



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 05:26 AM UTC

PDB ID : 7YMY / pdb_00007ymy
EMDB ID : EMD-33947
Title : Cryo-EM structure of MERS-CoV spike protein, One RBD-up conformation 1
Authors : Hsu, S.T.D.; Chang, N.E.; Weng, Z.W.; Yang, T.J.; Draczkowski, P.
Deposited on : 2022-07-29
Resolution : 4.96 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

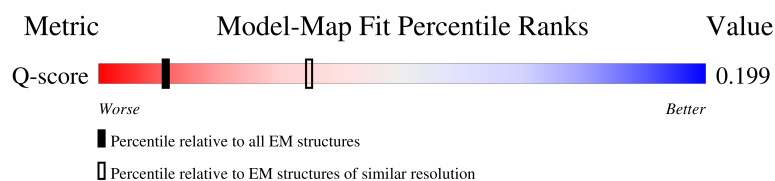
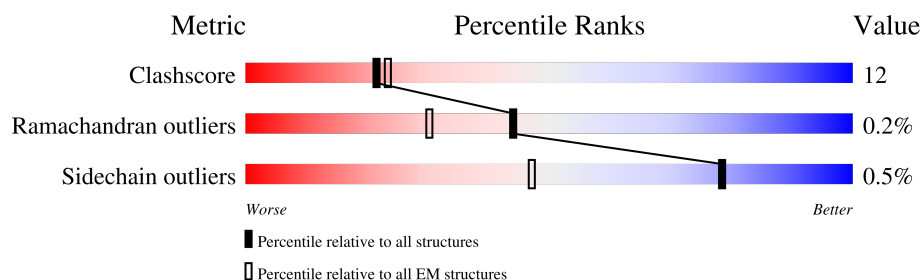
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.96 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



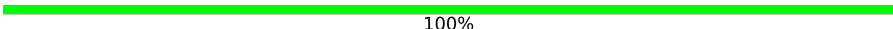
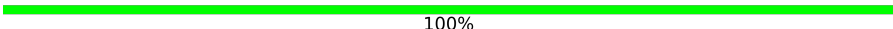
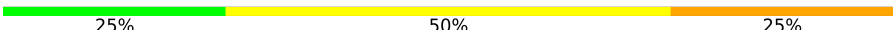
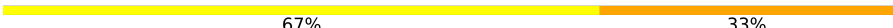
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1045 (4.46 - 5.45)

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	1369	
1	B	1369	
1	C	1369	
2	D	2	

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Mol	Chain	Length	Quality of chain
2	H	2	 50% 50%
2	I	2	 100%
2	J	2	 100%
2	K	2	 50% 50%
3	E	4	 25% 50% 25%
4	F	3	 67% 33%
5	G	5	 40% 40% 20%
5	L	5	 20% 80%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 27677 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1166	Total	C	N	O	S	0	0
			9020	5732	1489	1748	51		
1	B	1166	Total	C	N	O	S	0	0
			9020	5732	1489	1748	51		
1	C	1166	Total	C	N	O	S	0	0
			9020	5732	1489	1748	51		

There are 294 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP K0BRG7
A	-1	ASP	-	expression tag	UNP K0BRG7
A	0	SER	-	expression tag	UNP K0BRG7
A	1	TRP	-	expression tag	UNP K0BRG7
A	2	PHE	-	expression tag	UNP K0BRG7
A	3	ILE	-	expression tag	UNP K0BRG7
A	4	LEU	-	expression tag	UNP K0BRG7
A	5	VAL	-	expression tag	UNP K0BRG7
A	6	LEU	-	expression tag	UNP K0BRG7
A	7	LEU	-	expression tag	UNP K0BRG7
A	8	GLY	-	expression tag	UNP K0BRG7
A	9	SER	-	expression tag	UNP K0BRG7
A	10	GLY	-	expression tag	UNP K0BRG7
A	11	LEU	-	expression tag	UNP K0BRG7
A	12	ILE	-	expression tag	UNP K0BRG7
A	13	CYS	-	expression tag	UNP K0BRG7
A	14	VAL	-	expression tag	UNP K0BRG7
A	15	SER	-	expression tag	UNP K0BRG7
A	16	ALA	-	expression tag	UNP K0BRG7
A	748	ALA	ARG	engineered mutation	UNP K0BRG7
A	751	GLY	ARG	engineered mutation	UNP K0BRG7
A	1060	PRO	VAL	engineered mutation	UNP K0BRG7
A	1061	PRO	LEU	engineered mutation	UNP K0BRG7
A	1292	GLU	-	expression tag	UNP K0BRG7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1293	PHE	-	expression tag	UNP K0BRG7
A	1294	GLY	-	expression tag	UNP K0BRG7
A	1295	SER	-	expression tag	UNP K0BRG7
A	1296	GLY	-	expression tag	UNP K0BRG7
A	1297	GLY	-	expression tag	UNP K0BRG7
A	1298	TYR	-	expression tag	UNP K0BRG7
A	1299	ILE	-	expression tag	UNP K0BRG7
A	1300	PRO	-	expression tag	UNP K0BRG7
A	1301	GLU	-	expression tag	UNP K0BRG7
A	1302	ALA	-	expression tag	UNP K0BRG7
A	1303	PRO	-	expression tag	UNP K0BRG7
A	1304	ARG	-	expression tag	UNP K0BRG7
A	1305	ASP	-	expression tag	UNP K0BRG7
A	1306	GLY	-	expression tag	UNP K0BRG7
A	1307	GLN	-	expression tag	UNP K0BRG7
A	1308	ALA	-	expression tag	UNP K0BRG7
A	1309	TYR	-	expression tag	UNP K0BRG7
A	1310	VAL	-	expression tag	UNP K0BRG7
A	1311	ARG	-	expression tag	UNP K0BRG7
A	1312	LYS	-	expression tag	UNP K0BRG7
A	1313	ASP	-	expression tag	UNP K0BRG7
A	1314	GLY	-	expression tag	UNP K0BRG7
A	1315	GLU	-	expression tag	UNP K0BRG7
A	1316	TRP	-	expression tag	UNP K0BRG7
A	1317	VAL	-	expression tag	UNP K0BRG7
A	1318	LEU	-	expression tag	UNP K0BRG7
A	1319	LEU	-	expression tag	UNP K0BRG7
A	1320	SER	-	expression tag	UNP K0BRG7
A	1321	THR	-	expression tag	UNP K0BRG7
A	1322	PHE	-	expression tag	UNP K0BRG7
A	1323	LEU	-	expression tag	UNP K0BRG7
A	1324	LYS	-	expression tag	UNP K0BRG7
A	1325	GLY	-	expression tag	UNP K0BRG7
A	1326	GLN	-	expression tag	UNP K0BRG7
A	1327	ASP	-	expression tag	UNP K0BRG7
A	1328	ASN	-	expression tag	UNP K0BRG7
A	1329	SER	-	expression tag	UNP K0BRG7
A	1330	ALA	-	expression tag	UNP K0BRG7
A	1331	ASP	-	expression tag	UNP K0BRG7
A	1332	ILE	-	expression tag	UNP K0BRG7
A	1333	GLN	-	expression tag	UNP K0BRG7
A	1334	HIS	-	expression tag	UNP K0BRG7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1335	SER	-	expression tag	UNP K0BRG7
A	1336	GLY	-	expression tag	UNP K0BRG7
A	1337	ARG	-	expression tag	UNP K0BRG7
A	1338	PRO	-	expression tag	UNP K0BRG7
A	1339	LEU	-	expression tag	UNP K0BRG7
A	1340	GLU	-	expression tag	UNP K0BRG7
A	1341	SER	-	expression tag	UNP K0BRG7
A	1342	ARG	-	expression tag	UNP K0BRG7
A	1343	GLY	-	expression tag	UNP K0BRG7
A	1344	PRO	-	expression tag	UNP K0BRG7
A	1345	PHE	-	expression tag	UNP K0BRG7
A	1346	GLU	-	expression tag	UNP K0BRG7
A	1347	GLN	-	expression tag	UNP K0BRG7
A	1348	LYS	-	expression tag	UNP K0BRG7
A	1349	LEU	-	expression tag	UNP K0BRG7
A	1350	ILE	-	expression tag	UNP K0BRG7
A	1351	SER	-	expression tag	UNP K0BRG7
A	1352	GLU	-	expression tag	UNP K0BRG7
A	1353	GLU	-	expression tag	UNP K0BRG7
A	1354	ASP	-	expression tag	UNP K0BRG7
A	1355	LEU	-	expression tag	UNP K0BRG7
A	1356	ASN	-	expression tag	UNP K0BRG7
A	1357	MET	-	expression tag	UNP K0BRG7
A	1358	HIS	-	expression tag	UNP K0BRG7
A	1359	THR	-	expression tag	UNP K0BRG7
A	1360	GLY	-	expression tag	UNP K0BRG7
A	1361	HIS	-	expression tag	UNP K0BRG7
A	1362	HIS	-	expression tag	UNP K0BRG7
A	1363	HIS	-	expression tag	UNP K0BRG7
A	1364	HIS	-	expression tag	UNP K0BRG7
A	1365	HIS	-	expression tag	UNP K0BRG7
A	1366	HIS	-	expression tag	UNP K0BRG7
B	-2	MET	-	initiating methionine	UNP K0BRG7
B	-1	ASP	-	expression tag	UNP K0BRG7
B	0	SER	-	expression tag	UNP K0BRG7
B	1	TRP	-	expression tag	UNP K0BRG7
B	2	PHE	-	expression tag	UNP K0BRG7
B	3	ILE	-	expression tag	UNP K0BRG7
B	4	LEU	-	expression tag	UNP K0BRG7
B	5	VAL	-	expression tag	UNP K0BRG7
B	6	LEU	-	expression tag	UNP K0BRG7
B	7	LEU	-	expression tag	UNP K0BRG7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	8	GLY	-	expression tag	UNP K0BRG7
B	9	SER	-	expression tag	UNP K0BRG7
B	10	GLY	-	expression tag	UNP K0BRG7
B	11	LEU	-	expression tag	UNP K0BRG7
B	12	ILE	-	expression tag	UNP K0BRG7
B	13	CYS	-	expression tag	UNP K0BRG7
B	14	VAL	-	expression tag	UNP K0BRG7
B	15	SER	-	expression tag	UNP K0BRG7
B	16	ALA	-	expression tag	UNP K0BRG7
B	748	ALA	ARG	engineered mutation	UNP K0BRG7
B	751	GLY	ARG	engineered mutation	UNP K0BRG7
B	1060	PRO	VAL	engineered mutation	UNP K0BRG7
B	1061	PRO	LEU	engineered mutation	UNP K0BRG7
B	1292	GLU	-	expression tag	UNP K0BRG7
B	1293	PHE	-	expression tag	UNP K0BRG7
B	1294	GLY	-	expression tag	UNP K0BRG7
B	1295	SER	-	expression tag	UNP K0BRG7
B	1296	GLY	-	expression tag	UNP K0BRG7
B	1297	GLY	-	expression tag	UNP K0BRG7
B	1298	TYR	-	expression tag	UNP K0BRG7
B	1299	ILE	-	expression tag	UNP K0BRG7
B	1300	PRO	-	expression tag	UNP K0BRG7
B	1301	GLU	-	expression tag	UNP K0BRG7
B	1302	ALA	-	expression tag	UNP K0BRG7
B	1303	PRO	-	expression tag	UNP K0BRG7
B	1304	ARG	-	expression tag	UNP K0BRG7
B	1305	ASP	-	expression tag	UNP K0BRG7
B	1306	GLY	-	expression tag	UNP K0BRG7
B	1307	GLN	-	expression tag	UNP K0BRG7
B	1308	ALA	-	expression tag	UNP K0BRG7
B	1309	TYR	-	expression tag	UNP K0BRG7
B	1310	VAL	-	expression tag	UNP K0BRG7
B	1311	ARG	-	expression tag	UNP K0BRG7
B	1312	LYS	-	expression tag	UNP K0BRG7
B	1313	ASP	-	expression tag	UNP K0BRG7
B	1314	GLY	-	expression tag	UNP K0BRG7
B	1315	GLU	-	expression tag	UNP K0BRG7
B	1316	TRP	-	expression tag	UNP K0BRG7
B	1317	VAL	-	expression tag	UNP K0BRG7
B	1318	LEU	-	expression tag	UNP K0BRG7
B	1319	LEU	-	expression tag	UNP K0BRG7
B	1320	SER	-	expression tag	UNP K0BRG7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1321	THR	-	expression tag	UNP K0BRG7
B	1322	PHE	-	expression tag	UNP K0BRG7
B	1323	LEU	-	expression tag	UNP K0BRG7
B	1324	LYS	-	expression tag	UNP K0BRG7
B	1325	GLY	-	expression tag	UNP K0BRG7
B	1326	GLN	-	expression tag	UNP K0BRG7
B	1327	ASP	-	expression tag	UNP K0BRG7
B	1328	ASN	-	expression tag	UNP K0BRG7
B	1329	SER	-	expression tag	UNP K0BRG7
B	1330	ALA	-	expression tag	UNP K0BRG7
B	1331	ASP	-	expression tag	UNP K0BRG7
B	1332	ILE	-	expression tag	UNP K0BRG7
B	1333	GLN	-	expression tag	UNP K0BRG7
B	1334	HIS	-	expression tag	UNP K0BRG7
B	1335	SER	-	expression tag	UNP K0BRG7
B	1336	GLY	-	expression tag	UNP K0BRG7
B	1337	ARG	-	expression tag	UNP K0BRG7
B	1338	PRO	-	expression tag	UNP K0BRG7
B	1339	LEU	-	expression tag	UNP K0BRG7
B	1340	GLU	-	expression tag	UNP K0BRG7
B	1341	SER	-	expression tag	UNP K0BRG7
B	1342	ARG	-	expression tag	UNP K0BRG7
B	1343	GLY	-	expression tag	UNP K0BRG7
B	1344	PRO	-	expression tag	UNP K0BRG7
B	1345	PHE	-	expression tag	UNP K0BRG7
B	1346	GLU	-	expression tag	UNP K0BRG7
B	1347	GLN	-	expression tag	UNP K0BRG7
B	1348	LYS	-	expression tag	UNP K0BRG7
B	1349	LEU	-	expression tag	UNP K0BRG7
B	1350	ILE	-	expression tag	UNP K0BRG7
B	1351	SER	-	expression tag	UNP K0BRG7
B	1352	GLU	-	expression tag	UNP K0BRG7
B	1353	GLU	-	expression tag	UNP K0BRG7
B	1354	ASP	-	expression tag	UNP K0BRG7
B	1355	LEU	-	expression tag	UNP K0BRG7
B	1356	ASN	-	expression tag	UNP K0BRG7
B	1357	MET	-	expression tag	UNP K0BRG7
B	1358	HIS	-	expression tag	UNP K0BRG7
B	1359	THR	-	expression tag	UNP K0BRG7
B	1360	GLY	-	expression tag	UNP K0BRG7
B	1361	HIS	-	expression tag	UNP K0BRG7
B	1362	HIS	-	expression tag	UNP K0BRG7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1363	HIS	-	expression tag	UNP K0BRG7
B	1364	HIS	-	expression tag	UNP K0BRG7
B	1365	HIS	-	expression tag	UNP K0BRG7
B	1366	HIS	-	expression tag	UNP K0BRG7
C	-2	MET	-	initiating methionine	UNP K0BRG7
C	-1	ASP	-	expression tag	UNP K0BRG7
C	0	SER	-	expression tag	UNP K0BRG7
C	1	TRP	-	expression tag	UNP K0BRG7
C	2	PHE	-	expression tag	UNP K0BRG7
C	3	ILE	-	expression tag	UNP K0BRG7
C	4	LEU	-	expression tag	UNP K0BRG7
C	5	VAL	-	expression tag	UNP K0BRG7
C	6	LEU	-	expression tag	UNP K0BRG7
C	7	LEU	-	expression tag	UNP K0BRG7
C	8	GLY	-	expression tag	UNP K0BRG7
C	9	SER	-	expression tag	UNP K0BRG7
C	10	GLY	-	expression tag	UNP K0BRG7
C	11	LEU	-	expression tag	UNP K0BRG7
C	12	ILE	-	expression tag	UNP K0BRG7
C	13	CYS	-	expression tag	UNP K0BRG7
C	14	VAL	-	expression tag	UNP K0BRG7
C	15	SER	-	expression tag	UNP K0BRG7
C	16	ALA	-	expression tag	UNP K0BRG7
C	748	ALA	ARG	engineered mutation	UNP K0BRG7
C	751	GLY	ARG	engineered mutation	UNP K0BRG7
C	1060	PRO	VAL	engineered mutation	UNP K0BRG7
C	1061	PRO	LEU	engineered mutation	UNP K0BRG7
C	1292	GLU	-	expression tag	UNP K0BRG7
C	1293	PHE	-	expression tag	UNP K0BRG7
C	1294	GLY	-	expression tag	UNP K0BRG7
C	1295	SER	-	expression tag	UNP K0BRG7
C	1296	GLY	-	expression tag	UNP K0BRG7
C	1297	GLY	-	expression tag	UNP K0BRG7
C	1298	TYR	-	expression tag	UNP K0BRG7
C	1299	ILE	-	expression tag	UNP K0BRG7
C	1300	PRO	-	expression tag	UNP K0BRG7
C	1301	GLU	-	expression tag	UNP K0BRG7
C	1302	ALA	-	expression tag	UNP K0BRG7
C	1303	PRO	-	expression tag	UNP K0BRG7
C	1304	ARG	-	expression tag	UNP K0BRG7
C	1305	ASP	-	expression tag	UNP K0BRG7
C	1306	GLY	-	expression tag	UNP K0BRG7

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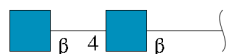
Chain	Residue	Modelled	Actual	Comment	Reference
C	1307	GLN	-	expression tag	UNP K0BRG7
C	1308	ALA	-	expression tag	UNP K0BRG7
C	1309	TYR	-	expression tag	UNP K0BRG7
C	1310	VAL	-	expression tag	UNP K0BRG7
C	1311	ARG	-	expression tag	UNP K0BRG7
C	1312	LYS	-	expression tag	UNP K0BRG7
C	1313	ASP	-	expression tag	UNP K0BRG7
C	1314	GLY	-	expression tag	UNP K0BRG7
C	1315	GLU	-	expression tag	UNP K0BRG7
C	1316	TRP	-	expression tag	UNP K0BRG7
C	1317	VAL	-	expression tag	UNP K0BRG7
C	1318	LEU	-	expression tag	UNP K0BRG7
C	1319	LEU	-	expression tag	UNP K0BRG7
C	1320	SER	-	expression tag	UNP K0BRG7
C	1321	THR	-	expression tag	UNP K0BRG7
C	1322	PHE	-	expression tag	UNP K0BRG7
C	1323	LEU	-	expression tag	UNP K0BRG7
C	1324	LYS	-	expression tag	UNP K0BRG7
C	1325	GLY	-	expression tag	UNP K0BRG7
C	1326	GLN	-	expression tag	UNP K0BRG7
C	1327	ASP	-	expression tag	UNP K0BRG7
C	1328	ASN	-	expression tag	UNP K0BRG7
C	1329	SER	-	expression tag	UNP K0BRG7
C	1330	ALA	-	expression tag	UNP K0BRG7
C	1331	ASP	-	expression tag	UNP K0BRG7
C	1332	ILE	-	expression tag	UNP K0BRG7
C	1333	GLN	-	expression tag	UNP K0BRG7
C	1334	HIS	-	expression tag	UNP K0BRG7
C	1335	SER	-	expression tag	UNP K0BRG7
C	1336	GLY	-	expression tag	UNP K0BRG7
C	1337	ARG	-	expression tag	UNP K0BRG7
C	1338	PRO	-	expression tag	UNP K0BRG7
C	1339	LEU	-	expression tag	UNP K0BRG7
C	1340	GLU	-	expression tag	UNP K0BRG7
C	1341	SER	-	expression tag	UNP K0BRG7
C	1342	ARG	-	expression tag	UNP K0BRG7
C	1343	GLY	-	expression tag	UNP K0BRG7
C	1344	PRO	-	expression tag	UNP K0BRG7
C	1345	PHE	-	expression tag	UNP K0BRG7
C	1346	GLU	-	expression tag	UNP K0BRG7
C	1347	GLN	-	expression tag	UNP K0BRG7
C	1348	LYS	-	expression tag	UNP K0BRG7

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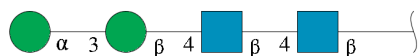
Chain	Residue	Modelled	Actual	Comment	Reference
C	1349	LEU	-	expression tag	UNP K0BRG7
C	1350	ILE	-	expression tag	UNP K0BRG7
C	1351	SER	-	expression tag	UNP K0BRG7
C	1352	GLU	-	expression tag	UNP K0BRG7
C	1353	GLU	-	expression tag	UNP K0BRG7
C	1354	ASP	-	expression tag	UNP K0BRG7
C	1355	LEU	-	expression tag	UNP K0BRG7
C	1356	ASN	-	expression tag	UNP K0BRG7
C	1357	MET	-	expression tag	UNP K0BRG7
C	1358	HIS	-	expression tag	UNP K0BRG7
C	1359	THR	-	expression tag	UNP K0BRG7
C	1360	GLY	-	expression tag	UNP K0BRG7
C	1361	HIS	-	expression tag	UNP K0BRG7
C	1362	HIS	-	expression tag	UNP K0BRG7
C	1363	HIS	-	expression tag	UNP K0BRG7
C	1364	HIS	-	expression tag	UNP K0BRG7
C	1365	HIS	-	expression tag	UNP K0BRG7
C	1366	HIS	-	expression tag	UNP K0BRG7

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



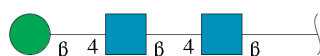
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



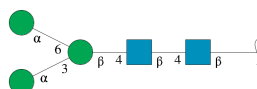
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	4	Total	C	N	O	0	0
			50	28	2	20		

- 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.



