wwPDB EM Validation Summary Report (i)

Dec 17, 2022 – 09:44 pm GMT

PDB ID	:	6ZOW
EMDB ID	:	EMD-11328
Title	:	SARS-CoV-2 spike in prefusion state
Authors	:	Martinez, M.; Marabini, R.; Carazo, J.M.
Deposited on	:	2020-07-07
Resolution	:	3.00 Å(reported)
Based on initial models	:	6VSB, 6VYB, 6YLA

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 (i) 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 (i)) were used in the production of this report:

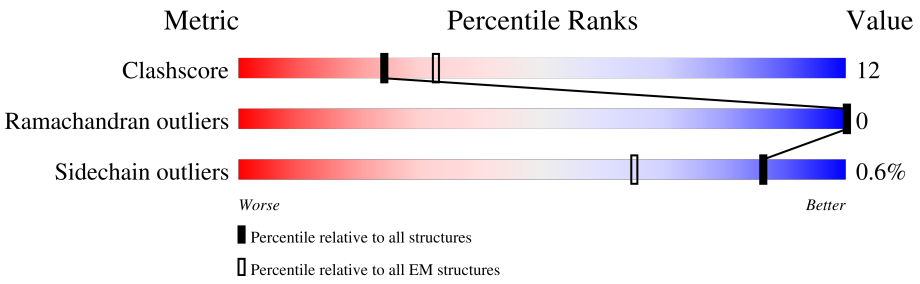
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1288	48% 15% 38%
1	B	1288	51% 21% 28%
1	C	1288	52% 21% 27%
1	a	1288	14% • 85%
2	D	2	100%
2	G	2	50% 50%
2	H	2	100%
2	I	2	100%

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Mol	Chain	Length	Quality of chain
2	J	2	100%
2	K	2	100%
2	L	2	100%
2	M	2	50% 50%
2	P	2	100%
2	S	2	50% 50%
2	T	2	50% 50%
2	V	2	50% 50%
2	X	2	50% 50%
2	Z	2	50% 50%
2	d	2	50% 50%
2	e	2	50% 100%
3	E	4	75% 25%
3	F	4	75% 25%
3	R	4	50% 50%
3	U	4	50% 50%
4	N	3	67% 33%
4	O	3	100%
4	W	3	100%
4	Y	3	100%
4	b	3	100%
4	c	3	33% 67%
5	Q	3	67% 33%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 23534 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
			Total	C	N	O	S		
1	A	801	6212	3957	1033	1196	26	0	0
1	C	943	7367	4704	1223	1408	32	0	0
1	B	930	7243	4621	1203	1387	32	0	0
1	a	188	1501	964	249	280	8	0	0

There are 340 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	GLY	-	expression tag	UNP P0DTC2
A	1239	ARG	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	PHE	-	expression tag	UNP P0DTC2
A	1246	GLN	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	PRO	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	ALA	-	expression tag	UNP P0DTC2
A	1260	TRP	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
A	1263	PRO	-	expression tag	UNP P0DTC2
A	1264	GLN	-	expression tag	UNP P0DTC2
A	1265	PHE	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1268	GLY	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	GLY	-	expression tag	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	ALA	-	expression tag	UNP P0DTC2
A	1281	TRP	-	expression tag	UNP P0DTC2
A	1282	SER	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	PRO	-	expression tag	UNP P0DTC2
A	1285	GLN	-	expression tag	UNP P0DTC2
A	1286	PHE	-	expression tag	UNP P0DTC2
A	1287	GLU	-	expression tag	UNP P0DTC2
A	1288	LYS	-	expression tag	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	GLY	-	expression tag	UNP P0DTC2
C	1239	ARG	-	expression tag	UNP P0DTC2
C	1240	SER	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	GLU	-	expression tag	UNP P0DTC2
C	1243	VAL	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	PHE	-	expression tag	UNP P0DTC2
C	1246	GLN	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2
C	1248	PRO	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2
C	1259	ALA	-	expression tag	UNP P0DTC2
C	1260	TRP	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	HIS	-	expression tag	UNP P0DTC2
C	1263	PRO	-	expression tag	UNP P0DTC2
C	1264	GLN	-	expression tag	UNP P0DTC2
C	1265	PHE	-	expression tag	UNP P0DTC2
C	1266	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1267	LYS	-	expression tag	UNP P0DTC2
C	1268	GLY	-	expression tag	UNP P0DTC2
C	1269	GLY	-	expression tag	UNP P0DTC2
C	1270	GLY	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	GLY	-	expression tag	UNP P0DTC2
C	1273	GLY	-	expression tag	UNP P0DTC2
C	1274	GLY	-	expression tag	UNP P0DTC2
C	1275	GLY	-	expression tag	UNP P0DTC2
C	1276	SER	-	expression tag	UNP P0DTC2
C	1277	GLY	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	SER	-	expression tag	UNP P0DTC2
C	1280	ALA	-	expression tag	UNP P0DTC2
C	1281	TRP	-	expression tag	UNP P0DTC2
C	1282	SER	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	PRO	-	expression tag	UNP P0DTC2
C	1285	GLN	-	expression tag	UNP P0DTC2
C	1286	PHE	-	expression tag	UNP P0DTC2
C	1287	GLU	-	expression tag	UNP P0DTC2
C	1288	LYS	-	expression tag	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	GLY	-	expression tag	UNP P0DTC2
B	1239	ARG	-	expression tag	UNP P0DTC2
B	1240	SER	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	GLU	-	expression tag	UNP P0DTC2
B	1243	VAL	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	PHE	-	expression tag	UNP P0DTC2
B	1246	GLN	-	expression tag	UNP P0DTC2
B	1247	GLY	-	expression tag	UNP P0DTC2
B	1248	PRO	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	SER	-	expression tag	UNP P0DTC2
B	1259	ALA	-	expression tag	UNP P0DTC2
B	1260	TRP	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
B	1263	PRO	-	expression tag	UNP P0DTC2
B	1264	GLN	-	expression tag	UNP P0DTC2
B	1265	PHE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	LYS	-	expression tag	UNP P0DTC2
B	1268	GLY	-	expression tag	UNP P0DTC2
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	GLY	-	expression tag	UNP P0DTC2
B	1274	GLY	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	SER	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	SER	-	expression tag	UNP P0DTC2
B	1280	ALA	-	expression tag	UNP P0DTC2
B	1281	TRP	-	expression tag	UNP P0DTC2
B	1282	SER	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	PRO	-	expression tag	UNP P0DTC2
B	1285	GLN	-	expression tag	UNP P0DTC2
B	1286	PHE	-	expression tag	UNP P0DTC2
B	1287	GLU	-	expression tag	UNP P0DTC2
B	1288	LYS	-	expression tag	UNP P0DTC2
a	682	GLY	ARG	engineered mutation	UNP P0DTC2
a	683	SER	ARG	engineered mutation	UNP P0DTC2
a	685	SER	ARG	engineered mutation	UNP P0DTC2
a	986	PRO	LYS	engineered mutation	UNP P0DTC2
a	987	PRO	VAL	engineered mutation	UNP P0DTC2
a	1209	GLY	-	expression tag	UNP P0DTC2
a	1210	SER	-	expression tag	UNP P0DTC2
a	1211	GLY	-	expression tag	UNP P0DTC2
a	1212	TYR	-	expression tag	UNP P0DTC2
a	1213	ILE	-	expression tag	UNP P0DTC2
a	1214	PRO	-	expression tag	UNP P0DTC2
a	1215	GLU	-	expression tag	UNP P0DTC2
a	1216	ALA	-	expression tag	UNP P0DTC2
a	1217	PRO	-	expression tag	UNP P0DTC2
a	1218	ARG	-	expression tag	UNP P0DTC2
a	1219	ASP	-	expression tag	UNP P0DTC2
a	1220	GLY	-	expression tag	UNP P0DTC2
a	1221	GLN	-	expression tag	UNP P0DTC2
a	1222	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
a	1223	TYR	-	expression tag	UNP P0DTC2
a	1224	VAL	-	expression tag	UNP P0DTC2
a	1225	ARG	-	expression tag	UNP P0DTC2
a	1226	LYS	-	expression tag	UNP P0DTC2
a	1227	ASP	-	expression tag	UNP P0DTC2
a	1228	GLY	-	expression tag	UNP P0DTC2
a	1229	GLU	-	expression tag	UNP P0DTC2
a	1230	TRP	-	expression tag	UNP P0DTC2
a	1231	VAL	-	expression tag	UNP P0DTC2
a	1232	LEU	-	expression tag	UNP P0DTC2
a	1233	LEU	-	expression tag	UNP P0DTC2
a	1234	SER	-	expression tag	UNP P0DTC2
a	1235	THR	-	expression tag	UNP P0DTC2
a	1236	PHE	-	expression tag	UNP P0DTC2
a	1237	LEU	-	expression tag	UNP P0DTC2
a	1238	GLY	-	expression tag	UNP P0DTC2
a	1239	ARG	-	expression tag	UNP P0DTC2
a	1240	SER	-	expression tag	UNP P0DTC2
a	1241	LEU	-	expression tag	UNP P0DTC2
a	1242	GLU	-	expression tag	UNP P0DTC2
a	1243	VAL	-	expression tag	UNP P0DTC2
a	1244	LEU	-	expression tag	UNP P0DTC2
a	1245	PHE	-	expression tag	UNP P0DTC2
a	1246	GLN	-	expression tag	UNP P0DTC2
a	1247	GLY	-	expression tag	UNP P0DTC2
a	1248	PRO	-	expression tag	UNP P0DTC2
a	1249	GLY	-	expression tag	UNP P0DTC2
a	1250	HIS	-	expression tag	UNP P0DTC2
a	1251	HIS	-	expression tag	UNP P0DTC2
a	1252	HIS	-	expression tag	UNP P0DTC2
a	1253	HIS	-	expression tag	UNP P0DTC2
a	1254	HIS	-	expression tag	UNP P0DTC2
a	1255	HIS	-	expression tag	UNP P0DTC2
a	1256	HIS	-	expression tag	UNP P0DTC2
a	1257	HIS	-	expression tag	UNP P0DTC2
a	1258	SER	-	expression tag	UNP P0DTC2
a	1259	ALA	-	expression tag	UNP P0DTC2
a	1260	TRP	-	expression tag	UNP P0DTC2
a	1261	SER	-	expression tag	UNP P0DTC2
a	1262	HIS	-	expression tag	UNP P0DTC2
a	1263	PRO	-	expression tag	UNP P0DTC2
a	1264	GLN	-	expression tag	UNP P0DTC2

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

- 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
			Total	C	N	O		
2	D	2	28	16	2	10	0	0
			Total	C	N	O		
2	G	2	28	16	2	10	0	0
			Total	C	N	O		
2	H	2	28	16	2	10	0	0
			Total	C	N	O		
2	I	2	28	16	2	10	0	0

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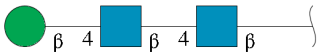
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	J	2	28	16	2	10	0	0
2	K	2	28	16	2	10	0	0
2	L	2	28	16	2	10	0	0
2	M	2	28	16	2	10	0	0
2	P	2	28	16	2	10	0	0
2	S	2	28	16	2	10	0	0
2	T	2	28	16	2	10	0	0
2	V	2	28	16	2	10	0	0
2	X	2	28	16	2	10	0	0
2	Z	2	28	16	2	10	0	0
2	d	2	28	16	2	10	0	0
2	e	2	28	16	2	10	0	0

- 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.

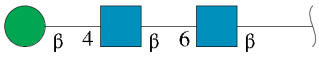
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	E	4	50	28	2	20	0	0
3	F	4	50	28	2	20	0	0
3	R	4	50	28	2	20	0	0
3	U	4	50	28	2	20	0	0

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



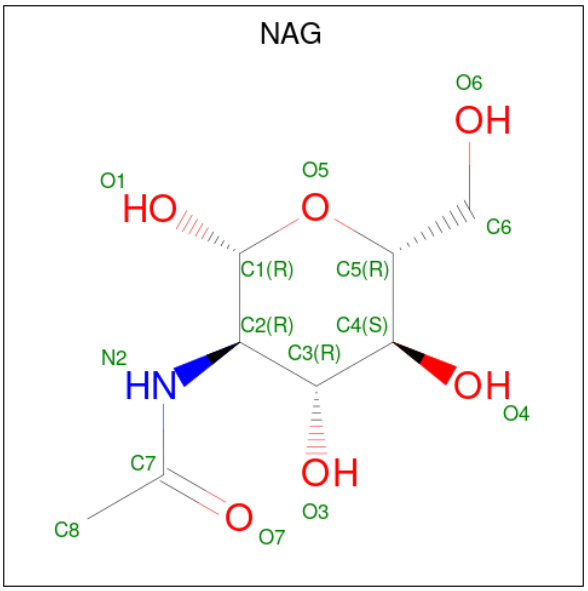
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	N	3	39	22	2	15	0	0
4	O	3	39	22	2	15	0	0
4	W	3	39	22	2	15	0	0
4	Y	3	39	22	2	15	0	0
4	b	3	39	22	2	15	0	0
4	c	3	39	22	2	15	0	0

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			70	40	5	25	
6	A	1	Total	C	N	O	0
			70	40	5	25	
6	A	1	Total	C	N	O	0
			70	40	5	25	
6	A	1	Total	C	N	O	0
			70	40	5	25	
6	A	1	Total	C	N	O	0
			70	40	5	25	
6	C	1	Total	C	N	O	0
			112	64	8	40	
6	C	1	Total	C	N	O	0
			112	64	8	40	
6	C	1	Total	C	N	O	0
			112	64	8	40	
6	C	1	Total	C	N	O	0
			112	64	8	40	
6	C	1	Total	C	N	O	0
			112	64	8	40	
6	C	1	Total	C	N	O	0
			112	64	8	40	
6	C	1	Total	C	N	O	0
			112	64	8	40	
6	C	1	Total	C	N	O	0
			112	64	8	40	
6	B	1	Total	C	N	O	0
			56	32	4	20	

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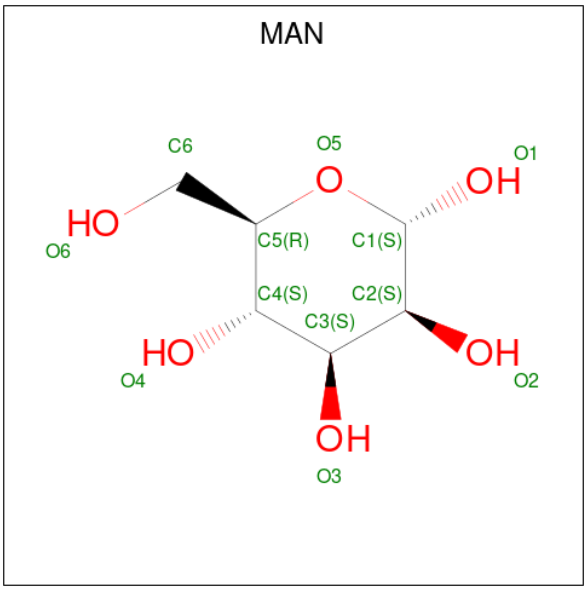
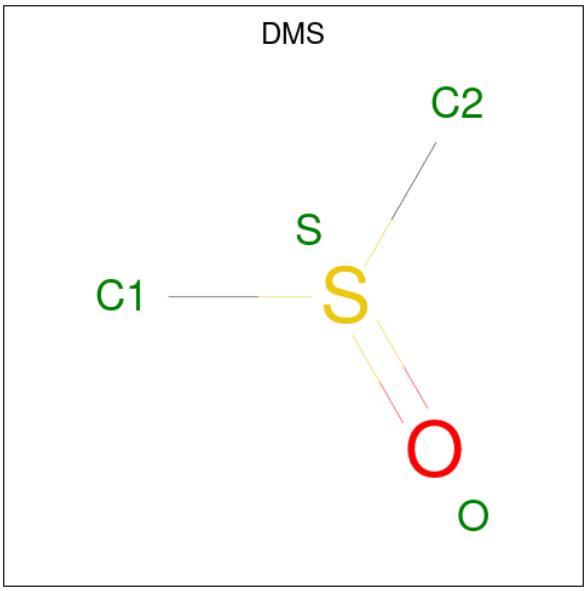
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	B	1	56	32	4	20	0
6	B	1	56	32	4	20	0
6	B	1	56	32	4	20	0
6	a	1	14	8	1	5	0

- Molecule 7 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
7	A	1	11	6	5	0
7	B	1	11	6	5	0

- Molecule 8 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				AltConf
8	a	1	Total	C	O	S	0
			12	6	3	3	
8	a	1	Total	C	O	S	0
			12	6	3	3	
8	a	1	Total	C	O	S	0
			12	6	3	3	

- Molecule 9 is water.

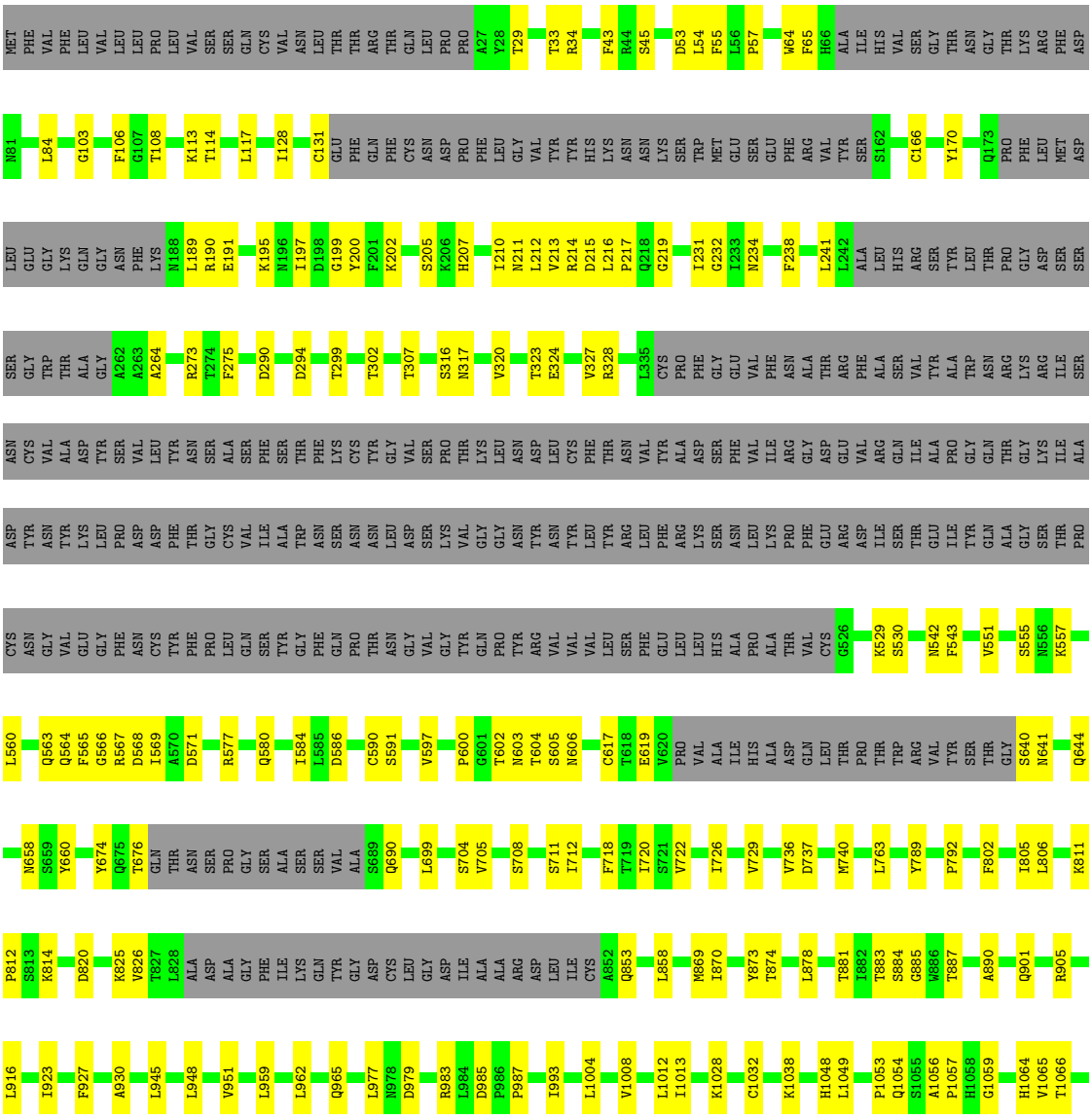
Mol	Chain	Residues	Atoms		AltConf
9	a	4	Total	O	0
			4	4	

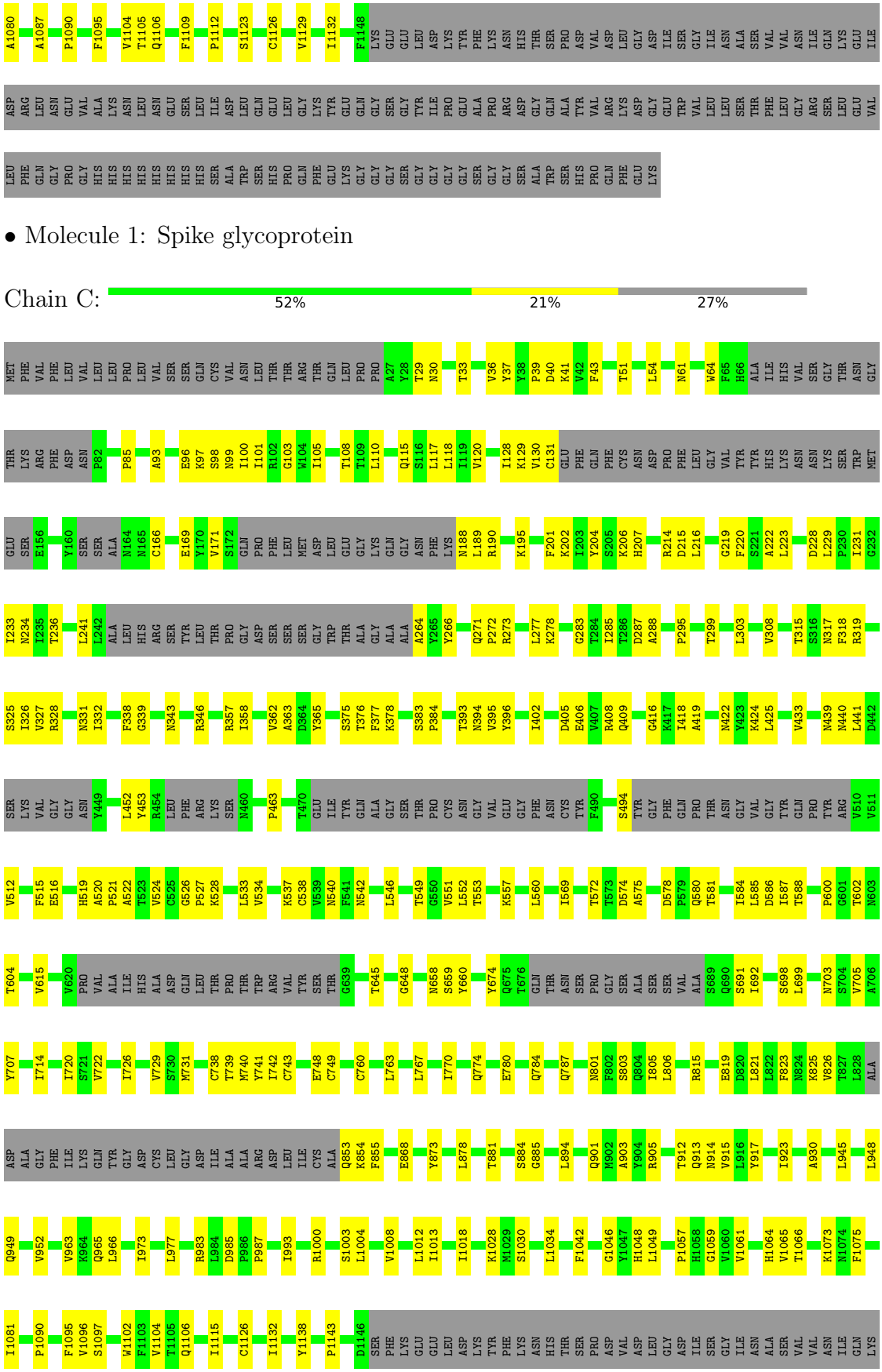
3 Residue-property plots (i)

