wwPDB EM Validation Summary Report ⓘ

Oct 14, 2024 – 08:54 PM JST

PDB ID	:	7YMV
EMDB ID	:	EMD-33943
Title	:	Cryo-EM structure of MERS-CoV spike protein, Two 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	:	6.74 Å(reported)

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

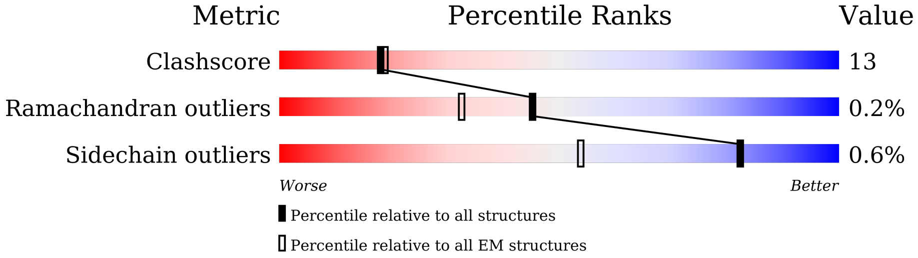
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance ⓘ

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

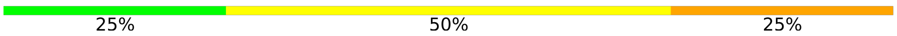
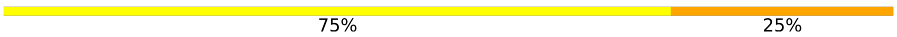
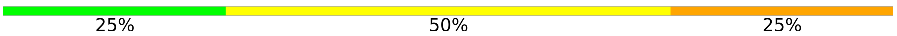
The reported resolution of this entry is 6.74 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	4	
2	F	4	
2	N	4	
2	X	4	
3	E	5	

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Mol	Chain	Length	Quality of chain
4	G	2	🟨 100%
4	H	2	🟩 100%
4	J	2	🟩 50% 🟨 50%
4	L	2	🟩 100%
4	M	2	🟩 100%
4	R	2	🟩 100%
4	S	2	🟩 50% 🟨 50%
4	U	2	🟩 100%
5	I	3	🟩 33% 🟨 67%
5	P	3	🟩 33% 🟨 67%
6	K	3	🟨 100%
6	O	3	🟨 67% 🟧 33%
6	Q	3	🟩 33% 🟨 67%
6	T	3	🟩 100%
6	V	3	🟨 100%
6	W	3	🟩 67% 🟨 33%
7	Y	2	🟨 100%

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 28075 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 9020	C 5732	N 1489	O 1748	S 51	0	0
1	B	1166	Total 9020	C 5732	N 1489	O 1748	S 51	0	0
1	C	1166	Total 9020	C 5732	N 1489	O 1748	S 51	0	0

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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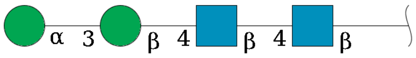
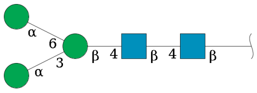
Chain	Residue	Modelled	Actual	Comment	Reference
C	1349	LEU	-	expression tag	UNP K0BRG7
C	1350	ILE	-	expression tag	UNP K0BRG7
C	1351	SER	-	expression tag	UNP K0BRG7
C	1352	GLU	-	expression tag	UNP K0BRG7
C	1353	GLU	-	expression tag	UNP K0BRG7
C	1354	ASP	-	expression tag	UNP K0BRG7
C	1355	LEU	-	expression 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 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.



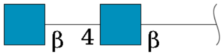
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	D	4	50	28	2	20	0	0
2	F	4	50	28	2	20	0	0
2	N	4	50	28	2	20	0	0
2	X	4	50	28	2	20	0	0

- Molecule 3 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.



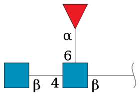
Mol	Chain	Residues	Atoms	AltConf	Trace
3	E	5	Total C N O 61 34 2 25	0	0

- Molecule 4 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
4	G	2	Total C N O 28 16 2 10	0	0
4	H	2	Total C N O 28 16 2 10	0	0
4	J	2	Total C N O 28 16 2 10	0	0
4	L	2	Total C N O 28 16 2 10	0	0
4	M	2	Total C N O 28 16 2 10	0	0
4	R	2	Total C N O 28 16 2 10	0	0
4	S	2	Total C N O 28 16 2 10	0	0
4	U	2	Total C N O 28 16 2 10	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	AltConf	Trace
5	I	3	Total C N O 38 22 2 14	0	0

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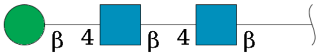
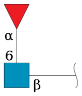
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	P	3	38	22	2	14	0	0

- Molecule 6 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.



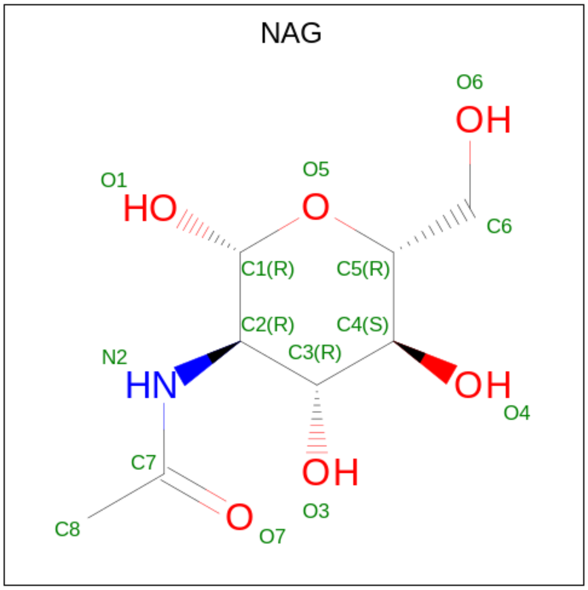
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	K	3	39	22	2	15	0	0
6	O	3	39	22	2	15	0	0
6	Q	3	39	22	2	15	0	0
6	T	3	39	22	2	15	0	0
6	V	3	39	22	2	15	0	0
6	W	3	39	22	2	15	0	0

- Molecule 7 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	Y	2	24	14	1	9	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



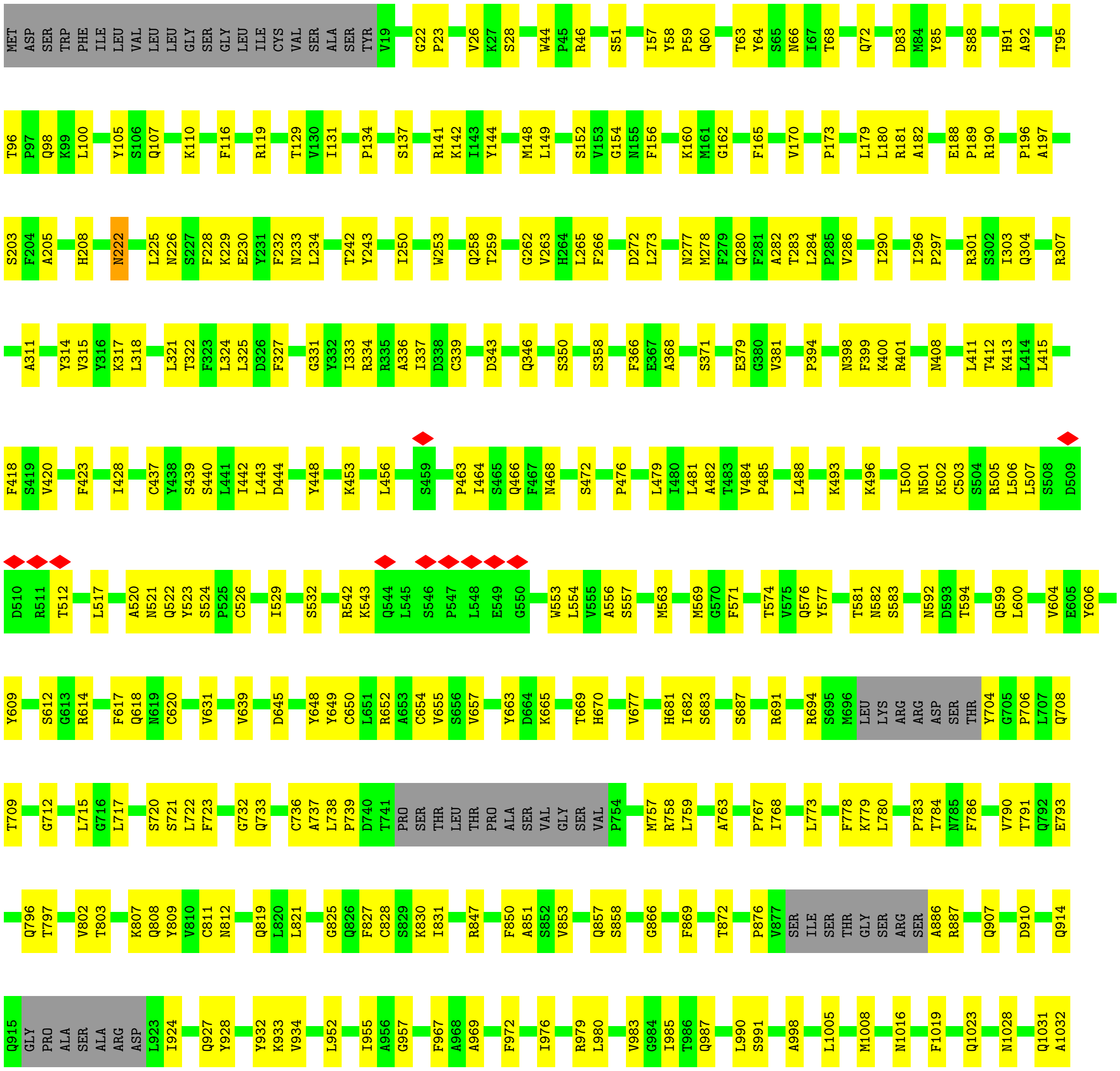
Mol	Chain	Residues	Atoms	AltConf
8	A	1	Total C N O 14 8 1 5	0
8	A	1	Total C N O 14 8 1 5	0
8	A	1	Total C N O 14 8 1 5	0
8	B	1	Total C N O 14 8 1 5	0
8	B	1	Total C N O 14 8 1 5	0
8	B	1	Total C N O 14 8 1 5	0
8	B	1	Total C N O 14 8 1 5	0
8	B	1	Total C N O 14 8 1 5	0
8	B	1	Total C N O 14 8 1 5	0
8	B	1	Total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

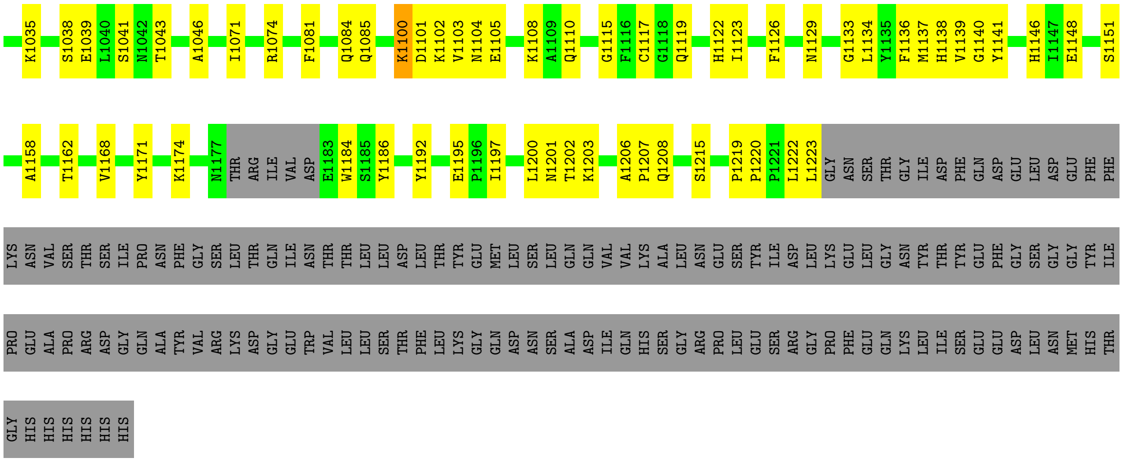
3 Residue-property plots ⓘ

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.

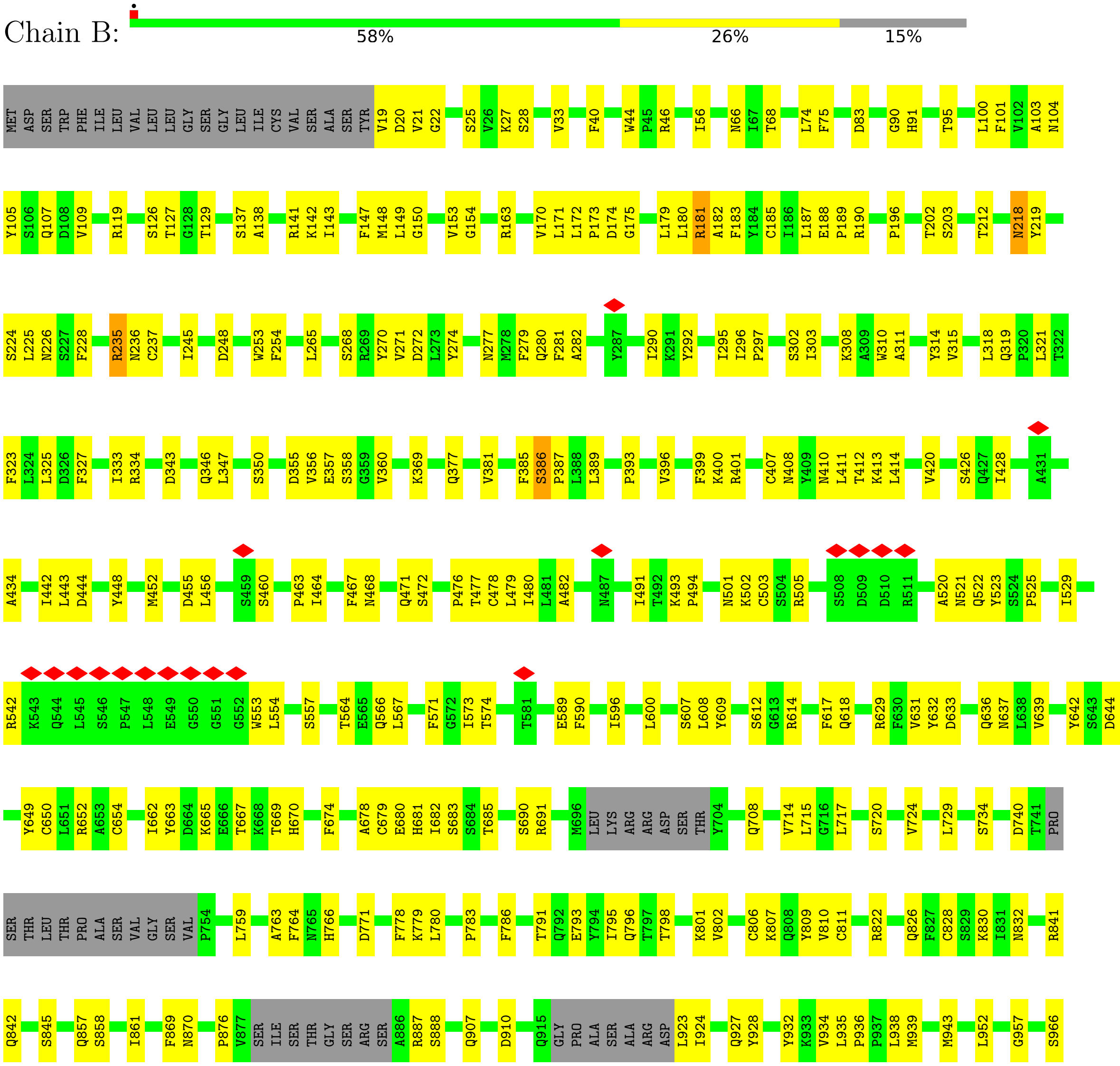
- Molecule 1: Spike glycoprotein

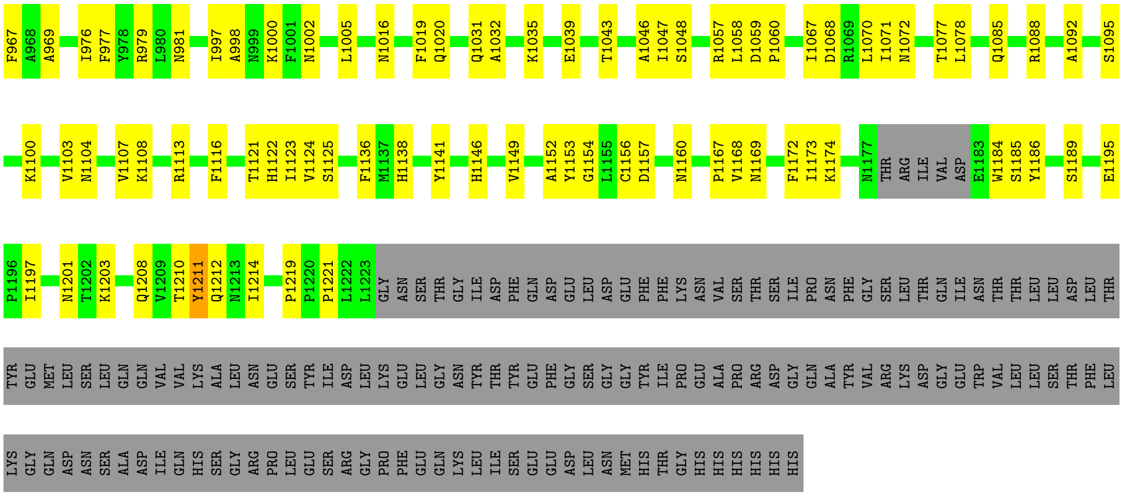
Chain A:





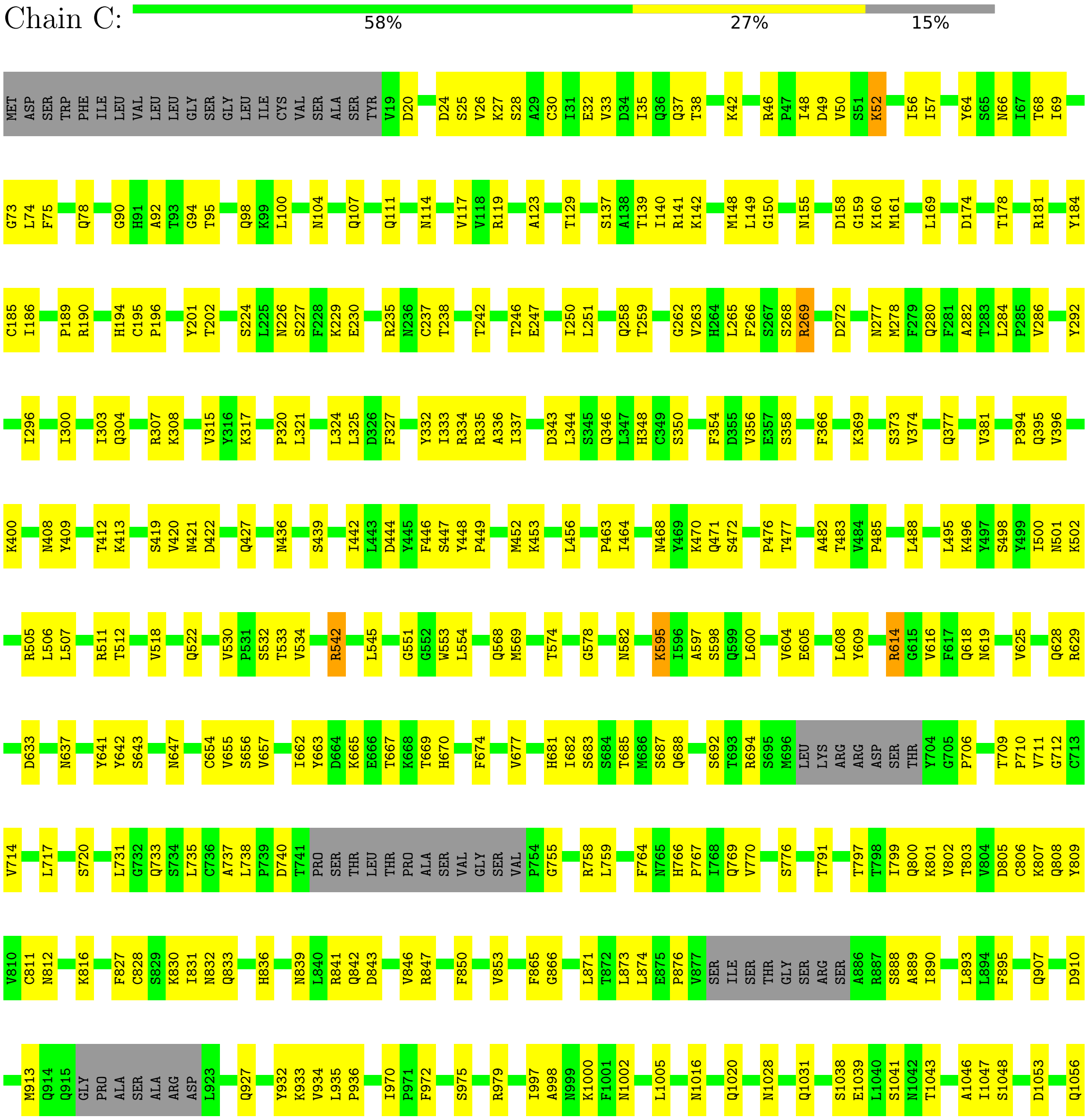
- Molecule 1: Spike glycoprotein

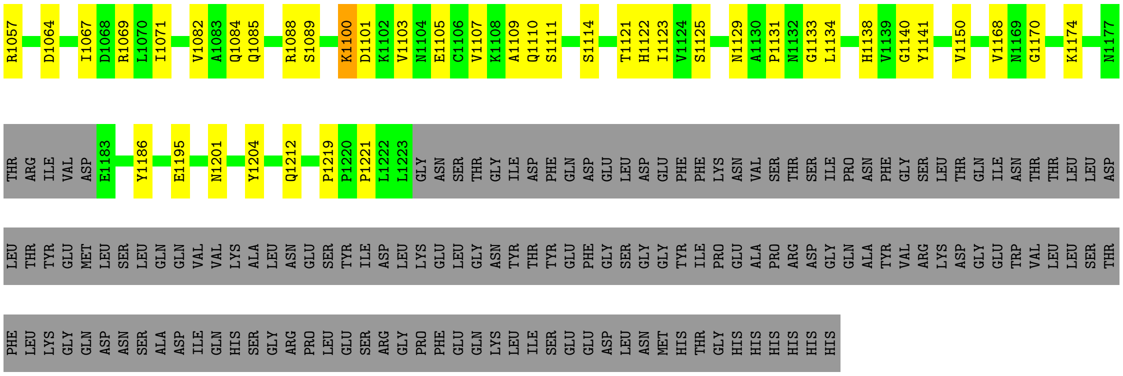




- Molecule 1: Spike glycoprotein

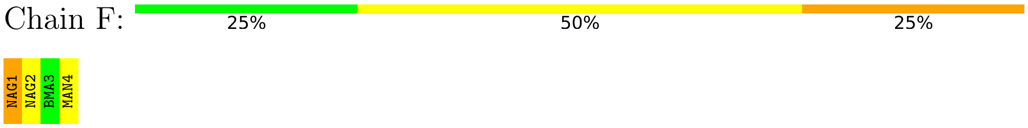
Chain C:



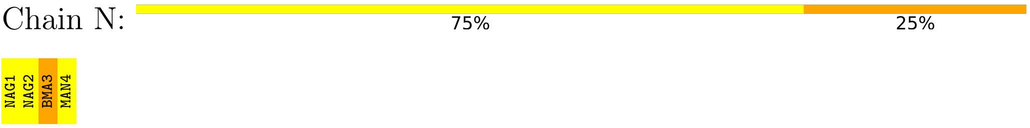


- Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

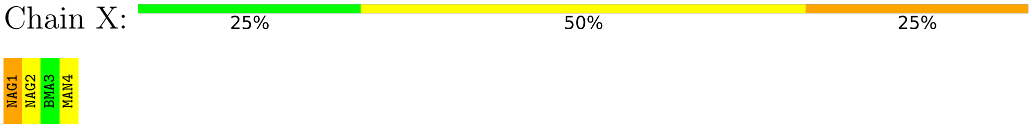
- Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: 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



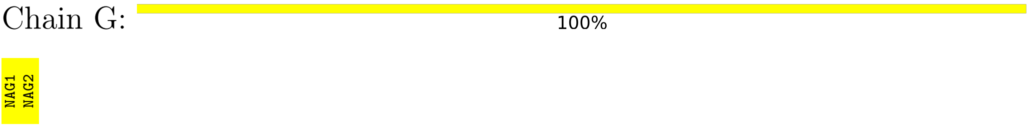
- Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 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

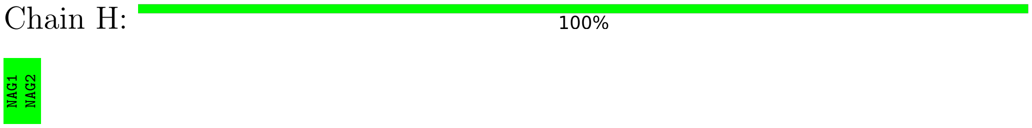
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

Chain H:

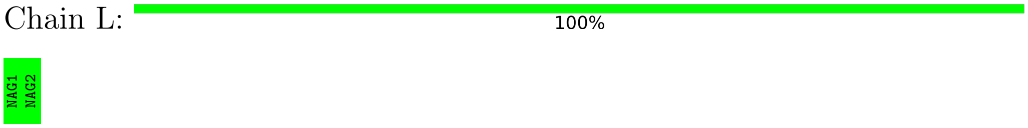


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

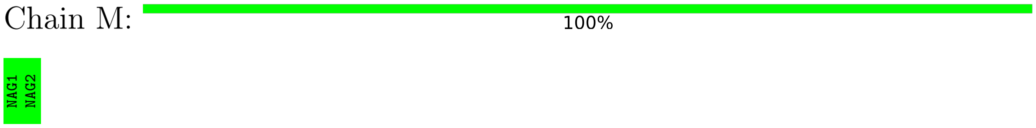
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



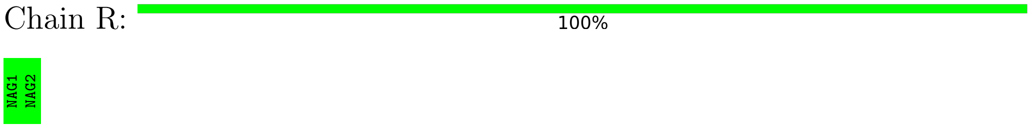
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



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

Chain R:

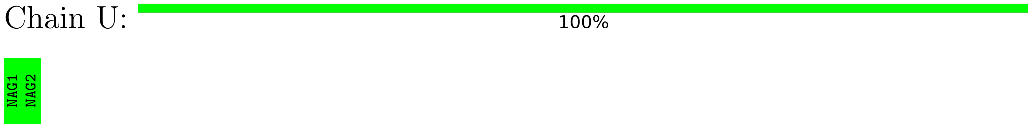


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

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

Chain U:



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

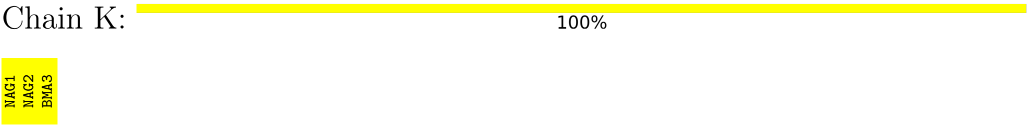
Chain I:

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

Chain P:

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

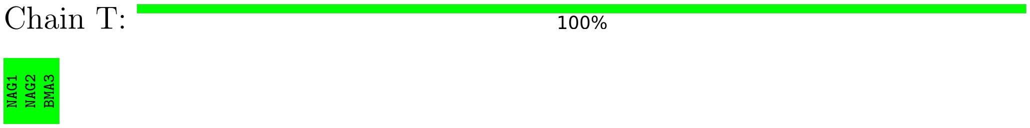
Chain O:

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

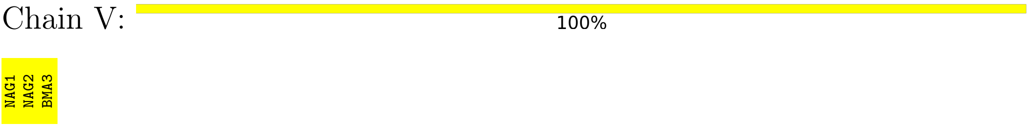
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



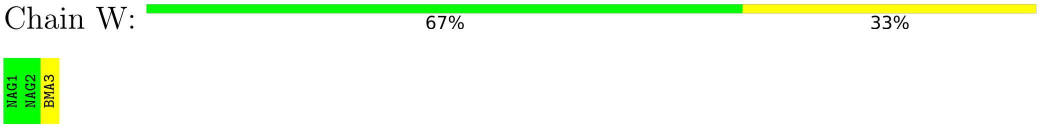
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



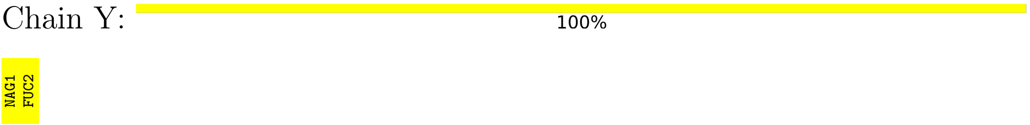
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



- Molecule 7: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:



4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21273	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 ($e^-/\text{Å}^2$)	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	1.370	Depositor
Minimum map value	-0.438	Depositor
Average map value	-0.005	Depositor
Map value standard deviation	0.117	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	281.6, 281.6, 281.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.30	0/9230	0.58	0/12557
1	B	0.29	0/9230	0.57	0/12557
1	C	0.29	0/9230	0.58	0/12557
All	All	0.29	0/27690	0.58	0/37671

There are no bond length outliers.