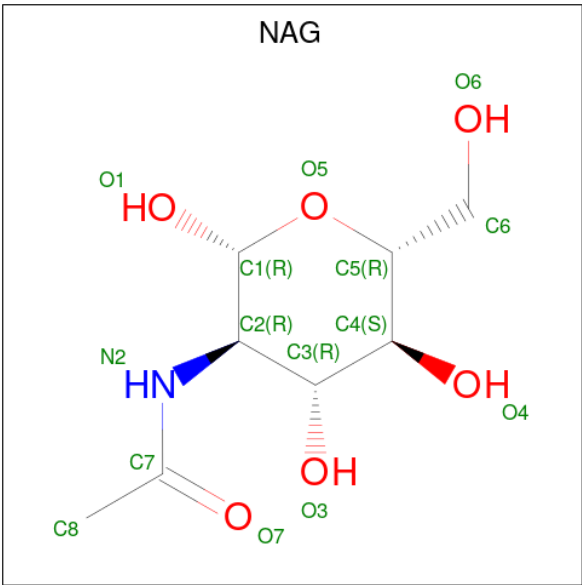
Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
5	G	5	Total	C	N	O	0	0
			61	34	2	25		
5	L	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

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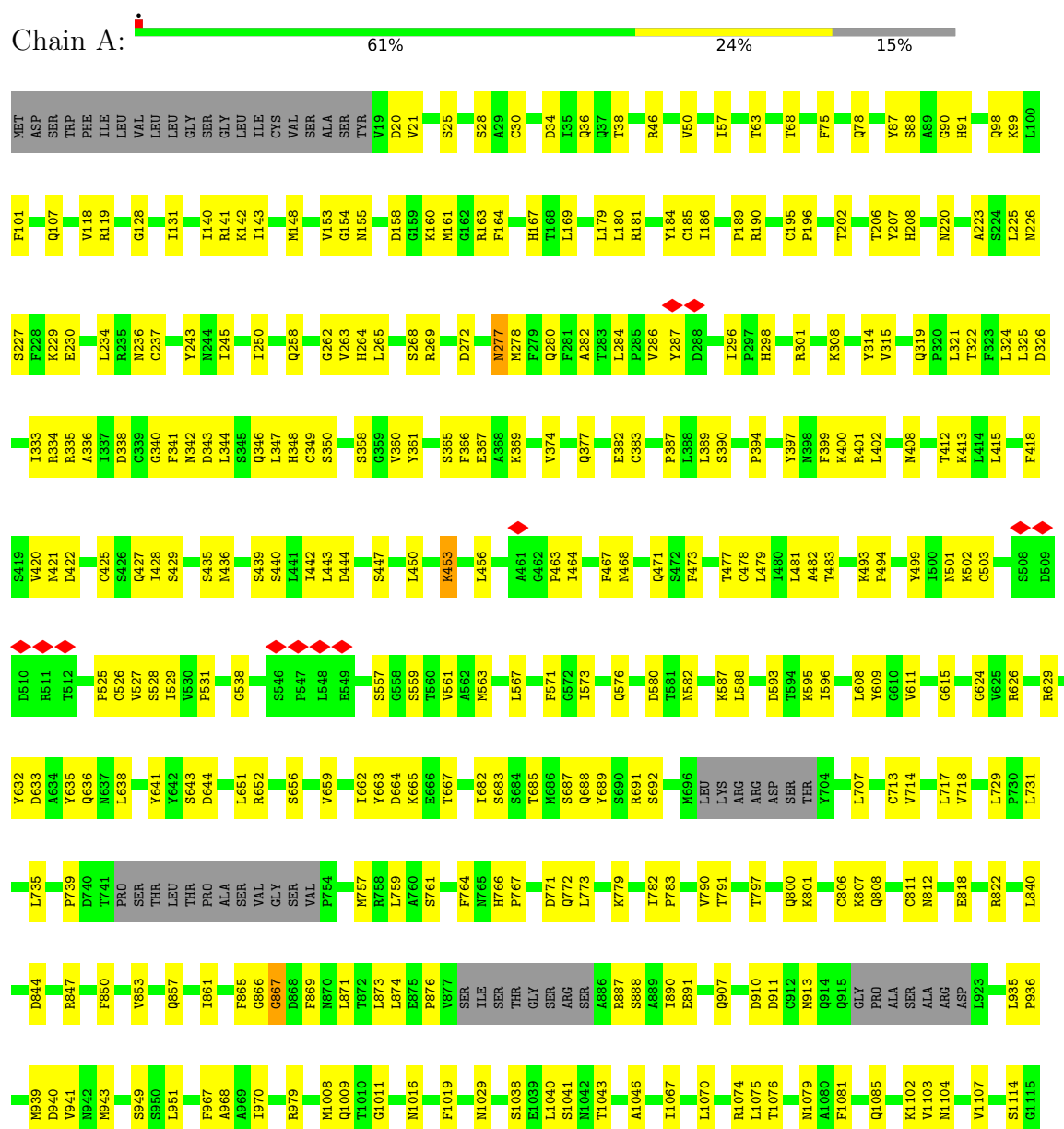
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Mol	Chain	Residues	Atoms				AltConf
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots

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

• Molecule 1: Spike glycoprotein



LEU SER
ASP
THR
LEU
THR
LYS
TYR
GLY
MET
LEU
SER
LEU
ASN
SER
LEU
ALA
GLN
GLN
VAL
VAL
LYS
LYS
SER
ALA
GLY
GLY
ASN
ASN
GLY
PRO
SER
SER
TYR
GLY
LEU
LYS
GLY
PHE
GLY
LEU
GLN
LYS
ASN
TYR
THR
TYR
GLY
PHE
GLY
LEU
SER
GLY
GLY
MET
GLY
THR
ILE
GLY
PRO
GLY
ALA
ALA
PRO
ARG
VAL
TYR
ALA
GLY
GLY
HIS
HIS
HIS
HIS
HIS
HIS

SER
THR
PHE
LEU
LEU
LYS
TYR
GLY
GLN
ASP
ASN
SER
LEU
ALA
GLY
SER
ASP
ILE
GLY
LEU
LYS
PRO
PHE
GLY
LEU
GLY
ASN
LYS
LEU
TYR
ILE
SER
GLY
LEU
ASP
LEU
ASN
MET
GLY
HIS
THR
ILE
GLY
HIS
HIS
HIS
HIS
HIS
HIS

● Molecule 1: Spike glycoprotein

Chain C:  61% 24% 15%

MET	A122	C237	L325	S447	N519	Y606	D740	Q857	A969	S1114	GLY
ASP	A123	T238	D326	S448	A520	R614	I741	L873	T986	C1117	THR
TRP	S126	T242	F327	P449	N521	G615	PRD	L874	S986	S1117	ILE
PHE	G128	Y243	D330	M452	Y523	V616	THR	E875	V989	H1122	GLY
ILE	G128	Y245	R335	D455	S524	F617	THR	E876	I987	H1123	VAL
LEU	A138	T246	A336	D455	P525	Q628	PRO	U877	K1000	V1124	SER
VAL	T139	D247	D338	S459	C526	S643	ALA	ILE	M1008	S1125	THR
ASN	I140	D248	C339	A460	Y527	D644	SER	THR	M1008	V1128	ILE
SER	R141	D248	C339	A461	Y527	D645	VAL	GLY	M1008	V1128	PRO
ASP	K142	Y253	L344	A462	S528	D646	GLY	SER	M1028	L1134	ALA
GLY	N155	Q258	L347	G462	D537	R647	VAL	ARG	S1034	Y1135	TYR
ILE	F156	T259	L347	P463	D537	L651	P754	ARG	S1034	H1138	VAL
HIS	F156	T259	L347	P463	D539	L651	P754	SER	S1034	H1138	ARG
LYS	M161	Q261	S358	S465	Y540	V659	M757	R887	S1038	G1139	LYS
GLY	G162	Q261	G359	S466	Y540	V659	M757	R888	E1039	G1140	ASP
ASN	R163	V263	V360	S467	Y541	V661	S761	S889	L1040	Y1141	GLY
PRO	F164	H264	Y361	N468	S542	R661	S761	S890	L1040	Y1141	ILE
SER	F165	L265	S365	Y469	Q544	V662	F764	T890	T1043	H1146	ASN
TYR	N166	F266	F366	K470	Q544	V663	H765	C904	F1044	G1146	THR
GLY	H167	S267	S366	S471	L545	D664	H766	S908	G1045	A1158	LEU
LEU	T168	S268	F366	S472	S546	R665	P767	Y908	A1046	T1162	SER
LYS	L169	R269	K369	F473	P547	T667	S776	D910	I1047	T1162	THR
GLY	T43	D272	S373	S474	L548	T668	I782	N913	D1053	H1177	PHE
PHE	W44	L273	V374	C478	Q550	T669	I782	Y914	I1054	THR	LEU
LEU	R46	L273	V375	L481	Q551	V790	V790	Q915	I1055	ARG	TYR
ASN	D49	Y277	L389	A482	Q552	T682	T791	Q915	Q1056	ILE	GLY
TYR	R181	L180	P393	P485	Y553	S683	Q792	PRO	R1057	VAL	LEU
GLY	Y184	L181	P394	L488	Y555	S684	Q793	ALA	L1058	ASP	THR
SER	G185	L182	P394	L488	Y555	T685	Q794	ALA	Q1063	E1183	LEU
LEU	N186	L183	P396	L488	Y555	T686	Q795	ALA	Q1066	E1195	GLN
GLY	L187	L183	V396	L488	Y555	T687	Q796	ARG	Q1067	N1201	VAL
MET	T67	V286	F399	L491	S557	Q688	T797	ASP	I1067	M1201	GLN
THR	P189	Y292	R401	K496	S558	R691	R801	L923	D1068	P1207	LYS
PRO	Q78	L296	F404	Y497	S559	S692	T803	Y932	R1069	Q1208	ALA
ALA	D83	R301	L411	N501	L567	S692	Q808	L938	L1070	Y1211	LEU
PRO	R84	H209	L414	K502	Q568	S692	Q808	N939	G1073	Q1212	SER
ARG	Y85	L303	L414	C503	G572	S692	Q808	D940	R1074	P1220	GLY
GLY	Y86	L303	L414	C503	G572	S692	Q808	E944	T1077	L1223	ARG
GLN	Y87	L303	L414	C503	G572	S692	Q808	Y947	V1082	L1223	PHE
ALA	L100	R307	D422	R505	L573	Y704	Q808	L951	R1088	GLY	THR
TYR	R220	R308	D422	R505	L573	Y704	Q808	L951	R1088	GLY	GLY
VAL	R221	R308	D422	R505	L573	Y704	Q808	L951	R1088	GLY	GLY
ARG	R222	R308	D422	R505	L573	Y704	Q808	L951	R1088	GLY	GLY
LYS	A223	A312	F438	S508	D580	L729	N839	P955	K1102	G1102	LYS
ASP	S106	F313	S439	S508	T581	L730	N839	A956	V1103	G1103	THR
GLY	Q107	S227	S440	D510	N582	L731	Q842	V958	E1105	G1105	THR
TRP	K110	N233	L441	R511	N582	L731	F850	L964	V1107	G1107	GLY
VAL	R119	L234	L442	R511	N582	L731	F850	L964	V1107	G1107	PHE
LEU	N236	R235	F323	R511	N582	L731	F850	L964	V1107	G1107	GLY
ASN			L324	R511	N582	L731	F850	L964	V1107	G1107	ASN

MET
HIS
THR
GLY
HIS
HIS
HIS
HIS
HIS

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

Chain D:  100%

NAG1
NAG2

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

Chain H:  50% 50%

NAG1
NAG2

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

Chain I:  100%

NAG1
NAG2

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

Chain J:  100%

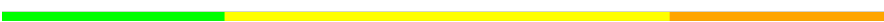
NAG1
NAG2

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

Chain K:  50% 50%

NAG1
NAG2

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

Chain E:  25% 50% 25%

NAG1
NAG2
MAN3
MAN4

- 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:  67% 33%

MAG1
MAG2
BMA3

- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  40% 40% 20%

MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  20% 80%

MAG1
MAG2
BMA3
MAN4
MAN5

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60257	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.6	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	92000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.488	Depositor
Minimum map value	-0.445	Depositor
Average map value	-0.005	Depositor
Map value standard deviation	0.118	Depositor
Recommended contour level	0.25	Depositor
Map size ($\text{\AA}$)	281.6, 281.6, 281.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	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: MAN, BMA, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.24	0/9230	0.51	4/12557 (0.0%)
1	B	0.31	7/9230 (0.1%)	0.55	5/12557 (0.0%)
1	C	0.32	3/9230 (0.0%)	0.59	7/12557 (0.1%)
All	All	0.29	10/27690 (0.0%)	0.55	16/37671 (0.0%)

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	221	ARG	CA-C	-7.76	1.42	1.52
1	B	270	TYR	CA-C	-7.25	1.43	1.52
1	B	268	SER	CA-C	-6.72	1.45	1.53
1	C	220	ASN	CA-C	-6.16	1.44	1.52
1	B	271	VAL	N-CA	-5.36	1.39	1.46

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	269	ARG	N-CA-C	-9.24	100.13	111.40
1	A	866	GLY	N-CA-C	-8.78	102.29	114.67
1	C	57	ILE	CA-C-N	7.82	132.57	120.68
1	C	57	ILE	C-N-CA	7.82	132.57	120.68
1	A	453	LYS	N-CA-C	6.74	120.37	111.75

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	9020	0	8705	229	0
1	B	9020	0	8707	209	0
1	C	9020	0	8704	221	0
2	D	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	1	0
3	E	50	0	43	1	0
4	F	39	0	34	1	0
5	G	61	0	52	1	0
5	L	61	0	52	0	0
6	A	98	0	91	3	0
6	B	70	0	65	0	0
6	C	98	0	91	2	0
All	All	27677	0	26669	637	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 637 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:497:TYR:HB3	1:B:561:VAL:O	1.76	0.85
1:A:21:VAL:HG12	1:A:237:CYS:H	1.49	0.76
1:B:427:GLN:NE2	1:B:475:ASN:O	2.21	0.73
1:C:169:LEU:HB3	1:C:184:TYR:HD1	1.53	0.72
1:C:237:CYS:SG	1:C:238:THR:N	2.63	0.72

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	1154/1369 (84%)	1053 (91%)	100 (9%)	1 (0%)	48	83
1	B	1154/1369 (84%)	1058 (92%)	93 (8%)	3 (0%)	36	72
1	C	1154/1369 (84%)	1046 (91%)	106 (9%)	2 (0%)	43	77
All	All	3462/4107 (84%)	3157 (91%)	299 (9%)	6 (0%)	44	77

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	272	ASP
1	C	220	ASN
1	A	867	GLY
1	B	876	PRO
1	C	218	ASN

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	1003/1180 (85%)	1000 (100%)	3 (0%)	86	84
1	B	1003/1180 (85%)	999 (100%)	4 (0%)	84	83
1	C	1003/1180 (85%)	995 (99%)	8 (1%)	73	78
All	All	3009/3540 (85%)	2994 (100%)	15 (0%)	78	82

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	163	ARG
1	C	875	GLU
1	C	167	HIS
1	C	877	VAL
1	C	188	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	981	ASN
1	C	427	GLN
1	B	988	GLN
1	B	1066	GLN
1	C	475	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 ⓘ

27 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	D	1	2,1	14,14,15	0.32	0	17,19,21	0.51	0
2	NAG	D	2	2	14,14,15	0.26	0	17,19,21	0.45	0
3	NAG	E	1	1,3	14,14,15	0.37	0	17,19,21	0.91	1 (5%)
3	NAG	E	2	3	14,14,15	0.31	0	17,19,21	0.71	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	E	3	3	11,11,12	0.66	0	15,15,17	0.84	0
3	MAN	E	4	3	11,11,12	0.78	1 (9%)	15,15,17	1.34	2 (13%)
4	NAG	F	1	4,1	14,14,15	1.34	2 (14%)	17,19,21	1.31	3 (17%)
4	NAG	F	2	4	14,14,15	0.31	0	17,19,21	1.05	2 (11%)
4	BMA	F	3	4	11,11,12	0.60	0	15,15,17	1.06	1 (6%)
5	NAG	G	1	5,1	14,14,15	1.47	2 (14%)	17,19,21	1.31	2 (11%)
5	NAG	G	2	5	14,14,15	0.29	0	17,19,21	0.53	0
5	BMA	G	3	5	11,11,12	0.87	0	15,15,17	0.78	0
5	MAN	G	4	5	11,11,12	0.93	0	15,15,17	1.13	2 (13%)
5	MAN	G	5	5	11,11,12	0.70	0	15,15,17	0.92	1 (6%)
2	NAG	H	1	2,1	14,14,15	0.94	1 (7%)	17,19,21	0.80	0
2	NAG	H	2	2	14,14,15	0.31	0	17,19,21	0.35	0
2	NAG	I	1	2,1	14,14,15	0.31	0	17,19,21	0.49	0
2	NAG	I	2	2	14,14,15	0.26	0	17,19,21	0.47	0
2	NAG	J	1	2,1	14,14,15	0.32	0	17,19,21	0.51	0
2	NAG	J	2	2	14,14,15	0.35	0	17,19,21	0.44	0
2	NAG	K	1	2,1	14,14,15	0.69	1 (7%)	17,19,21	0.99	0
2	NAG	K	2	2	14,14,15	0.39	0	17,19,21	0.46	0
5	NAG	L	1	5,1	14,14,15	0.93	1 (7%)	17,19,21	1.06	2 (11%)
5	NAG	L	2	5	14,14,15	0.26	0	17,19,21	0.95	2 (11%)
5	BMA	L	3	5	11,11,12	0.51	0	15,15,17	0.88	0
5	MAN	L	4	5	11,11,12	0.97	0	15,15,17	1.13	2 (13%)
5	MAN	L	5	5	11,11,12	0.62	0	15,15,17	1.09	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
4	NAG	F	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	2/2/19/22	0/1/1/1
5	MAN	G	4	5	-	2/2/19/22	1/1/1/1
5	MAN	G	5	5	-	0/2/19/22	0/1/1/1
2	NAG	H	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
5	NAG	L	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	L	2	5	-	3/6/23/26	0/1/1/1
5	BMA	L	3	5	-	0/2/19/22	0/1/1/1
5	MAN	L	4	5	-	2/2/19/22	1/1/1/1
5	MAN	L	5	5	-	0/2/19/22	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	1	NAG	O5-C1	-4.89	1.35	1.43
4	F	1	NAG	O5-C1	-3.80	1.37	1.43
2	H	1	NAG	C1-C2	3.32	1.56	1.52
5	L	1	NAG	O5-C1	-3.07	1.38	1.43
4	F	1	NAG	C1-C2	2.74	1.56	1.52

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	1	NAG	C3-C4-C5	3.93	117.36	110.23
3	E	4	MAN	C1-O5-C5	3.69	117.13	112.19
4	F	1	NAG	C4-C3-C2	3.47	116.10	111.02
5	G	4	MAN	C1-O5-C5	3.29	116.59	112.19
5	L	4	MAN	C1-O5-C5	3.13	116.38	112.19

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

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

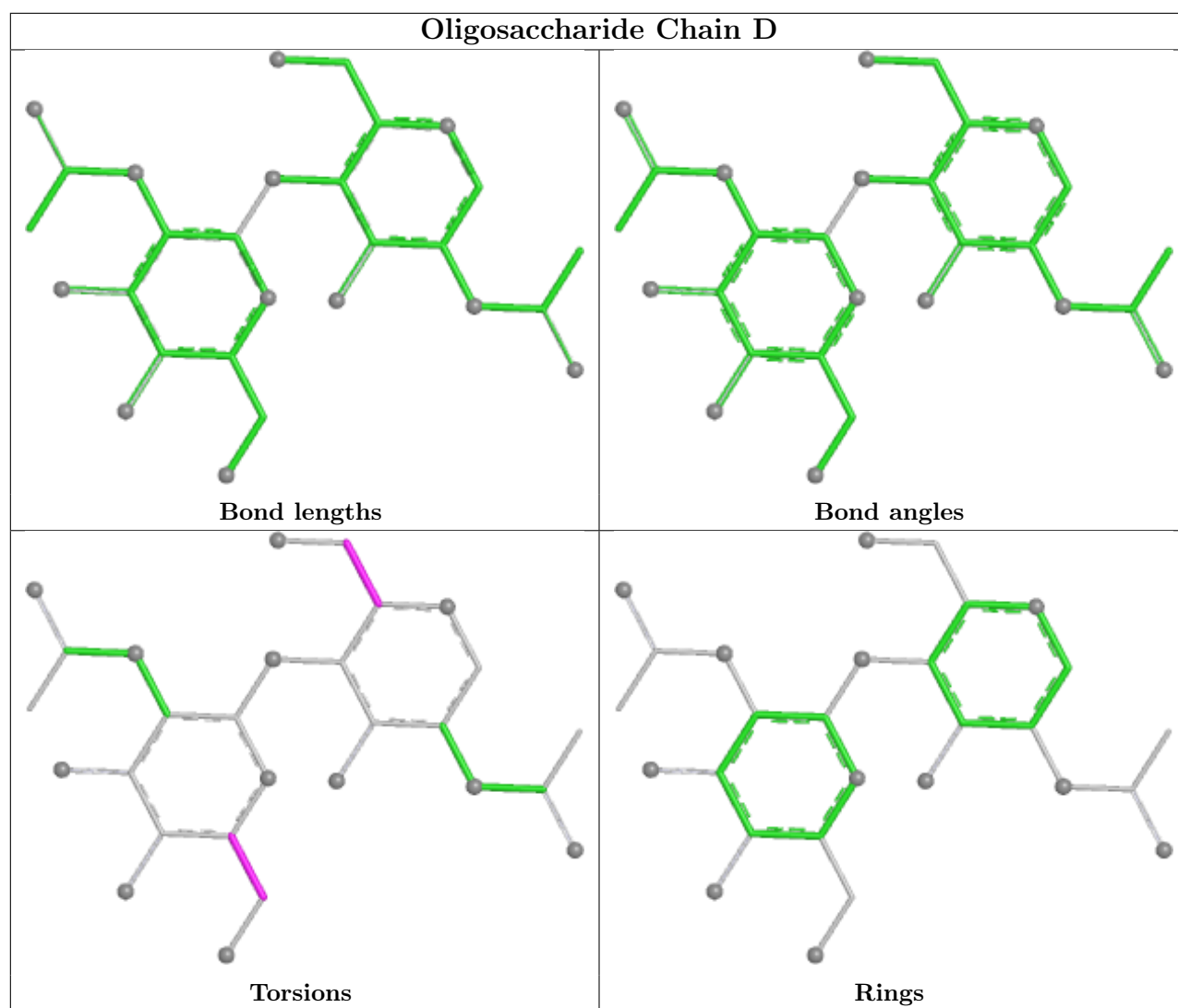
All (2) ring outliers are listed below:

