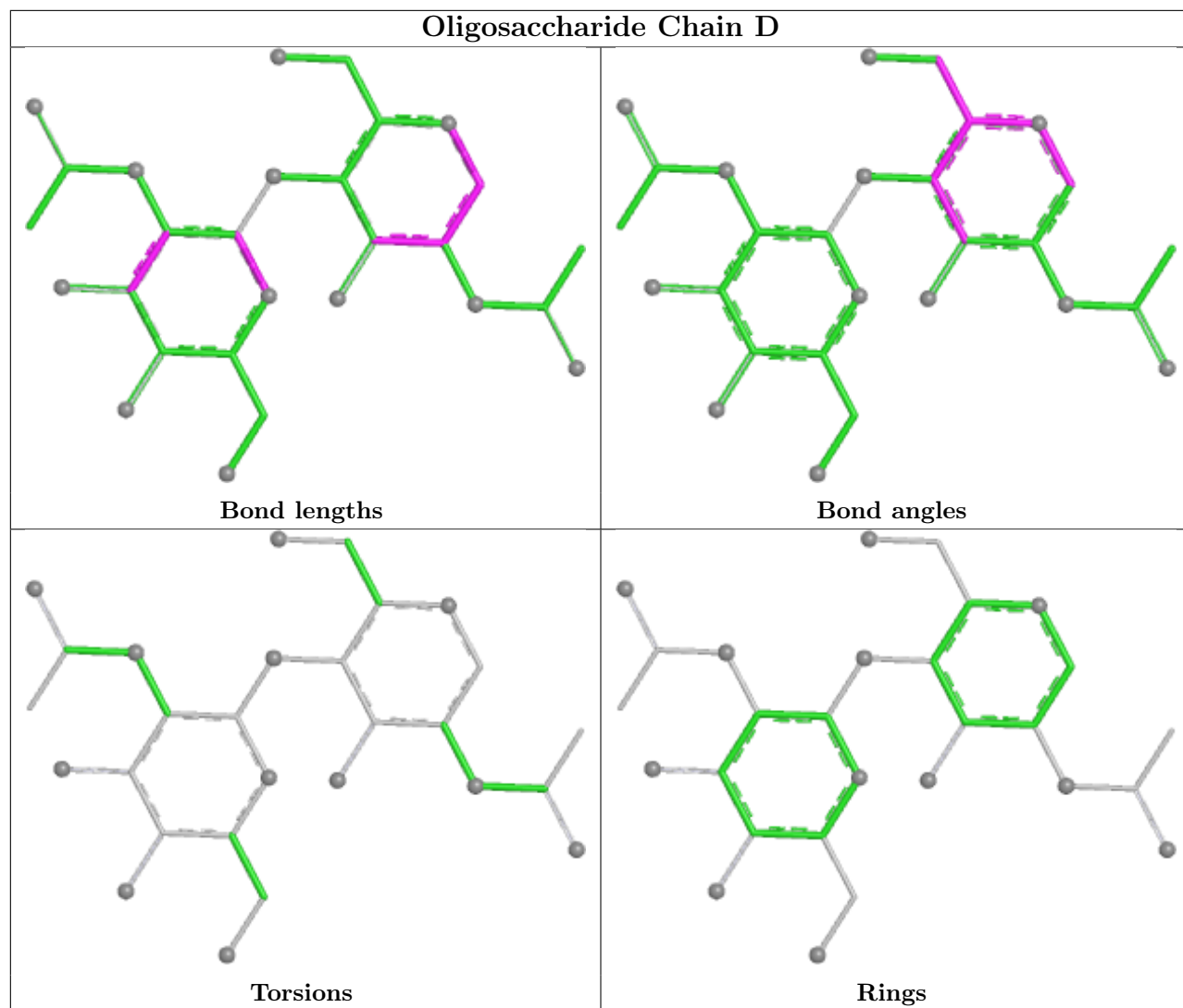
There are no ring outliers.

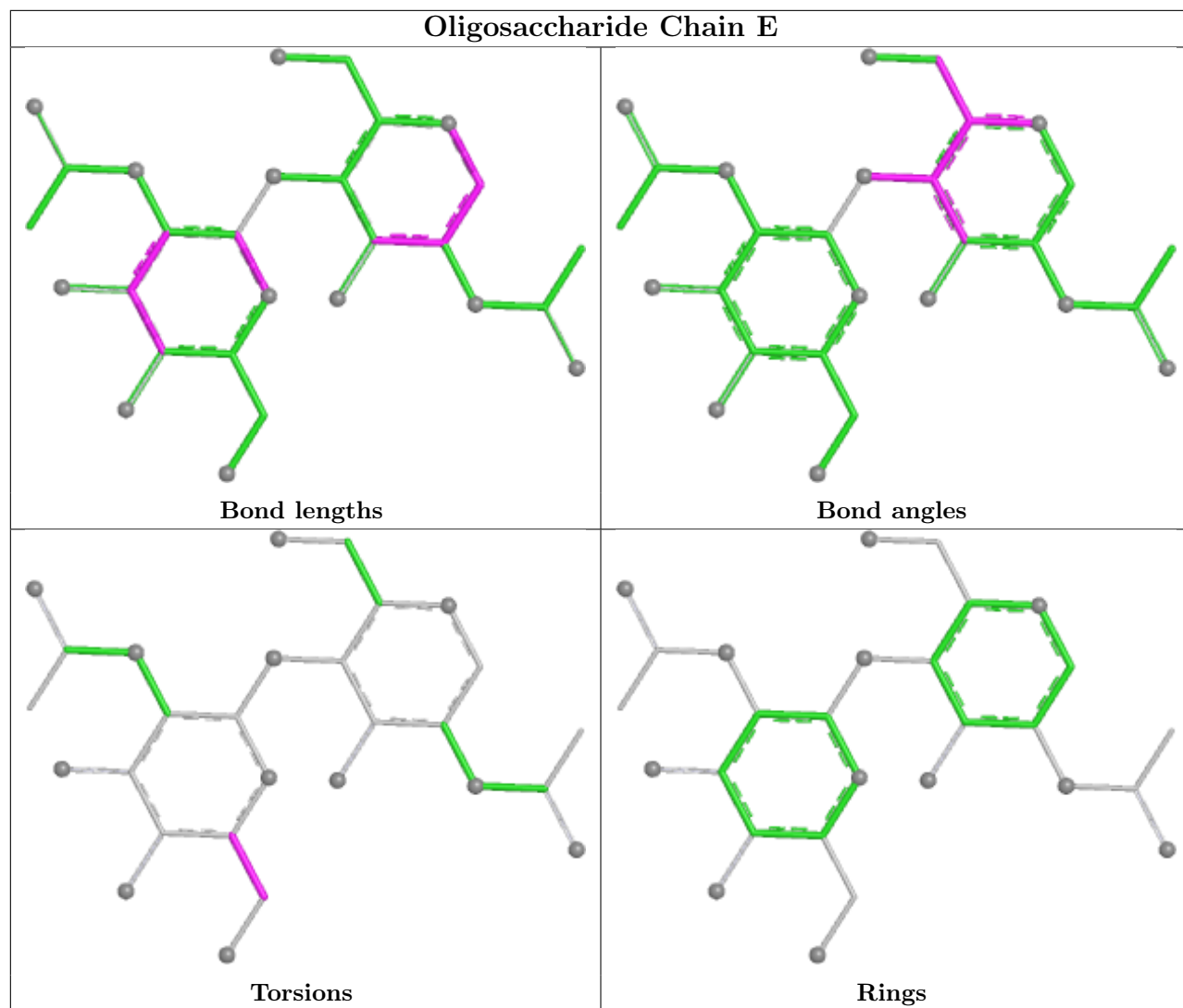
1 monomer is involved in 1 short contact:

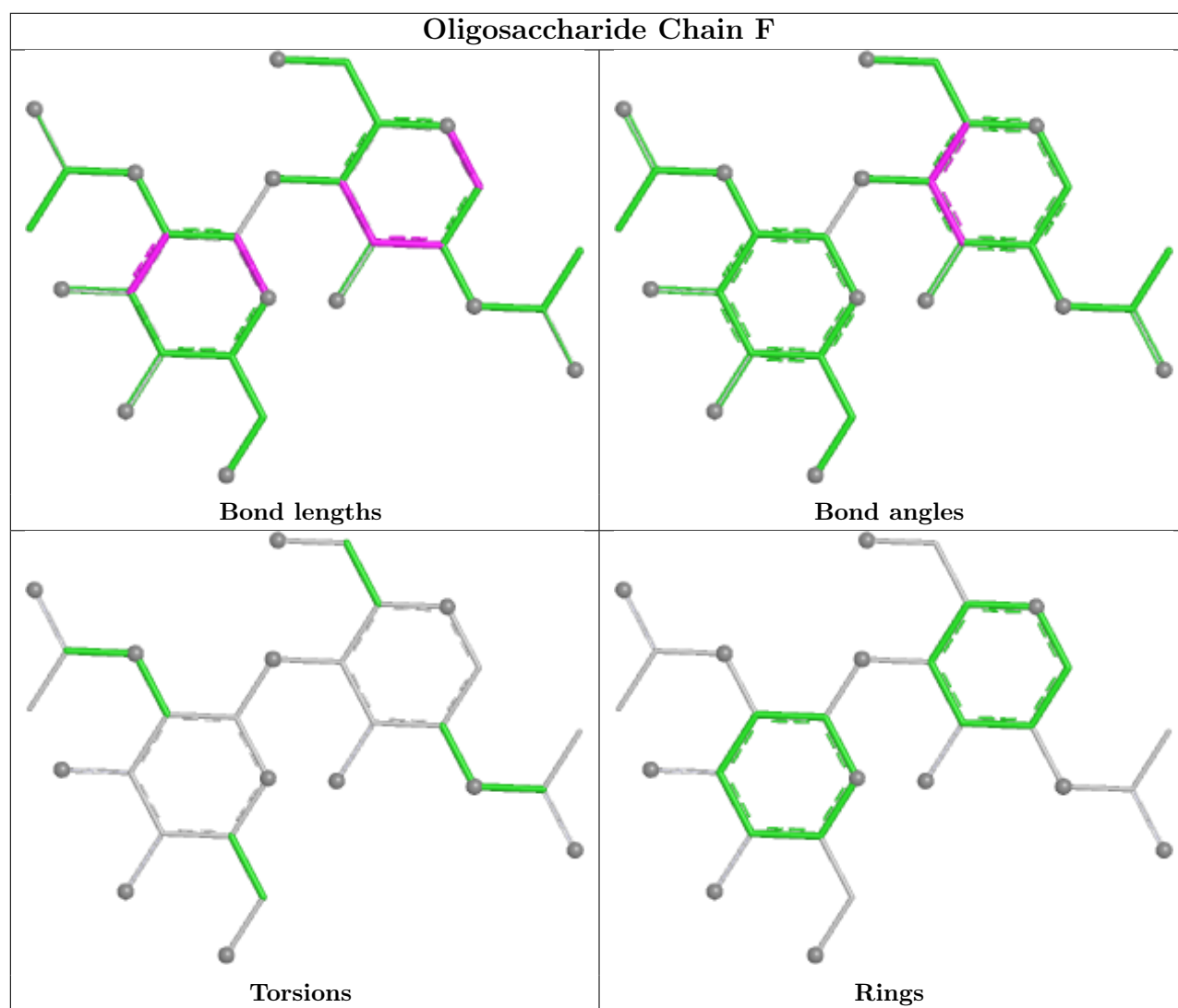
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	T	1	NAG	1	0

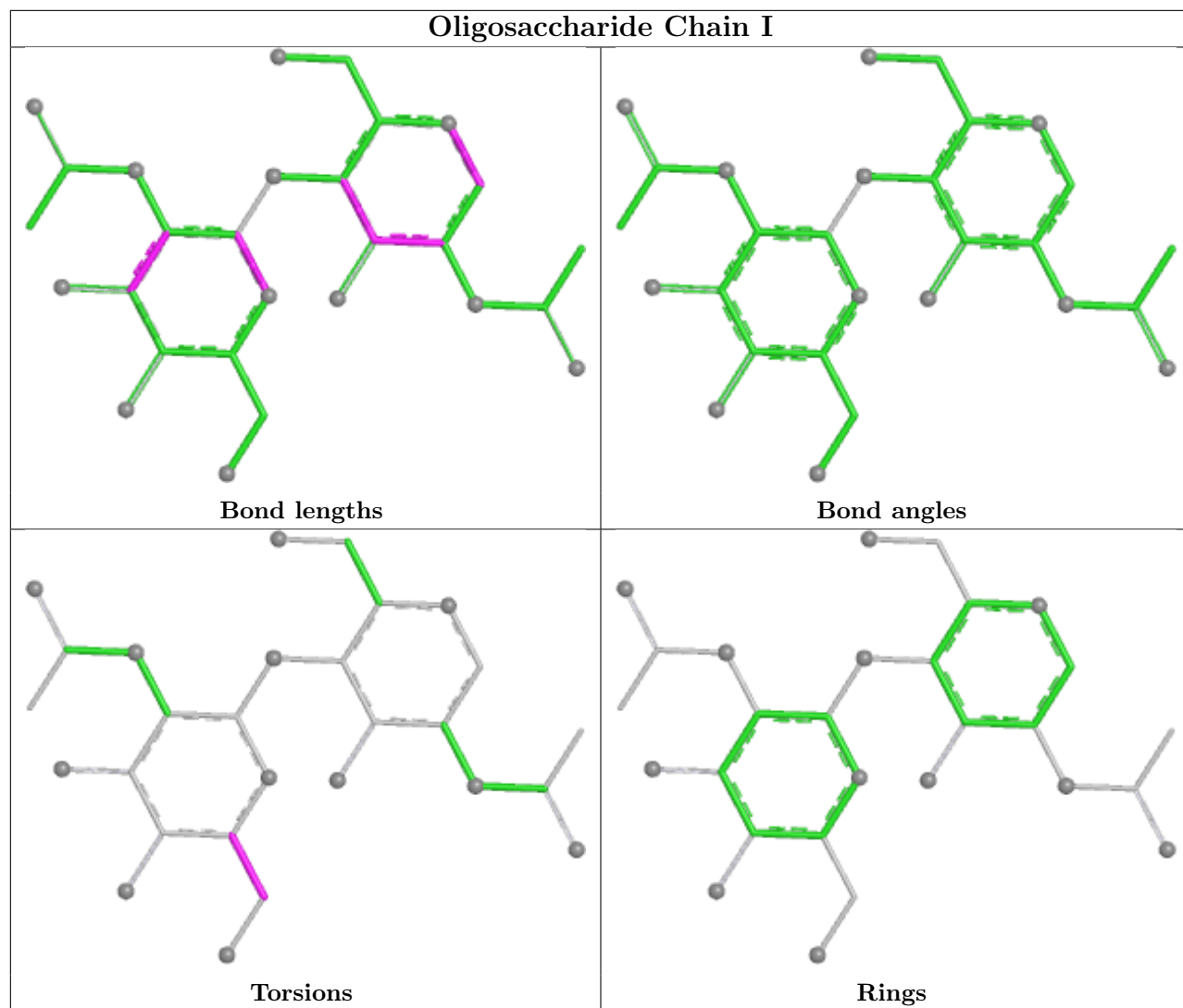
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

