



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 07:53 AM EST

PDB ID : 7SB3
EMDB ID : EMD-24968
Title : Structure of OC43 spike in complex with polyclonal Fab1 (Donor 269)
Authors : Ward, A.; Bangaru, S.; Antanasijevic, A.
Deposited on : 2021-09-23
Resolution : 3.30 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

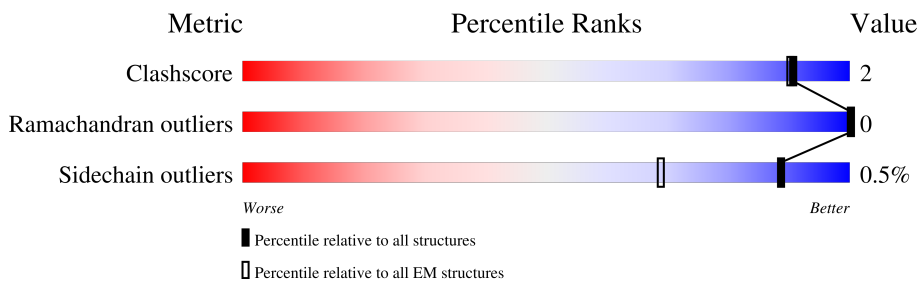
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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% 14%
1	B	1367	81% 5% 14%
1	J	1367	82% 13%
2	H	122	83% 8% 9%
2	L	122	83% 16%
3	C	2	50% 50%
3	D	2	50% 50%
3	E	2	100%

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Mol	Chain	Length	Quality of chain
3	G	2	 100%
3	I	2	 100%
3	K	2	 100%
3	M	2	 50% 50%
3	N	2	 100%
3	O	2	 100%
3	P	2	 100%
3	Q	2	 100%
3	R	2	 50% 50%
3	S	2	 50% 100%
4	F	3	 33% 67%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 29451 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
			Total	C	N	O	S		
1	J	1183	9198	5859	1514	1762	63	0	0
1	A	1178	9168	5842	1508	1755	63	0	0
1	B	1182	9185	5857	1507	1758	63	0	0

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

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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

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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

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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

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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

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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

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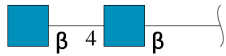
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Chain	Residue	Modelled	Actual	Comment	Reference
B	1338	ALA	-	expression tag	UNP A0A7U1BGV5
B	1339	TRP	-	expression tag	UNP A0A7U1BGV5
B	1340	SER	-	expression tag	UNP A0A7U1BGV5
B	1341	HIS	-	expression tag	UNP A0A7U1BGV5
B	1342	PRO	-	expression tag	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	111	Total	C	N	O	0	0
			555	333	111	111		
2	L	102	Total	C	N	O	0	0
			510	306	102	102		

- 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
			Total	C	N	O		
3	C	2	28	16	2	10	0	0
3	D	2	28	16	2	10	0	0
3	E	2	28	16	2	10	0	0
3	G	2	28	16	2	10	0	0
3	I	2	28	16	2	10	0	0
3	K	2	28	16	2	10	0	0
3	M	2	28	16	2	10	0	0
3	N	2	28	16	2	10	0	0
3	O	2	28	16	2	10	0	0
3	P	2	28	16	2	10	0	0
3	Q	2	28	16	2	10	0	0
3	R	2	28	16	2	10	0	0
3	S	2	28	16	2	10	0	0

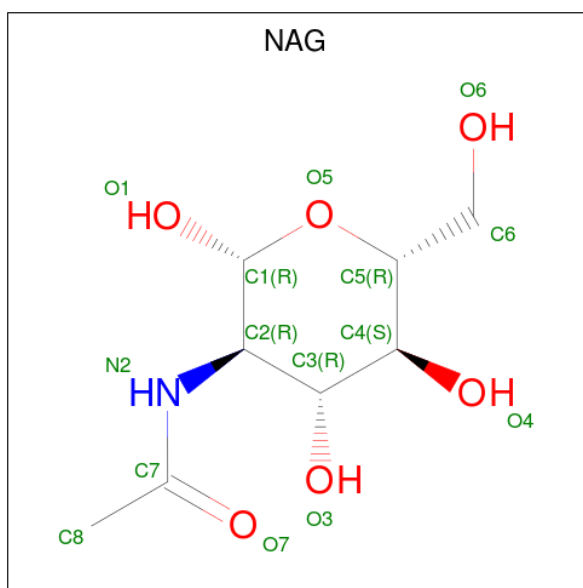
- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

C₈H₁₅NO₆).



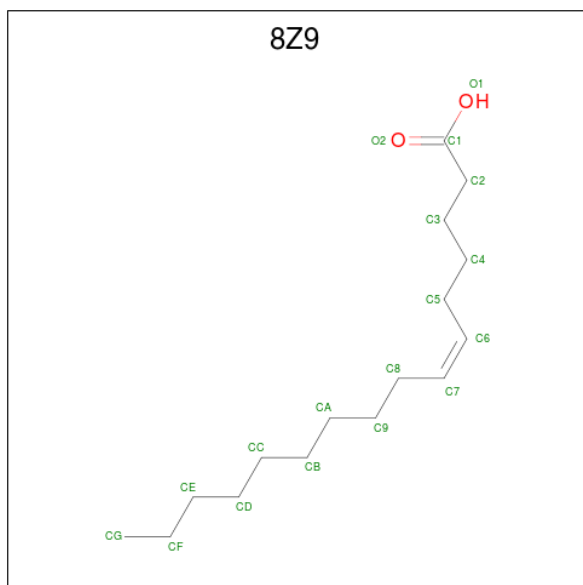
Mol	Chain	Residues	Atoms			AltConf	
			Total	C	N		O
5	J	1	126	72	9	45	0
5	J	1	126	72	9	45	0
5	J	1	126	72	9	45	0
5	J	1	126	72	9	45	0
5	J	1	126	72	9	45	0
5	J	1	126	72	9	45	0
5	J	1	126	72	9	45	0
5	J	1	126	72	9	45	0
5	J	1	126	72	9	45	0
5	A	1	126	72	9	45	0
5	A	1	126	72	9	45	0
5	A	1	126	72	9	45	0
5	A	1	126	72	9	45	0

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Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			126	72	9	45	
5	A	1	Total	C	N	O	0
			126	72	9	45	
5	A	1	Total	C	N	O	0
			126	72	9	45	
5	A	1	Total	C	N	O	0
			126	72	9	45	
5	A	1	Total	C	N	O	0
			126	72	9	45	
5	B	1	Total	C	N	O	0
			126	72	9	45	
5	B	1	Total	C	N	O	0
			126	72	9	45	
5	B	1	Total	C	N	O	0
			126	72	9	45	
5	B	1	Total	C	N	O	0
			126	72	9	45	
5	B	1	Total	C	N	O	0
			126	72	9	45	
5	B	1	Total	C	N	O	0
			126	72	9	45	
5	B	1	Total	C	N	O	0
			126	72	9	45	
5	B	1	Total	C	N	O	0
			126	72	9	45	

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

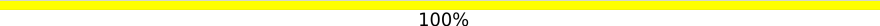


Mol	Chain	Residues	Atoms			AltConf
6	J	1	Total	C	O	0
			36	32	4	
6	J	1	Total	C	O	0
			36	32	4	
6	B	1	Total	C	O	0
			18	16	2	

Chain D:  50% 50%

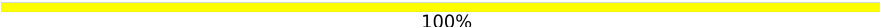
MAG1
MAG2

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

Chain E:  100%

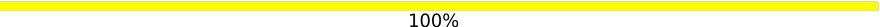
MAG1
MAG2

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

Chain G:  100%

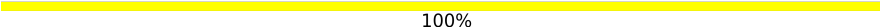
MAG1
MAG2

- 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%

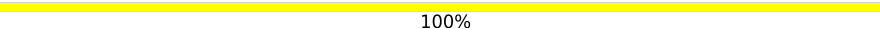
MAG1
MAG2

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

Chain M:  50% 50%

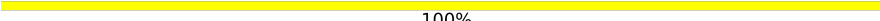
MAG1
MAG2

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

Chain N:  100%

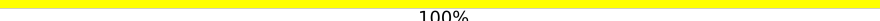
MAG1
MAG2

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

Chain O:  100%

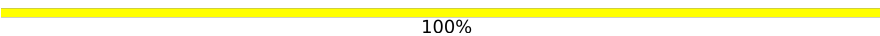
MAG1
MAG2

- 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:  50% 50%

MAG1
MAG2

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

Chain S:  50% 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 F:  33% 67%

MAG1
MAG2
BMA3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	25472	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)	1500	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.086	Depositor
Minimum map value	-0.032	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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 8Z9, 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	A	1.01	7/9379 (0.1%)	0.88	8/12766 (0.1%)
1	B	1.03	17/9399 (0.2%)	0.89	11/12798 (0.1%)
1	J	1.03	16/9410 (0.2%)	0.90	13/12809 (0.1%)
All	All	1.02	40/28188 (0.1%)	0.89	32/38373 (0.1%)

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

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	669	PHE	CB-CG	-9.36	1.35	1.51
1	J	293	PHE	CB-CG	-8.18	1.37	1.51
1	B	192	TRP	CB-CG	-7.56	1.36	1.50
1	B	667	TYR	CE2-CZ	-7.01	1.29	1.38
1	A	528	TYR	CB-CG	-6.69	1.41	1.51
1	J	528	TYR	CB-CG	-6.68	1.41	1.51
1	B	1203	TYR	CB-CG	-6.47	1.42	1.51
1	B	811	GLU	CG-CD	-6.36	1.42	1.51
1	A	756	CYS	CB-SG	-6.36	1.71	1.82
1	A	273	TRP	CB-CG	-6.36	1.38	1.50
1	B	667	TYR	CG-CD2	-6.20	1.31	1.39
1	J	67	PHE	CB-CG	-5.99	1.41	1.51
1	B	1154	TYR	CB-CG	-5.84	1.42	1.51
1	B	756	CYS	CB-SG	-5.82	1.72	1.81
1	J	260	CYS	CB-SG	-5.80	1.72	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	725	TYR	CB-CG	-5.80	1.43	1.51
1	J	1203	TYR	CB-CG	-5.78	1.43	1.51
1	B	260	CYS	CB-SG	-5.76	1.72	1.81
1	B	667	TYR	CD2-CE2	-5.49	1.31	1.39
1	J	282	TYR	CB-CG	-5.48	1.43	1.51
1	A	1203	TYR	CB-CG	-5.46	1.43	1.51
1	J	725	TYR	CB-CG	-5.44	1.43	1.51
1	J	346	GLU	CD-OE2	-5.32	1.19	1.25
1	J	608	VAL	CB-CG1	-5.32	1.41	1.52
1	B	240	PHE	CB-CG	-5.29	1.42	1.51
1	B	203	TYR	CB-CG	-5.24	1.43	1.51
1	A	444	ASN	CB-CG	-5.23	1.39	1.51
1	B	282	TYR	CB-CG	-5.22	1.43	1.51
1	J	170	TYR	CB-CG	-5.21	1.43	1.51
1	B	667	TYR	CB-CG	-5.20	1.43	1.51
1	J	684	TYR	CE2-CZ	-5.19	1.31	1.38
1	B	934	TYR	CB-CG	-5.18	1.43	1.51
1	B	430	TYR	CG-CD1	-5.18	1.32	1.39
1	J	321	GLU	CD-OE1	-5.16	1.20	1.25
1	J	798	GLU	CD-OE2	-5.16	1.20	1.25
1	B	1062	ARG	CB-CG	-5.15	1.38	1.52
1	J	843	TYR	CE2-CZ	-5.12	1.31	1.38
1	J	485	VAL	CB-CG1	-5.07	1.42	1.52
1	A	485	VAL	CB-CG1	-5.04	1.42	1.52
1	J	79	TYR	CB-CG	-5.02	1.44	1.51

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	282	TYR	CB-CG-CD2	-9.40	115.36	121.00
1	J	912	ARG	NE-CZ-NH2	-9.05	115.78	120.30
1	B	282	TYR	CB-CG-CD2	-8.87	115.68	121.00
1	A	282	TYR	CB-CG-CD2	-8.48	115.91	121.00
1	B	413	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	B	687	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	J	1088	ARG	NE-CZ-NH2	7.20	123.90	120.30
1	A	1062	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	B	667	TYR	CB-CG-CD2	-6.78	116.94	121.00
1	J	280	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	A	660	TYR	CB-CG-CD2	-6.57	117.06	121.00
1	B	660	TYR	CB-CG-CD2	-6.54	117.07	121.00
1	A	670	ARG	NE-CZ-NH2	-6.28	117.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	676	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	B	684	TYR	CB-CG-CD1	-6.05	117.37	121.00
1	A	952	TYR	CB-CG-CD2	-5.80	117.52	121.00
1	J	660	TYR	CB-CG-CD2	-5.78	117.53	121.00
1	A	528	TYR	CB-CG-CD2	-5.74	117.55	121.00
1	B	528	TYR	CB-CG-CD2	-5.63	117.62	121.00
1	J	430	TYR	CB-CG-CD1	-5.48	117.71	121.00
1	B	704	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	1224	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	J	997	TYR	CB-CG-CD2	-5.41	117.75	121.00
1	B	215	TYR	CB-CG-CD2	-5.39	117.77	121.00
1	A	424	TYR	CB-CG-CD2	-5.39	117.77	121.00
1	J	528	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	J	704	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	J	833	TYR	CB-CG-CD1	-5.25	117.85	121.00
1	A	413	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	J	1198	TYR	CB-CG-CD2	-5.23	117.86	121.00
1	B	1198	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	J	265	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	936	ASN	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9168	0	8854	16	0
1	B	9185	0	8877	41	0
1	J	9198	0	8887	25	0
2	H	555	0	139	9	0
2	L	510	0	131	3	0
3	C	28	0	25	0	0
3	D	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	28	0	25	0	0
3	G	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	O	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
4	F	39	0	33	0	0
5	A	126	0	117	0	0
5	B	126	0	117	0	0
5	J	126	0	117	0	0
6	B	18	0	0	0	0
6	J	36	0	0	3	0
All	All	29451	0	27597	91	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (91) 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:23:LEU:HD11	1:B:188:PHE:HB3	1.77	0.67
1:B:258:LEU:HD23	1:B:268:PHE:CE1	2.33	0.64
1:J:192:TRP:CE3	1:J:193:HIS:N	2.66	0.64
1:A:371:ASN:N	1:A:371:ASN:OD1	2.32	0.62
1:B:188:PHE:CD2	1:B:259:THR:HG21	2.34	0.62
1:B:258:LEU:CD2	1:B:268:PHE:CE1	2.85	0.60
1:B:266:ILE:HG12	2:L:26:UNK:HA	1.82	0.60
1:J:85:LYS:NZ	1:J:87:THR:OG1	2.34	0.59
1:B:258:LEU:HD23	1:B:268:PHE:HE1	1.67	0.59
1:B:185:GLY:HA3	1:B:261:ILE:HB	1.86	0.58
2:H:33:UNK:N	2:H:94:UNK:O	2.37	0.58
1:J:192:TRP:CZ3	1:J:193:HIS:HB2	2.39	0.57
2:H:6:UNK:HA	2:H:22:UNK:HA	1.85	0.57
1:B:371:ASN:N	1:B:371:ASN:OD1	2.40	0.55
1:B:266:ILE:HG13	1:B:266:ILE:O	2.07	0.54
1:A:429:ASN:ND2	1:A:487:TYR:HB2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:371:ASN:N	1:J:371:ASN:OD1	2.41	0.53
1:J:667:TYR:HD2	1:J:679:MET:HE1	1.74	0.53
1:J:900:GLY:O	1:J:901:CYS:C	2.47	0.53
1:B:125:GLU:OE1	1:B:268:PHE:HZ	1.92	0.53
1:B:258:LEU:CD2	1:B:268:PHE:HE1	2.21	0.53
1:J:659:LEU:HD21	1:J:667:TYR:CE2	2.44	0.53
1:B:185:GLY:CA	1:B:261:ILE:HB	2.38	0.53
1:B:188:PHE:HD2	1:B:259:THR:HG21	1.72	0.53
1:A:829:VAL:HG22	1:A:1093:ARG:HB3	1.91	0.53
1:J:505:SER:O	1:J:506:SER:C	2.48	0.52
1:A:233:ASP:OD1	1:A:233:ASP:N	2.42	0.52
1:B:258:LEU:HD21	1:B:268:PHE:CZ	2.46	0.51
1:B:266:ILE:CG1	2:L:26:UNK:HA	2.42	0.50
1:A:829:VAL:HA	1:A:1093:ARG:HG2	1.93	0.50
1:B:262:SER:HB2	1:B:265:ASP:O	2.11	0.50
1:J:193:HIS:CG	1:J:193:HIS:O	2.62	0.49
1:A:28:GLY:HA3	1:A:188:PHE:CZ	2.47	0.49
2:H:6:UNK:CB	2:H:109:UNK:HA	2.41	0.49
1:B:300:SER:OG	1:B:301:ASP:N	2.44	0.49
1:B:505:SER:O	1:B:506:SER:C	2.50	0.49
1:B:187:HIS:CE1	1:B:261:ILE:HG12	2.48	0.49
1:B:944:ARG:O	1:B:944:ARG:HG3	2.12	0.49
1:B:125:GLU:OE1	1:B:268:PHE:CZ	2.66	0.48
1:A:983:TRP:CE2	1:A:990:PRO:HA	2.48	0.48
1:B:301:ASP:OD1	1:B:302:PHE:N	2.46	0.48
1:B:87:THR:OG1	1:B:88:ASP:N	2.47	0.48
1:A:23:LEU:HB3	1:A:25:SER:HB3	1.95	0.47
1:J:133:SER:OG	1:J:134:THR:N	2.46	0.47
1:B:504:ASN:OD1	1:B:504:ASN:N	2.47	0.47
1:B:233:ASP:N	1:B:233:ASP:OD1	2.40	0.47
2:H:6:UNK:HA	2:H:22:UNK:CB	2.44	0.47
1:J:787:ASN:OD1	1:J:787:ASN:N	2.48	0.47
1:J:899:LEU:HD22	1:J:972:LEU:HD11	1.97	0.47
1:B:267:GLY:O	1:B:268:PHE:C	2.53	0.47
1:J:402:ILE:HD13	6:J:1410:8Z9:CG	2.45	0.46
1:B:1130:SER:OG	1:B:1131:SER:N	2.47	0.46
1:J:892:ASP:OD2	1:J:1014:LYS:NZ	2.47	0.46
1:B:64:THR:OG1	1:B:65:THR:N	2.49	0.46
1:B:787:ASN:OD1	1:B:787:ASN:N	2.48	0.46
2:H:101:UNK:O	2:H:103:UNK:N	2.49	0.46
1:A:133:SER:OG	1:A:134:THR:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:ASN:OD1	1:A:504:ASN:N	2.48	0.45
1:J:375:LEU:HD21	6:J:1410:8Z9:CB	2.46	0.45
1:B:1113:PHE:CE2	1:B:1117:GLN:NE2	2.84	0.45
1:B:187:HIS:CD2	1:B:261:ILE:HD11	2.52	0.45
1:J:180:CYS:O	1:J:181:HIS:C	2.54	0.45
1:J:375:LEU:HD21	6:J:1410:8Z9:CC	2.46	0.45
1:B:160:GLN:O	1:B:160:GLN:HG2	2.17	0.44
2:H:108:UNK:O	2:H:109:UNK:C	2.65	0.44
1:B:137:ASN:OD1	1:B:137:ASN:C	2.54	0.44
1:B:258:LEU:HD21	1:B:268:PHE:CE1	2.52	0.44
1:J:738:ASN:OD1	1:J:738:ASN:C	2.55	0.44
1:J:901:CYS:SG	1:J:901:CYS:O	2.77	0.43
1:B:755:TYR:CD2	1:B:775:PHE:CE2	3.07	0.43
1:A:64:THR:OG1	1:A:65:THR:N	2.51	0.43
1:A:891:ASP:OD2	1:A:992:TYR:HB3	2.18	0.43
1:B:738:ASN:OD1	1:B:738:ASN:C	2.57	0.43
1:J:574:ASN:HB3	1:J:575:PRO:HD3	2.01	0.43
1:A:300:SER:OG	1:A:301:ASP:N	2.49	0.42
1:B:901:CYS:SG	1:B:901:CYS:O	2.76	0.42
1:J:536:ASN:N	1:J:537:PRO:CD	2.82	0.42
1:J:212:ASN:OD1	1:J:212:ASN:N	2.52	0.42
2:H:6:UNK:HA	2:H:22:UNK:CA	2.48	0.42
1:A:285:ALA:HB1	1:A:293:PHE:CE2	2.55	0.42
1:J:351:ASP:OD1	1:J:352:LYS:N	2.51	0.42
1:A:429:ASN:HD21	1:A:487:TYR:HB2	1.85	0.42
1:A:771:THR:HG22	1:A:773:TYR:H	1.86	0.41
1:B:133:SER:OG	1:B:134:THR:N	2.52	0.41
1:B:258:LEU:CD2	1:B:268:PHE:CZ	3.04	0.41
2:H:101:UNK:C	2:H:103:UNK:N	2.83	0.41
1:J:667:TYR:O	1:J:679:MET:HE3	2.20	0.41
1:B:573:GLY:O	1:B:574:ASN:C	2.58	0.41
1:B:266:ILE:CB	2:L:26:UNK:HA	2.51	0.40
2:H:81:UNK:O	2:H:82:UNK:C	2.67	0.40
1:J:170:TYR:CD2	1:J:193:HIS:CD2	3.10	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1164/1367 (85%)	1142 (98%)	22 (2%)	0	100	100
1	B	1170/1367 (86%)	1149 (98%)	21 (2%)	0	100	100
1	J	1171/1367 (86%)	1148 (98%)	23 (2%)	0	100	100
All	All	3505/4101 (86%)	3439 (98%)	66 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1026/1182 (87%)	1022 (100%)	4 (0%)	91	95
1	B	1028/1182 (87%)	1022 (99%)	6 (1%)	86	91
1	J	1029/1182 (87%)	1024 (100%)	5 (0%)	88	93
All	All	3083/3546 (87%)	3068 (100%)	15 (0%)	89	93