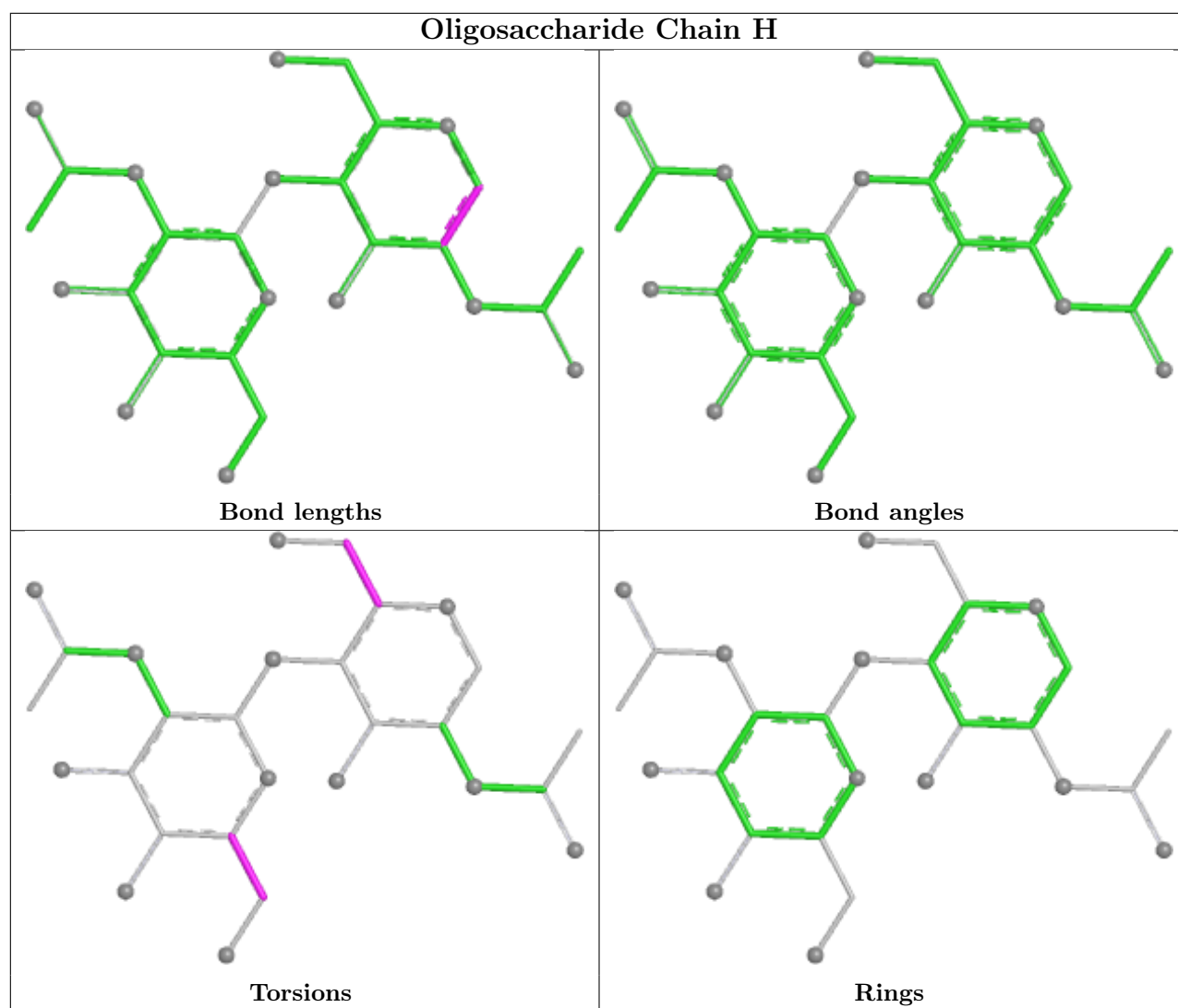
Mol	Chain	Res	Type	Atoms
5	G	4	MAN	C1-C2-C3-C4-C5-O5
5	L	4	MAN	C1-C2-C3-C4-C5-O5

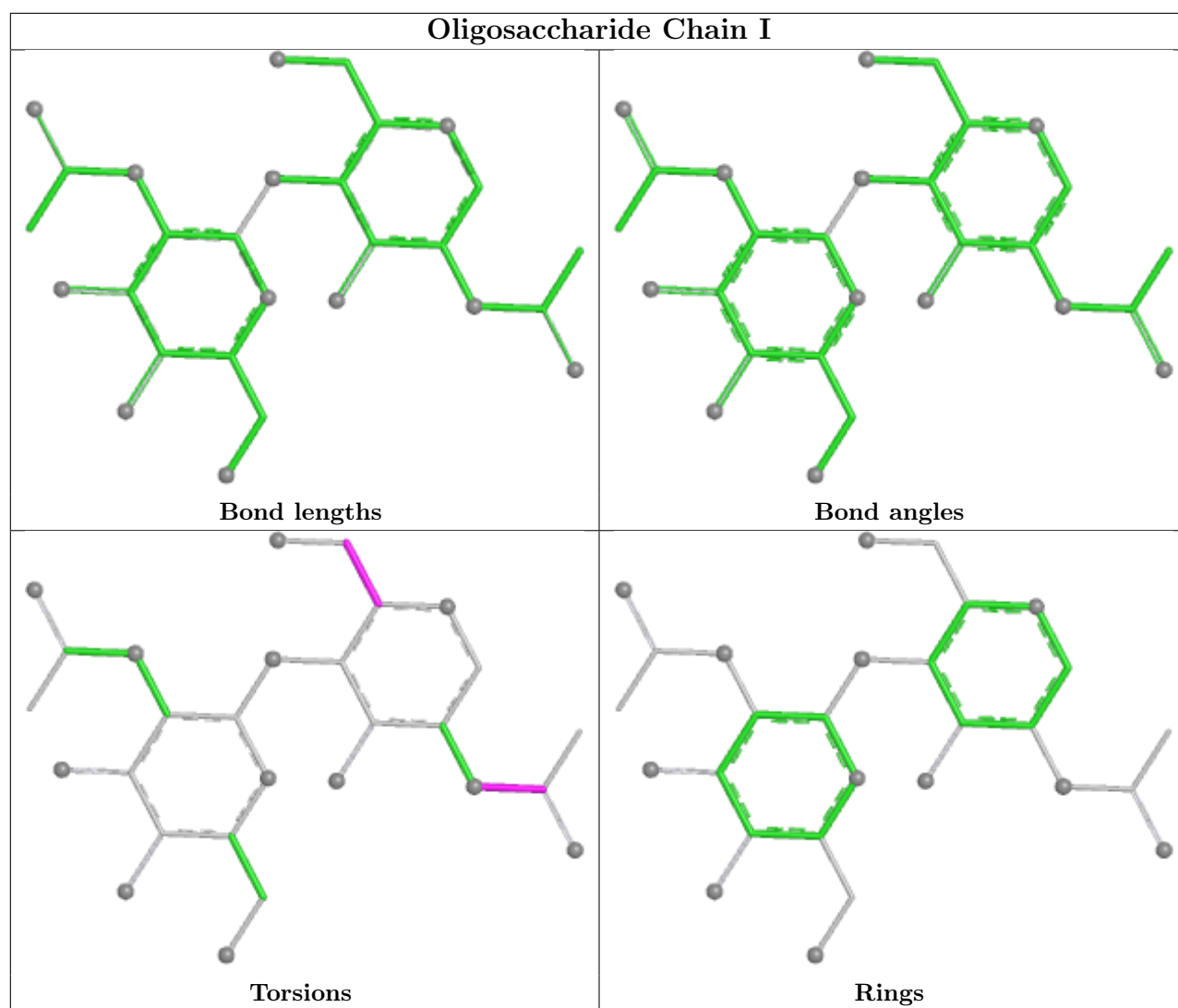
4 monomers are involved in 4 short contacts:

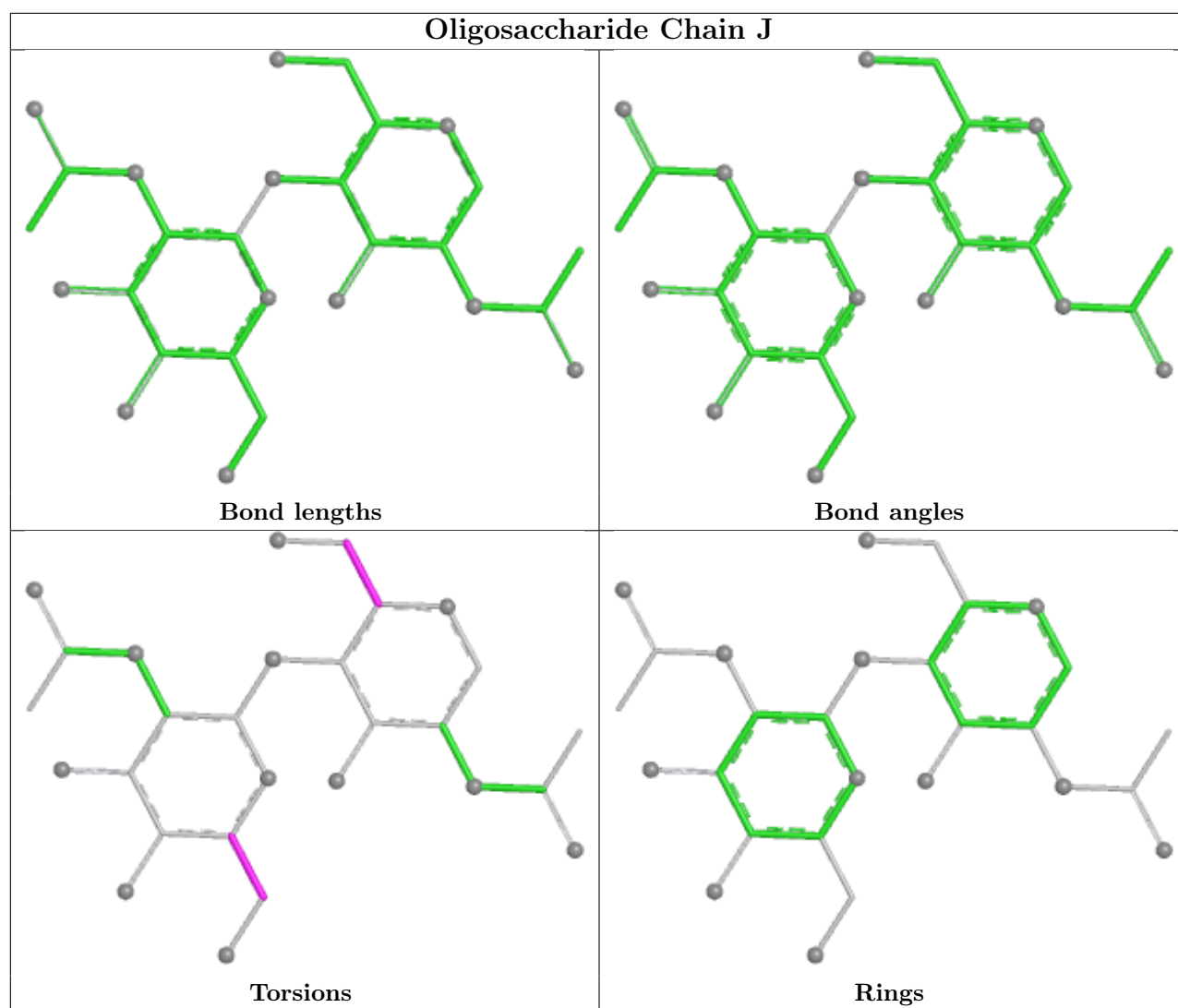
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	1	NAG	1	0
5	G	4	MAN	1	0
3	E	1	NAG	1	0
4	F	1	NAG	1	0

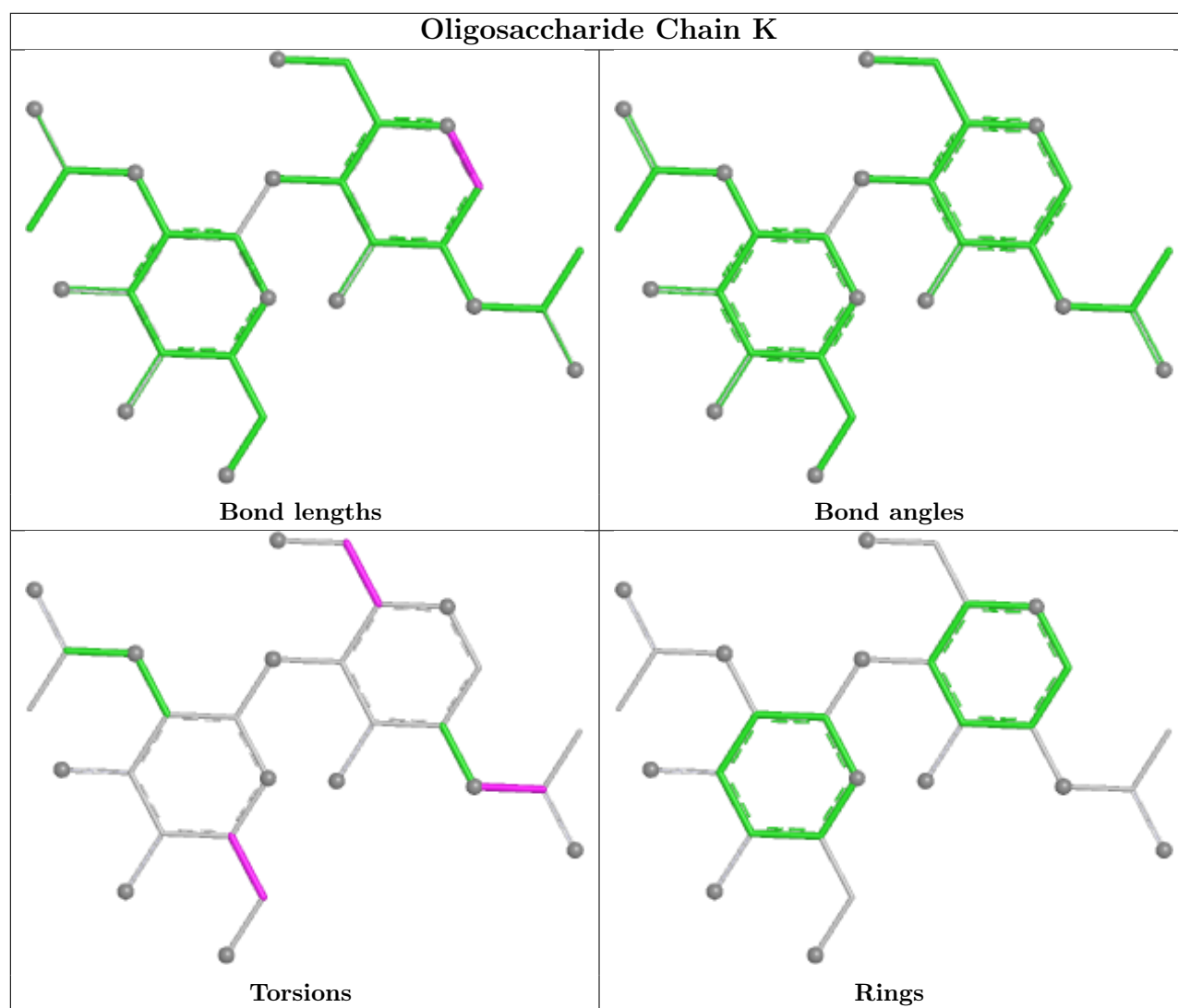
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

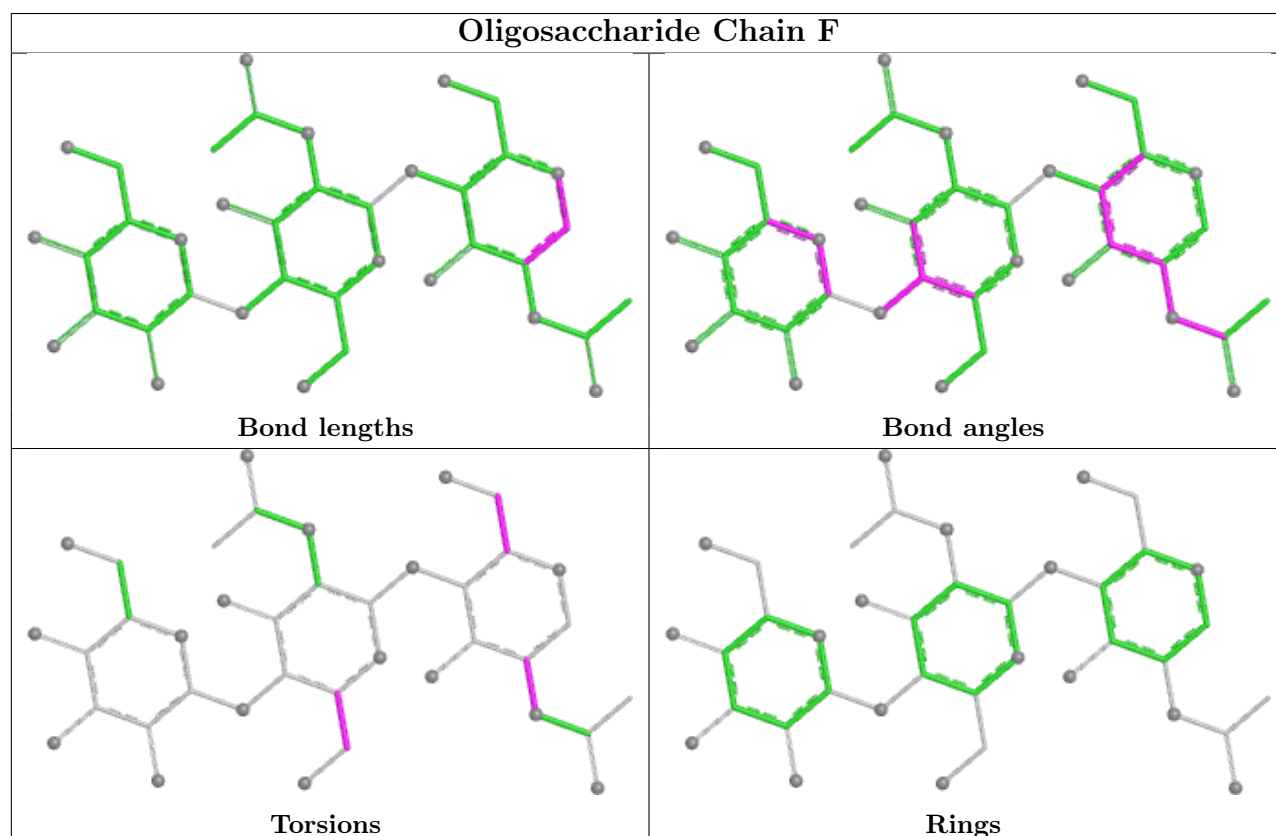
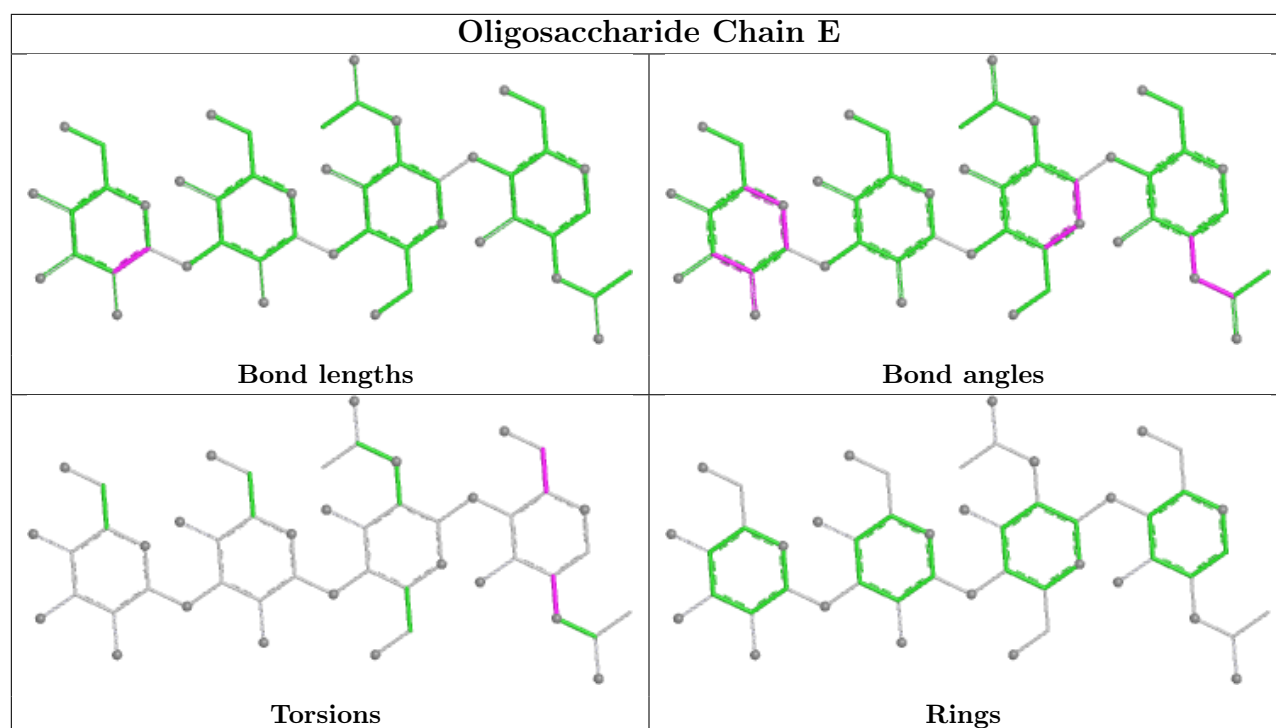