There are no bond angle outliers.

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	8703	246	0
1	B	9020	0	8701	244	0
1	C	9020	0	8704	240	0
2	D	50	0	43	0	0
2	F	50	0	43	2	0
2	N	50	0	43	1	0
2	X	50	0	43	2	0
3	E	61	0	52	0	0
4	G	28	0	25	1	0
4	H	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	28	0	25	0	0
4	L	28	0	25	0	0
4	M	28	0	25	0	0
4	R	28	0	25	0	0
4	S	28	0	25	0	0
4	U	28	0	25	0	0
5	I	38	0	34	1	0
5	P	38	0	34	0	0
6	K	39	0	34	1	0
6	O	39	0	34	3	0
6	Q	39	0	34	1	0
6	T	39	0	34	0	0
6	V	39	0	34	1	0
6	W	39	0	34	0	0
7	Y	24	0	22	0	0
8	A	42	0	39	0	0
8	B	98	0	91	0	0
8	C	56	0	52	0	0
All	All	28075	0	27008	717	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 13.

The worst 5 of 717 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:358:SER:HA	1:B:663:TYR:O	1.72	0.90
1:B:173:PRO:HA	1:B:179:LEU:O	1.72	0.88
1:A:778:PHE:HB3	1:A:1151:SER:O	1.80	0.81
1:C:150:GLY:O	1:C:292:TYR:HB2	1.80	0.81
1:C:706:PRO:HA	1:C:714:VAL:O	1.85	0.75

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%)	1073 (93%)	78 (7%)	3 (0%)	37	73
1	B	1154/1369 (84%)	1064 (92%)	85 (7%)	5 (0%)	30	68
1	C	1154/1369 (84%)	1064 (92%)	90 (8%)	0	100	100
All	All	3462/4107 (84%)	3201 (92%)	253 (7%)	8 (0%)	45	78

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	592	ASN
1	B	386	SER
1	B	589	GLU
1	B	1211	TYR
1	B	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%)	998 (100%)	5 (0%)	86	89
1	B	1003/1180 (85%)	1000 (100%)	3 (0%)	91	92
1	C	1003/1180 (85%)	994 (99%)	9 (1%)	75	83
All	All	3009/3540 (85%)	2992 (99%)	17 (1%)	82	88

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	847	ARG
1	C	1100	LYS
1	B	887	ARG
1	C	52	LYS
1	C	141	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	800	GLN
1	C	1031	GLN
1	B	796	GLN
1	B	800	GLN
1	B	842	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

63 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	0.57	1 (7%)	17,19,21	0.62	0
2	NAG	D	2	2	14,14,15	0.21	0	17,19,21	0.44	0
2	BMA	D	3	2	11,11,12	0.56	0	15,15,17	0.73	0
2	MAN	D	4	2	11,11,12	0.66	0	15,15,17	1.02	2 (13%)
3	NAG	E	1	3,1	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	E	2	3	14,14,15	0.19	0	17,19,21	0.45	0
3	BMA	E	3	3	11,11,12	0.59	0	15,15,17	0.97	0
3	MAN	E	4	3	11,11,12	0.70	0	15,15,17	1.00	2 (13%)
3	MAN	E	5	3	11,11,12	0.70	0	15,15,17	1.02	2 (13%)
2	NAG	F	1	2,1	14,14,15	0.62	1 (7%)	17,19,21	0.97	2 (11%)
2	NAG	F	2	2	14,14,15	0.42	0	17,19,21	0.51	0

Mol	**Type**	**Chain**	**Res**	**Link**	**Bond lengths**			**Bond angles**		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	BMA	F	3	2	11,11,12	0.74	0	15,15,17	0.87	0
2	MAN	F	4	2	11,11,12	0.96	1 (9%)	15,15,17	1.28	2 (13%)
4	NAG	G	1	4,1	14,14,15	0.28	0	17,19,21	0.59	0
4	NAG	G	2	4	14,14,15	0.26	0	17,19,21	0.59	1 (5%)
4	NAG	H	1	4,1	14,14,15	0.18	0	17,19,21	0.47	0
4	NAG	H	2	4	14,14,15	0.23	0	17,19,21	0.51	0
5	NAG	I	1	5,1	14,14,15	0.36	0	17,19,21	0.63	0
5	NAG	I	2	5	14,14,15	0.28	0	17,19,21	0.49	0
5	FUC	I	3	5	10,10,11	0.64	0	14,14,16	0.87	1 (7%)
4	NAG	J	1	4,1	14,14,15	0.47	0	17,19,21	0.69	1 (5%)
4	NAG	J	2	4	14,14,15	0.27	0	17,19,21	0.45	0
6	NAG	K	1	6,1	14,14,15	0.26	0	17,19,21	0.64	0
6	NAG	K	2	6	14,14,15	0.35	0	17,19,21	0.81	1 (5%)
6	BMA	K	3	6	11,11,12	0.62	0	15,15,17	0.99	1 (6%)
4	NAG	L	1	4,1	14,14,15	0.57	0	17,19,21	0.58	0
4	NAG	L	2	4	14,14,15	0.35	0	17,19,21	0.52	0
4	NAG	M	1	4,1	14,14,15	0.29	0	17,19,21	0.41	0
4	NAG	M	2	4	14,14,15	0.30	0	17,19,21	0.47	0
2	NAG	N	1	2,1	14,14,15	0.70	1 (7%)	17,19,21	0.83	0
2	NAG	N	2	2	14,14,15	0.60	0	17,19,21	1.03	2 (11%)
2	BMA	N	3	2	11,11,12	1.20	1 (9%)	15,15,17	0.90	0
2	MAN	N	4	2	11,11,12	0.71	0	15,15,17	1.02	2 (13%)
6	NAG	O	1	6,1	14,14,15	0.82	1 (7%)	17,19,21	0.70	0
6	NAG	O	2	6	14,14,15	0.22	0	17,19,21	0.50	0
6	BMA	O	3	6	11,11,12	0.82	0	15,15,17	0.73	0
5	NAG	P	1	5,1	14,14,15	0.18	0	17,19,21	0.99	1 (5%)
5	NAG	P	2	5	14,14,15	0.26	0	17,19,21	0.47	0
5	FUC	P	3	5	10,10,11	1.02	0	14,14,16	1.08	2 (14%)
6	NAG	Q	1	6,1	14,14,15	0.25	0	17,19,21	0.43	0
6	NAG	Q	2	6	14,14,15	0.20	0	17,19,21	0.54	0
6	BMA	Q	3	6	11,11,12	0.58	0	15,15,17	0.89	1 (6%)
4	NAG	R	1	4,1	14,14,15	0.18	0	17,19,21	0.50	0
4	NAG	R	2	4	14,14,15	0.27	0	17,19,21	0.44	0
4	NAG	S	1	4,1	14,14,15	0.37	0	17,19,21	0.78	1 (5%)
4	NAG	S	2	4	14,14,15	0.29	0	17,19,21	0.47	0
6	NAG	T	1	6,1	14,14,15	0.20	0	17,19,21	0.48	0
6	NAG	T	2	6	14,14,15	0.26	0	17,19,21	0.46	0
6	BMA	T	3	6	11,11,12	0.65	0	15,15,17	0.78	0
4	NAG	U	1	4,1	14,14,15	0.33	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	NAG	U	2	4	14,14,15	0.26	0	17,19,21	0.51	0
6	NAG	V	1	6,1	14,14,15	0.39	0	17,19,21	0.66	0
6	NAG	V	2	6	14,14,15	0.38	0	17,19,21	1.00	1 (5%)
6	BMA	V	3	6	11,11,12	0.65	0	15,15,17	1.01	1 (6%)
6	NAG	W	1	6,1	14,14,15	0.26	0	17,19,21	0.72	0
6	NAG	W	2	6	14,14,15	0.28	0	17,19,21	0.69	0
6	BMA	W	3	6	11,11,12	0.62	0	15,15,17	1.08	1 (6%)
2	NAG	X	1	2,1	14,14,15	1.29	1 (7%)	17,19,21	2.72	1 (5%)
2	NAG	X	2	2	14,14,15	0.38	0	17,19,21	0.49	0
2	BMA	X	3	2	11,11,12	0.55	0	15,15,17	0.85	0
2	MAN	X	4	2	11,11,12	0.64	0	15,15,17	1.17	2 (13%)
7	NAG	Y	1	7,1	14,14,15	0.19	0	17,19,21	0.73	1 (5%)
7	FUC	Y	2	7	10,10,11	0.89	0	14,14,16	1.33	2 (14%)

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	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	MAN	D	4	2	-	0/2/19/22	0/1/1/1
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	2/2/19/22	0/1/1/1
3	MAN	E	4	3	-	2/2/19/22	0/1/1/1
3	MAN	E	5	3	-	0/2/19/22	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1
2	MAN	F	4	2	-	2/2/19/22	1/1/1/1
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	NAG	H	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
5	NAG	I	1	5,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
5	FUC	I	3	5	-	-	0/1/1/1
4	NAG	J	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	4/6/23/26	0/1/1/1
6	NAG	K	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	K	2	6	-	0/6/23/26	0/1/1/1
6	BMA	K	3	6	-	2/2/19/22	0/1/1/1
4	NAG	L	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1
4	NAG	M	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	N	2	2	-	3/6/23/26	0/1/1/1
2	BMA	N	3	2	-	0/2/19/22	0/1/1/1
2	MAN	N	4	2	-	0/2/19/22	0/1/1/1
6	NAG	O	1	6,1	-	3/6/23/26	0/1/1/1
6	NAG	O	2	6	-	0/6/23/26	0/1/1/1
6	BMA	O	3	6	-	1/2/19/22	0/1/1/1
5	NAG	P	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	P	2	5	-	2/6/23/26	0/1/1/1
5	FUC	P	3	5	-	-	0/1/1/1
6	NAG	Q	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	2/6/23/26	0/1/1/1
6	BMA	Q	3	6	-	2/2/19/22	0/1/1/1
4	NAG	R	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	R	2	4	-	2/6/23/26	0/1/1/1
4	NAG	S	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	S	2	4	-	4/6/23/26	0/1/1/1
6	NAG	T	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	T	2	6	-	1/6/23/26	0/1/1/1
6	BMA	T	3	6	-	0/2/19/22	0/1/1/1
4	NAG	U	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	U	2	4	-	2/6/23/26	0/1/1/1
6	NAG	V	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	V	2	6	-	2/6/23/26	0/1/1/1
6	BMA	V	3	6	-	2/2/19/22	0/1/1/1
6	NAG	W	1	6,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	W	2	6	-	0/6/23/26	0/1/1/1
6	BMA	W	3	6	-	2/2/19/22	0/1/1/1
2	NAG	X	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	X	2	2	-	0/6/23/26	0/1/1/1
2	BMA	X	3	2	-	1/2/19/22	0/1/1/1
2	MAN	X	4	2	-	0/2/19/22	0/1/1/1
7	NAG	Y	1	7,1	-	2/6/23/26	0/1/1/1
7	FUC	Y	2	7	-	-	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	1	NAG	O5-C1	4.72	1.51	1.43
6	O	1	NAG	C1-C2	2.72	1.56	1.52
2	N	3	BMA	C2-C3	2.38	1.56	1.52
2	N	1	NAG	O5-C1	2.32	1.47	1.43
2	F	4	MAN	C1-C2	2.15	1.57	1.52

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	1	NAG	C1-O5-C5	10.89	126.95	112.19
2	F	4	MAN	C1-O5-C5	3.92	117.51	112.19
6	V	2	NAG	C1-O5-C5	3.49	116.92	112.19
5	P	1	NAG	C1-O5-C5	3.47	116.89	112.19
2	X	4	MAN	C1-O5-C5	3.43	116.84	112.19

There are no chirality outliers.

5 of 92 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C4-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6

All (1) ring outliers are listed below:

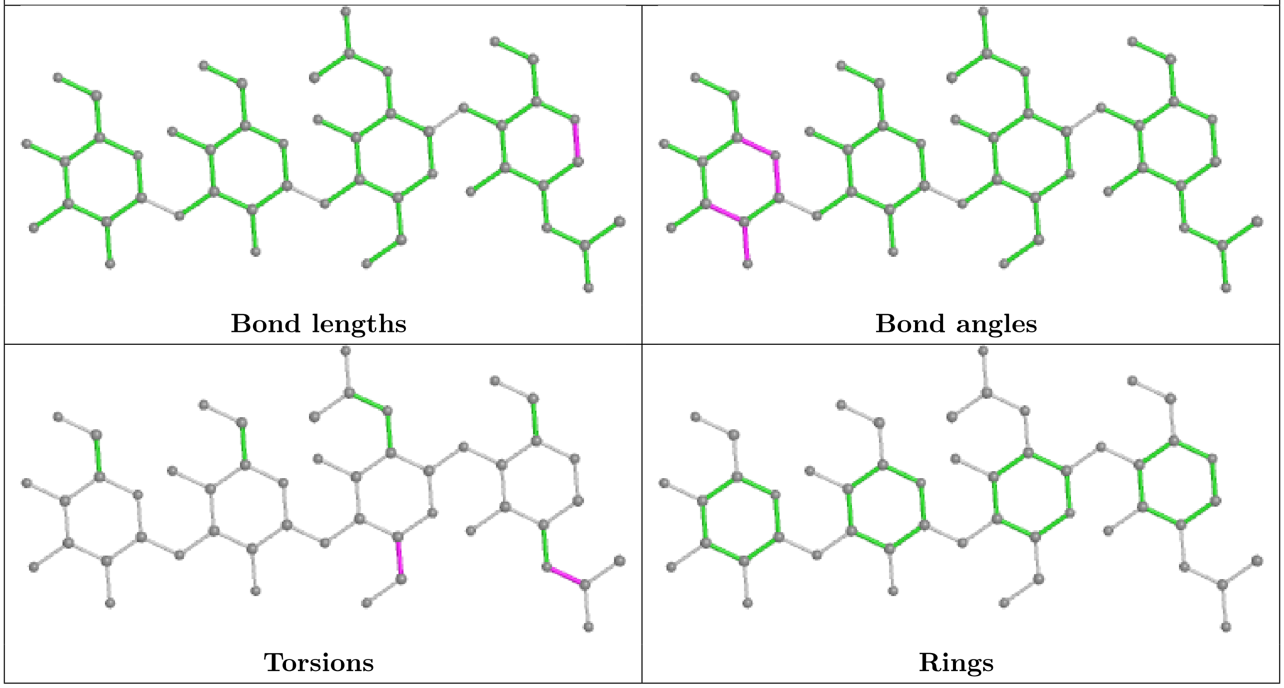
Mol	Chain	Res	Type	Atoms
2	F	4	MAN	C1-C2-C3-C4-C5-O5

13 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2	NAG	2	0
2	X	1	NAG	1	0
6	Q	1	NAG	1	0
6	O	1	NAG	1	0
2	N	3	BMA	1	0
2	F	1	NAG	1	0
5	I	1	NAG	1	0
6	O	3	BMA	1	0
2	X	2	NAG	1	0
4	G	1	NAG	1	0
6	K	1	NAG	1	0
6	V	1	NAG	1	0
6	O	2	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.