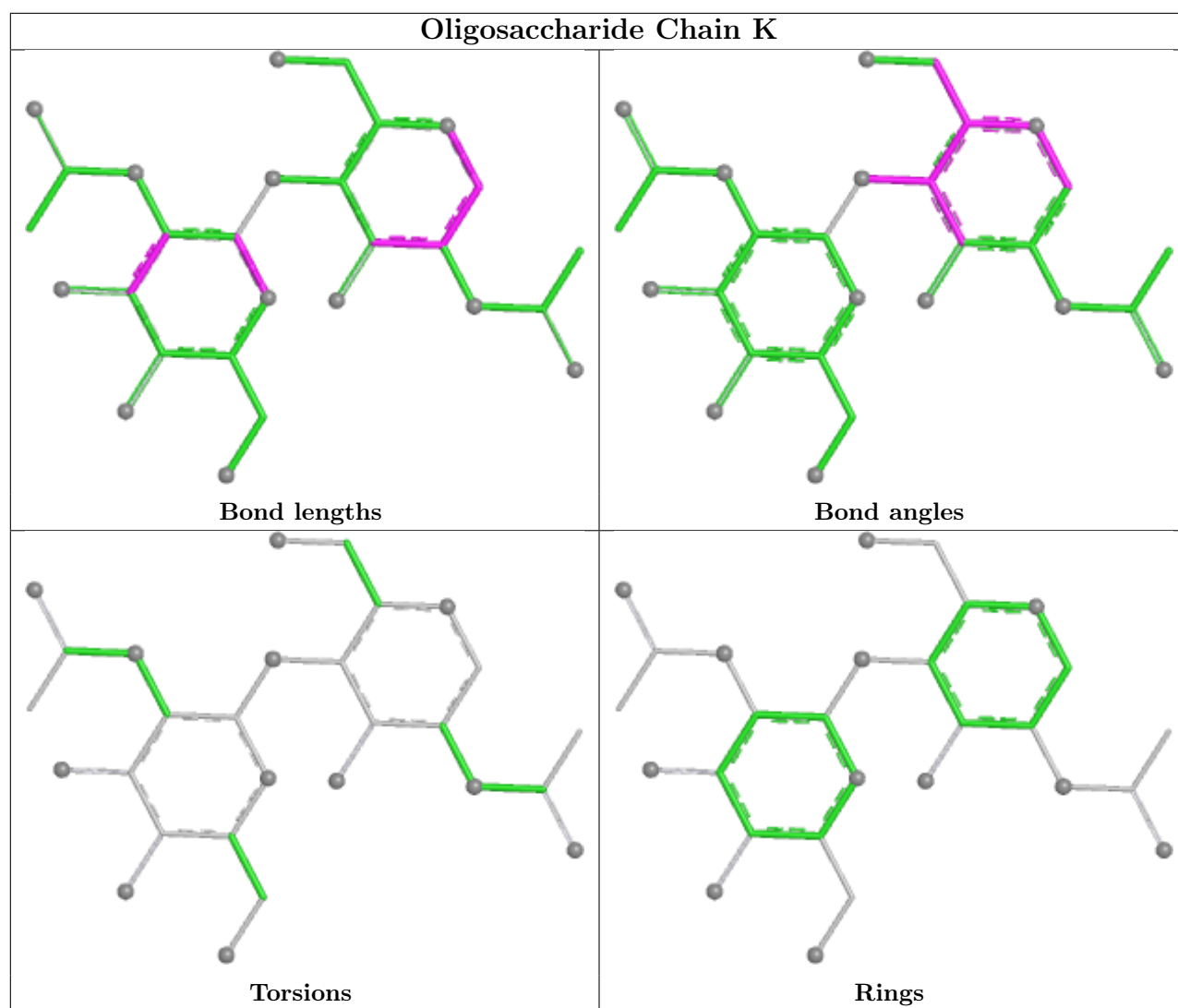


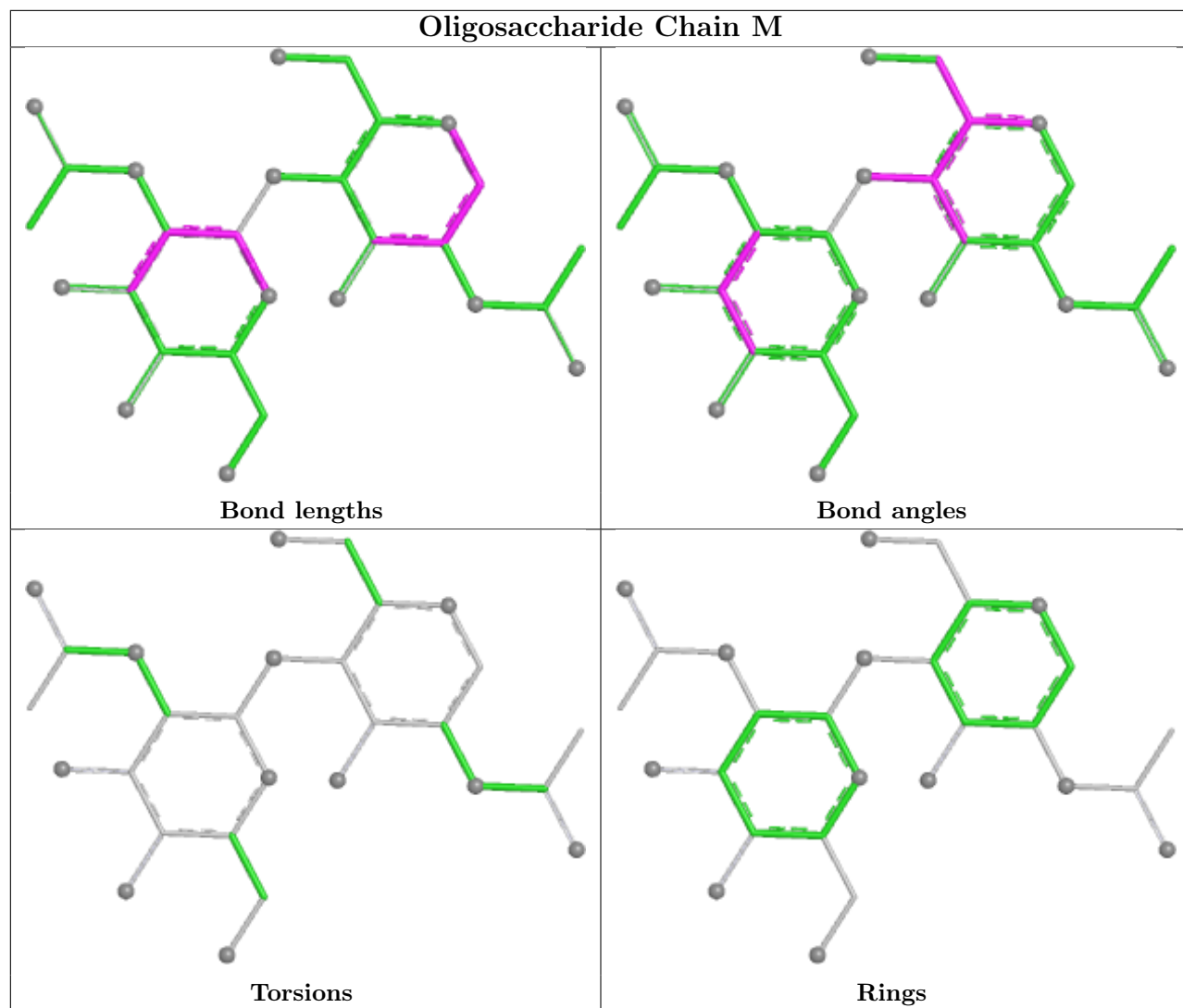


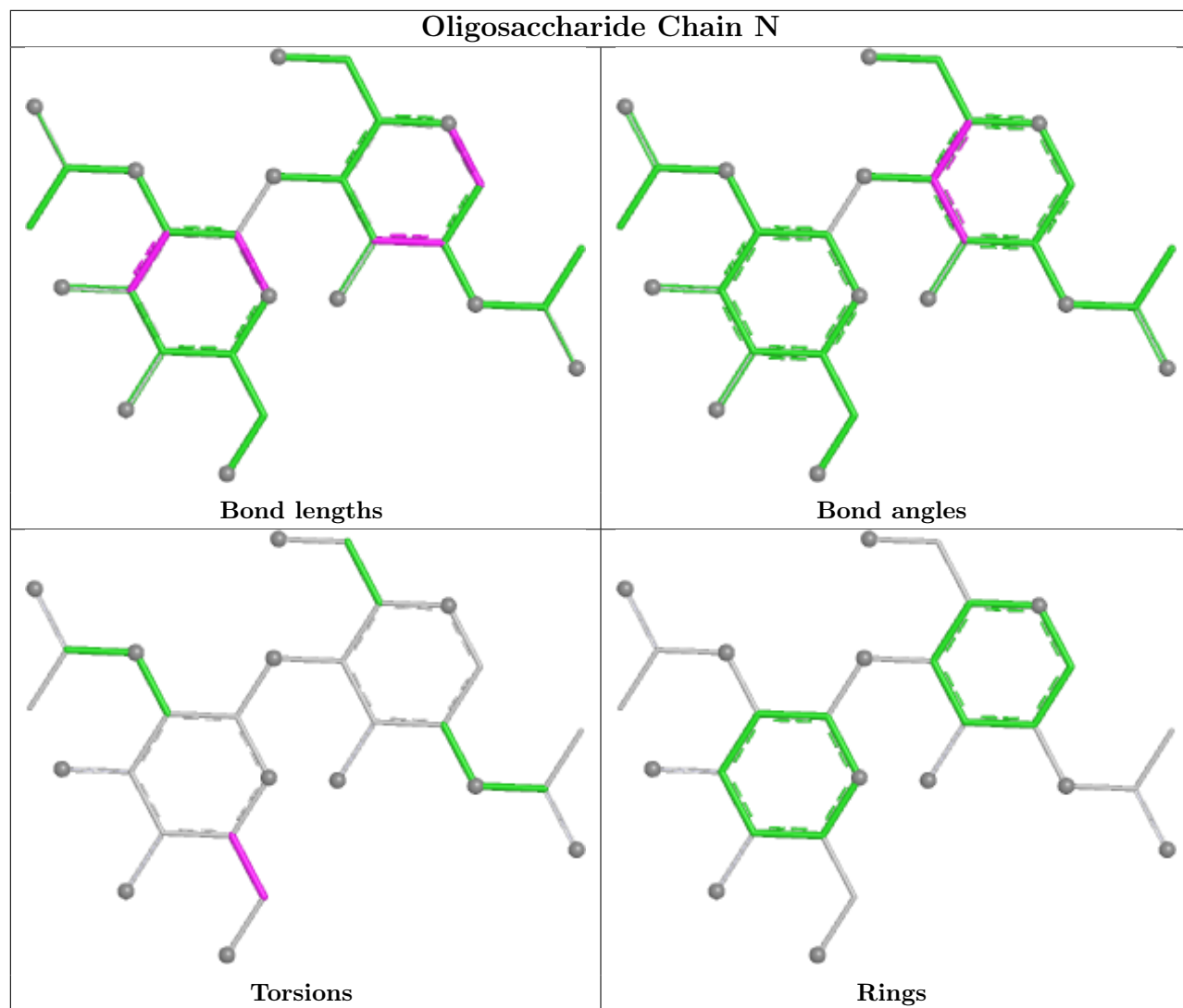


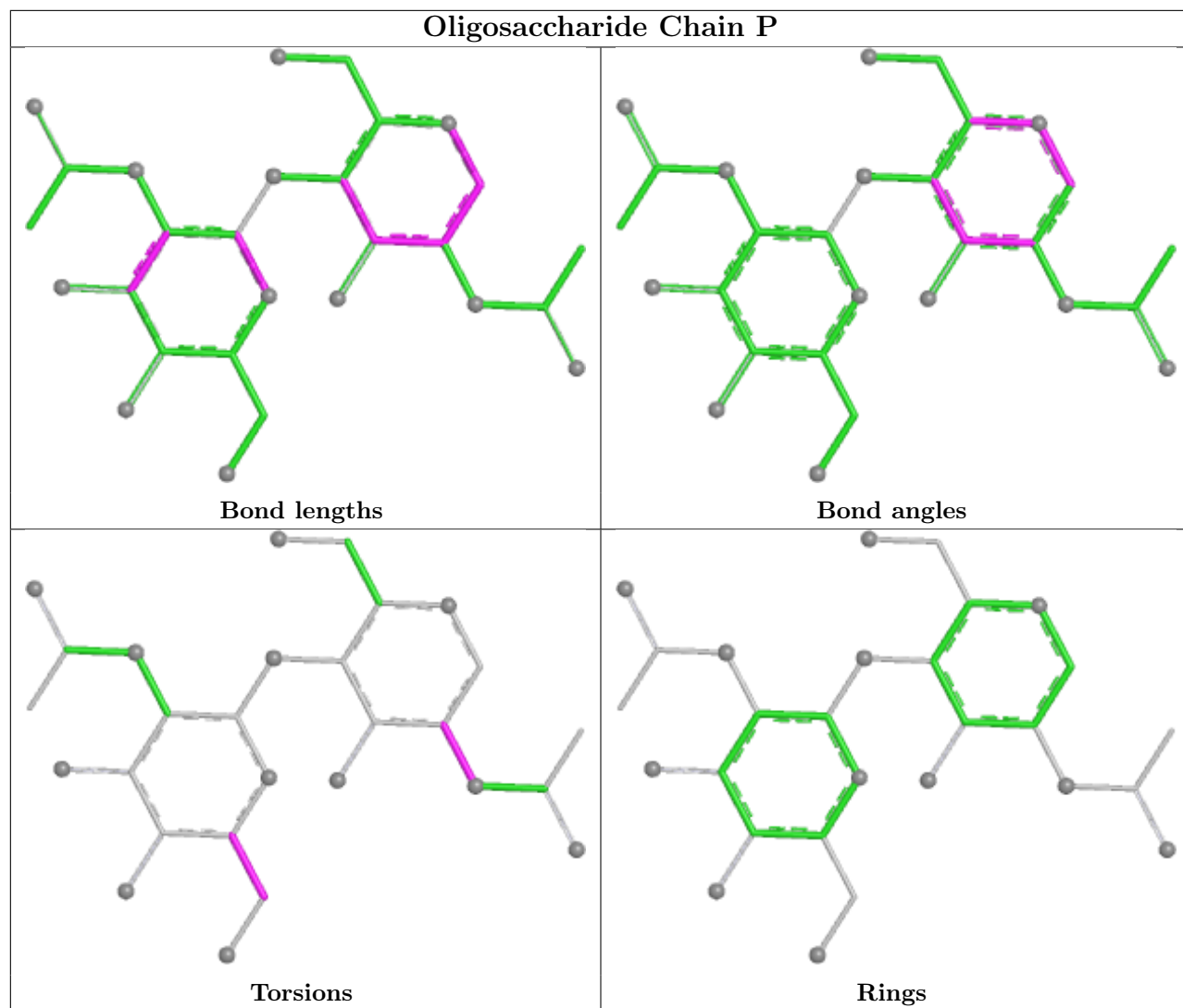


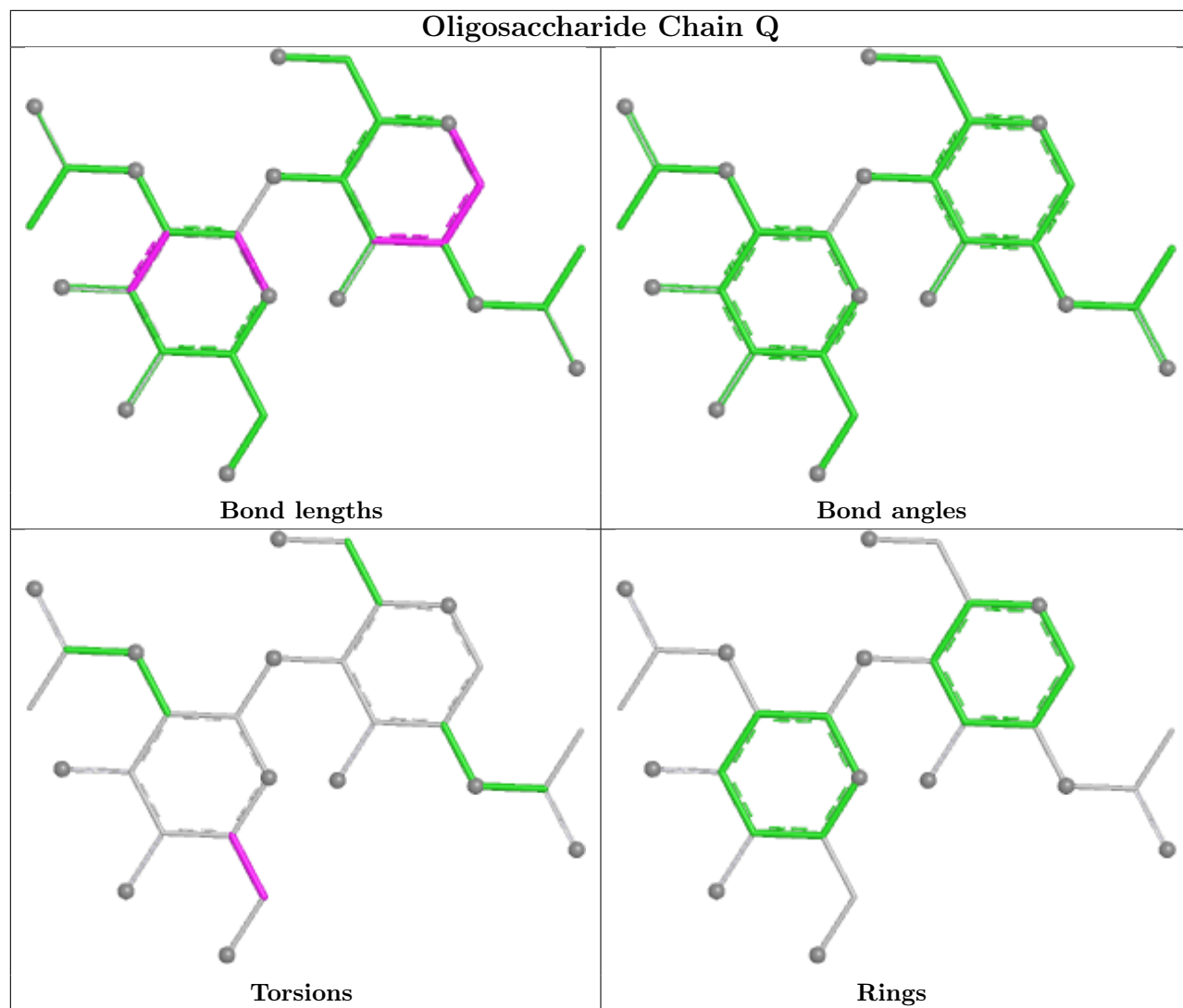


