Full wwPDB EM Validation Report (i)

Nov 22, 2022 – 12:00 PM JST

PDB ID	:	7EDJ
EMDB ID	:	EMD-31073
Title	:	Cryo-EM structure of SARS-CoV-2 S-UK variant (B.1.1.7) in complex with A ngiotensin-converting enzyme 2 (ACE2) ectodomain
Authors	:	Yang, T.J.; Yu, P.Y.; Chang, Y.C.; Wu, H.C.; Hsu, S.T.D.
Deposited on	:	2021-03-16
Resolution	:	3.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (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:

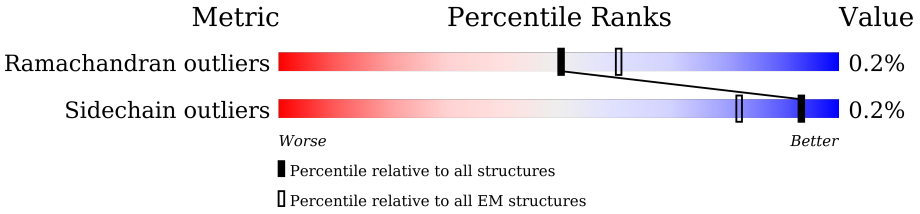
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	1286	79% 20%
1	B	1286	5% 79% 21%
1	C	1286	• 78% 22%
2	I	861	9% 69% 31%
2	J	861	60% 69% 31%
2	K	861	45% 69% 31%
3	D	2	50% 100%
3	E	2	100%
3	F	2	100%

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Mol	Chain	Length	Quality of chain
3	G	2	100%
3	H	2	50% 50%
3	L	2	100%
3	M	2	100%
3	N	2	50% 50% 50%
3	O	2	100%
3	P	2	50% 50%
3	Q	2	100%
3	R	2	100%
3	S	2	100%
3	T	2	50% 50%
3	U	2	50% 50%
3	V	2	100%
3	W	2	100%
3	X	2	50% 100%
3	Y	2	100%
3	Z	2	100%
3	a	2	50% 100%
3	b	2	100%
3	c	2	100%
3	d	2	50% 100%
3	e	2	100%
3	f	2	100%
3	g	2	50% 50% 50%
3	h	2	100%

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Mol	Chain	Length	Quality of chain
3	i	2	100%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 39565 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	1024	7992	5104	1329	1523	36	0	0
1	B	1016	7933	5070	1319	1508	36	0	0
1	C	1008	7878	5037	1308	1497	36	0	0