Oligosaccharide Chain D



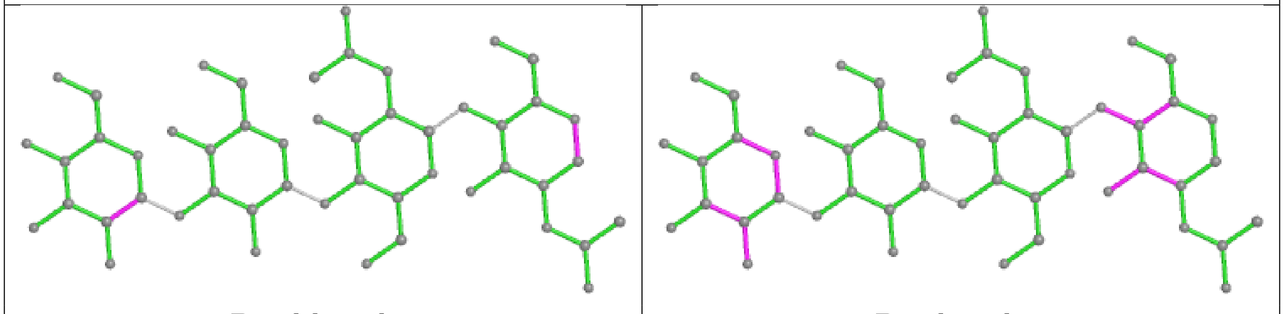
Bond lengths

Bond angles

Torsions

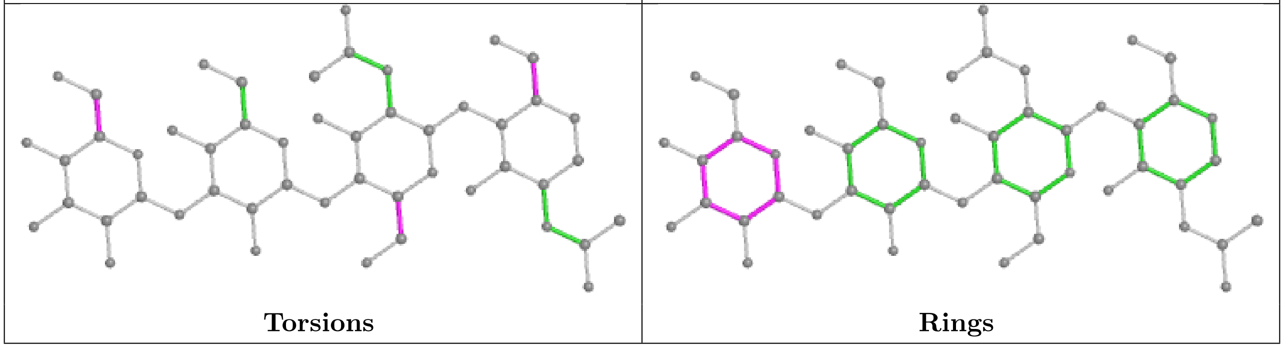
Rings

Oligosaccharide Chain F



Bond lengths

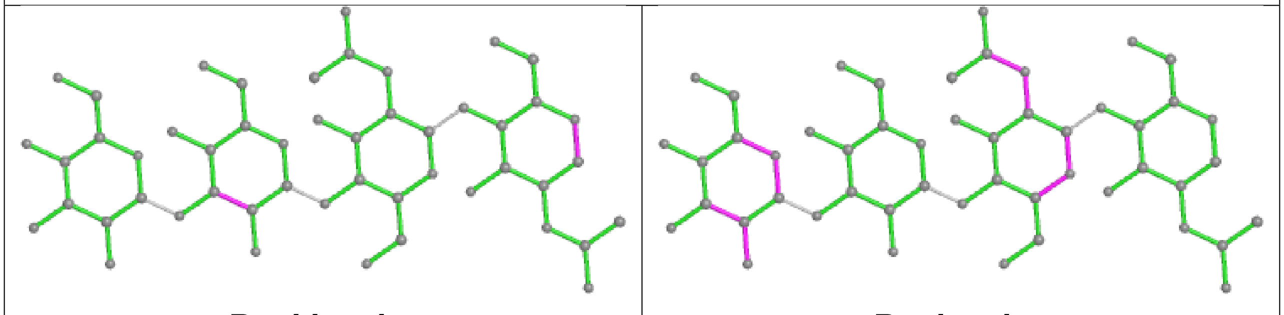
Bond angles



Torsions

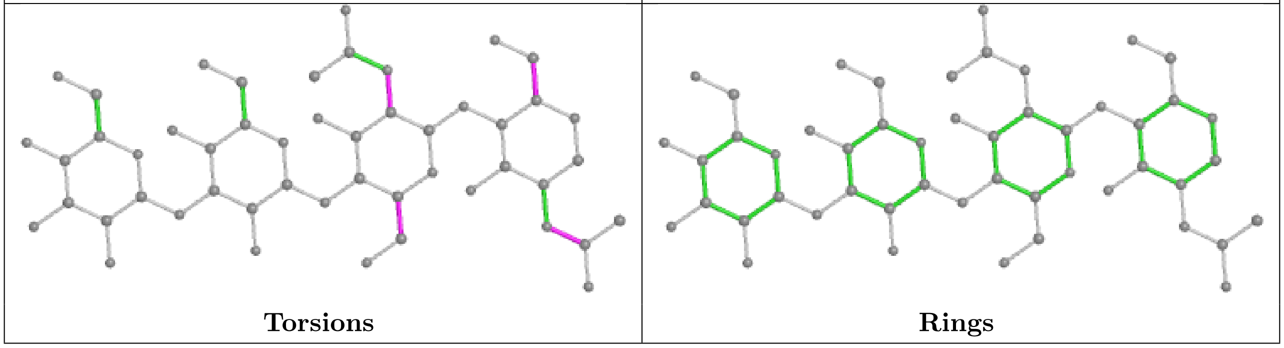
Rings

Oligosaccharide Chain N



Bond lengths

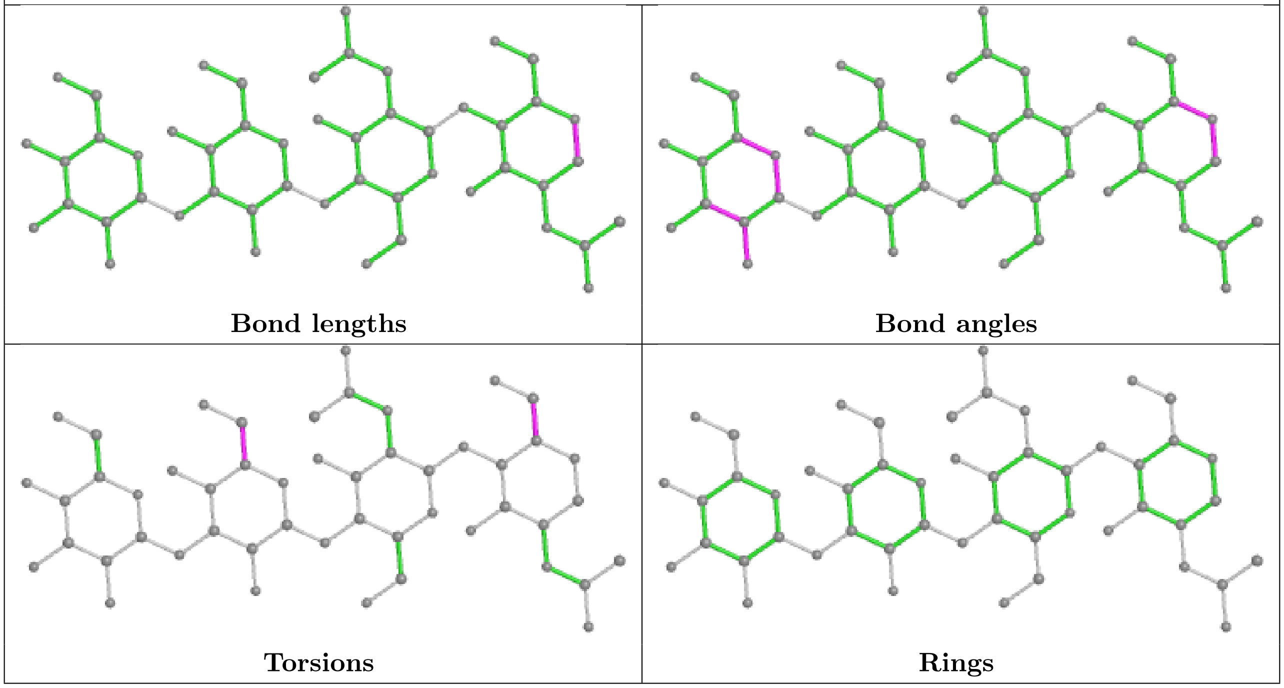
Bond angles



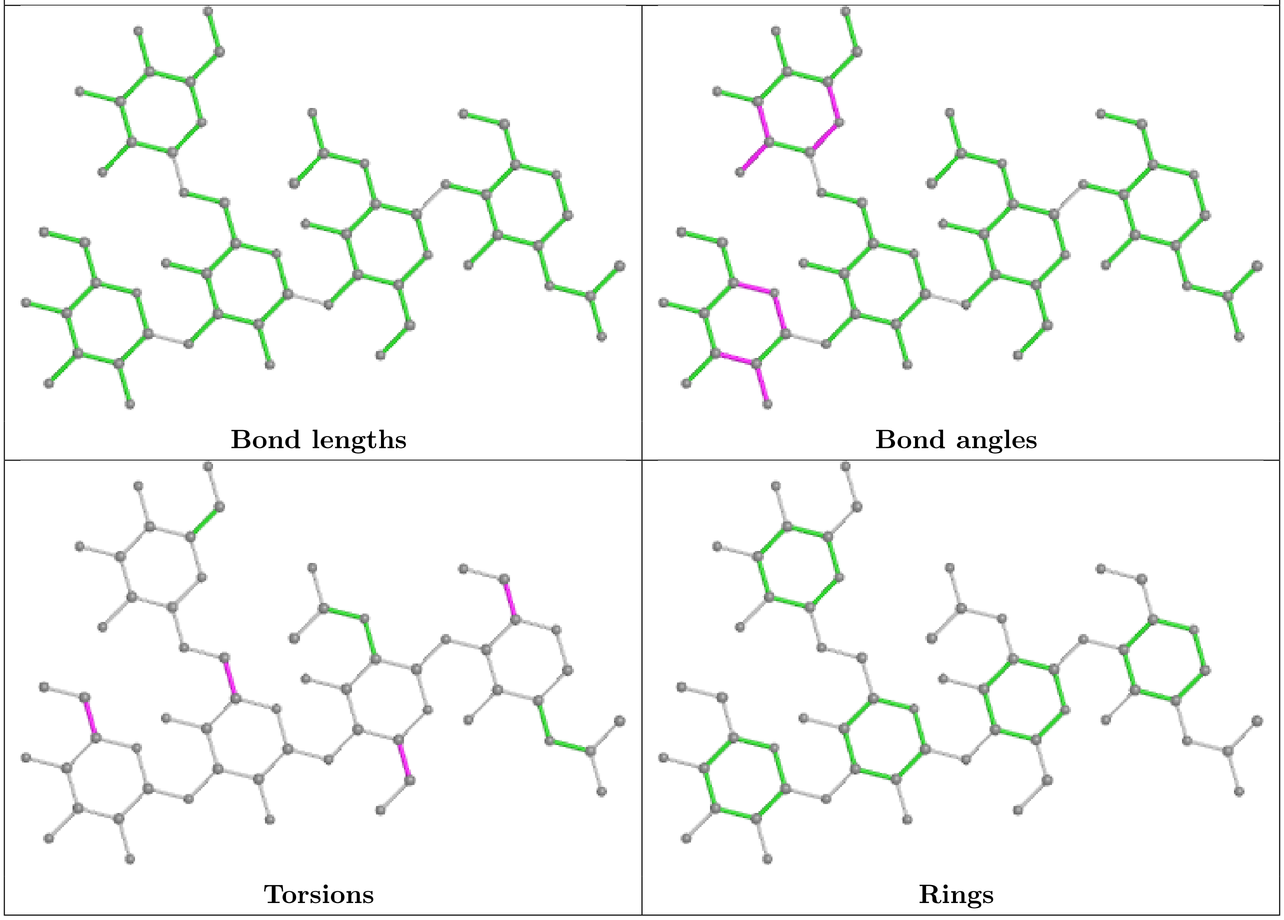
Torsions

Rings

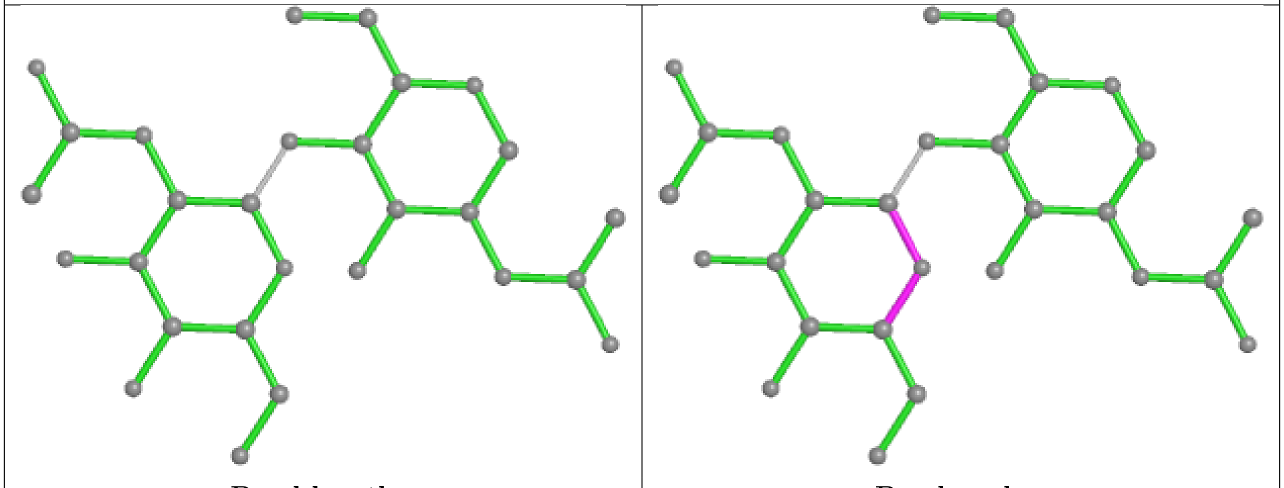
Oligosaccharide Chain X


Bond lengths
Bond angles
Torsions
Rings

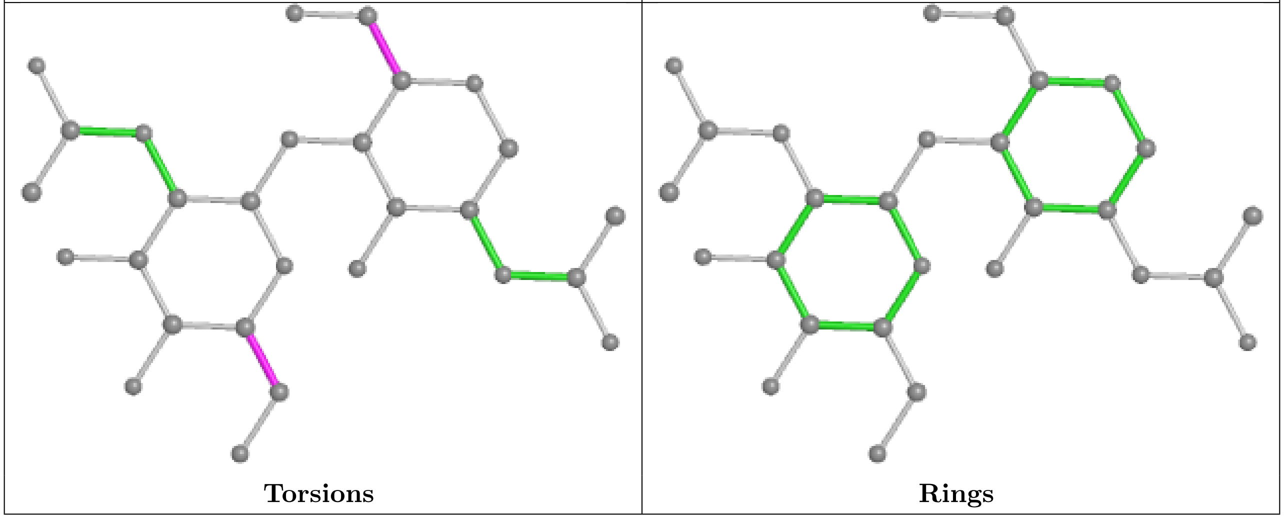
Oligosaccharide Chain E


Bond lengths
Bond angles
Torsions
Rings

Oligosaccharide Chain G

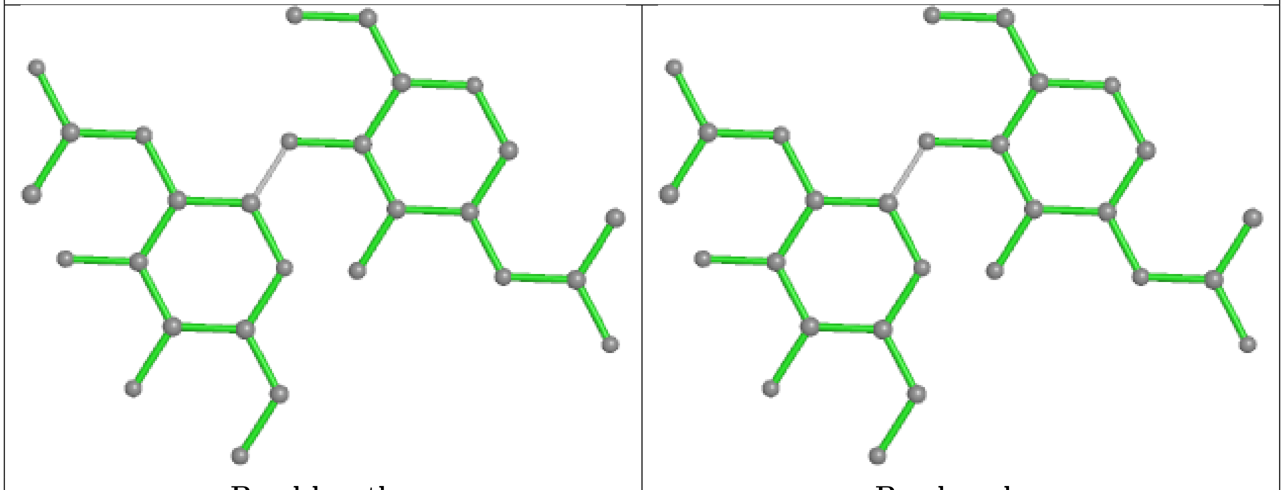


Bond lengths Bond angles



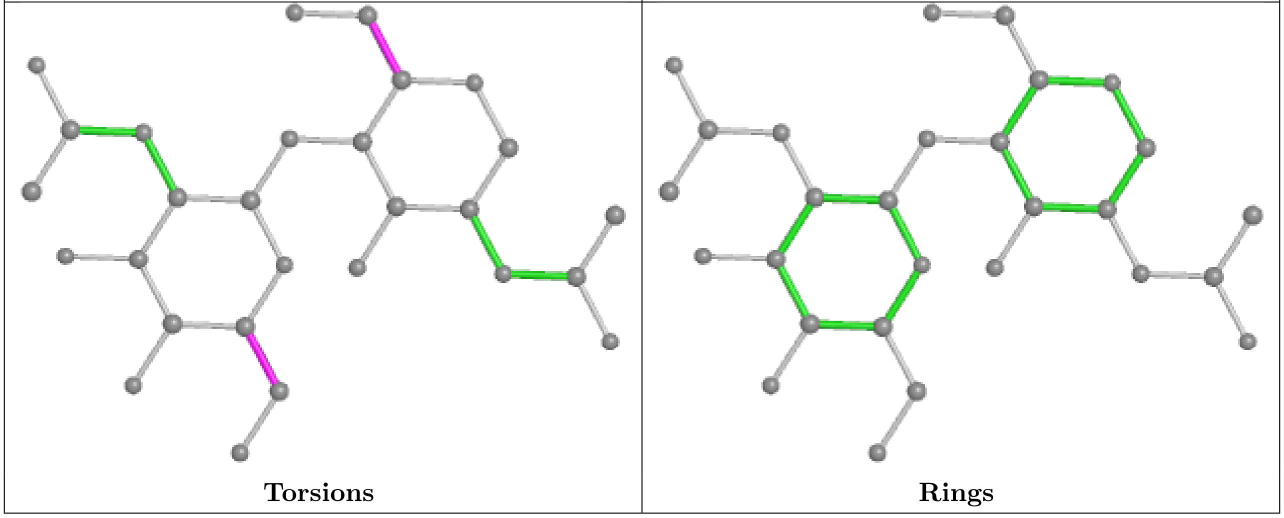
Torsions Rings

Oligosaccharide Chain H



Bond lengths

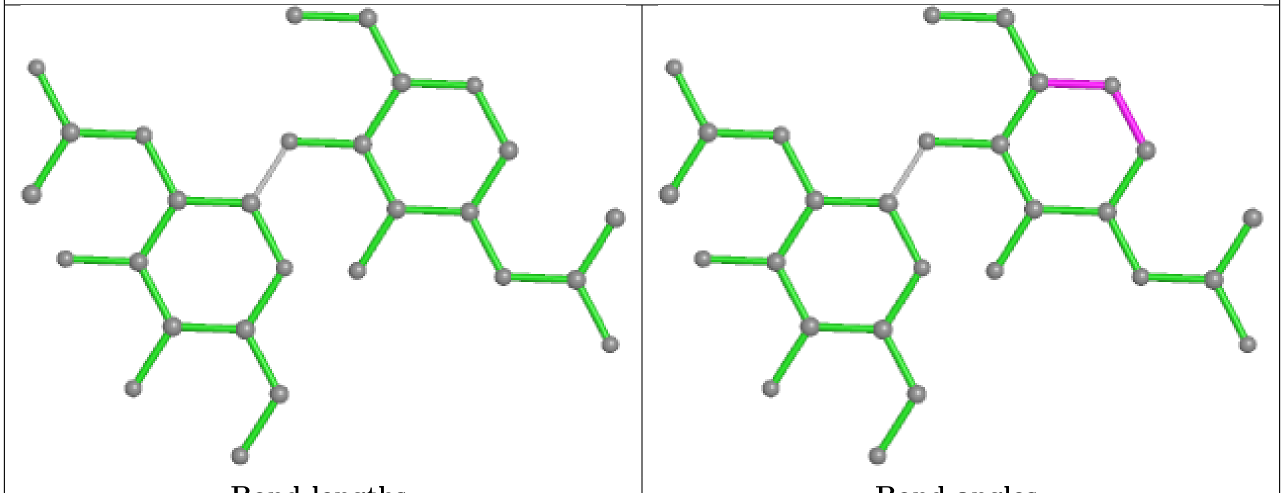
Bond angles



Torsions

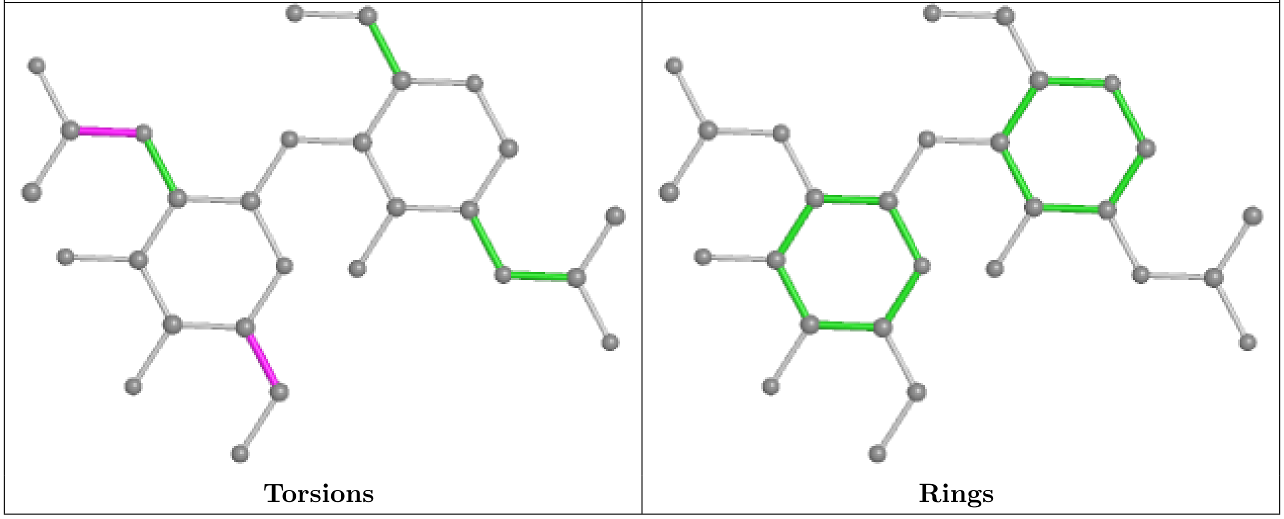
Rings

Oligosaccharide Chain J



Bond lengths

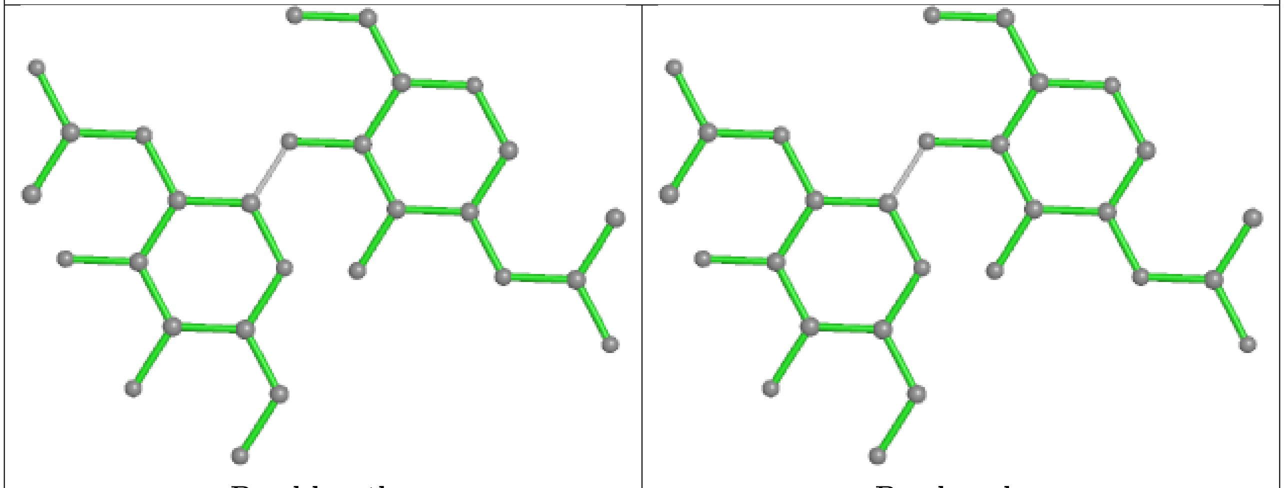
Bond angles



Torsions

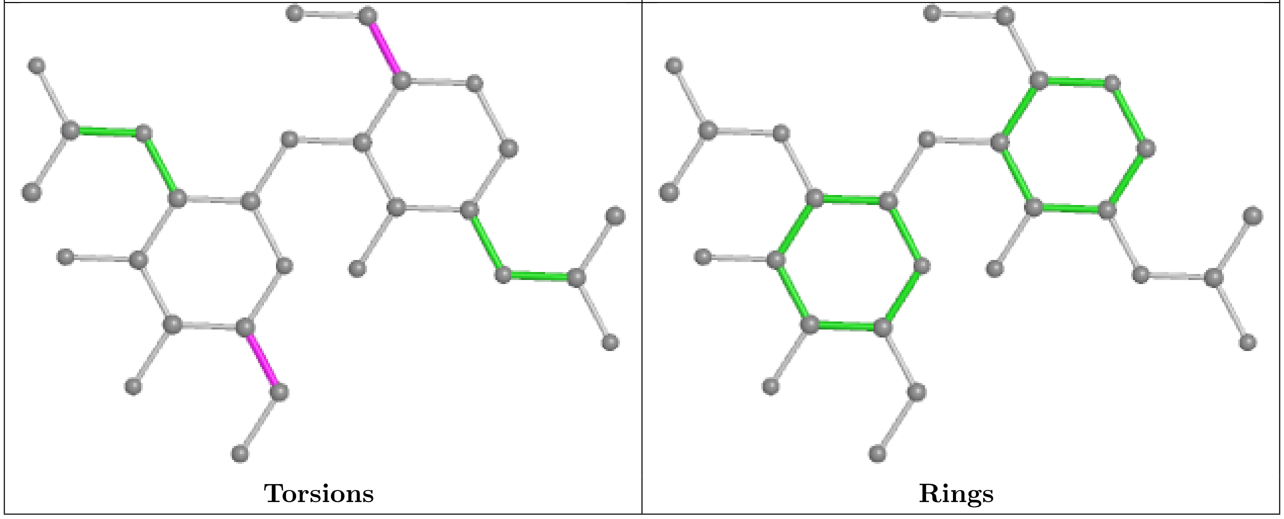
Rings

Oligosaccharide Chain L



Bond lengths

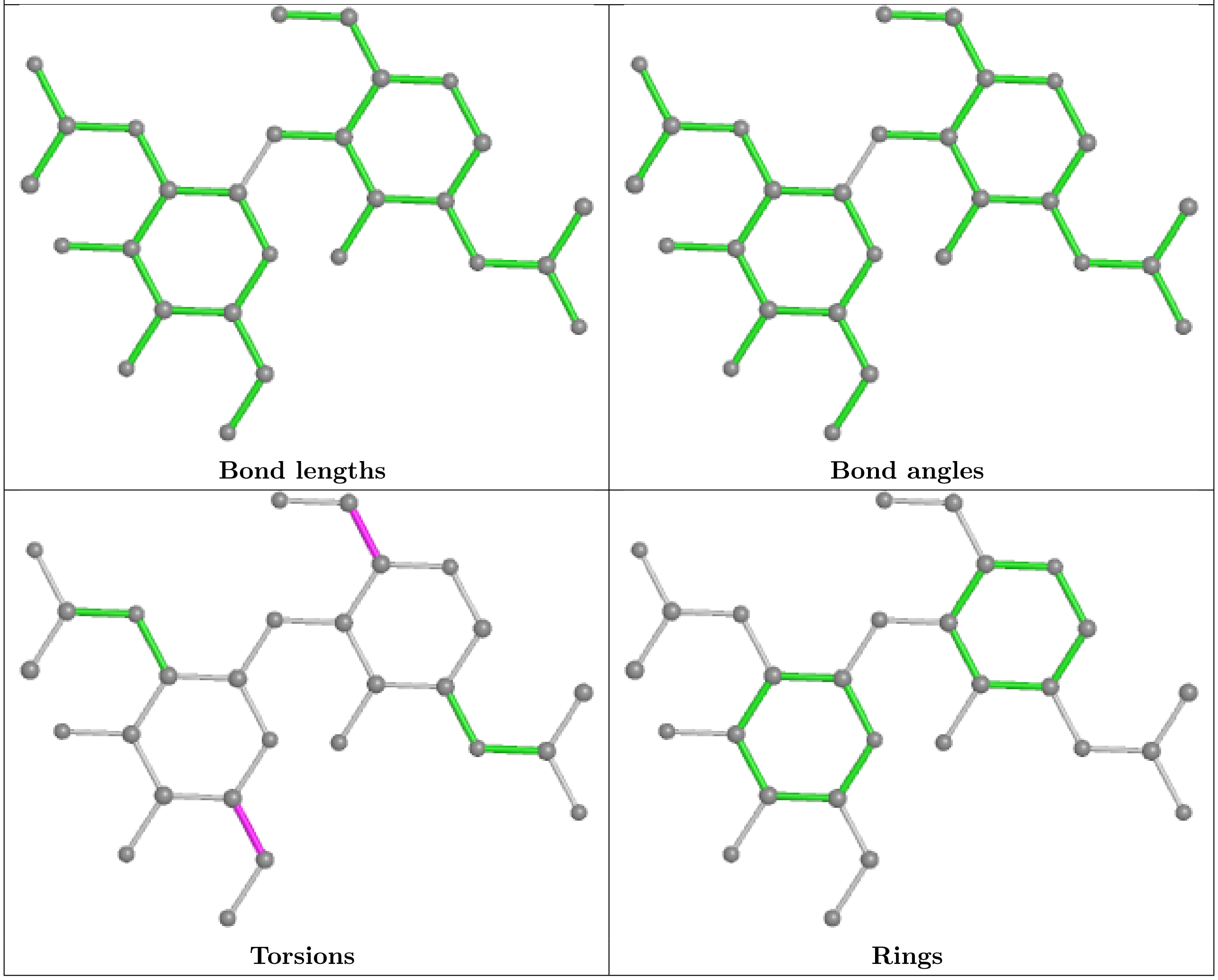
Bond angles



Torsions

Rings

Oligosaccharide Chain M



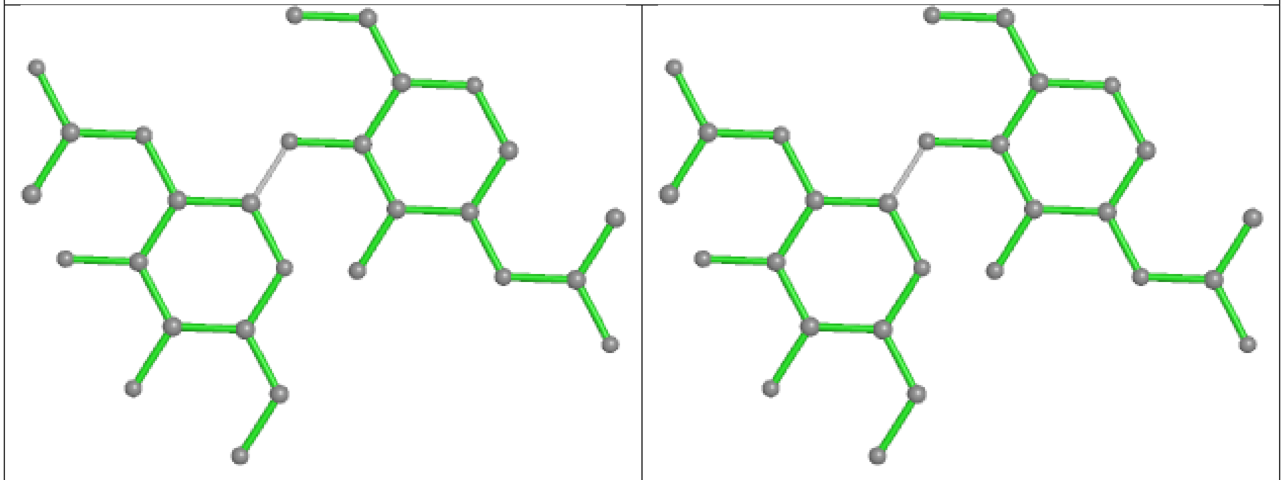
Bond lengths

Bond angles

Torsions

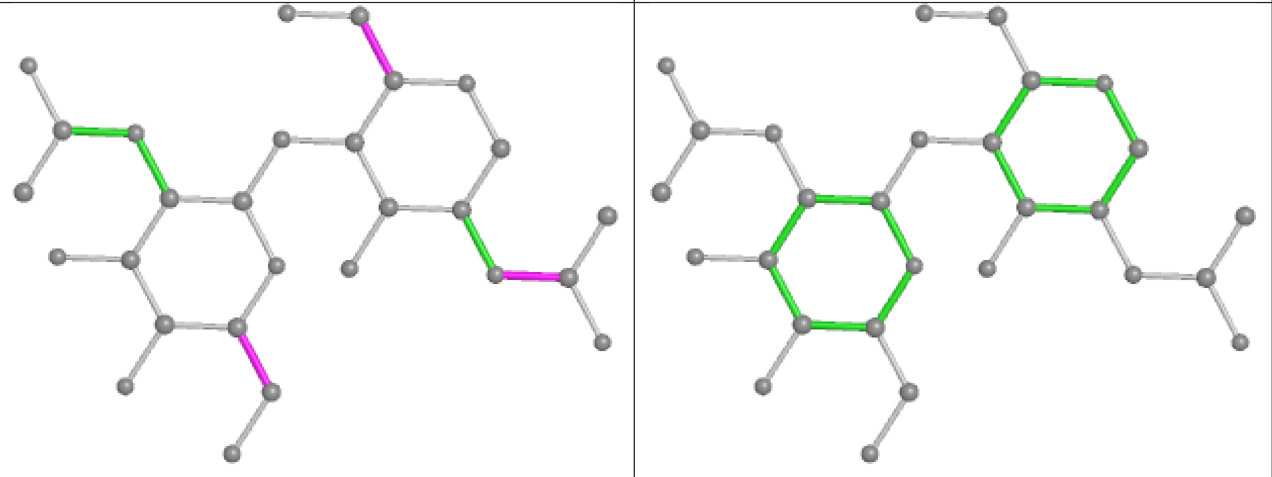
Rings

Oligosaccharide Chain R



Bond lengths

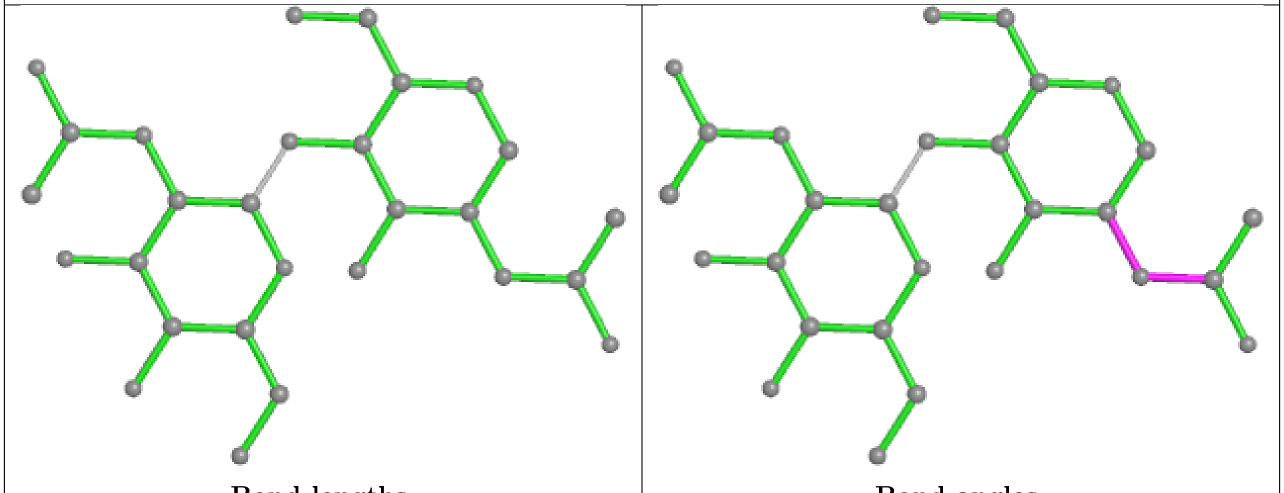
Bond angles



Torsions

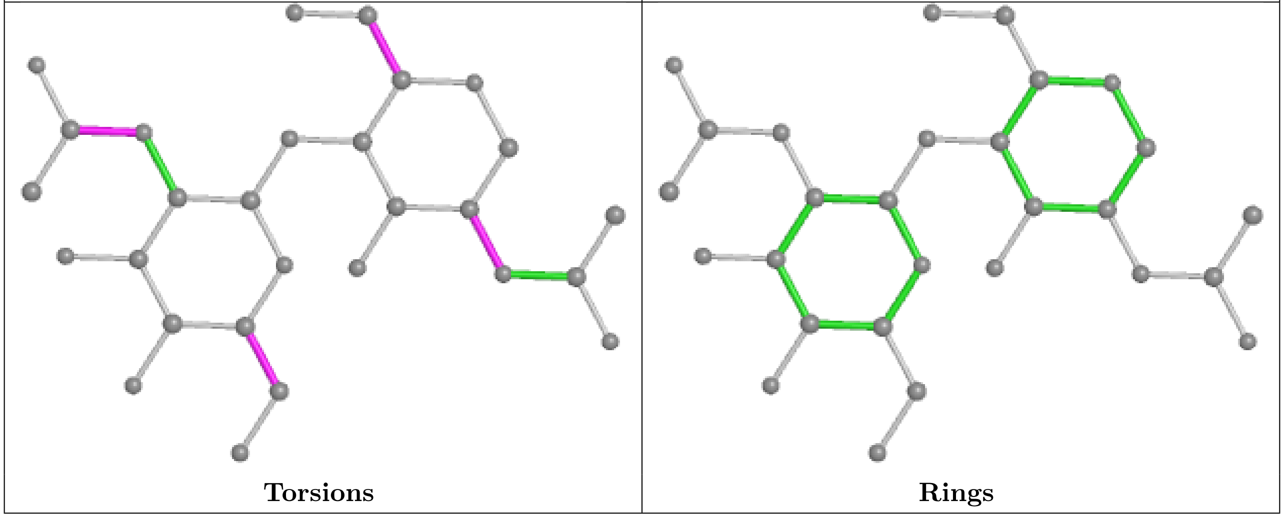
Rings

Oligosaccharide Chain S