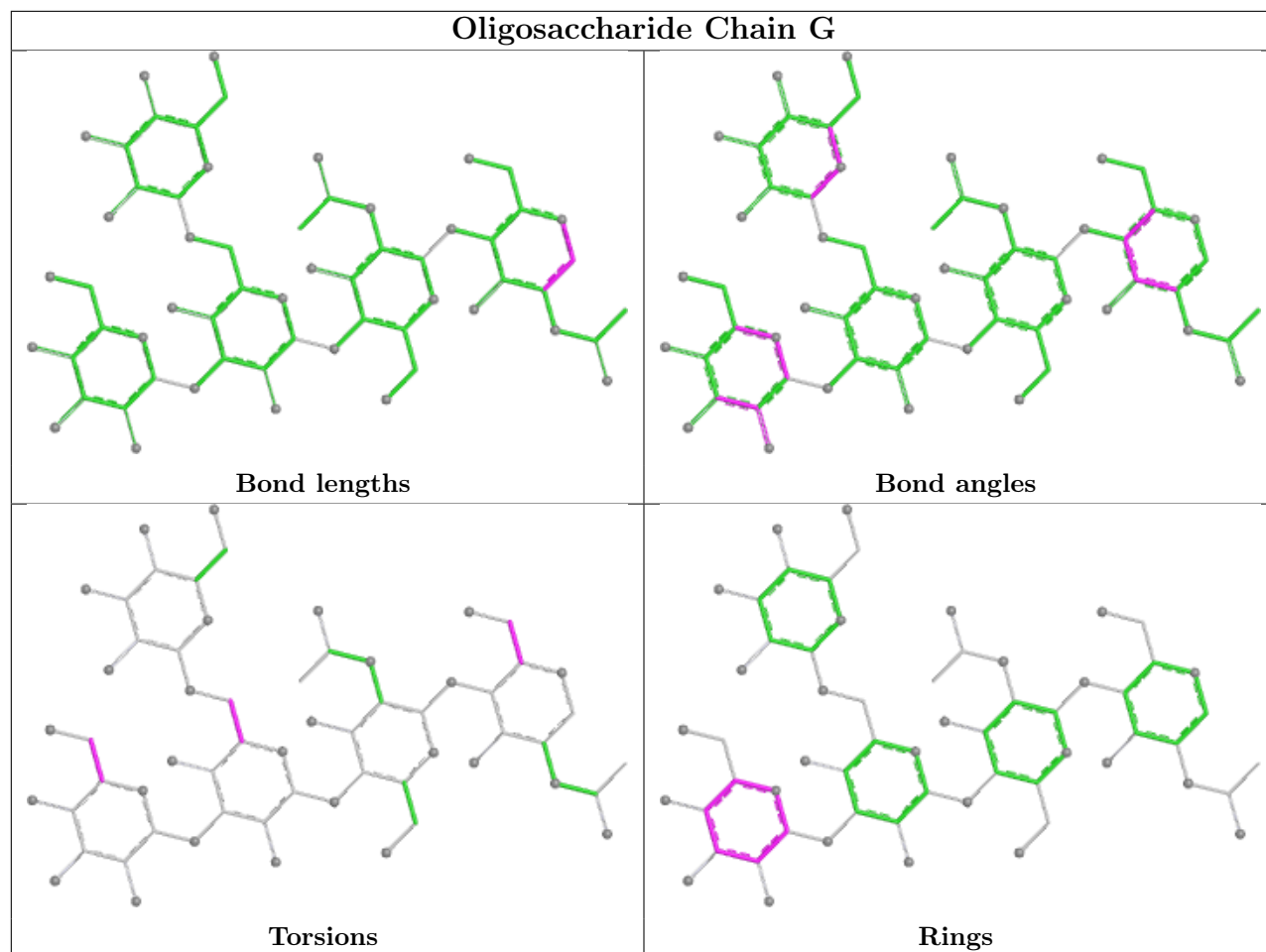


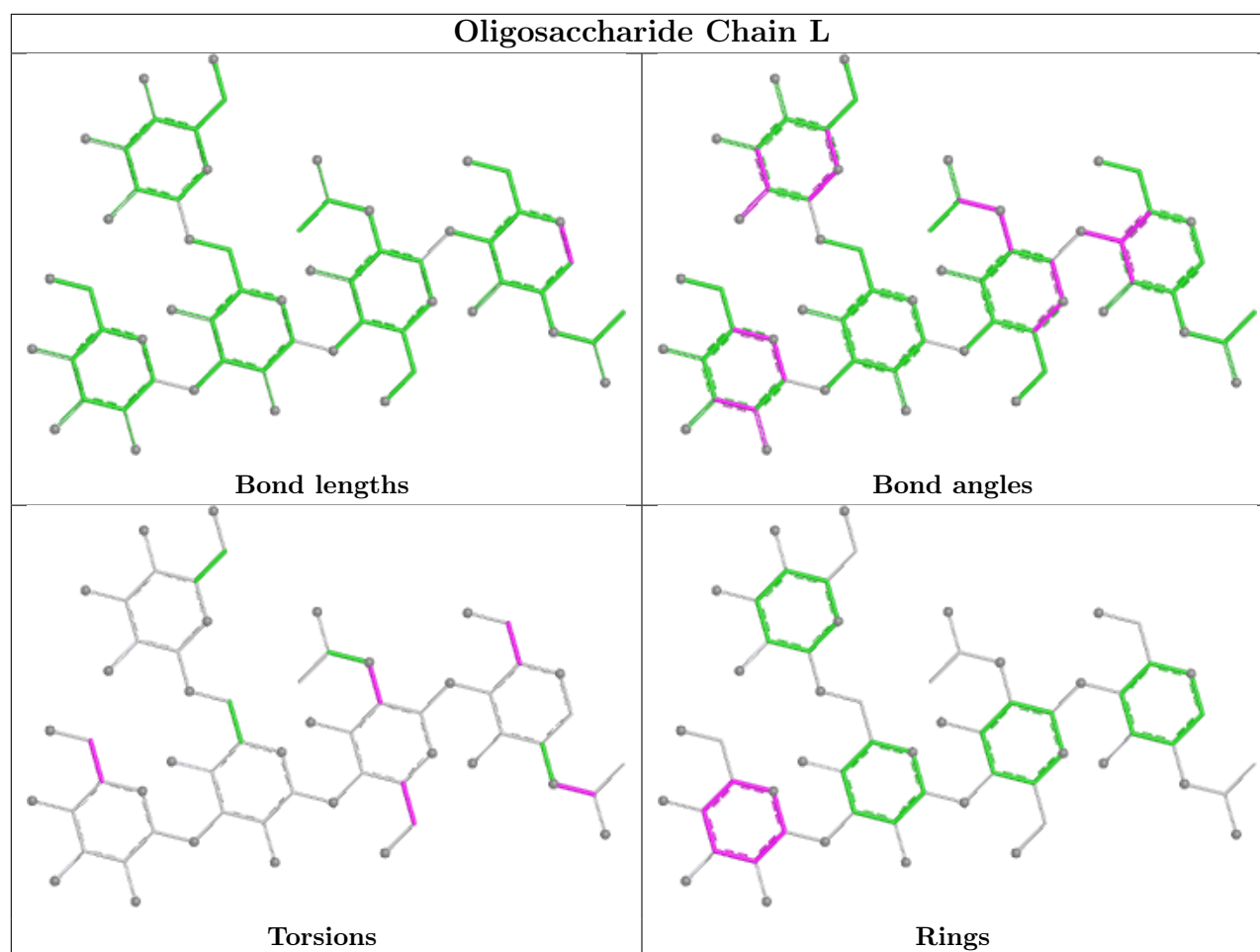












5.6 Ligand geometry [i](#)

19 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	C	1405	1	14,14,15	0.18	0	17,19,21	0.55	0
6	NAG	B	1402	1	14,14,15	0.17	0	17,19,21	0.50	0
6	NAG	A	1402	1	14,14,15	0.38	0	17,19,21	0.52	0
6	NAG	C	1401	1	14,14,15	0.31	0	17,19,21	0.43	0
6	NAG	C	1406	1	14,14,15	0.18	0	17,19,21	0.41	0
6	NAG	A	1404	1	14,14,15	0.21	0	17,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	B	1403	1	14,14,15	0.31	0	17,19,21	0.53	0
6	NAG	A	1403	1	14,14,15	0.26	0	17,19,21	0.48	0
6	NAG	C	1404	1	14,14,15	0.25	0	17,19,21	0.47	0
6	NAG	C	1403	1	14,14,15	0.90	2 (14%)	17,19,21	1.05	2 (11%)
6	NAG	A	1407	1	14,14,15	0.43	0	17,19,21	0.70	1 (5%)
6	NAG	A	1401	1	14,14,15	0.37	0	17,19,21	0.41	0
6	NAG	B	1405	1	14,14,15	0.35	0	17,19,21	0.41	0
6	NAG	B	1401	1	14,14,15	0.28	0	17,19,21	0.52	0
6	NAG	C	1407	1	14,14,15	0.19	0	17,19,21	0.54	0
6	NAG	A	1405	1	14,14,15	0.27	0	17,19,21	0.55	0
6	NAG	B	1404	1	14,14,15	0.39	0	17,19,21	0.43	0
6	NAG	C	1402	1	14,14,15	0.34	0	17,19,21	0.40	0
6	NAG	A	1406	1	14,14,15	0.29	0	17,19,21	0.47	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	1405	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1402	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1401	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1406	1	-	3/6/23/26	0/1/1/1
6	NAG	A	1404	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1403	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1403	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1404	1	-	3/6/23/26	0/1/1/1
6	NAG	C	1403	1	-	3/6/23/26	0/1/1/1
6	NAG	A	1407	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1401	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1405	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1407	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1405	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1404	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1402	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1406	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1403	NAG	O5-C1	2.33	1.47	1.43
6	C	1403	NAG	C1-C2	2.31	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1403	NAG	C2-N2-C7	3.03	126.96	122.90
6	A	1407	NAG	C1-O5-C5	2.30	115.27	112.19
6	C	1403	NAG	C1-C2-N2	2.01	113.60	110.43

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1403	NAG	C4-C5-C6-O6
6	A	1406	NAG	C4-C5-C6-O6
6	C	1404	NAG	C4-C5-C6-O6
6	B	1401	NAG	O5-C5-C6-O6
6	C	1405	NAG	O5-C5-C6-O6

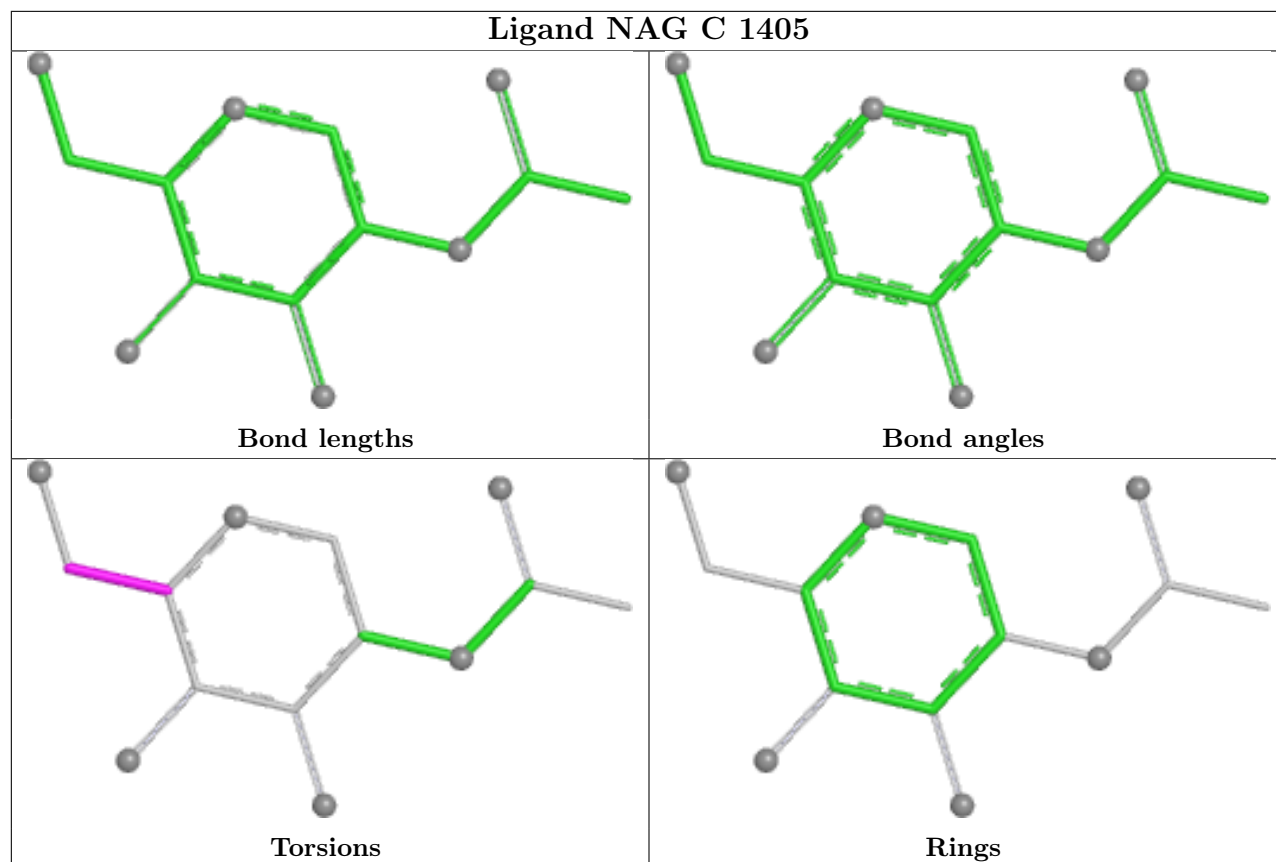
There are no ring outliers.

4 monomers are involved in 5 short contacts:

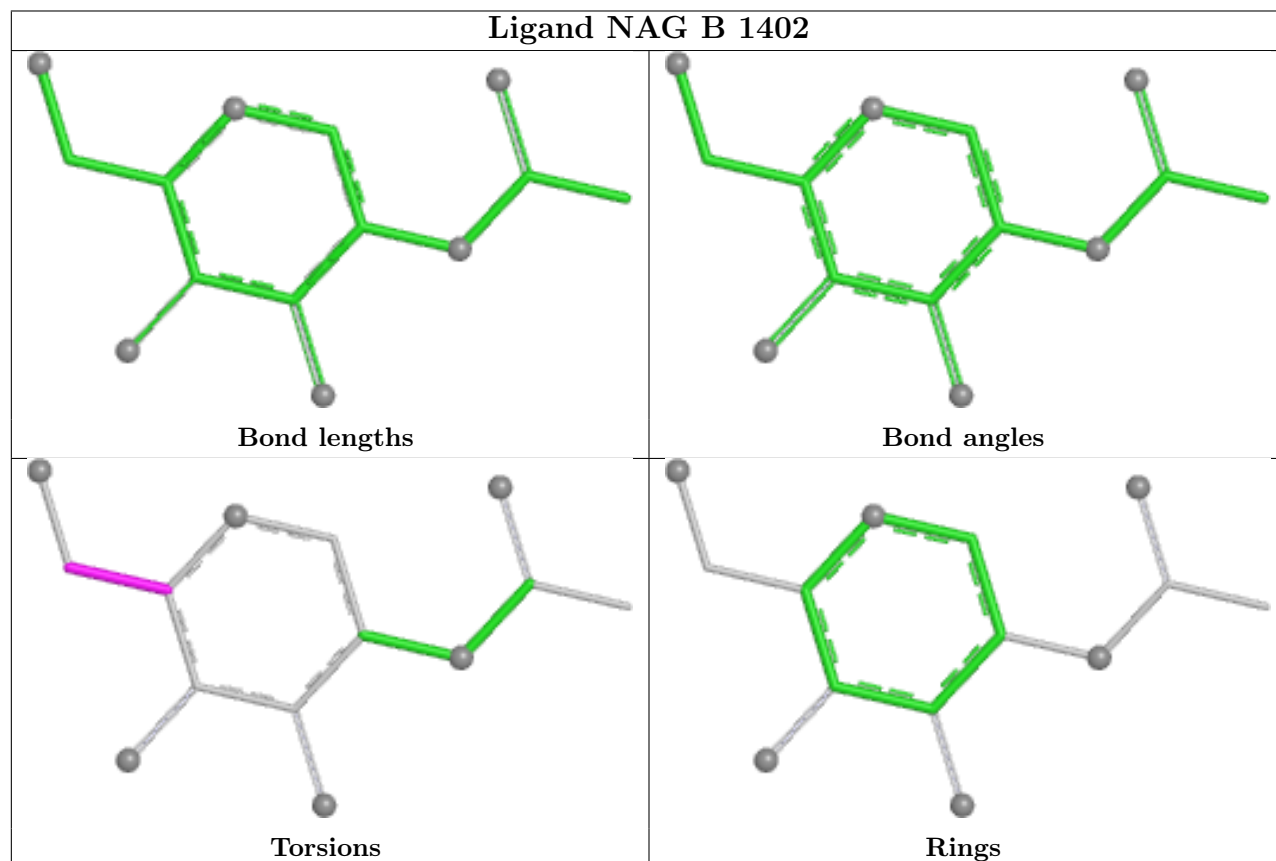
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1404	NAG	1	0
6	A	1407	NAG	1	0
6	A	1401	NAG	1	0
6	C	1402	NAG	2	0

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.