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	212	ASN
1	J	248	MET
1	J	655	TRP
1	J	787	ASN
1	J	846	PHE

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Mol	Chain	Res	Type
1	A	248	MET
1	A	787	ASN
1	A	1093	ARG
1	A	1223	ASN
1	B	63	ASN
1	B	137	ASN
1	B	187	HIS
1	B	239	LYS
1	B	449	ASN
1	B	787	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	193	HIS
1	J	252	HIS
1	J	1011	GLN
1	A	252	HIS
1	A	444	ASN
1	A	598	ASN
1	B	187	HIS
1	B	252	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

29 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	3,1	14,14,15	0.74	0	17,19,21	0.88	0
3	NAG	C	2	3	14,14,15	0.76	0	17,19,21	0.95	1 (5%)
3	NAG	D	1	3,1	14,14,15	0.77	0	17,19,21	1.11	0
3	NAG	D	2	3	14,14,15	0.79	0	17,19,21	0.92	1 (5%)
3	NAG	E	1	3,1	14,14,15	0.78	0	17,19,21	1.17	2 (11%)
3	NAG	E	2	3	14,14,15	0.78	0	17,19,21	1.13	1 (5%)
4	NAG	F	1	1,4	14,14,15	0.76	0	17,19,21	0.83	0
4	NAG	F	2	4	14,14,15	0.81	0	17,19,21	0.78	1 (5%)
4	BMA	F	3	4	11,11,12	1.80	2 (18%)	15,15,17	1.01	1 (6%)
3	NAG	G	1	3,1	14,14,15	0.83	0	17,19,21	1.15	1 (5%)
3	NAG	G	2	3	14,14,15	0.77	0	17,19,21	0.86	1 (5%)
3	NAG	I	1	3,1	14,14,15	0.76	0	17,19,21	1.27	2 (11%)
3	NAG	I	2	3	14,14,15	0.82	0	17,19,21	0.96	1 (5%)
3	NAG	K	1	3,1	14,14,15	0.79	0	17,19,21	0.84	1 (5%)
3	NAG	K	2	3	14,14,15	0.84	0	17,19,21	0.88	1 (5%)
3	NAG	M	1	3,1	14,14,15	0.80	0	17,19,21	1.12	2 (11%)
3	NAG	M	2	3	14,14,15	0.87	0	17,19,21	0.86	0
3	NAG	N	1	3,1	14,14,15	0.78	0	17,19,21	1.05	1 (5%)
3	NAG	N	2	3	14,14,15	0.81	0	17,19,21	0.85	1 (5%)
3	NAG	O	1	3,1	14,14,15	0.76	0	17,19,21	1.51	4 (23%)
3	NAG	O	2	3	14,14,15	0.79	0	17,19,21	1.09	1 (5%)
3	NAG	P	1	3,1	14,14,15	0.83	1 (7%)	17,19,21	1.33	3 (17%)
3	NAG	P	2	3	14,14,15	0.77	0	17,19,21	0.97	1 (5%)
3	NAG	Q	1	3,1	14,14,15	0.83	0	17,19,21	1.07	1 (5%)
3	NAG	Q	2	3	14,14,15	0.84	0	17,19,21	0.84	1 (5%)
3	NAG	R	1	3,1	14,14,15	0.81	0	17,19,21	1.21	3 (17%)
3	NAG	R	2	3	14,14,15	0.85	0	17,19,21	0.88	0
3	NAG	S	1	3,1	14,14,15	0.87	1 (7%)	17,19,21	0.82	0
3	NAG	S	2	3	14,14,15	0.76	0	17,19,21	0.92	1 (5%)

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

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	3	BMA	O2-C2	-4.06	1.34	1.43
4	F	3	BMA	C2-C3	-2.35	1.49	1.52
3	P	1	NAG	C3-C2	-2.13	1.48	1.52
3	S	1	NAG	C3-C2	-2.11	1.48	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	1	NAG	O4-C4-C3	-3.51	102.24	110.35
3	E	2	NAG	C4-C3-C2	-3.48	105.91	111.02
3	G	1	NAG	C4-C3-C2	-3.31	106.16	111.02
3	O	2	NAG	C4-C3-C2	-3.25	106.26	111.02
3	O	1	NAG	C4-C3-C2	-3.24	106.27	111.02
3	E	1	NAG	O4-C4-C3	-3.05	103.29	110.35
3	R	1	NAG	O5-C5-C6	-2.95	102.58	107.20
3	I	1	NAG	C4-C3-C2	-2.93	106.72	111.02
3	P	2	NAG	C4-C3-C2	-2.88	106.79	111.02
3	C	2	NAG	C4-C3-C2	-2.81	106.91	111.02
3	P	1	NAG	O5-C5-C6	-2.68	103.00	107.20
3	S	2	NAG	C4-C3-C2	-2.68	107.09	111.02
3	D	2	NAG	C4-C3-C2	-2.66	107.12	111.02
3	N	1	NAG	C4-C3-C2	-2.43	107.45	111.02
3	R	1	NAG	C3-C4-C5	-2.43	105.91	110.24
3	M	1	NAG	O5-C5-C6	-2.42	103.42	107.20
3	K	1	NAG	C3-C4-C5	-2.41	105.94	110.24
3	M	1	NAG	C3-C4-C5	-2.37	106.02	110.24
3	K	2	NAG	C4-C3-C2	-2.36	107.56	111.02
3	N	2	NAG	C4-C3-C2	-2.31	107.64	111.02
3	I	2	NAG	C4-C3-C2	-2.29	107.66	111.02
3	O	1	NAG	O5-C1-C2	-2.27	107.71	111.29
3	P	1	NAG	C3-C4-C5	-2.25	106.23	110.24
3	E	1	NAG	O5-C5-C6	-2.23	103.70	107.20
4	F	2	NAG	C3-C4-C5	-2.22	106.28	110.24
3	R	1	NAG	O4-C4-C3	-2.17	105.34	110.35
3	I	1	NAG	O5-C5-C6	-2.15	103.83	107.20
3	Q	1	NAG	O5-C1-C2	-2.14	107.91	111.29
4	F	3	BMA	C2-C3-C4	-2.12	107.23	110.89
3	O	1	NAG	O4-C4-C5	-2.11	104.05	109.30
3	O	1	NAG	C6-C5-C4	-2.07	108.15	113.00
3	G	2	NAG	C4-C3-C2	-2.07	107.99	111.02
3	Q	2	NAG	C4-C3-C2	-2.06	108.00	111.02

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	O5-C5-C6-O6
3	O	2	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	S	1	NAG	O5-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6

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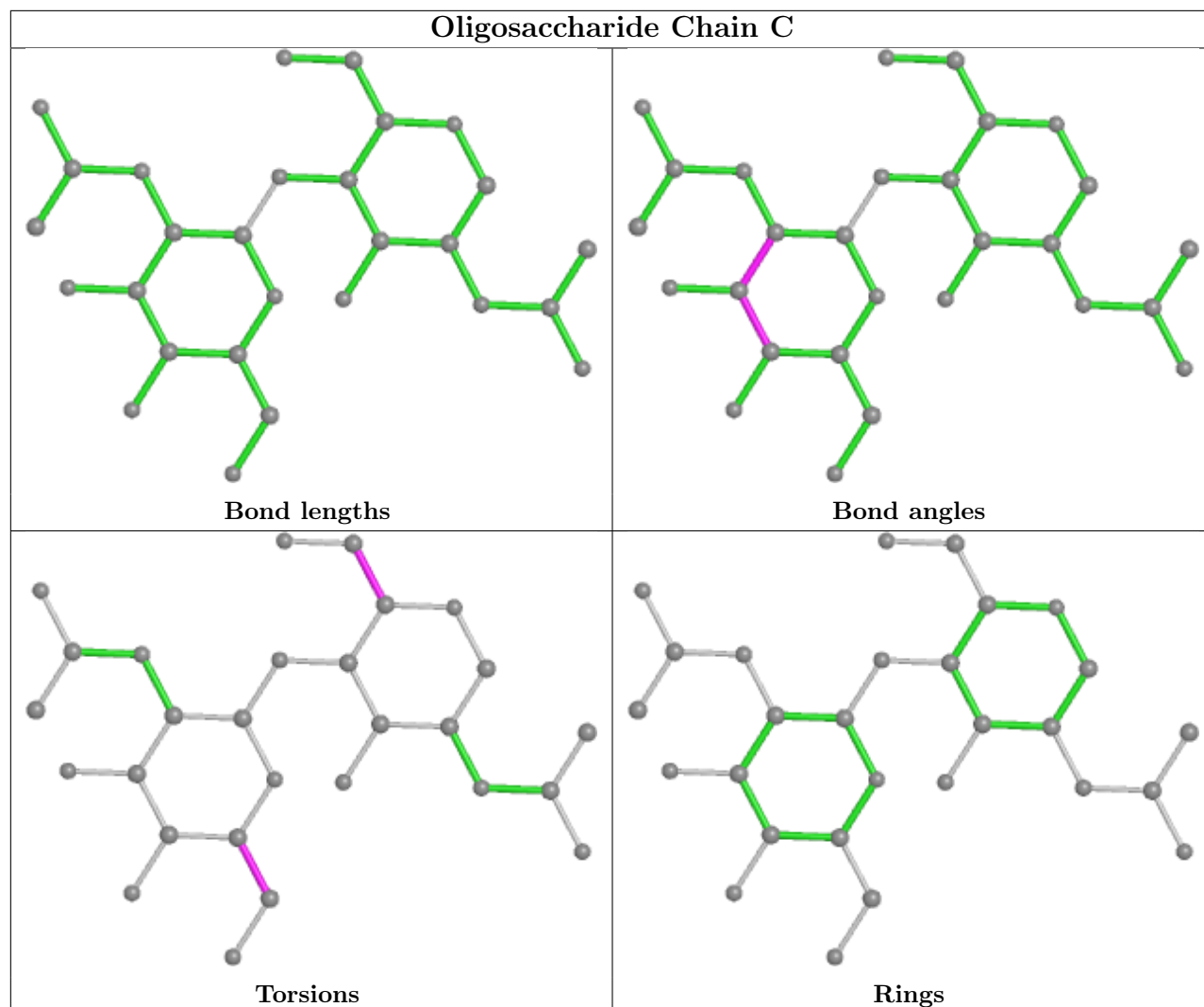
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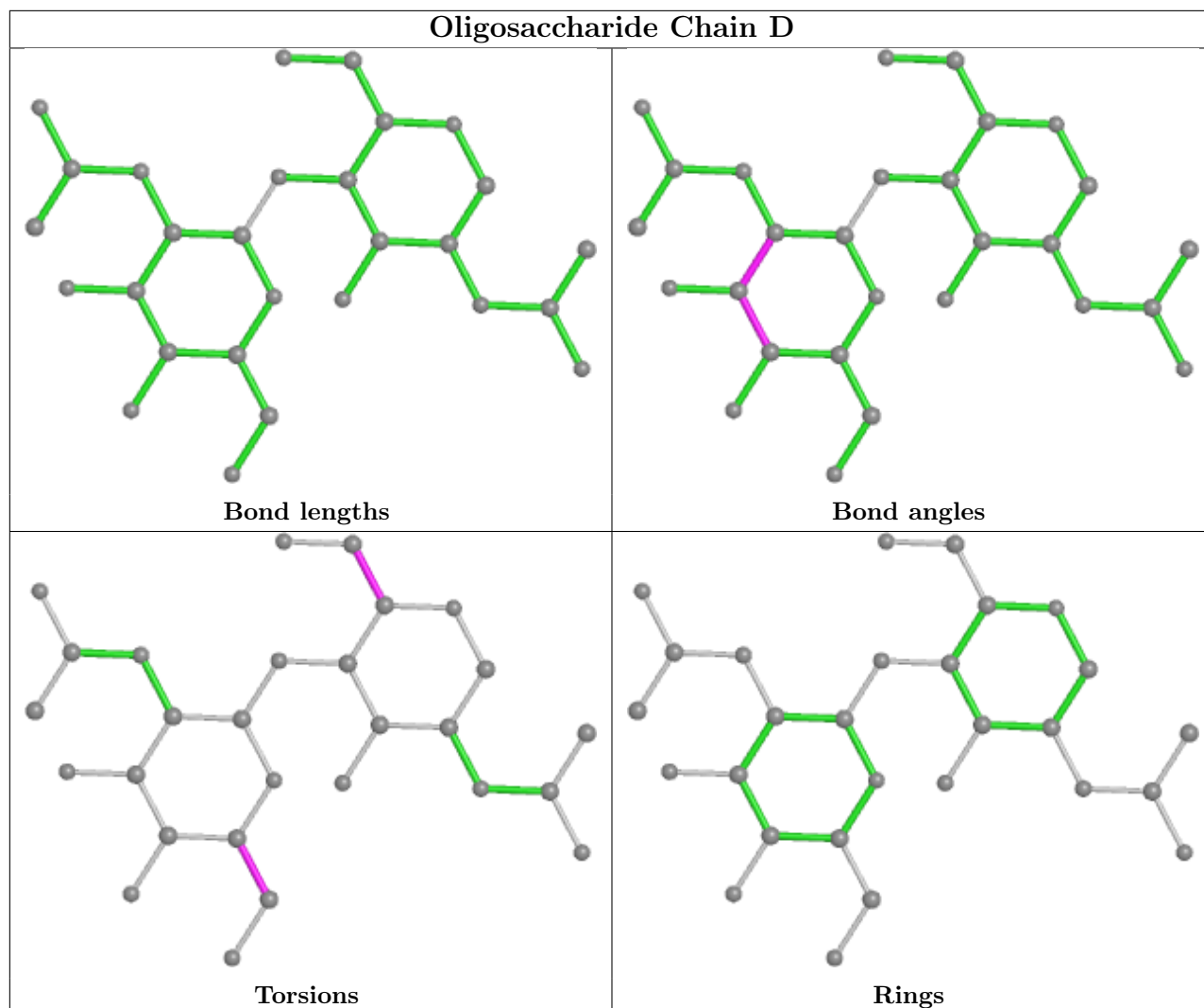
Mol	Chain	Res	Type	Atoms
3	D	2	NAG	O5-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	S	1	NAG	C4-C5-C6-O6
3	R	2	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6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