There are 330 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP P0DTC2
A	-4	GLU	-	expression tag	UNP P0DTC2
A	-3	THR	-	expression tag	UNP P0DTC2
A	-2	ASP	-	expression tag	UNP P0DTC2
A	-1	THR	-	expression tag	UNP P0DTC2
A	0	LEU	-	expression tag	UNP P0DTC2
A	1	LEU	-	expression tag	UNP P0DTC2
A	2	LEU	-	expression tag	UNP P0DTC2
A	3	TRP	-	expression tag	UNP P0DTC2
A	4	VAL	-	expression tag	UNP P0DTC2
A	5	LEU	-	expression tag	UNP P0DTC2
A	6	LEU	-	expression tag	UNP P0DTC2
A	7	LEU	-	expression tag	UNP P0DTC2
A	8	TRP	-	expression tag	UNP P0DTC2
A	9	VAL	-	expression tag	UNP P0DTC2
A	10	PRO	-	expression tag	UNP P0DTC2
A	11	GLY	-	expression tag	UNP P0DTC2
A	12	SER	-	expression tag	UNP P0DTC2
A	13	THR	-	expression tag	UNP P0DTC2
A	14	GLY	-	expression tag	UNP P0DTC2
A	15	ASP	-	expression tag	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	498	TYR	ASN	conflict	UNP P0DTC2
A	567	ASP	ALA	conflict	UNP P0DTC2
A	611	GLY	ASP	conflict	UNP P0DTC2
A	678	HIS	PRO	conflict	UNP P0DTC2
A	680	ALA	ARG	conflict	UNP P0DTC2
A	682	ALA	ARG	conflict	UNP P0DTC2
A	713	ILE	THR	conflict	UNP P0DTC2
A	979	ALA	SER	conflict	UNP P0DTC2
A	983	PRO	LYS	conflict	UNP P0DTC2
A	984	PRO	VAL	conflict	UNP P0DTC2
A	1115	HIS	ASP	conflict	UNP P0DTC2
A	1206	GLU	-	expression tag	UNP P0DTC2
A	1207	PHE	-	expression tag	UNP P0DTC2
A	1208	GLY	-	expression tag	UNP P0DTC2
A	1209	SER	-	expression tag	UNP P0DTC2
A	1210	GLY	-	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	LYS	-	expression tag	UNP P0DTC2
A	1239	GLY	-	expression tag	UNP P0DTC2
A	1240	GLN	-	expression tag	UNP P0DTC2
A	1241	ASP	-	expression tag	UNP P0DTC2
A	1242	ASN	-	expression tag	UNP P0DTC2
A	1243	SER	-	expression tag	UNP P0DTC2
A	1244	ALA	-	expression tag	UNP P0DTC2
A	1245	ASP	-	expression tag	UNP P0DTC2
A	1246	ILE	-	expression tag	UNP P0DTC2
A	1247	GLN	-	expression tag	UNP P0DTC2
A	1248	HIS	-	expression tag	UNP P0DTC2
A	1249	SER	-	expression tag	UNP P0DTC2
A	1250	GLY	-	expression tag	UNP P0DTC2
A	1251	ARG	-	expression tag	UNP P0DTC2
A	1252	PRO	-	expression tag	UNP P0DTC2
A	1253	LEU	-	expression tag	UNP P0DTC2
A	1254	GLU	-	expression tag	UNP P0DTC2
A	1255	SER	-	expression tag	UNP P0DTC2
A	1256	ARG	-	expression tag	UNP P0DTC2
A	1257	GLY	-	expression tag	UNP P0DTC2
A	1258	PRO	-	expression tag	UNP P0DTC2
A	1259	PHE	-	expression tag	UNP P0DTC2
A	1260	GLU	-	expression tag	UNP P0DTC2
A	1261	GLN	-	expression tag	UNP P0DTC2
A	1262	LYS	-	expression tag	UNP P0DTC2
A	1263	LEU	-	expression tag	UNP P0DTC2
A	1264	ILE	-	expression tag	UNP P0DTC2
A	1265	SER	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	GLU	-	expression tag	UNP P0DTC2
A	1268	ASP	-	expression tag	UNP P0DTC2
A	1269	LEU	-	expression tag	UNP P0DTC2
A	1270	ASN	-	expression tag	UNP P0DTC2
A	1271	MET	-	expression tag	UNP P0DTC2
A	1272	HIS	-	expression tag	UNP P0DTC2
A	1273	THR	-	expression tag	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	HIS	-	expression tag	UNP P0DTC2
A	1276	HIS	-	expression tag	UNP P0DTC2
A	1277	HIS	-	expression tag	UNP P0DTC2
A	1278	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1279	HIS	-	expression tag	UNP P0DTC2
A	1280	HIS	-	expression tag	UNP P0DTC2
B	-5	MET	-	initiating methionine	UNP P0DTC2
B	-4	GLU	-	expression tag	UNP P0DTC2
B	-3	THR	-	expression tag	UNP P0DTC2
B	-2	ASP	-	expression tag	UNP P0DTC2
B	-1	THR	-	expression tag	UNP P0DTC2
B	0	LEU	-	expression tag	UNP P0DTC2
B	1	LEU	-	expression tag	UNP P0DTC2
B	2	LEU	-	expression tag	UNP P0DTC2
B	3	TRP	-	expression tag	UNP P0DTC2
B	4	VAL	-	expression tag	UNP P0DTC2
B	5	LEU	-	expression tag	UNP P0DTC2
B	6	LEU	-	expression tag	UNP P0DTC2
B	7	LEU	-	expression tag	UNP P0DTC2
B	8	TRP	-	expression tag	UNP P0DTC2
B	9	VAL	-	expression tag	UNP P0DTC2
B	10	PRO	-	expression tag	UNP P0DTC2
B	11	GLY	-	expression tag	UNP P0DTC2
B	12	SER	-	expression tag	UNP P0DTC2
B	13	THR	-	expression tag	UNP P0DTC2
B	14	GLY	-	expression tag	UNP P0DTC2
B	15	ASP	-	expression tag	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	498	TYR	ASN	conflict	UNP P0DTC2
B	567	ASP	ALA	conflict	UNP P0DTC2
B	611	GLY	ASP	conflict	UNP P0DTC2
B	678	HIS	PRO	conflict	UNP P0DTC2
B	680	ALA	ARG	conflict	UNP P0DTC2
B	682	ALA	ARG	conflict	UNP P0DTC2
B	713	ILE	THR	conflict	UNP P0DTC2
B	979	ALA	SER	conflict	UNP P0DTC2
B	983	PRO	LYS	conflict	UNP P0DTC2
B	984	PRO	VAL	conflict	UNP P0DTC2
B	1115	HIS	ASP	conflict	UNP P0DTC2
B	1206	GLU	-	expression tag	UNP P0DTC2
B	1207	PHE	-	expression tag	UNP P0DTC2
B	1208	GLY	-	expression tag	UNP P0DTC2
B	1209	SER	-	expression tag	UNP P0DTC2
B	1210	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	LYS	-	expression tag	UNP P0DTC2
B	1239	GLY	-	expression tag	UNP P0DTC2
B	1240	GLN	-	expression tag	UNP P0DTC2
B	1241	ASP	-	expression tag	UNP P0DTC2
B	1242	ASN	-	expression tag	UNP P0DTC2
B	1243	SER	-	expression tag	UNP P0DTC2
B	1244	ALA	-	expression tag	UNP P0DTC2
B	1245	ASP	-	expression tag	UNP P0DTC2
B	1246	ILE	-	expression tag	UNP P0DTC2
B	1247	GLN	-	expression tag	UNP P0DTC2
B	1248	HIS	-	expression tag	UNP P0DTC2
B	1249	SER	-	expression tag	UNP P0DTC2
B	1250	GLY	-	expression tag	UNP P0DTC2
B	1251	ARG	-	expression tag	UNP P0DTC2
B	1252	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1253	LEU	-	expression tag	UNP P0DTC2