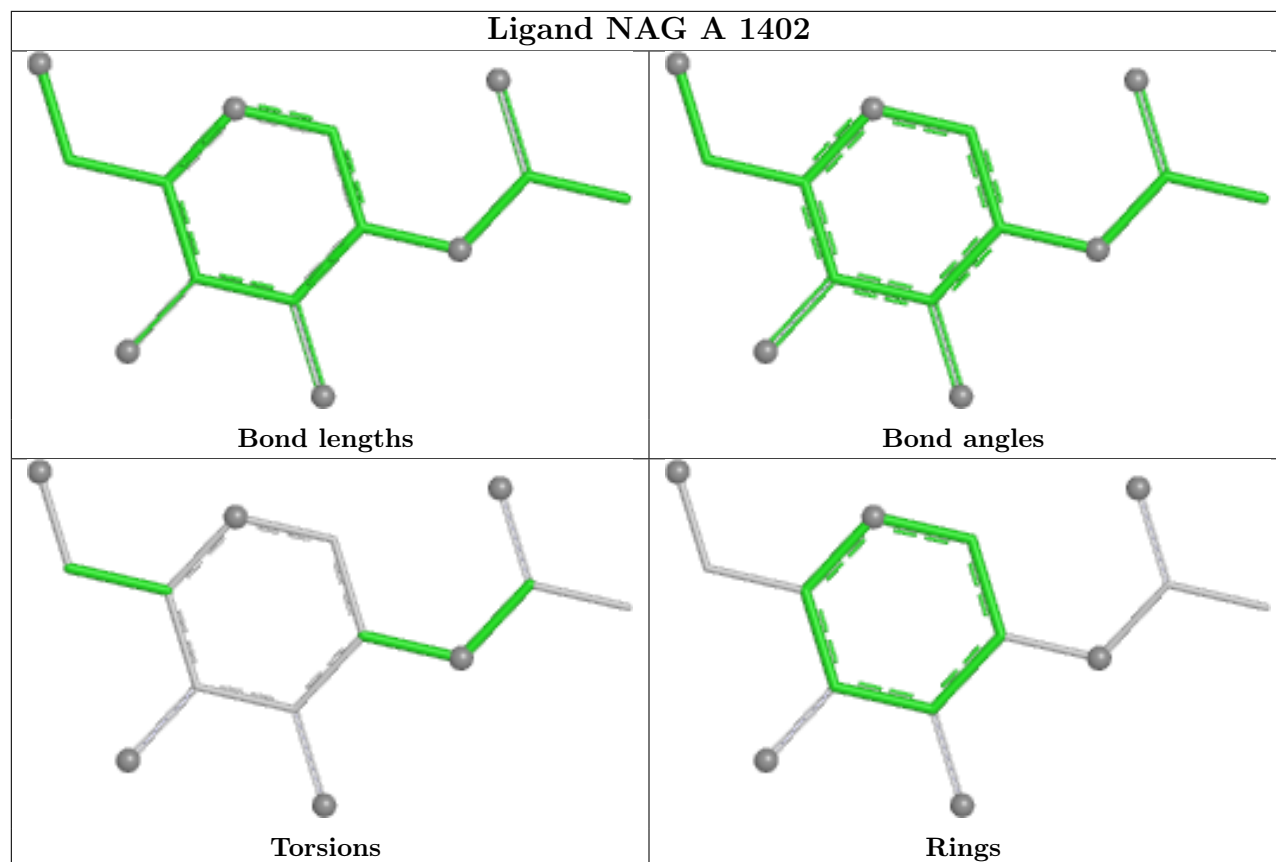
Ligand NAG C 1405



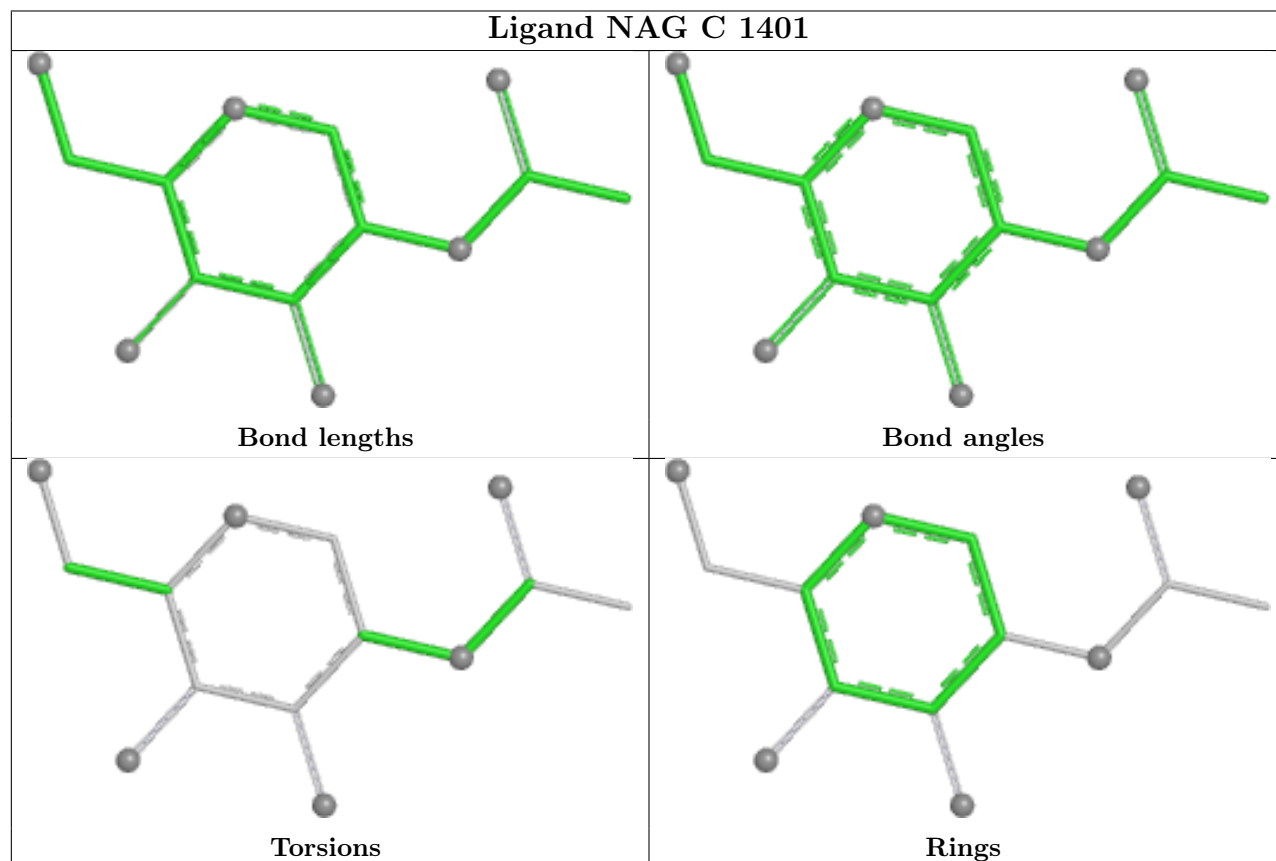
Ligand NAG B 1402

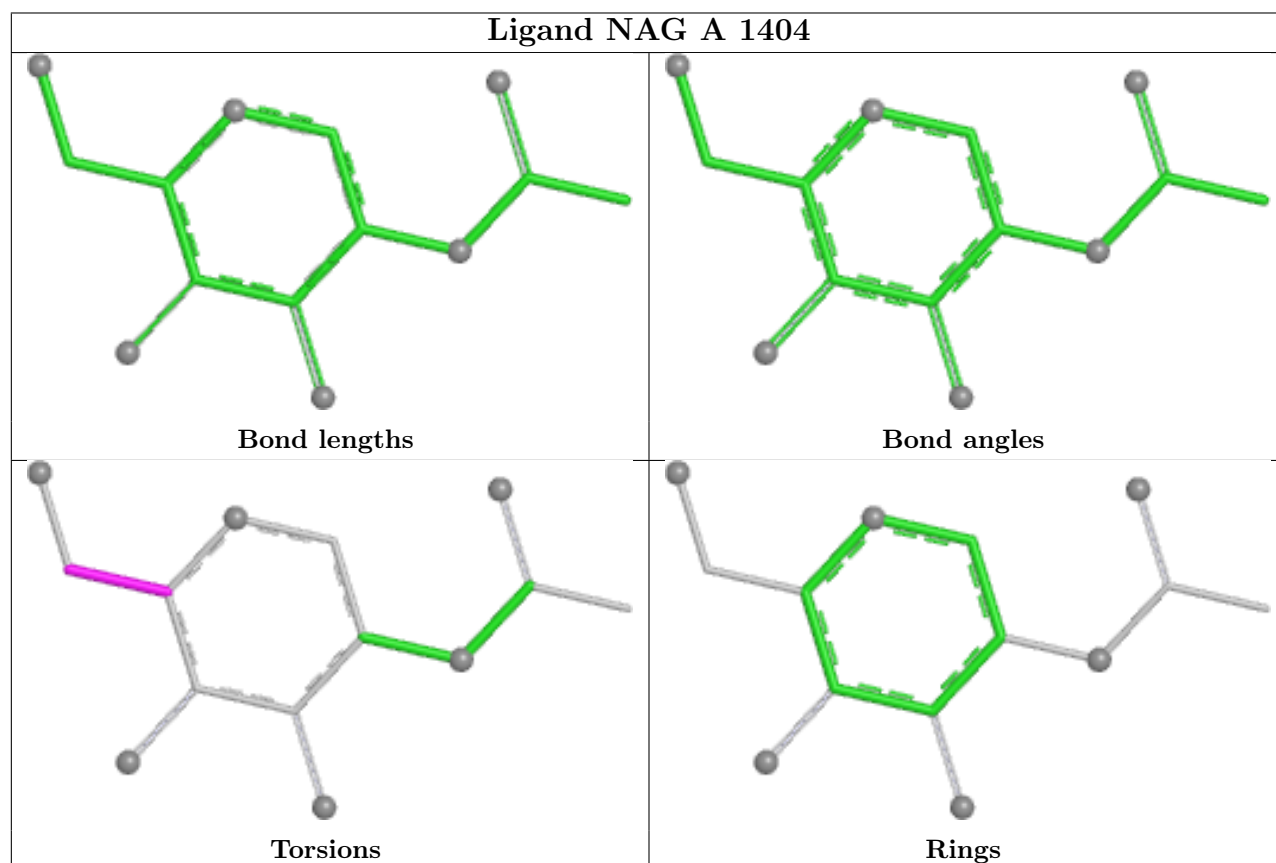
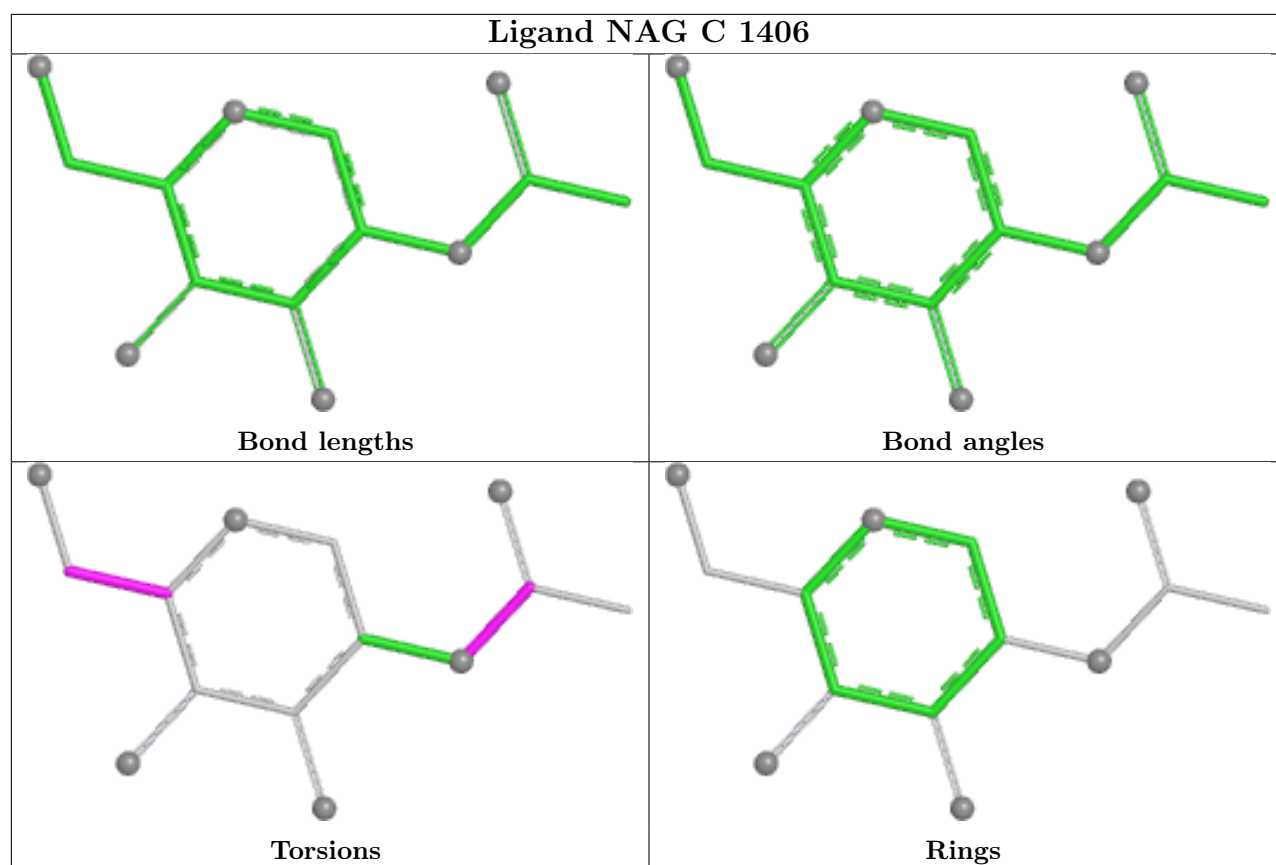


Ligand NAG A 1402

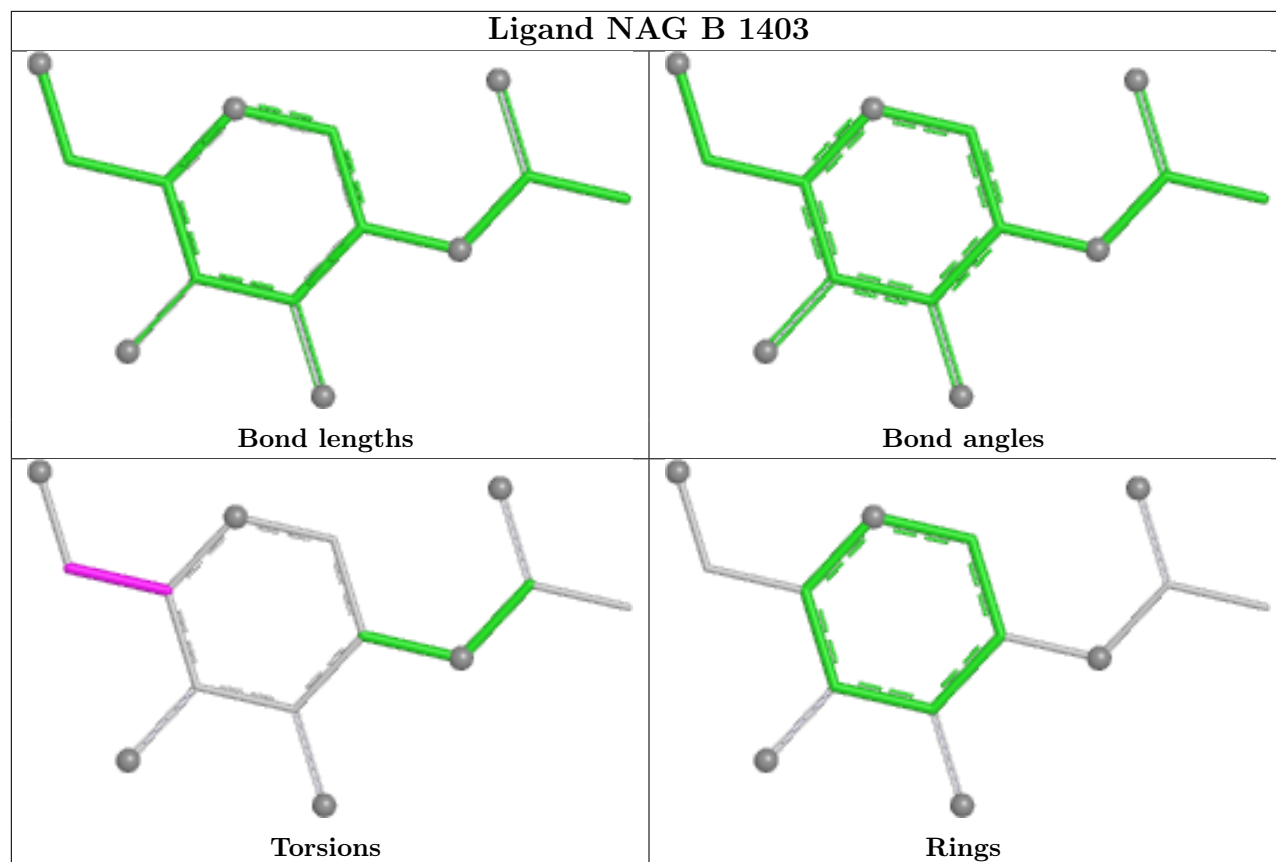


Ligand NAG C 1401

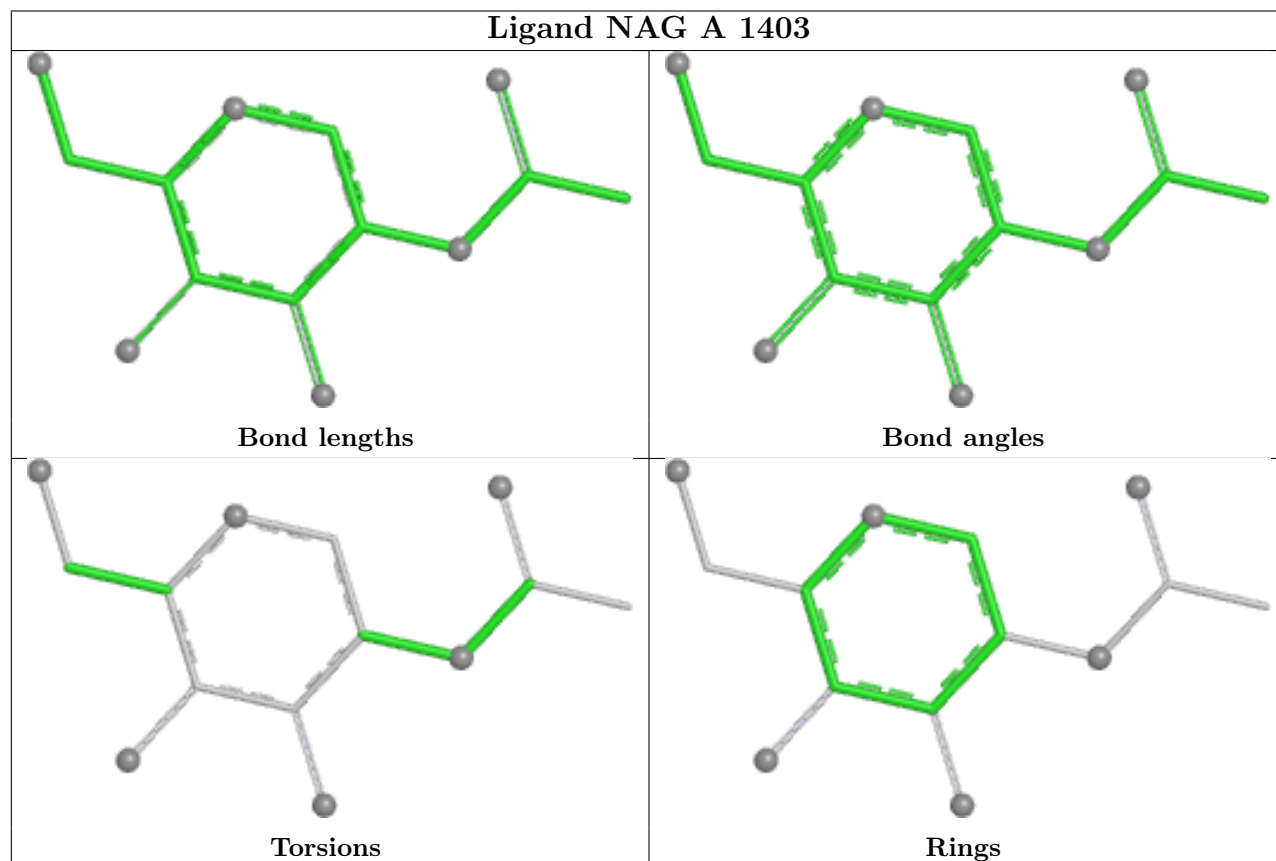


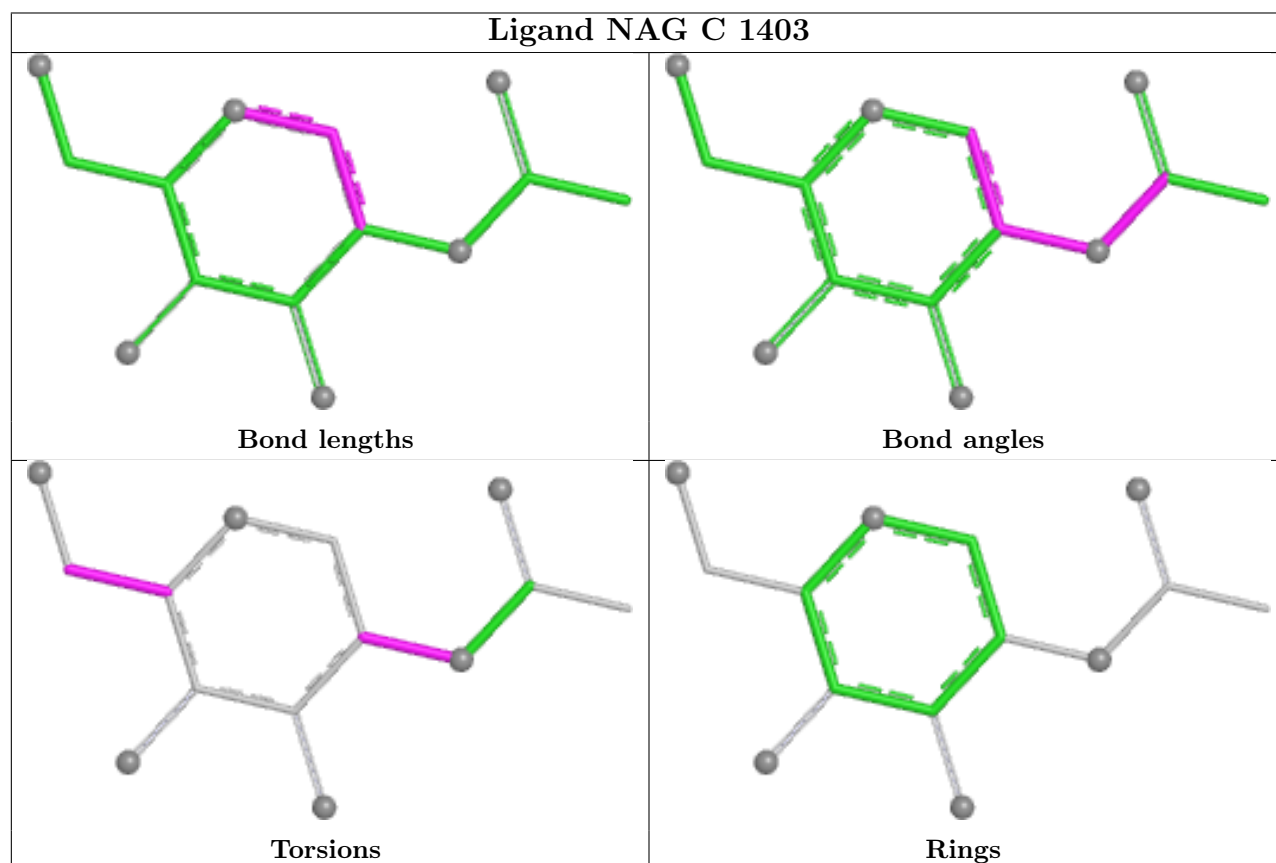
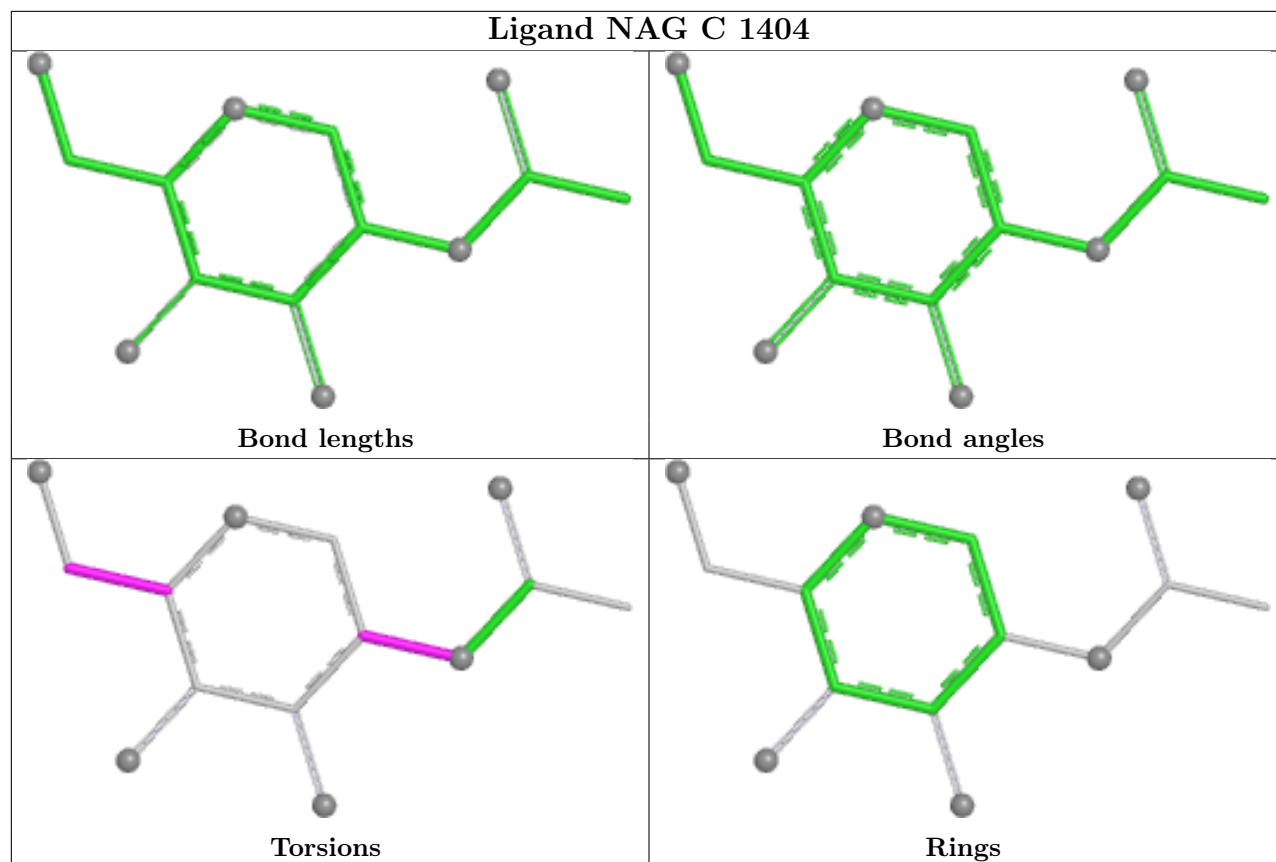