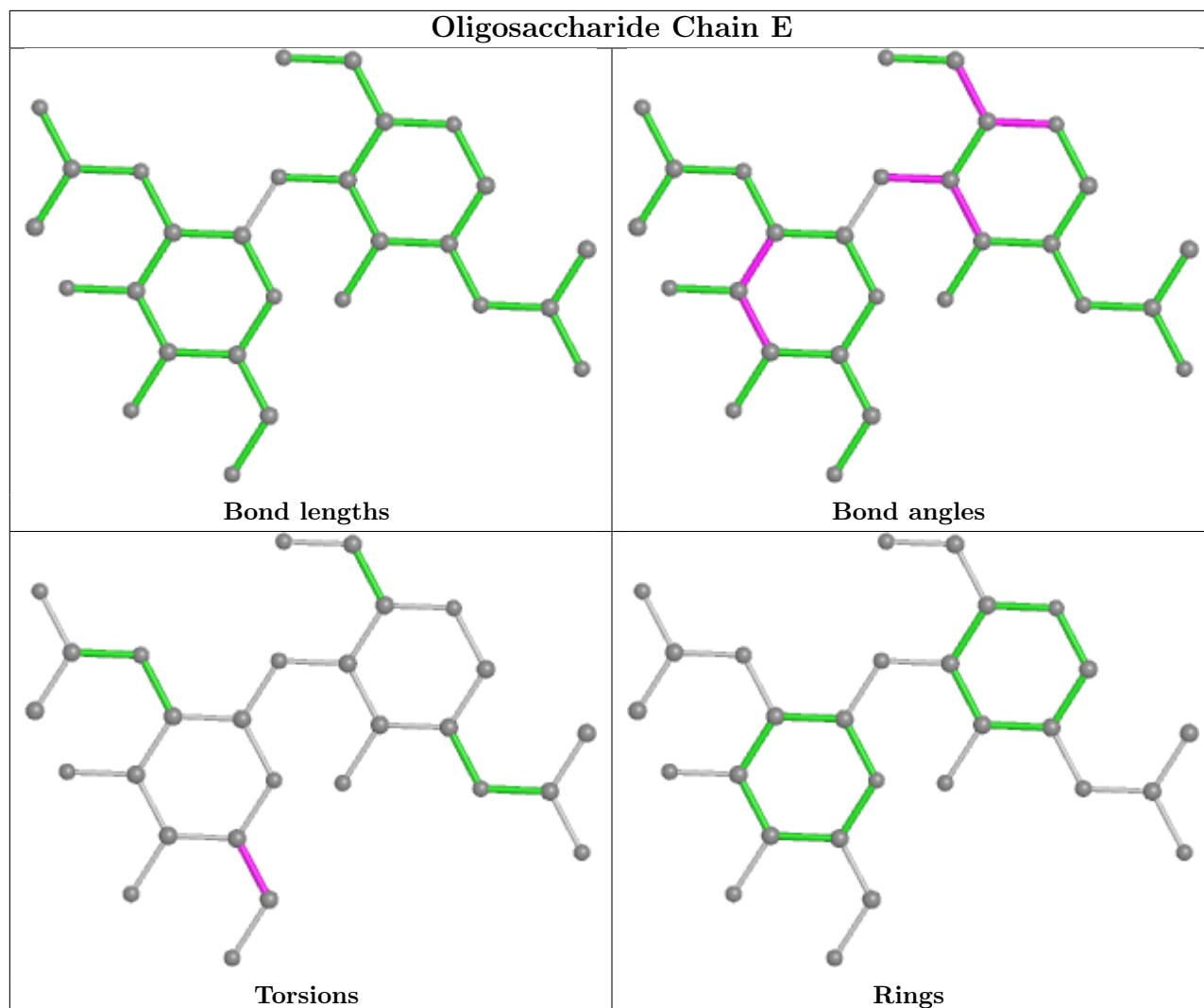
There are no ring outliers.

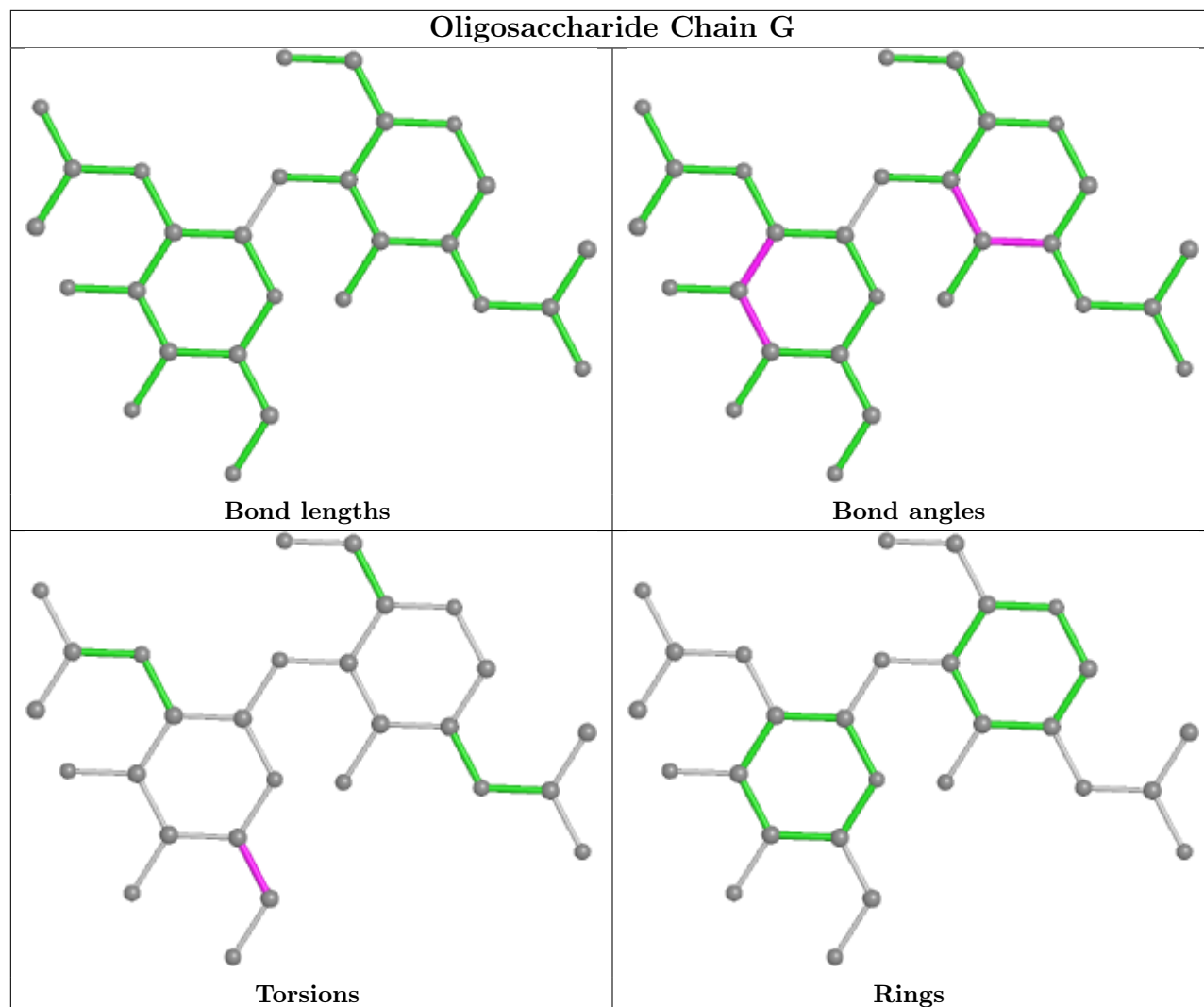
No monomer is involved in short contacts.

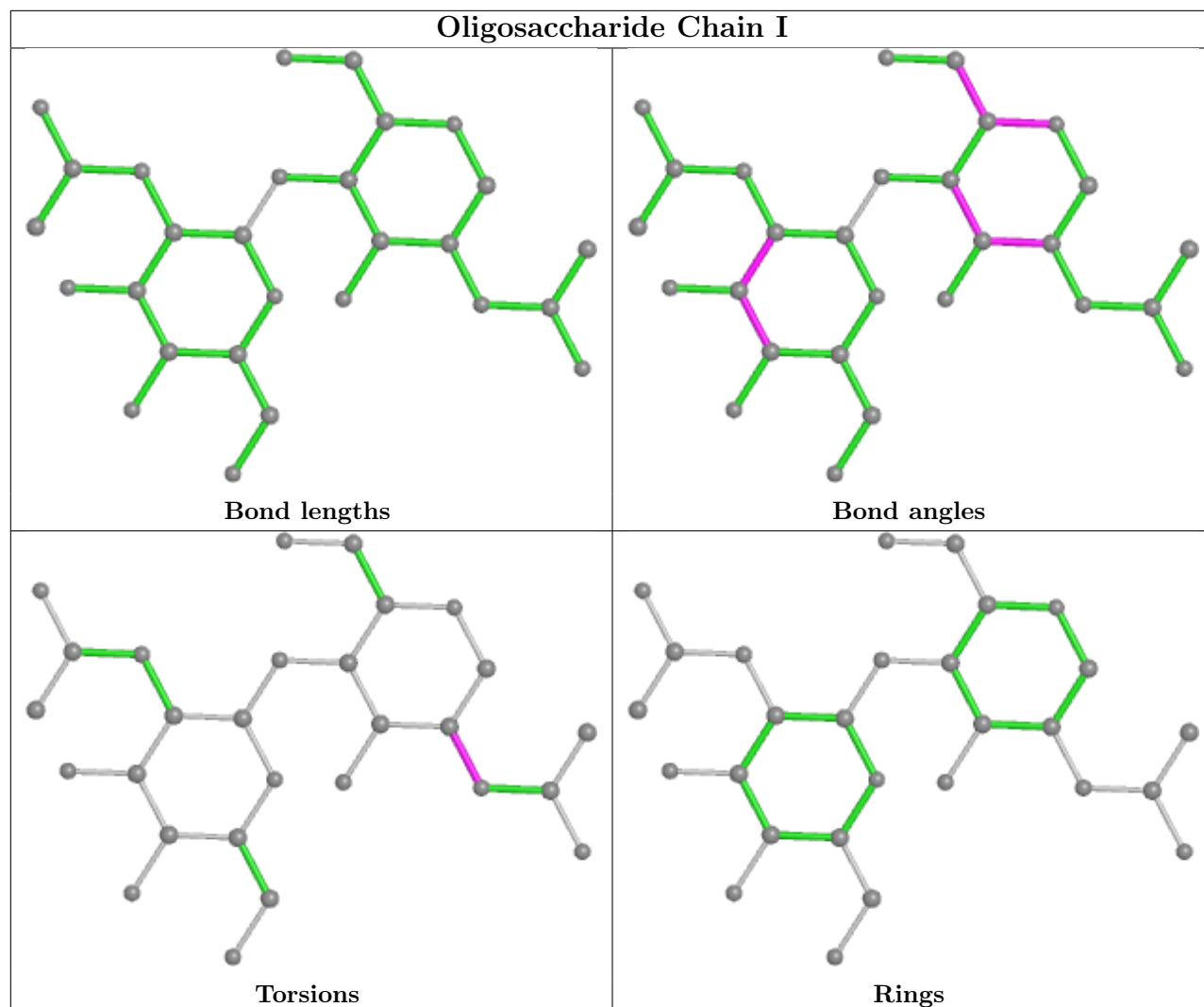
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