B	1254	GLU	-	expression tag	UNP P0DTC2
B	1255	SER	-	expression tag	UNP P0DTC2
B	1256	ARG	-	expression tag	UNP P0DTC2
B	1257	GLY	-	expression tag	UNP P0DTC2
B	1258	PRO	-	expression tag	UNP P0DTC2
B	1259	PHE	-	expression tag	UNP P0DTC2
B	1260	GLU	-	expression tag	UNP P0DTC2
B	1261	GLN	-	expression tag	UNP P0DTC2
B	1262	LYS	-	expression tag	UNP P0DTC2
B	1263	LEU	-	expression tag	UNP P0DTC2
B	1264	ILE	-	expression tag	UNP P0DTC2
B	1265	SER	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	GLU	-	expression tag	UNP P0DTC2
B	1268	ASP	-	expression tag	UNP P0DTC2
B	1269	LEU	-	expression tag	UNP P0DTC2
B	1270	ASN	-	expression tag	UNP P0DTC2
B	1271	MET	-	expression tag	UNP P0DTC2
B	1272	HIS	-	expression tag	UNP P0DTC2
B	1273	THR	-	expression tag	UNP P0DTC2
B	1274	GLY	-	expression tag	UNP P0DTC2
B	1275	HIS	-	expression tag	UNP P0DTC2
B	1276	HIS	-	expression tag	UNP P0DTC2
B	1277	HIS	-	expression tag	UNP P0DTC2
B	1278	HIS	-	expression tag	UNP P0DTC2
B	1279	HIS	-	expression tag	UNP P0DTC2
B	1280	HIS	-	expression tag	UNP P0DTC2
C	-5	MET	-	initiating methionine	UNP P0DTC2
C	-4	GLU	-	expression tag	UNP P0DTC2
C	-3	THR	-	expression tag	UNP P0DTC2
C	-2	ASP	-	expression tag	UNP P0DTC2
C	-1	THR	-	expression tag	UNP P0DTC2
C	0	LEU	-	expression tag	UNP P0DTC2
C	1	LEU	-	expression tag	UNP P0DTC2
C	2	LEU	-	expression tag	UNP P0DTC2
C	3	TRP	-	expression tag	UNP P0DTC2
C	4	VAL	-	expression tag	UNP P0DTC2
C	5	LEU	-	expression tag	UNP P0DTC2
C	6	LEU	-	expression tag	UNP P0DTC2
C	7	LEU	-	expression tag	UNP P0DTC2
C	8	TRP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	9	VAL	-	expression tag	UNP P0DTC2
C	10	PRO	-	expression tag	UNP P0DTC2
C	11	GLY	-	expression tag	UNP P0DTC2
C	12	SER	-	expression tag	UNP P0DTC2
C	13	THR	-	expression tag	UNP P0DTC2
C	14	GLY	-	expression tag	UNP P0DTC2
C	15	ASP	-	expression tag	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	498	TYR	ASN	conflict	UNP P0DTC2
C	567	ASP	ALA	conflict	UNP P0DTC2
C	611	GLY	ASP	conflict	UNP P0DTC2
C	678	HIS	PRO	conflict	UNP P0DTC2
C	680	ALA	ARG	conflict	UNP P0DTC2
C	682	ALA	ARG	conflict	UNP P0DTC2
C	713	ILE	THR	conflict	UNP P0DTC2
C	979	ALA	SER	conflict	UNP P0DTC2
C	983	PRO	LYS	conflict	UNP P0DTC2
C	984	PRO	VAL	conflict	UNP P0DTC2
C	1115	HIS	ASP	conflict	UNP P0DTC2
C	1206	GLU	-	expression tag	UNP P0DTC2
C	1207	PHE	-	expression tag	UNP P0DTC2
C	1208	GLY	-	expression tag	UNP P0DTC2
C	1209	SER	-	expression tag	UNP P0DTC2
C	1210	GLY	-	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
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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	LYS	-	expression tag	UNP P0DTC2
C	1239	GLY	-	expression tag	UNP P0DTC2
C	1240	GLN	-	expression tag	UNP P0DTC2
C	1241	ASP	-	expression tag	UNP P0DTC2
C	1242	ASN	-	expression tag	UNP P0DTC2
C	1243	SER	-	expression tag	UNP P0DTC2
C	1244	ALA	-	expression tag	UNP P0DTC2
C	1245	ASP	-	expression tag	UNP P0DTC2
C	1246	ILE	-	expression tag	UNP P0DTC2
C	1247	GLN	-	expression tag	UNP P0DTC2
C	1248	HIS	-	expression tag	UNP P0DTC2
C	1249	SER	-	expression tag	UNP P0DTC2
C	1250	GLY	-	expression tag	UNP P0DTC2
C	1251	ARG	-	expression tag	UNP P0DTC2
C	1252	PRO	-	expression tag	UNP P0DTC2
C	1253	LEU	-	expression tag	UNP P0DTC2
C	1254	GLU	-	expression tag	UNP P0DTC2
C	1255	SER	-	expression tag	UNP P0DTC2
C	1256	ARG	-	expression tag	UNP P0DTC2
C	1257	GLY	-	expression tag	UNP P0DTC2
C	1258	PRO	-	expression tag	UNP P0DTC2
C	1259	PHE	-	expression tag	UNP P0DTC2
C	1260	GLU	-	expression tag	UNP P0DTC2
C	1261	GLN	-	expression tag	UNP P0DTC2
C	1262	LYS	-	expression tag	UNP P0DTC2
C	1263	LEU	-	expression tag	UNP P0DTC2
C	1264	ILE	-	expression tag	UNP P0DTC2
C	1265	SER	-	expression tag	UNP P0DTC2
C	1266	GLU	-	expression tag	UNP P0DTC2
C	1267	GLU	-	expression tag	UNP P0DTC2
C	1268	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1269	LEU	-	expression tag	UNP P0DTC2
C	1270	ASN	-	expression tag	UNP P0DTC2
C	1271	MET	-	expression tag	UNP P0DTC2
C	1272	HIS	-	expression tag	UNP P0DTC2
C	1273	THR	-	expression tag	UNP P0DTC2
C	1274	GLY	-	expression tag	UNP P0DTC2
C	1275	HIS	-	expression tag	UNP P0DTC2
C	1276	HIS	-	expression tag	UNP P0DTC2
C	1277	HIS	-	expression tag	UNP P0DTC2
C	1278	HIS	-	expression tag	UNP P0DTC2
C	1279	HIS	-	expression tag	UNP P0DTC2
C	1280	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Angiotensin-converting enzyme 2 (ACE2) ectodomain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	I	596	4862	3111	805	917	29	0	0
2	J	596	4862	3111	805	917	29	0	0
2	K	596	4862	3111	805	917	29	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	D	2	28	16	2	10	0	0
3	E	2	28	16	2	10	0	0
3	F	2	28	16	2	10	0	0
3	G	2	28	16	2	10	0	0
3	H	2	28	16	2	10	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	L	2	28	16	2	10	0	0
3	M	2	28	16	2	10	0	0
3	N	2	28	16	2	10	0	0
3	O	2	28	16	2	10	0	0
3	P	2	28	16	2	10	0	0
3	Q	2	28	16	2	10	0	0
3	R	2	28	16	2	10	0	0
3	S	2	28	16	2	10	0	0
3	T	2	28	16	2	10	0	0
3	U	2	28	16	2	10	0	0
3	V	2	28	16	2	10	0	0
3	W	2	28	16	2	10	0	0
3	X	2	28	16	2	10	0	0
3	Y	2	28	16	2	10	0	0
3	Z	2	28	16	2	10	0	0
3	a	2	28	16	2	10	0	0
3	b	2	28	16	2	10	0	0
3	c	2	28	16	2	10	0	0
3	d	2	28	16	2	10	0	0
3	e	2	28	16	2	10	0	0
3	f	2	28	16	2	10	0	0