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

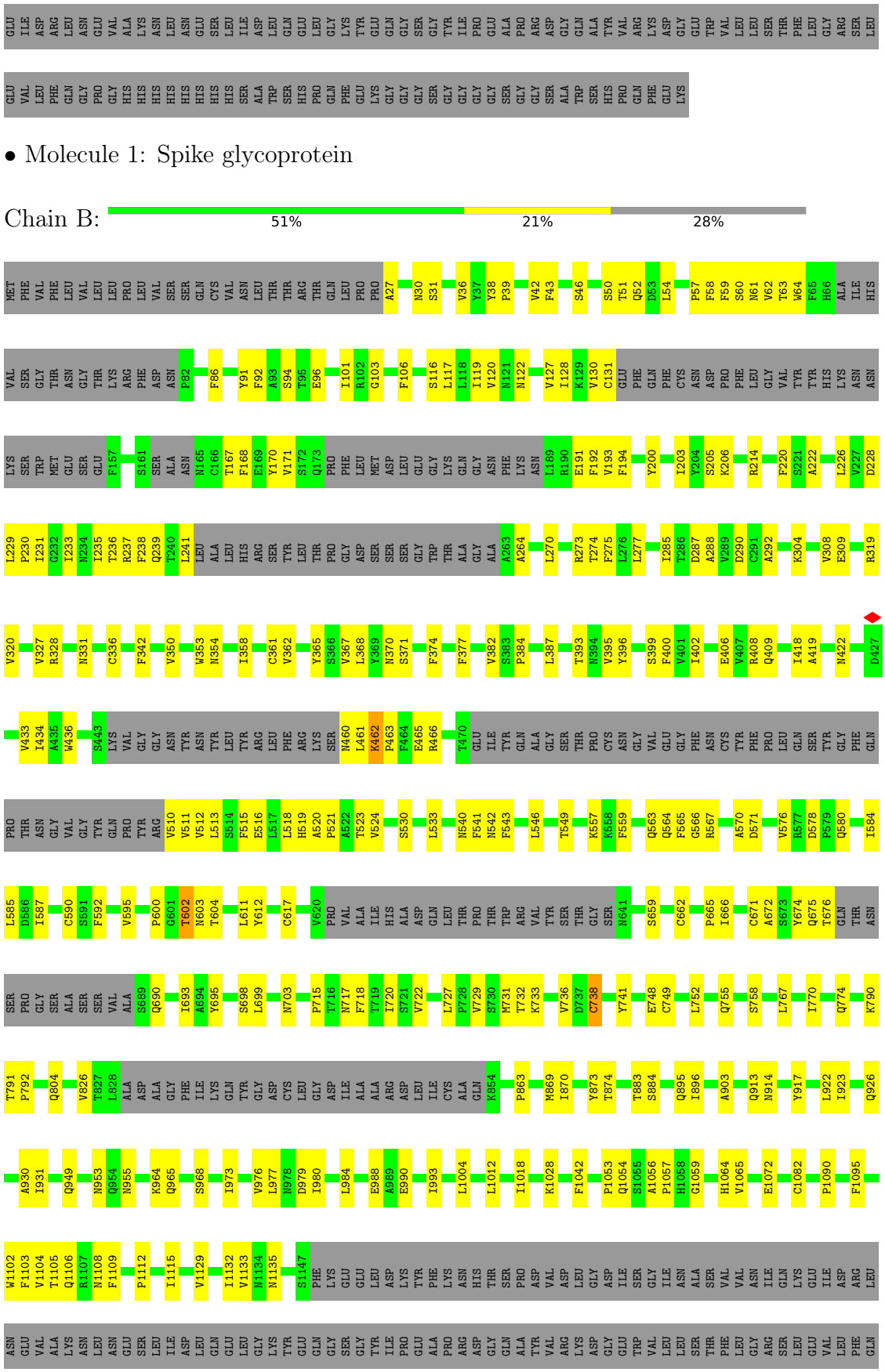
Chain A: 48% 15% 38%

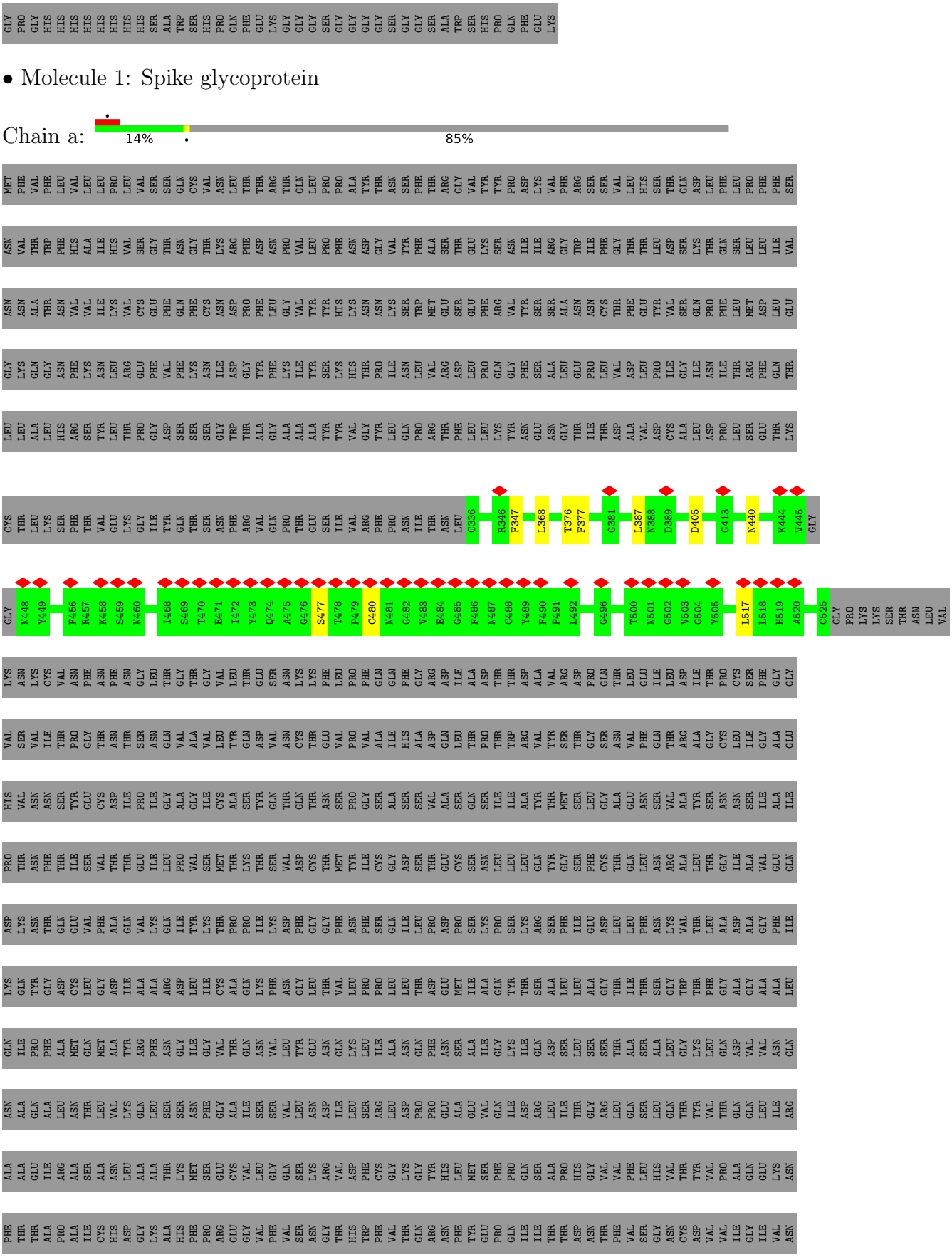




- Molecule 1: Spike glycoprotein

Chain C: 52% 21% 27%


GLU ILE ASP ARG LEU ASN GLU VAL ALA LYS ASN LEU ASN GLU SER LEU ILE ASP LEU GLN GLU LEU GLY LYS TYR GLU GLN GLY SER GLY TYR ILE PRO GLU ALA PRO ARG ASP GLY GLN ALA TYR VAL ARG LYS ASP GLY GLU TRP VAL LEU LEU SER THR PHE LEU GLY ARG SER LEU
GLU VAL LEU PHE GLN GLY PRO GLY HIS HIS HIS HIS HIS HIS HIS HIS HIS SER ALA TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLY GLY GLY GLY SER GLY GLY SER ALA TRP SER HIS PRO GLN PHE GLU LYS
• Molecule 1: Spike glycoprotein
Chain B:
51%
21%
28%
MET PHE VAL PHE LEU VAL LEU LEU PRO LEU VAL SER SER GLN CYS VAL ASN LEU THR THR ARG THR GLN LEU PRO PRO A27 N30 S31 V36 Y37 Y38 P39 V42 F43 S46 S50 T51 Q52 D53 L54 P57 F58 F59 S60 N61 V62 T63 W64 F65 H66 ALA ILE HIS
VAL SER GLY THR ASN GLY THR LYS ARG PHE ASP ASN P82 F86 Y91 F92 A93 S94 T95 E96 I101 R102 G103 F106 S116 L117 L118 I119 V120 N121 N122 V127 I128 K129 V130 C131 GLU PHE GLN PHE CYS ASN ASP PRO PHE LEU GLY VAL TYR TYR HIS LYS ASN ASN
LYS SER TRP MET GLU SER GLU F157 S161 SER ALA ASN N165 C166 T167 F168 E169 Y170 V171 S172 Q173 PRO PHE LEU MET ASP LEU GLU GLY LYS GLN GLY ASN PHE LYS ASN L189 R190 E191 F192 V193 F194 Y200 I203 Y204 S205 K206 R214 F220 S221 A222 L226 V227 D228
L229 P230 I231 G232 I233 N234 I235 T236 R237 F238 Q239 T240 L241 LEU ALA LEU HIS ARG SER TYR LEU THR PRO GLY ASP SER SER SER GLY TRP THR ALA GLY ALA A263 A264 L270 R273 T274 F275 L276 L277 I285 T286 D287 A288 V289 D290 C291 A292 K304 V308 E309 R319
V320 V327 R328 N331 G336 F342 V350 W353 N354 I358 C361 V362 Y365 S366 V367 L368 Y369 N370 S371 F374 F377 V382 S383 P384 L387 T393 N394 V395 Y396 S399 F400 V401 I402 E406 V407 R408 Q409 I418 A419 N422 D427
V433 I434 A435 W436 S443 LYS VAL GLY GLY ASN TYR ASN TYR LEU TYR ARG LEU PHE ARG LYS SER N460 L461 K462 P463 F464 E465 R466 T470 GLU ILE TYR GLN ALA GLY SER THR PRO CYS ASN GLY VAL GLU GLY PHE ASN CYS TYR PHE PRO LEU GLN SER TYR GLY PHE GLN
PRO THR ASN GLY VAL GLY TYR GLN PRO TYR ARG V510 V511 V512 L513 S514 F515 E516 L517 L518 H519 A520 P521 A522 T523 V524 S530 L533 N540 F541 N542 F543 L546 T549 K557 K558 F559 Q563 Q564 F565 G566 R567 A570 D571 V576 R577 D578 P579 Q580 I584
L585 D586 I587 C590 S591 F592 V595 P600 G601 T602 N603 T604 L611 Y612 C617 V620 PRO VAL ALA ILE HIS ALA ASP GLN LEU THR PRO THR TRP ARG VAL TYR SER THR GLY SER N641 S659 C662 P665 I666 C671 A672 S673 Y674 Q675 T676 GLN THR ASN
SER PRO GLY SER ALA SER SER VAL ALA S689 Q690 I693 A694 Y695 S698 L699 N703 P715 T716 N717 F718 T719 I720 S721 V722 L727 P728 V729 S730 M731 T732 K733 V736 D737 C738 Y741 E748 C749 L752 Q755 S758 L767 I770 Q774 K790
T791 P792 Q804 V826 T827 L828 ALA ASP ALA GLY PHE ILE LYS GLN TYR GLY ASP CYS LEU GLY ASP ILE ALA ALA ARG ASP LEU ILE CYS ALA GLN K854 P863 M869 I870 Y873 T874 T883 S884 Q895 I896 A903 Q913 N914 Y917 L922 I923 Q926
A930 I931 Q949 N953 Q954 N955 K964 Q965 S968 I973 V976 L977 N978 D979 I980 L984 E988 A989 E990 I993 L1004 L1012 I1018 K1028 F1042 P1053 Q1054 S1055 A1056 P1057 H1058 G1059 H1064 V1065 E1072 C1082 P1090 F1095
W1102 F1103 V1104 T1105 Q1106 R1107 N1108 F1109 P1112 I1115 V1129 I1132 V1133 N1134 N1135 S1147 PHE LYS GLU GLU LEU ASP LYS PHE LYS ASN HIS THR SER PRO ASP VAL ASP LEU GLY ASP ILE SER GLY ILE ASN ALA SER VAL VAL ASN ILE GLN LYS GLU ILE ASP ARG LEU
ASN GLU VAL ALA LYS ASN LEU ASN GLU SER LEU ILE ASP LEU GLN GLU LEU GLY LYS TYR GLU GLN GLY SER GLY TYR ILE PRO GLU ALA PRO ARG ASP GLY GLN ALA TYR VAL ARG LYS ASP GLY GLU TRP VAL LEU LEU SER THR PHE LEU GLY ARG SER LEU GLU VAL LEU PHE GLN


GLY PRO GLY HIS HIS HIS HIS HIS HIS HIS HIS SER ALA TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLY GLY GLY GLY GLY SER GLY GLY SER ALA TRP SER HIS PRO GLN PHE GLU LYS
• Molecule 1: Spike glycoprotein
Chain a:
14%
85%
MET PHE VAL PHE LEU VAL LEU LEU LEU PRO LEU VAL SER SER GLN CYS VAL ASN LEU THR THR ARG THR GLN LEU PRO PRO ALA TYR THR ASN SER PHE THR ARG GLY VAL TYR TYR PRO ASP LYS VAL PHE ARG SER SER LEU HIS SER THR GLN ASP LEU PHE LEU PRO PHE PHE SER
ASN VAL THR TRP PHE HIS ALA ILE HIS VAL SER GLY THR ASN GLY THR LYS ARG PHE ASP ASN PRO VAL LEU PRO PHE ASN ASP GLY VAL TYR PHE ALA SER THR GLU LYS SER ASN ILE ILE ARG GLY TRP ILE PHE GLY THR THR LEU ASP SER LYS THR GLN SER LEU LEU ILE VAL
ASN ASN ALA THR ASN VAL VAL ILE LYS VAL CYS GLU PHE GLN PHE CYS ASN ASP PRO PHE LEU GLY VAL TYR TYR HIS LYS ASN ASN LYS SER TRP MET GLU SER GLU PHE ARG VAL TYR SER SER ALA ASN ASN CYS THR PHE GLU TYR VAL SER GLN PRO PHE LEU MET ASP LEU GLU
GLY LYS GLN GLY ASN PHE LYS ASN LEU ARG GLU PHE VAL PHE LYS ASN ILE ASP GLY TYR PHE LYS ILE TYR SER LYS HIS THR PRO ILE ASN LEU VAL ARG ASP LEU PRO GLN GLY PHE SER SER ALA LEU GLU PRO LEU VAL ASP LEU PRO ILE GLY ILE ASN ILE THR ARG PHE GLN THR
LEU LEU ALA LEU HIS ARG SER TYR LEU THR PRO GLY ASP SER SER SER GLY TRP THR ALA LEU ALA ALA ALA TYR TYR LEU GLN PRO ARG THR PHE LEU LEU LYS TYR ASN GLU ASN GLY THR ILE THR ASP ALA VAL ASP CYS PRO ALA LEU SER GLU THR LYS
CYS THR LEU LYS SER PHE THR VAL GLU LYS GLY ILE TYR GLN THR SER ASN PHE ARG VAL GLN PRO THR GLU SER ILE VAL ARG PHE PRO ASN ILE THR ASN LEU C336 R346 F347 L368 T376 F377 G381 L387 N388 D389 D405 G413 N440 K444 V445 GLY
GLY N448 Y449 F456 R457 K458 S459 N460 I468 S469 T470 E471 I472 V473 Q474 A475 G476 S477 T478 P479 C480 N481 G482 V483 E484 G485 F486 N487 C488 Y489 F490 P491 L492 G496 T500 N501 G502 V503 G504 Y505 L517 L518 H519 A520 C525 GLY PRO LYS LYS SER THR ASN LEU VAL
LYS ASN LYS CYS VAL ASN PHE ASN PHE ASN GLY LEU THR GLY THR GLY VAL LEU THR GLU SER ASN LYS LYS PHE LEU PRO PHE GLN GLN PHE GLY ARG ASP ILE ALA ASP THR THR ASP ALA VAL ARG ASP PRO GLN THR LEU GLU ILE LEU ASP ILE THR PRO CYS SER PHE GLY GLY
VAL SER VAL ILE THR PRO GLY THR ASN THR SER ASN GLN VAL ALA VAL LEU TYR GLN ASP VAL ASN CYS THR GLU VAL PRO VAL ALA ILE HIS ALA ASP GLN LEU THR PRO THR TRP ARG VAL TYR SER THR GLY SER ASN VAL PHE GLN THR ARG ALA GLY CYS LEU ILE GLY ALA GLU
HIS VAL ASN ASN SER TYR GLU CYS ASP ILE PRO ILE GLY ALA GLY ILE CYS ALA SER TYR GLN THR GLN THR ASN SER PRO GLY SER ALA SER SER VAL ALA SER GLN SER ILE ILE ALA TYR THR MET SER LEU GLY ALA GLU ASN SER VAL ALA TYR SER ASN ASN SER ILE ALA ILE
PRO THR ASN PHE THR ILE SER VAL THR THR GLU ILE LEU PRO VAL SER MET THR LYS THR SER VAL ASP CYS THR MET TYR ILE CYS GLY ASP SER SER THR GLU CYS SER ASN LEU LEU LEU GLN TYR GLY SER PHE CYS THR GLN LEU ASN ARG ALA LEU GLY ILE ALA VAL GLN
ASP LYS ASN THR GLN GLU VAL PHE ALA GLN VAL LYS GLN ILE TYR LYS THR PRO PRO ILE LYS ASP PHE GLY GLY PHE ASN PHE SER GLN ILE LEU PRO ASP PRO SER LYS PRO SER LYS ARG SER PHE ILE GLU ASP LEU LEU PHE ASN LYS VAL THR LEU ALA ASP ALA GLY PHE ILE
LYS GLN TYR GLY ASP CYS LEU GLY ASP ILE ALA ALA ARG ASP LEU ILE CYS ALA GLN LYS PHE ASN GLY LEU THR VAL LEU PRO PRO LEU LEU THR ASP GLU MET ILE ALA GLN TYR THR SER ALA LEU LEU ALA GLY TYR THR ILE THR SER GLY TRP THR PHE GLY ALA GLY ALA LEU
GLN ILE PRO PHE ALA MET GLN MET ALA TYR ARG PHE ASN GLY ILE GLY VAL THR GLN LYS VAL ASN VAL LEU TYR GLU ASN GLN LYS LEU ILE ALA ASN GLN PHE ASN SER ILE ILE GLY LYS ILE GLN ASP SER LEU SER SER THR ALA SER ALA LEU GLY VAL VAL ASN GLN
ASN ALA GLN ALA LEU ASN THR LEU VAL LYS GLN LEU SER SER ASN PHE GLY ALA ILE SER VAL LEU ASN ASP ILE LEU SER ARG LEU ASP PRO PRO GLU ALA GLU VAL CYS GLN ILE ILE ASP ARG LEU ILE THR GLY ILE GLN GLN SER ALA LEU GLN ASP VAL THR GLN GLN ILE LEU ARG
ALA ALA GLU ILE ARG ALA ALA SER LEU ALA ALA ALA THR LYS MET SER GLU CYS VAL LEU GLY GLN SER SER LYS ARG VAL ASP PHE PRO ARG GLU GLY VAL LYS GLY TYR HIS LEU MET SER PHE PRO GLN SER SER ALA PRO HIS GLY VAL VAL PHE LEU HIS VAL THR TYR VAL PRO ALA GLN GLU VAL ASN LYS ILE
PHE THR THR ALA PRO ALA ILE CYS HIS ASP GLY LYS ALA HIS PHE PRO ARG GLU GLY VAL PHE VAL SER ASN GLY THR HIS TRP PHE VAL THR GLN ARG ASN PHE TYR GLU PRO GLN ILE ILE THR THR ASP ASN THR PHE VAL SER GLY ASN THR ASP ASN THR PHE VAL PHE ILE VAL ASP

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

GLU SER LEU ILE ASP LEU GLN GLU LEU GLY LYS TYR GLU GLN GLY SER GLY TYR ILE PRO GLU ALA PRO ARG ASP GLY GLN ALA TYR VAL ARG LYS ASP GLY GLU TRP VAL LEU LEU SER THR PHE LEU GLY ARG SER LEU GLU VAL LEU PHE GLN GLY PRO GLY HIS HIS HIS HIS HIS

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

• 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 G: 50% 50%

NAG1 NAG2

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

Chain H: 100%

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

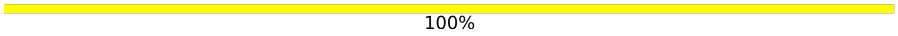
Chain J: 100%

NAG1 NAG2

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

Chain K: 100%

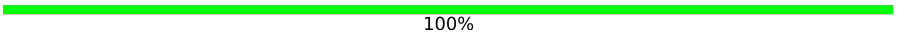
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L: 

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

Chain M:

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

Chain P: 

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

Chain S:

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

Chain T:

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

Chain V:

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

Chain X:

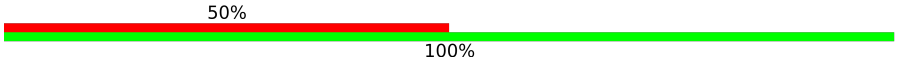
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:

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

Chain d:

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

Chain e: 

• 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:

• 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 F:

• 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 R: 50% 50%

NAG1 NAG2 BMA3 MAN4

• 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 U: 50% 50%

NAG1 NAG2 BMA3 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 N: 67% 33%

NAG1 NAG2 BMA3

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

Chain O: 100%

NAG1 NAG2 BMA3

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

Chain W: 100%

NAG1 NAG2 BMA3

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

Chain Y: 100%

NAG1 NAG2 BMA3

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

Chain b: 100%

NAG1 NAG2 BMA3

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

Chain c:

• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	203000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	36	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.612	Depositor
Minimum map value	-0.570	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.129	Depositor
Map size (Å)	452.30402, 452.30402, 452.30402	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.047, 1.047, 1.047	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: BMA, DMS, MAN, 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	0.36	0/6337	0.48	0/8620
1	B	0.36	0/7395	0.50	1/10059 (0.0%)
1	C	0.36	0/7522	0.48	0/10229
1	a	0.26	0/1543	0.45	0/2099
All	All	0.35	0/22797	0.48	1/31007 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	738	CYS	CA-CB-SG	5.18	123.32	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6212	0	6103	144	0
1	B	7243	0	7097	216	0
1	C	7367	0	7205	202	0
1	a	1501	0	1418	0	0
2	D	28	0	25	1	0
2	G	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0	0
2	L	28	0	25	1	0
2	M	28	0	25	1	0
2	P	28	0	25	0	0
2	S	28	0	25	1	0
2	T	28	0	25	1	0
2	V	28	0	25	2	0
2	X	28	0	25	1	0
2	Z	28	0	25	1	0
2	d	28	0	25	0	0
2	e	28	0	25	0	0
3	E	50	0	43	0	0
3	F	50	0	43	0	0
3	R	50	0	43	0	0
3	U	50	0	43	1	0
4	N	39	0	34	1	0
4	O	39	0	34	0	0
4	W	39	0	34	1	0
4	Y	39	0	34	0	0
4	b	39	0	34	0	0
4	c	39	0	34	0	0
5	Q	39	0	34	2	0
6	A	70	0	65	2	0
6	B	56	0	52	2	0
6	C	112	0	104	3	0
6	a	14	0	13	0	0
7	A	11	0	10	0	0
7	B	11	0	10	1	0
8	a	12	0	18	0	0
9	a	4	0	0	0	0
All	All	23534	0	22905	538	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 538 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:C:308:VAL:HG22	1:C:602:THR:HG23	1.52	0.89
1:C:190:ARG:HH11	1:C:207:HIS:HB3	1.41	0.86
1:B:57:PRO:HA	1:B:273:ARG:HH12	1.41	0.86
1:B:273:ARG:HD2	1:B:292:ALA:HB3	1.62	0.80
1:B:732:THR:OG1	1:B:955:ASN:ND2	2.16	0.79