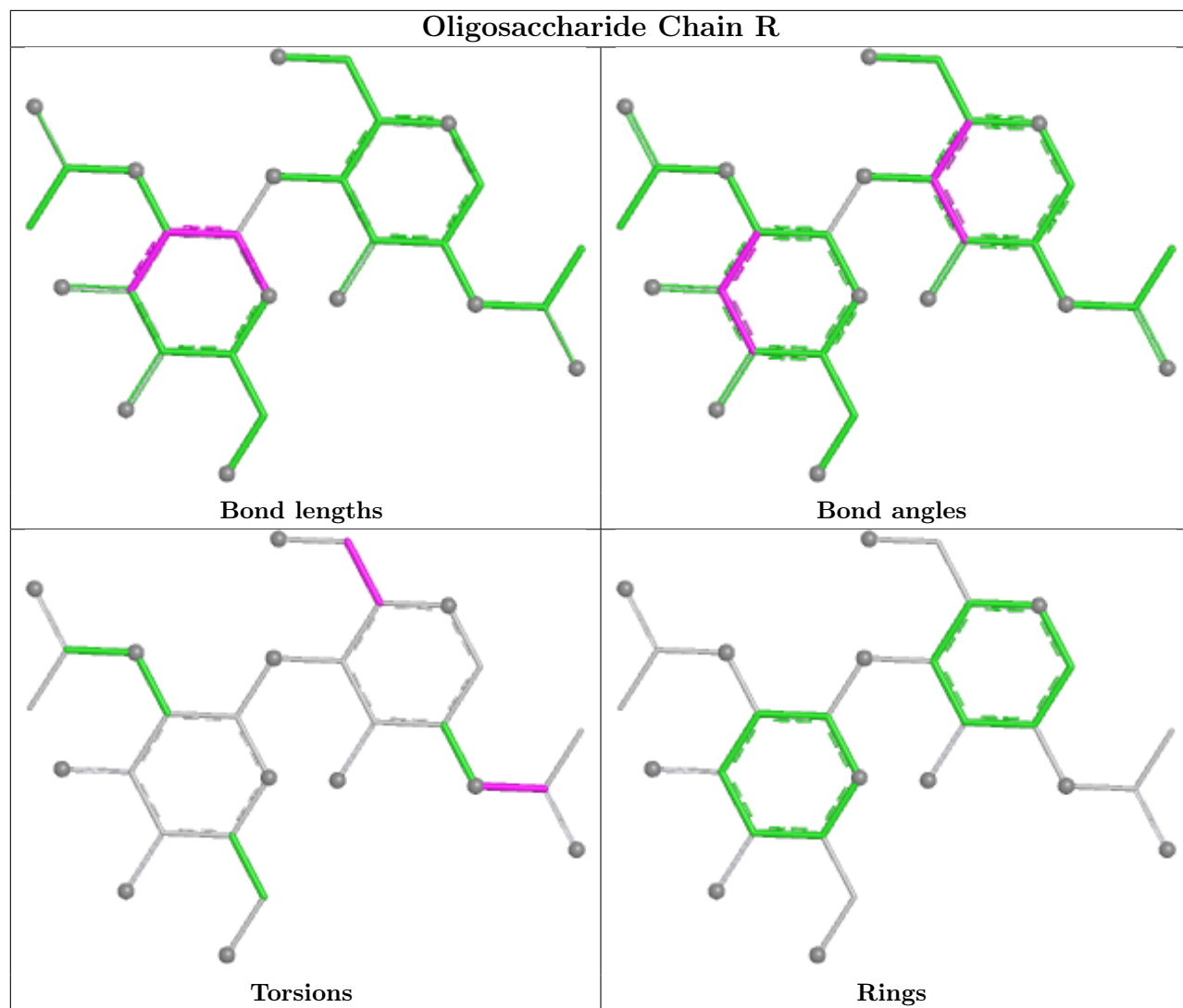


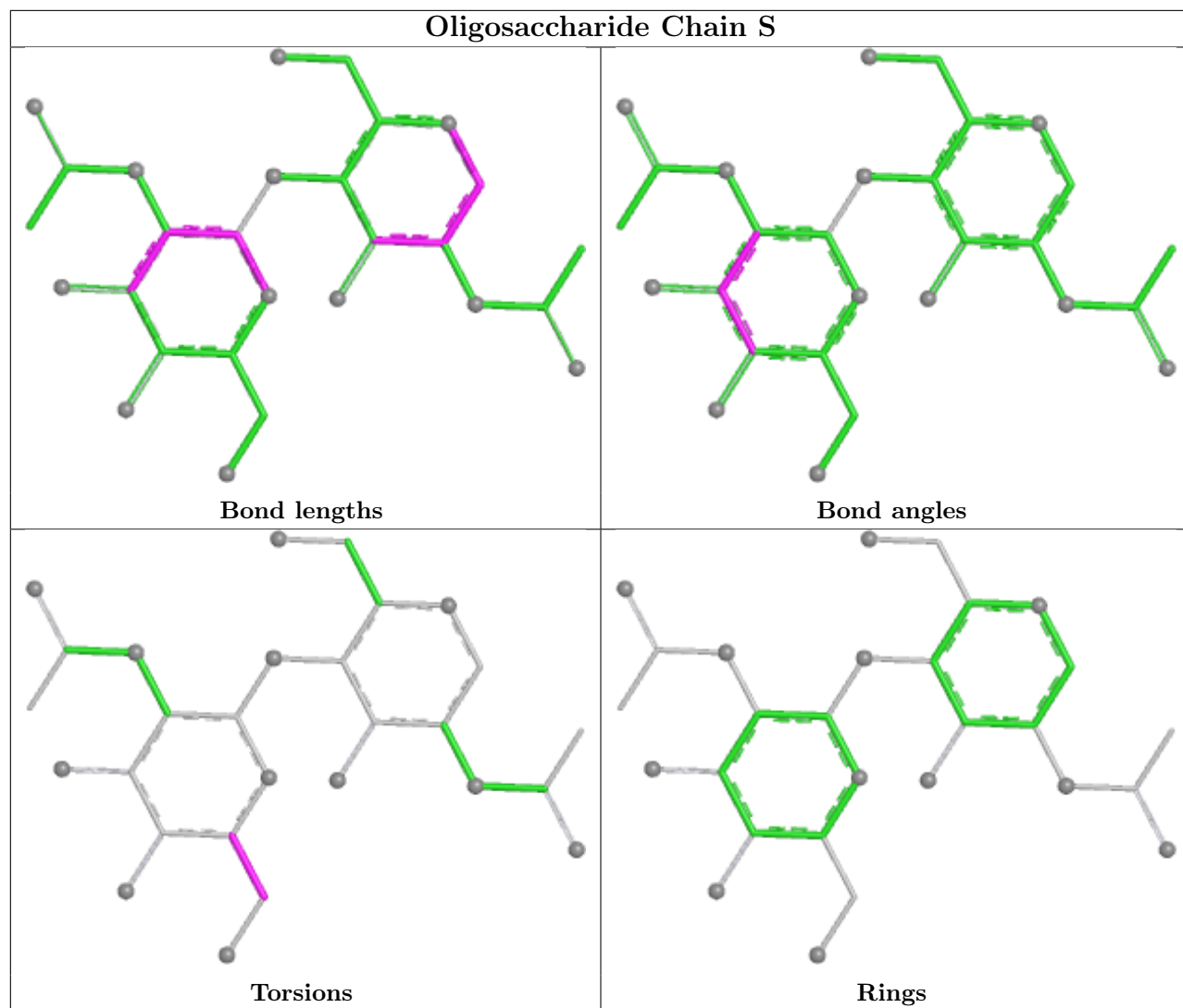


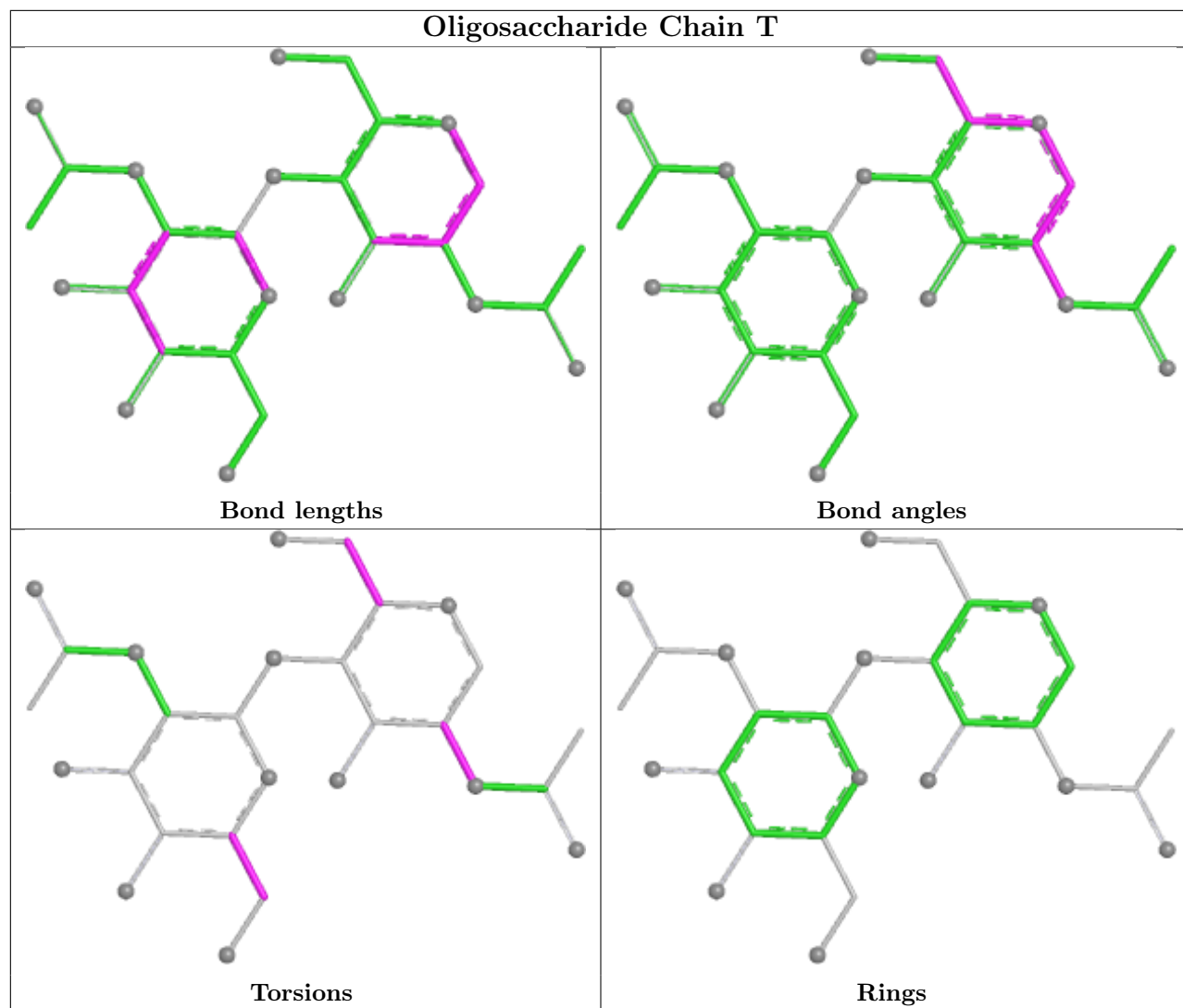


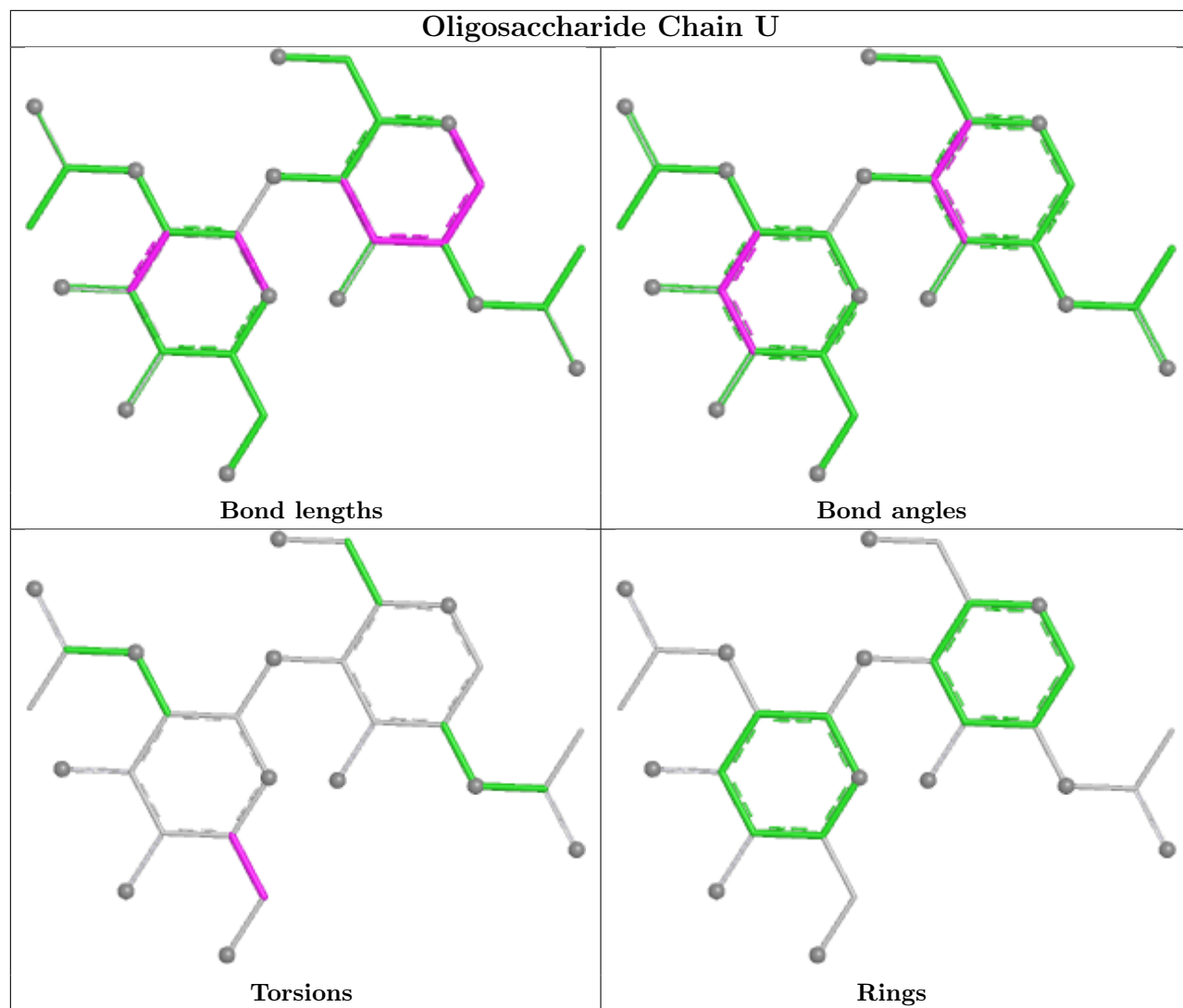