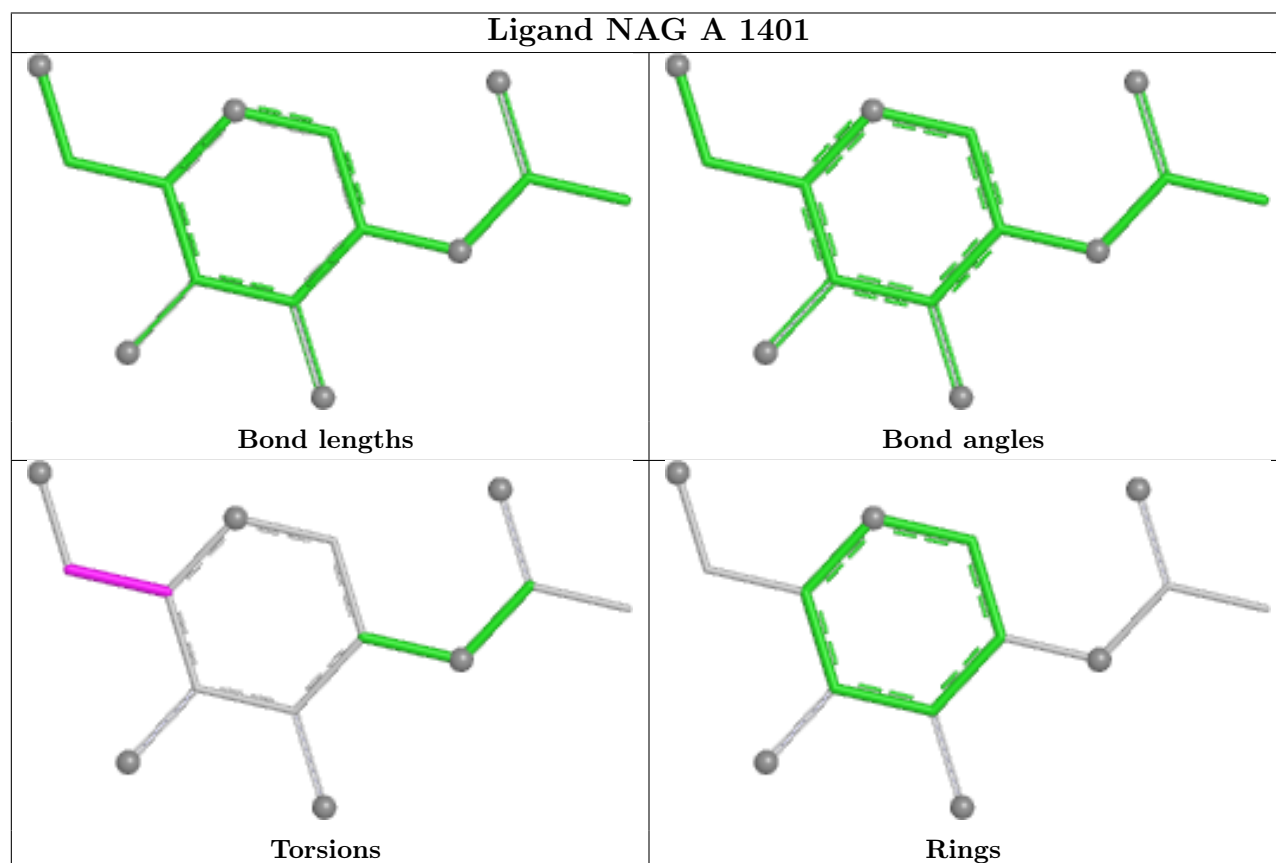
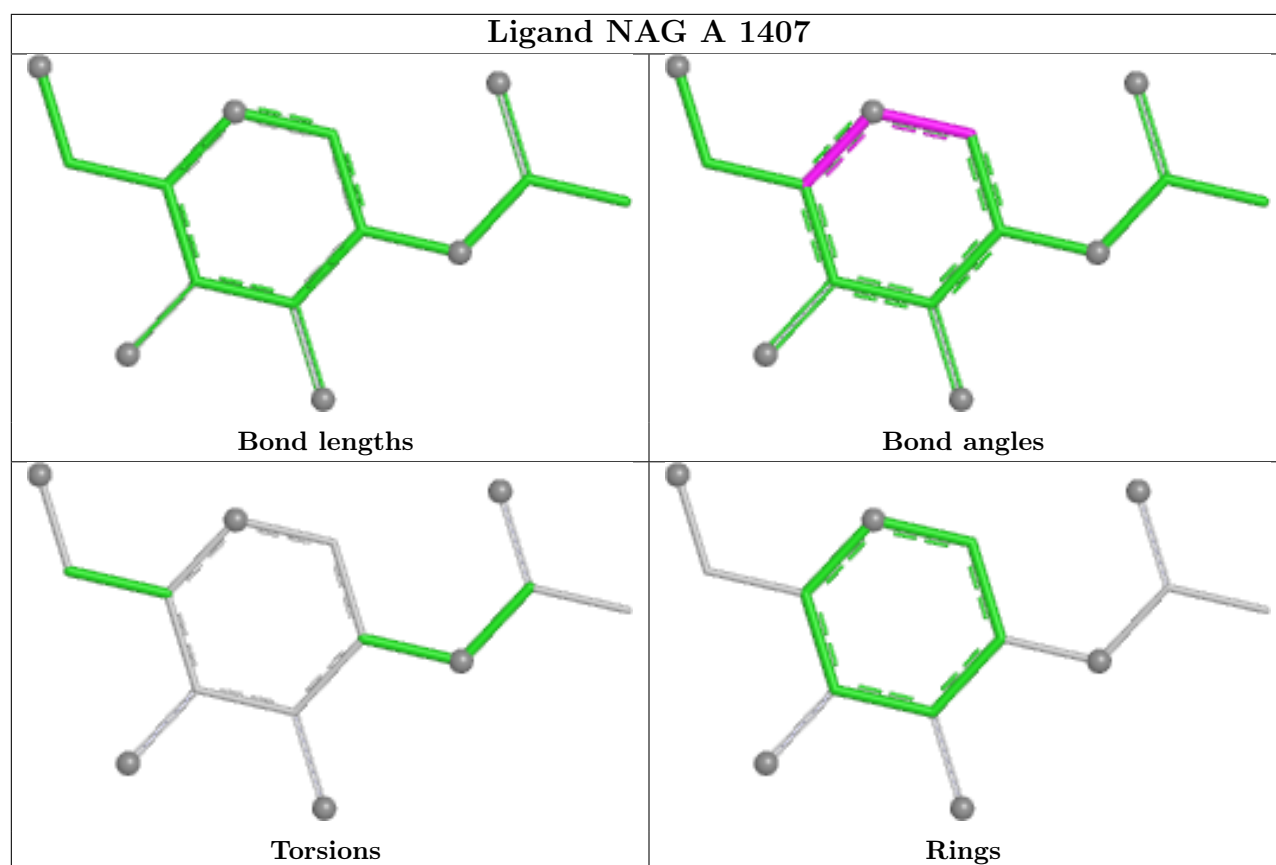
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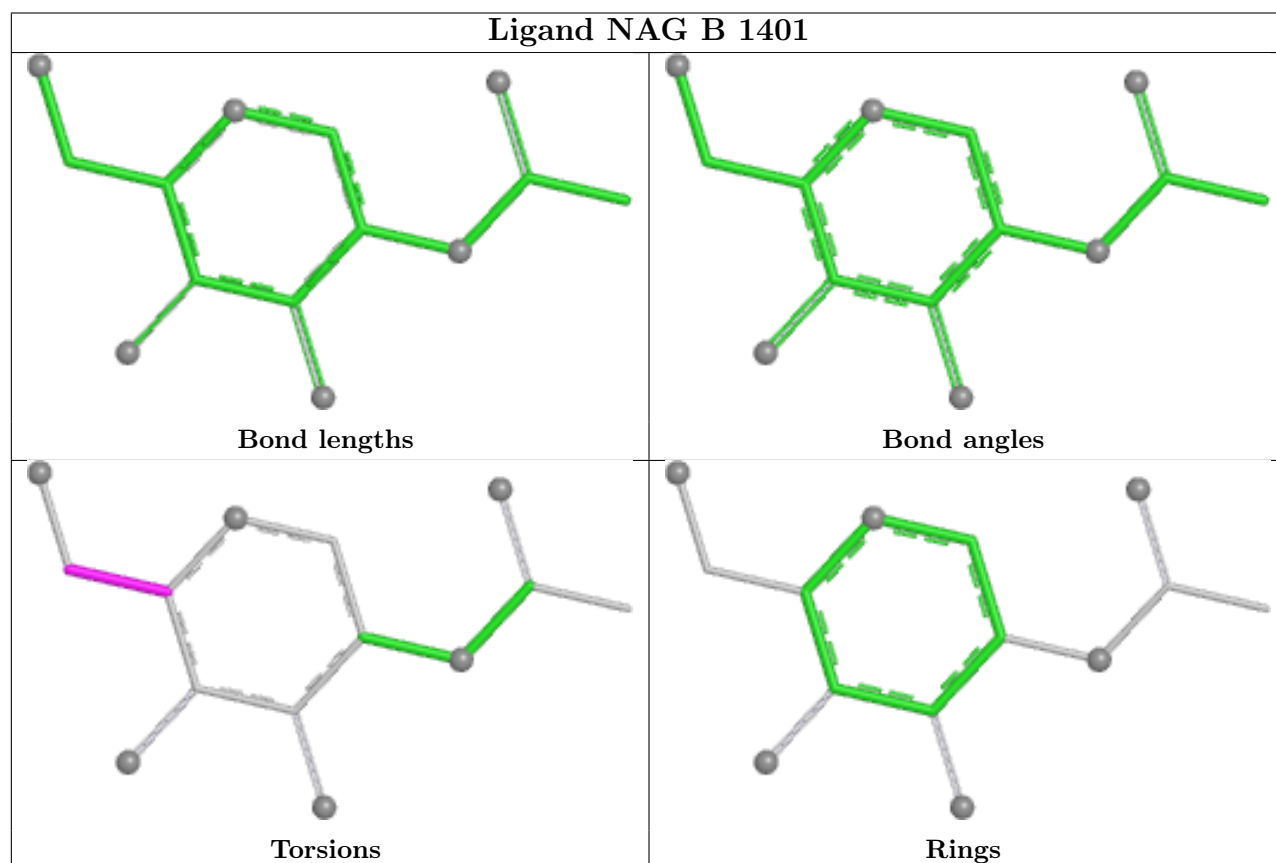
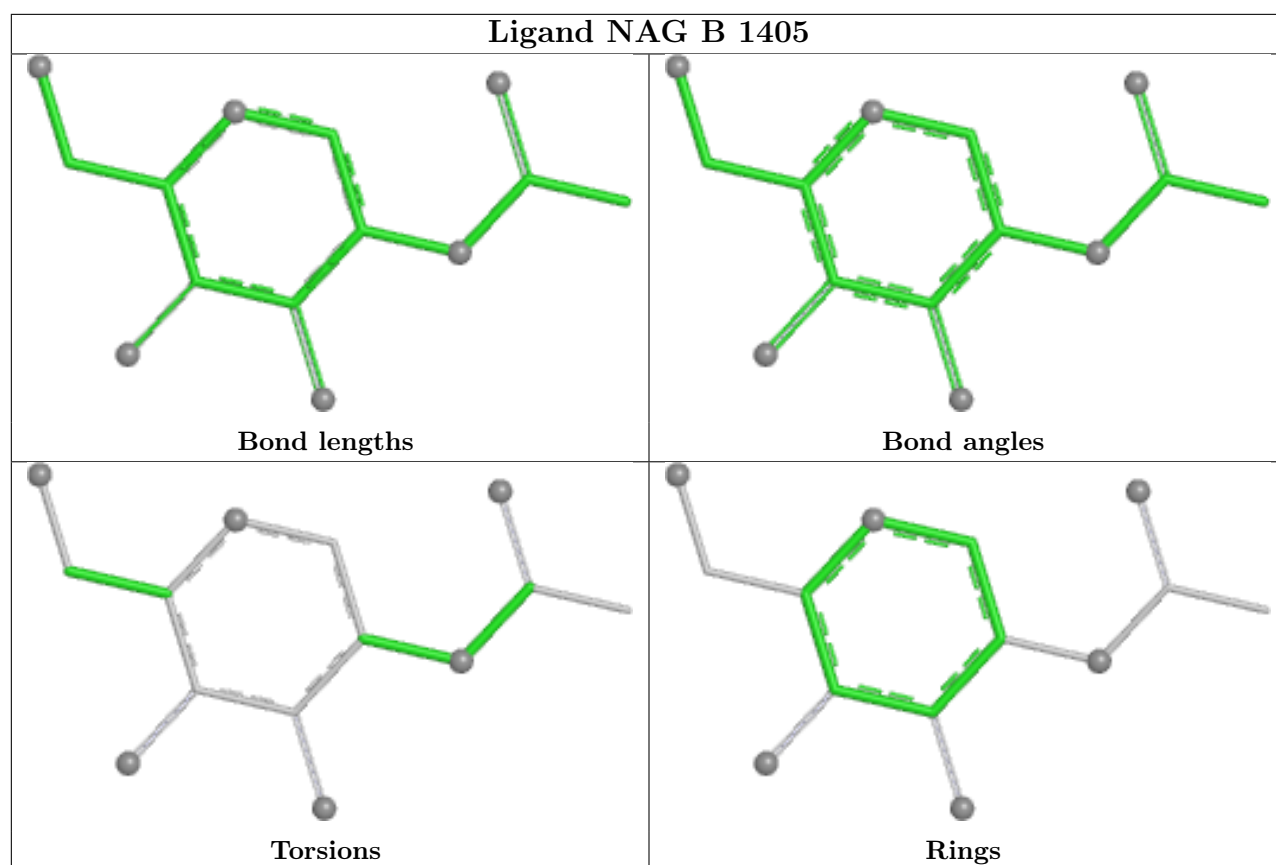


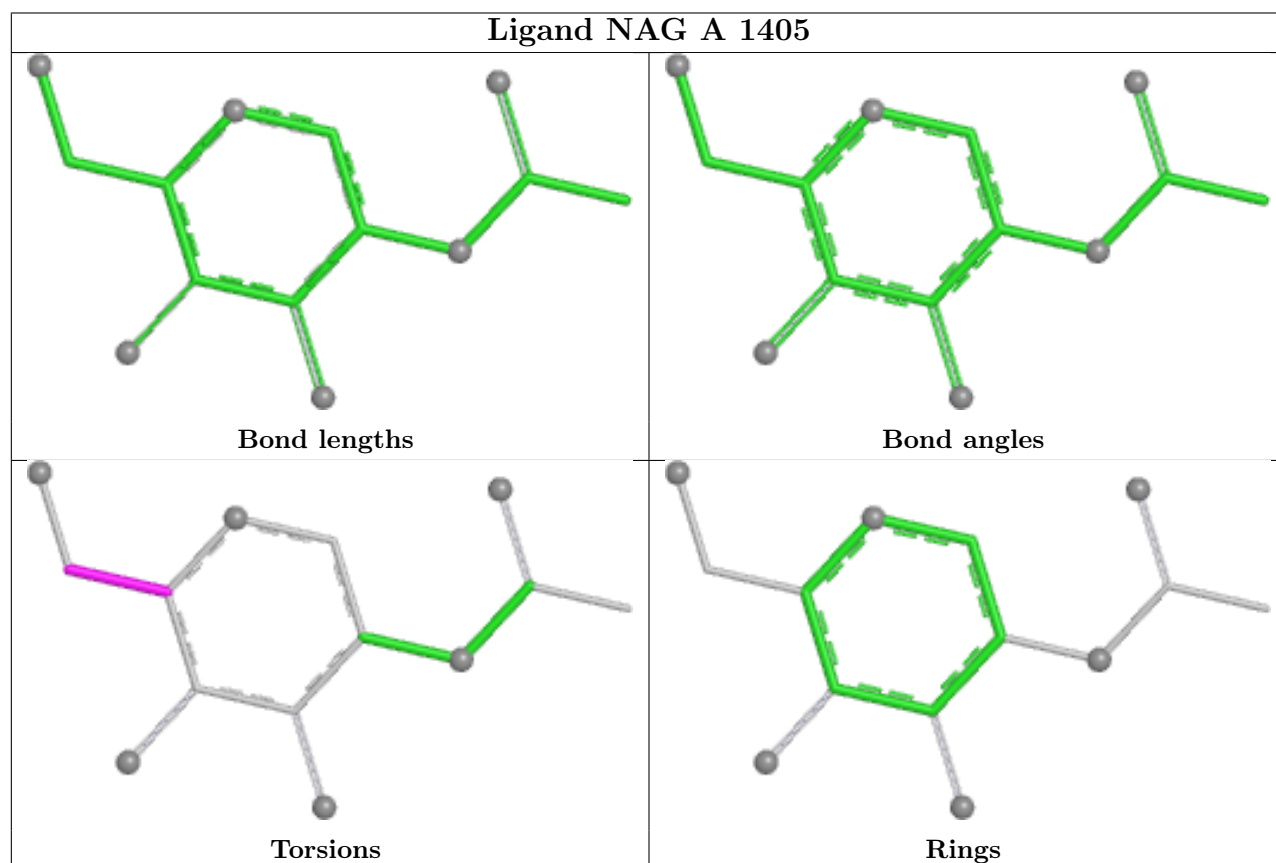
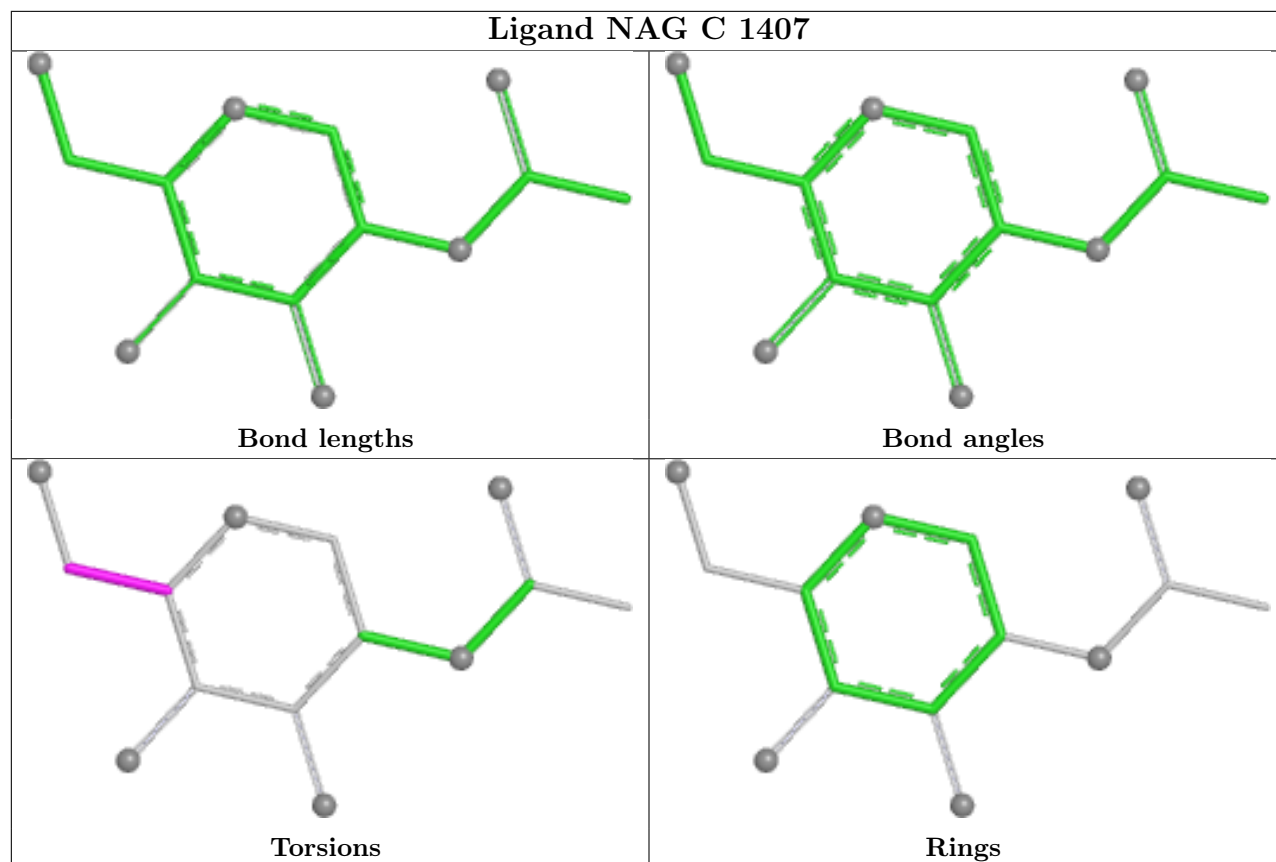
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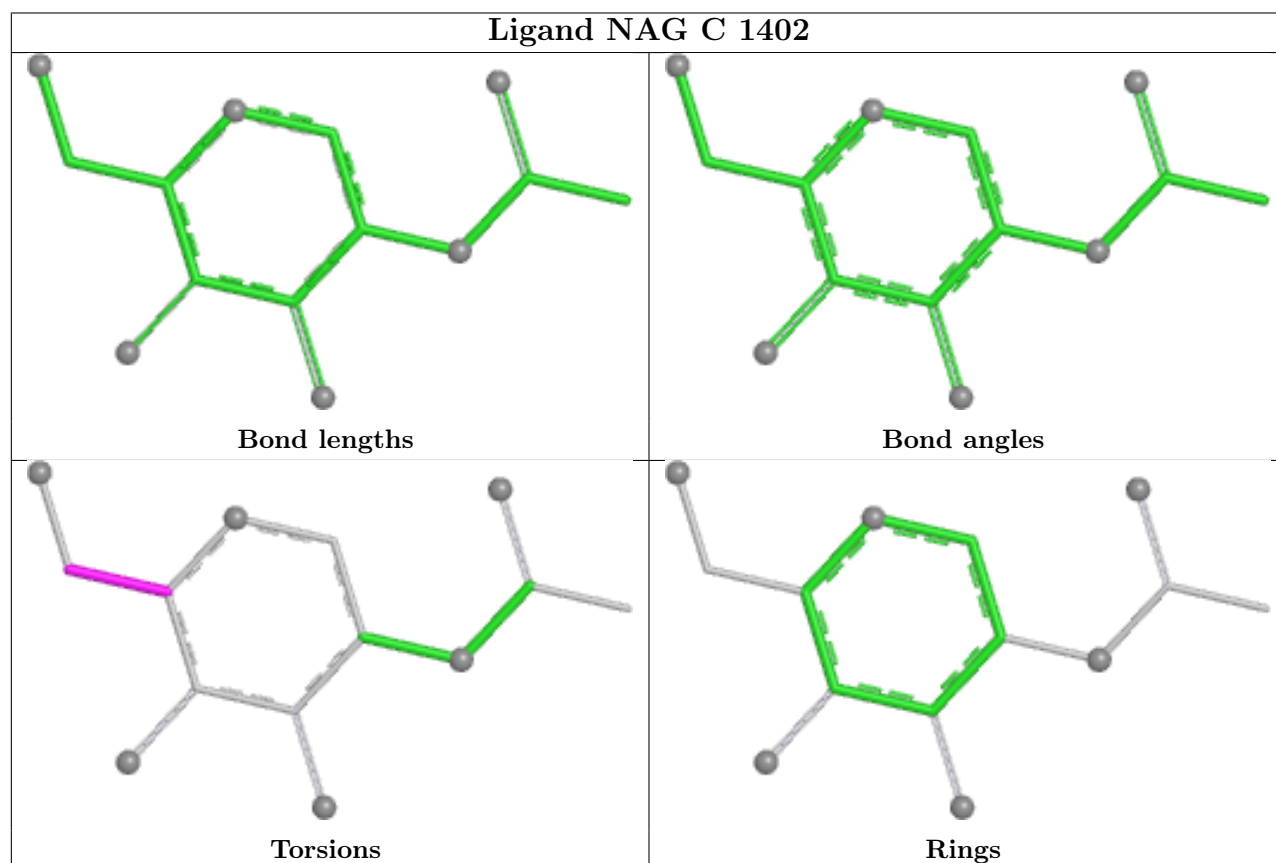
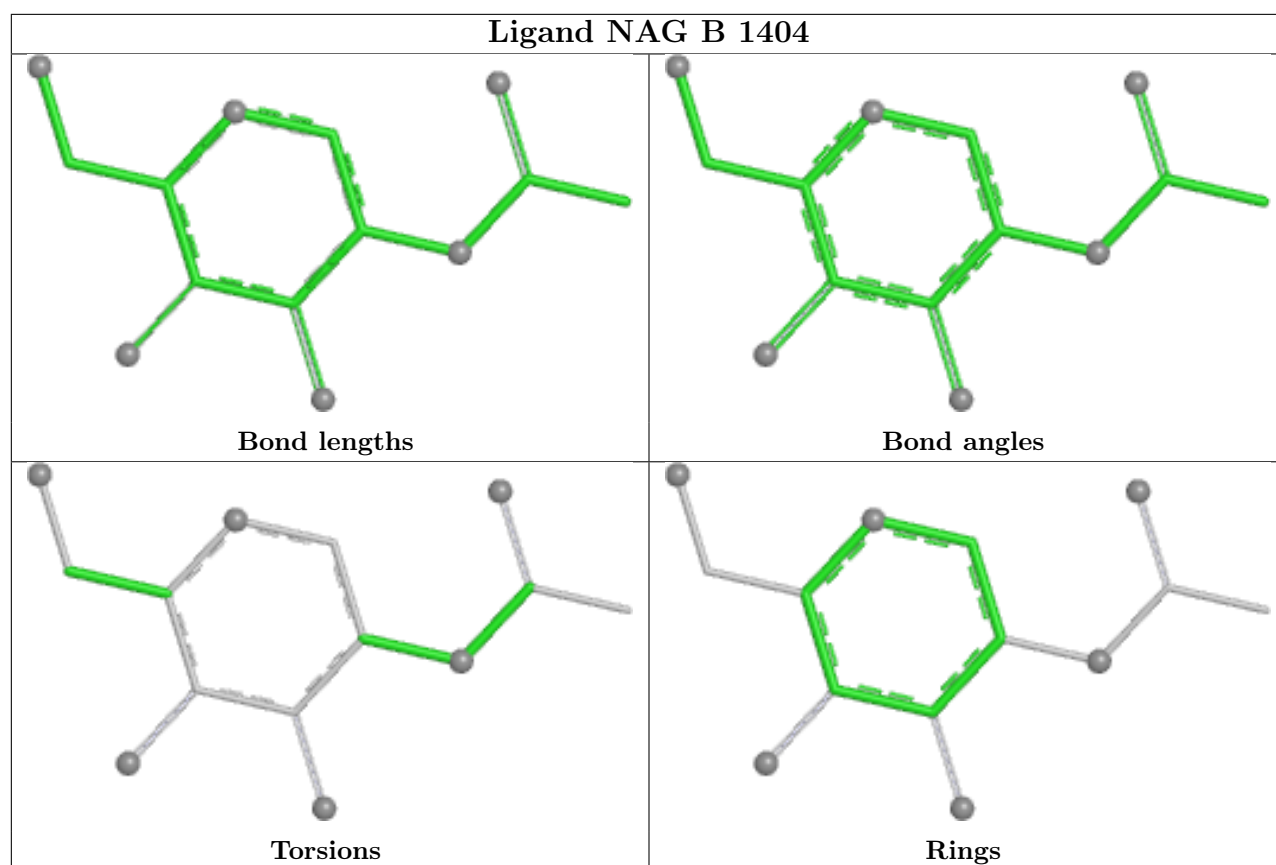