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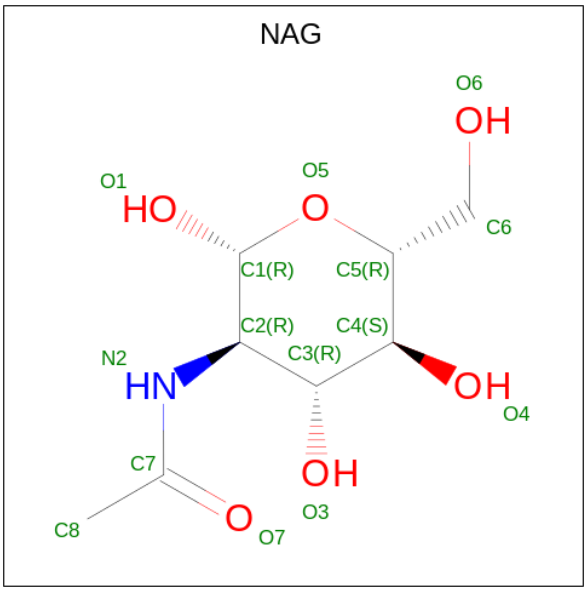
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	g	2	28	16	2	10	0	0
			Total	C	N	O		
3	h	2	28	16	2	10	0	0
			Total	C	N	O		
3	i	2	28	16	2	10	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	A	1	84	48	6	30	0
			Total	C	N	O	
4	A	1	84	48	6	30	0
			Total	C	N	O	
4	A	1	84	48	6	30	0
			Total	C	N	O	
4	A	1	84	48	6	30	0
			Total	C	N	O	
4	A	1	84	48	6	30	0
			Total	C	N	O	
4	A	1	84	48	6	30	0
			Total	C	N	O	
4	B	1	84	48	6	30	0
			Total	C	N	O	
4	B	1	84	48	6	30	0