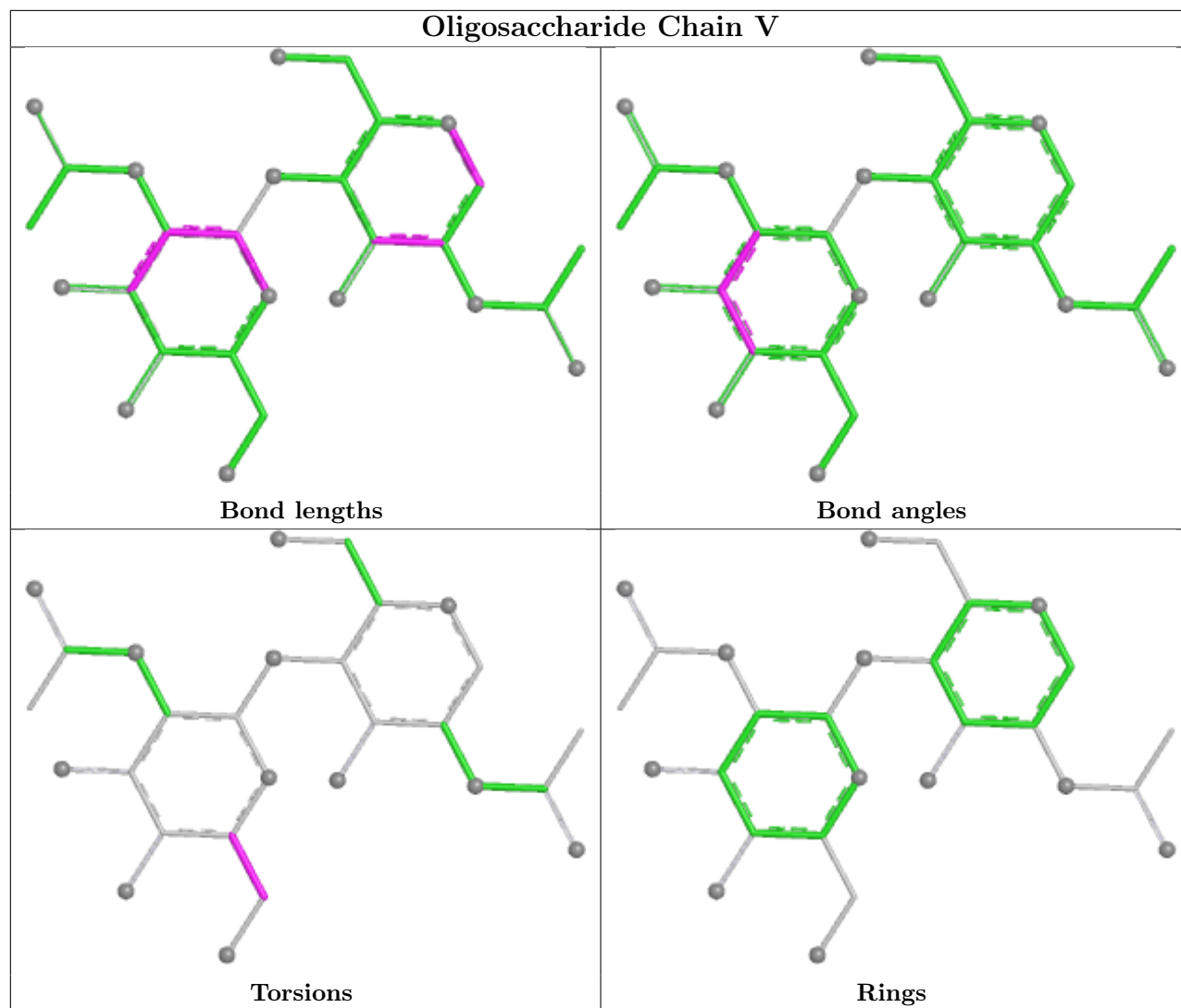


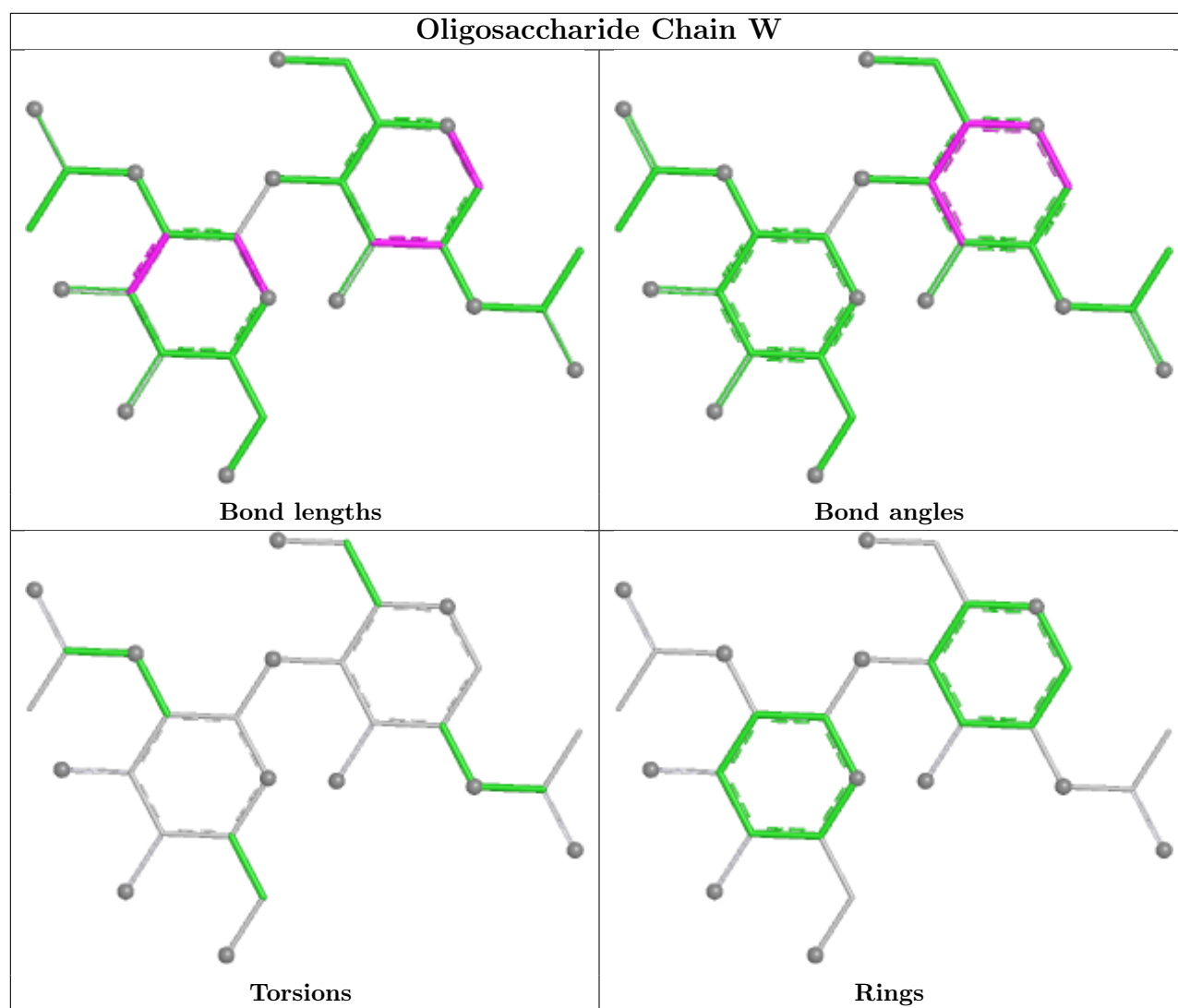


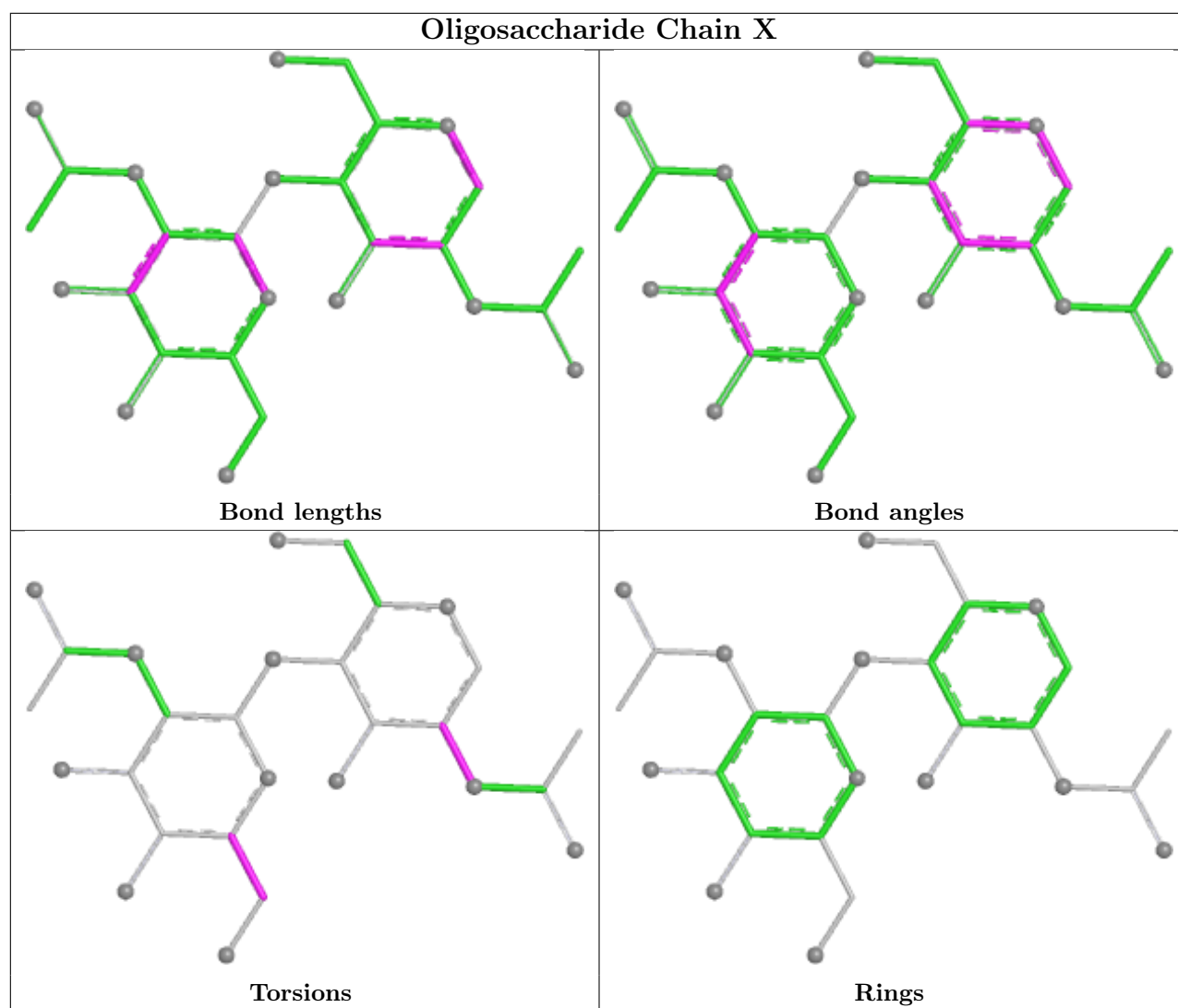


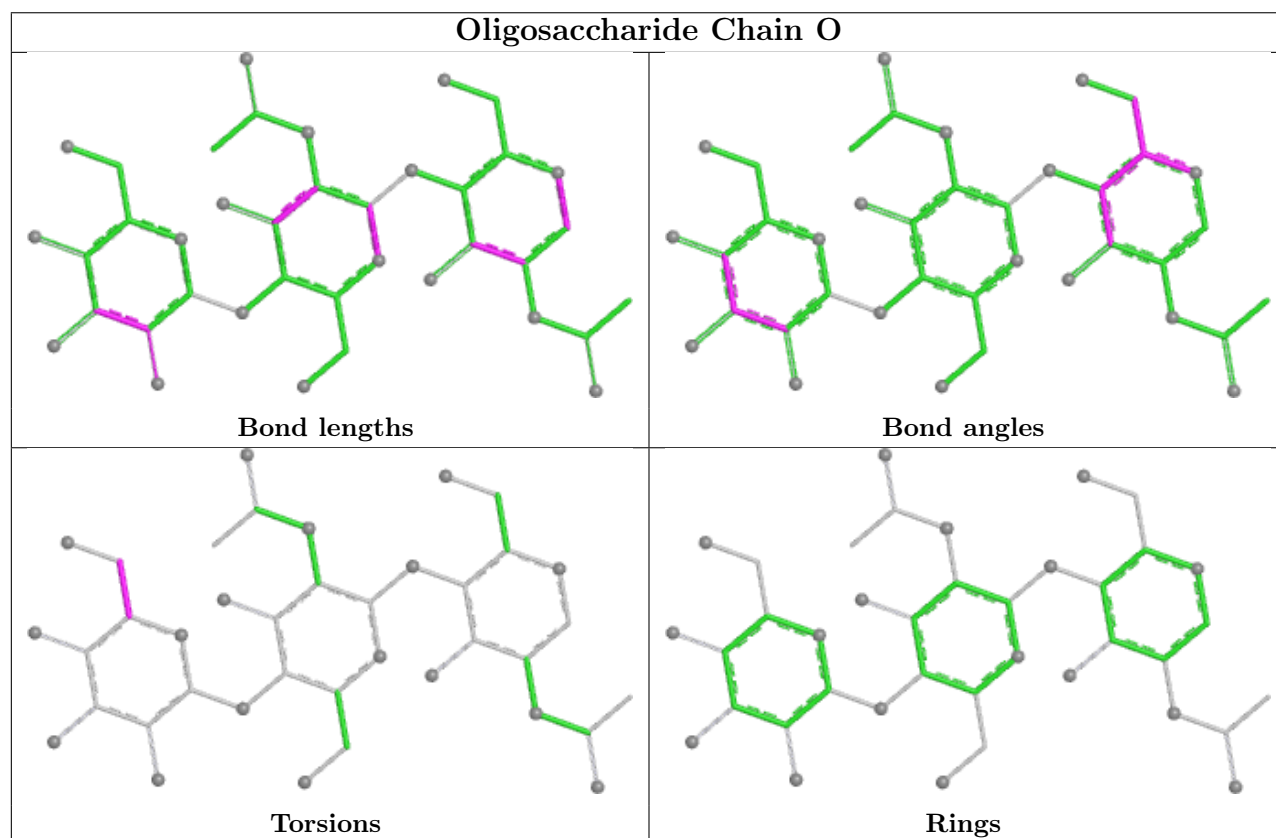
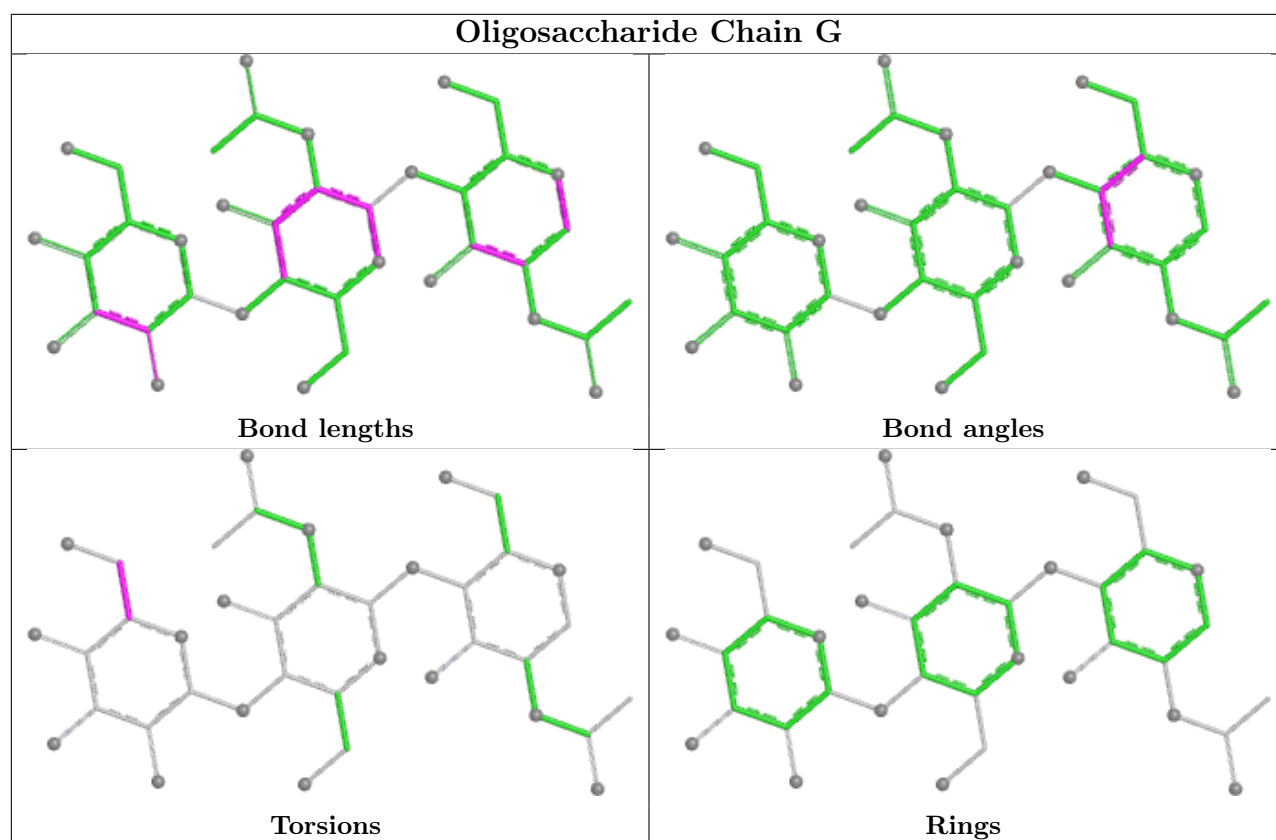