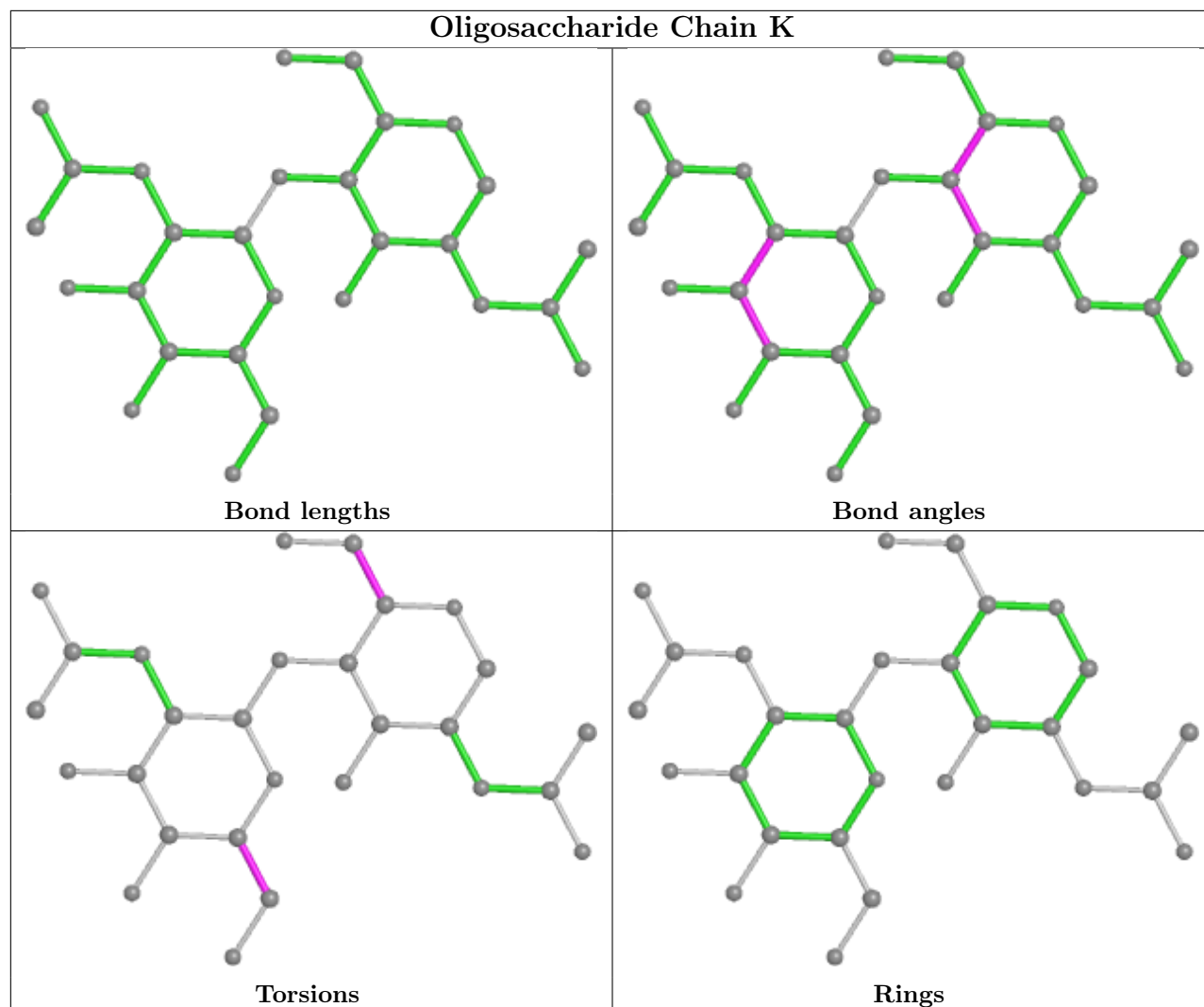


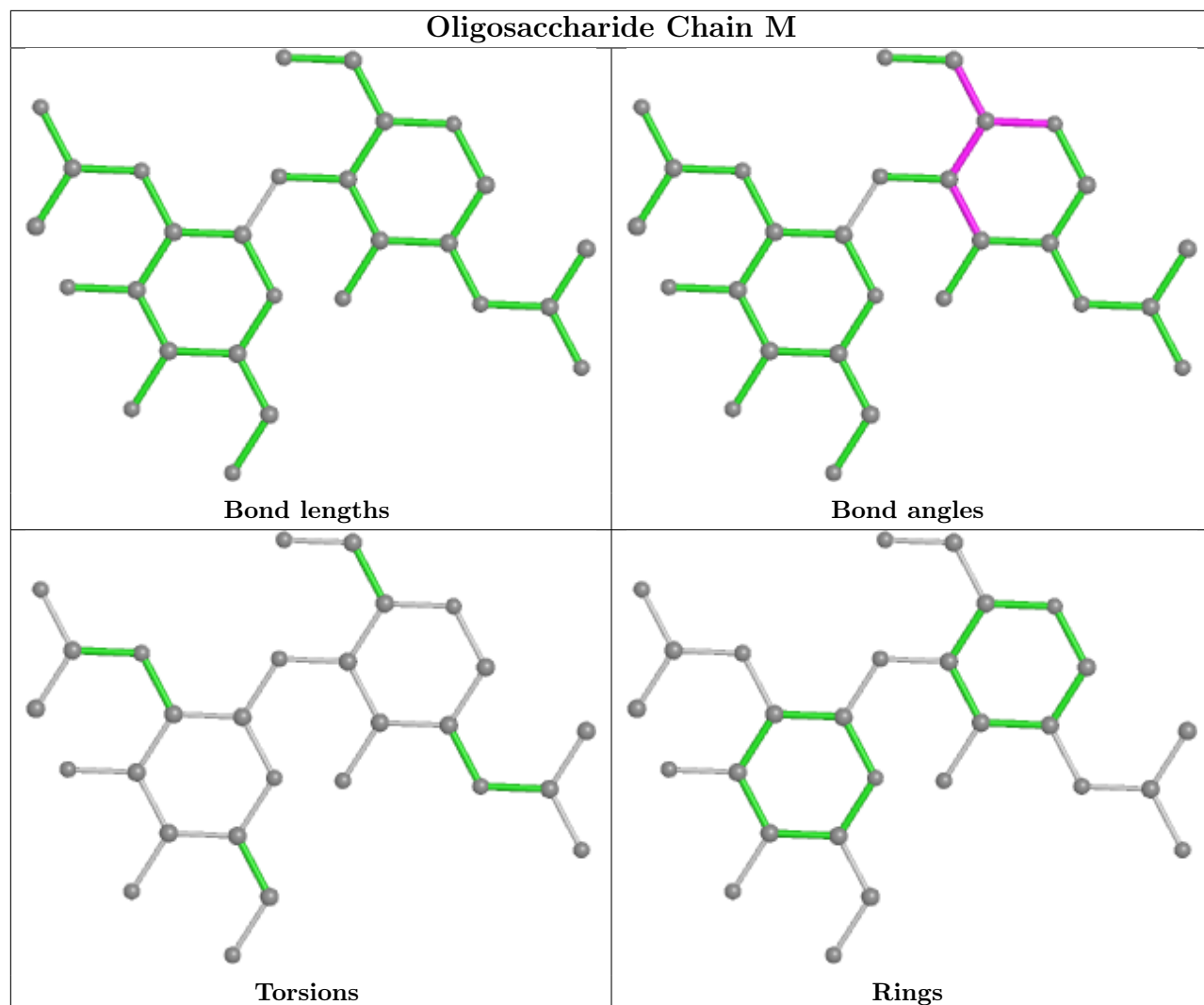


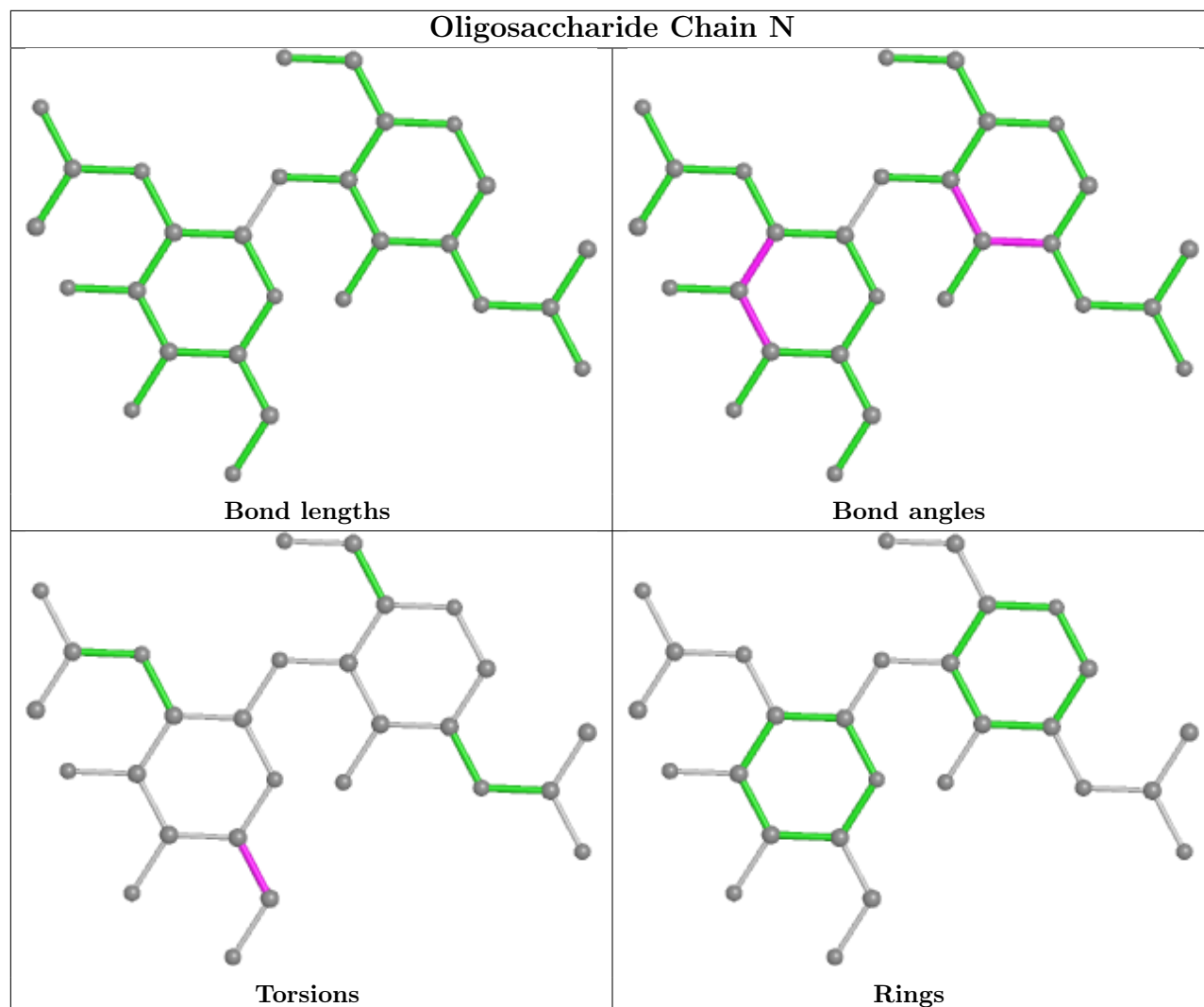


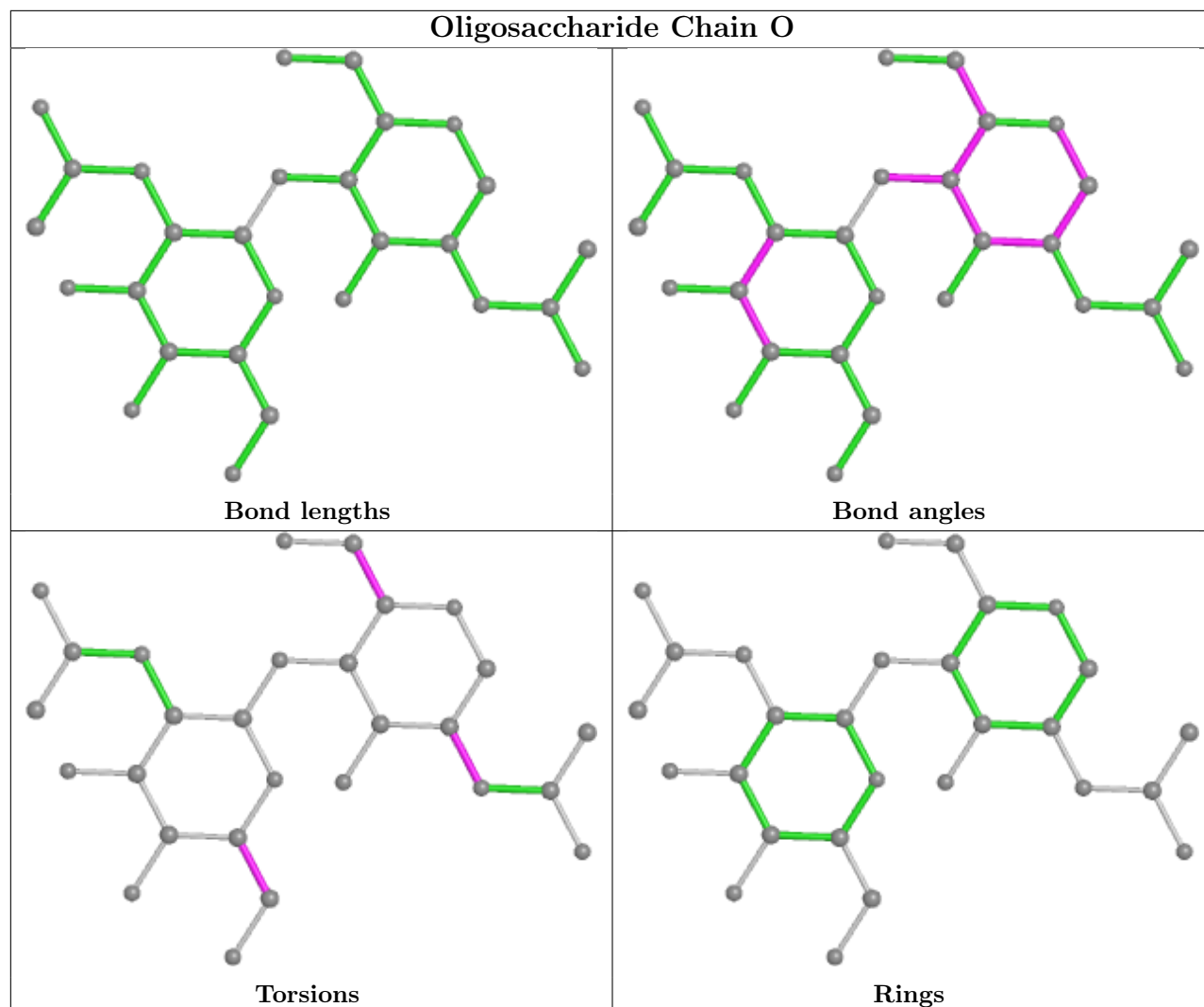


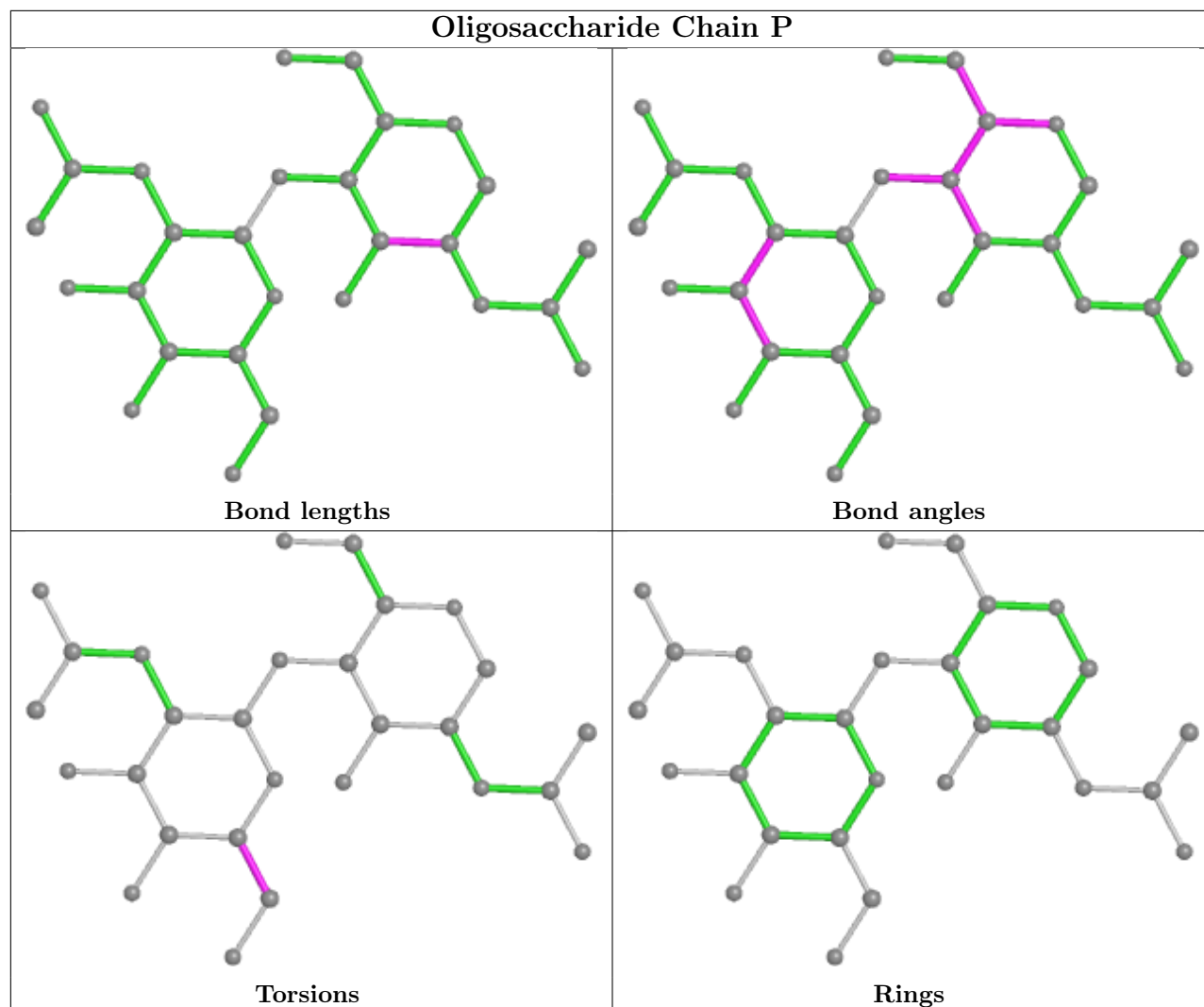


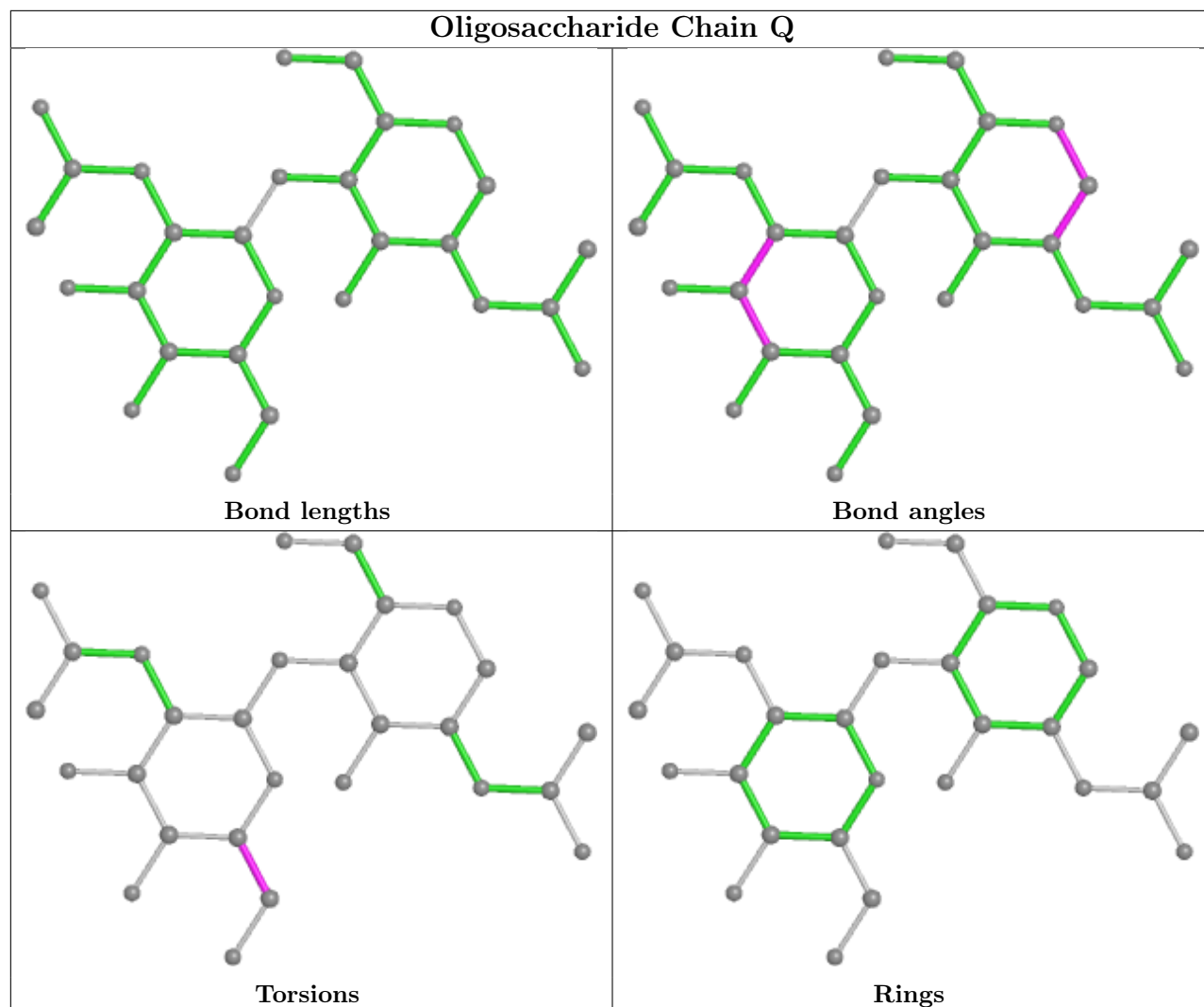


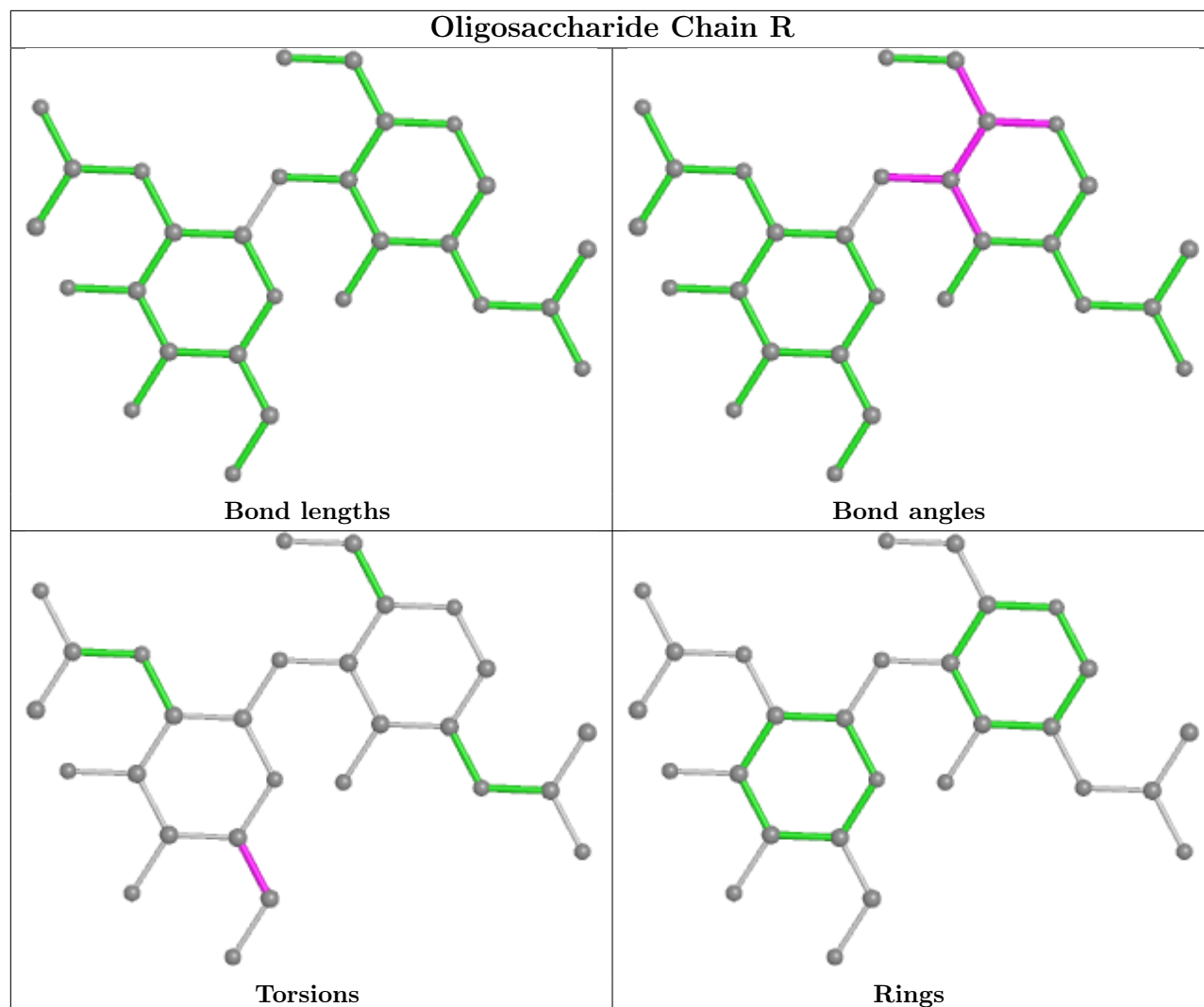


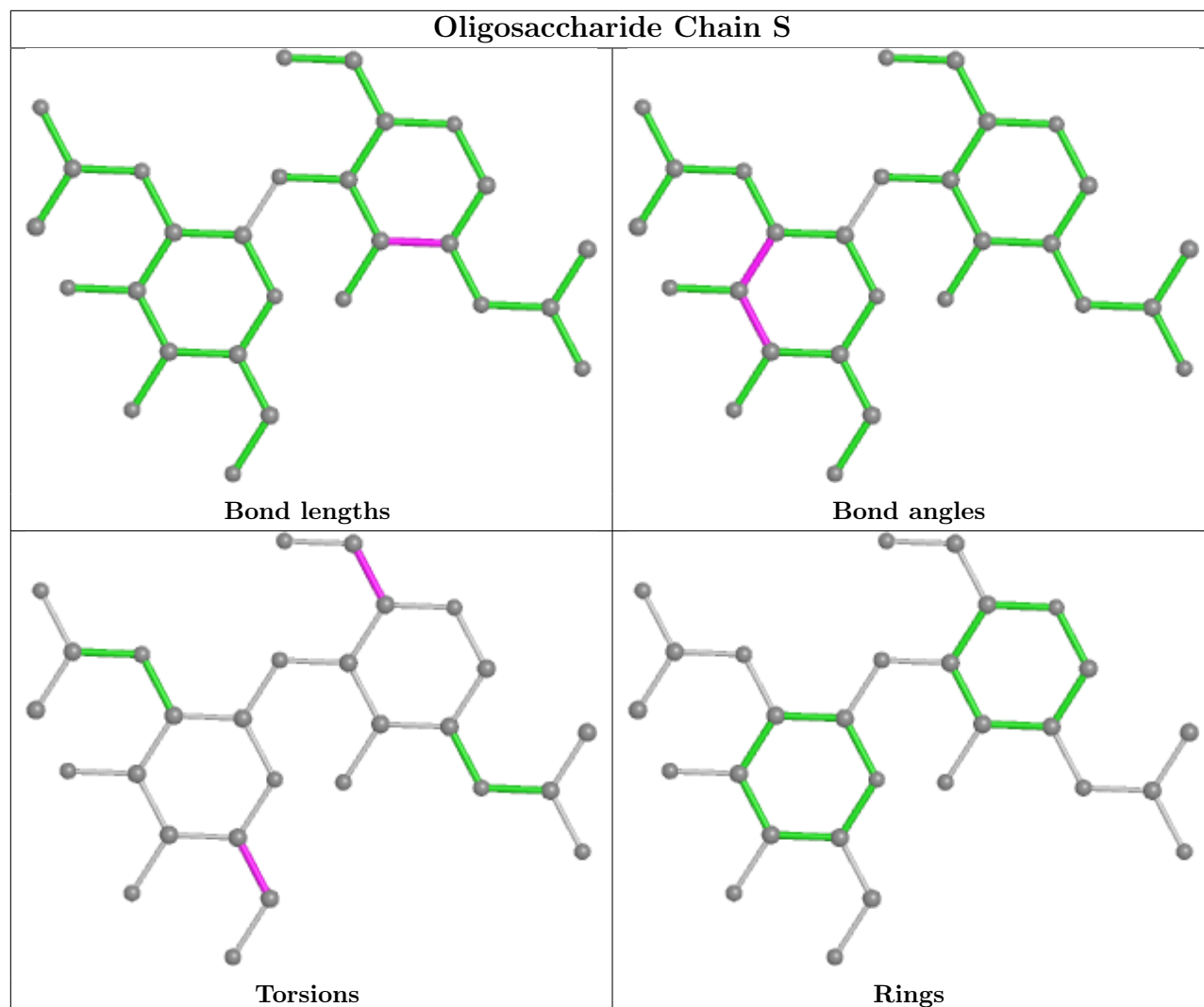


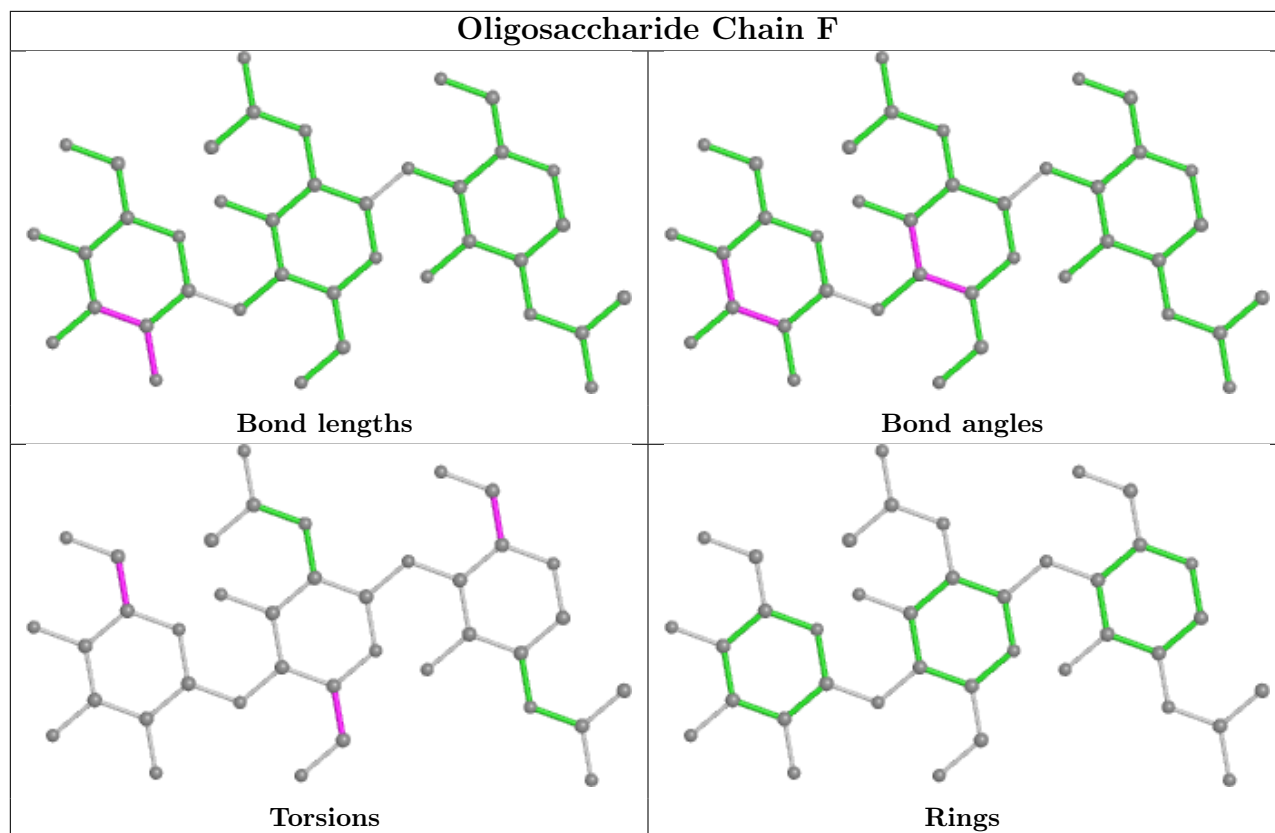












5.6 Ligand geometry [i](#)

30 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	1409	1	14,14,15	0.92	0	17,19,21	1.14	1 (5%)
6	8Z9	B	1410	-	17,17,17	0.96	1 (5%)	17,17,17	0.68	0
5	NAG	B	1405	1	14,14,15	0.31	0	17,19,21	0.65	0
6	8Z9	J	1410	-	17,17,17	0.97	1 (5%)	17,17,17	0.63	0
5	NAG	A	1402	1	14,14,15	0.83	0	17,19,21	1.31	2 (11%)
5	NAG	A	1408	1	14,14,15	0.83	0	17,19,21	0.85	1 (5%)
5	NAG	B	1404	1	14,14,15	0.83	0	17,19,21	1.03	1 (5%)
5	NAG	A	1403	1	14,14,15	0.82	0	17,19,21	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	J	1404	1	14,14,15	0.31	0	17,19,21	0.65	0
5	NAG	J	1407	1	14,14,15	0.92	1 (7%)	17,19,21	1.13	1 (5%)
5	NAG	B	1403	1	14,14,15	0.34	0	17,19,21	0.82	0
5	NAG	J	1409	1	14,14,15	0.88	0	17,19,21	0.90	1 (5%)
5	NAG	A	1404	1	14,14,15	0.86	0	17,19,21	1.03	2 (11%)
5	NAG	J	1402	1	14,14,15	0.80	0	17,19,21	1.45	3 (17%)
5	NAG	A	1406	1	14,14,15	0.81	0	17,19,21	0.95	1 (5%)
5	NAG	A	1401	1	14,14,15	0.76	0	17,19,21	0.95	1 (5%)
5	NAG	B	1402	1	14,14,15	0.78	0	17,19,21	0.97	1 (5%)
5	NAG	B	1408	1	14,14,15	0.82	1 (7%)	17,19,21	1.27	2 (11%)
5	NAG	J	1403	1	14,14,15	0.81	0	17,19,21	0.94	1 (5%)
5	NAG	J	1405	1	14,14,15	0.82	0	17,19,21	1.32	2 (11%)
5	NAG	A	1409	1	14,14,15	0.76	1 (7%)	17,19,21	1.19	2 (11%)
5	NAG	B	1401	1	14,14,15	0.74	0	17,19,21	1.01	2 (11%)
5	NAG	A	1405	1	14,14,15	0.82	0	17,19,21	0.90	1 (5%)
5	NAG	B	1407	1	14,14,15	0.89	0	17,19,21	0.87	1 (5%)
5	NAG	J	1406	1	14,14,15	0.91	0	17,19,21	1.04	1 (5%)
6	8Z9	J	1411	-	17,17,17	0.79	0	17,17,17	0.58	0
5	NAG	B	1406	1	14,14,15	0.79	0	17,19,21	1.00	1 (5%)
5	NAG	J	1401	1	14,14,15	0.82	0	17,19,21	1.09	1 (5%)
5	NAG	A	1407	1	14,14,15	0.93	0	17,19,21	1.20	1 (5%)
5	NAG	J	1408	1	14,14,15	0.73	0	17,19,21	1.11	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1409	1	-	2/6/23/26	0/1/1/1
6	8Z9	B	1410	-	-	6/15/15/15	-
5	NAG	B	1405	1	-	4/6/23/26	0/1/1/1
6	8Z9	J	1410	-	-	7/15/15/15	-
5	NAG	A	1402	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1408	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1404	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1403	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	J	1404	1	-	3/6/23/26	0/1/1/1