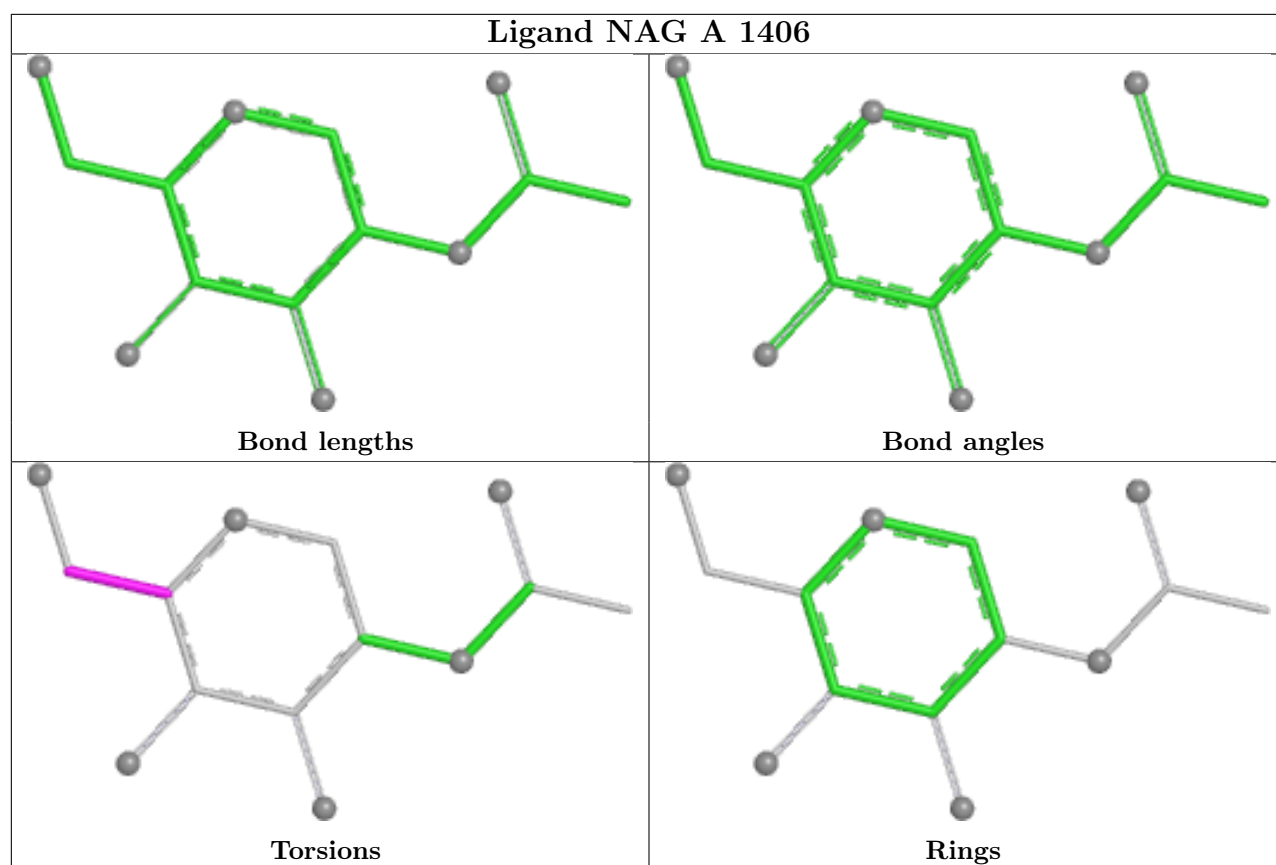












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

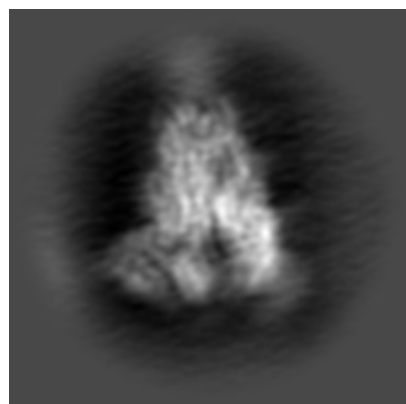
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33947. These allow visual inspection of the internal detail of the map and identification of artifacts.

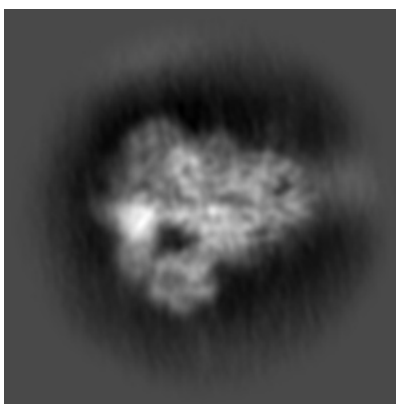
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

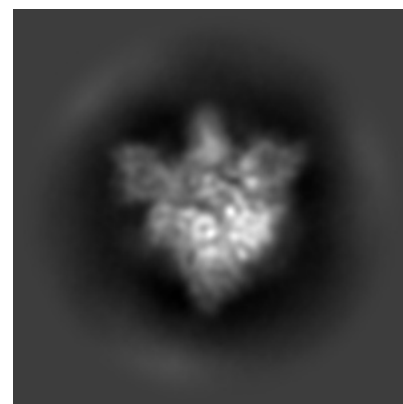
6.1.1 Primary map



X

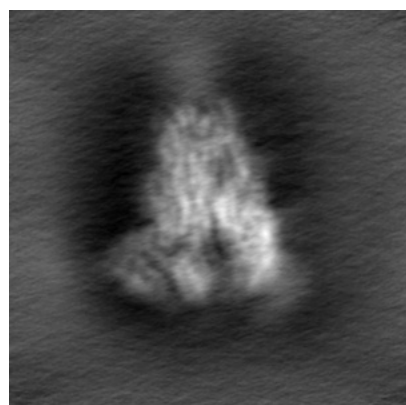


Y

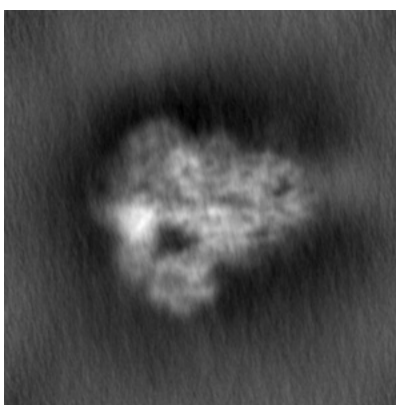


Z

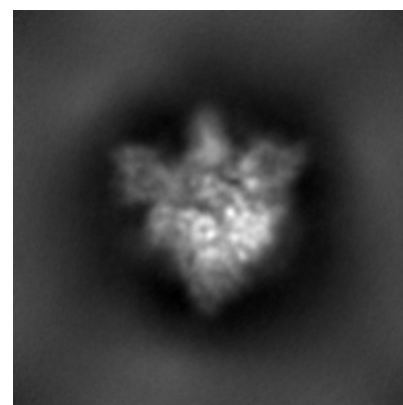
6.1.2 Raw map



X



Y

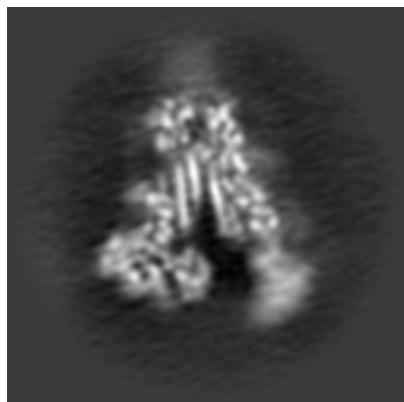


Z

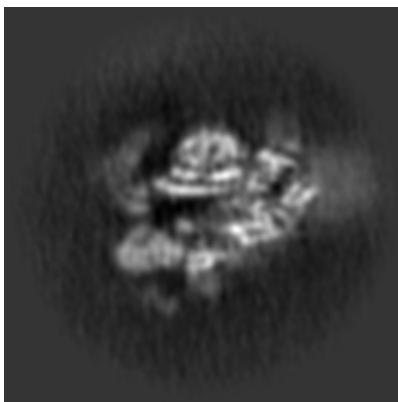
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

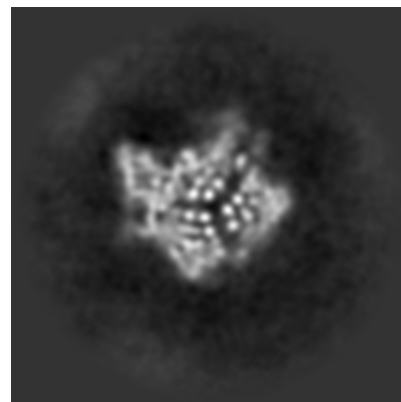
6.2.1 Primary map



X Index: 128

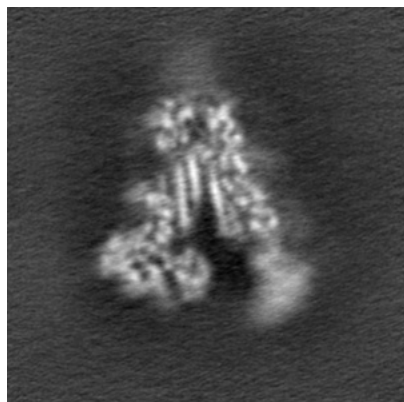


Y Index: 128

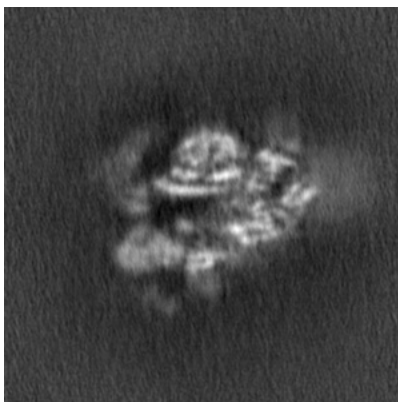


Z Index: 128

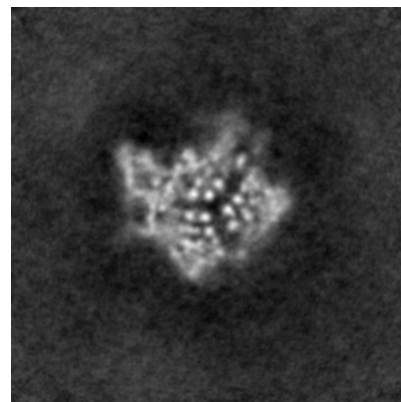
6.2.2 Raw map



X Index: 128



Y Index: 128

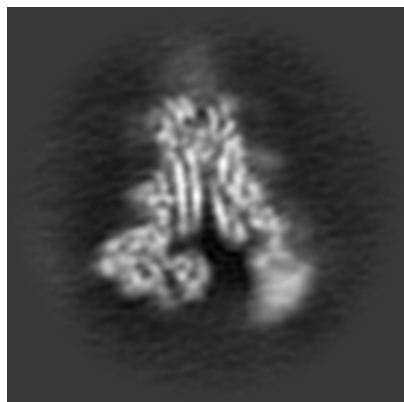


Z Index: 128

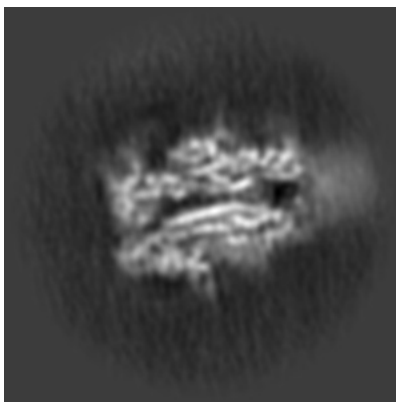
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

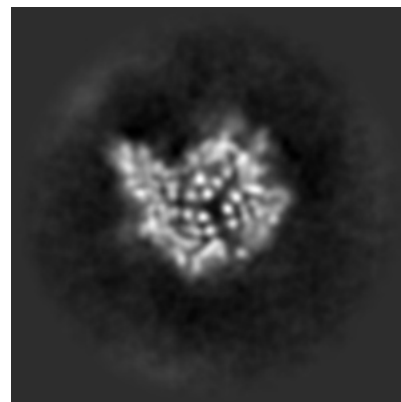
6.3.1 Primary map



X Index: 125

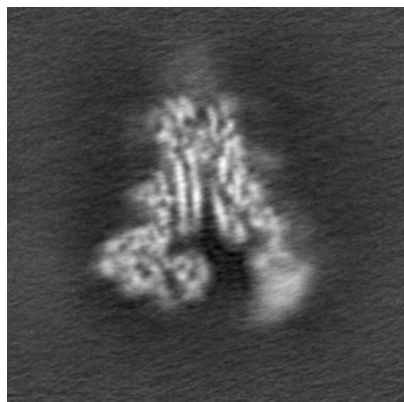


Y Index: 121

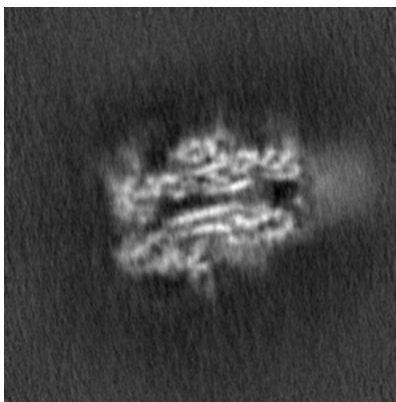


Z Index: 124

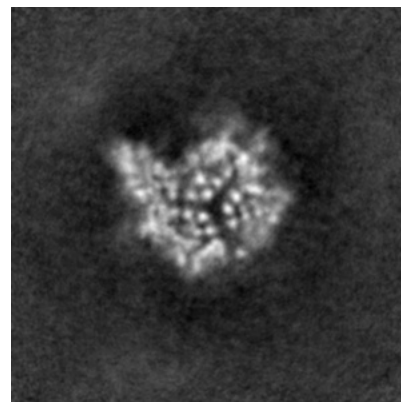
6.3.2 Raw map



X Index: 125



Y Index: 122

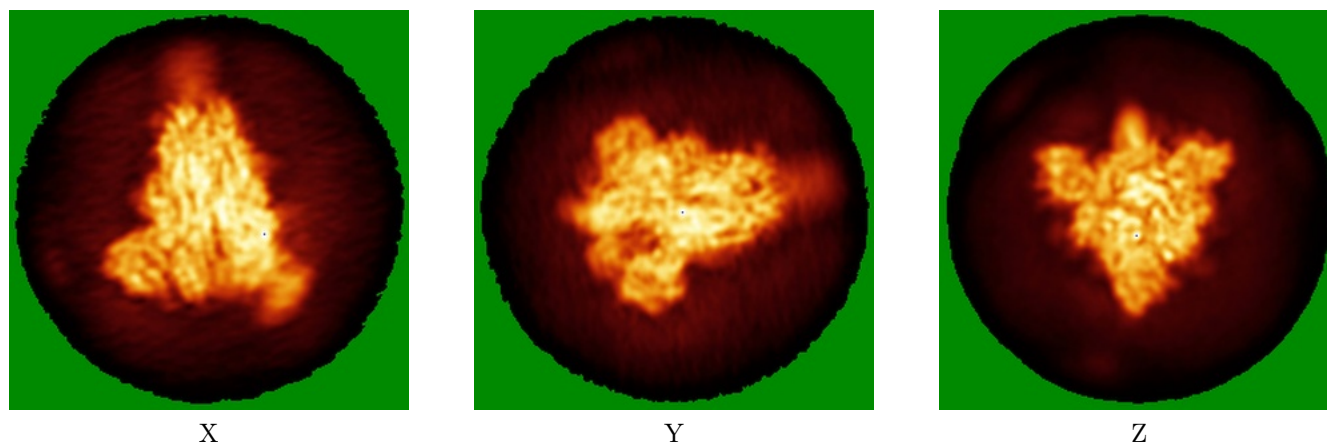


Z Index: 124

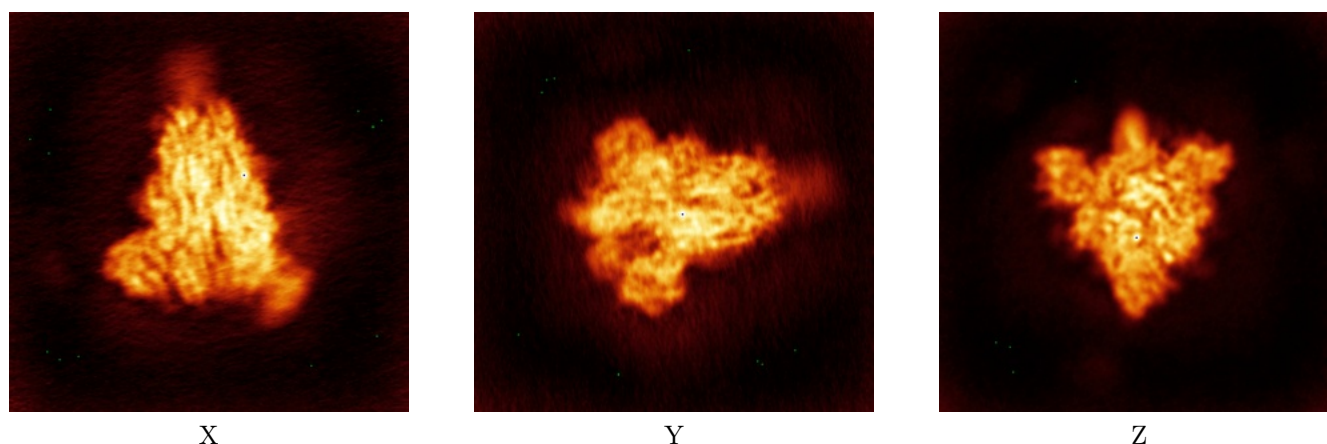
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