5.6 Ligand geometry

25 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	1404	1	14,14,15	0.46	0	17,19,21	0.92	1 (5%)
5	NAG	A	1408	1	14,14,15	2.02	3 (21%)	17,19,21	0.79	0
6	8Z9	A	1410	-	17,17,17	0.85	0	17,17,17	0.68	0
5	NAG	J	1405	1	14,14,15	1.93	3 (21%)	17,19,21	0.94	1 (5%)
5	NAG	A	1405	1	14,14,15	2.04	2 (14%)	17,19,21	0.81	0
5	NAG	J	1401	1	14,14,15	1.96	1 (7%)	17,19,21	0.96	2 (11%)
5	NAG	B	1402	1	14,14,15	2.08	4 (28%)	17,19,21	0.97	0
5	NAG	B	1403	1	14,14,15	2.04	2 (14%)	17,19,21	0.96	1 (5%)
5	NAG	J	1402	1	14,14,15	1.96	2 (14%)	17,19,21	1.05	3 (17%)
5	NAG	J	1406	1	14,14,15	2.04	2 (14%)	17,19,21	0.94	1 (5%)
5	NAG	A	1403	1	14,14,15	0.39	0	17,19,21	0.60	0
5	NAG	J	1407	1	14,14,15	1.99	3 (21%)	17,19,21	1.19	3 (17%)
5	NAG	A	1404	1	14,14,15	1.99	2 (14%)	17,19,21	0.72	0
5	NAG	J	1409	1	14,14,15	2.03	2 (14%)	17,19,21	0.84	0
5	NAG	A	1401	1	14,14,15	2.01	1 (7%)	17,19,21	1.07	2 (11%)
5	NAG	J	1403	1	14,14,15	2.09	2 (14%)	17,19,21	0.84	0
5	NAG	B	1401	1	14,14,15	2.09	2 (14%)	17,19,21	0.71	0
5	NAG	J	1404	1	14,14,15	1.96	2 (14%)	17,19,21	0.68	0
5	NAG	A	1406	1	14,14,15	0.36	0	17,19,21	0.85	1 (5%)
5	NAG	A	1402	1	14,14,15	2.05	2 (14%)	17,19,21	0.83	0
5	NAG	A	1407	1	14,14,15	2.05	3 (21%)	17,19,21	0.78	1 (5%)
6	8Z9	A	1409	-	17,17,17	0.82	1 (5%)	17,17,17	0.67	0
5	NAG	J	1408	1	14,14,15	2.07	2 (14%)	17,19,21	0.62	0
6	8Z9	J	1410	-	17,17,17	0.79	0	17,17,17	0.60	0
5	NAG	B	1405	1	14,14,15	2.10	2 (14%)	17,19,21	0.64	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
5	NAG	B	1404	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1408	1	-	1/6/23/26	0/1/1/1
6	8Z9	A	1410	-	-	10/15/15/15	-
5	NAG	J	1405	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1405	1	-	1/6/23/26	0/1/1/1
5	NAG	J	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1402	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1403	1	-	2/6/23/26	0/1/1/1
5	NAG	J	1402	1	-	0/6/23/26	0/1/1/1
5	NAG	J	1406	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1403	1	-	2/6/23/26	0/1/1/1
5	NAG	J	1407	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1404	1	-	2/6/23/26	0/1/1/1
5	NAG	J	1409	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1401	1	-	1/6/23/26	0/1/1/1
5	NAG	J	1403	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1401	1	-	1/6/23/26	0/1/1/1
5	NAG	J	1404	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1406	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1402	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1407	1	-	2/6/23/26	0/1/1/1
6	8Z9	A	1409	-	-	10/15/15/15	-
5	NAG	J	1408	1	-	2/6/23/26	0/1/1/1
6	8Z9	J	1410	-	-	10/15/15/15	-
5	NAG	B	1405	1	-	1/6/23/26	0/1/1/1

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1405	NAG	O5-C1	6.74	1.55	1.43
5	B	1401	NAG	O5-C1	6.72	1.55	1.43
5	J	1408	NAG	O5-C1	6.64	1.54	1.43
5	J	1403	NAG	O5-C1	6.54	1.54	1.43
5	J	1409	NAG	O5-C1	6.51	1.54	1.43
5	A	1405	NAG	O5-C1	6.43	1.54	1.43
5	J	1406	NAG	O5-C1	6.43	1.54	1.43
5	A	1408	NAG	O5-C1	6.39	1.54	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1401	NAG	O5-C1	6.35	1.54	1.43
5	J	1401	NAG	O5-C1	6.30	1.54	1.43
5	A	1402	NAG	O5-C1	6.30	1.54	1.43
5	B	1403	NAG	O5-C1	6.28	1.54	1.43
5	B	1402	NAG	O5-C1	6.20	1.54	1.43
5	J	1404	NAG	O5-C1	6.17	1.54	1.43
5	A	1407	NAG	O5-C1	6.14	1.54	1.43
5	J	1407	NAG	O5-C1	6.12	1.54	1.43
5	A	1404	NAG	O5-C1	6.09	1.53	1.43
5	J	1402	NAG	O5-C1	5.90	1.53	1.43
5	J	1405	NAG	O5-C1	5.66	1.53	1.43
5	B	1403	NAG	C3-C2	-2.69	1.46	1.52
5	A	1405	NAG	C3-C2	-2.53	1.47	1.52
5	A	1408	NAG	C3-C2	-2.51	1.47	1.52
5	J	1405	NAG	C4-C3	2.49	1.58	1.52
5	J	1402	NAG	C3-C2	-2.48	1.47	1.52
5	A	1407	NAG	C3-C2	-2.48	1.47	1.52
5	J	1403	NAG	C3-C2	-2.47	1.47	1.52
5	A	1402	NAG	C3-C2	-2.46	1.47	1.52
5	J	1407	NAG	C3-C2	-2.44	1.47	1.52
5	A	1404	NAG	C3-C2	-2.42	1.47	1.52
5	J	1406	NAG	C3-C2	-2.33	1.47	1.52
5	B	1402	NAG	C4-C3	2.29	1.58	1.52
5	B	1402	NAG	C1-C2	-2.28	1.49	1.52
5	J	1408	NAG	C3-C2	-2.26	1.47	1.52
5	B	1402	NAG	C3-C2	-2.25	1.47	1.52
5	B	1401	NAG	C3-C2	-2.21	1.47	1.52
5	B	1405	NAG	C3-C2	-2.20	1.47	1.52
5	J	1409	NAG	C3-C2	-2.19	1.47	1.52
5	J	1405	NAG	C1-C2	-2.16	1.49	1.52
5	A	1408	NAG	C4-C3	2.13	1.57	1.52
5	A	1407	NAG	C4-C3	2.12	1.57	1.52
6	A	1409	8Z9	C2-C1	2.12	1.55	1.50
5	J	1407	NAG	C4-C5	2.04	1.57	1.53
5	J	1404	NAG	C3-C2	-2.01	1.48	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1401	NAG	C1-O5-C5	-2.97	108.21	112.19
5	J	1406	NAG	C1-O5-C5	-2.75	108.50	112.19
5	B	1403	NAG	C1-O5-C5	-2.74	108.51	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	1401	NAG	C1-O5-C5	-2.57	108.74	112.19
5	J	1402	NAG	C1-O5-C5	-2.36	109.02	112.19
5	A	1401	NAG	C4-C3-C2	-2.36	107.56	111.02
5	J	1407	NAG	C3-C4-C5	-2.30	106.06	110.23
5	J	1407	NAG	O4-C4-C3	-2.23	105.11	110.38
5	J	1401	NAG	C4-C3-C2	-2.23	107.75	111.02
5	J	1407	NAG	C1-O5-C5	-2.19	109.25	112.19
5	B	1404	NAG	C1-C2-N2	-2.19	106.98	110.43
5	J	1405	NAG	C3-C4-C5	-2.18	106.27	110.23
5	J	1402	NAG	O5-C5-C6	-2.14	103.50	107.66
5	J	1402	NAG	C3-C4-C5	-2.02	106.57	110.23
5	A	1407	NAG	C3-C4-C5	-2.01	106.59	110.23
5	A	1406	NAG	C2-N2-C7	2.01	125.59	122.90

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1403	NAG	C8-C7-N2-C2
5	A	1403	NAG	O7-C7-N2-C2
5	J	1406	NAG	O5-C5-C6-O6
5	J	1401	NAG	O5-C5-C6-O6
5	A	1406	NAG	C8-C7-N2-C2
5	A	1406	NAG	O7-C7-N2-C2
5	J	1408	NAG	O5-C5-C6-O6
5	B	1403	NAG	C4-C5-C6-O6
5	A	1407	NAG	C4-C5-C6-O6
6	A	1409	8Z9	C1-C2-C3-C4
5	A	1401	NAG	O5-C5-C6-O6
5	B	1403	NAG	O5-C5-C6-O6
5	J	1407	NAG	O5-C5-C6-O6
6	A	1410	8Z9	C1-C2-C3-C4
6	J	1410	8Z9	C1-C2-C3-C4
5	A	1407	NAG	O5-C5-C6-O6
5	B	1401	NAG	O5-C5-C6-O6
5	J	1409	NAG	O5-C5-C6-O6
5	J	1404	NAG	O5-C5-C6-O6
5	B	1405	NAG	O5-C5-C6-O6
6	A	1409	8Z9	CC-CD-CE-CF
6	A	1409	8Z9	CB-CC-CD-CE
6	J	1410	8Z9	C2-C3-C4-C5
5	A	1404	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

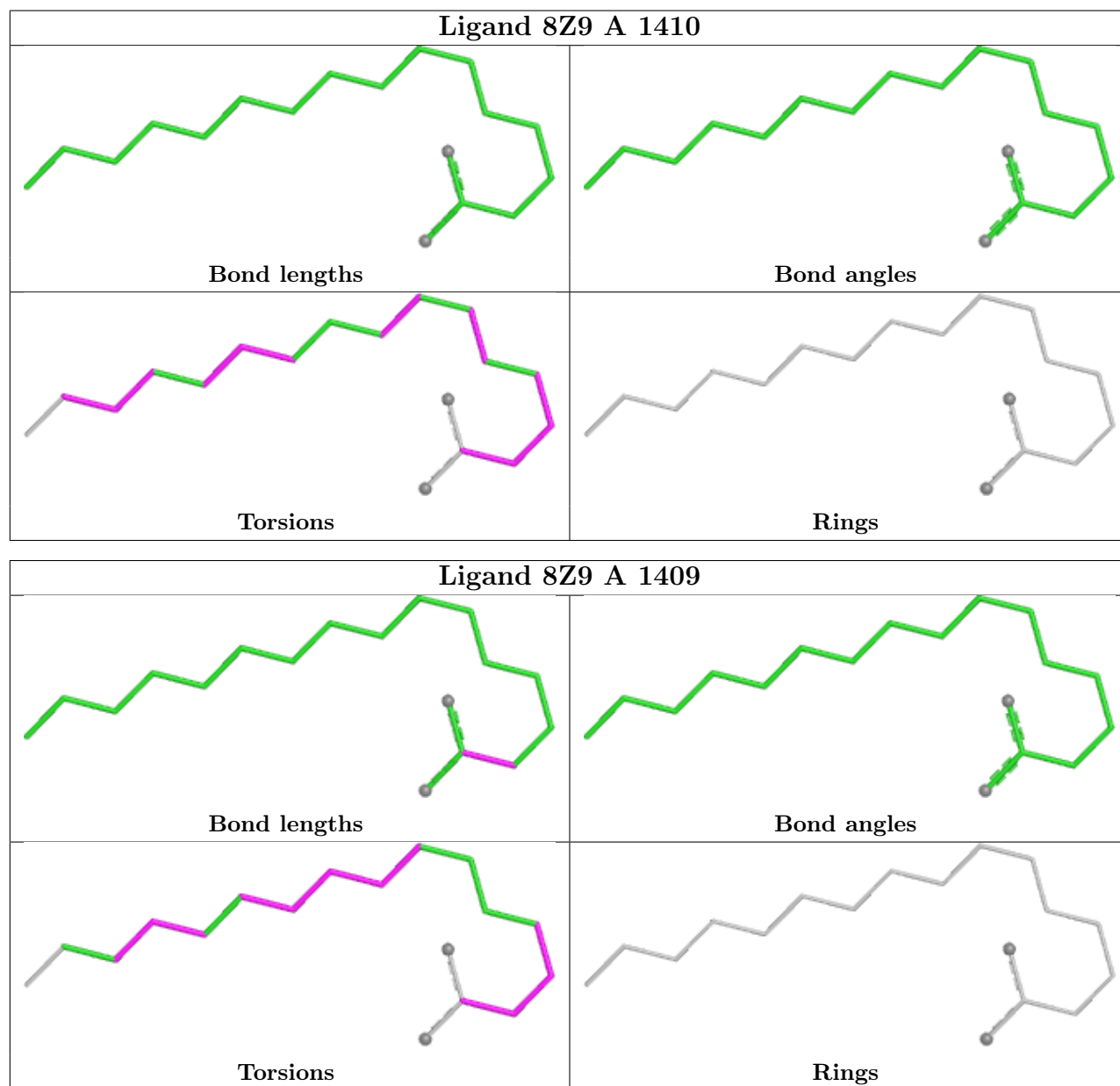
Mol	Chain	Res	Type	Atoms
5	J	1406	NAG	C4-C5-C6-O6
6	A	1410	8Z9	CD-CE-CF-CG
6	J	1410	8Z9	C9-CA-CB-CC
5	A	1406	NAG	O5-C5-C6-O6
6	A	1410	8Z9	C9-CA-CB-CC
5	A	1405	NAG	O5-C5-C6-O6
6	J	1410	8Z9	C7-C8-C9-CA
5	A	1402	NAG	O5-C5-C6-O6
6	A	1409	8Z9	C7-C8-C9-CA
6	A	1409	8Z9	C9-CA-CB-CC
5	J	1401	NAG	C4-C5-C6-O6
5	J	1407	NAG	C4-C5-C6-O6
5	J	1403	NAG	O5-C5-C6-O6
6	J	1410	8Z9	CA-CB-CC-CD
6	A	1409	8Z9	C2-C3-C4-C5
6	A	1410	8Z9	C2-C3-C4-C5
6	A	1410	8Z9	CA-CB-CC-CD
5	A	1404	NAG	C4-C5-C6-O6
6	J	1410	8Z9	C4-C5-C6-C7
6	A	1410	8Z9	C6-C7-C8-C9
6	J	1410	8Z9	CB-CC-CD-CE
6	A	1409	8Z9	C8-C9-CA-CB
6	A	1409	8Z9	O2-C1-C2-C3
6	J	1410	8Z9	O1-C1-C2-C3
6	J	1410	8Z9	O2-C1-C2-C3
5	J	1408	NAG	C4-C5-C6-O6
6	A	1409	8Z9	O1-C1-C2-C3
6	A	1410	8Z9	O1-C1-C2-C3
5	A	1408	NAG	O5-C5-C6-O6
6	A	1410	8Z9	O2-C1-C2-C3
6	A	1409	8Z9	C6-C7-C8-C9
6	A	1410	8Z9	C4-C5-C6-C7
6	J	1410	8Z9	C6-C7-C8-C9
6	A	1410	8Z9	CC-CD-CE-CF