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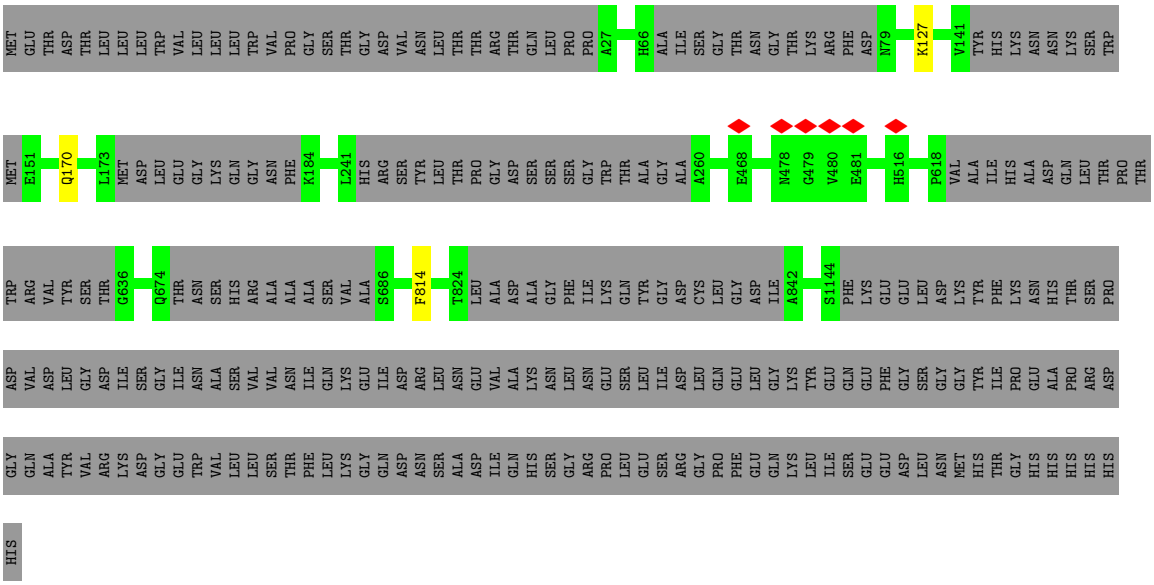
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	B	1	84	48	6	30	0
4	B	1	84	48	6	30	0
4	B	1	84	48	6	30	0
4	B	1	84	48	6	30	0
4	C	1	98	56	7	35	0
4	C	1	98	56	7	35	0
4	C	1	98	56	7	35	0
4	C	1	98	56	7	35	0
4	C	1	98	56	7	35	0
4	C	1	98	56	7	35	0
4	C	1	98	56	7	35	0
4	I	1	84	48	6	30	0
4	I	1	84	48	6	30	0
4	I	1	84	48	6	30	0
4	I	1	84	48	6	30	0
4	I	1	84	48	6	30	0
4	I	1	84	48	6	30	0
4	J	1	14	8	1	5	0