5	NAG	J	1407	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1403	1	-	3/6/23/26	0/1/1/1
5	NAG	J	1409	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1404	1	-	0/6/23/26	0/1/1/1
5	NAG	J	1402	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1406	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1401	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1402	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1408	1	-	2/6/23/26	0/1/1/1
5	NAG	J	1403	1	-	0/6/23/26	0/1/1/1
5	NAG	J	1405	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1409	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1401	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1405	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1407	1	-	1/6/23/26	0/1/1/1
5	NAG	J	1406	1	-	1/6/23/26	0/1/1/1
6	8Z9	J	1411	-	-	8/15/15/15	-
5	NAG	B	1406	1	-	1/6/23/26	0/1/1/1
5	NAG	J	1401	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1407	1	-	1/6/23/26	0/1/1/1
5	NAG	J	1408	1	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1410	8Z9	C2-C1	2.58	1.56	1.50
6	J	1410	8Z9	C2-C1	2.18	1.55	1.50
5	J	1407	NAG	C3-C2	-2.14	1.48	1.52
5	B	1408	NAG	C3-C2	-2.01	1.48	1.52
5	A	1409	NAG	C3-C2	-2.01	1.48	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	1405	NAG	C4-C3-C2	-3.95	105.24	111.02
5	B	1408	NAG	C4-C3-C2	-3.78	105.48	111.02
5	J	1402	NAG	O5-C5-C6	-3.73	101.35	107.20
5	A	1407	NAG	C4-C3-C2	-3.65	105.67	111.02
5	B	1409	NAG	C4-C3-C2	-3.28	106.22	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	1401	NAG	C4-C3-C2	-3.28	106.22	111.02
5	B	1406	NAG	C4-C3-C2	-3.06	106.54	111.02
5	B	1404	NAG	C4-C3-C2	-3.04	106.56	111.02
5	B	1402	NAG	C4-C3-C2	-3.03	106.58	111.02
5	J	1408	NAG	C4-C3-C2	-2.99	106.63	111.02
5	J	1407	NAG	C4-C3-C2	-2.97	106.67	111.02
5	J	1402	NAG	O5-C1-C2	-2.92	106.68	111.29
5	A	1401	NAG	C4-C3-C2	-2.75	106.98	111.02
5	A	1409	NAG	O4-C4-C3	-2.45	104.68	110.35
5	A	1408	NAG	C4-C3-C2	-2.42	107.47	111.02
5	B	1408	NAG	O5-C1-C2	-2.41	107.48	111.29
5	A	1405	NAG	C4-C3-C2	-2.39	107.52	111.02
5	J	1405	NAG	O5-C1-C2	-2.38	107.52	111.29
5	B	1401	NAG	C3-C4-C5	-2.36	106.03	110.24
5	J	1406	NAG	C4-C3-C2	-2.33	107.61	111.02
5	A	1404	NAG	C3-C4-C5	-2.30	106.13	110.24
5	A	1402	NAG	C1-O5-C5	-2.30	109.08	112.19
5	A	1409	NAG	O5-C5-C6	-2.27	103.64	107.20
5	J	1403	NAG	C4-C3-C2	-2.24	107.73	111.02
5	J	1409	NAG	C4-C3-C2	-2.23	107.74	111.02
5	B	1407	NAG	C4-C3-C2	-2.20	107.80	111.02
5	B	1401	NAG	O5-C5-C6	-2.18	103.78	107.20
5	A	1406	NAG	C3-C4-C5	-2.10	106.49	110.24
5	J	1402	NAG	C3-C4-C5	-2.09	106.51	110.24
5	A	1404	NAG	C1-O5-C5	-2.07	109.39	112.19
5	A	1402	NAG	O4-C4-C5	-2.01	104.31	109.30