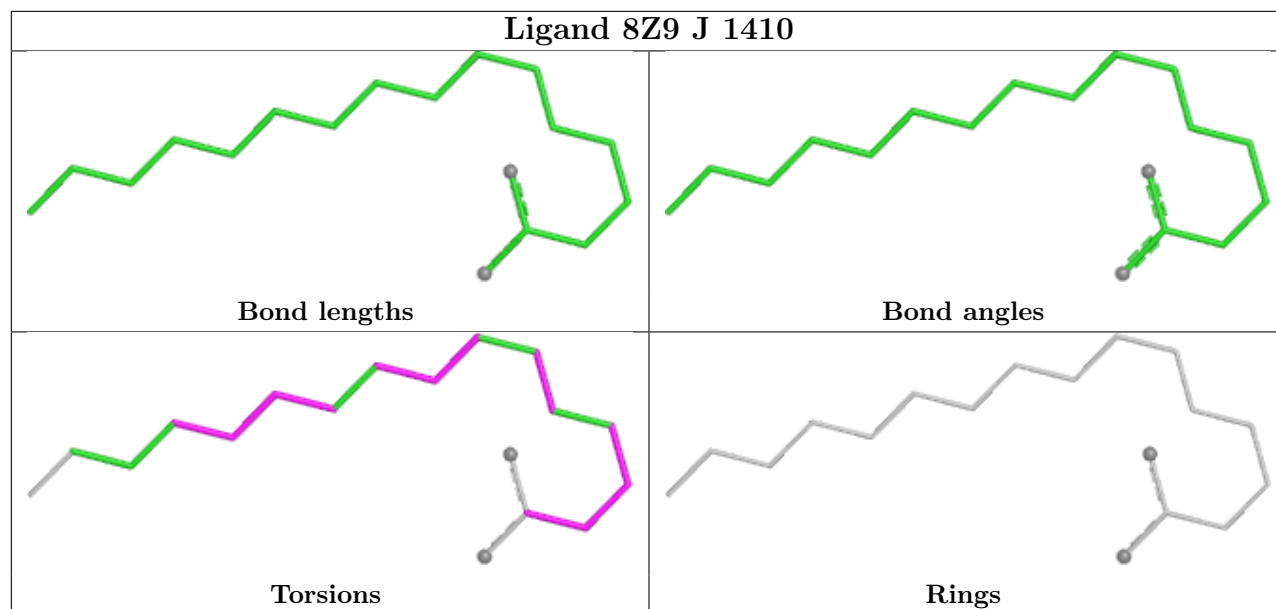
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1404	NAG	2	0
5	J	1403	NAG	1	0
5	A	1402	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

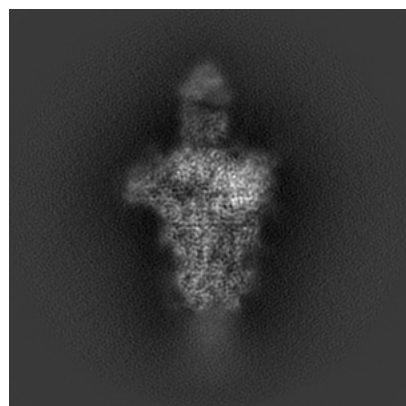
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24991. These allow visual inspection of the internal detail of the map and identification of artifacts.

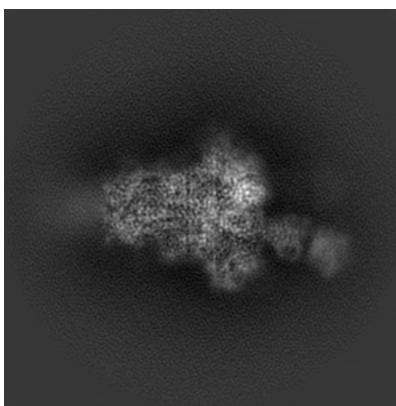
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

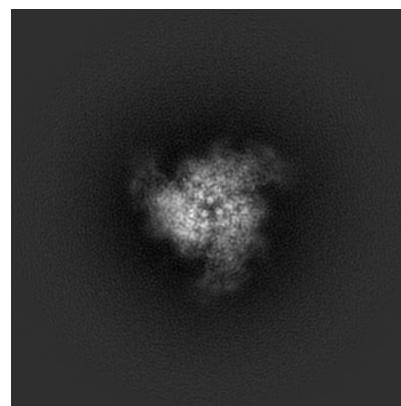
6.1.1 Primary map



X

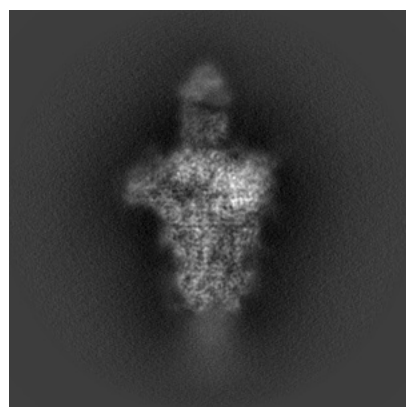


Y

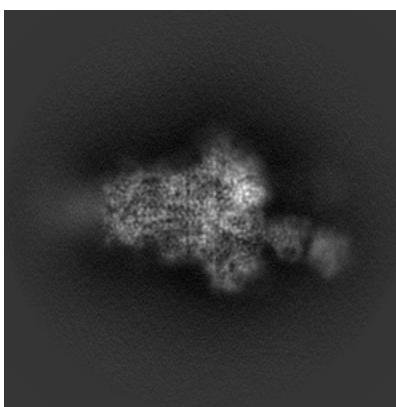


Z

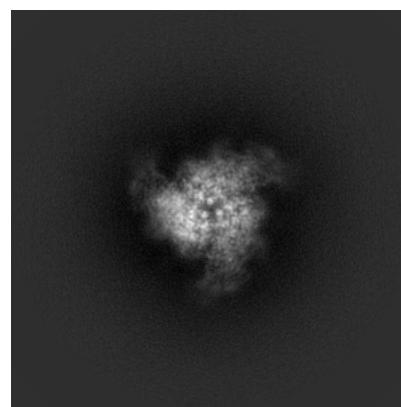
6.1.2 Raw map



X



Y

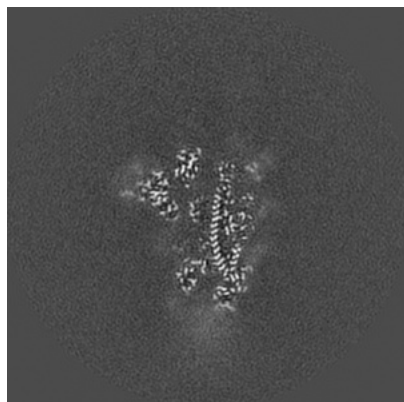


Z

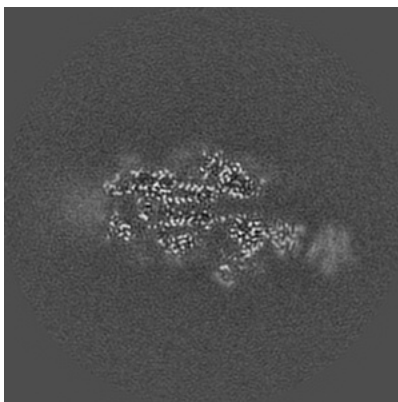
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

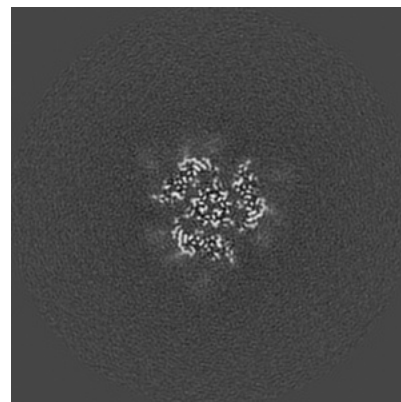
6.2.1 Primary map



X Index: 170

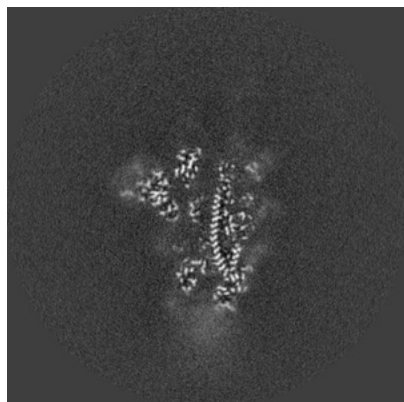


Y Index: 170

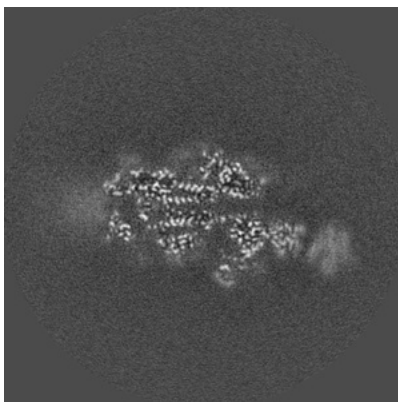


Z Index: 170

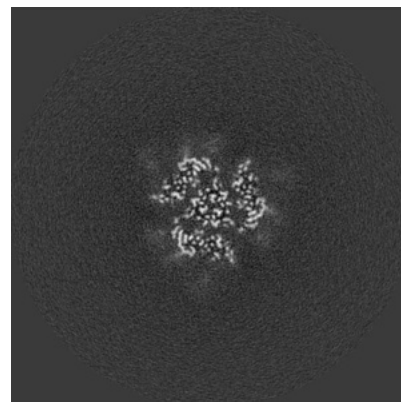
6.2.2 Raw map



X Index: 170



Y Index: 170

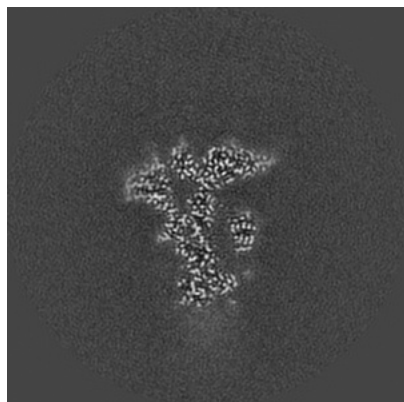


Z Index: 170

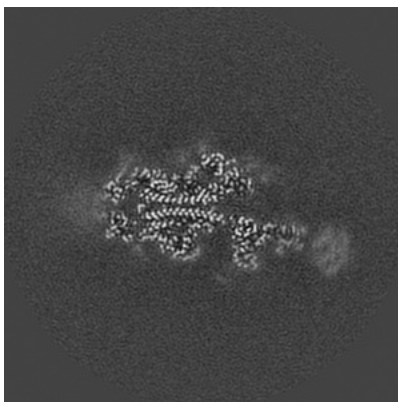
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

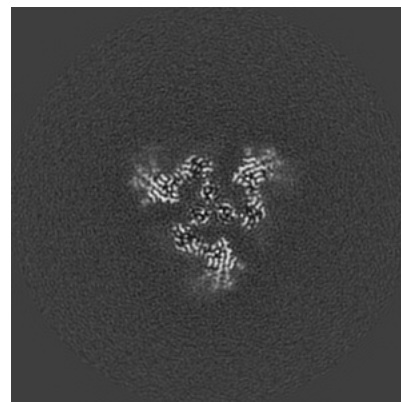
6.3.1 Primary map



X Index: 184

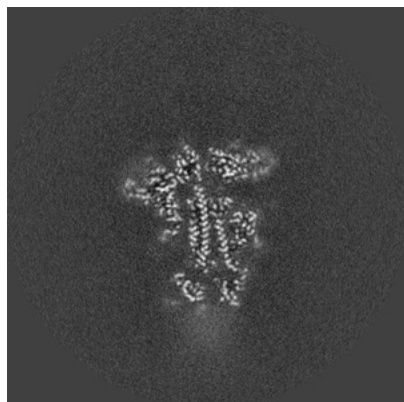


Y Index: 166

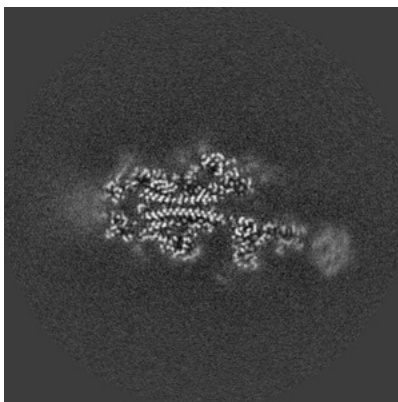


Z Index: 178

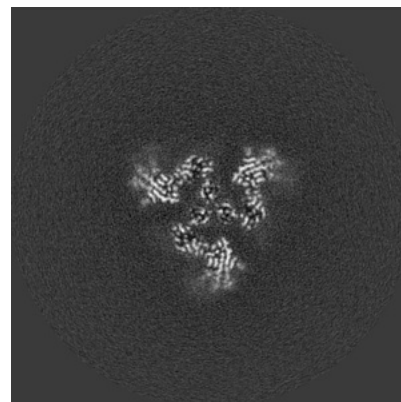
6.3.2 Raw map



X Index: 177



Y Index: 166

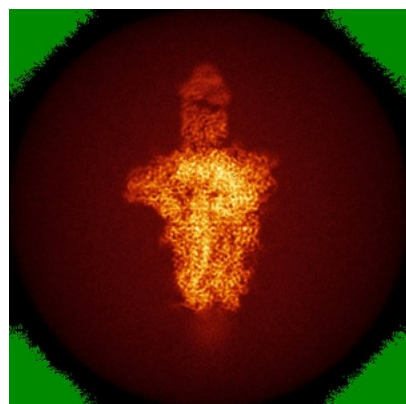


Z Index: 178

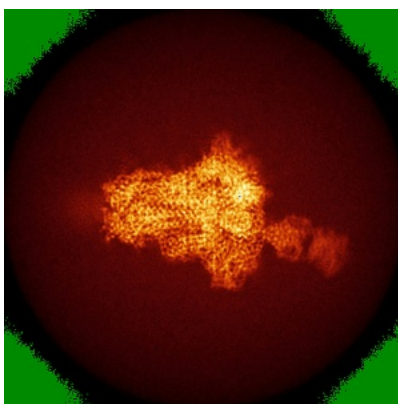
The images above show the largest variance slices of the map in three orthogonal directions.