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	783/1288 (61%)	752 (96%)	31 (4%)	0	100	100
1	B	908/1288 (70%)	882 (97%)	26 (3%)	0	100	100
1	C	917/1288 (71%)	903 (98%)	14 (2%)	0	100	100
1	a	184/1288 (14%)	173 (94%)	11 (6%)	0	100	100
All	All	2792/5152 (54%)	2710 (97%)	82 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	701/1113 (63%)	701 (100%)	0	100	100
1	B	816/1113 (73%)	812 (100%)	4 (0%)	88	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	829/1113 (74%)	829 (100%)	0	100	100
1	a	164/1113 (15%)	154 (94%)	10 (6%)	18	53
All	All	2510/4452 (56%)	2496 (99%)	14 (1%)	86	95

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	377	PHE
1	a	387	LEU
1	a	517	LEU
1	a	477	SER
1	a	480	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	563	GLN
1	B	955	ASN
1	B	703	ASN
1	B	935	GLN
1	B	1058	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

69 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	1,2	14,14,15	0.20	0	17,19,21	0.38	0
2	NAG	D	2	2	14,14,15	0.20	0	17,19,21	0.41	0
3	NAG	E	1	1,3	14,14,15	0.33	0	17,19,21	0.50	0
3	NAG	E	2	3	14,14,15	0.22	0	17,19,21	0.40	0
3	BMA	E	3	3	11,11,12	0.48	0	15,15,17	0.74	0
3	MAN	E	4	3	11,11,12	0.64	0	15,15,17	1.16	2 (13%)
3	NAG	F	1	1,3	14,14,15	0.31	0	17,19,21	0.41	0
3	NAG	F	2	3	14,14,15	0.49	0	17,19,21	0.73	0
3	BMA	F	3	3	11,11,12	0.53	0	15,15,17	0.75	0
3	MAN	F	4	3	11,11,12	0.63	0	15,15,17	1.03	2 (13%)
2	NAG	G	1	1,2	14,14,15	0.26	0	17,19,21	0.56	0
2	NAG	G	2	2	14,14,15	0.40	0	17,19,21	1.26	2 (11%)
2	NAG	H	1	1,2	14,14,15	0.29	0	17,19,21	0.44	0
2	NAG	H	2	2	14,14,15	0.23	0	17,19,21	0.50	0
2	NAG	I	1	1,2	14,14,15	0.19	0	17,19,21	0.43	0
2	NAG	I	2	2	14,14,15	0.21	0	17,19,21	0.41	0
2	NAG	J	1	1,2	14,14,15	0.24	0	17,19,21	0.36	0
2	NAG	J	2	2	14,14,15	0.23	0	17,19,21	0.43	0
2	NAG	K	1	1,2	14,14,15	0.25	0	17,19,21	0.42	0
2	NAG	K	2	2	14,14,15	0.22	0	17,19,21	0.46	0
2	NAG	L	1	1,2	14,14,15	0.17	0	17,19,21	0.54	0
2	NAG	L	2	2	14,14,15	0.55	0	17,19,21	0.53	0
2	NAG	M	1	1,2	14,14,15	0.60	1 (7%)	17,19,21	0.62	0
2	NAG	M	2	2	14,14,15	0.54	0	17,19,21	1.31	2 (11%)
4	NAG	N	1	1,4	14,14,15	0.31	0	17,19,21	0.42	0
4	NAG	N	2	4	14,14,15	0.45	0	17,19,21	1.24	1 (5%)
4	BMA	N	3	4	11,11,12	0.50	0	15,15,17	0.76	0
4	NAG	O	1	1,4	14,14,15	0.40	0	17,19,21	0.60	0
4	NAG	O	2	4	14,14,15	0.17	0	17,19,21	0.59	0
4	BMA	O	3	4	11,11,12	0.62	0	15,15,17	0.76	0
2	NAG	P	1	1,2	14,14,15	0.51	0	17,19,21	0.54	0
2	NAG	P	2	2	14,14,15	0.27	0	17,19,21	0.48	0
5	NAG	Q	1	1,5	14,14,15	0.42	0	17,19,21	1.28	2 (11%)
5	NAG	Q	2	5	14,14,15	0.39	0	17,19,21	0.90	0
5	BMA	Q	3	5	11,11,12	1.38	2 (18%)	15,15,17	0.88	0
3	NAG	R	1	1,3	14,14,15	0.35	0	17,19,21	0.55	0
3	NAG	R	2	3	14,14,15	0.24	0	17,19,21	0.45	0
3	BMA	R	3	3	11,11,12	0.83	1 (9%)	15,15,17	0.82	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	MAN	R	4	3	11,11,12	0.66	0	15,15,17	0.92	2 (13%)
2	NAG	S	1	1,2	14,14,15	1.32	1 (7%)	17,19,21	1.87	3 (17%)
2	NAG	S	2	2	14,14,15	0.47	0	17,19,21	0.61	0
2	NAG	T	1	1,2	14,14,15	0.45	0	17,19,21	1.24	1 (5%)
2	NAG	T	2	2	14,14,15	0.57	0	17,19,21	0.55	0
3	NAG	U	1	1,3	14,14,15	0.35	0	17,19,21	0.45	0
3	NAG	U	2	3	14,14,15	0.18	0	17,19,21	0.42	0
3	BMA	U	3	3	11,11,12	0.47	0	15,15,17	0.73	0
3	MAN	U	4	3	11,11,12	0.91	1 (9%)	15,15,17	1.44	2 (13%)
2	NAG	V	1	1,2	14,14,15	0.26	0	17,19,21	0.44	0
2	NAG	V	2	2	14,14,15	0.42	0	17,19,21	1.26	2 (11%)
4	NAG	W	1	1,4	14,14,15	0.39	0	17,19,21	0.51	0
4	NAG	W	2	4	14,14,15	0.51	0	17,19,21	0.59	0
4	BMA	W	3	4	11,11,12	0.71	0	15,15,17	0.93	1 (6%)
2	NAG	X	1	1,2	14,14,15	0.29	0	17,19,21	0.44	0
2	NAG	X	2	2	14,14,15	0.33	0	17,19,21	0.52	0
4	NAG	Y	1	1,4	14,14,15	0.21	0	17,19,21	0.56	0
4	NAG	Y	2	4	14,14,15	0.27	0	17,19,21	0.39	0
4	BMA	Y	3	4	11,11,12	0.64	0	15,15,17	0.71	0
2	NAG	Z	1	1,2	14,14,15	0.35	0	17,19,21	1.31	1 (5%)
2	NAG	Z	2	2	14,14,15	0.18	0	17,19,21	0.54	0
4	NAG	b	1	1,4	14,14,15	0.47	0	17,19,21	0.81	0
4	NAG	b	2	4	14,14,15	0.26	0	17,19,21	0.65	0
4	BMA	b	3	4	11,11,12	0.54	0	15,15,17	0.80	0
4	NAG	c	1	1,4	14,14,15	0.42	0	17,19,21	1.32	2 (11%)
4	NAG	c	2	4	14,14,15	0.17	0	17,19,21	0.67	1 (5%)
4	BMA	c	3	4	11,11,12	0.62	0	15,15,17	0.71	0
2	NAG	d	1	1,2	14,14,15	0.46	0	17,19,21	1.37	1 (5%)
2	NAG	d	2	2	14,14,15	0.26	0	17,19,21	0.55	0
2	NAG	e	1	1,2	14,14,15	0.23	0	17,19,21	0.51	0
2	NAG	e	2	2	14,14,15	0.38	0	17,19,21	0.54	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
2	NAG	D	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	S	2	2	-	1/6/23/26	0/1/1/1
2	NAG	T	1	1,2	-	5/6/23/26	0/1/1/1
2	NAG	T	2	2	-	1/6/23/26	0/1/1/1
3	NAG	U	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	U	2	3	-	0/6/23/26	0/1/1/1
3	BMA	U	3	3	-	2/2/19/22	0/1/1/1
3	MAN	U	4	3	-	0/2/19/22	0/1/1/1
2	NAG	V	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	V	2	2	-	5/6/23/26	0/1/1/1
4	NAG	W	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	W	2	4	-	4/6/23/26	0/1/1/1
4	BMA	W	3	4	-	2/2/19/22	0/1/1/1
2	NAG	X	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	X	2	2	-	3/6/23/26	0/1/1/1
4	NAG	Y	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	2/6/23/26	0/1/1/1
4	BMA	Y	3	4	-	1/2/19/22	0/1/1/1
2	NAG	Z	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	2/6/23/26	0/1/1/1
4	NAG	b	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	b	2	4	-	4/6/23/26	0/1/1/1
4	BMA	b	3	4	-	0/2/19/22	0/1/1/1
4	NAG	c	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	c	2	4	-	0/6/23/26	0/1/1/1
4	BMA	c	3	4	-	0/2/19/22	0/1/1/1
2	NAG	d	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	d	2	2	-	1/6/23/26	0/1/1/1
2	NAG	e	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	e	2	2	-	2/6/23/26	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	1	NAG	O5-C1	-4.82	1.36	1.43
5	Q	3	BMA	C4-C5	2.96	1.59	1.53
5	Q	3	BMA	O5-C1	2.67	1.48	1.43
3	R	3	BMA	C1-C2	2.25	1.57	1.52
3	U	4	MAN	C1-C2	2.09	1.57	1.52

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	d	1	NAG	C1-O5-C5	4.80	118.69	112.19
2	Z	1	NAG	C2-N2-C7	4.56	129.40	122.90
3	U	4	MAN	C1-O5-C5	4.55	118.36	112.19
2	V	2	NAG	C2-N2-C7	4.36	129.11	122.90
4	c	1	NAG	C2-N2-C7	4.35	129.09	122.90

There are no chirality outliers.

5 of 105 torsion outliers are listed below:

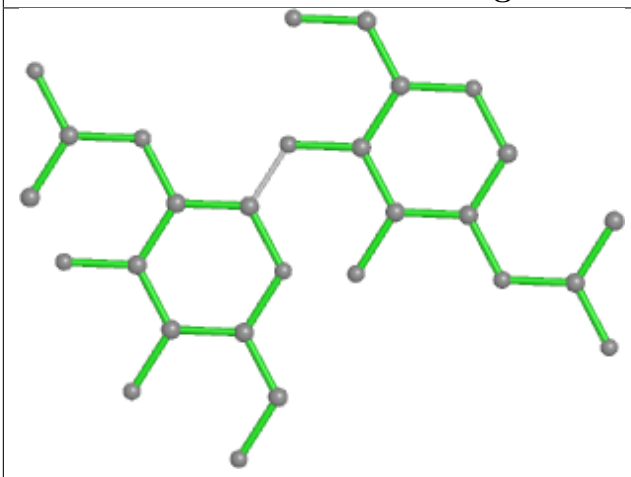
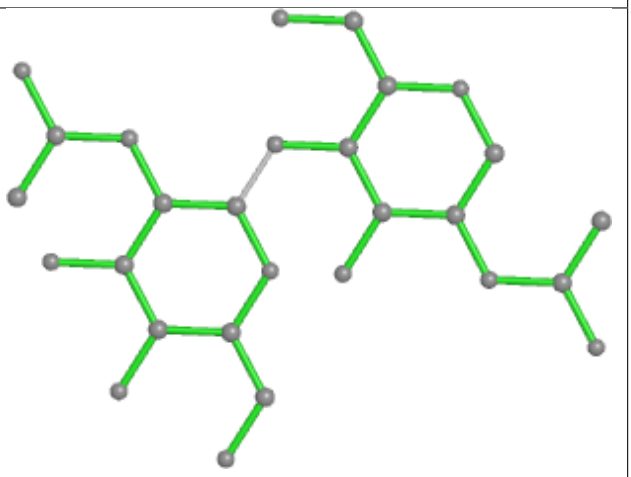
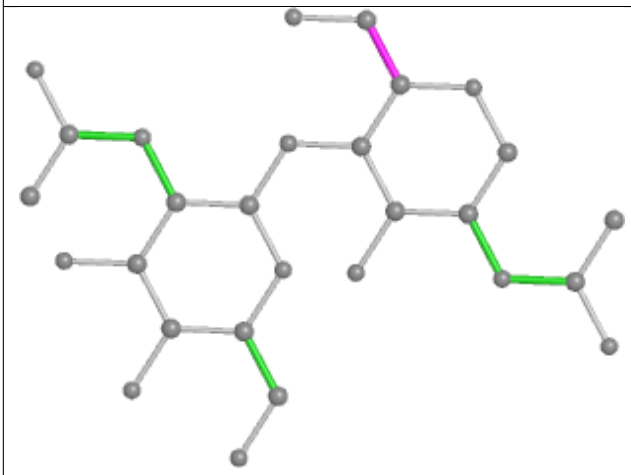
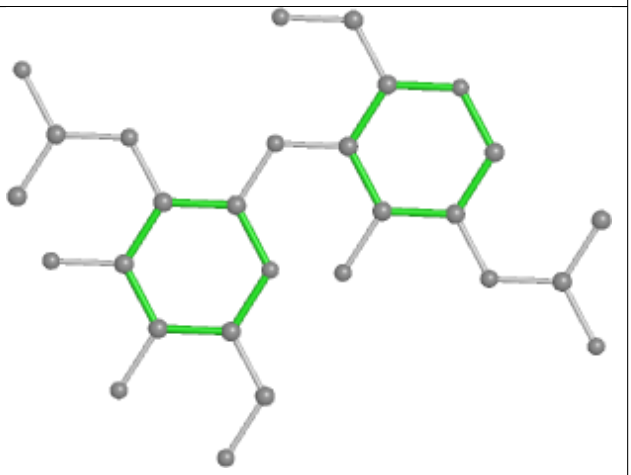
Mol	Chain	Res	Type	Atoms
2	K	1	NAG	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	T	1	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6

There are no ring outliers.

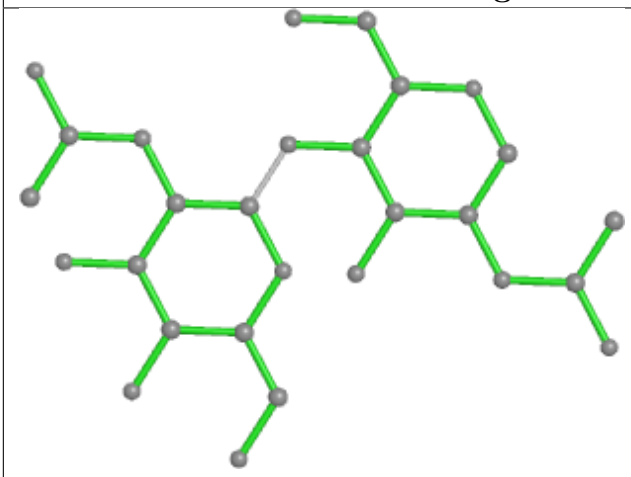
18 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	NAG	1	0
2	D	2	NAG	1	0
2	Z	1	NAG	1	0
2	S	1	NAG	1	0
2	L	1	NAG	1	0
2	T	1	NAG	1	0
5	Q	1	NAG	2	0
2	D	1	NAG	1	0
5	Q	2	NAG	1	0
4	N	2	NAG	1	0
4	W	2	NAG	1	0
3	U	3	BMA	1	0
2	L	2	NAG	1	0
4	W	1	NAG	1	0
2	V	1	NAG	1	0
2	V	2	NAG	1	0
2	X	1	NAG	1	0
2	M	2	NAG	1	0

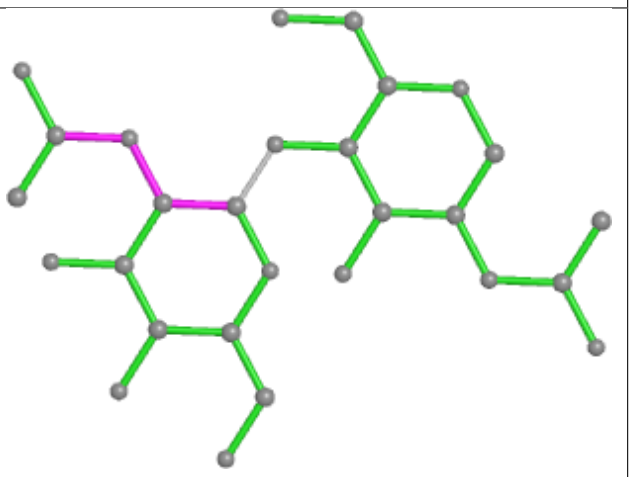
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain D	
 Bond lengths	 Bond angles
 Torsions	 Rings

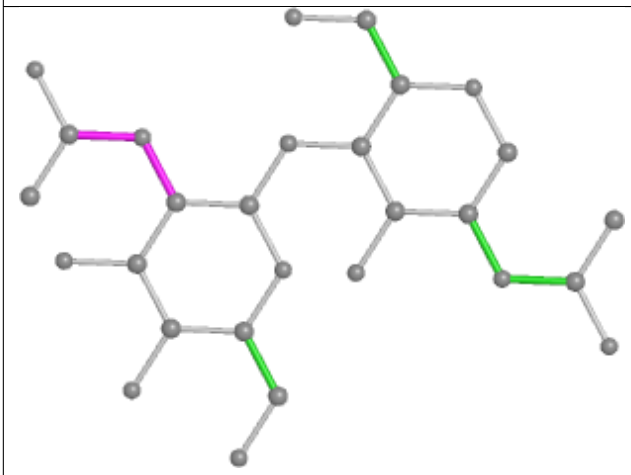
Oligosaccharide Chain G



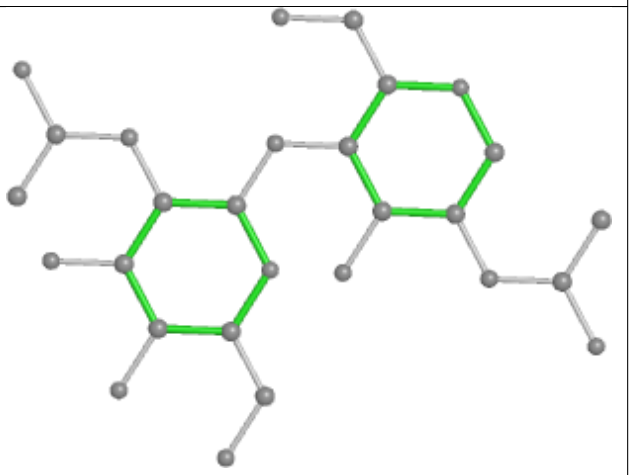
Bond lengths



Bond angles

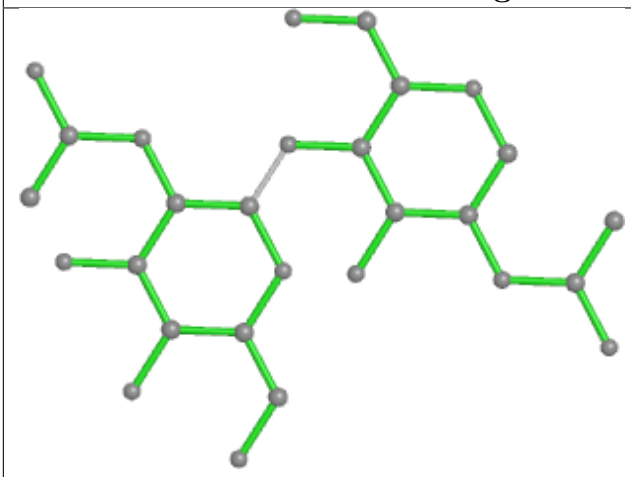


Torsions

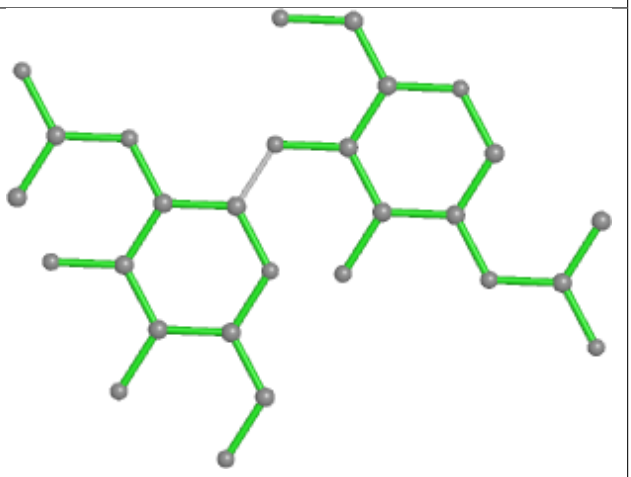


Rings

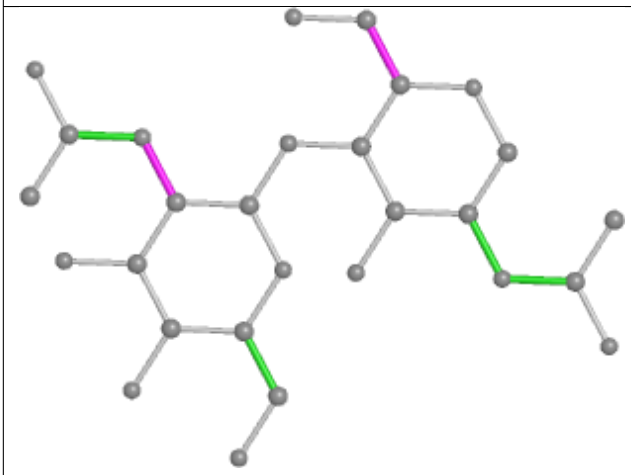
Oligosaccharide Chain H



Bond lengths



Bond angles



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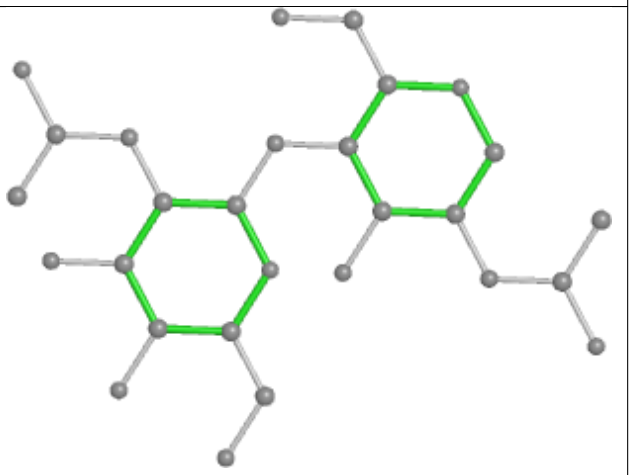
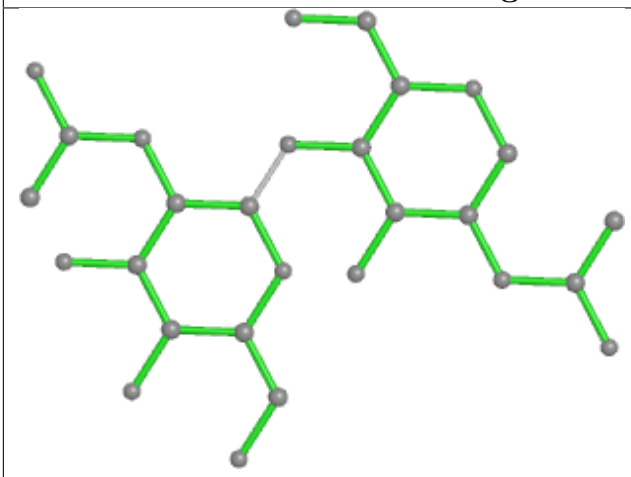
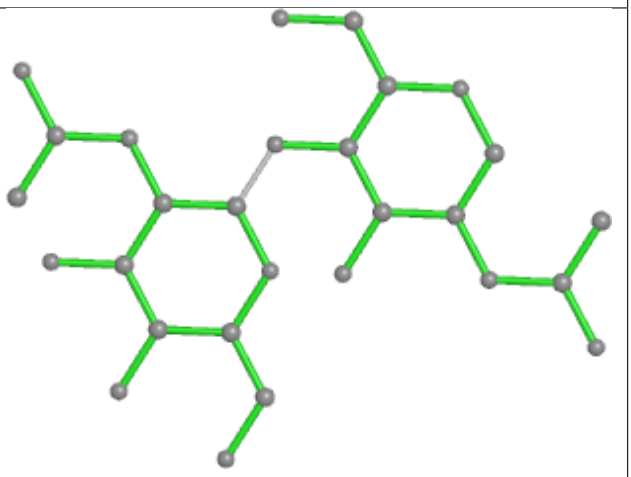