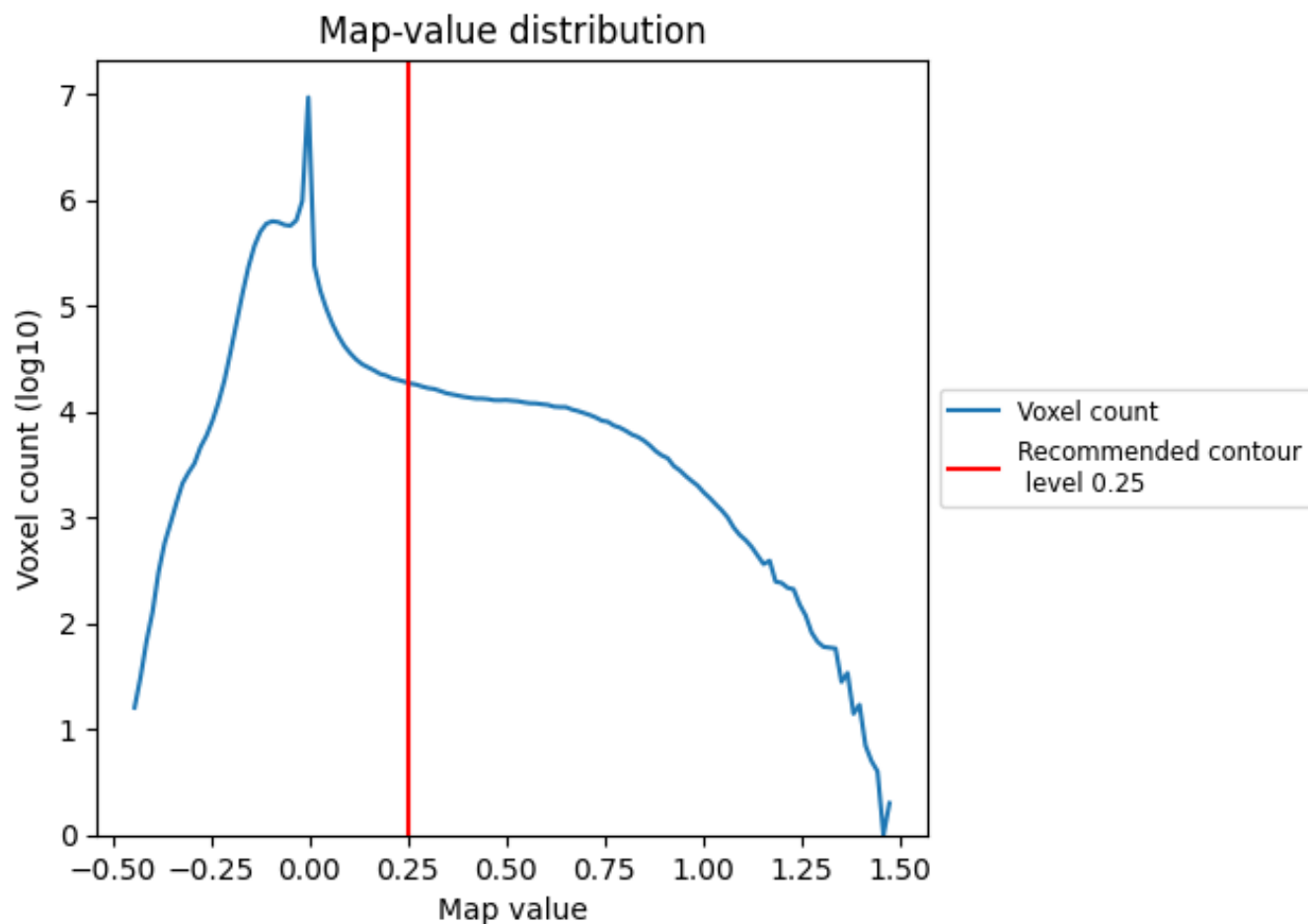
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

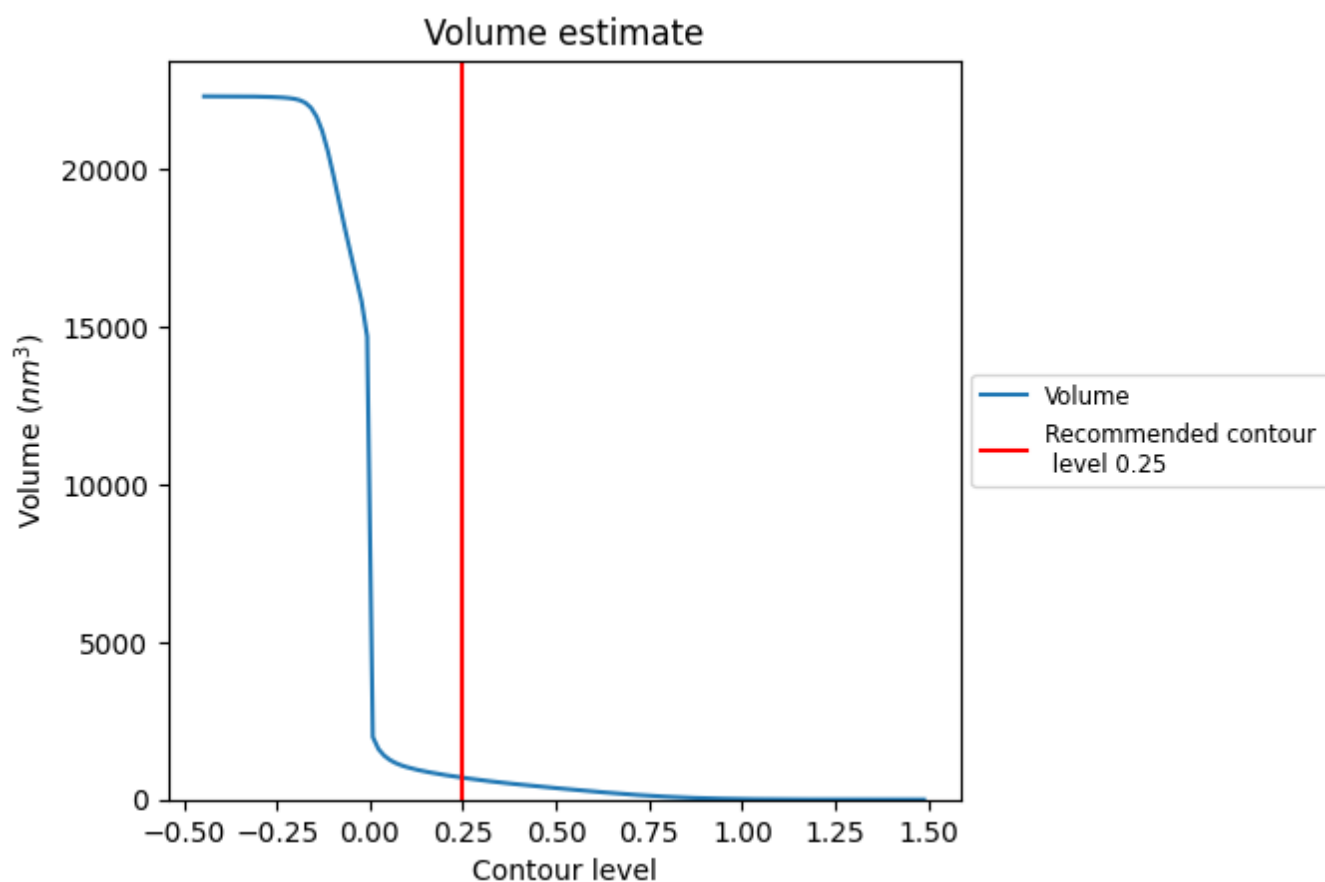
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

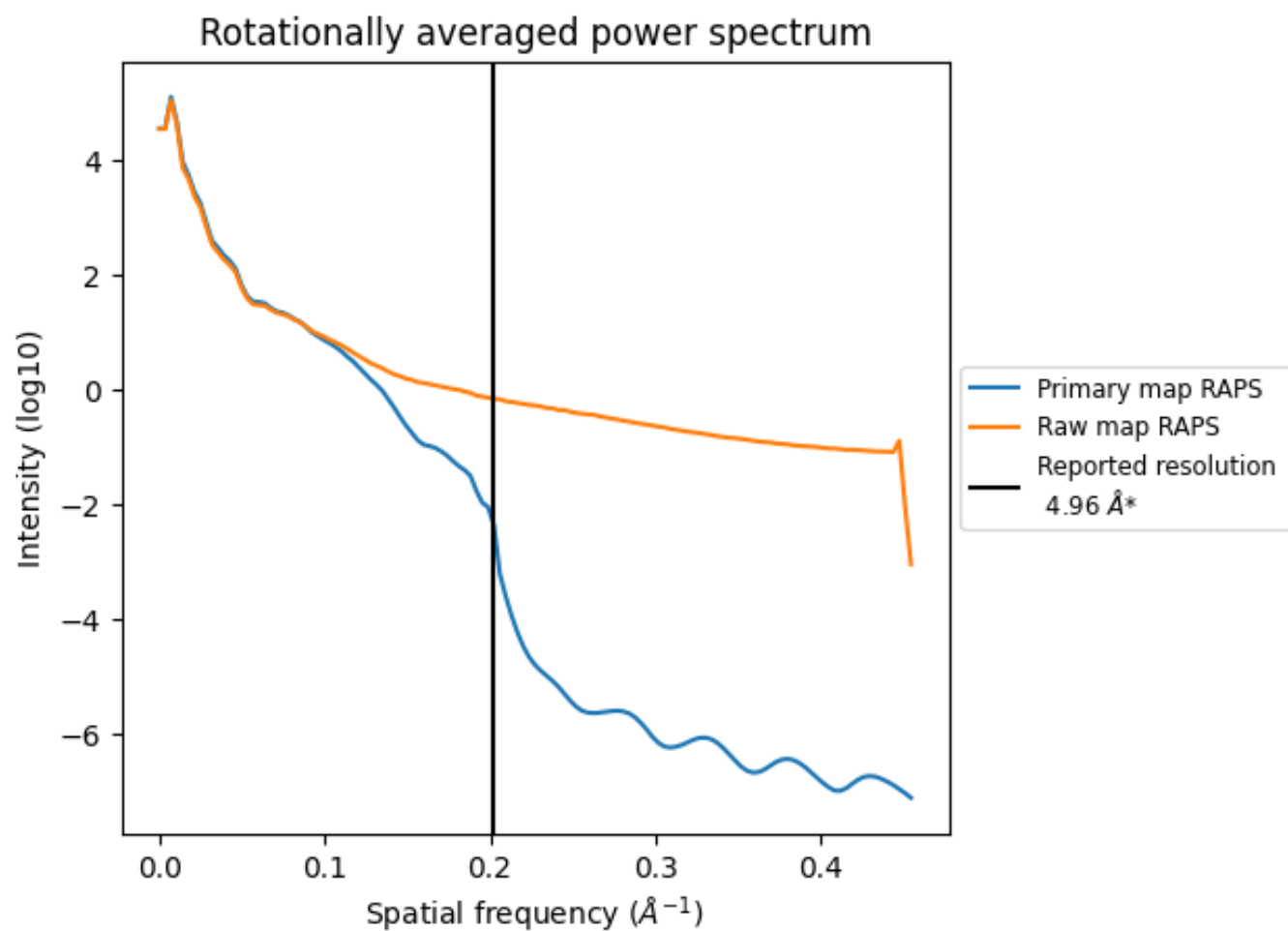
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 693 nm³; this corresponds to an approximate mass of 626 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](#)

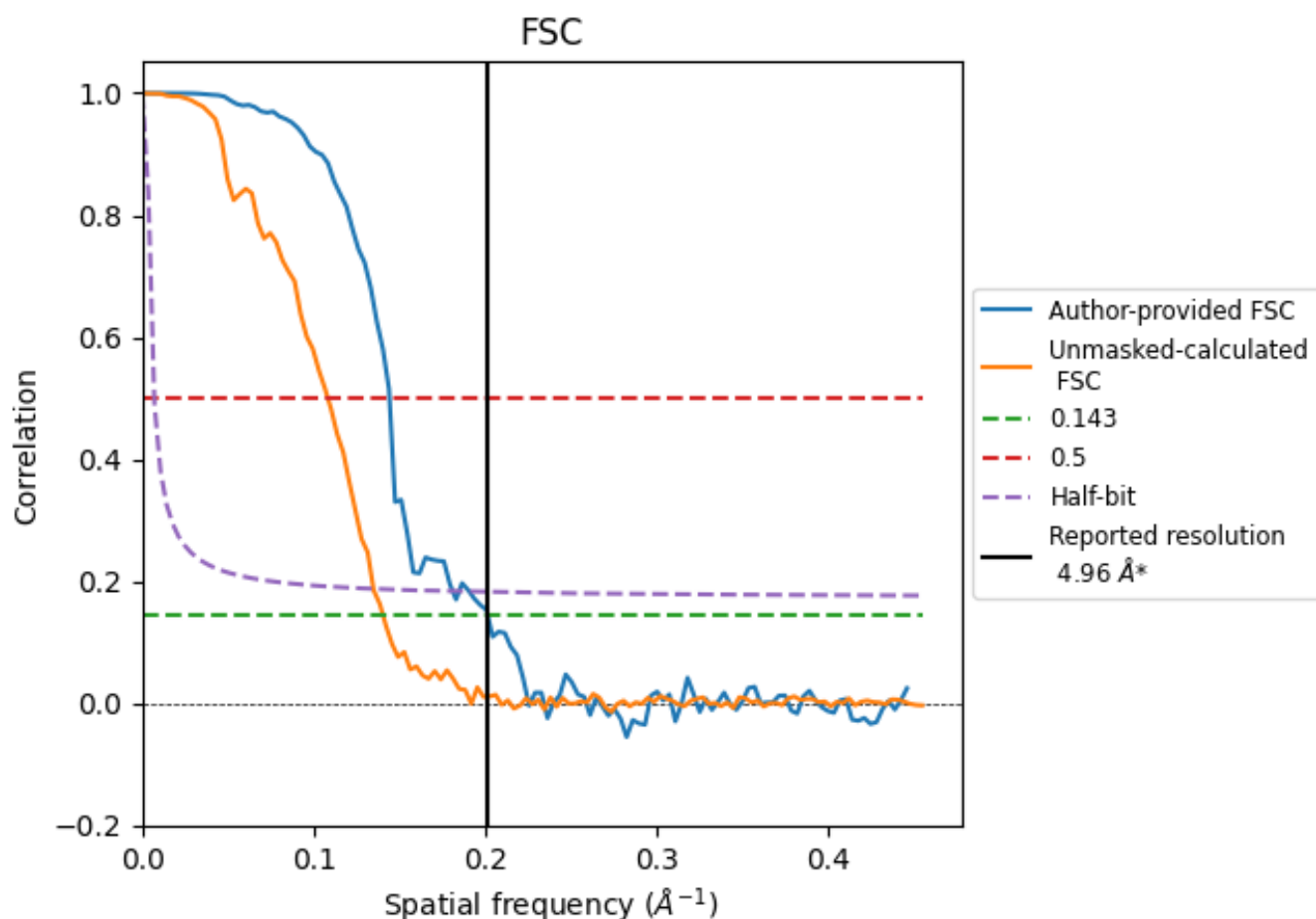


*Reported resolution corresponds to spatial frequency of 0.202 Å⁻¹

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 0.202 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

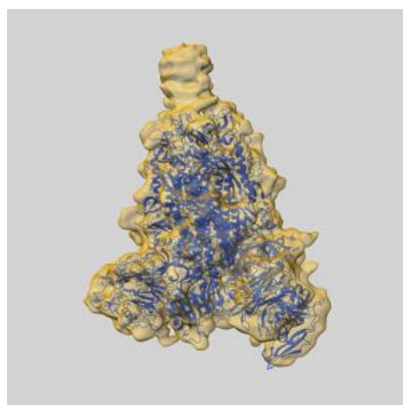
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.96	-	-
Author-provided FSC curve	4.97	6.94	5.52
Unmasked-calculated*	7.12	9.24	7.42

*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 7.12 differs from the reported value 4.96 by more than 10 %

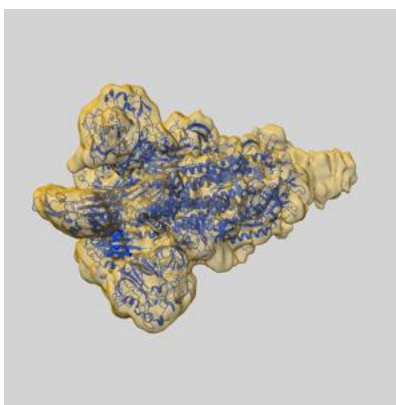
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33947 and PDB model 7YMY. Per-residue inclusion information can be found in section [3](#) on page [15](#).

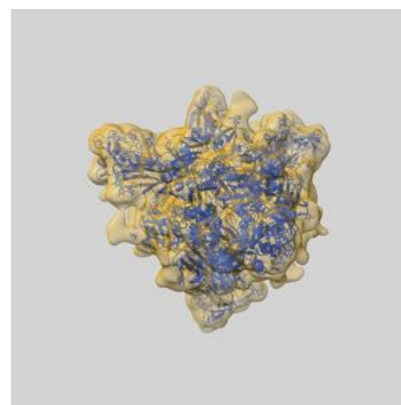
9.1 Map-model overlay [i](#)



X



Y



Z

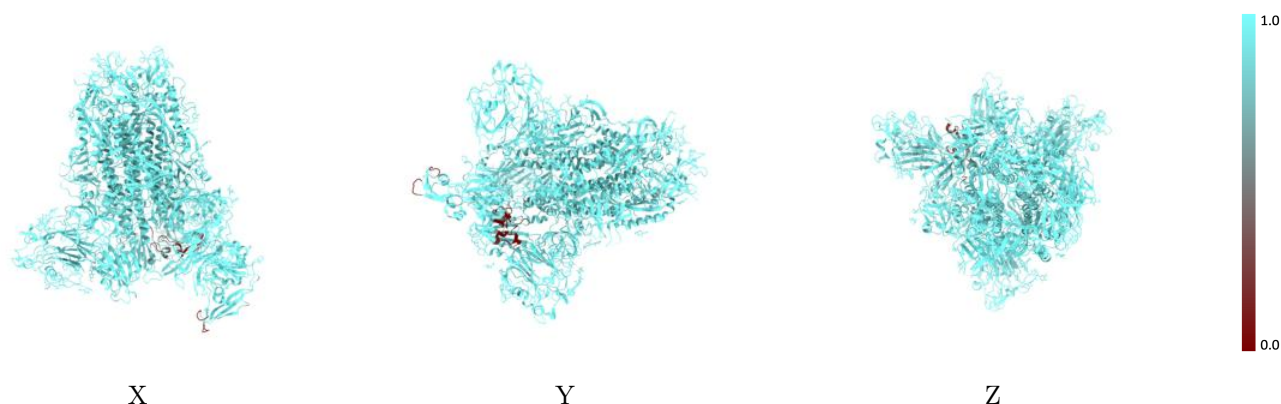
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



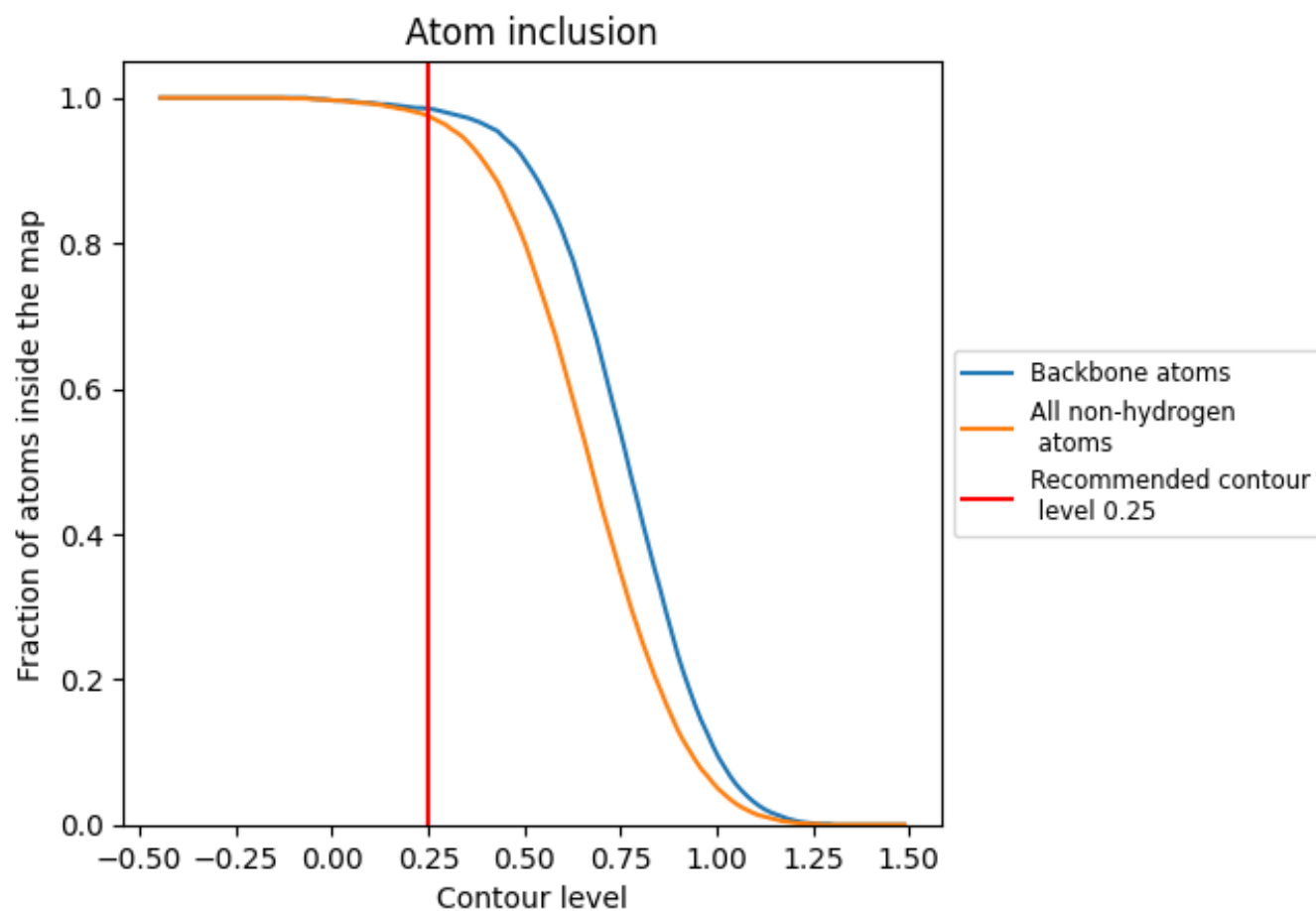
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

9.4 Atom inclusion ⓘ



At the recommended contour level, 98% of all backbone atoms, 98% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9750	0.1990
A	0.9800	0.1900
B	0.9880	0.2050
C	0.9560	0.1970
D	1.0000	0.3880
E	1.0000	0.2970
F	1.0000	0.2910
G	1.0000	0.2420
H	1.0000	0.2630
I	1.0000	0.3320
J	1.0000	0.3930
K	1.0000	0.2460
L	1.0000	0.3190

1.0

0.0

<0.0