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1405	NAG	C8-C7-N2-C2
5	B	1405	NAG	O7-C7-N2-C2
5	J	1402	NAG	O5-C5-C6-O6
6	J	1410	8Z9	CB-CC-CD-CE
5	B	1403	NAG	C8-C7-N2-C2
5	J	1405	NAG	O5-C5-C6-O6
5	B	1408	NAG	O5-C5-C6-O6
5	J	1402	NAG	C4-C5-C6-O6
5	B	1409	NAG	O5-C5-C6-O6
5	A	1405	NAG	O5-C5-C6-O6
6	B	1410	8Z9	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
5	B	1403	NAG	O7-C7-N2-C2
6	J	1410	8Z9	C2-C3-C4-C5
5	B	1402	NAG	O5-C5-C6-O6
5	B	1405	NAG	O5-C5-C6-O6
6	J	1411	8Z9	C1-C2-C3-C4
5	J	1409	NAG	O5-C5-C6-O6
5	A	1408	NAG	O5-C5-C6-O6
5	B	1404	NAG	O5-C5-C6-O6
5	A	1407	NAG	O5-C5-C6-O6
6	B	1410	8Z9	C1-C2-C3-C4
6	J	1411	8Z9	CD-CE-CF-CG
5	A	1401	NAG	O5-C5-C6-O6
6	J	1410	8Z9	C9-CA-CB-CC
5	J	1405	NAG	C4-C5-C6-O6
6	J	1411	8Z9	CA-CB-CC-CD
6	B	1410	8Z9	C9-CA-CB-CC
6	J	1410	8Z9	C7-C8-C9-CA
5	B	1406	NAG	O5-C5-C6-O6
6	B	1410	8Z9	CD-CE-CF-CG
5	J	1407	NAG	O5-C5-C6-O6
5	J	1401	NAG	O5-C5-C6-O6
6	J	1410	8Z9	CD-CE-CF-CG
5	J	1404	NAG	C1-C2-N2-C7
5	B	1407	NAG	O5-C5-C6-O6
6	B	1410	8Z9	C3-C4-C5-C6
5	B	1409	NAG	C4-C5-C6-O6
6	J	1411	8Z9	C7-C8-C9-CA
5	J	1404	NAG	O5-C5-C6-O6
5	J	1406	NAG	O5-C5-C6-O6
5	B	1403	NAG	O5-C5-C6-O6
6	J	1410	8Z9	CC-CD-CE-CF
6	B	1410	8Z9	CC-CD-CE-CF
5	B	1405	NAG	C4-C5-C6-O6
6	J	1411	8Z9	CC-CD-CE-CF
5	B	1408	NAG	C4-C5-C6-O6
6	J	1411	8Z9	C9-CA-CB-CC
5	A	1409	NAG	C1-C2-N2-C7
5	A	1409	NAG	C3-C2-N2-C7
5	A	1405	NAG	C4-C5-C6-O6
6	J	1410	8Z9	C4-C5-C6-C7
5	J	1404	NAG	C3-C2-N2-C7
6	J	1411	8Z9	O1-C1-C2-C3

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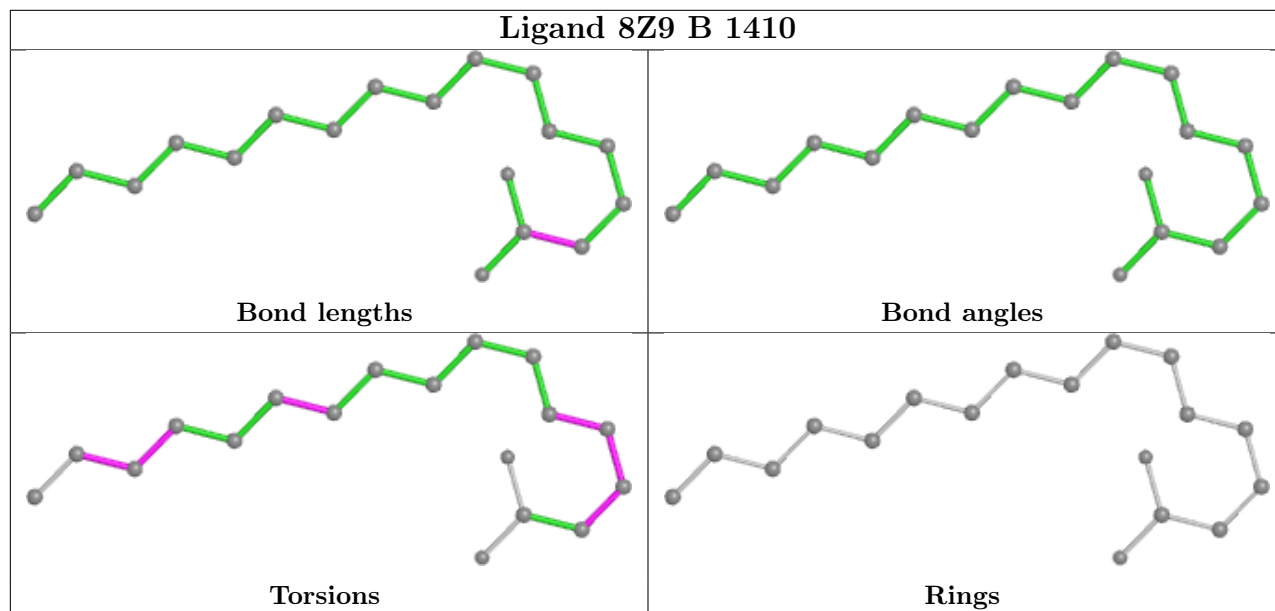
Mol	Chain	Res	Type	Atoms
6	J	1411	8Z9	O2-C1-C2-C3

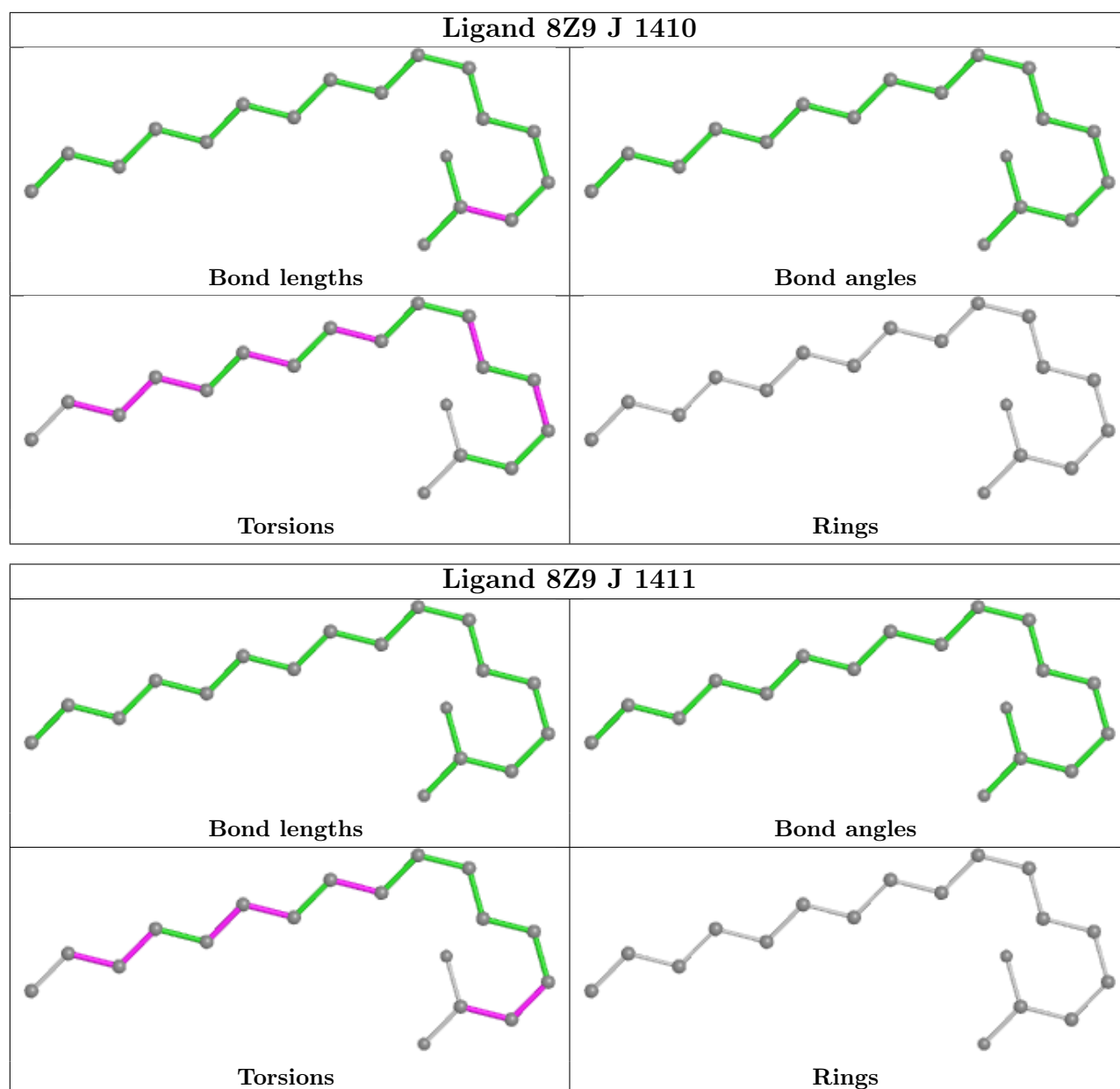
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	1410	8Z9	3	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.

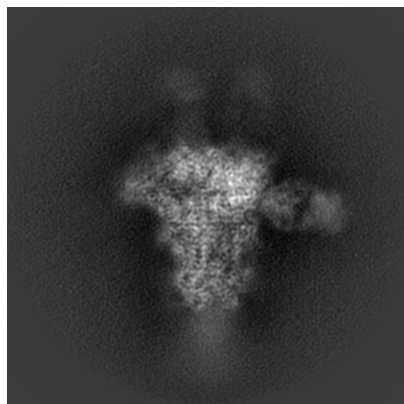
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24968. These allow visual inspection of the internal detail of the map and identification of artifacts.

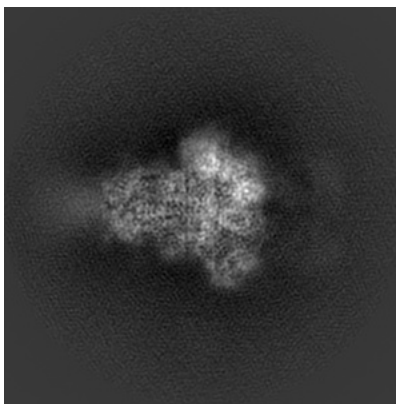
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

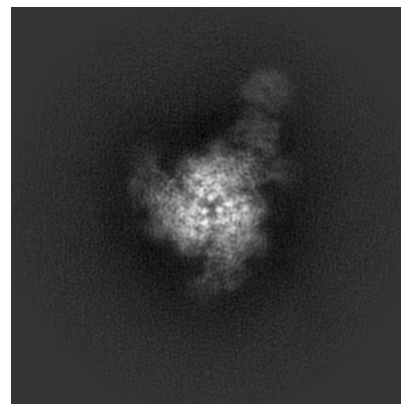
6.1.1 Primary map



X

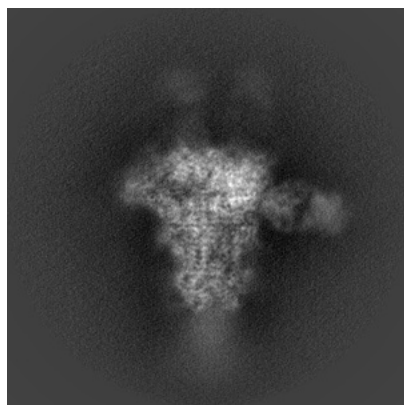


Y

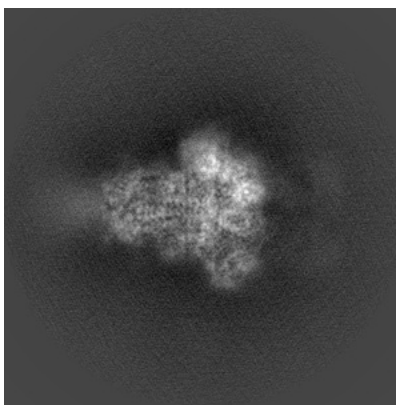


Z

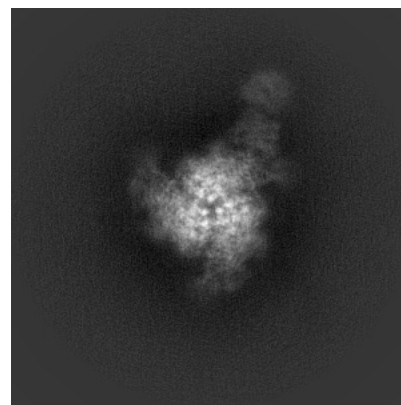
6.1.2 Raw map



X



Y

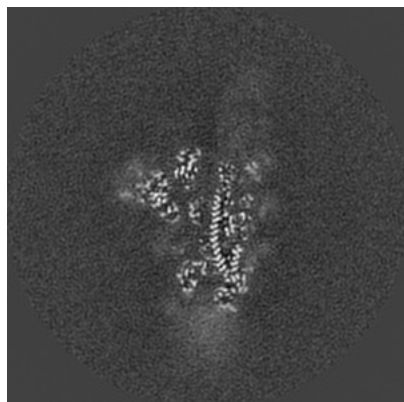


Z

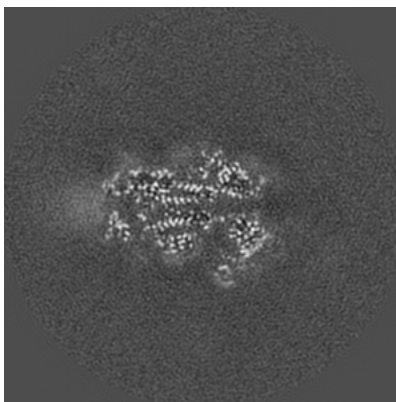
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