Rings

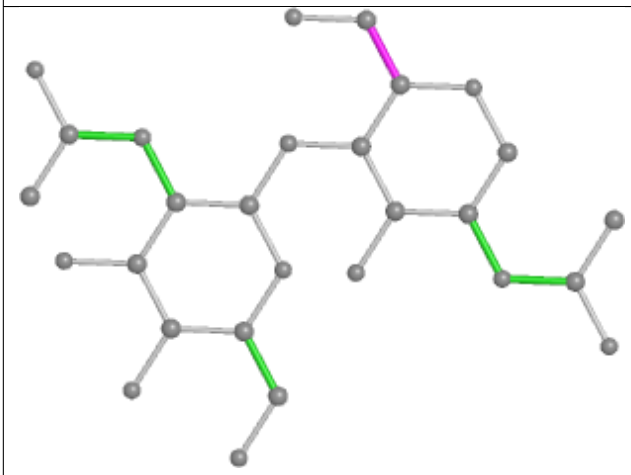
Oligosaccharide Chain I



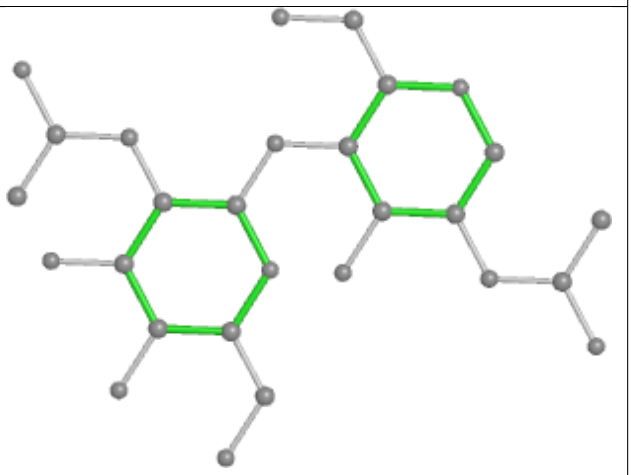
Bond lengths



Bond angles

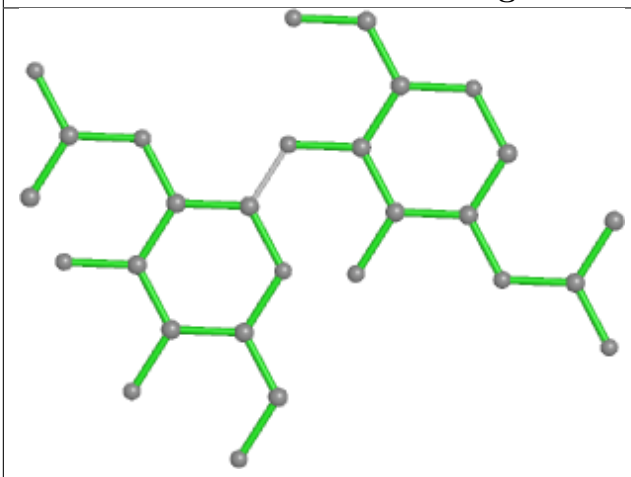


Torsions

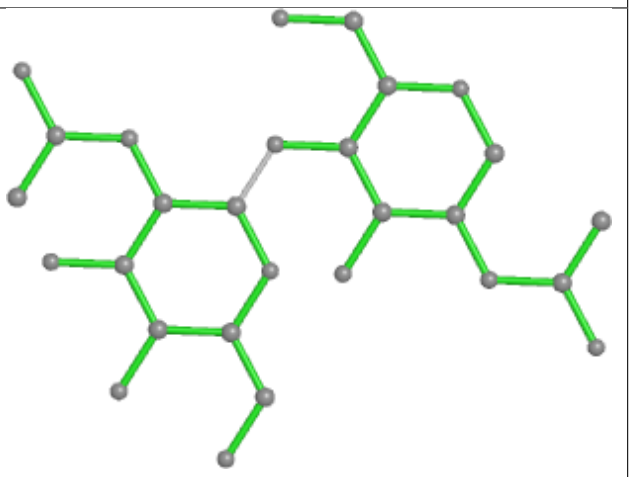


Rings

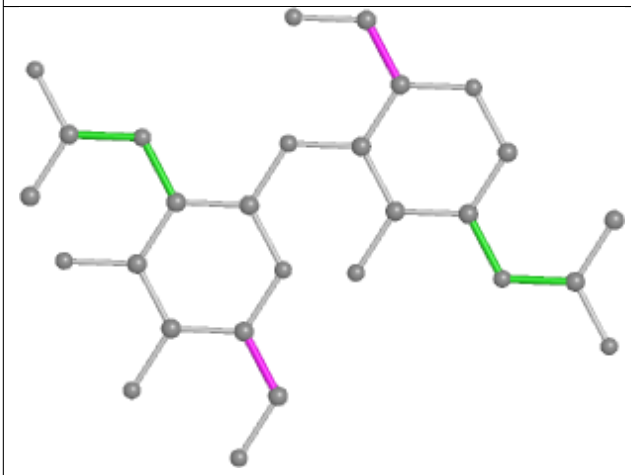
Oligosaccharide Chain J



Bond lengths



Bond angles



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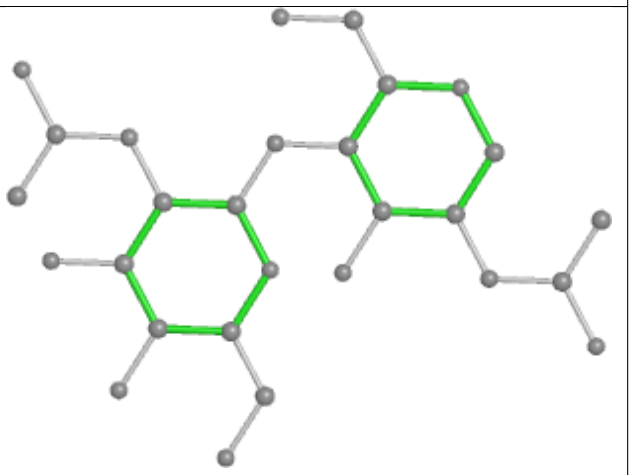
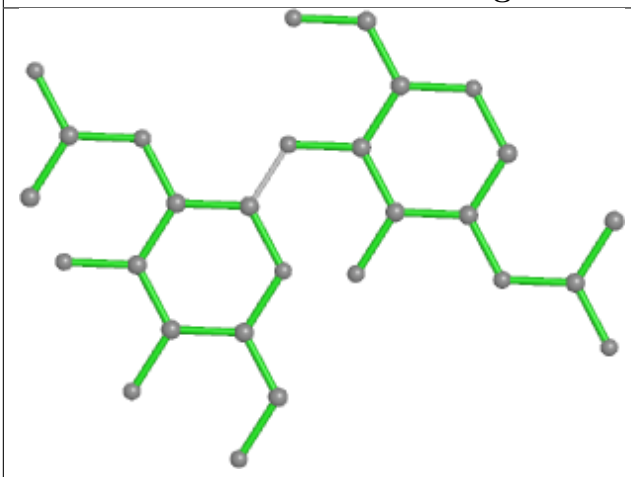
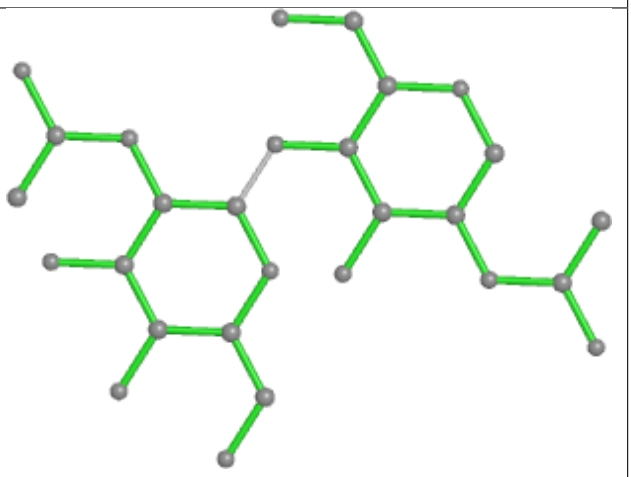
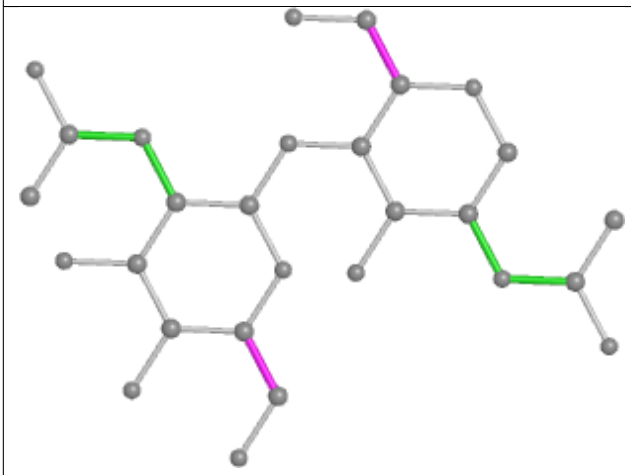
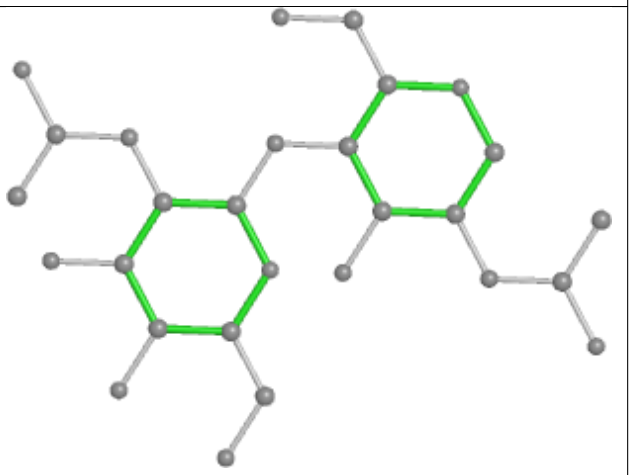
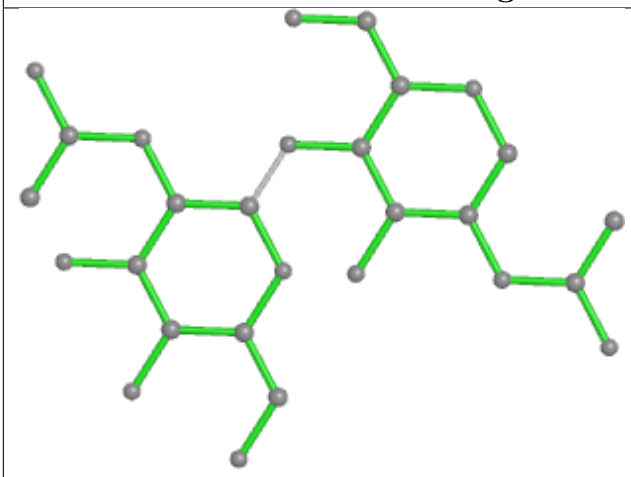


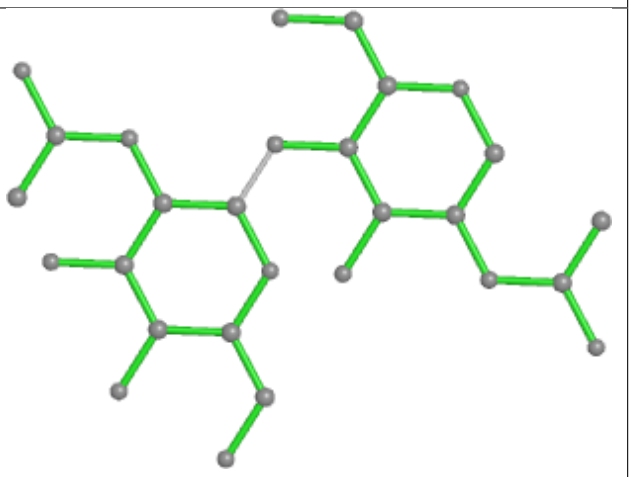
Rings

Oligosaccharide Chain K	
 Bond lengths	 Bond angles
 Torsions	 Rings

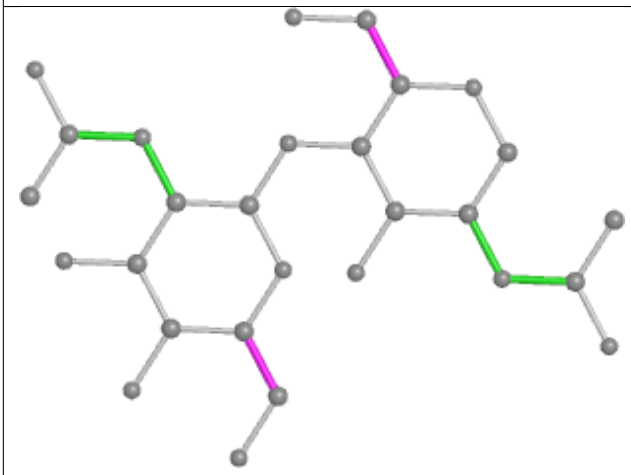
Oligosaccharide Chain L



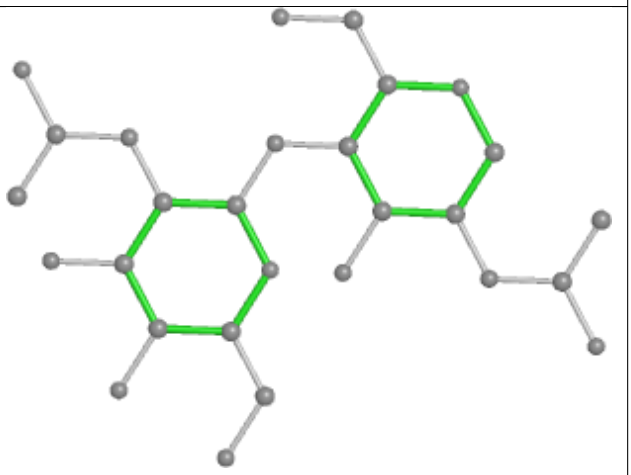
Bond lengths



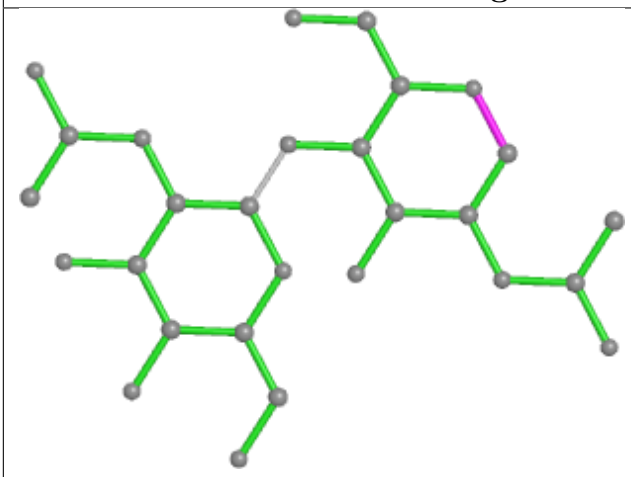
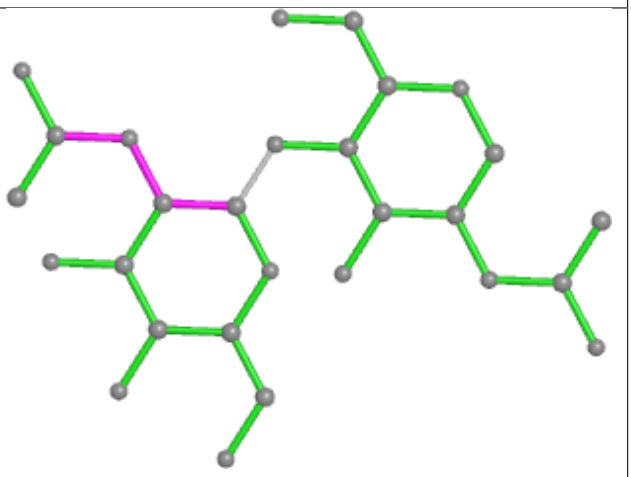
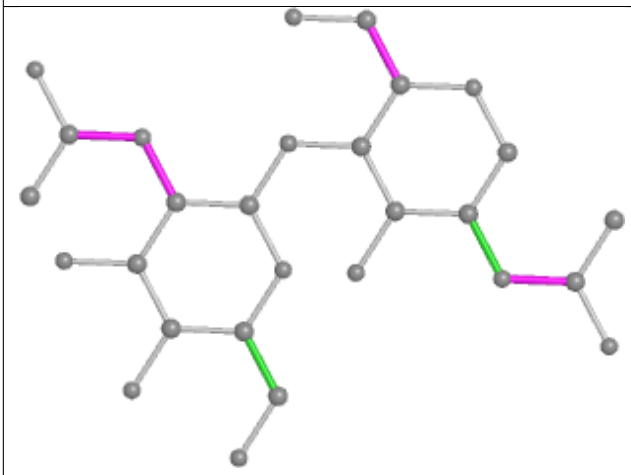
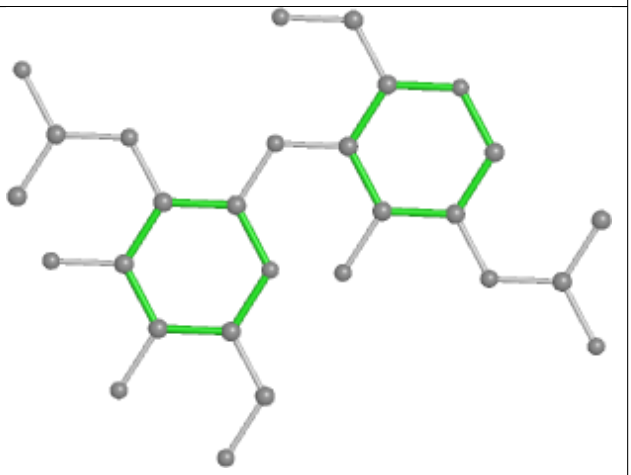
Bond angles



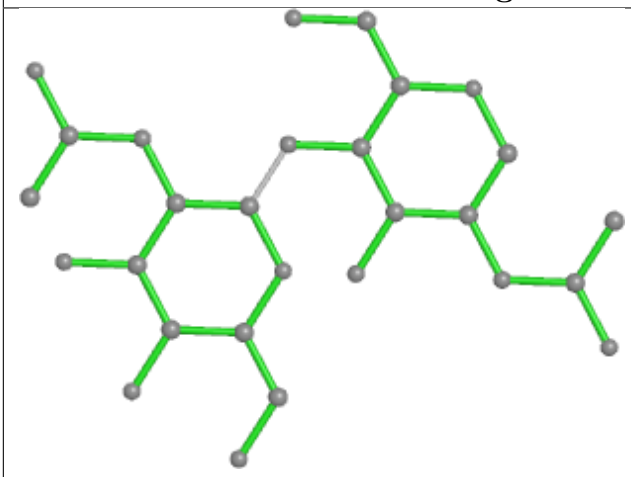
Torsions



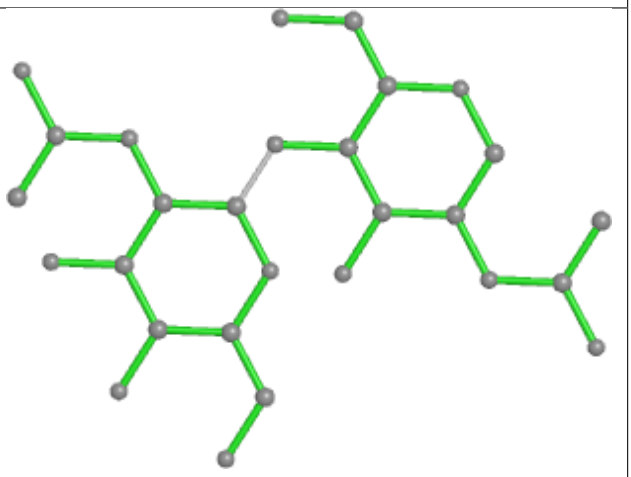
Rings

Oligosaccharide Chain M	
 Bond lengths	 Bond angles
 Torsions	 Rings

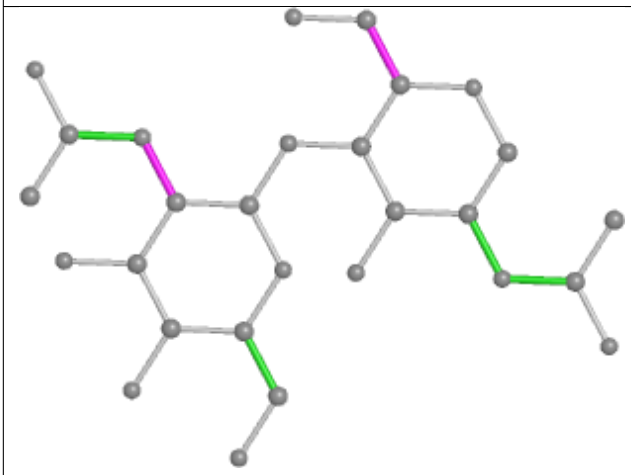
Oligosaccharide Chain P



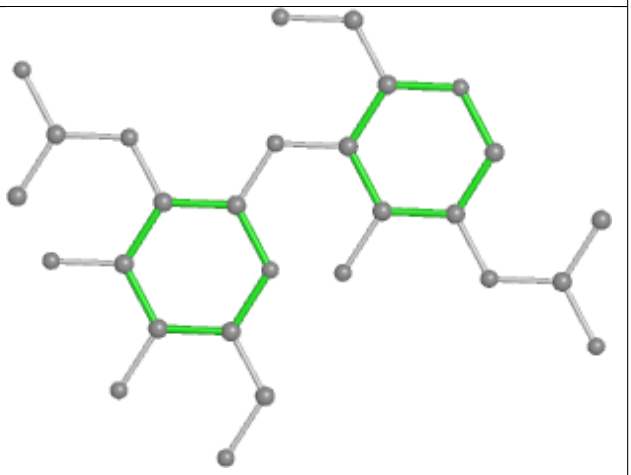
Bond lengths



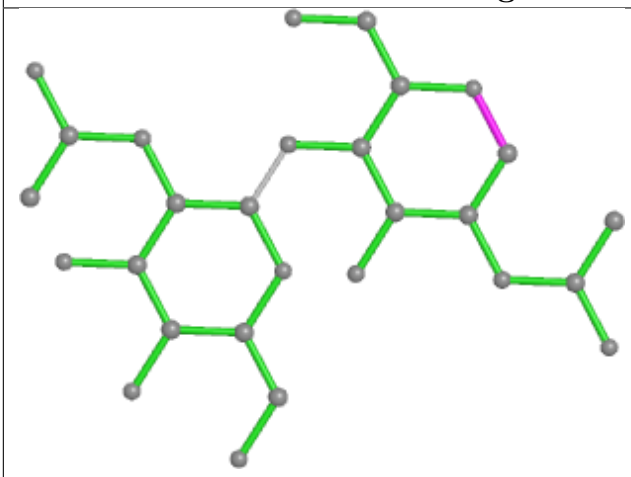
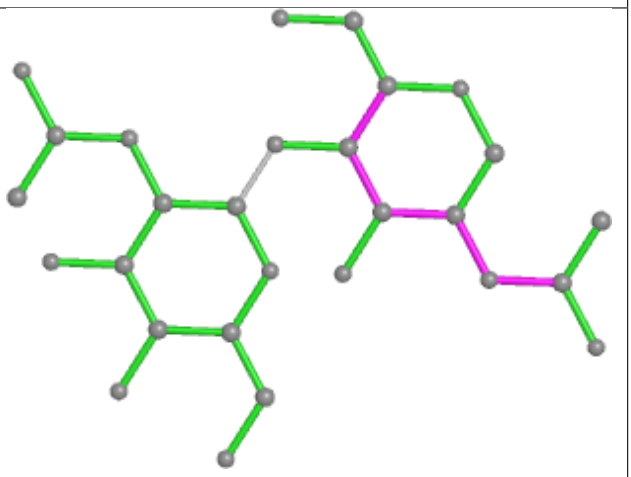
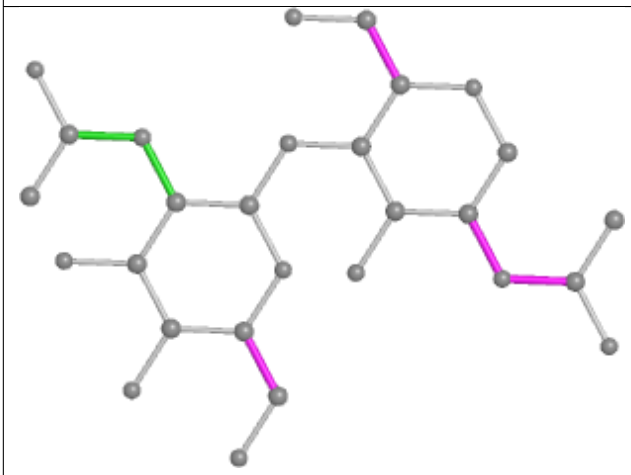
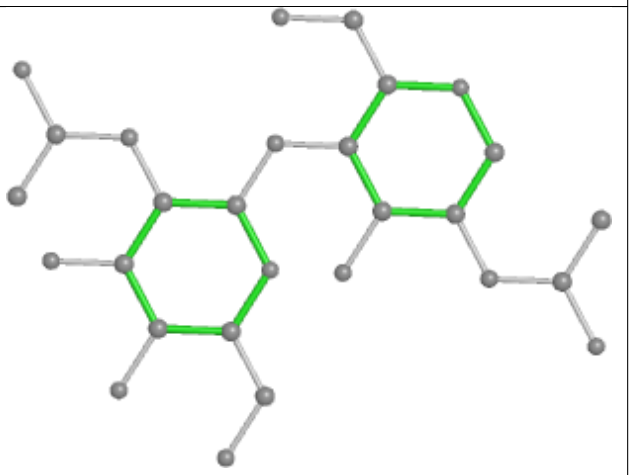
Bond angles