Bond lengths

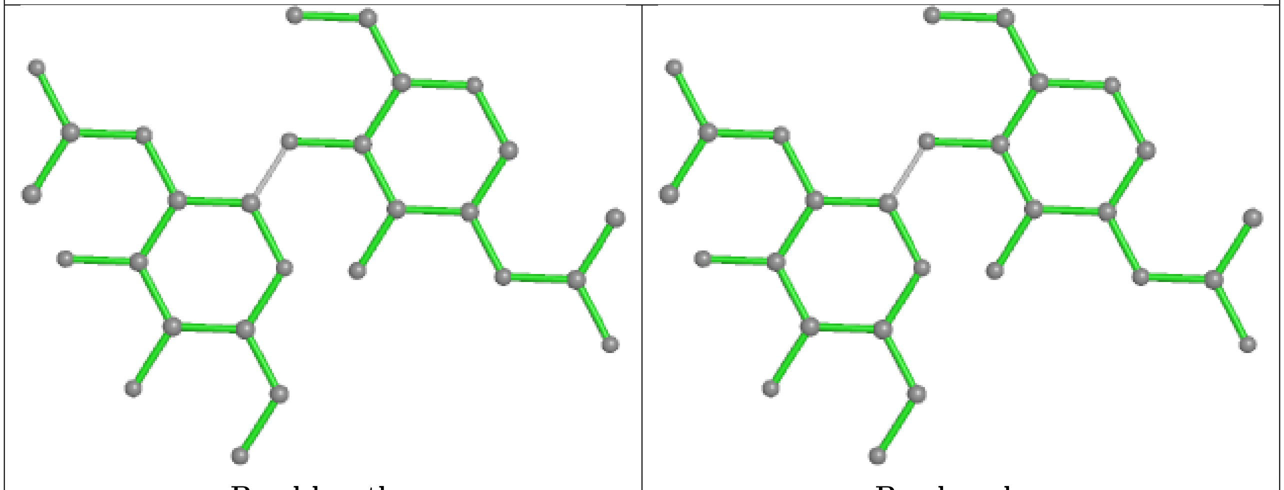
Bond angles



Torsions

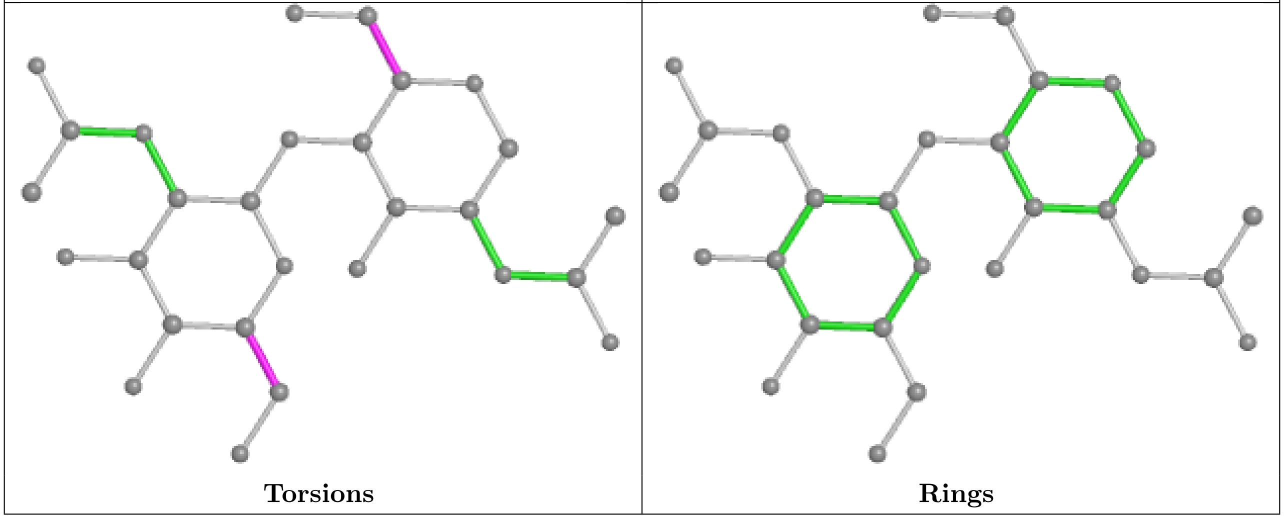
Rings

Oligosaccharide Chain U



Bond lengths

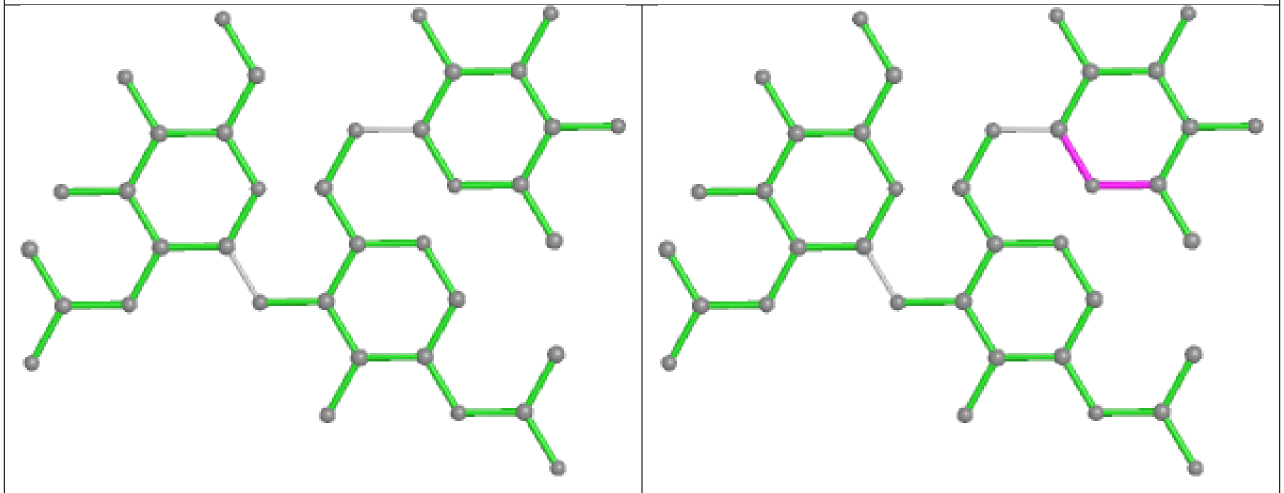
Bond angles



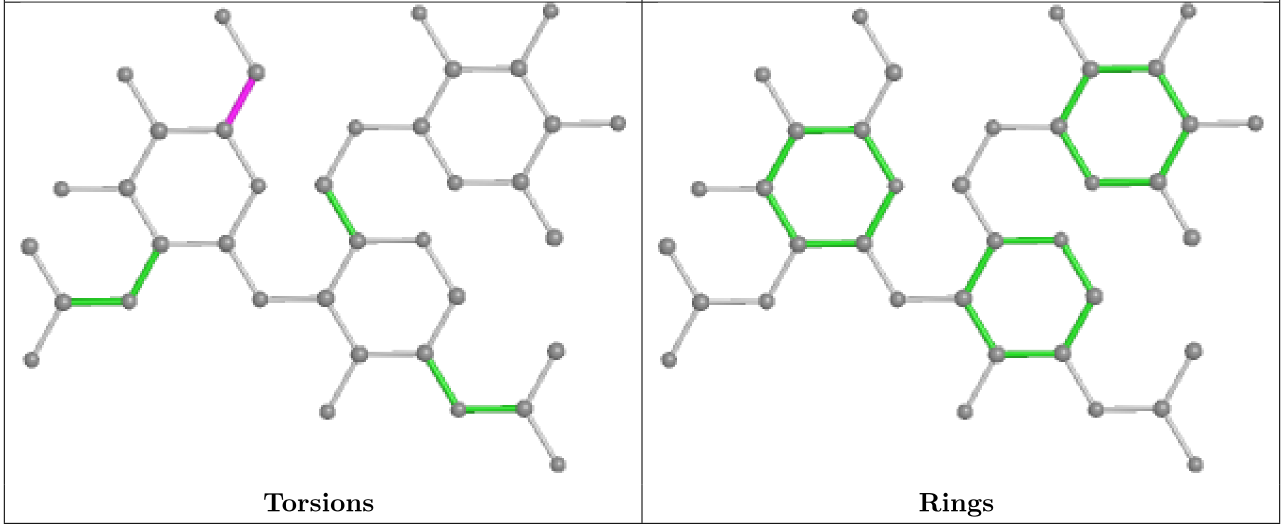
Torsions

Rings

Oligosaccharide Chain I

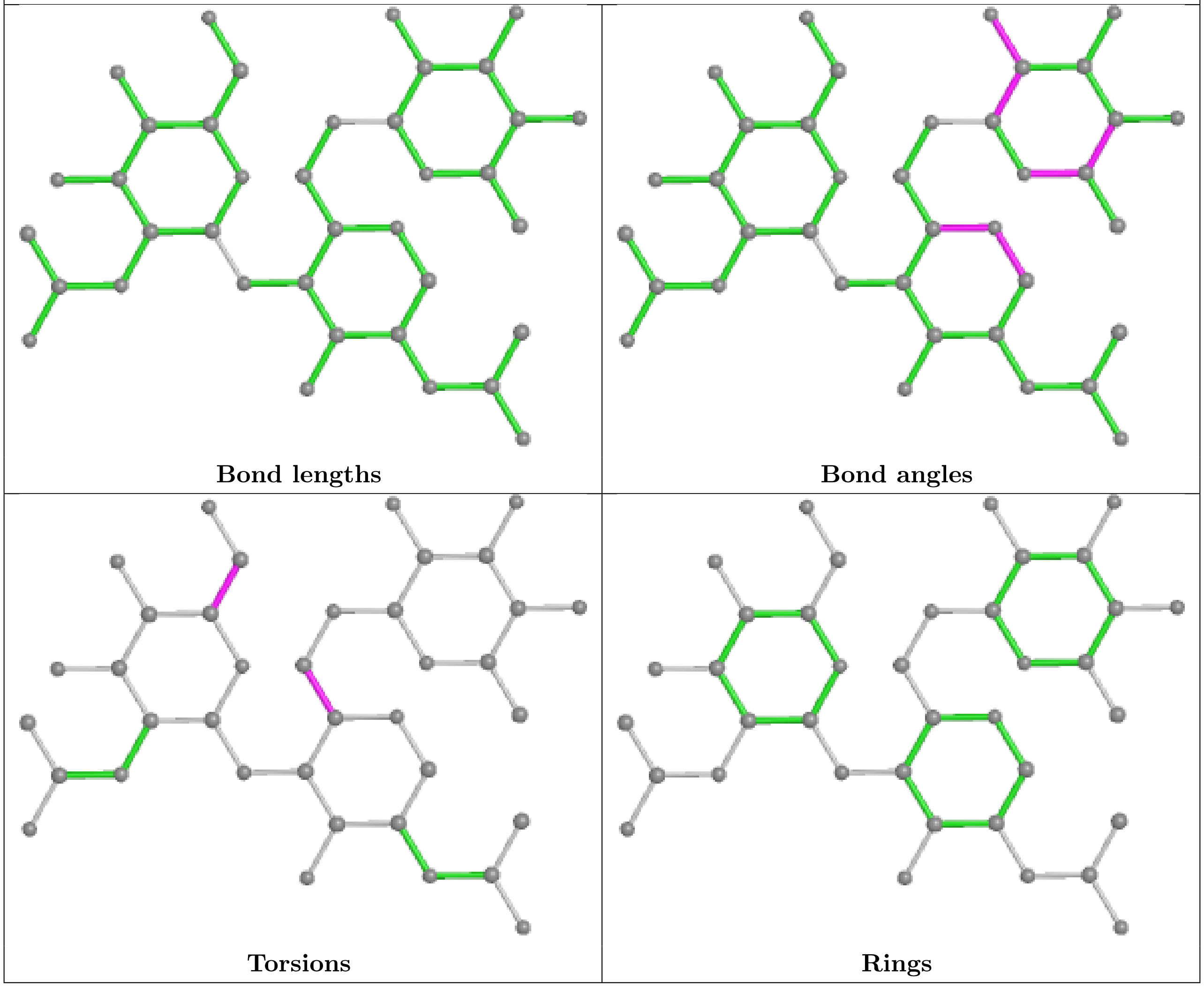


Bond lengths **Bond angles**



Torsions **Rings**

Oligosaccharide Chain P



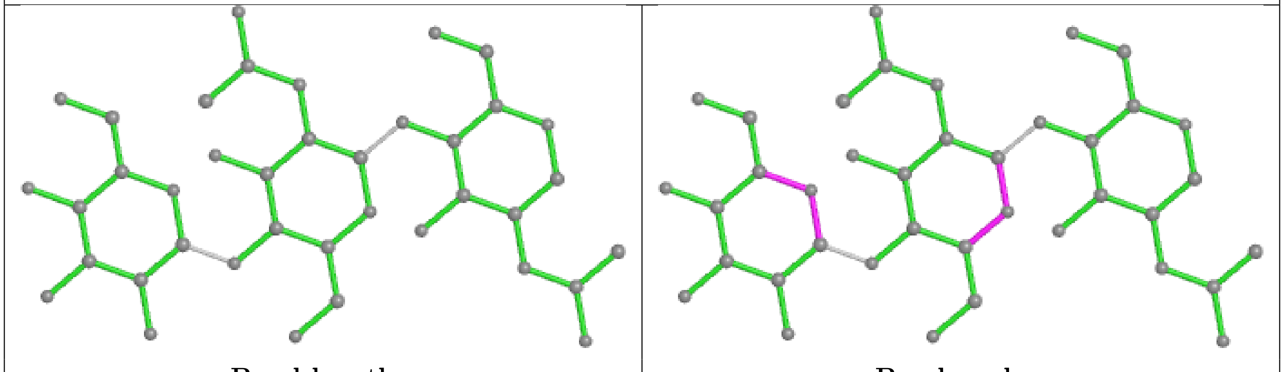
Bond lengths

Bond angles

Torsions

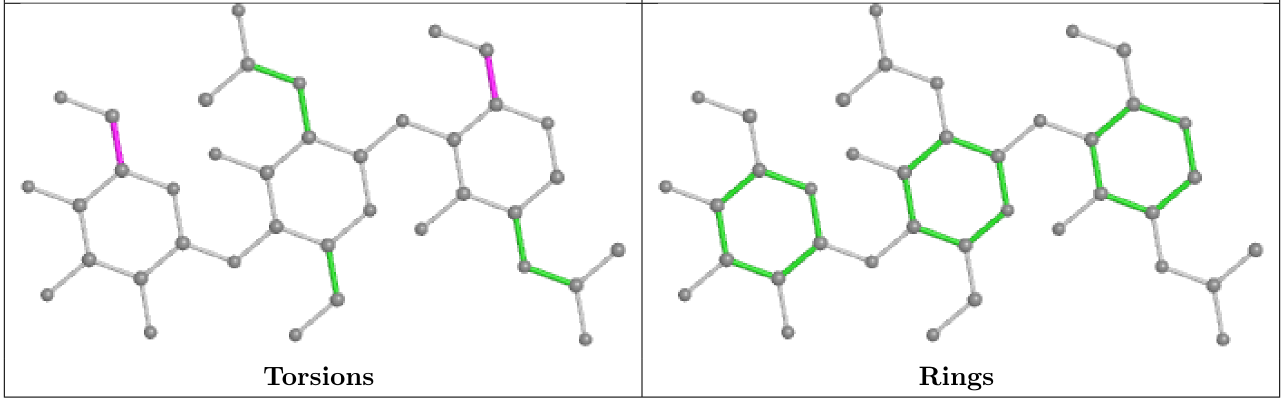
Rings

Oligosaccharide Chain K



Bond lengths

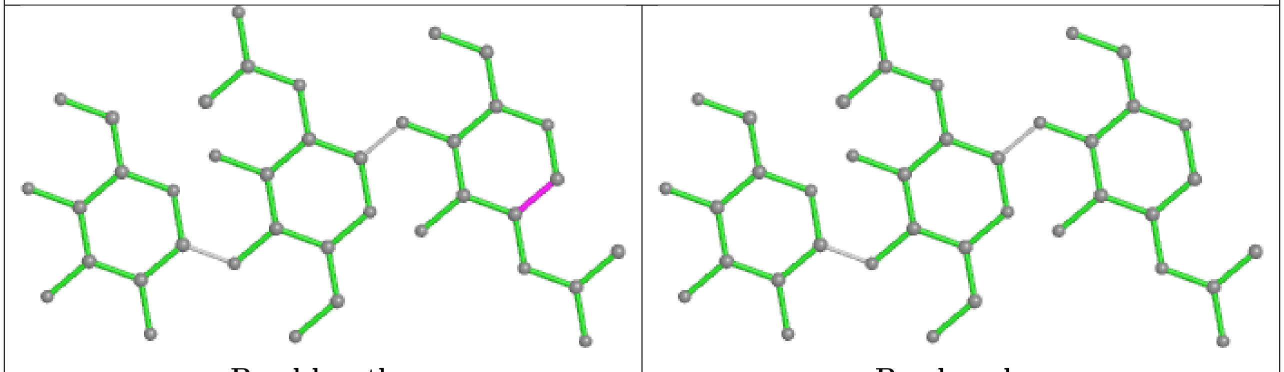
Bond angles



Torsions

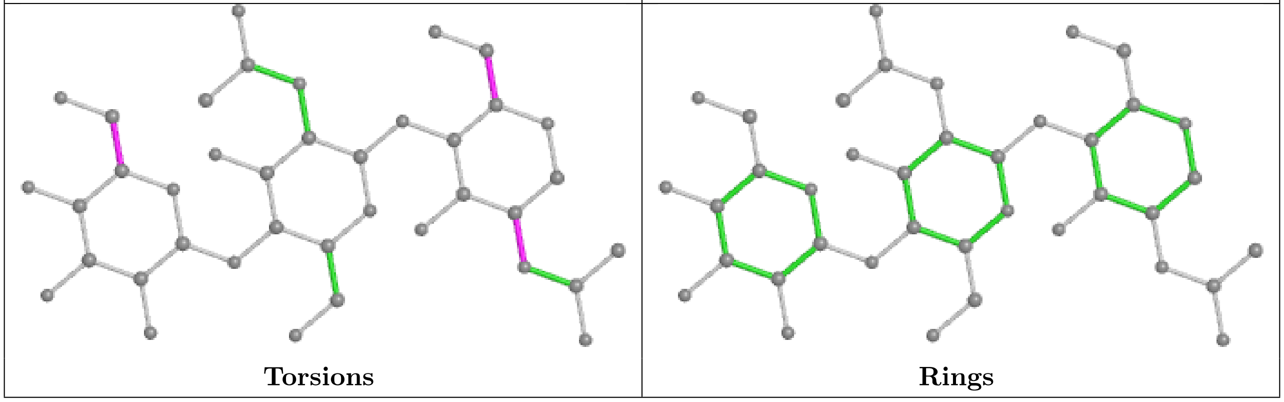
Rings

Oligosaccharide Chain O



Bond lengths

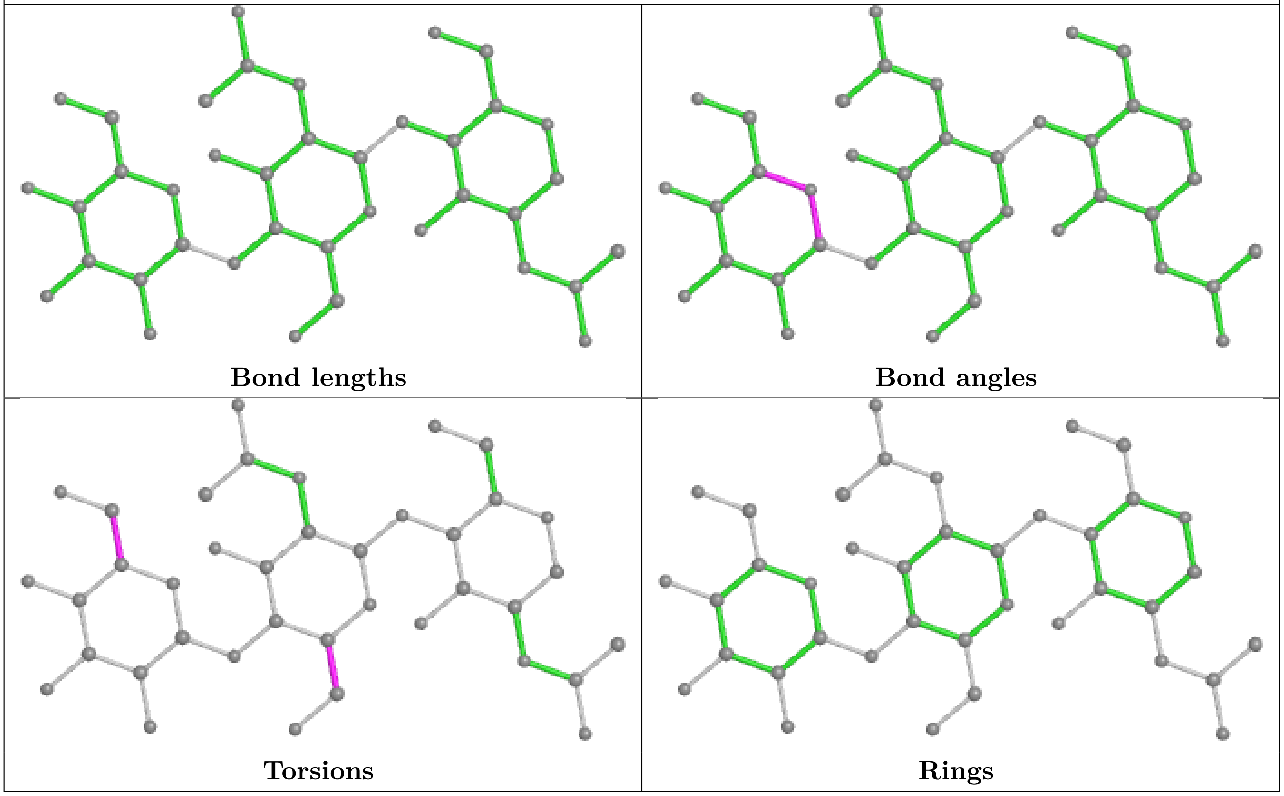
Bond angles



Torsions

Rings

Oligosaccharide Chain Q



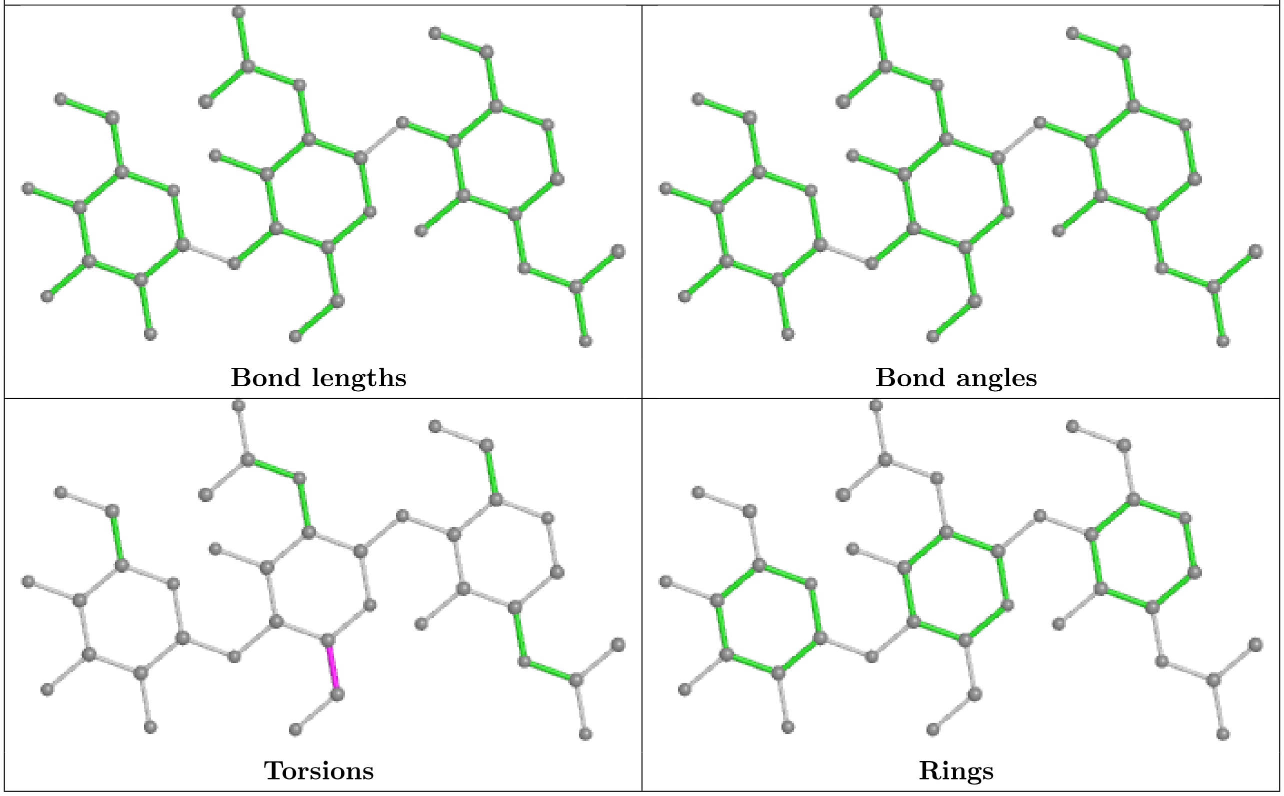
Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain T



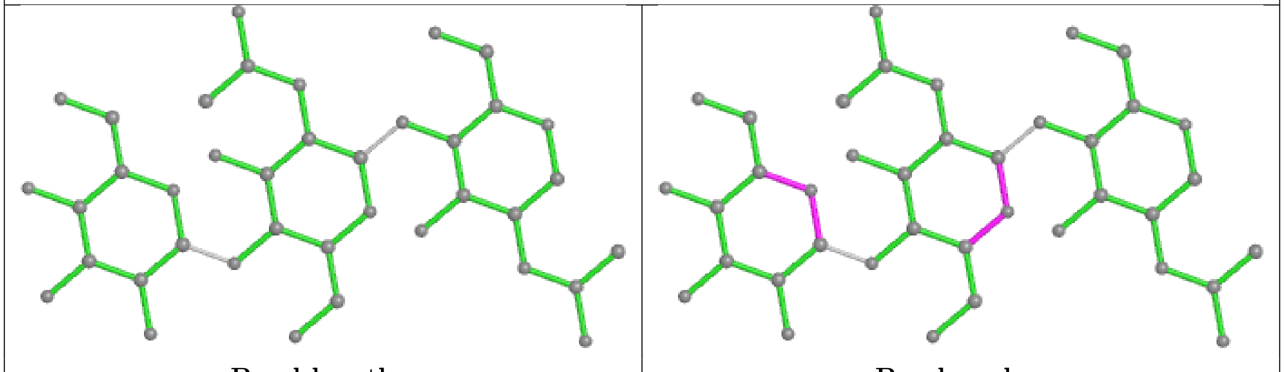
Bond lengths

Bond angles

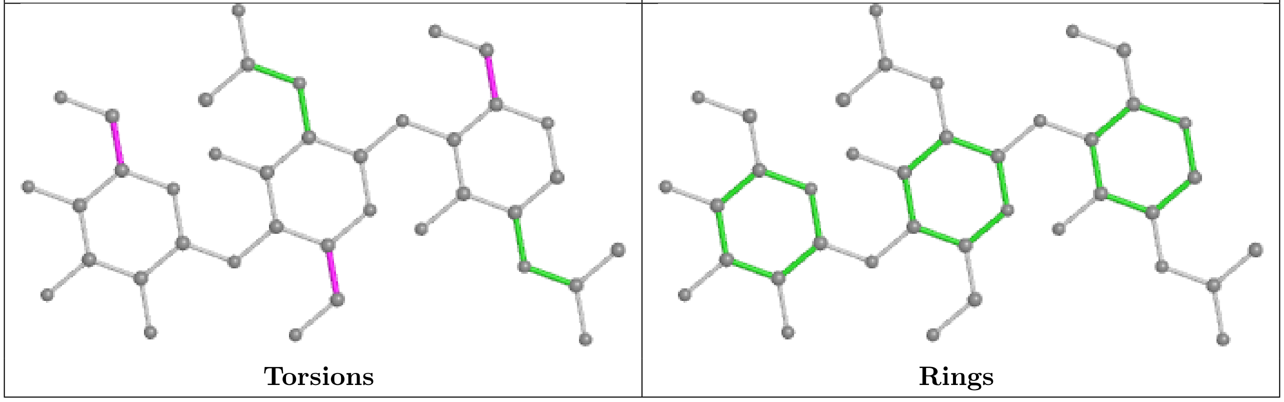
Torsions

Rings

Oligosaccharide Chain V

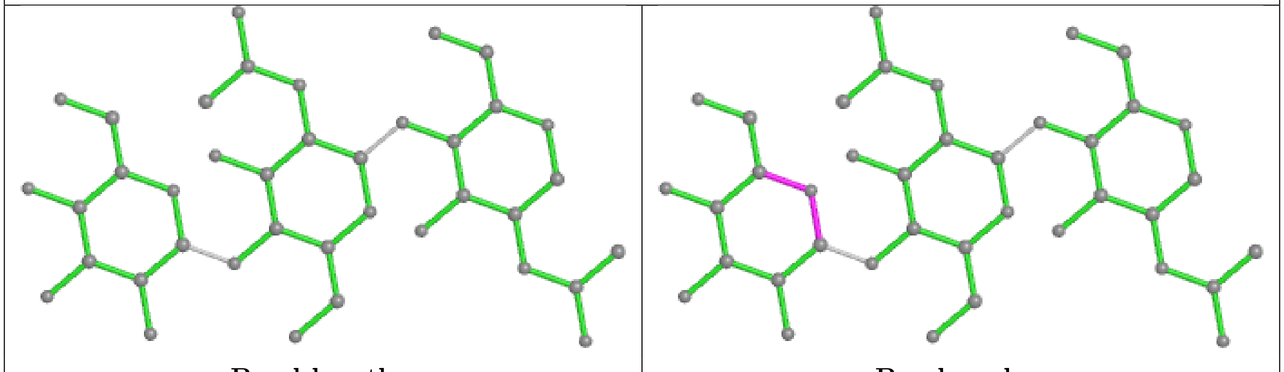


Bond lengths Bond angles

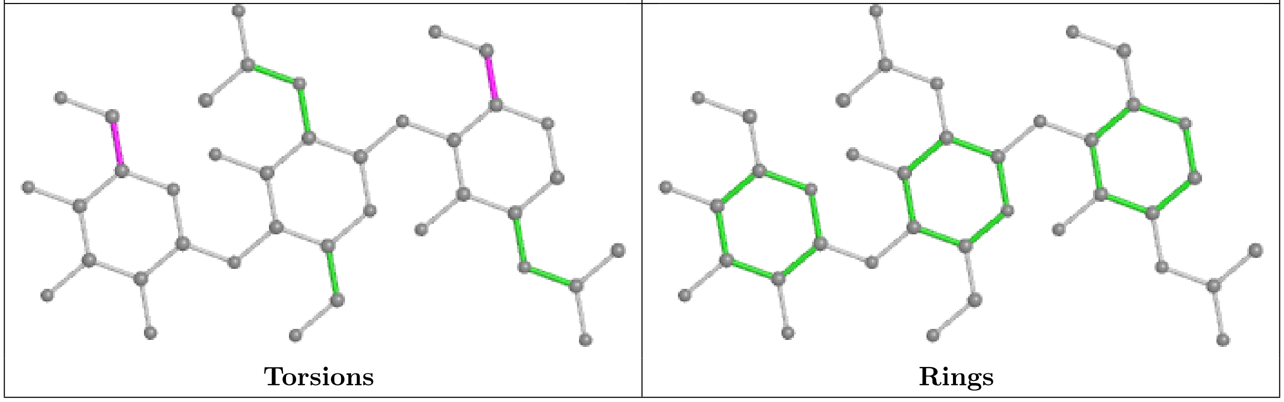


Torsions Rings

Oligosaccharide Chain W

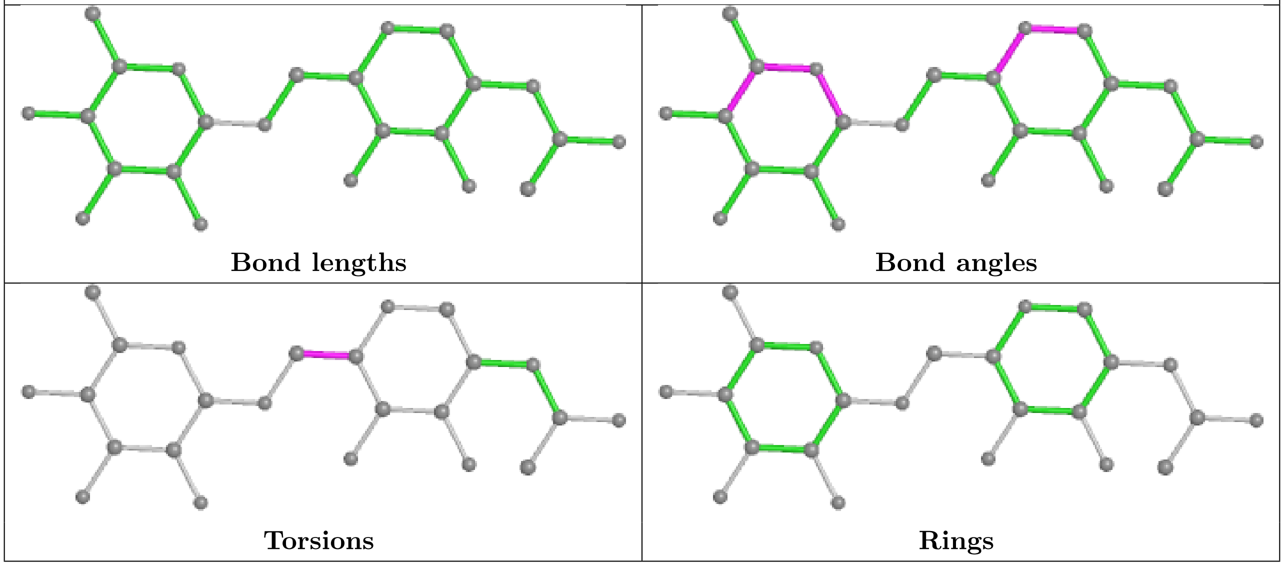


Bond lengths Bond angles



Torsions Rings

Oligosaccharide Chain Y



5.6 Ligand geometry (i)

14 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	$\#\|Z\| > 2$
8	NAG	A	1402	1	14,14,15	0.26	0	17,19,21	0.43	0
8	NAG	A	1403	1	14,14,15	0.24	0	17,19,21	0.45	0