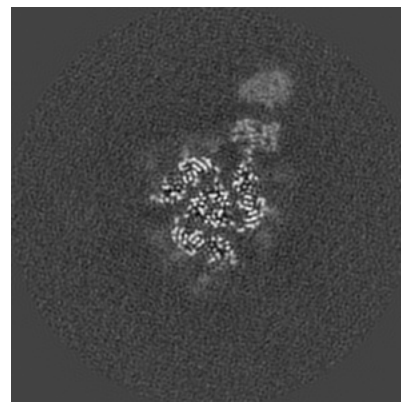
6.2.1 Primary map



X Index: 170

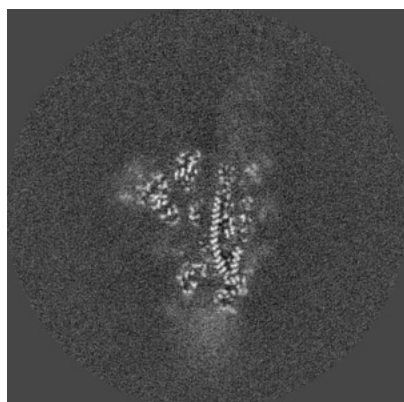


Y Index: 170

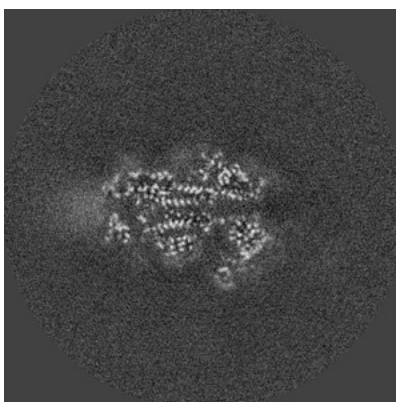


Z Index: 170

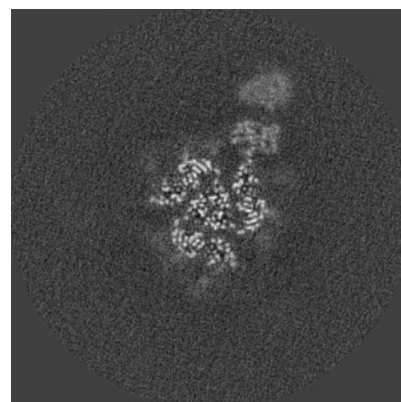
6.2.2 Raw map



X Index: 170



Y Index: 170

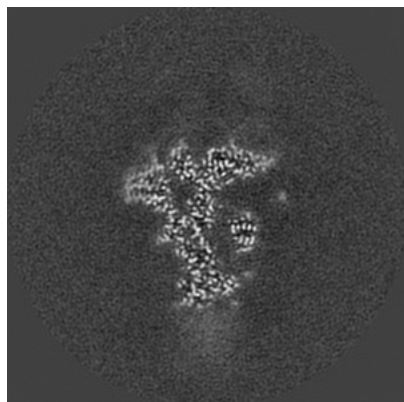


Z Index: 170

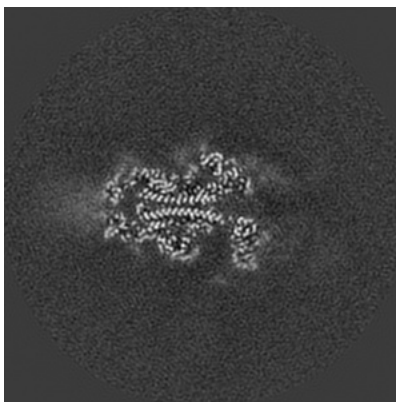
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

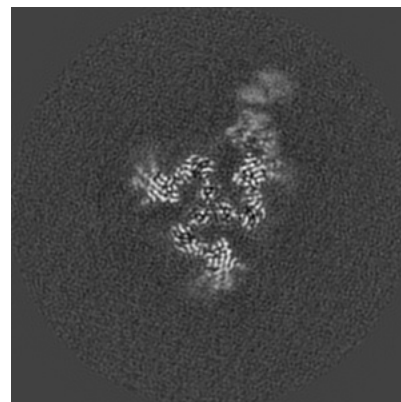
6.3.1 Primary map



X Index: 184

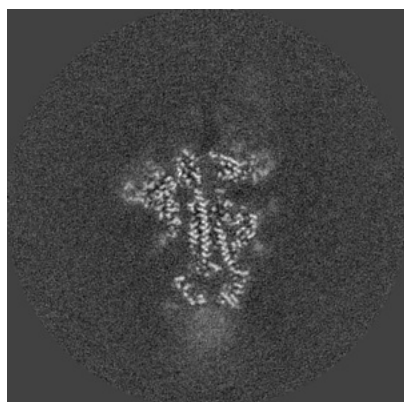


Y Index: 166

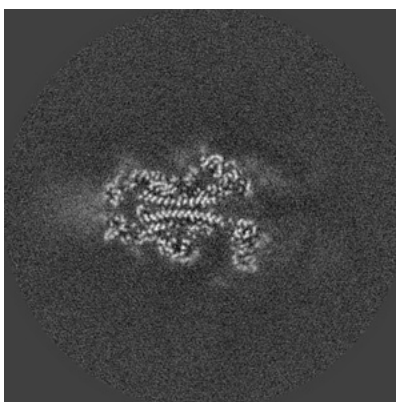


Z Index: 177

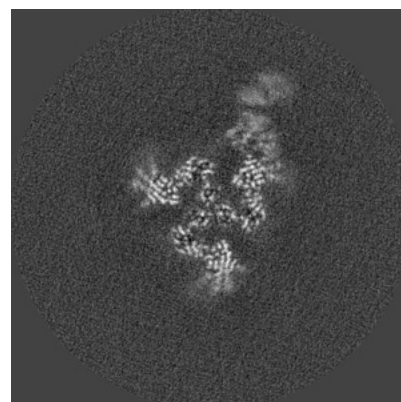
6.3.2 Raw map



X Index: 176



Y Index: 166

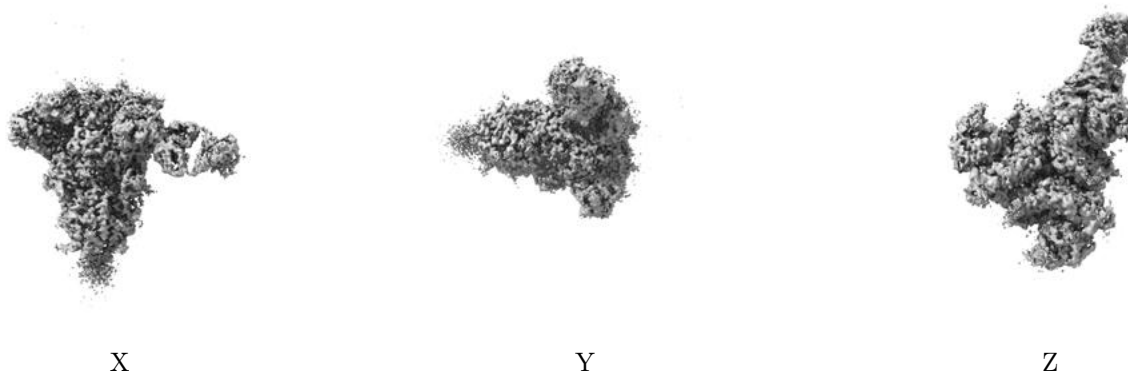


Z Index: 177

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

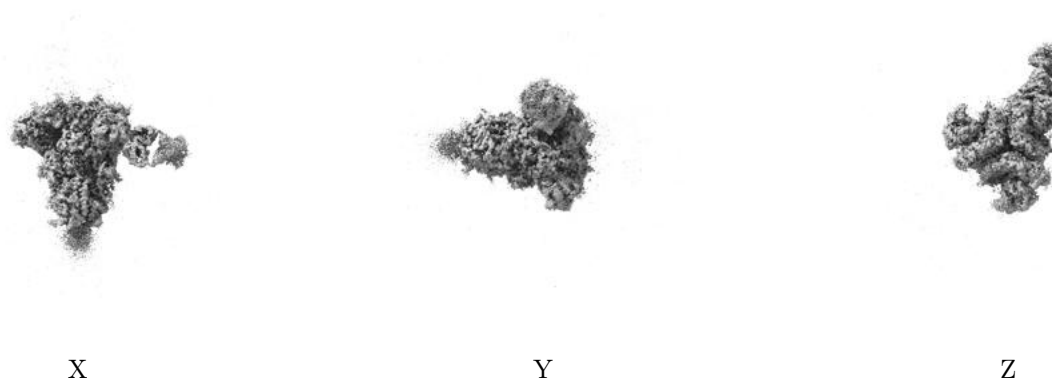
6.4 Orthogonal surface views [i](#)

6.4.1 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.

6.4.2 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.

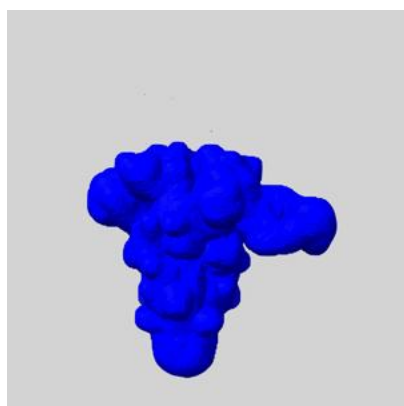
6.5 Mask visualisation [i](#)

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

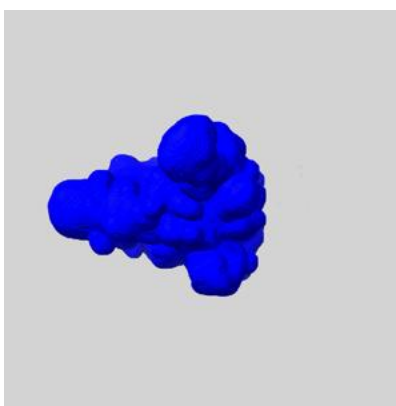
A mask typically either:

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

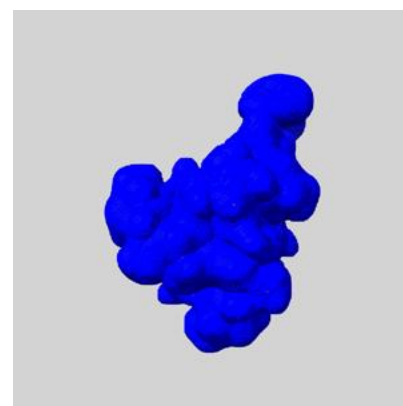
6.5.1 emd_24968_msk_1.map [i](#)



X



Y

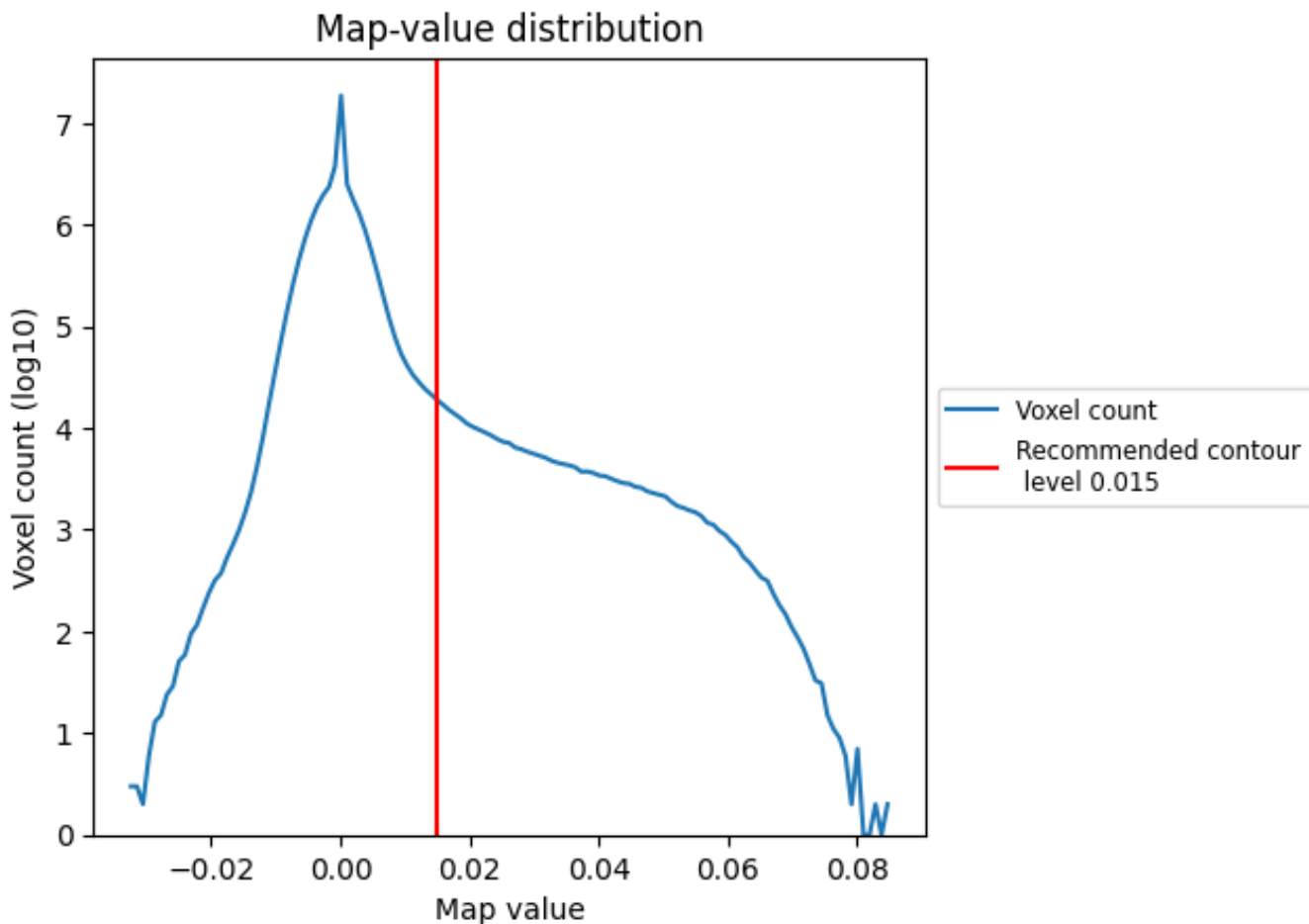


Z

7 Map analysis [i](#)

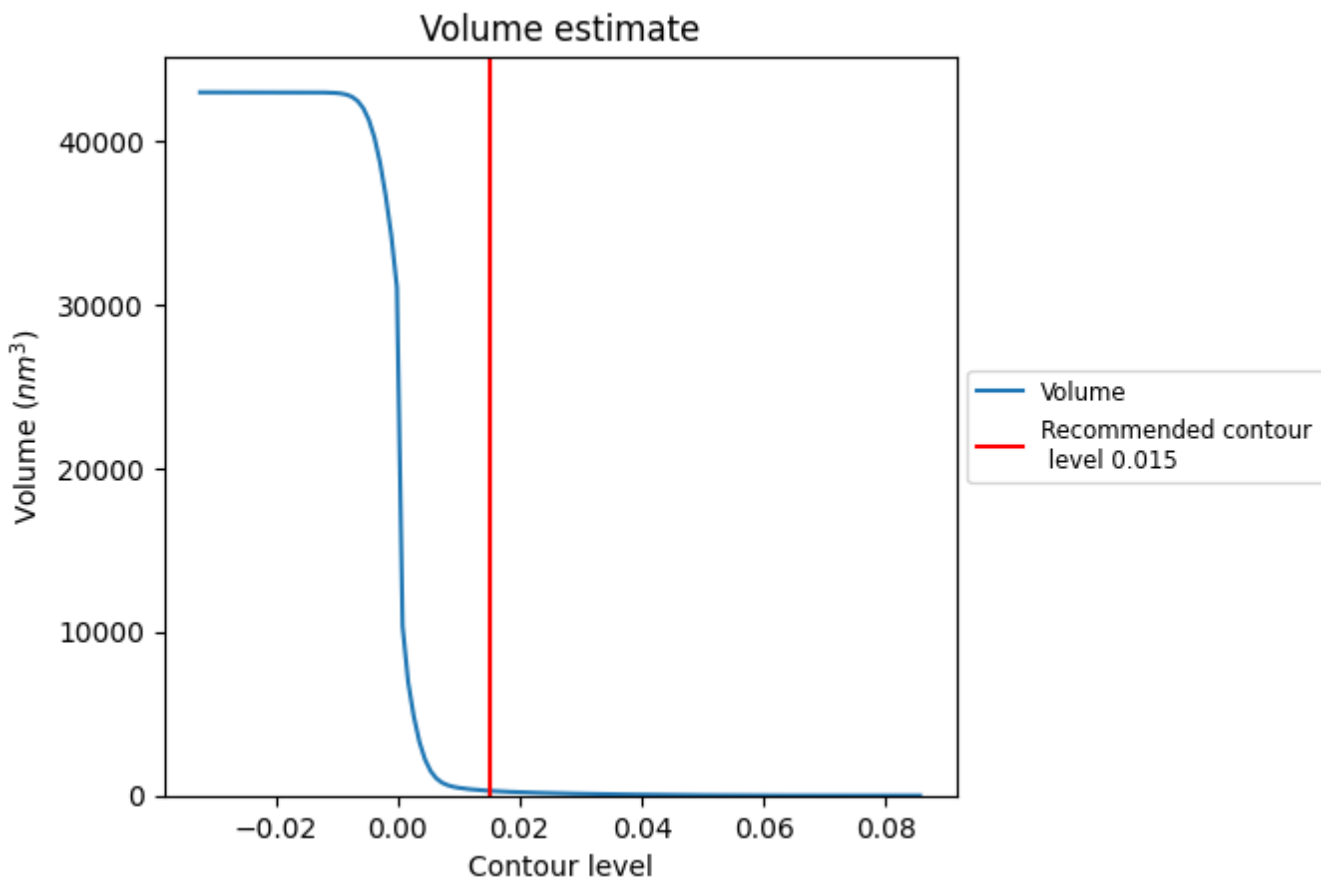
This section contains the results of statistical analysis of the map.

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.