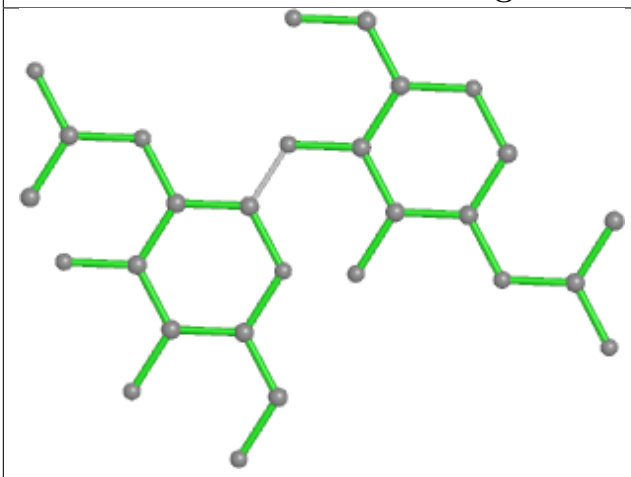
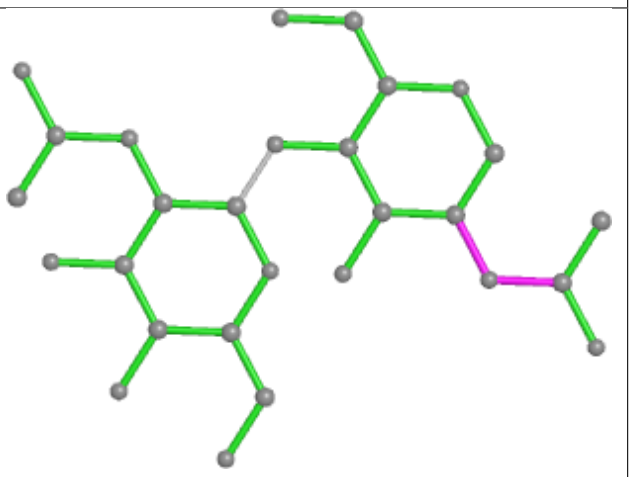
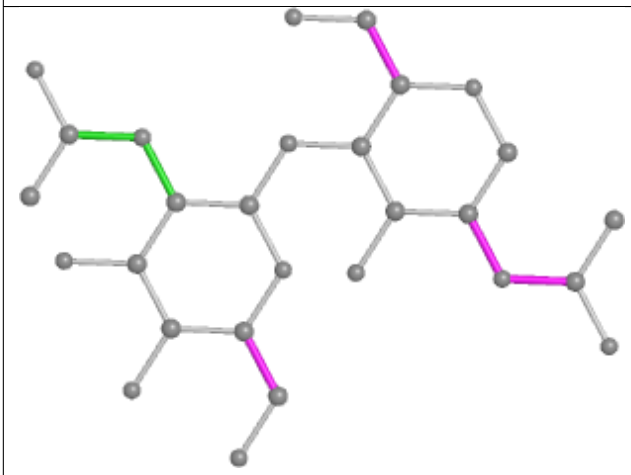
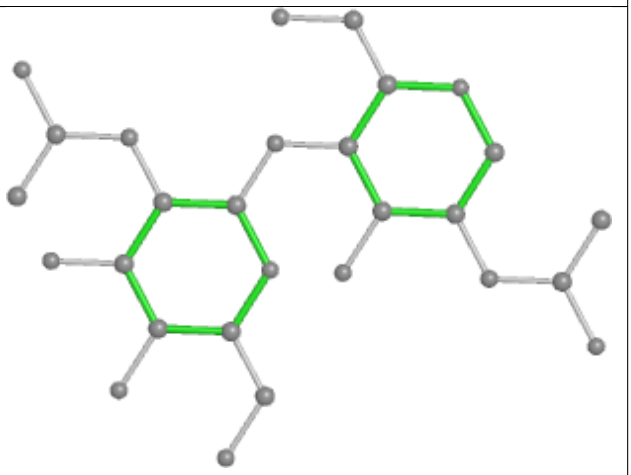


Torsions

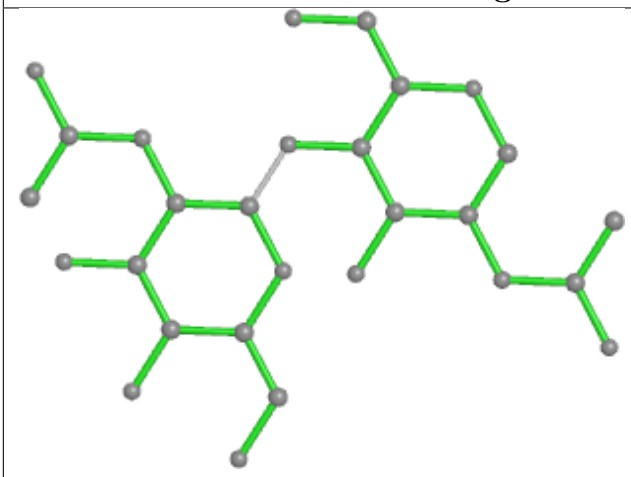


Rings

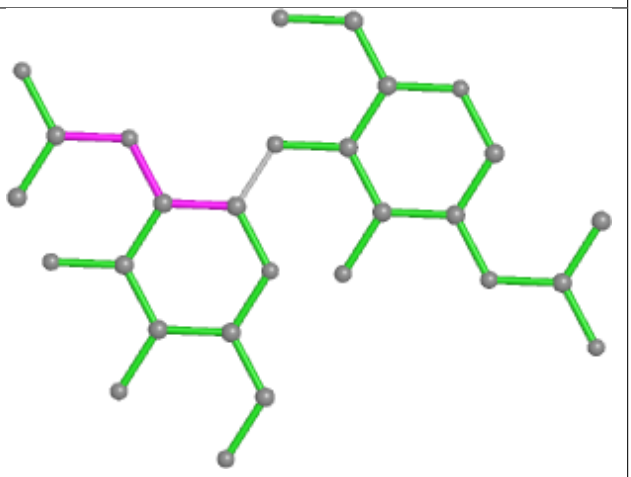
Oligosaccharide Chain S	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain T	
 Bond lengths	 Bond angles
 Torsions	 Rings

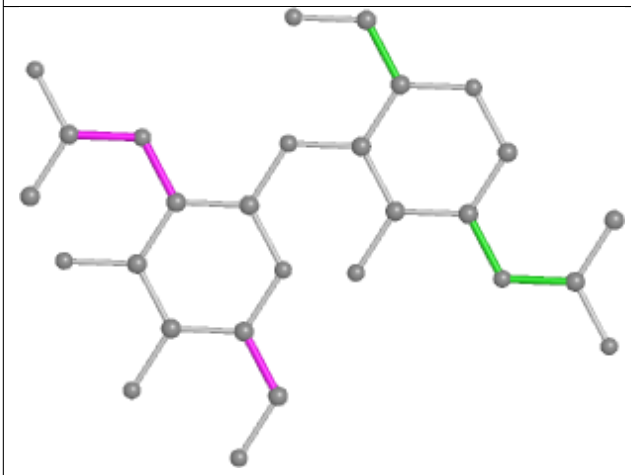
Oligosaccharide Chain V



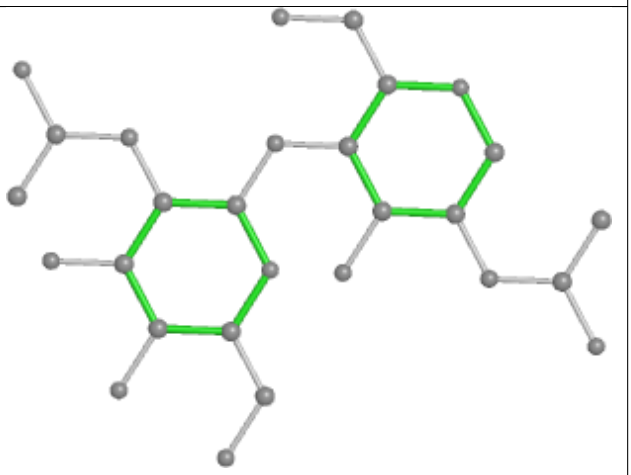
Bond lengths



Bond angles

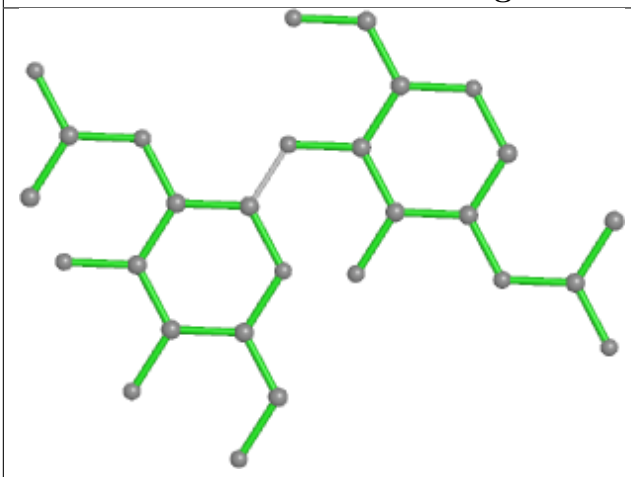


Torsions

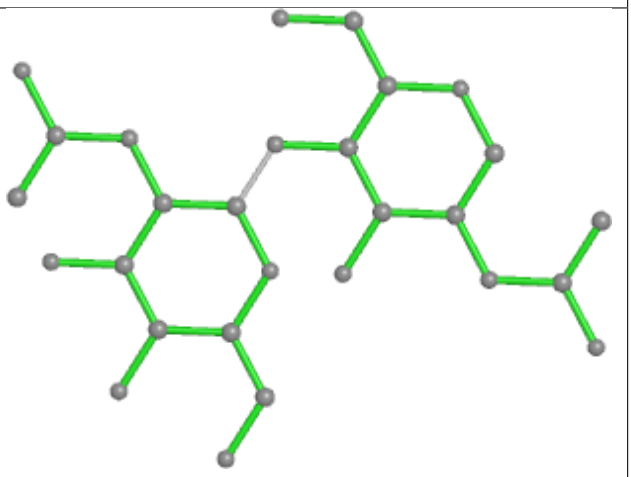


Rings

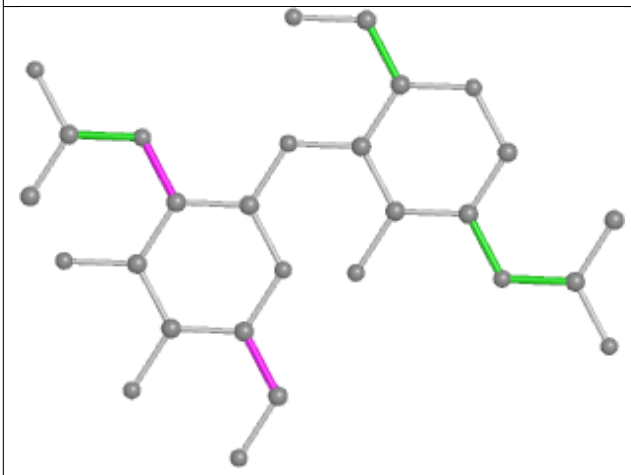
Oligosaccharide Chain X



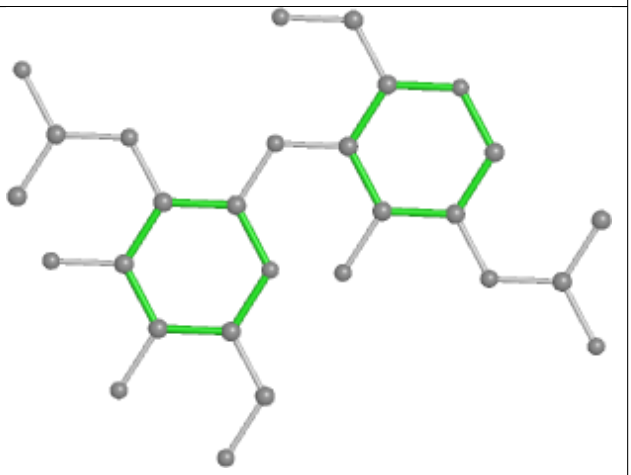
Bond lengths



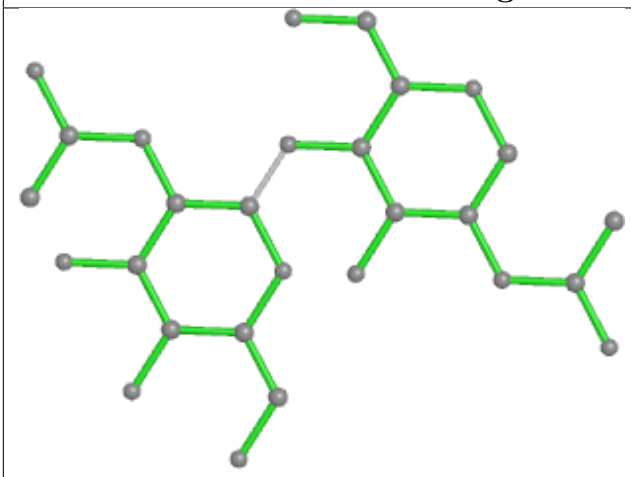
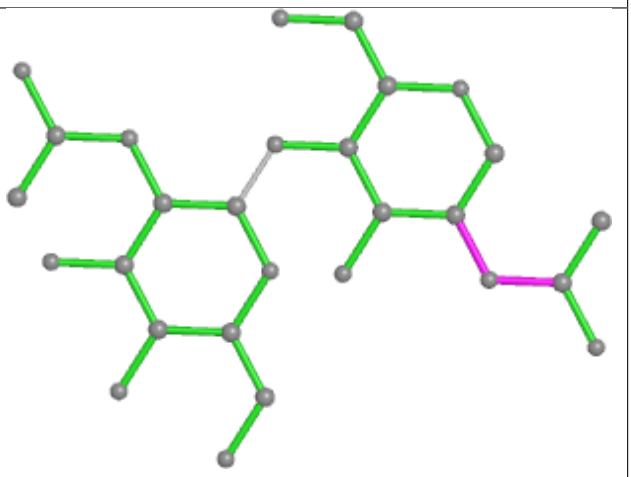
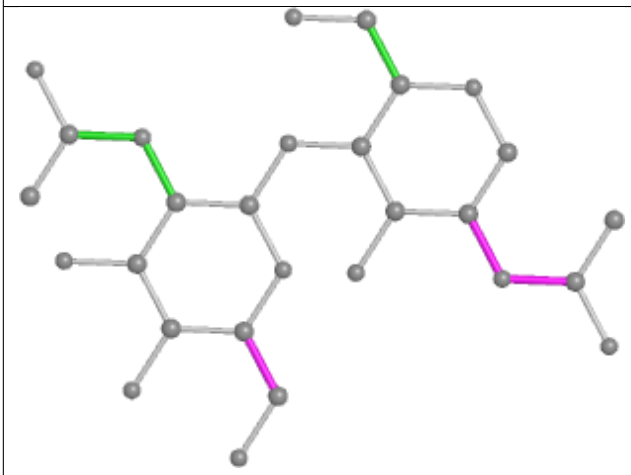
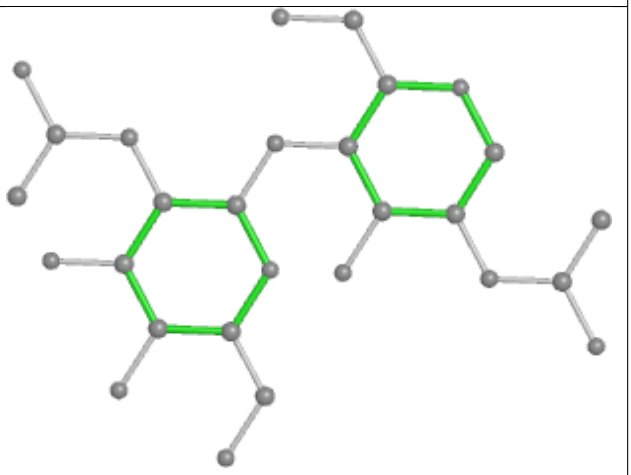
Bond angles