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

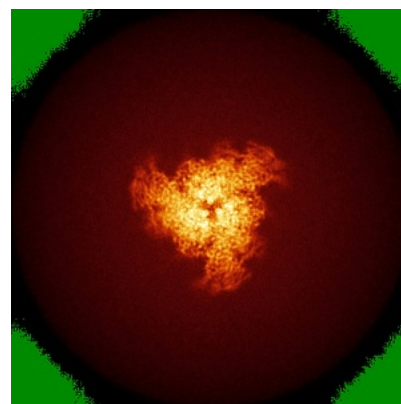
6.4.1 Primary map



X



Y

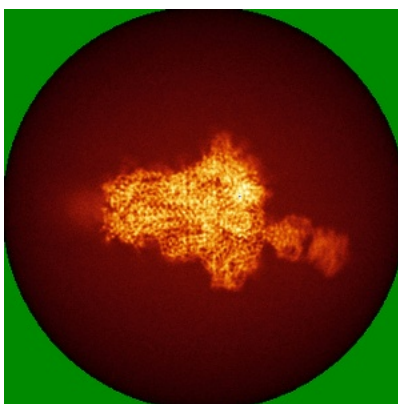


Z

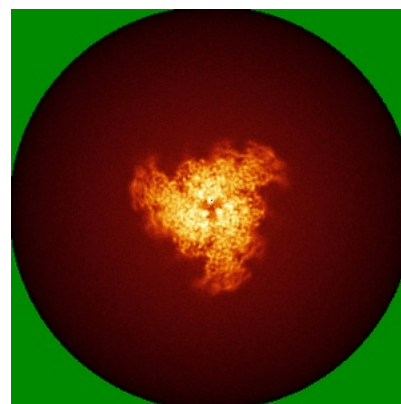
6.4.2 Raw map



X



Y

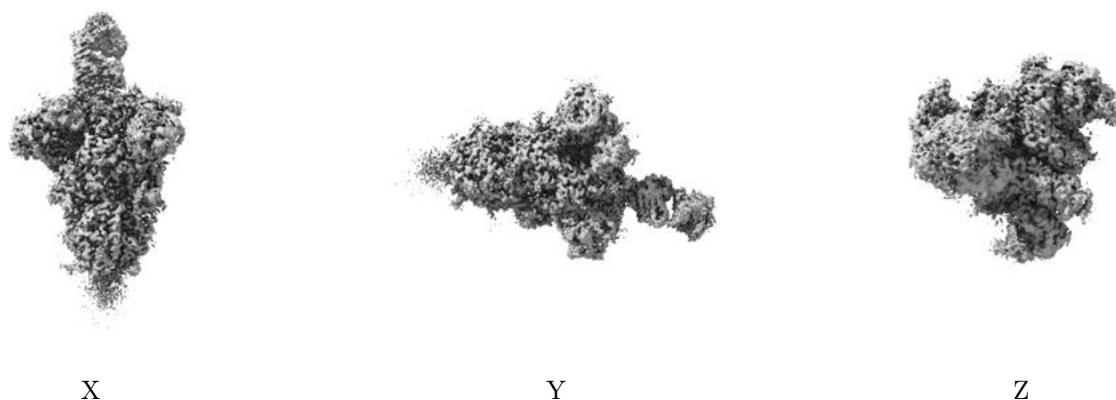


Z

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

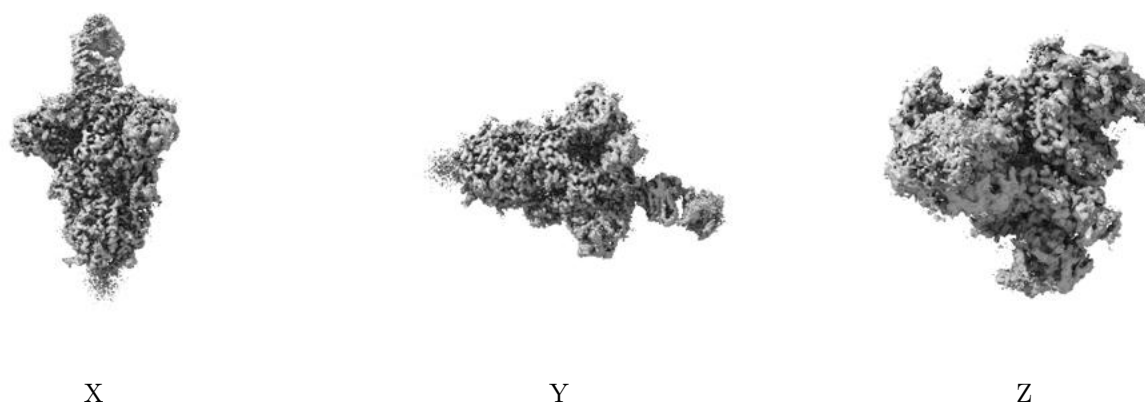
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

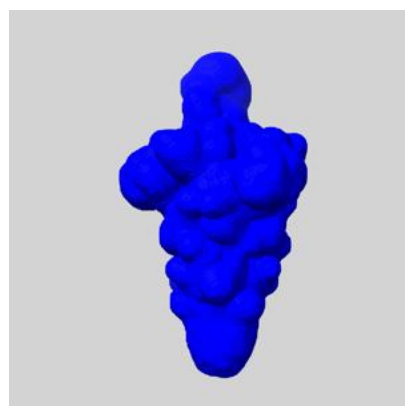
6.6 Mask visualisation [i](#)

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

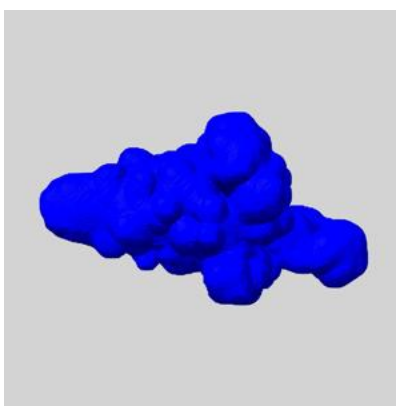
A mask typically either:

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

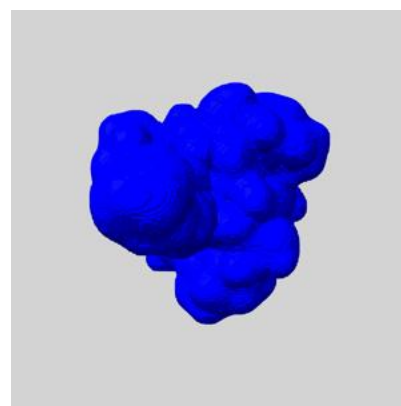
6.6.1 emd_24991_msk_1.map [i](#)



X



Y

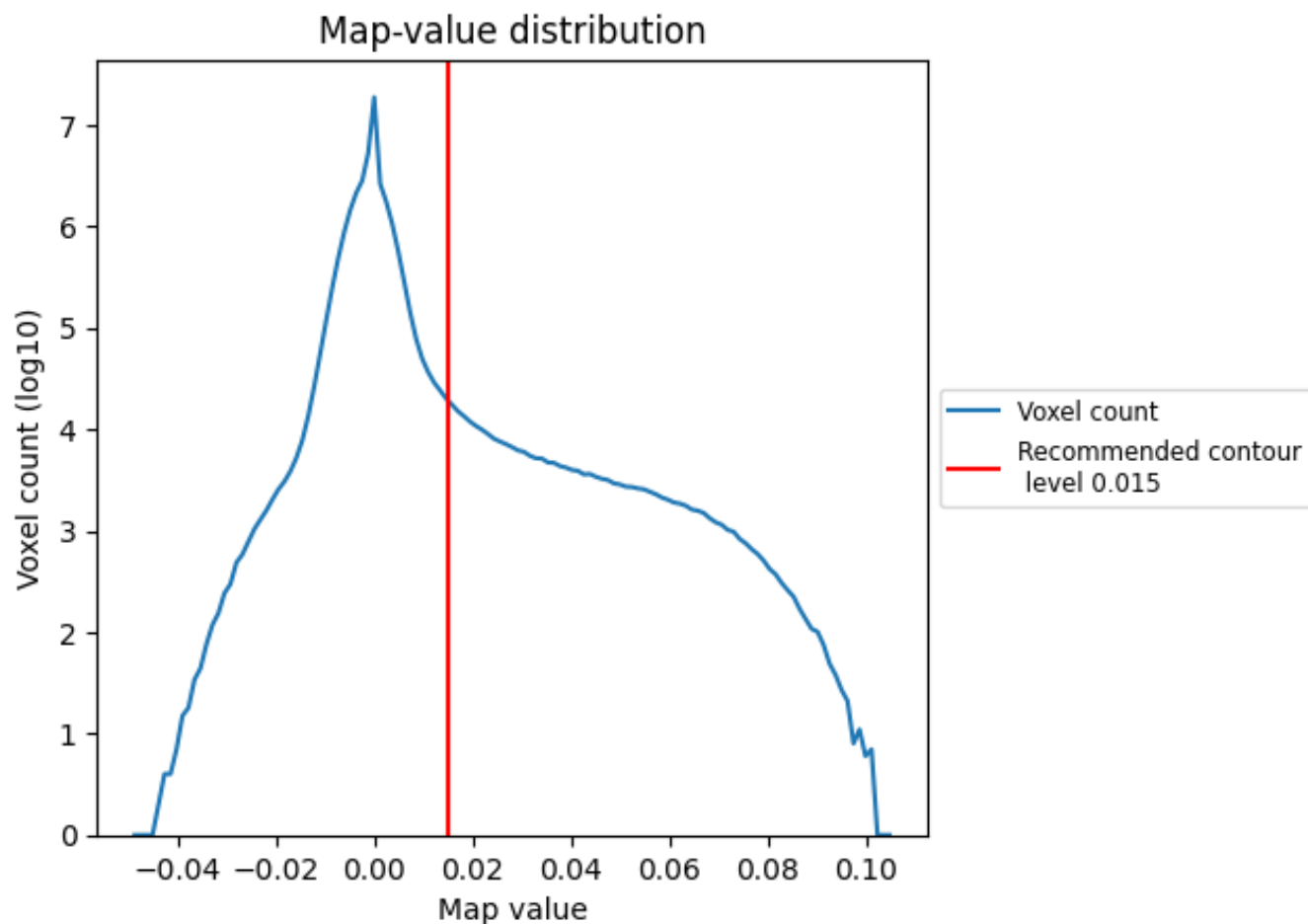


Z

7 Map analysis [i](#)

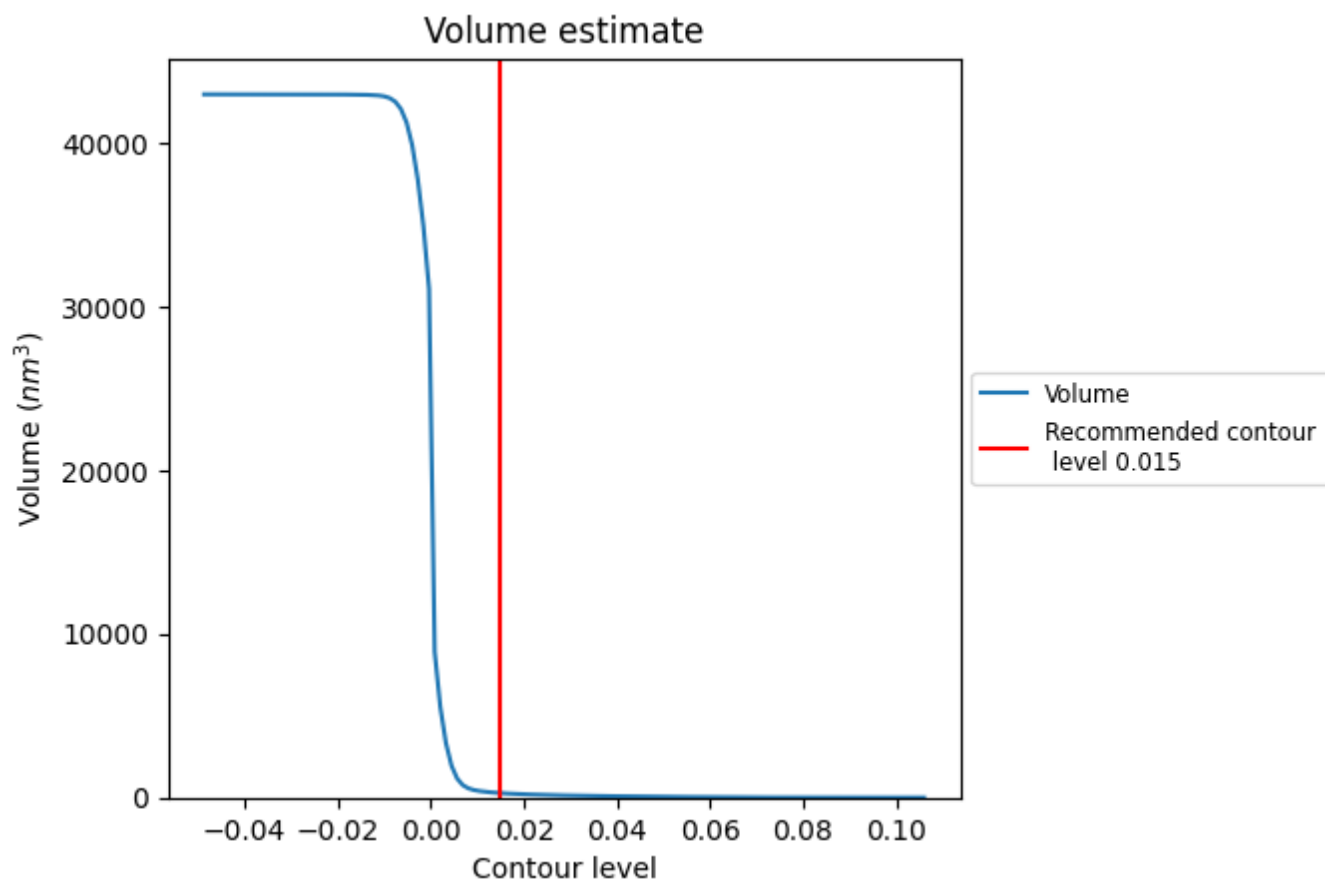
This section contains the results of statistical analysis of the map.

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.