8	NAG	B	1406	1	14,14,15	0.22	0	17,19,21	0.46	0
8	NAG	C	1401	1	14,14,15	0.28	0	17,19,21	0.49	0
8	NAG	C	1404	1	14,14,15	0.29	0	17,19,21	0.44	0
8	NAG	B	1403	1	14,14,15	0.25	0	17,19,21	0.47	0
8	NAG	B	1404	1	14,14,15	0.21	0	17,19,21	0.46	0
8	NAG	B	1402	1	14,14,15	0.26	0	17,19,21	0.47	0
8	NAG	B	1407	1	14,14,15	0.24	0	17,19,21	0.44	0
8	NAG	B	1405	1	14,14,15	0.25	0	17,19,21	0.43	0
8	NAG	C	1403	1	14,14,15	0.26	0	17,19,21	0.41	0
8	NAG	A	1401	1	14,14,15	0.37	0	17,19,21	0.45	0
8	NAG	B	1401	1	14,14,15	0.25	0	17,19,21	0.46	0
8	NAG	C	1402	1	14,14,15	0.28	0	17,19,21	0.37	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
8	NAG	A	1402	1	-	3/6/23/26	0/1/1/1
8	NAG	A	1403	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1406	1	-	4/6/23/26	0/1/1/1
8	NAG	C	1401	1	-	0/6/23/26	0/1/1/1
8	NAG	C	1404	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1403	1	-	4/6/23/26	0/1/1/1
8	NAG	B	1404	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1407	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1405	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1403	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1401	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1402	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

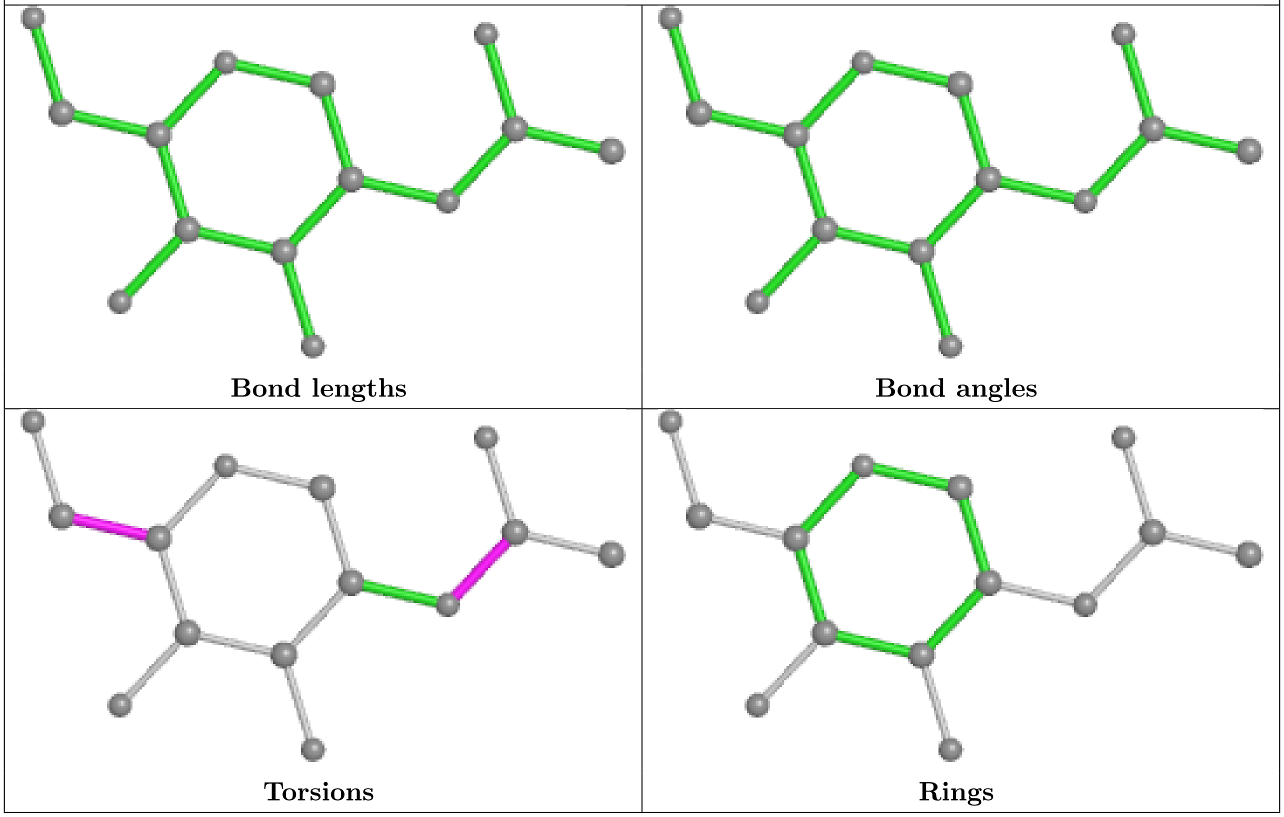
Mol	Chain	Res	Type	Atoms
8	B	1401	NAG	C4-C5-C6-O6
8	B	1406	NAG	C4-C5-C6-O6
8	B	1402	NAG	O5-C5-C6-O6
8	C	1404	NAG	C4-C5-C6-O6
8	B	1407	NAG	C4-C5-C6-O6

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 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 then 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 A 1402