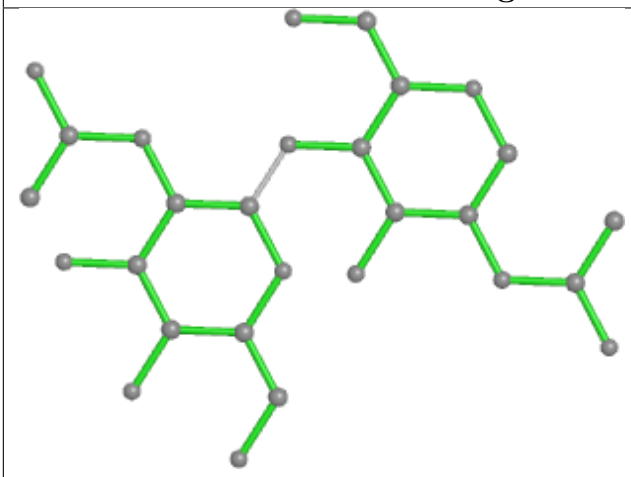
Torsions



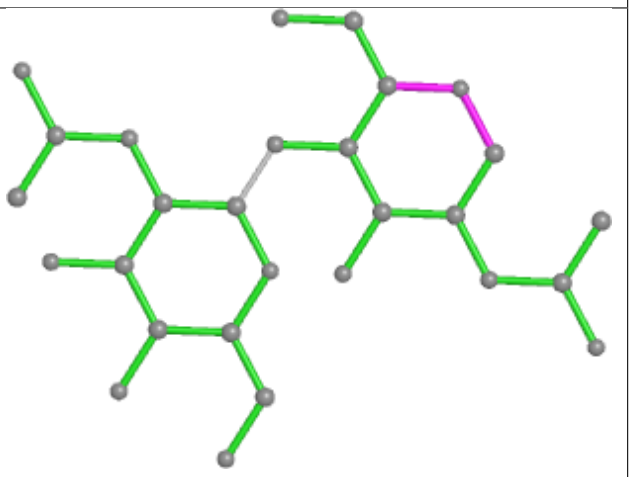
Rings

Oligosaccharide Chain Z	
 Bond lengths	 Bond angles
 Torsions	 Rings

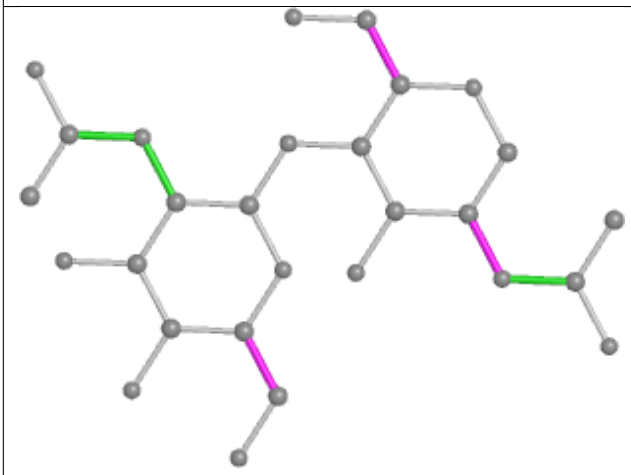
Oligosaccharide Chain d



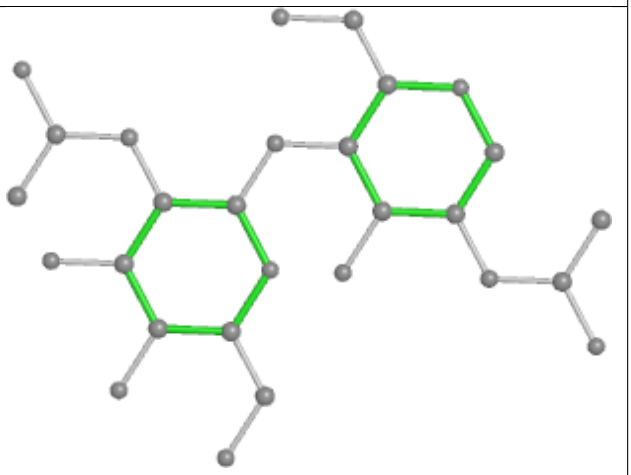
Bond lengths



Bond angles

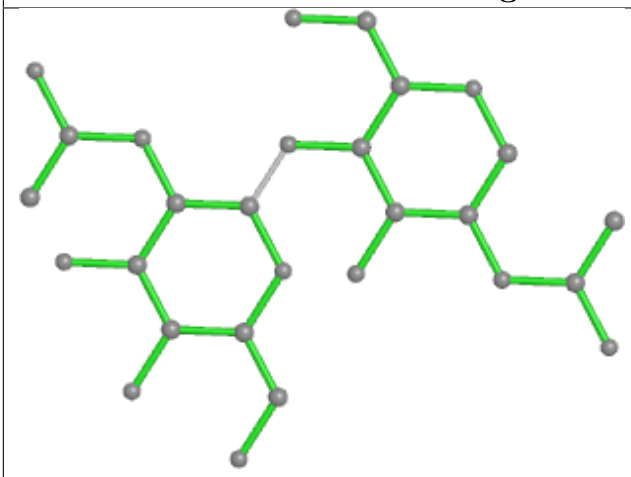


Torsions

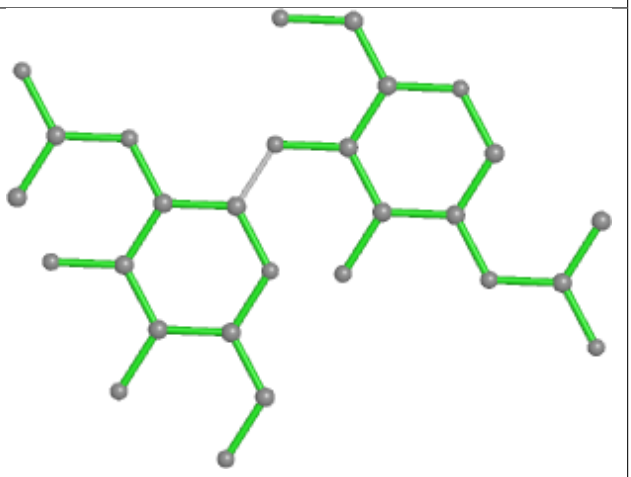


Rings

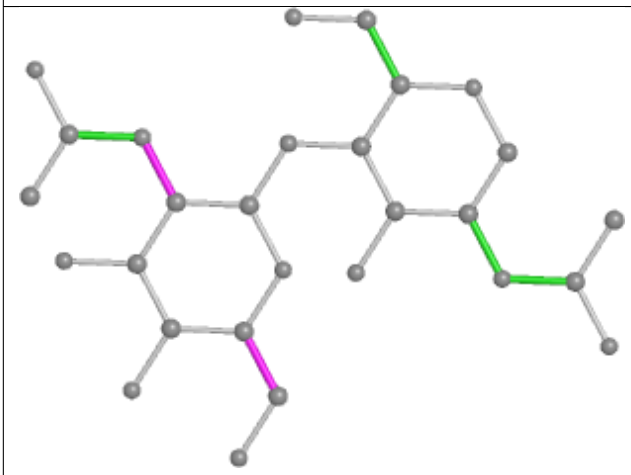
Oligosaccharide Chain e



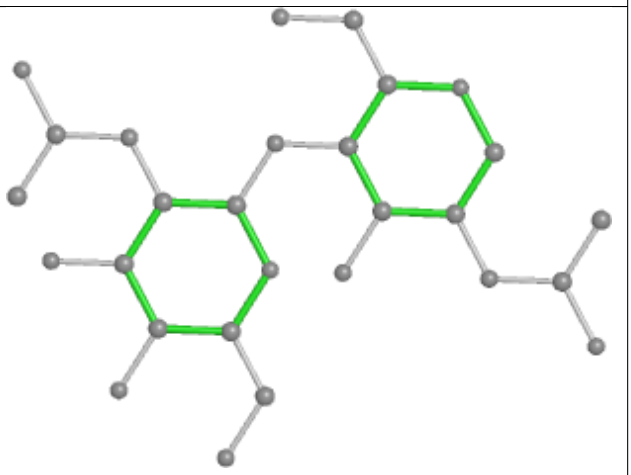
Bond lengths



Bond angles

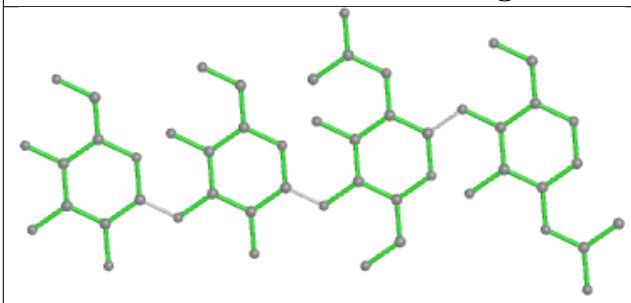


Torsions

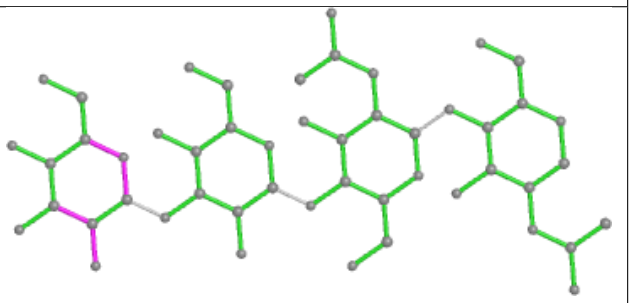


Rings

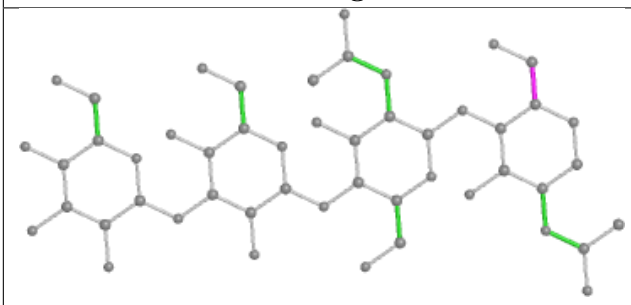
Oligosaccharide Chain E



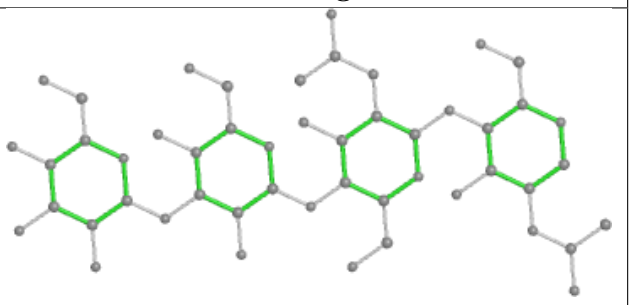
Bond lengths



Bond angles

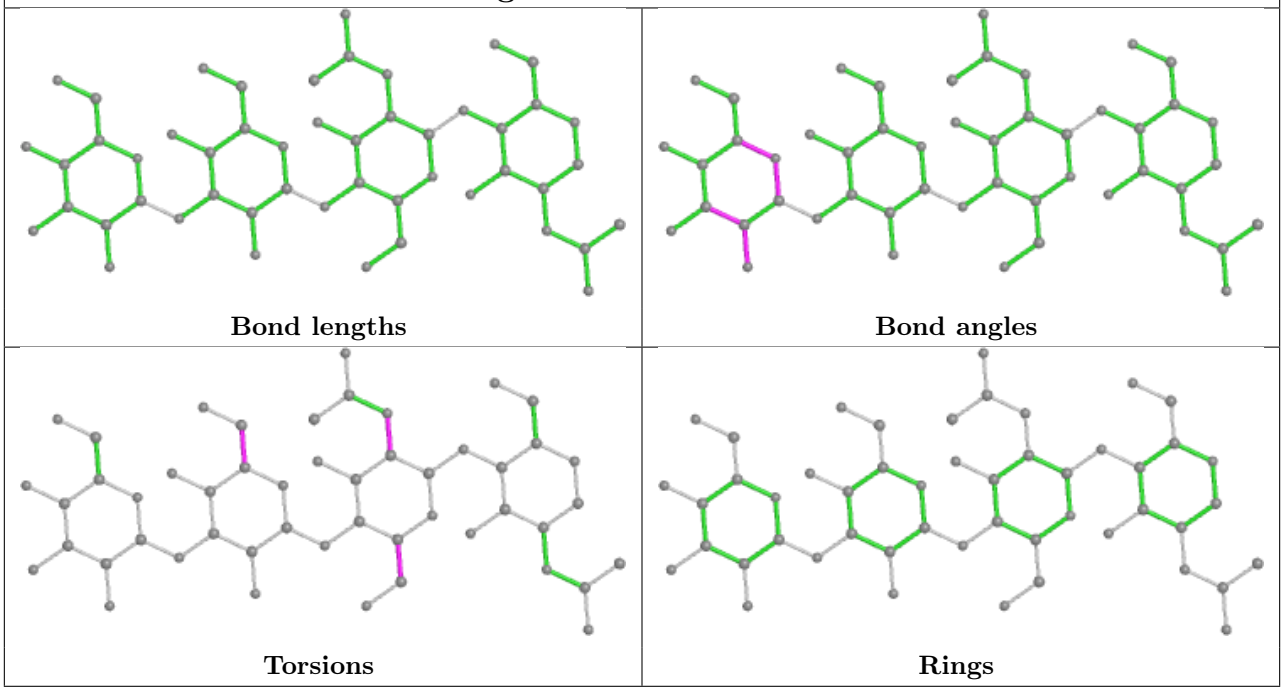


Torsions

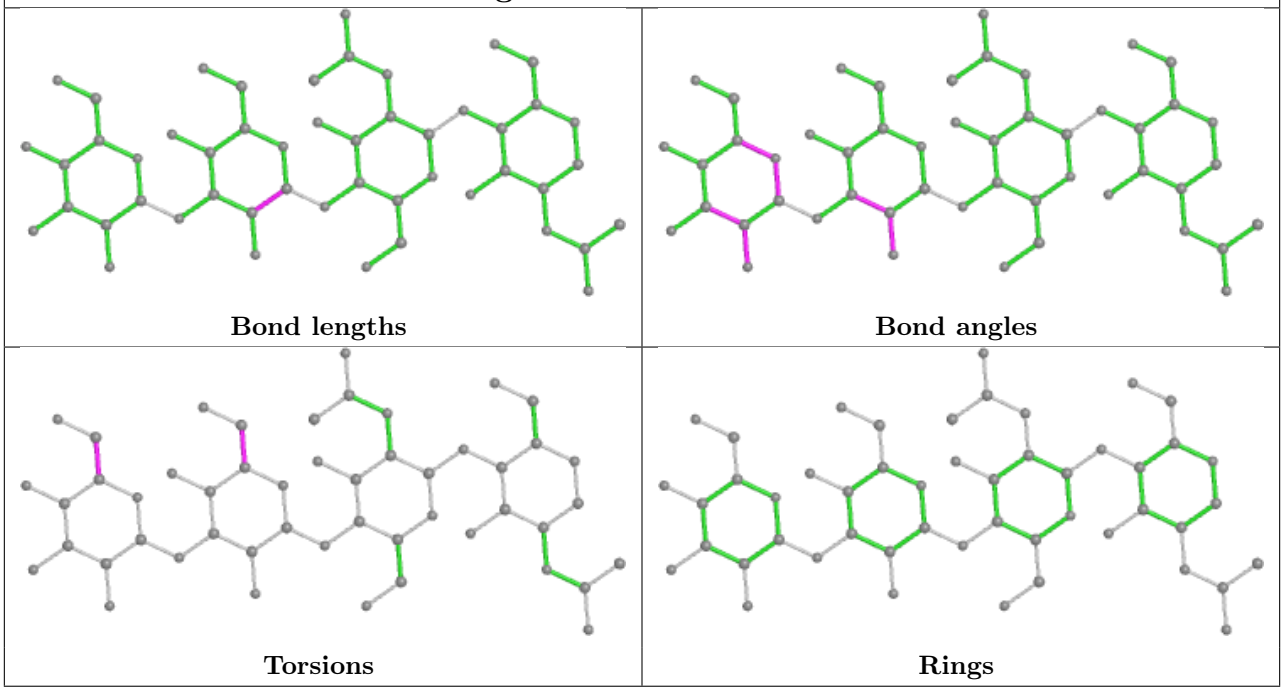


Rings

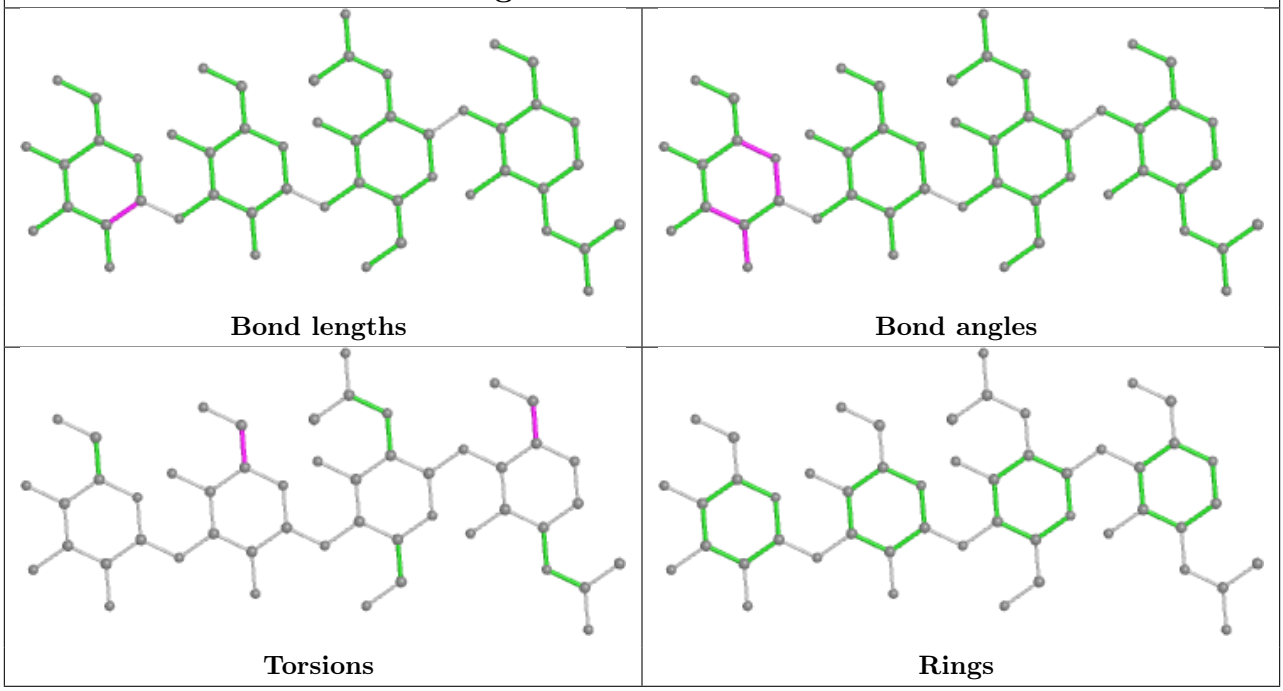
Oligosaccharide Chain F



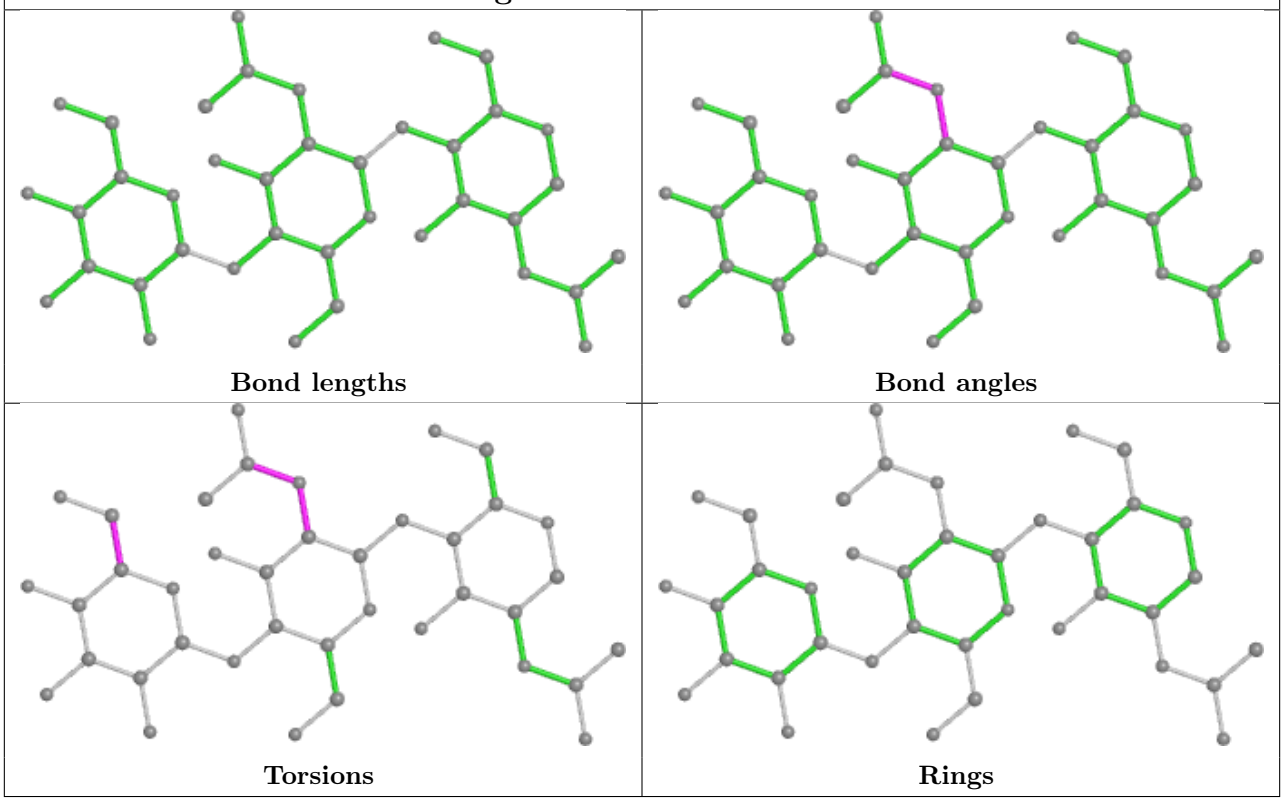
Oligosaccharide Chain R



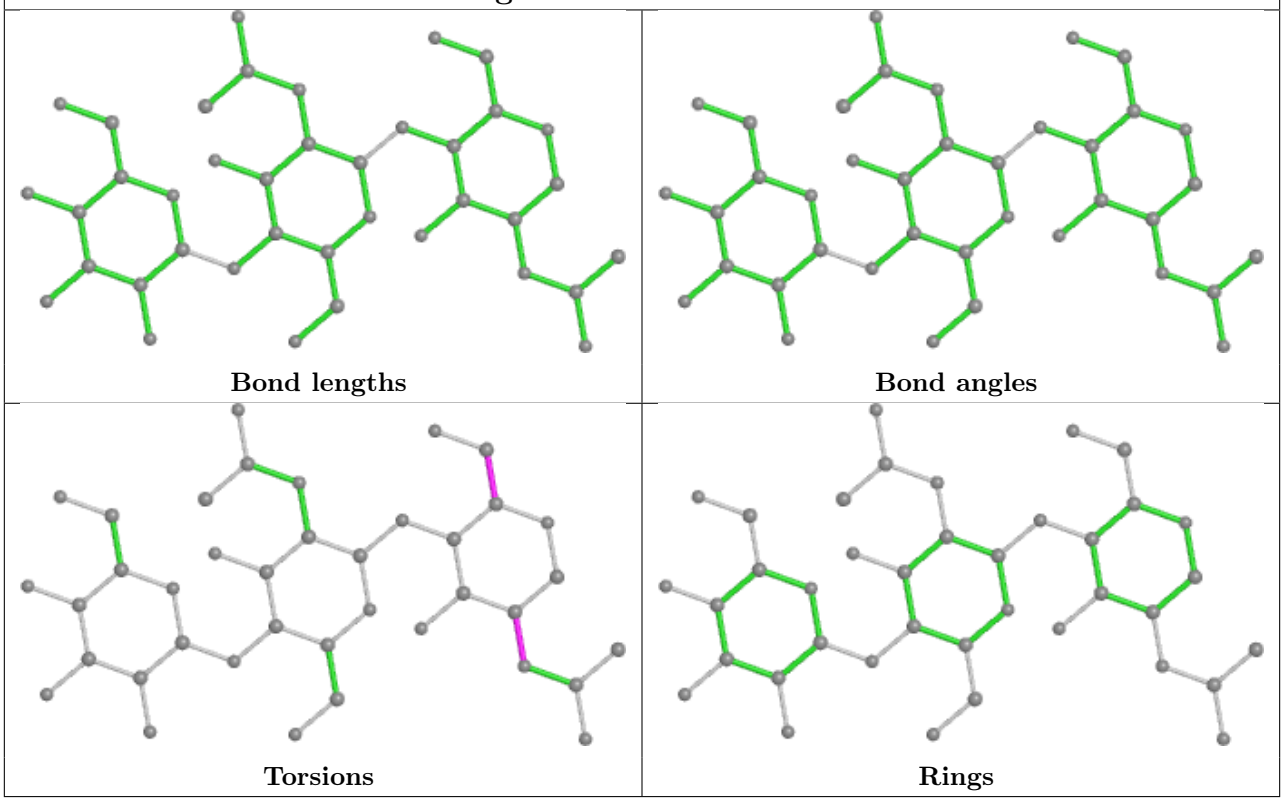
Oligosaccharide Chain U



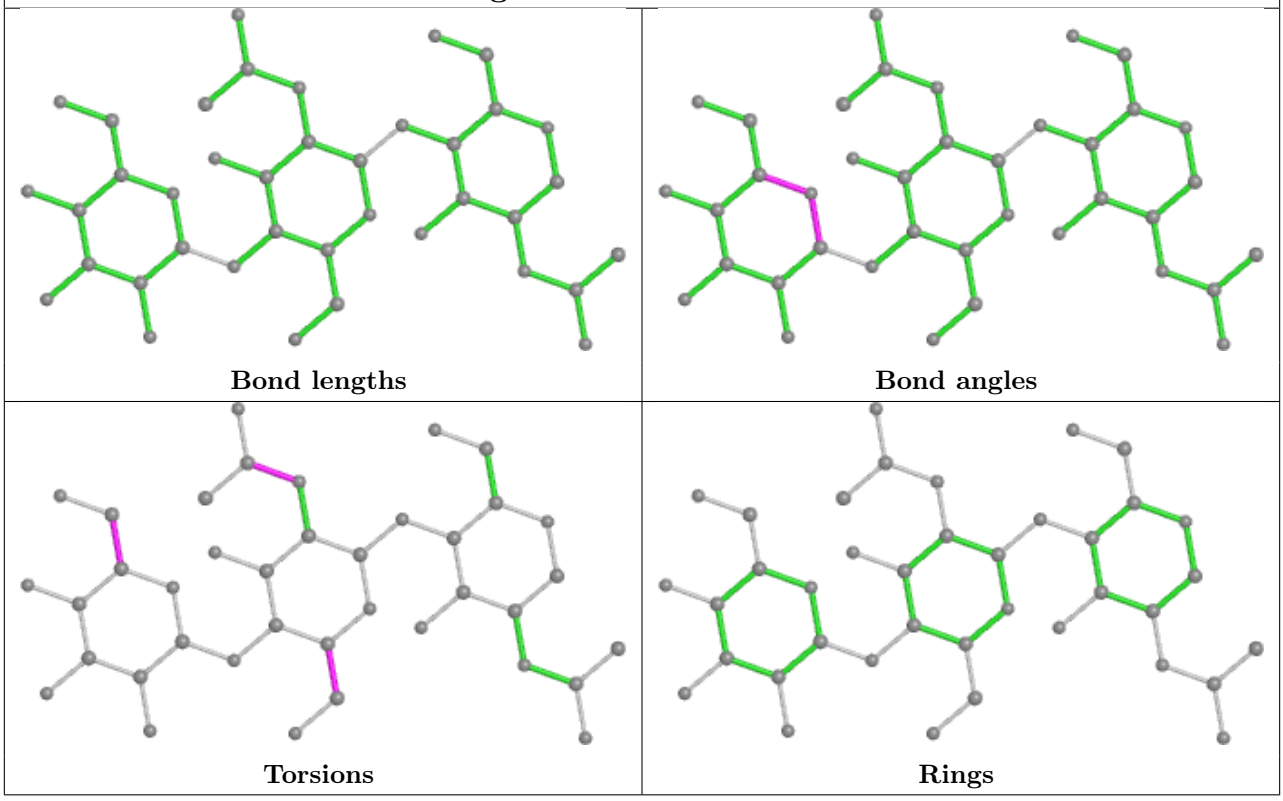
Oligosaccharide Chain N



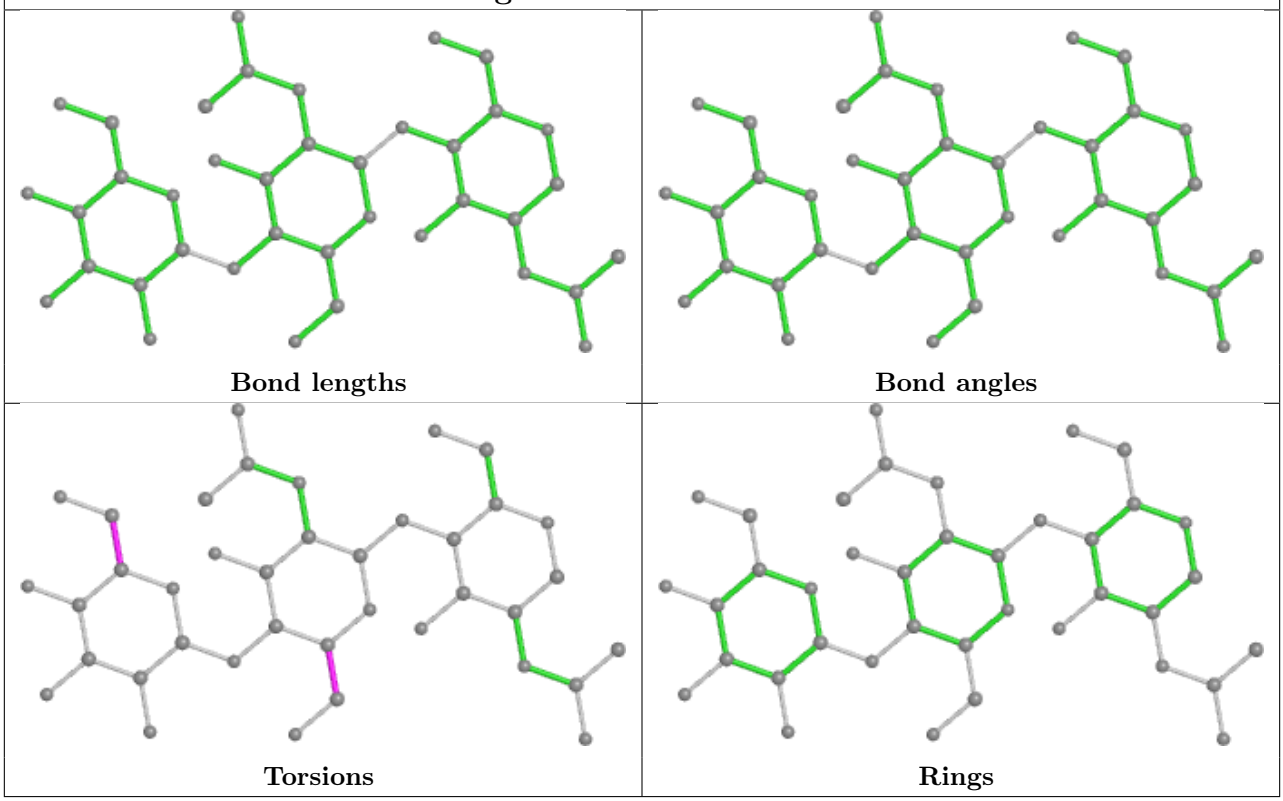
Oligosaccharide Chain O



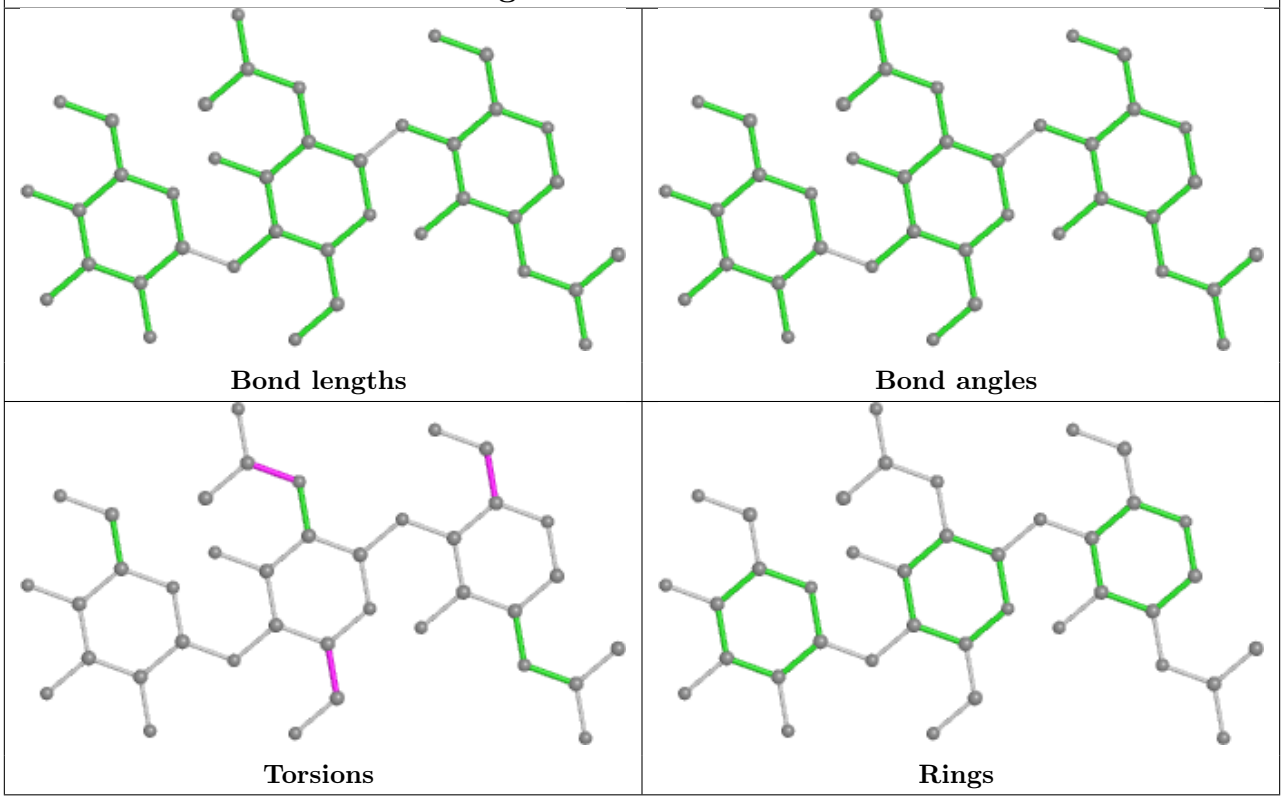
Oligosaccharide Chain W



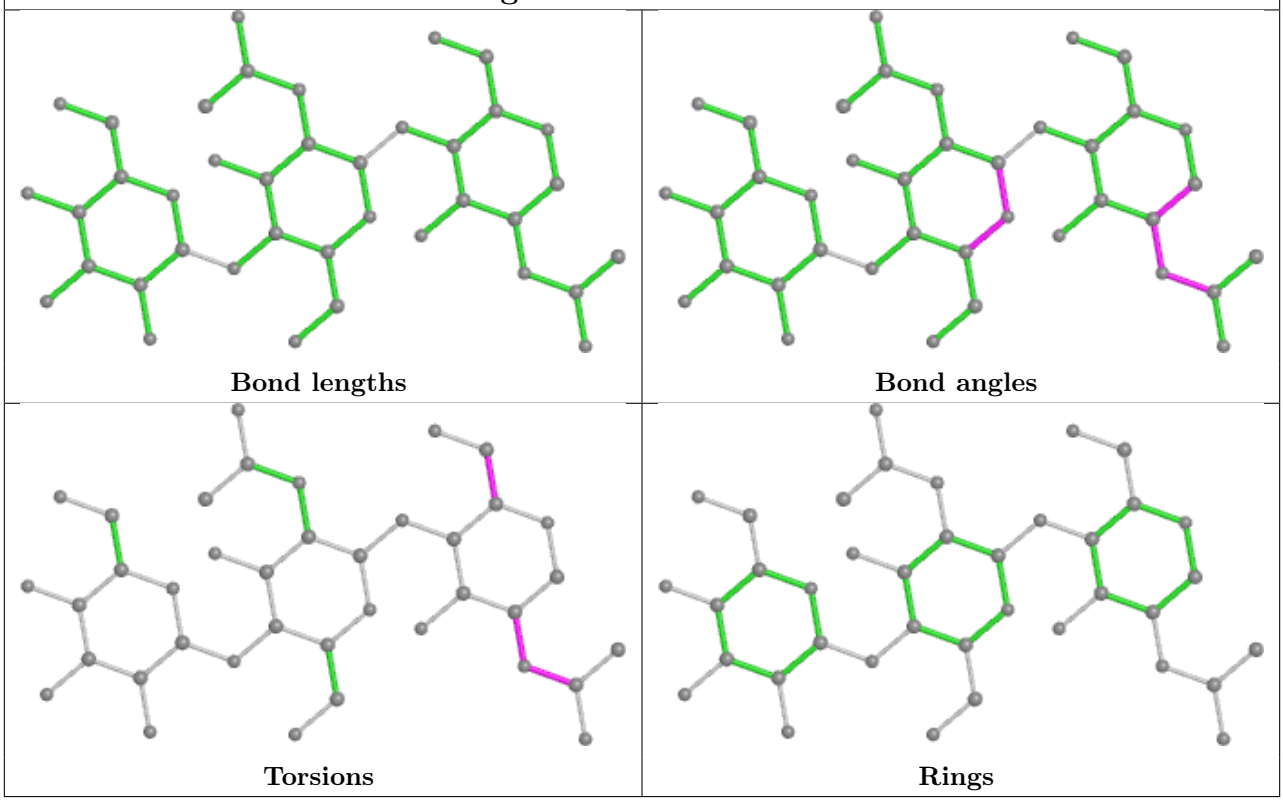
Oligosaccharide Chain Y



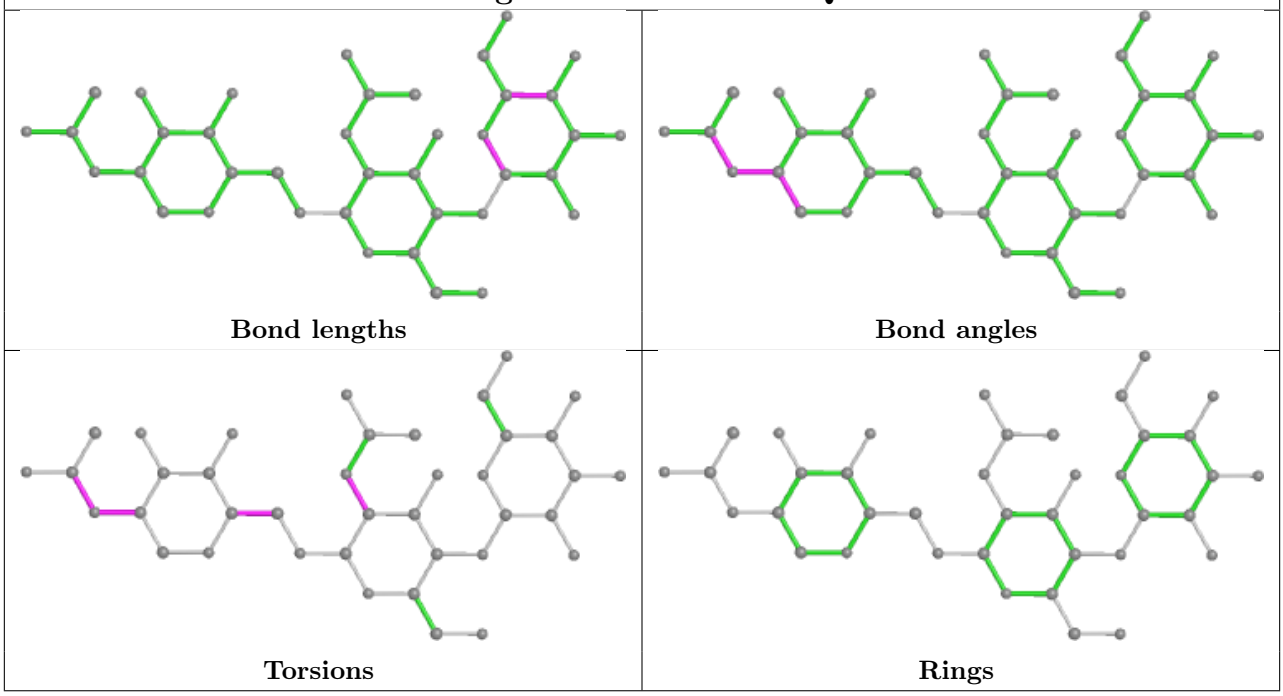
Oligosaccharide Chain b



Oligosaccharide Chain c



Oligosaccharide Chain Q



5.6 Ligand geometry (i)

23 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	a	1303	1	14,14,15	0.72	1 (7%)	17,19,21	0.63	0
6	NAG	A	1304	1	14,14,15	0.36	0	17,19,21	1.29	2 (11%)
6	NAG	A	1302	1	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	C	1302	1	14,14,15	0.38	0	17,19,21	0.59	1 (5%)
7	MAN	A	1306	-	11,11,12	0.71	0	15,15,17	1.08	2 (13%)
7	MAN	B	1304	-	11,11,12	0.70	0	15,15,17	1.07	2 (13%)
6	NAG	B	1301	1	14,14,15	0.24	0	17,19,21	0.44	0
8	DMS	a	1302	-	3,3,3	0.67	0	3,3,3	0.51	0
6	NAG	B	1305	1	14,14,15	0.51	0	17,19,21	0.63	0
6	NAG	B	1302	1	14,14,15	0.87	1 (7%)	17,19,21	0.82	1 (5%)
6	NAG	C	1308	1	14,14,15	0.20	0	17,19,21	0.55	0
6	NAG	A	1301	1	14,14,15	0.24	0	17,19,21	0.38	0
6	NAG	C	1301	1	14,14,15	0.17	0	17,19,21	0.51	0
8	DMS	a	1304	-	3,3,3	0.66	0	3,3,3	1.12	0
6	NAG	A	1303	1	14,14,15	0.21	0	17,19,21	0.45	0
6	NAG	C	1305	1	14,14,15	0.27	0	17,19,21	0.44	0
6	NAG	C	1303	1	14,14,15	0.34	0	17,19,21	1.27	2 (11%)
6	NAG	C	1307	1	14,14,15	0.58	0	17,19,21	0.45	0
6	NAG	B	1303	1	14,14,15	0.89	1 (7%)	17,19,21	0.72	1 (5%)
8	DMS	a	1301	-	3,3,3	0.67	0	3,3,3	0.48	0
6	NAG	A	1305	1	14,14,15	0.20	0	17,19,21	0.45	0
6	NAG	C	1306	1	14,14,15	0.67	1 (7%)	17,19,21	0.46	0
6	NAG	C	1304	1	14,14,15	0.42	0	17,19,21	0.64	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	1302	1	-	3/6/23/26	0/1/1/1