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.

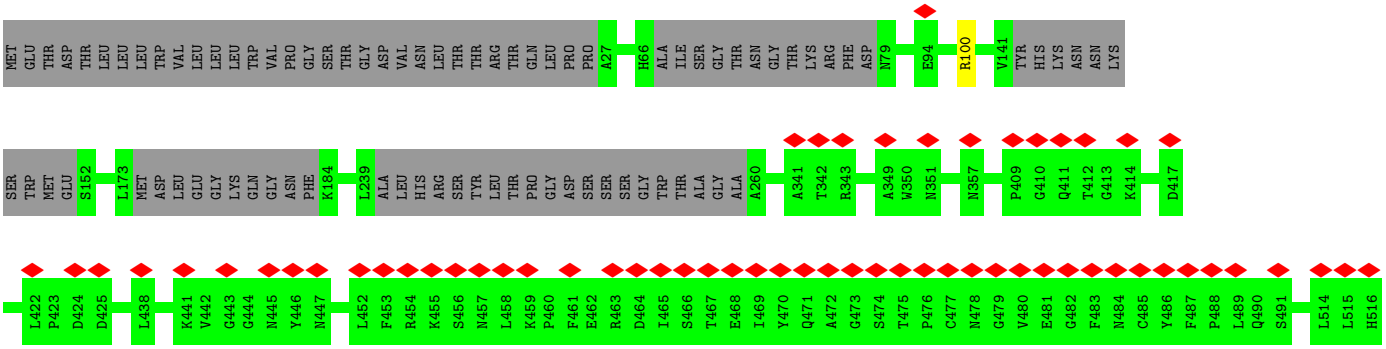
- Molecule 1: Spike glycoprotein

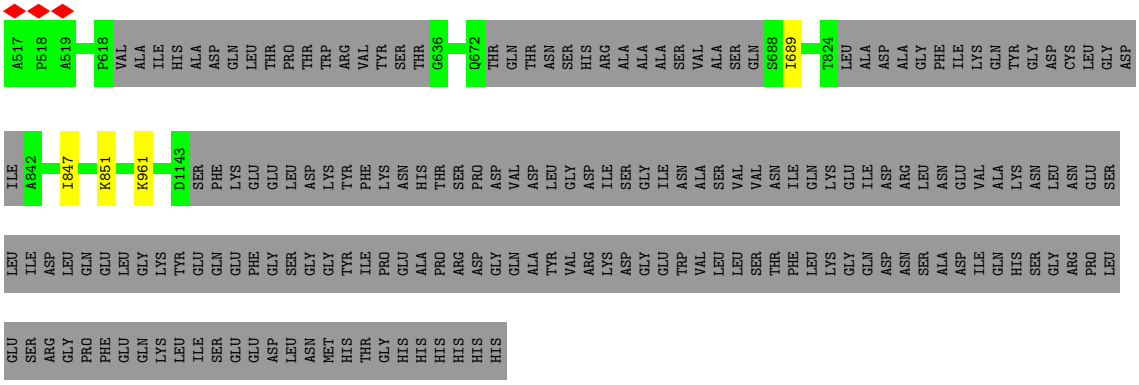
Chain A:



- Molecule 1: Spike glycoprotein

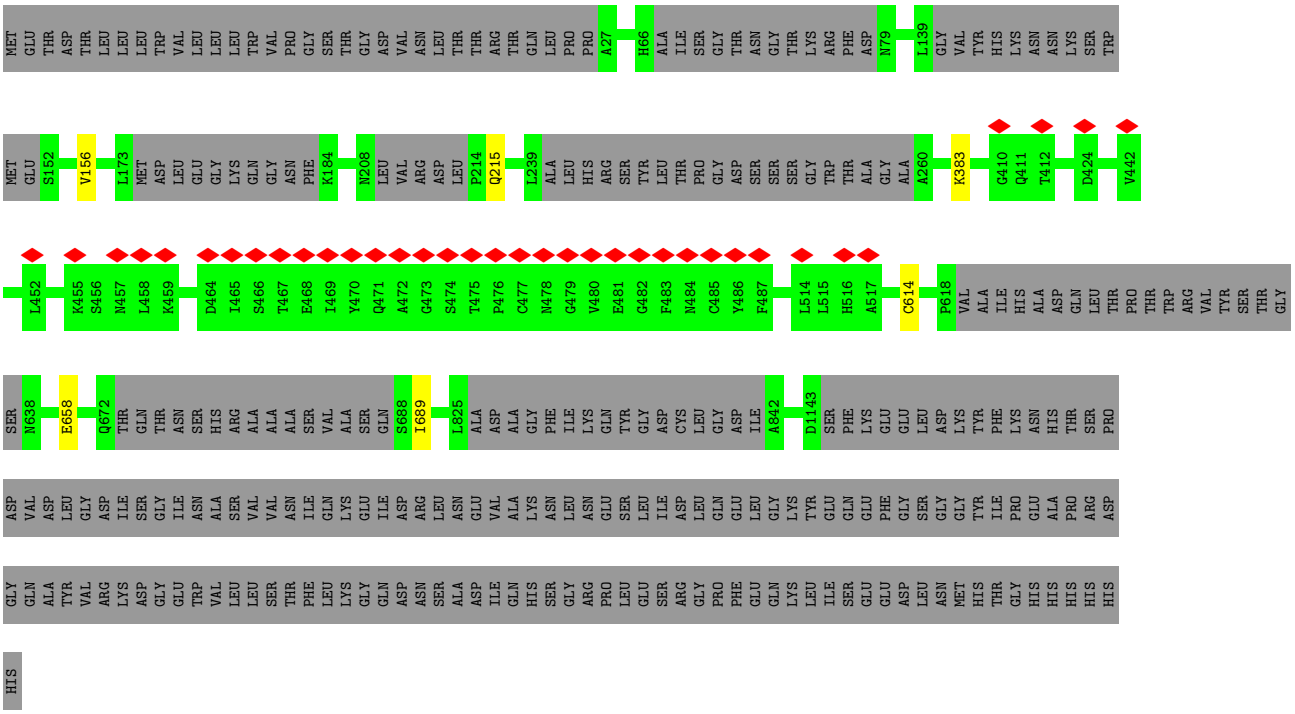
Chain B:





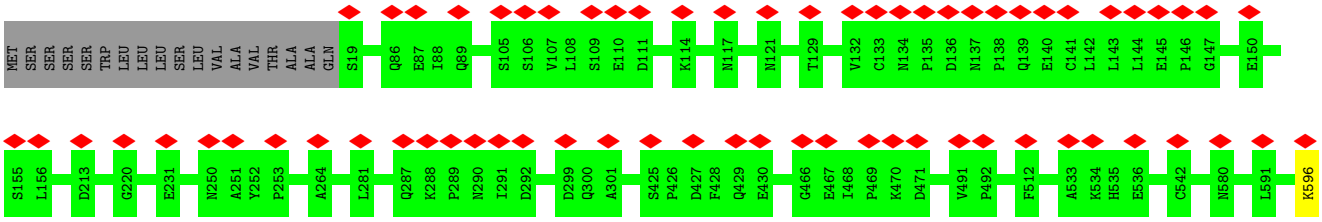
- Molecule 1: Spike glycoprotein

Chain C:



- Molecule 2: Angiotensin-converting enzyme 2 (ACE2) ectodomain

Chain I:



D597 Q598 N599 K600 N601 S602 S607 T608 Y613 A614 ASP GLY SER GLY GLY GLY SER GLY SER GLY GLY SER LYS GLY GLU GLU LEU PHE THR GLY VAL VAL PRO ILE LEU VAL GLU LEU ASP GLY ASP VAL ASN GLY HIS LYS PHE SER VAL ARG GLY GLU GLY GLU GLY ASP ALA THR ASN