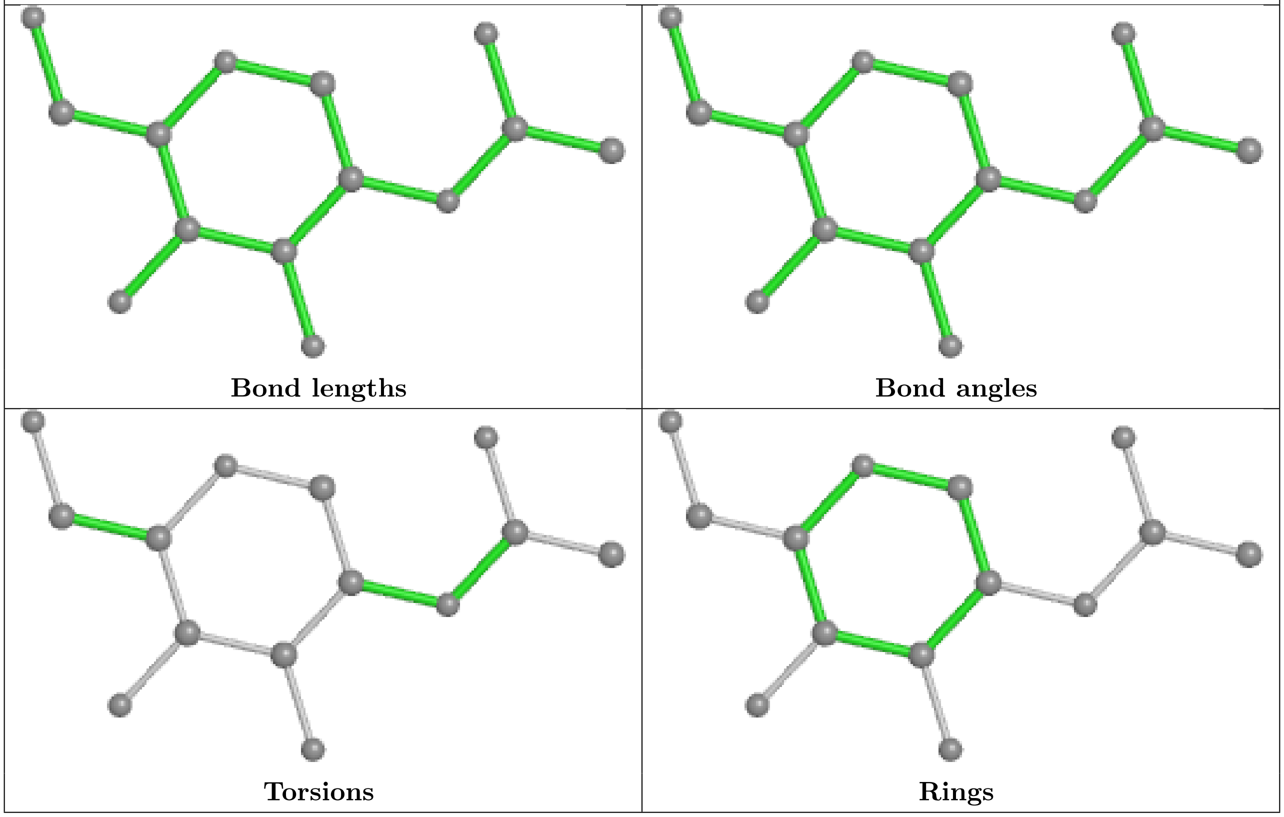
Bond lengths

Bond angles

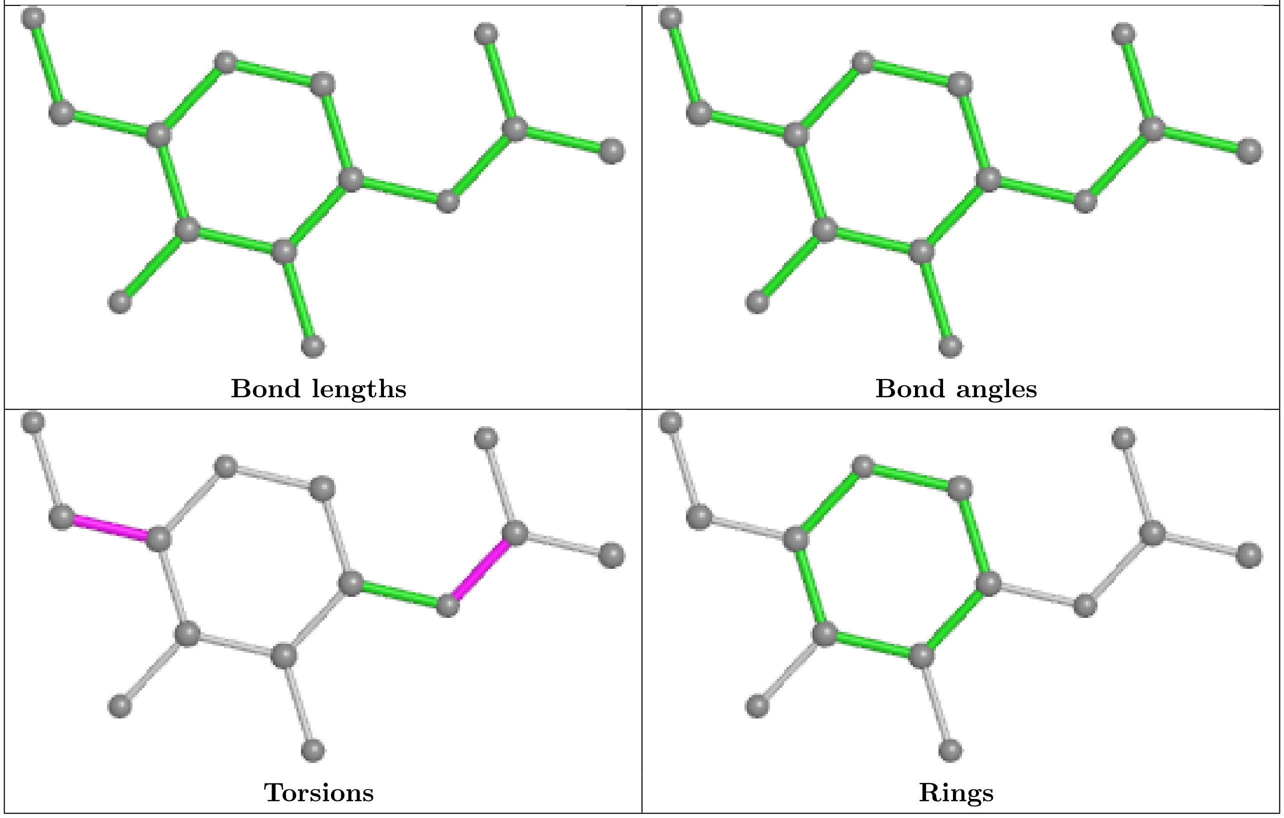
Torsions

Rings

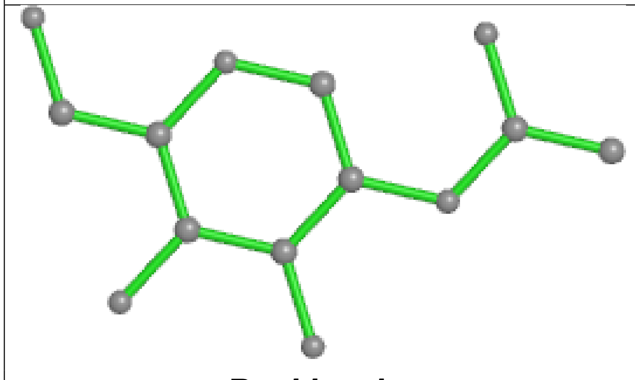
Ligand NAG A 1403

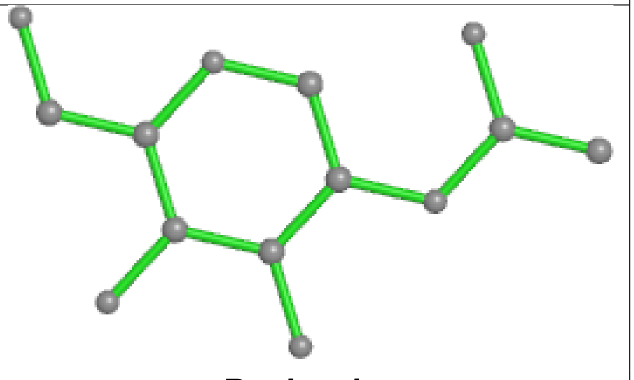


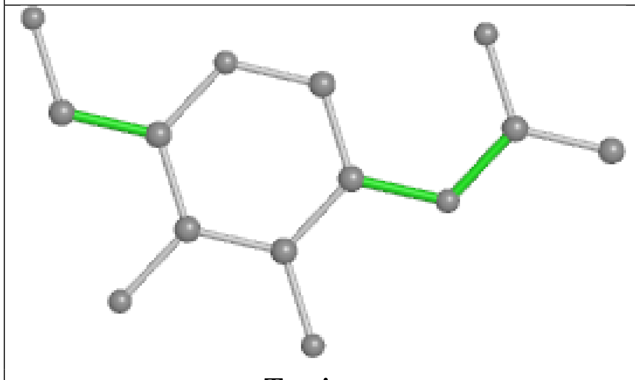
Ligand NAG B 1406

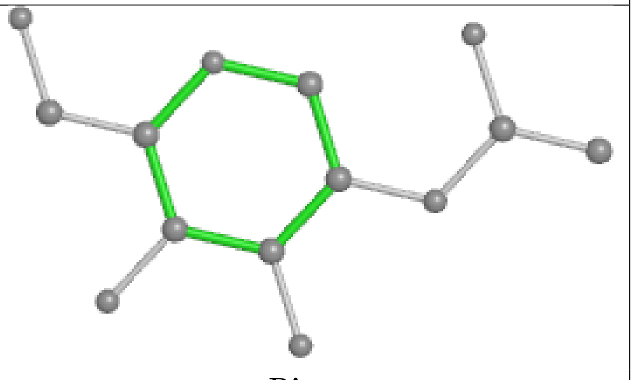


Ligand NAG C 1401

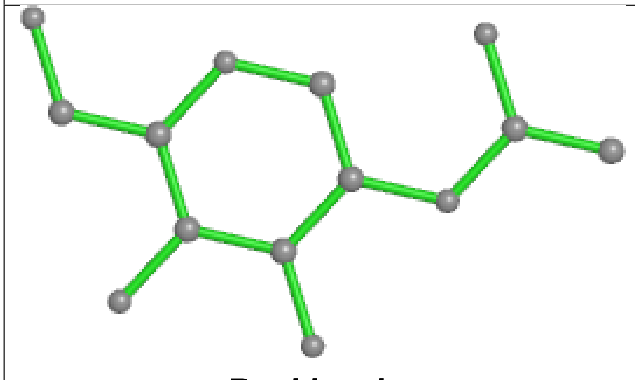

Bond lengths

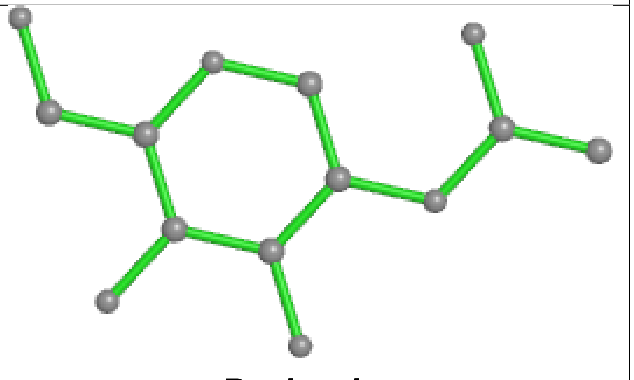

Bond angles

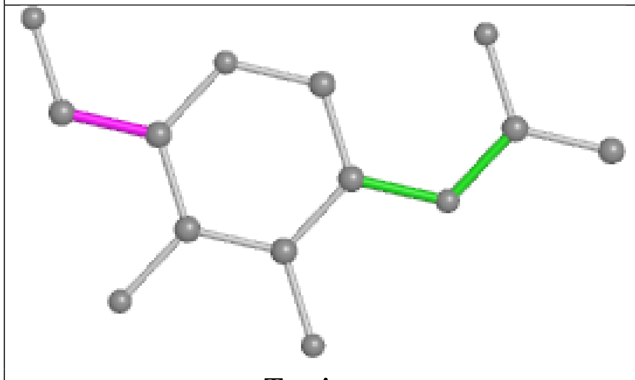

Torsions

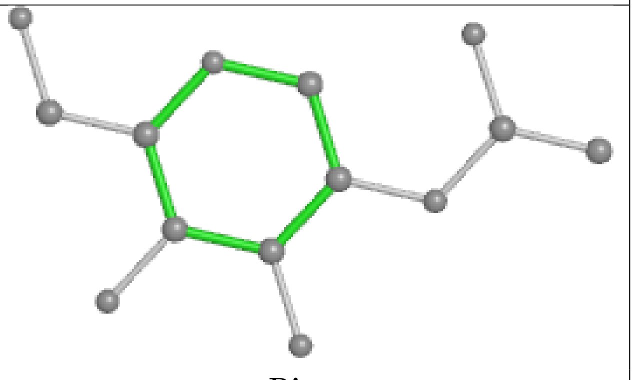

Rings

Ligand NAG C 1404

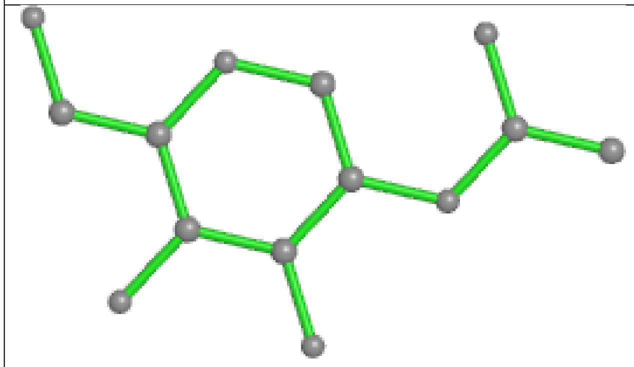

Bond lengths


Bond angles

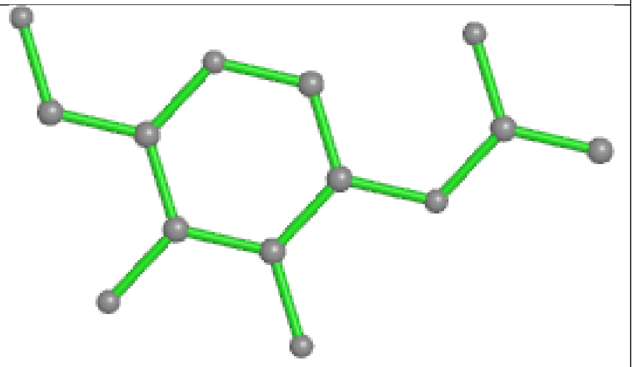

Torsions


Rings

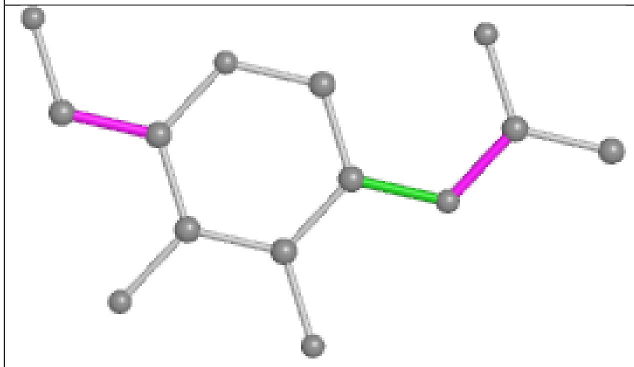
Ligand NAG B 1403



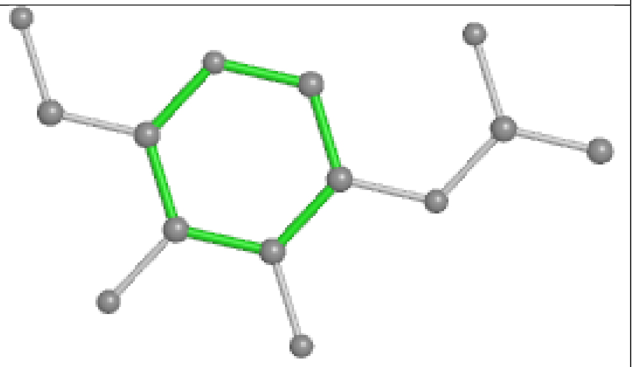
Bond lengths



Bond angles

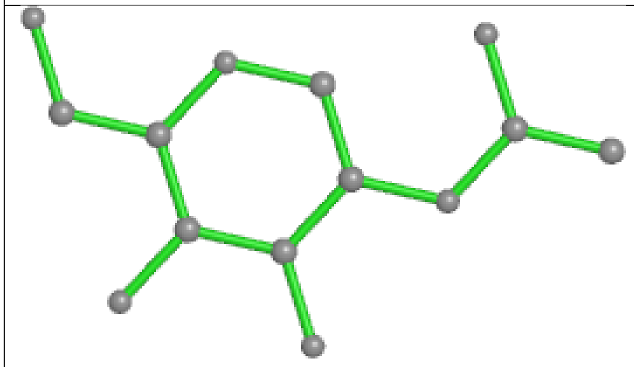


Torsions

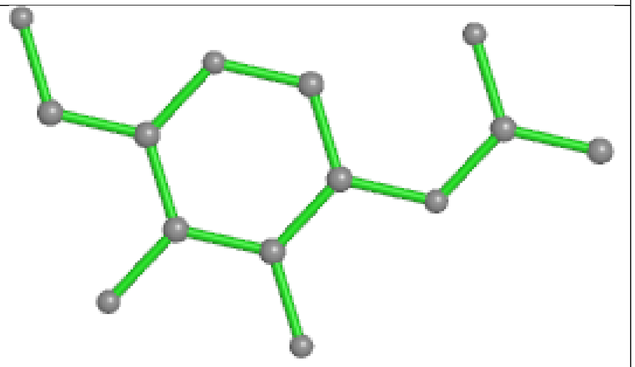


Rings

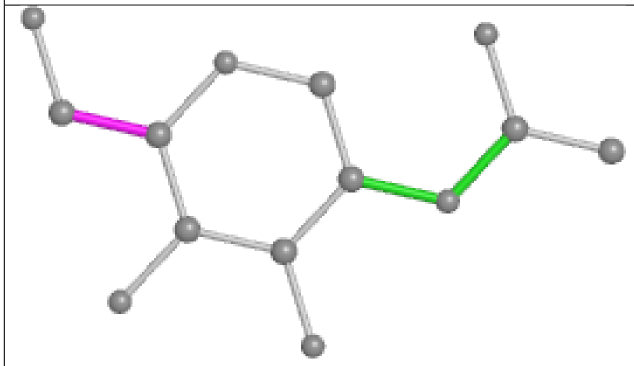
Ligand NAG B 1404



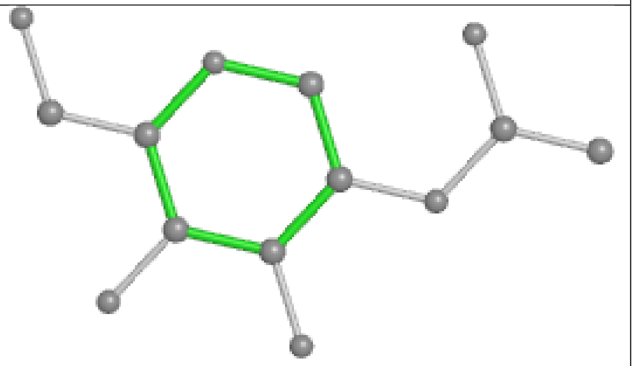
Bond lengths



Bond angles

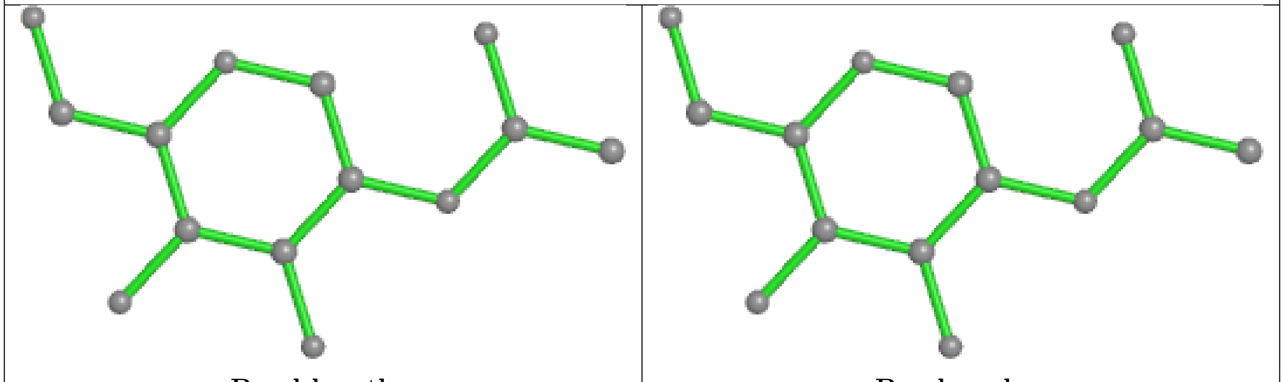


Torsions

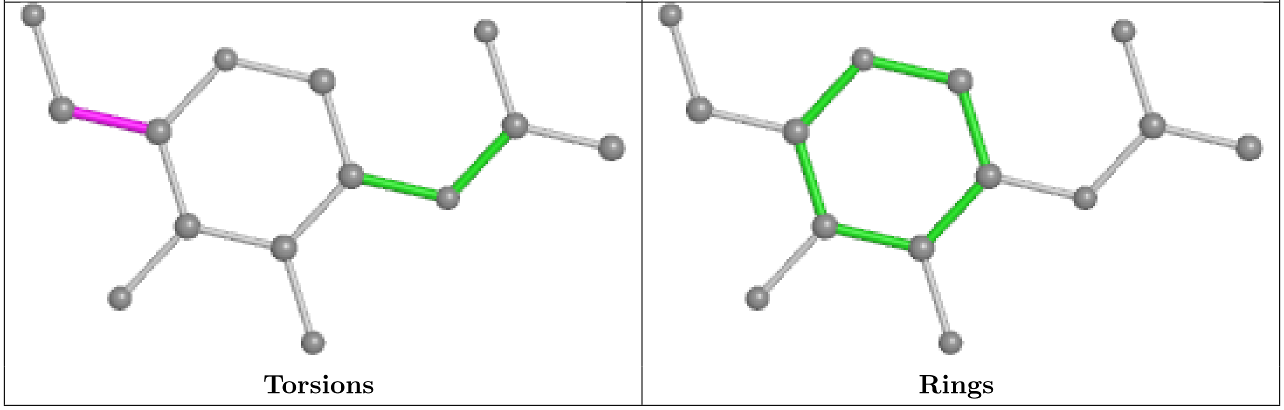


Rings

Ligand NAG B 1402

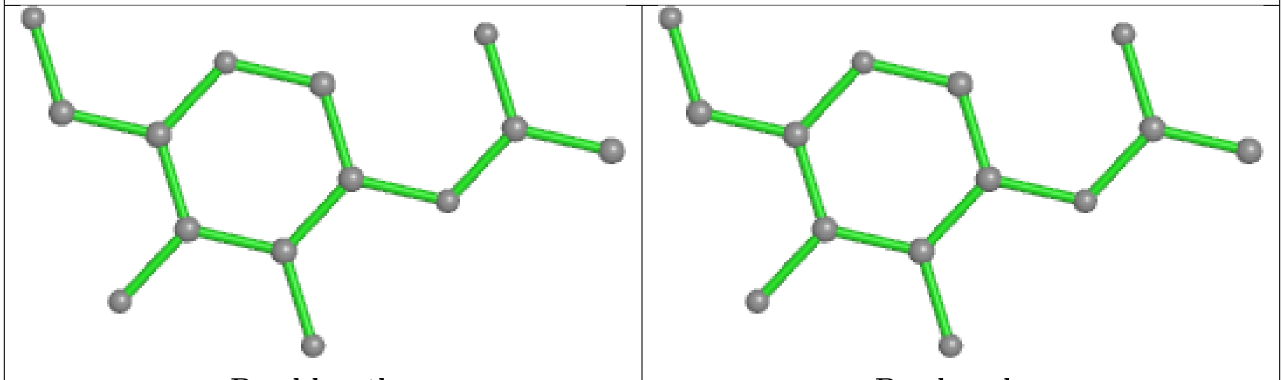


Bond lengths Bond angles

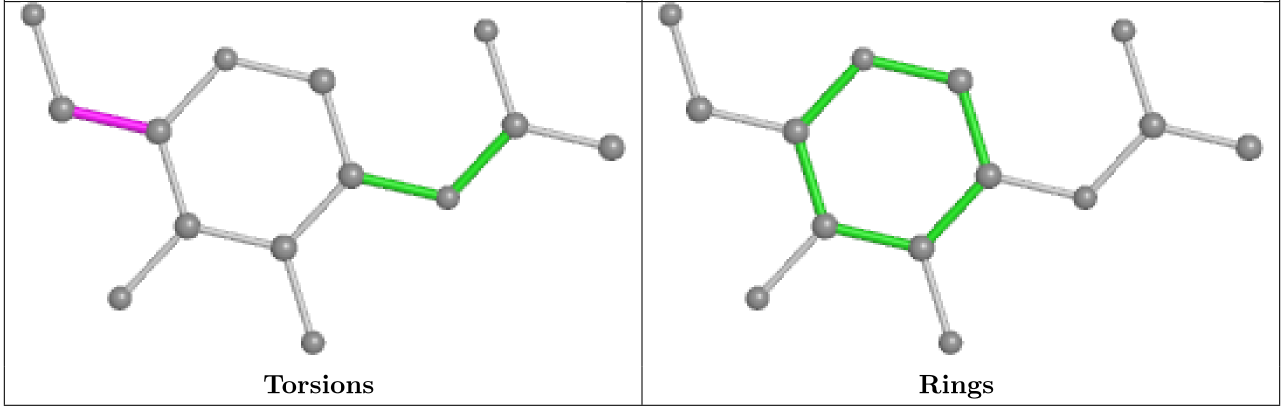


Torsions Rings

Ligand NAG B 1407

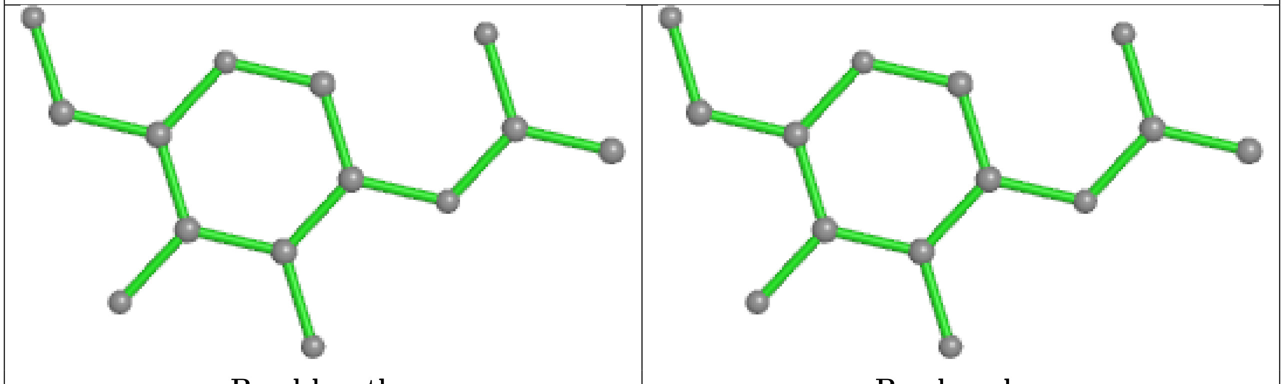


Bond lengths Bond angles



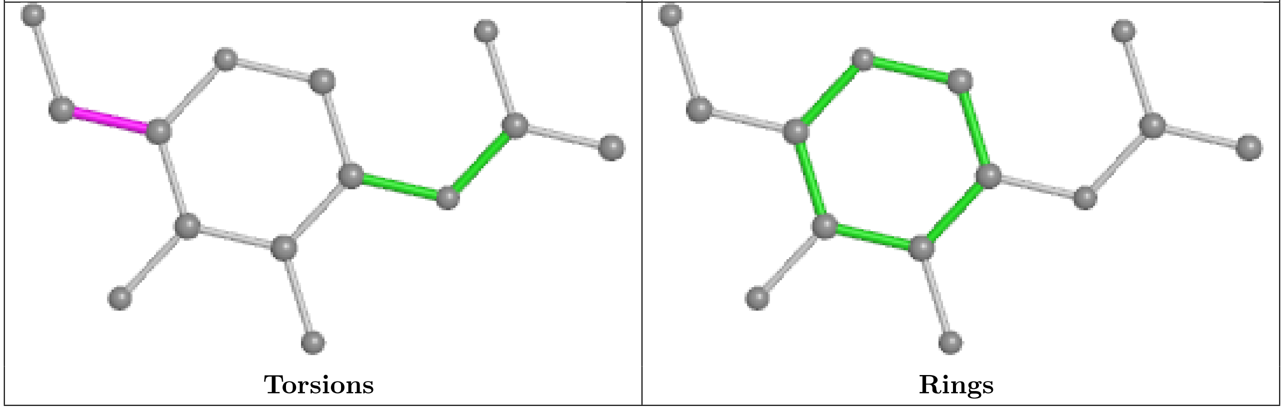
Torsions Rings

Ligand NAG B 1405



Bond lengths

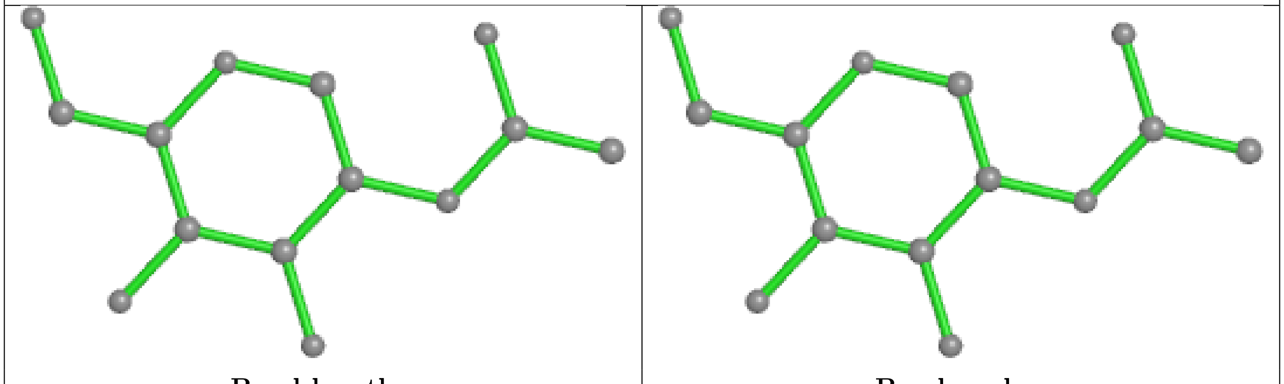
Bond angles



Torsions

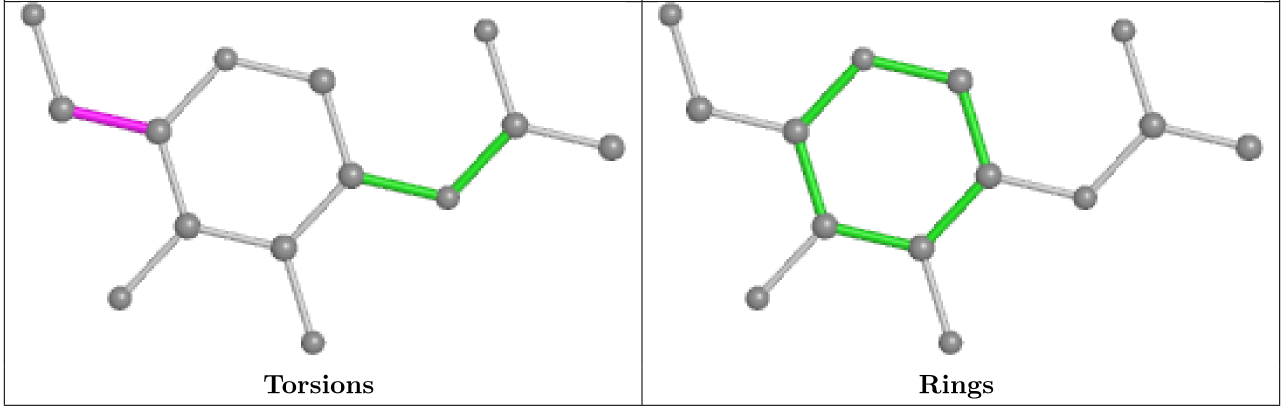
Rings

Ligand NAG C 1403



Bond lengths

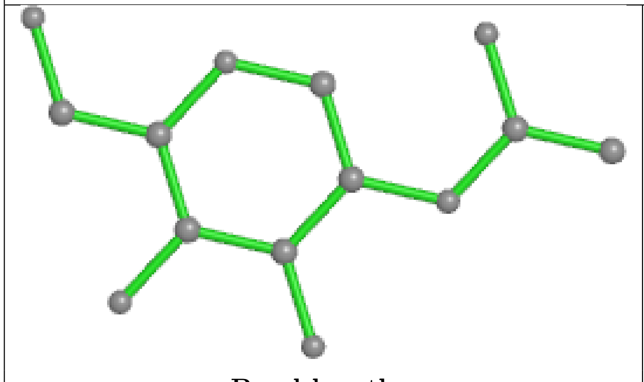
Bond angles

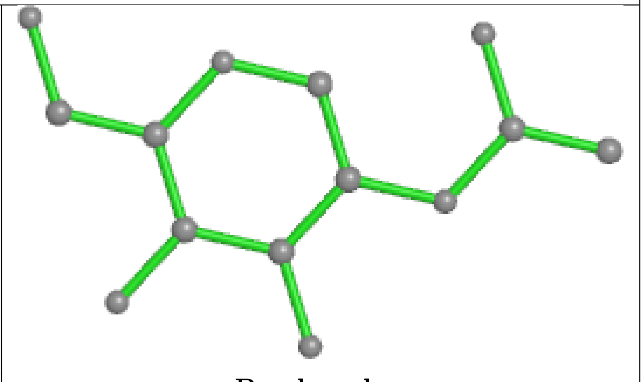


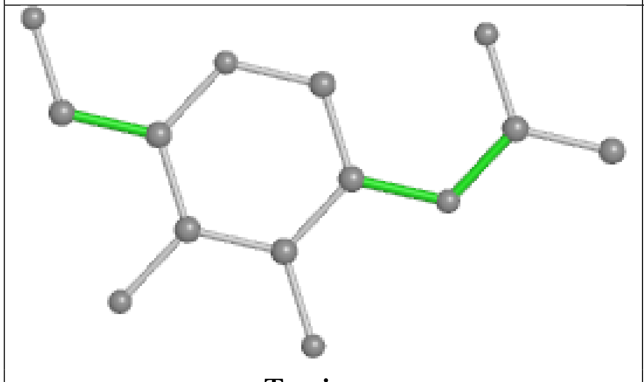
Torsions

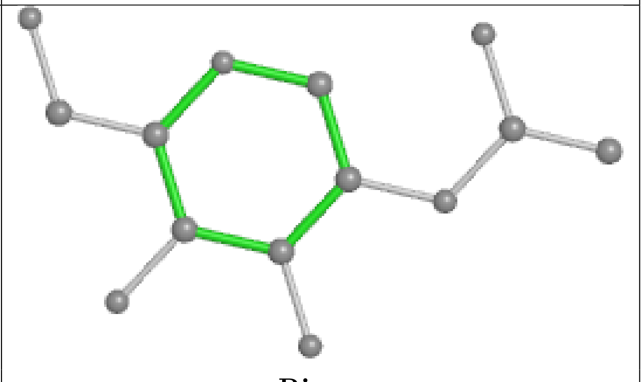
Rings

Ligand NAG A 1401

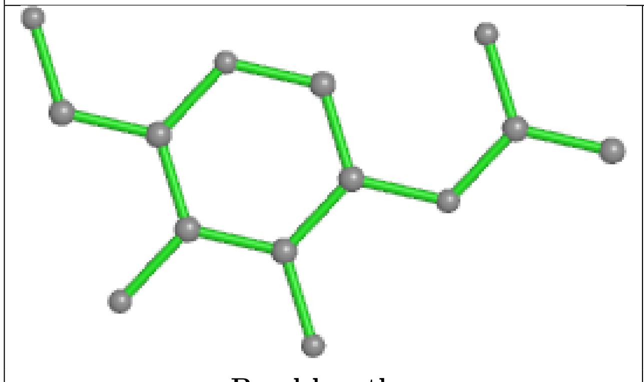

Bond lengths

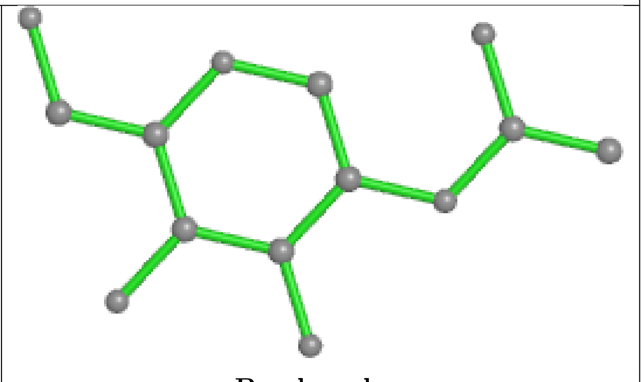

Bond angles

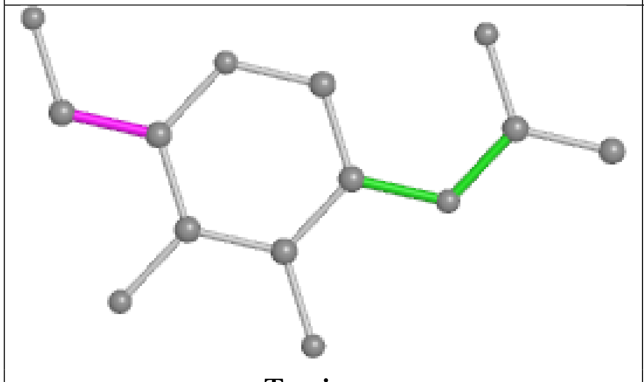

Torsions

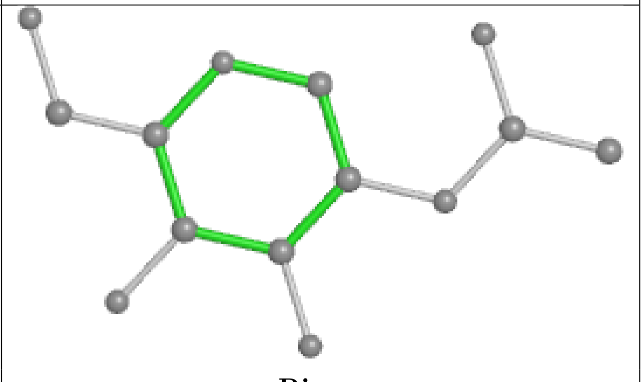

Rings

Ligand NAG B 1401