7	MAN	A	1306	-	-	0/2/19/22	0/1/1/1
7	MAN	B	1304	-	-	0/2/19/22	0/1/1/1
6	NAG	B	1301	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1301	1	-	4/6/23/26	0/1/1/1
6	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1303	1	-	5/6/23/26	0/1/1/1
6	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1306	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1304	1	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1303	NAG	C1-C2	2.73	1.56	1.52
6	B	1302	NAG	O5-C1	2.72	1.48	1.43
6	a	1303	NAG	C1-C2	2.42	1.56	1.52
6	C	1306	NAG	O5-C1	-2.11	1.40	1.43

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1304	NAG	C2-N2-C7	4.40	129.16	122.90
6	C	1303	NAG	C2-N2-C7	4.35	129.10	122.90
6	B	1302	NAG	C1-O5-C5	3.00	116.25	112.19
7	A	1306	MAN	C1-O5-C5	2.38	115.42	112.19
7	B	1304	MAN	C1-O5-C5	2.38	115.41	112.19

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1305	NAG	O5-C5-C6-O6
6	B	1303	NAG	O5-C5-C6-O6
6	A	1302	NAG	O5-C5-C6-O6
6	A	1303	NAG	O5-C5-C6-O6
6	A	1305	NAG	C4-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1304	NAG	1	0
7	B	1304	MAN	1	0
6	A	1301	NAG	1	0
6	C	1303	NAG	1	0
6	C	1307	NAG	1	0
6	B	1303	NAG	2	0
6	C	1306	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

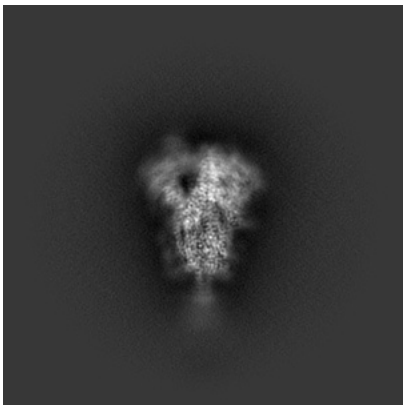
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11328. These allow visual inspection of the internal detail of the map and identification of artifacts.

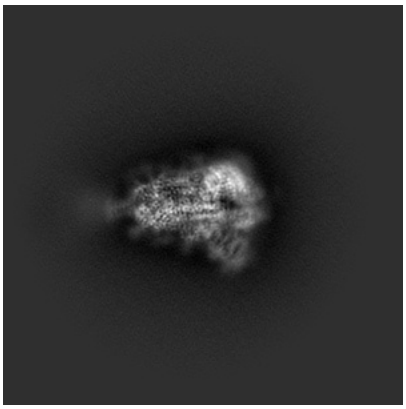
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

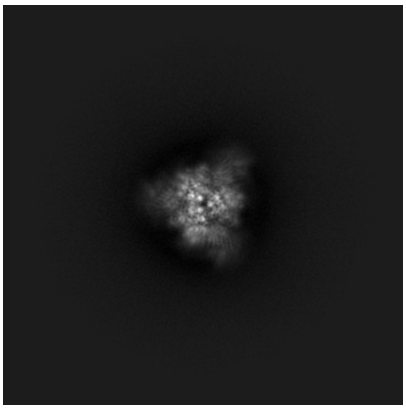
6.1.1 Primary map



X

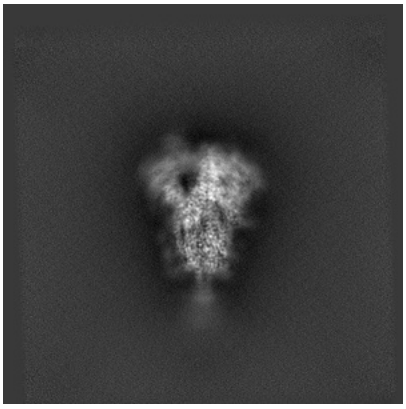


Y

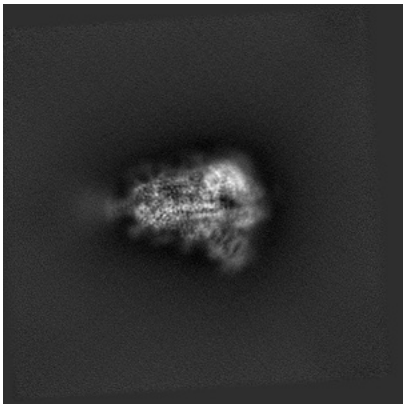


Z

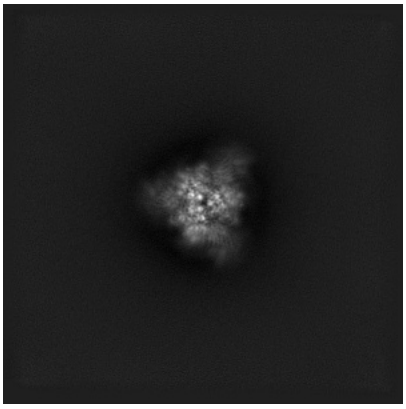
6.1.2 Raw map



X



Y



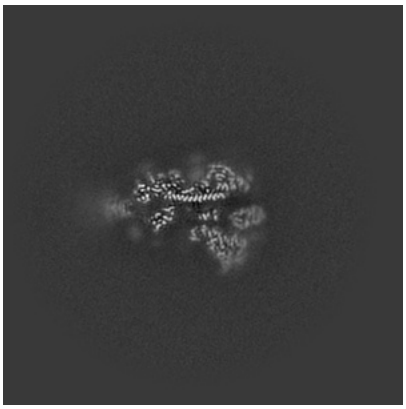
Z

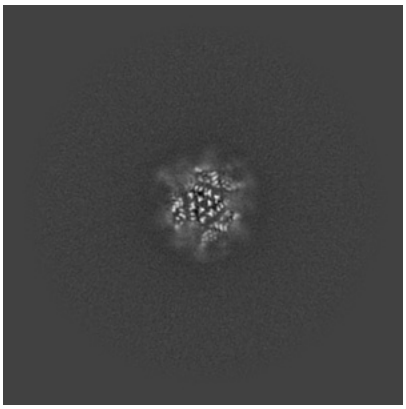
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

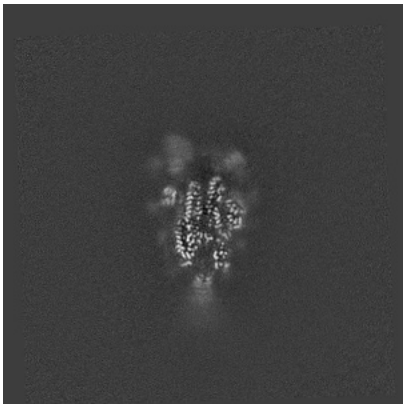
6.2.1 Primary map

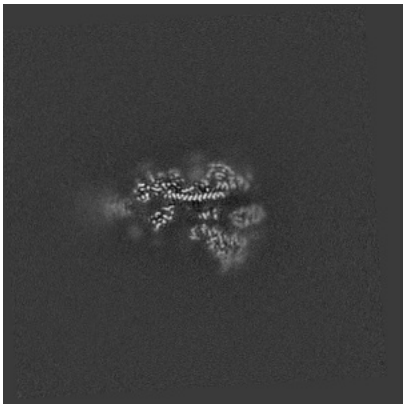
X Index: 216

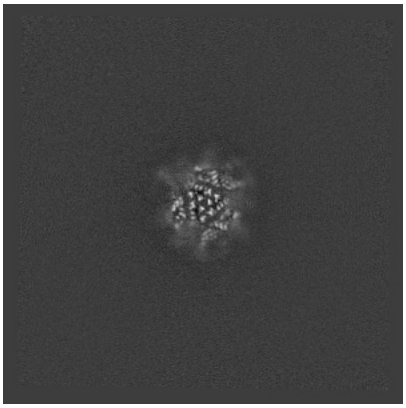

Y Index: 216


Z Index: 216

6.2.2 Raw map


X Index: 216

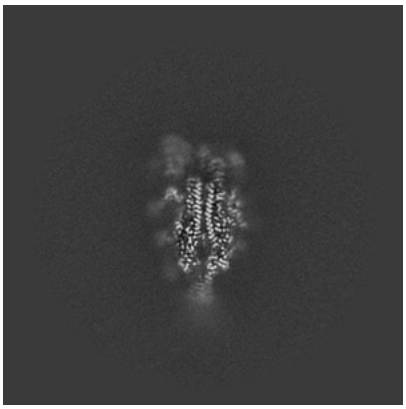

Y Index: 216


Z Index: 216

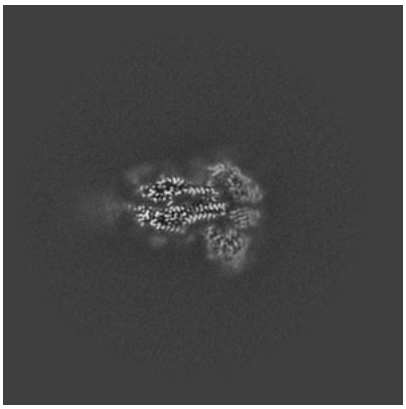
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

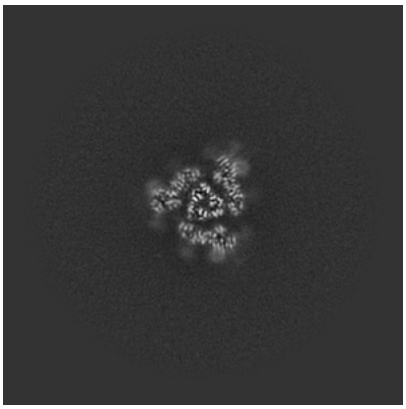
6.3.1 Primary map



X Index: 212

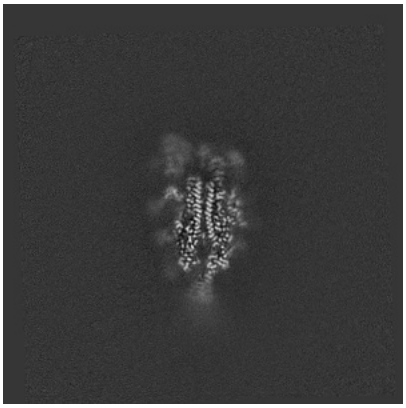


Y Index: 225

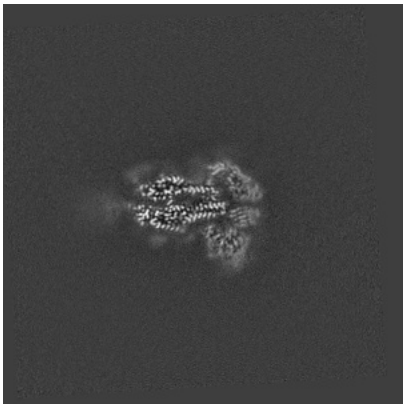


Z Index: 231

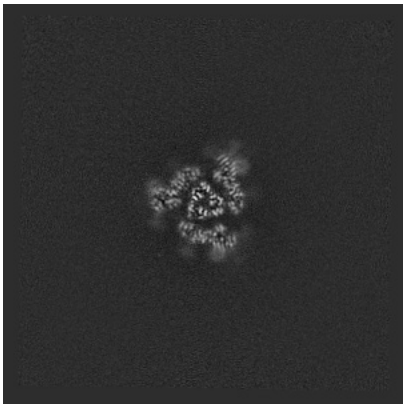
6.3.2 Raw map



X Index: 212



Y Index: 225



Z Index: 231

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

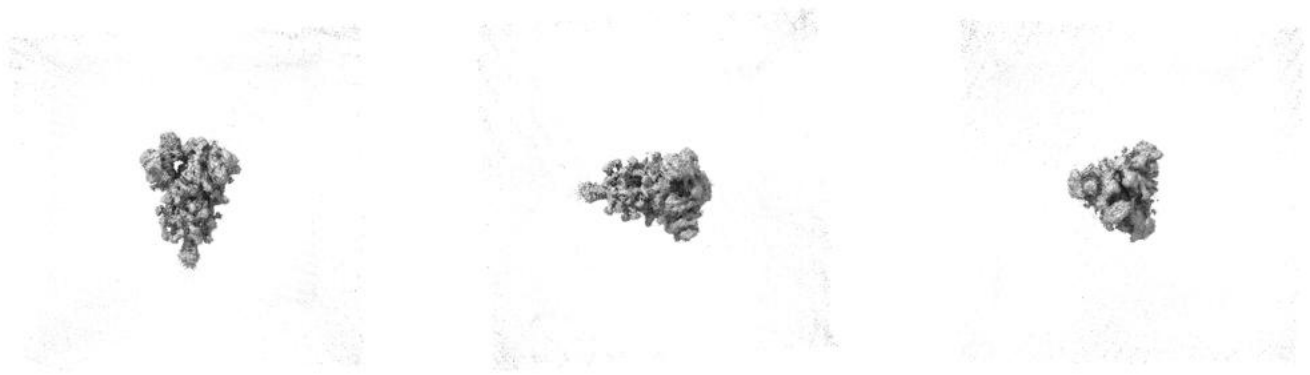
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.129. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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.