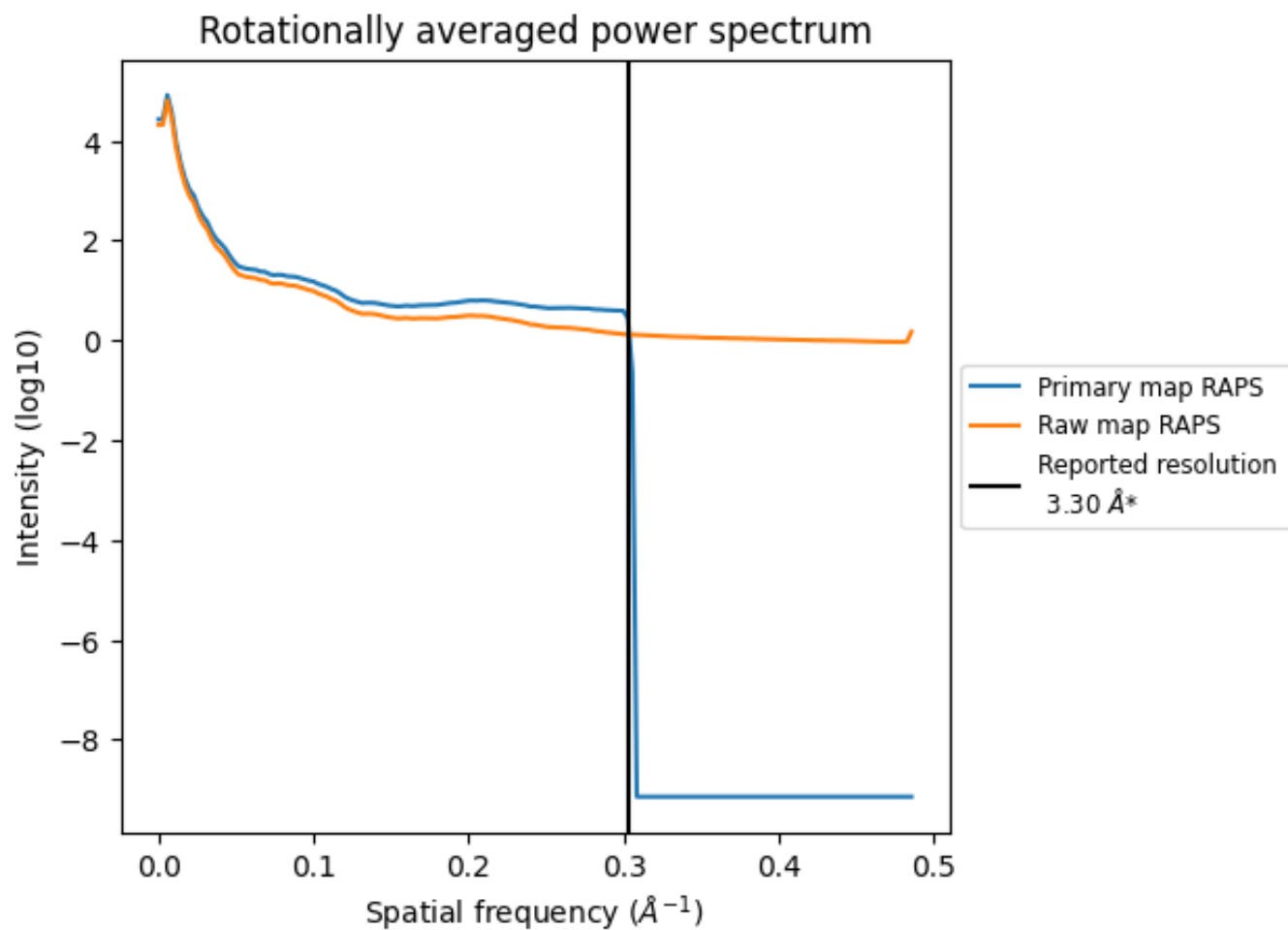
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 292 nm³; this corresponds to an approximate mass of 264 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

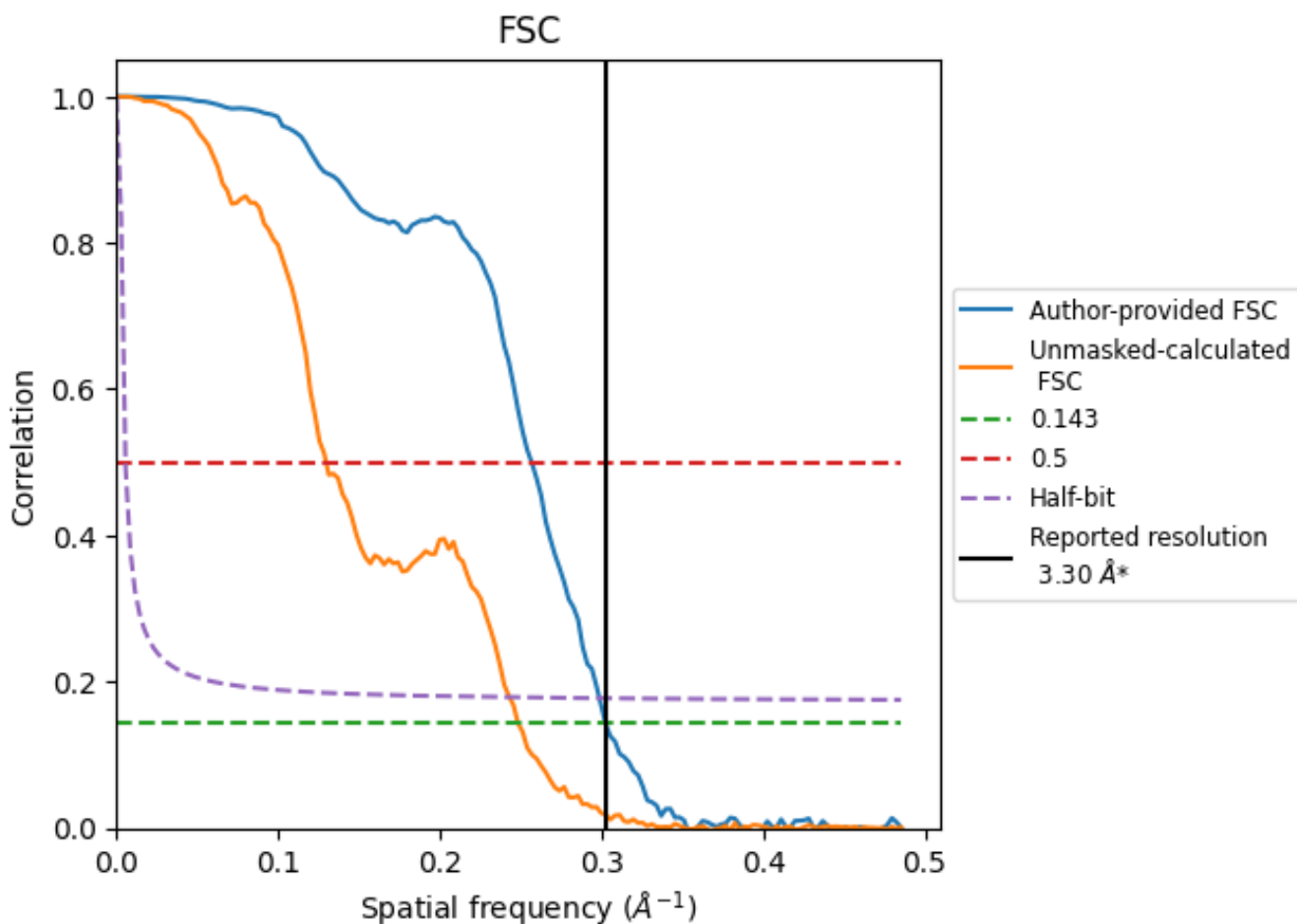


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

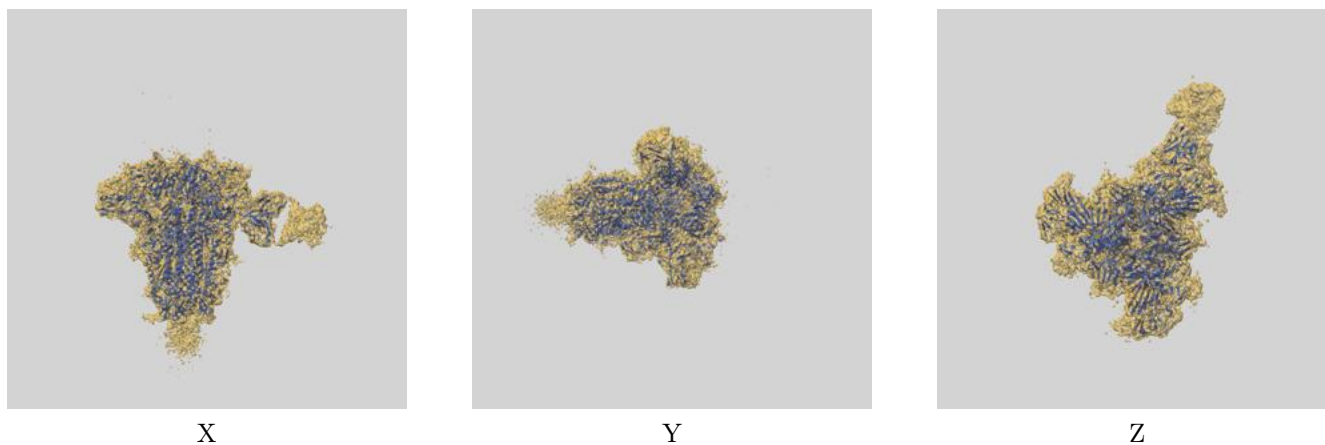
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.31	3.89	3.35
Unmasked-calculated*	4.02	7.71	4.11

*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 4.02 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

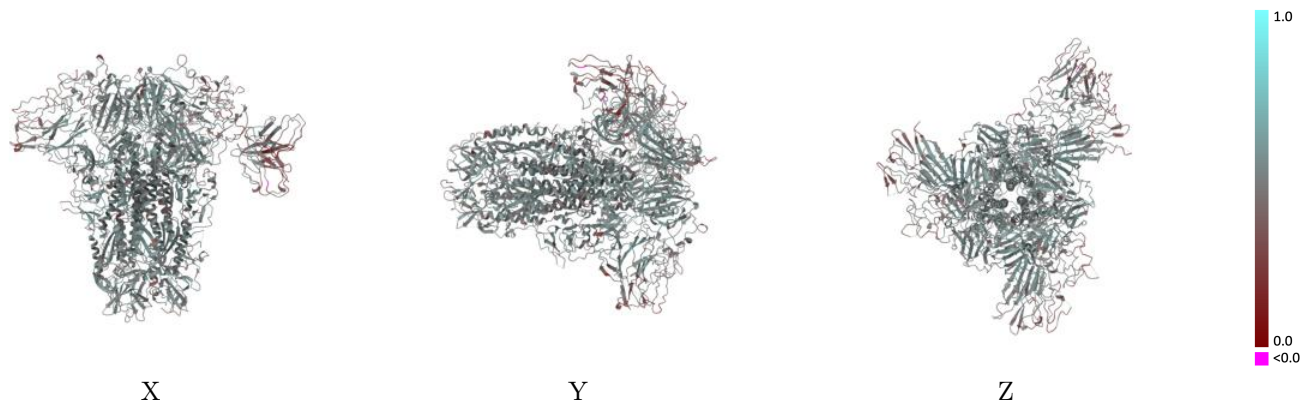
This section contains information regarding the fit between EMDB map EMD-24968 and PDB model 7SB3. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



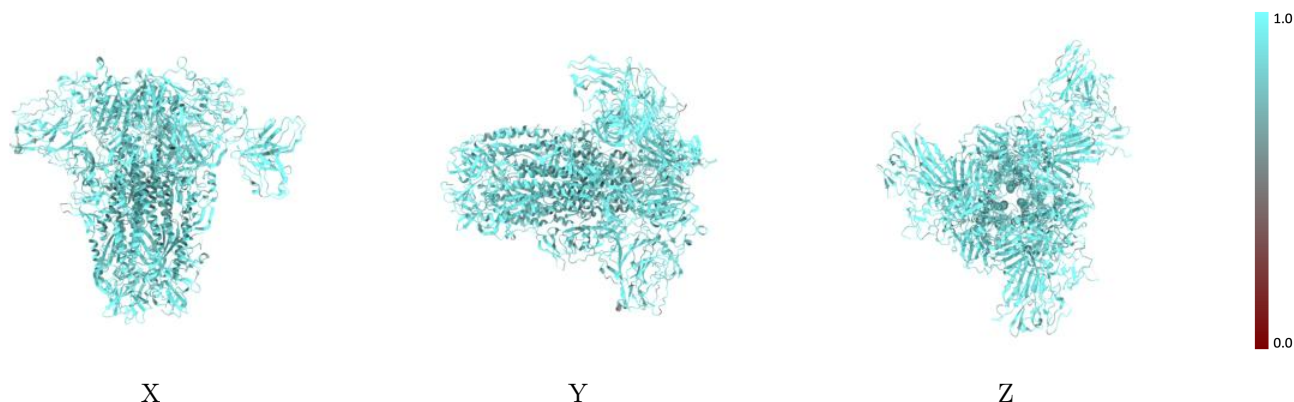
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



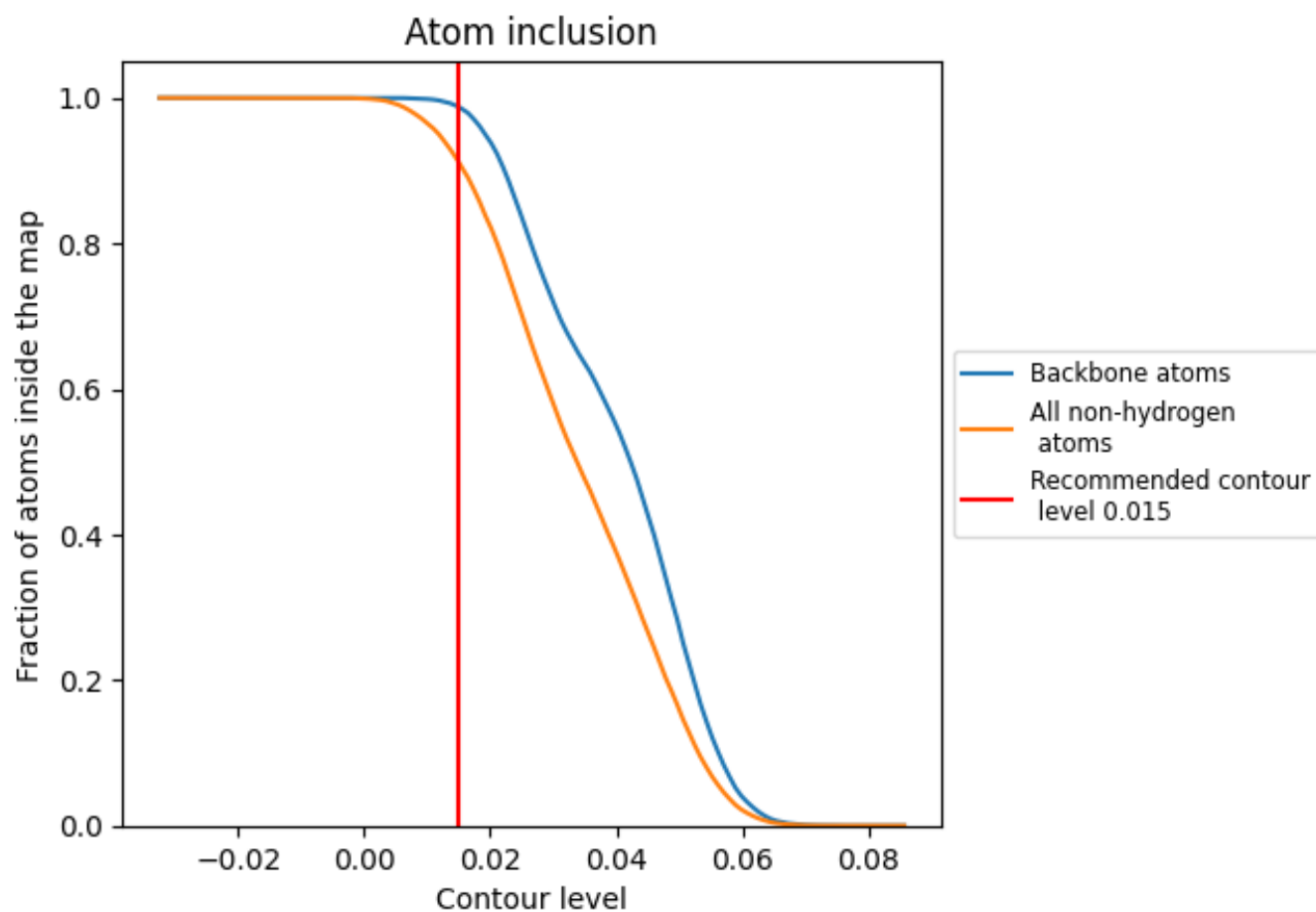
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 91% 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	 0.9119	 0.4960
A	 0.9129	 0.4990
B	 0.9136	 0.5030
C	 0.7857	 0.3110
D	 0.9286	 0.4480
E	 0.8929	 0.4320
F	 0.7949	 0.2160
G	 0.8571	 0.4510
H	 0.9369	 0.4200
I	 0.8214	 0.3730
J	 0.9139	 0.5030
K	 0.7500	 0.4270
L	 0.9039	 0.3930
M	 0.7500	 0.3100
N	 0.5714	 0.3660
O	 0.8571	 0.4060
P	 0.8571	 0.3930
Q	 0.6786	 0.3780
R	 0.8929	 0.3900
S	 0.5000	 0.3850