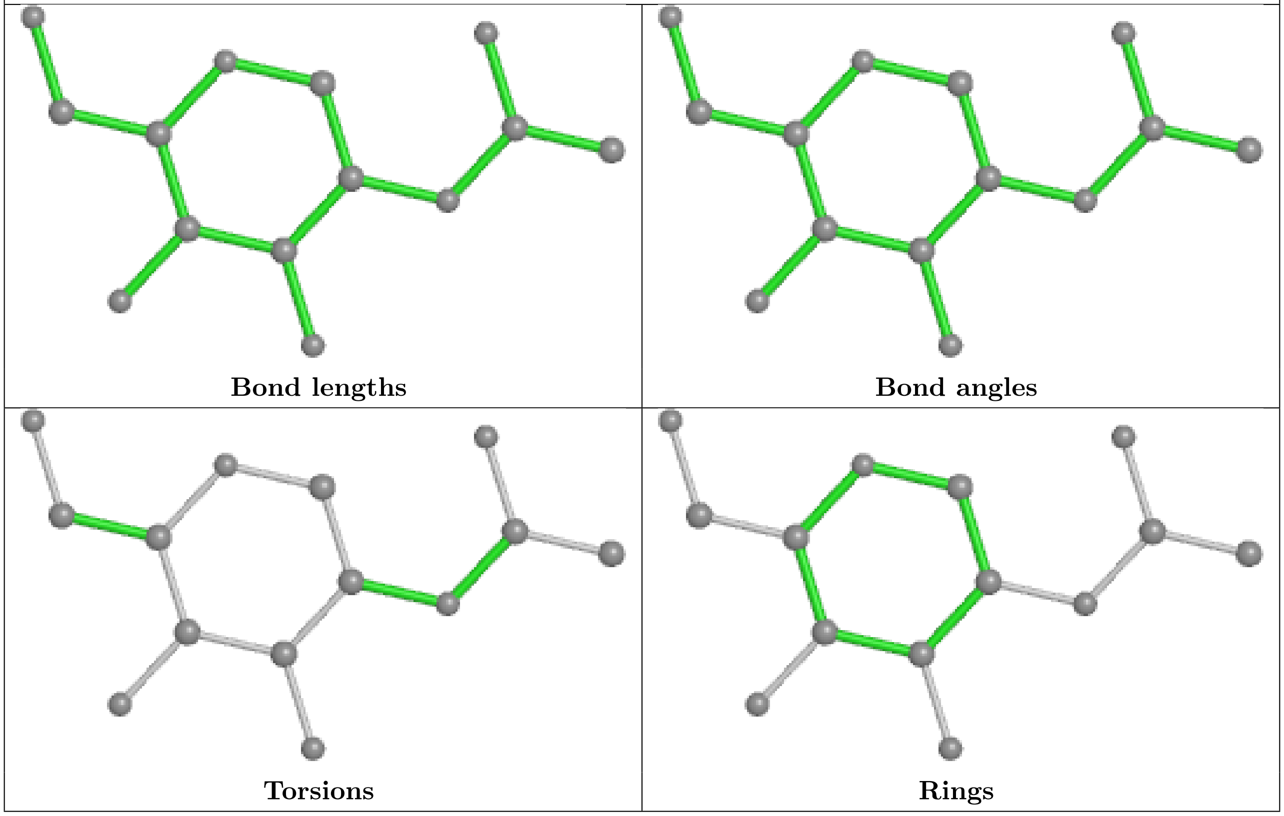

Bond lengths


Bond angles


Torsions


Rings

Ligand NAG C 1402



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

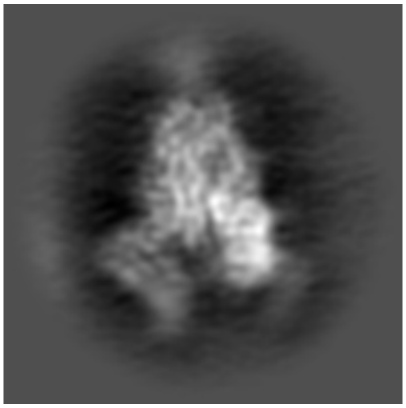
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33943. These allow visual inspection of the internal detail of the map and identification of artifacts.

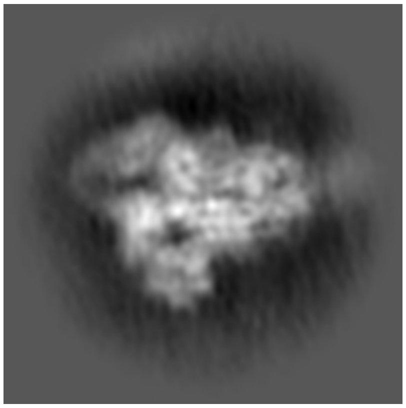
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

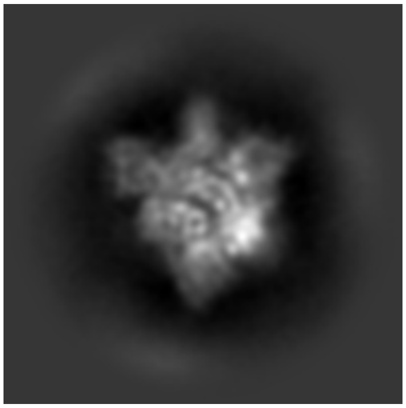
6.1.1 Primary map



X

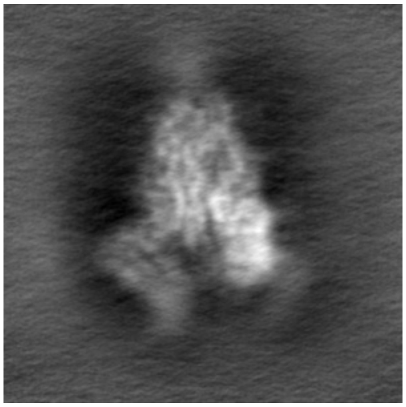


Y

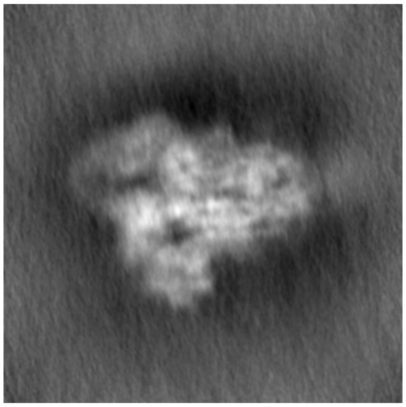


Z

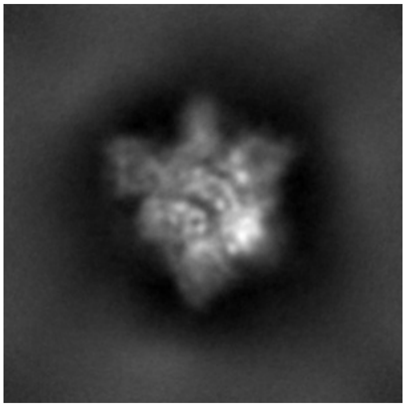
6.1.2 Raw map



X



Y

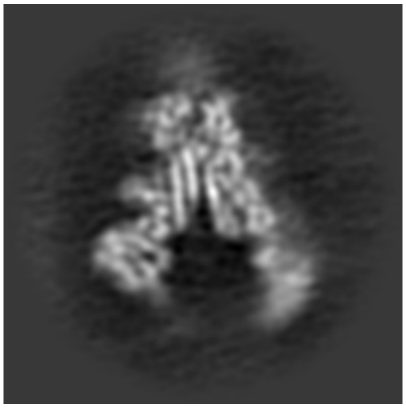


Z

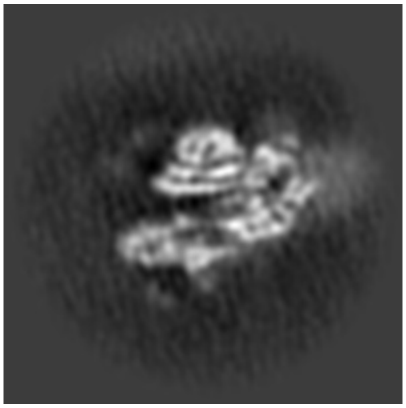
The images above show the map projected in three orthogonal directions.

6.2 Central slices

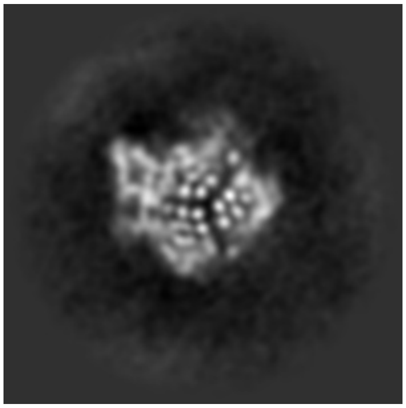
6.2.1 Primary map



X Index: 128

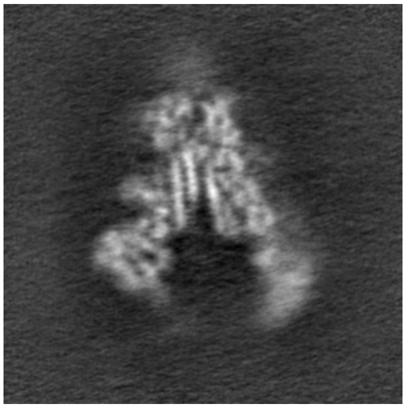


Y Index: 128

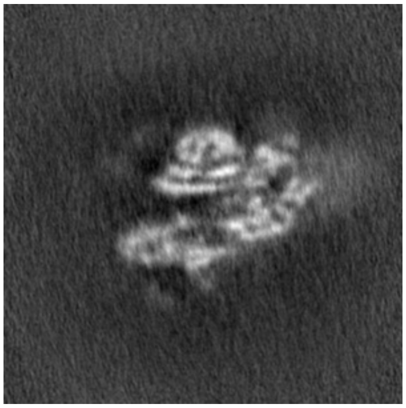


Z Index: 128

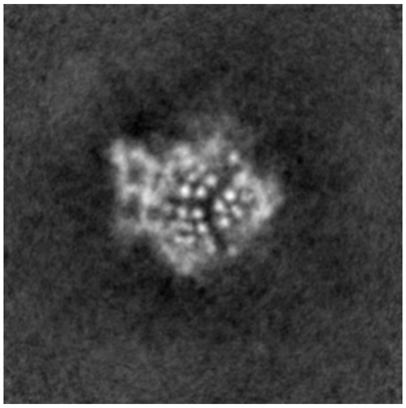
6.2.2 Raw map



X Index: 128



Y Index: 128

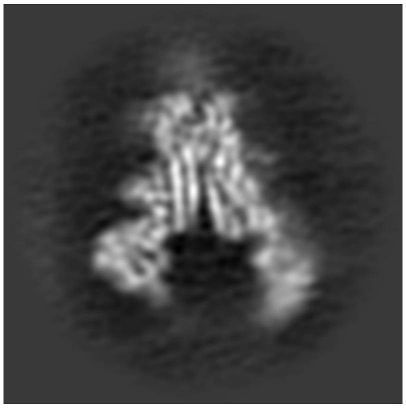


Z Index: 128

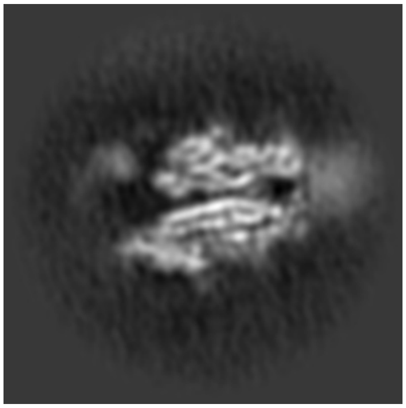
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

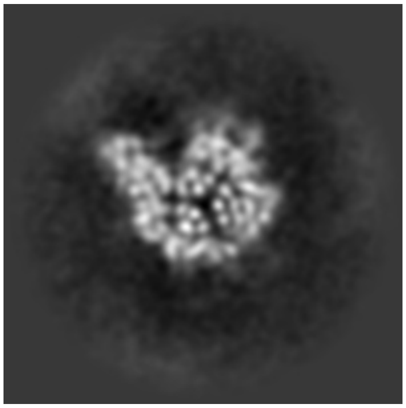
6.3.1 Primary map



X Index: 126

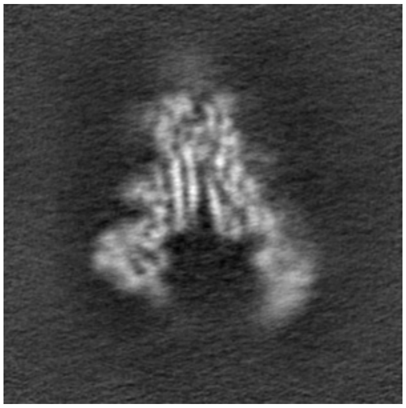


Y Index: 121

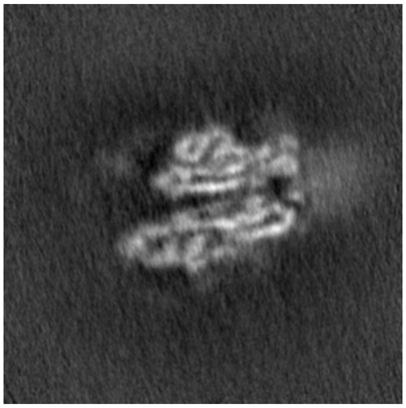


Z Index: 121

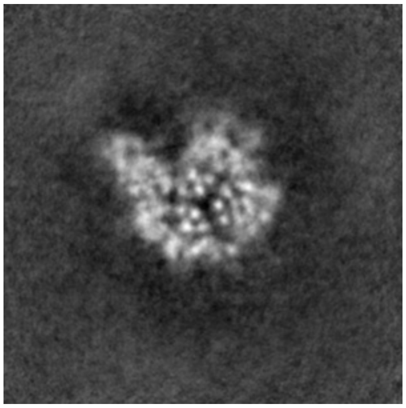
6.3.2 Raw map



X Index: 126



Y Index: 125

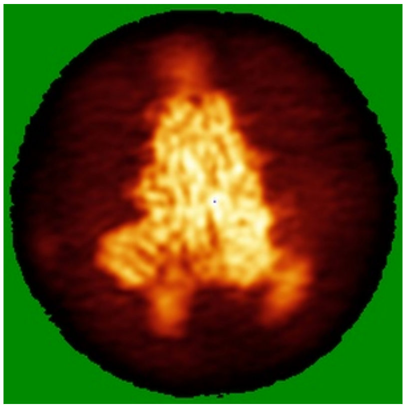


Z Index: 122

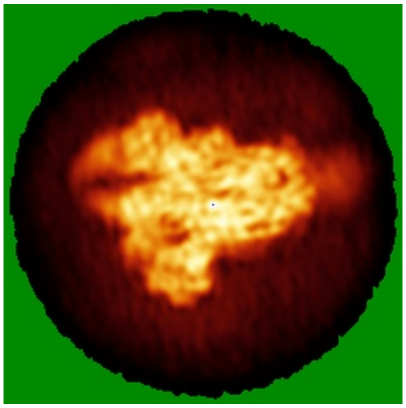
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

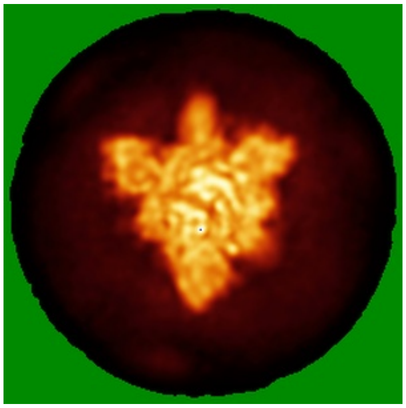
6.4.1 Primary map



X

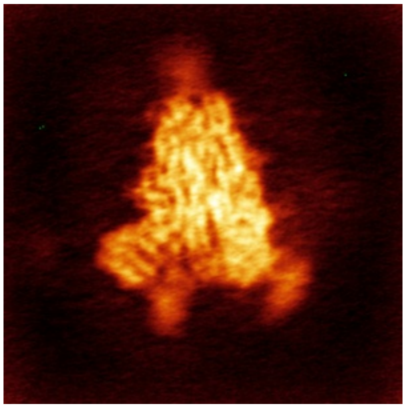


Y

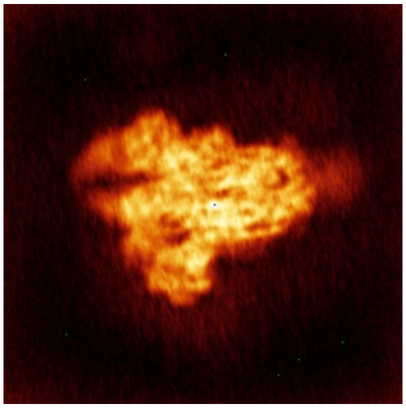


Z

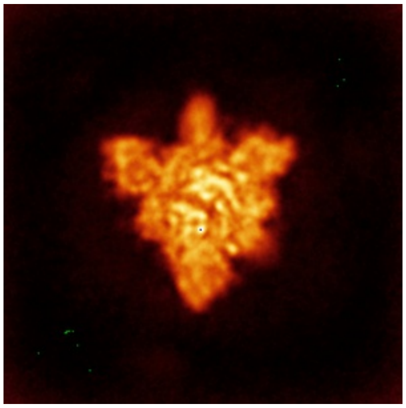
6.4.2 Raw map



X



Y

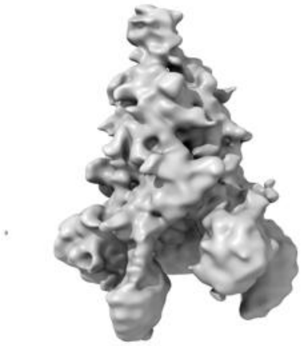


Z

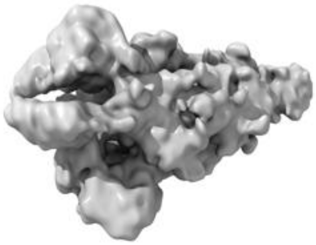
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