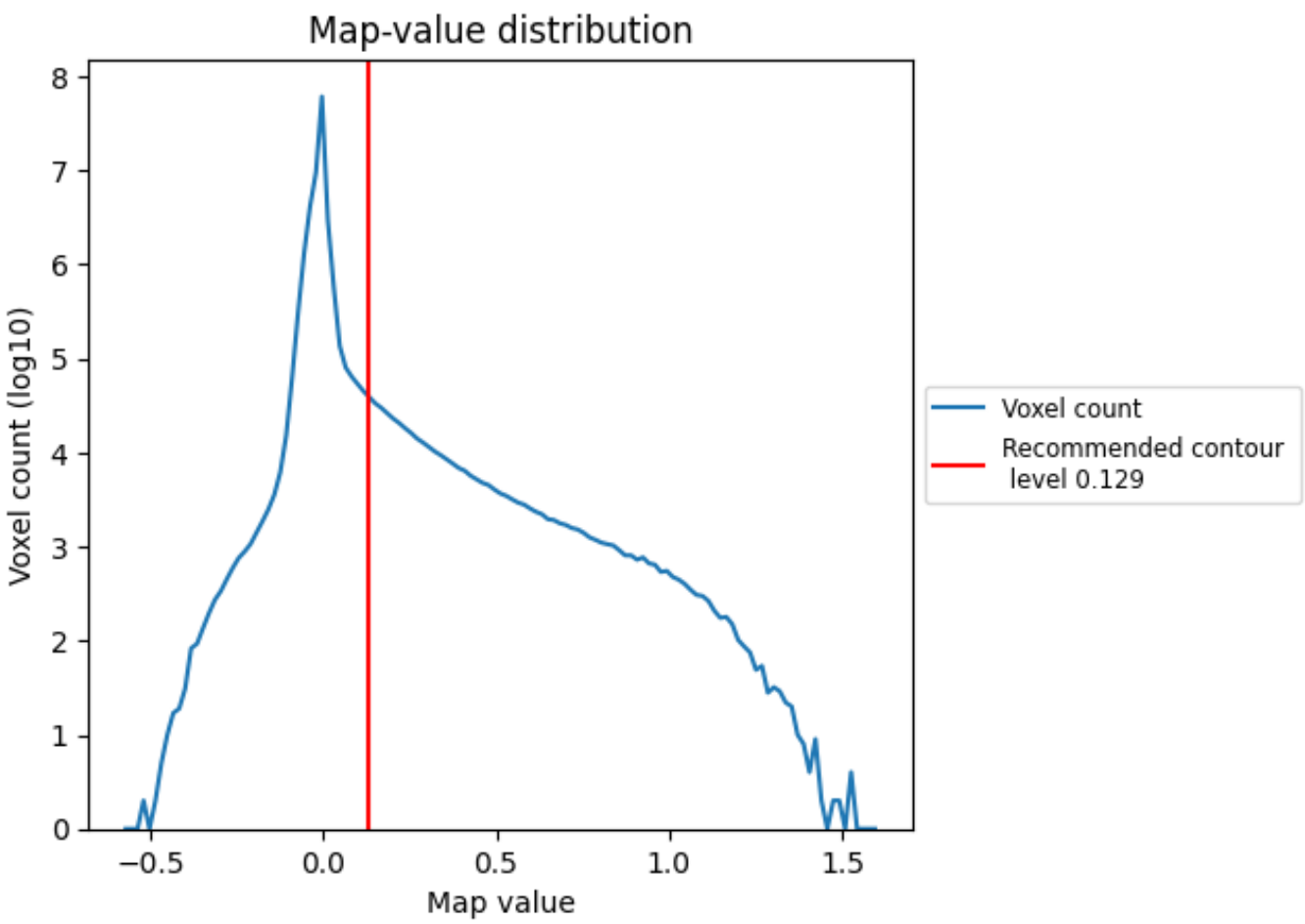
6.5 Mask visualisation (i)

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

7 Map analysis (i)

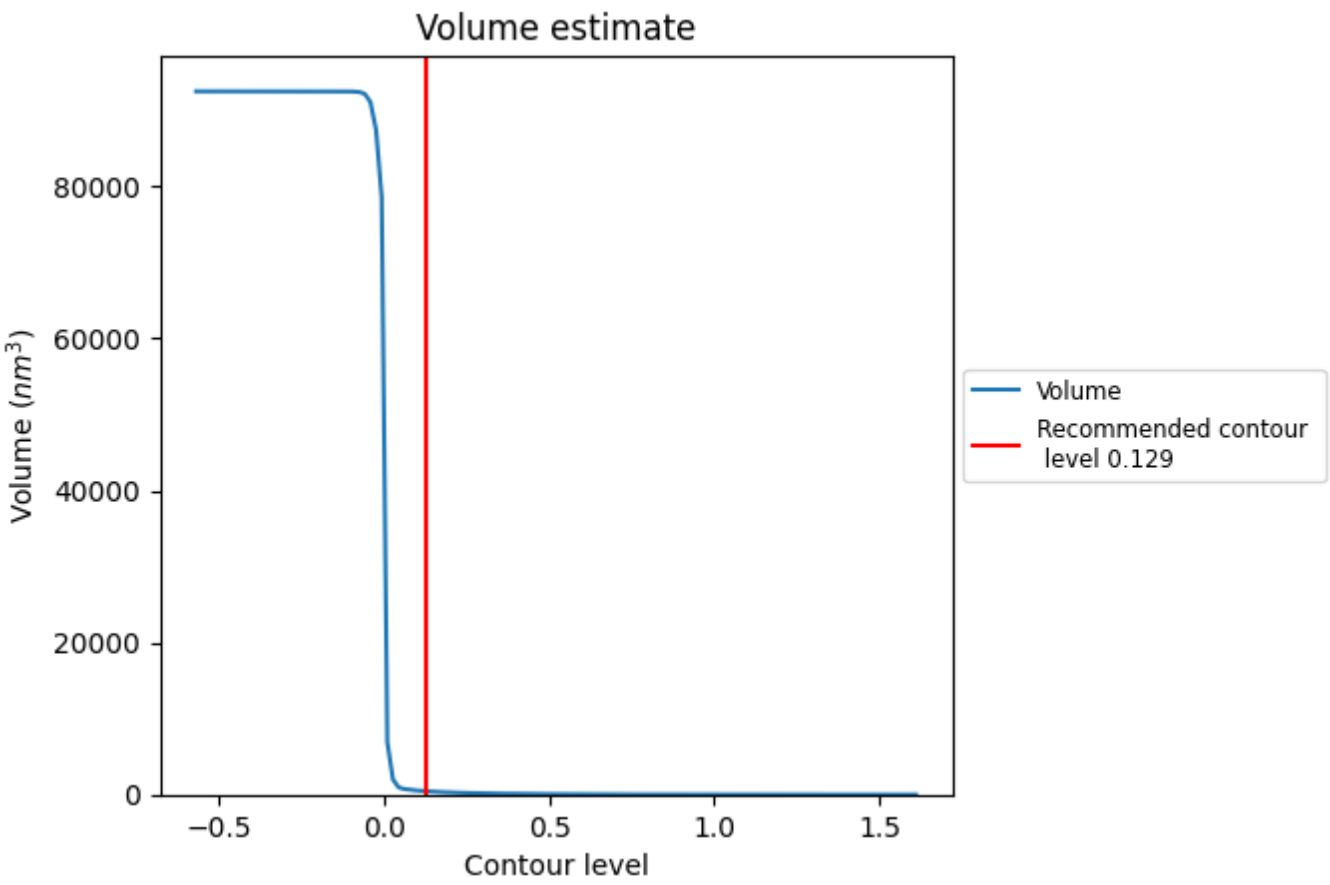
This section contains the results of statistical analysis of the map.

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.

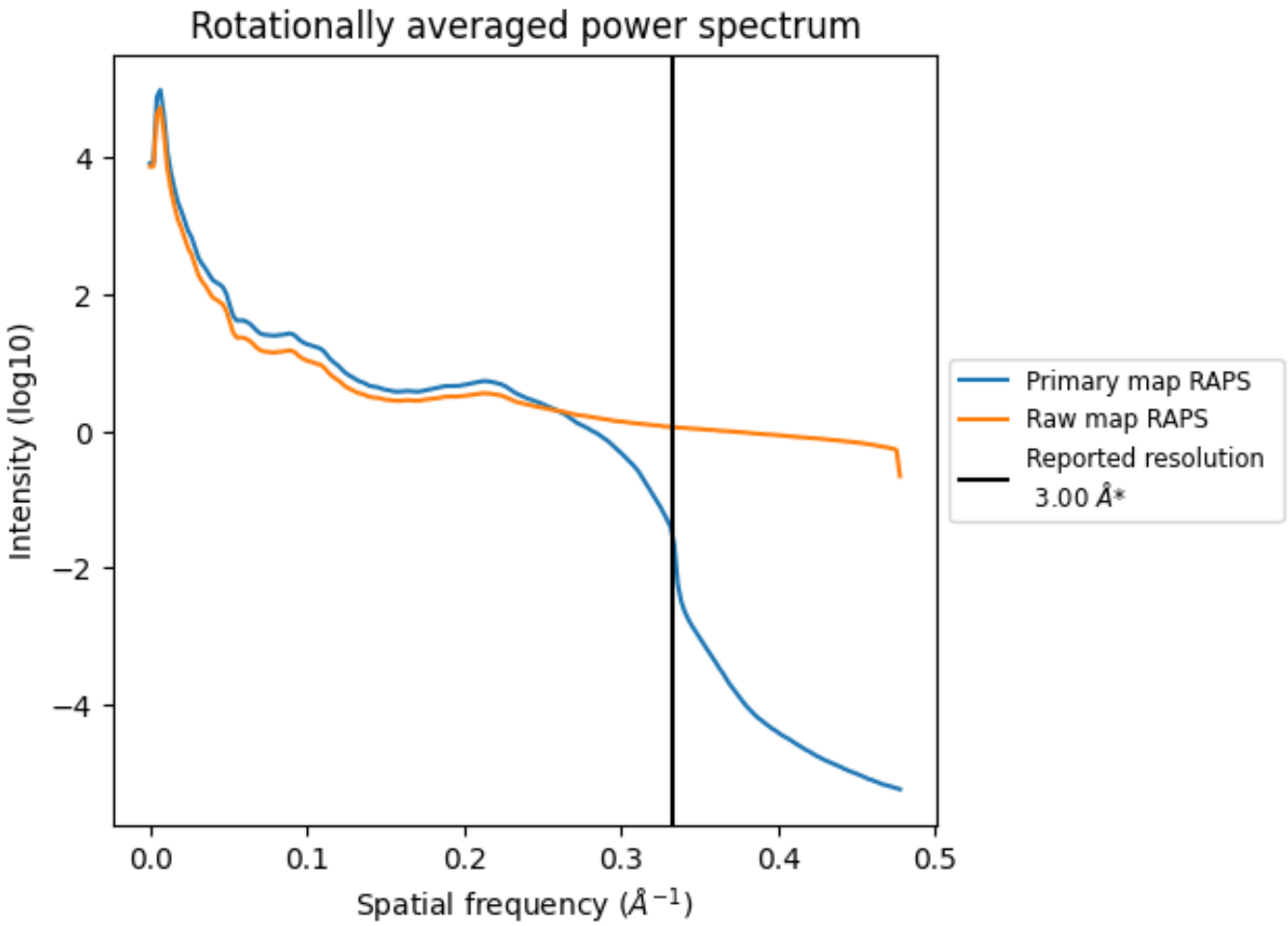
7.2 Volume estimate (i)



The volume at the recommended contour level is 437 nm^3; this corresponds to an approximate mass of 395 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)

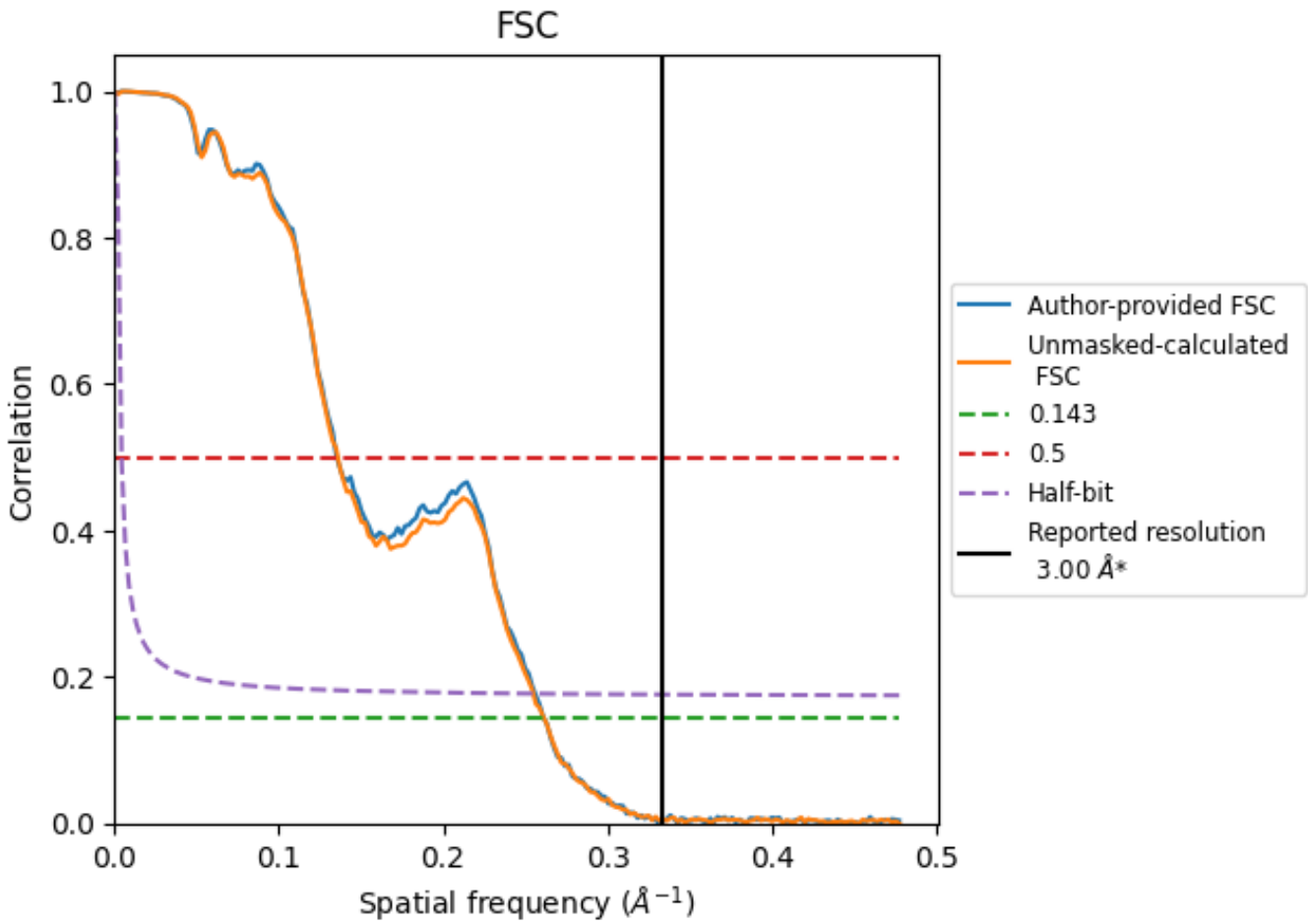


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

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 0.333 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.83	7.40	3.91
Unmasked-calculated*	3.83	7.36	3.92

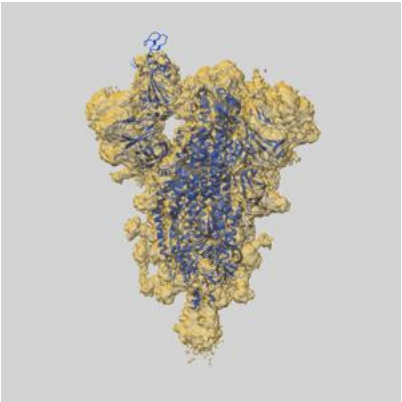
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.83 differs from the reported value 3.0 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.83 differs from the reported value 3.0 by more than 10 %

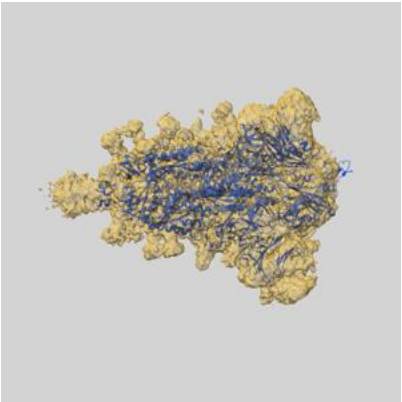
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11328 and PDB model 6ZOW. Per-residue inclusion information can be found in section 3 on page 18.

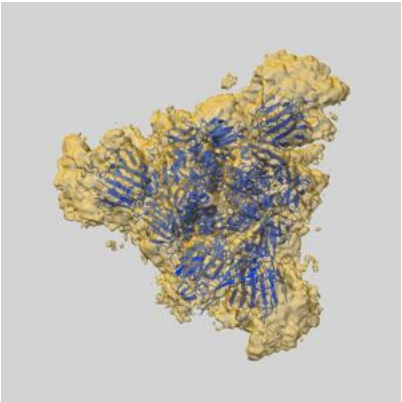
9.1 Map-model overlay (i)



X



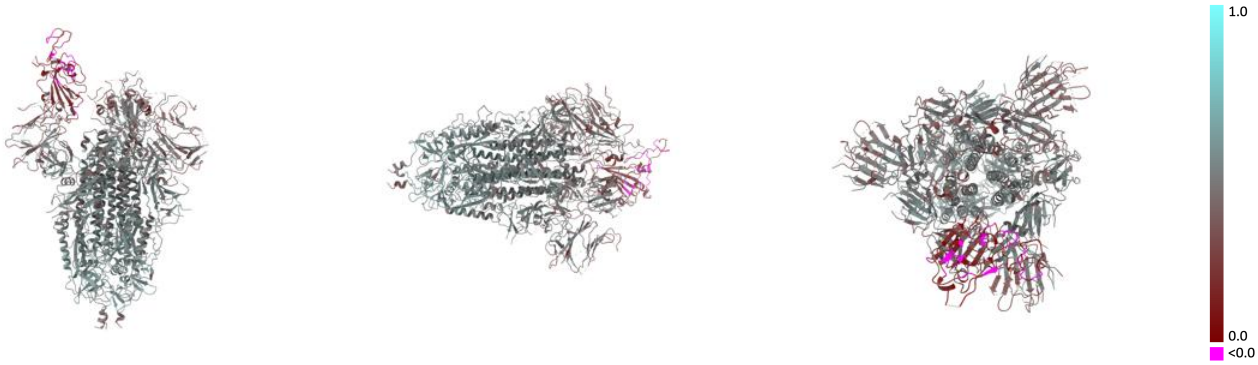
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.129 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.

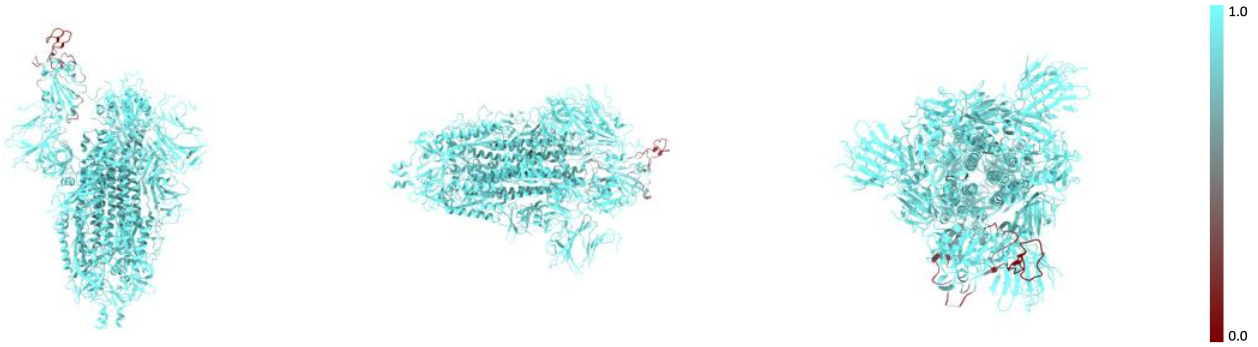
9.2 Q-score mapped to coordinate model (i)



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.

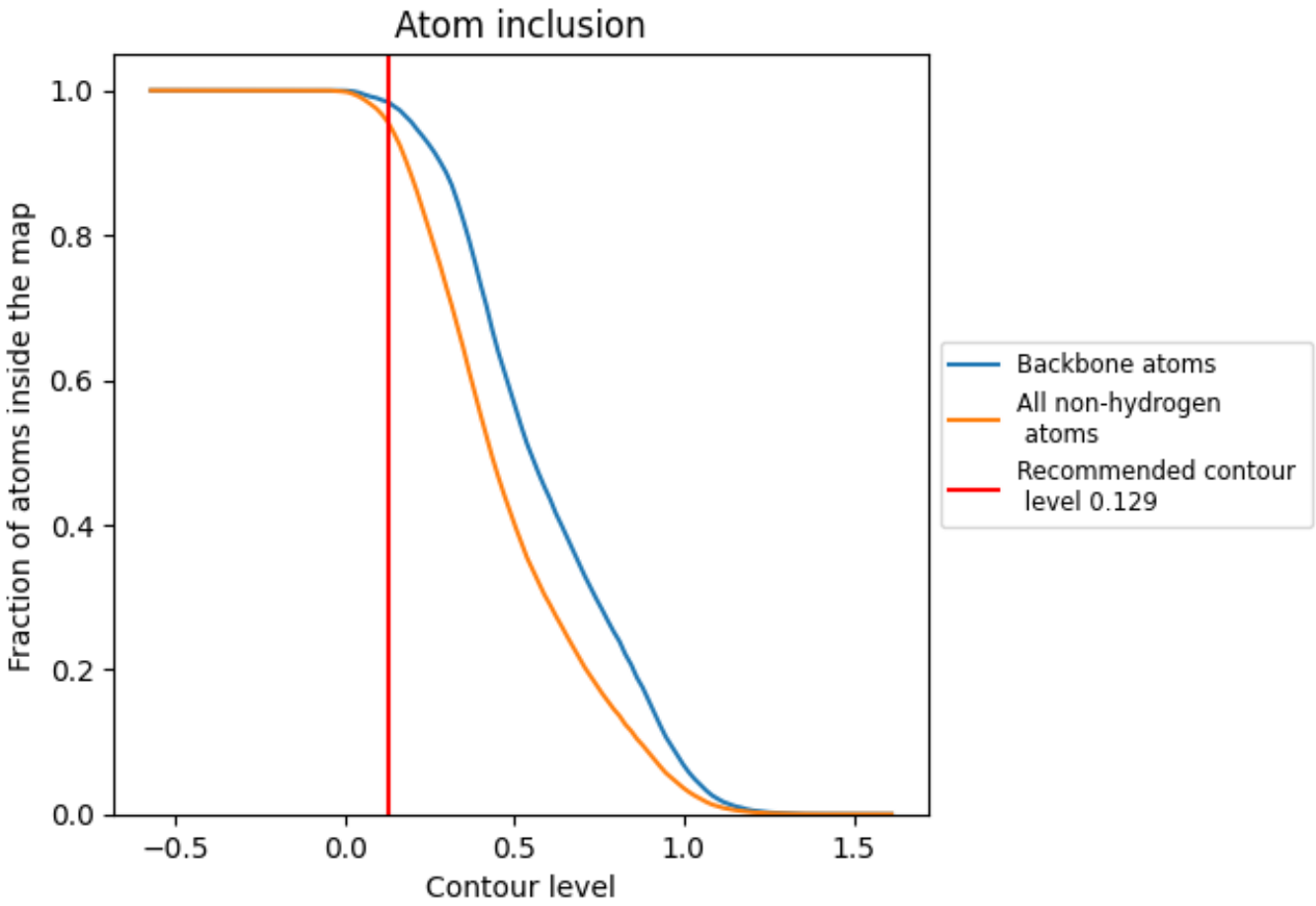
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.129).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.129) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9554	0.4510
A	0.9789	0.4930
B	0.9756	0.4710
C	0.9716	0.4660
D	0.6429	0.3870
E	0.9800	0.4370
F	0.9600	0.3690
G	0.9643	0.4940
H	1.0000	0.4600
I	1.0000	0.4620
J	0.7857	0.2550
K	0.9643	0.4180
L	0.8571	0.3000
M	1.0000	0.4410
N	0.9487	0.4220
O	0.8718	0.3640
P	1.0000	0.4510
Q	0.9744	0.4380
R	1.0000	0.4680
S	0.9643	0.3520
T	0.8571	0.2440
U	0.9800	0.4050
V	1.0000	0.4210
W	0.8462	0.3820
X	1.0000	0.4310
Y	1.0000	0.5110
Z	1.0000	0.4550
a	0.6930	0.1310
b	0.8718	0.3680
c	1.0000	0.4780
d	0.9643	0.3340
e	0.6786	0.3140