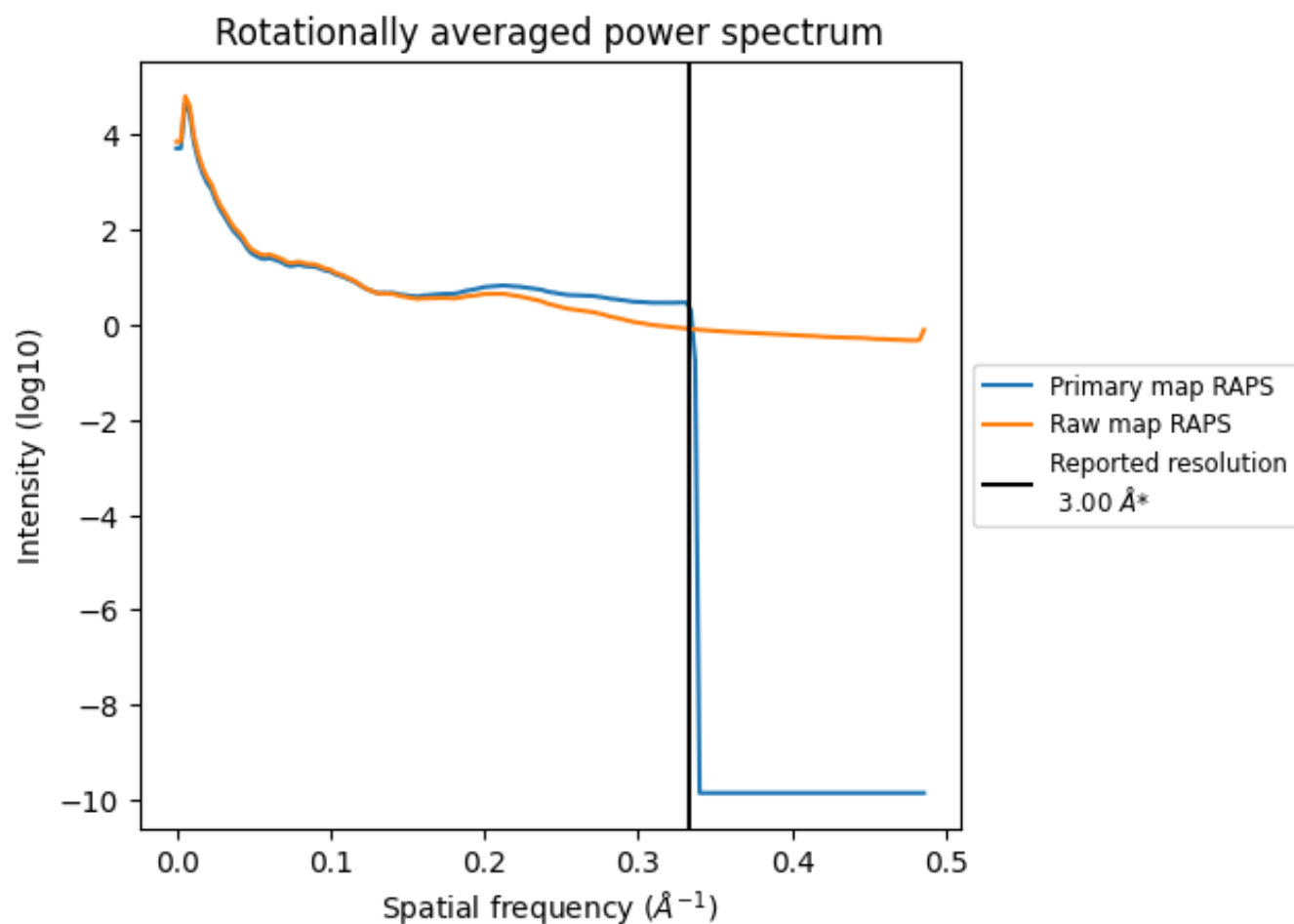
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 272 nm³; this corresponds to an approximate mass of 245 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 ⓘ

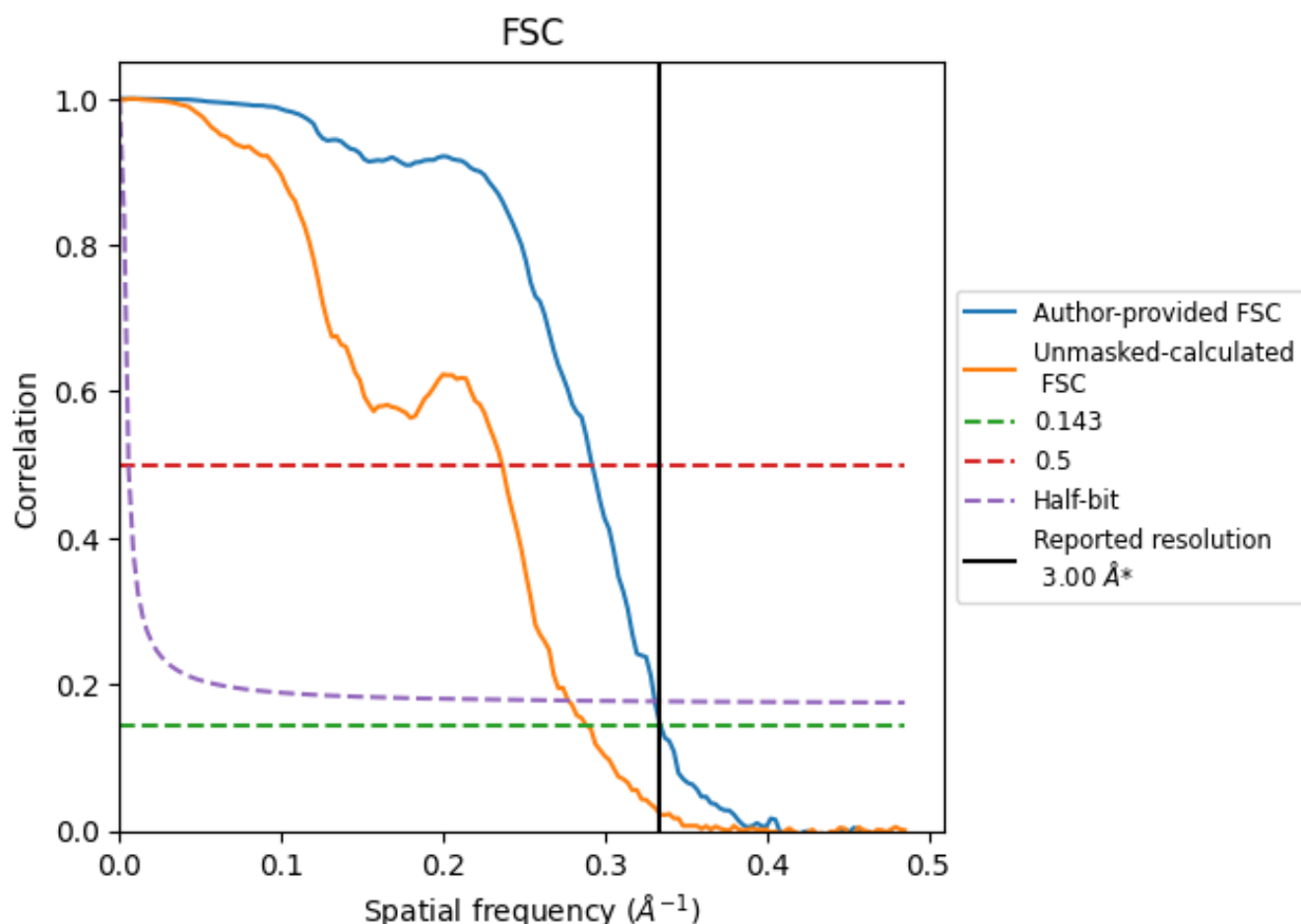


*Reported resolution corresponds to spatial frequency of 0.333 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

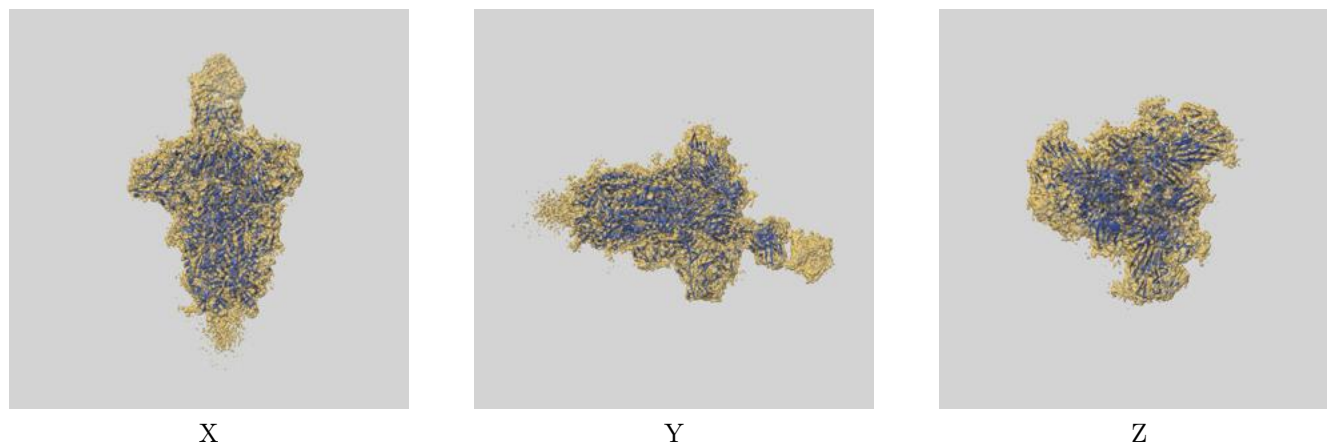
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.99	3.42	3.02
Unmasked-calculated*	3.46	4.23	3.60

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.46 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

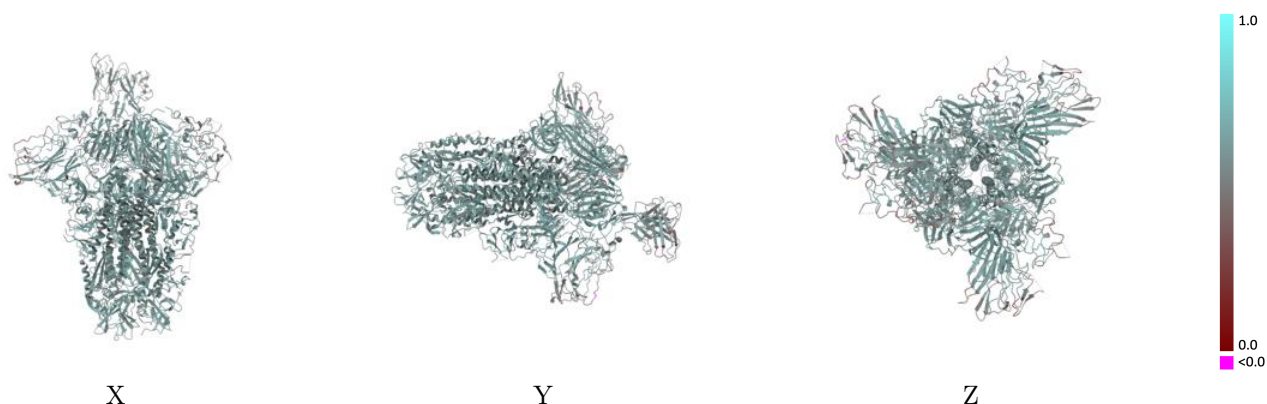
This section contains information regarding the fit between EMDB map EMD-24991 and PDB model 7SBX. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



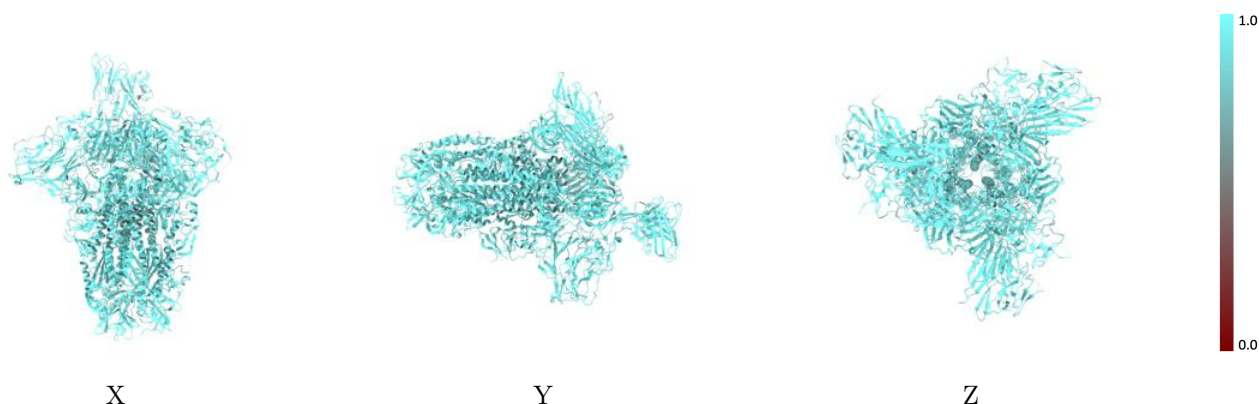
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



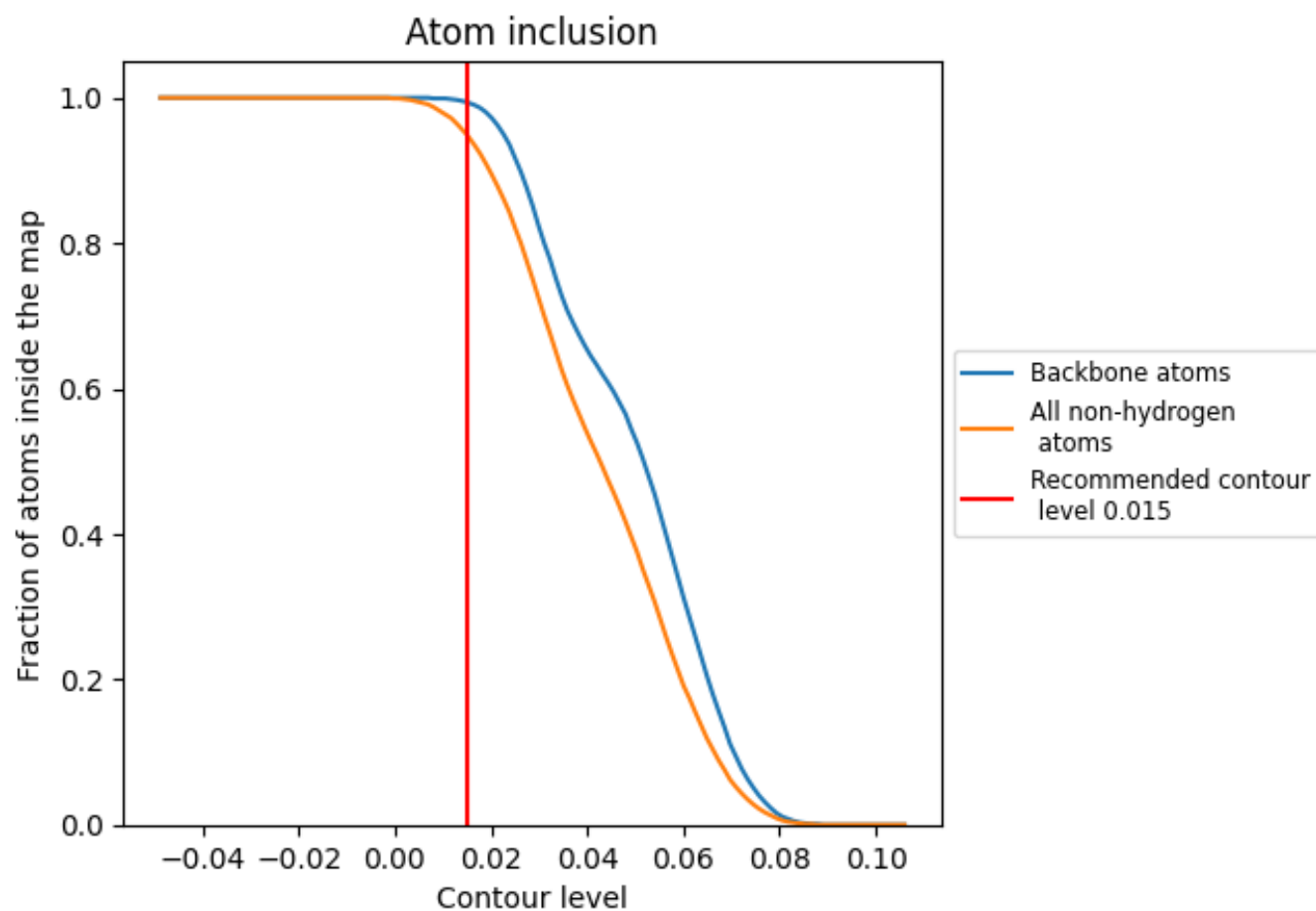
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 95% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9490	 0.5710
A	 0.9510	 0.5760
B	 0.9550	 0.5800
C	 0.7500	 0.4890
D	 0.8570	 0.4870
E	 0.8930	 0.5030
F	 0.7860	 0.4060
G	 0.8720	 0.4850
H	 0.9460	 0.5060
I	 0.7140	 0.4150
J	 0.9490	 0.5740
K	 0.8570	 0.4760
L	 0.9710	 0.4890
M	 0.7500	 0.4820
N	 0.7860	 0.4890
O	 0.8210	 0.4150
P	 0.6790	 0.4560
Q	 0.8570	 0.4410
R	 0.7860	 0.4370
S	 0.7500	 0.4360
T	 0.9290	 0.5010
U	 0.7140	 0.4130
V	 0.7500	 0.4830
W	 0.9290	 0.5060
X	 0.7140	 0.4890