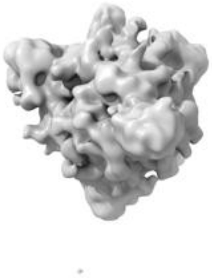
6.5.1 Primary map



X



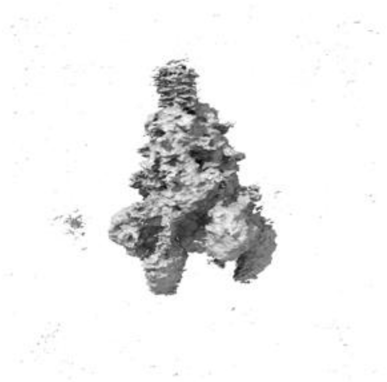
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X

Y

Z

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

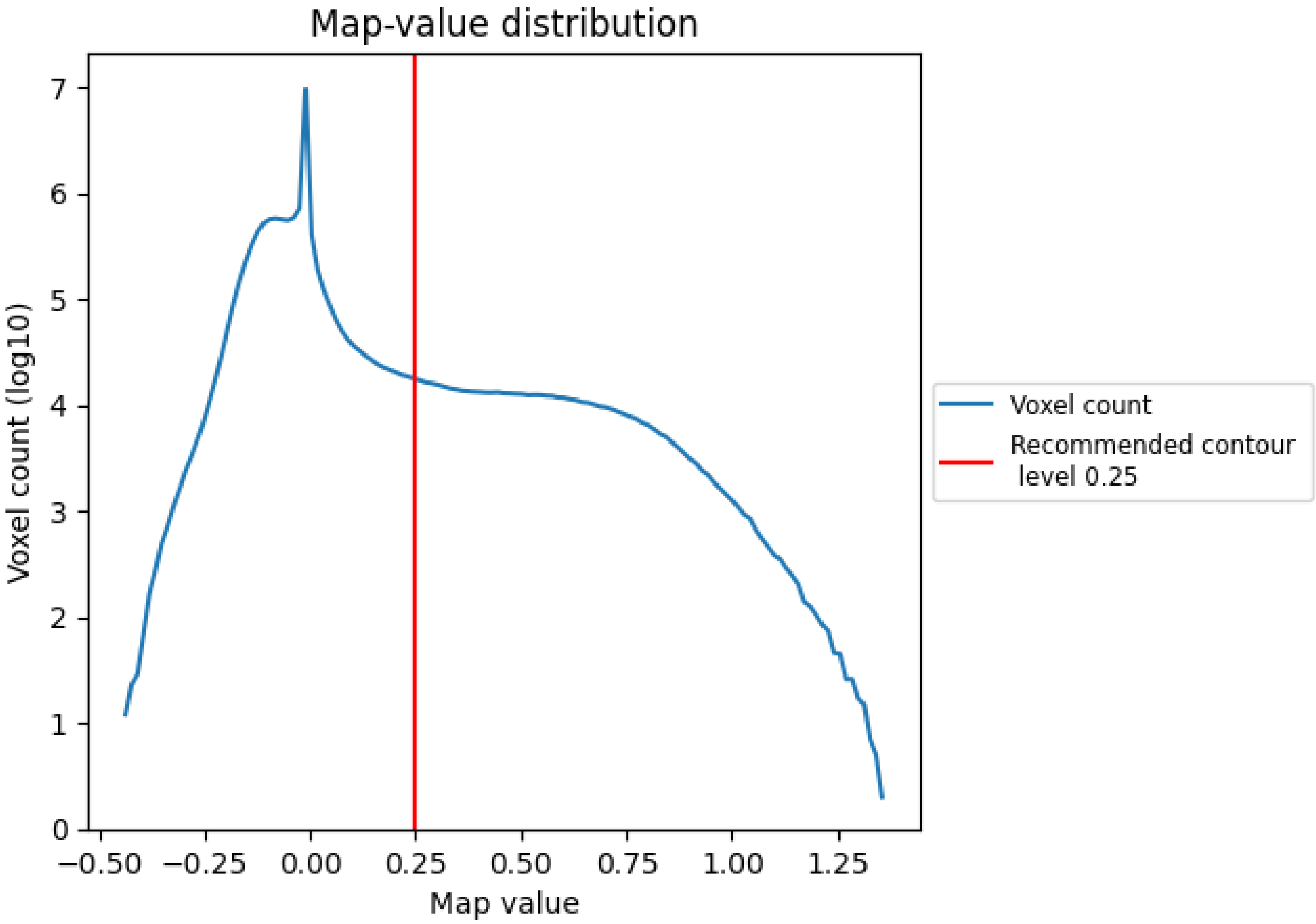
6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

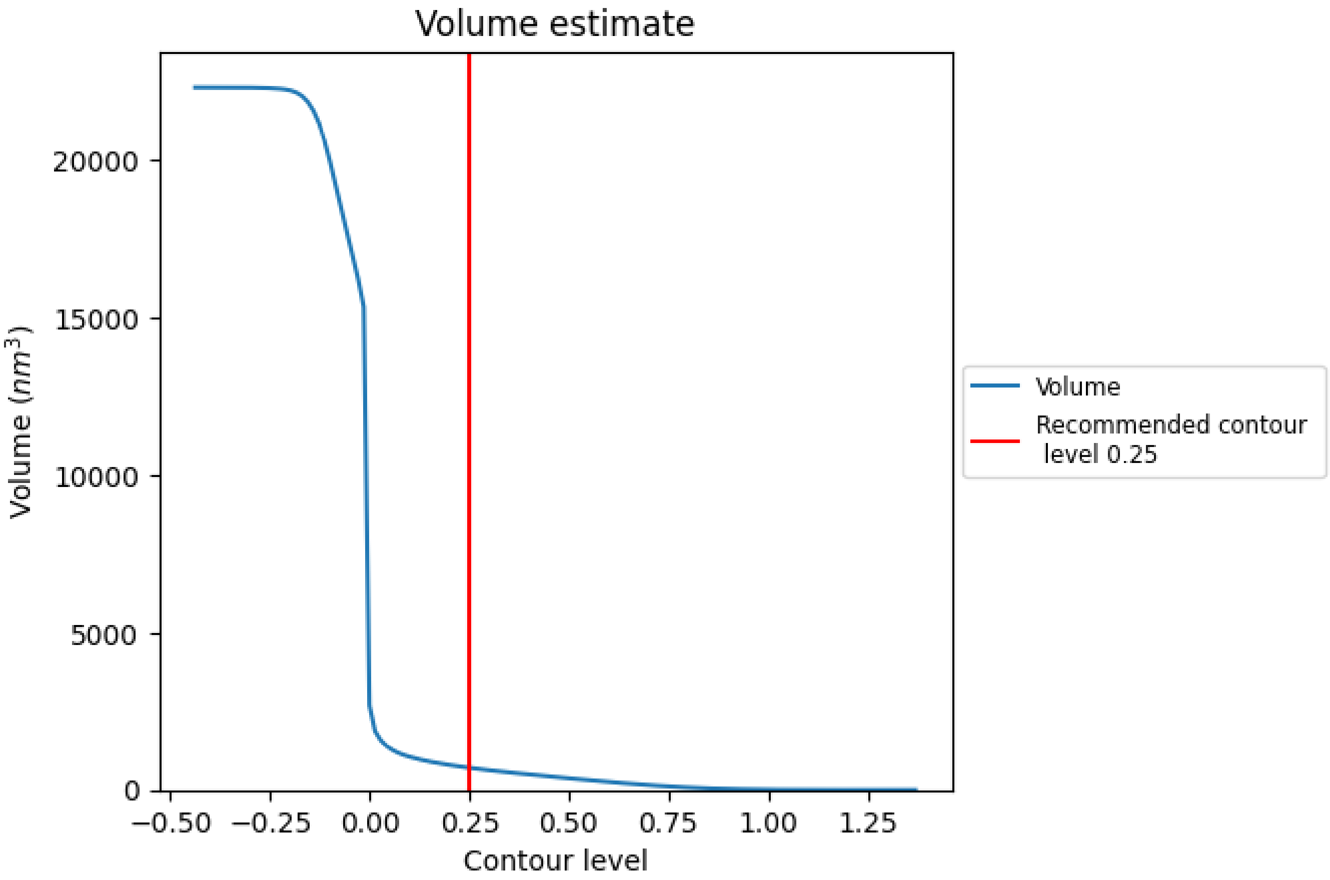
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

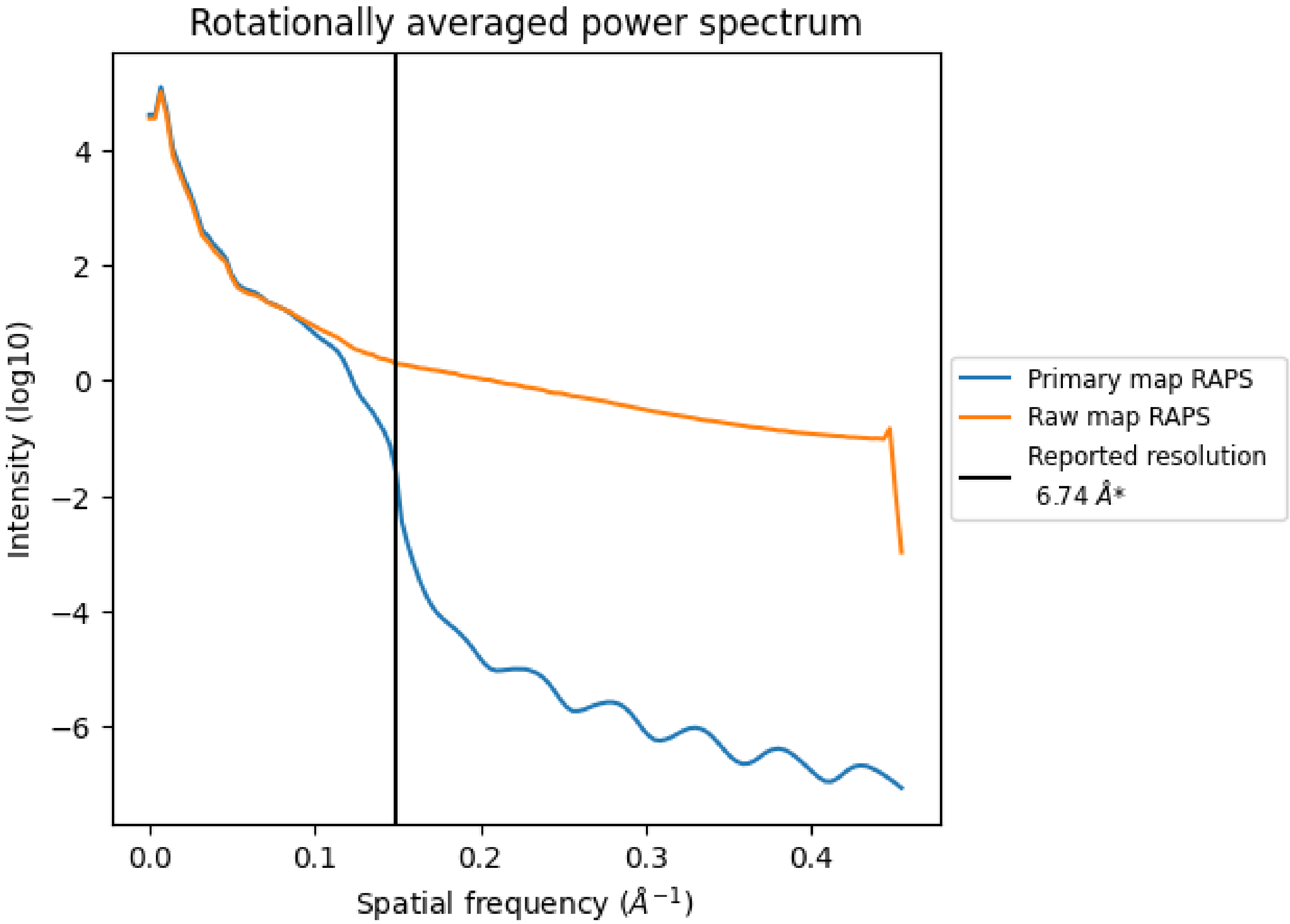
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 705 nm^3; this corresponds to an approximate mass of 637 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

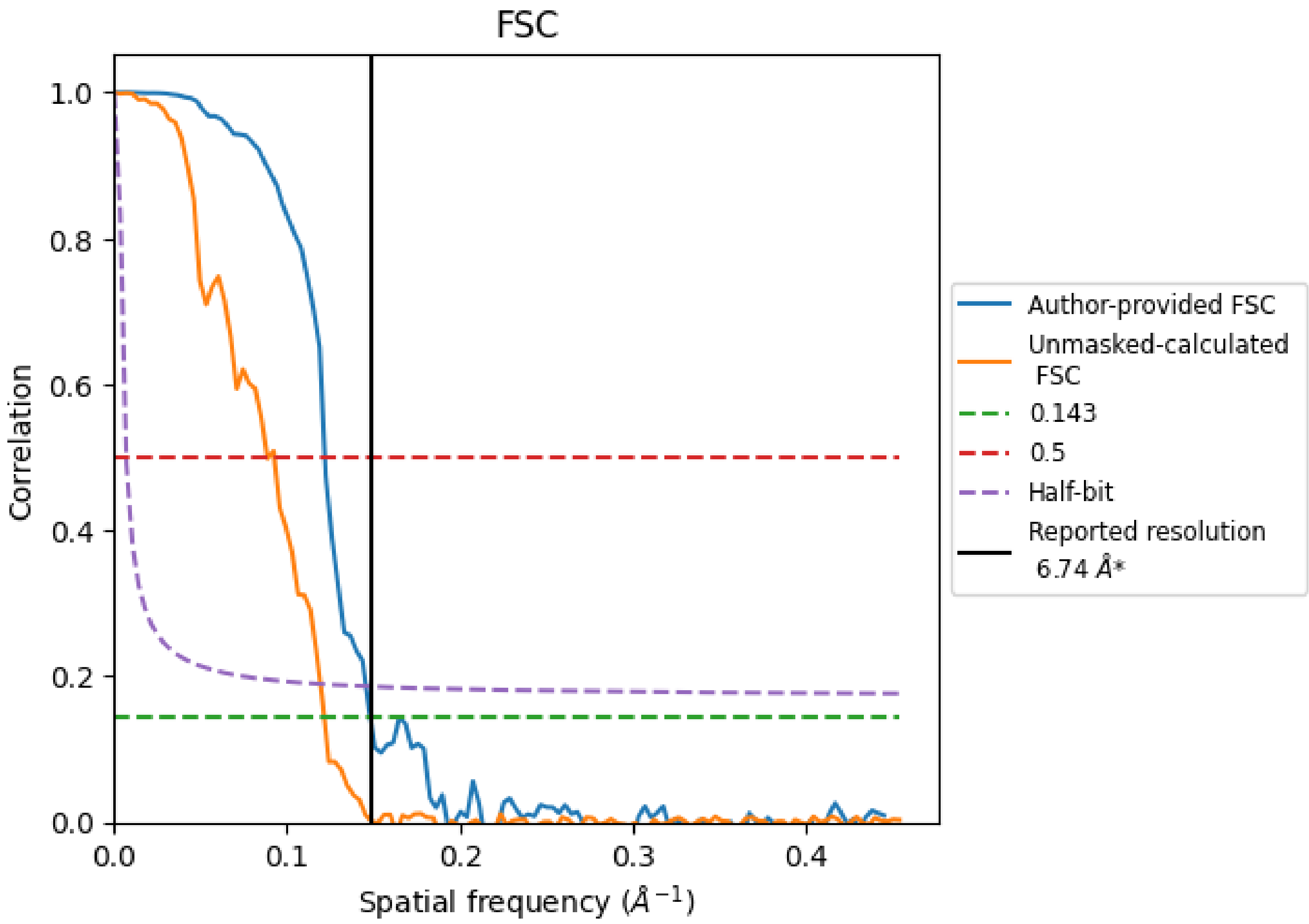


*Reported resolution corresponds to spatial frequency of 0.148 Å^{-1}

8 Fourier-Shell correlation ⓘ

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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.148 $Å^{-1}$

8.2 Resolution estimates

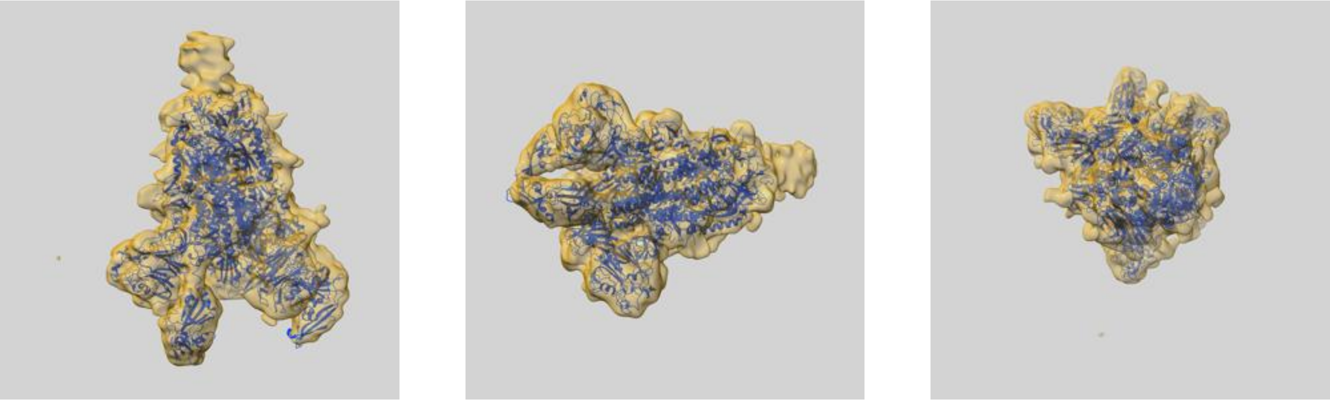
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	6.74	-	-
Author-provided FSC curve	6.74	8.20	6.86
Unmasked-calculated*	8.22	11.27	8.37

*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 8.22 differs from the reported value 6.74 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33943 and PDB model 7YMV. Per-residue inclusion information can be found in section 3 on page 15.

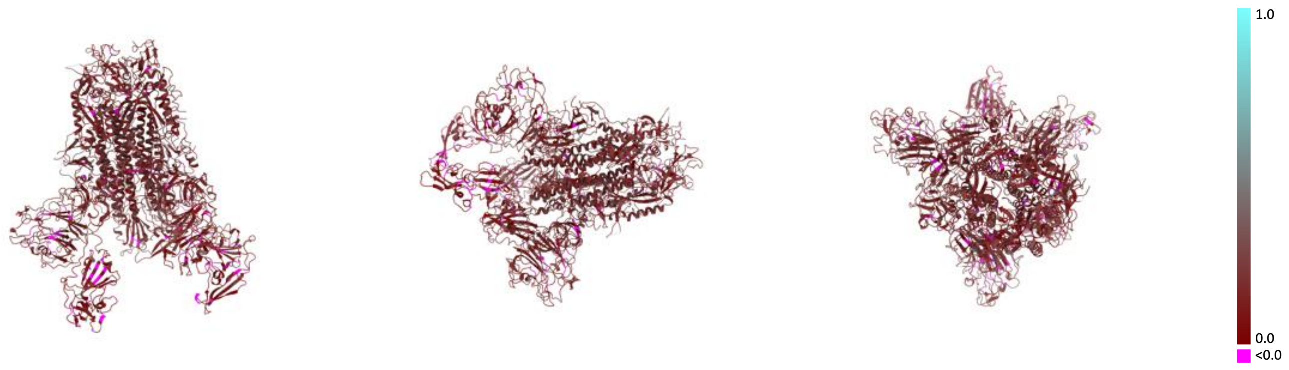
9.1 Map-model overlay



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.

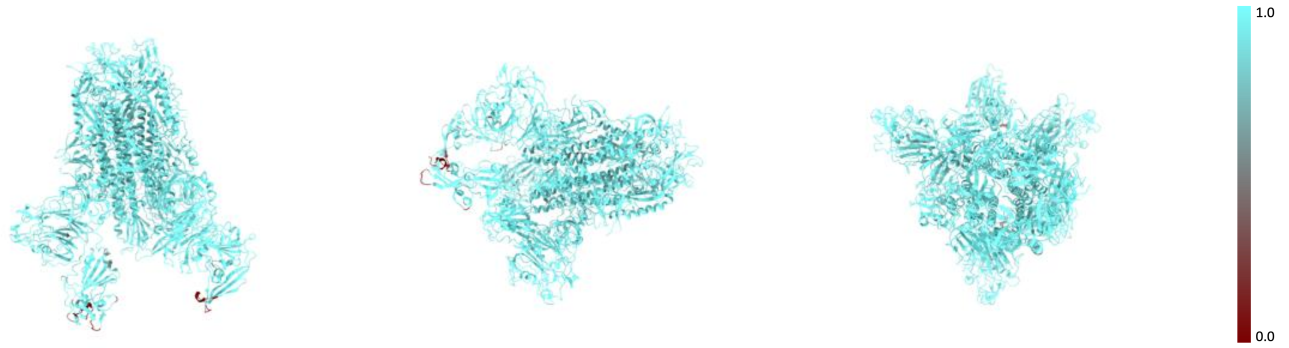
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

The images above show the model with each residue coloured according 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.

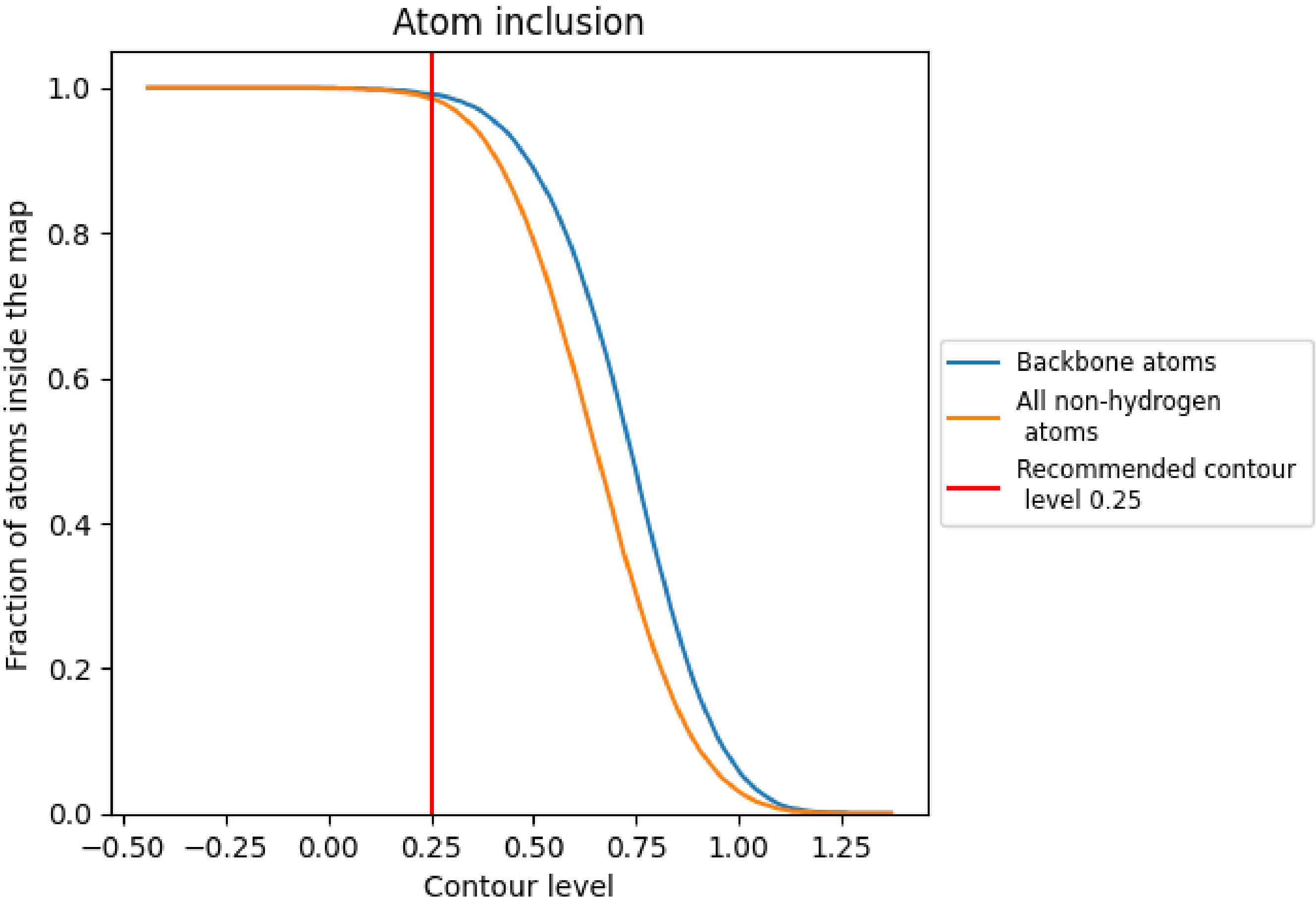
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

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, 99% 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	0.9850	0.1730
A	0.9840	0.1660
B	0.9780	0.1660
C	0.9930	0.1780
D	1.0000	0.3810
E	1.0000	0.2060
F	1.0000	0.2750
G	0.9640	0.2970
H	0.9640	0.3090
I	1.0000	0.2270
J	0.9640	0.2620
K	1.0000	0.2890
L	1.0000	0.2490
M	1.0000	0.3450
N	1.0000	0.2570
O	1.0000	0.2640
P	1.0000	0.2230
Q	1.0000	0.2090
R	1.0000	0.3880
S	0.9640	0.1540
T	1.0000	0.3710
U	0.9640	0.2700
V	1.0000	0.3060
W	0.9740	0.3730
X	1.0000	0.1930
Y	1.0000	0.2130