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

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

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

LEU LEU GLU PHE VAL THR ALA ALA GLY ILE THR HIS GLY MET ASP GLU LEU TYR LYS

- Molecule 2: Angiotensin-converting enzyme 2 (ACE2) ectodomain

Chain J: 60% 69% 31%

MET SER SER SER SER TRP LEU LEU LEU SER LEU VAL ALA VAL THR ALA ALA GLN S19 T20 I21 E22 E23 Q24 A25 K26 T27 F28 L29 D30 K31 H34 E35 A36 E37 D38 L39 F40 Y41 Q42 L45 N49 Y50 N53 I54 T55 E56 E57 N58 V59 Q60 N61 M62 N63 N64 A65

G66 D67 K68 W69 S70 A71 F72 L73 K74 E75 Q76 S77 T78 L79 A80 Q81 M82 Y83 P84 L85 Q86 E87 I88 Q89 N90 L91 T92 V93 K94 L95 Q96 L97 Q98 A99 L100 Q101 Q102 N103 G104 S105 S106 V107 L108 S109 E110 D111 K112 S113 K114 R115 L116 N117 T118 I119 L120 N121 T122 M123 S124 T125

I126 Y127 S128 T129 G130 K131 V132 C133 N134 P135 D136 N137 P138 Q139 E140 C141 L142 L143 L144 E145 P146 G147 L148 N149 E150 I151 M152 A153 N154 S155 L156 D157 Y158 N159 E160 R161 L162 W163 A164 W165 E166 S167 W168 R169 S170 E171 V172 G173 K174 Q175 L176 R177 P178 L179 Y180 E181 E182 Y183 V184 V185

L186 K187 N188 E189 M190 A191 R192 A193 N194 H195 Y196 E197 D198 Y199 G200 D201 Y202 W203 R204 G205 D206 Y207 E208 V209 N210 G211 V212 D213 G214 Y215 D216 Y217 S218 R219 G220 Q221 L222 I223 E224 D225 V226 E227 H228 T229 F230 E231 E232 I233 K234 P235 L236 Y237 E238 H239 L240 H241 A242 Y243 V244 R245

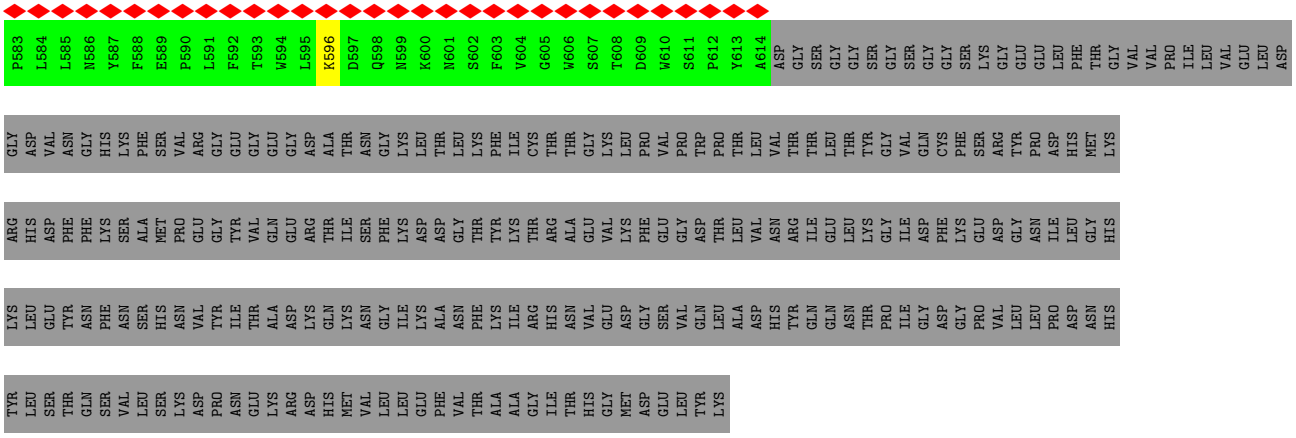
A246 K247 L248 M249 N250 A251 Y252 P253 S254 Y255 I256 S257 P258 I259 G260 C261 L262 P263 A264 H265 L266 L267 G268 D269 M270 W271 G272 R273 F274 W275 T276 N277 L278 Y279 S280 L281 T282 V283 P284 F285 G286 Q287 K288 P289 N290 I291 D292 V293 T294 D295 A296 M297 V298 D299 Q300 A301 W302 D303 A304 Q305

R306 I307 F308 K309 E310 A311 E312 K313 F314 F315 V316 S317 V318 G319 L320 P321 N322 M323 T324 Q325 G326 F327 W328 E329 N330 S331 M332 L333 T334 D335 P336 G337 N338 V339 Q340 K341 C344 H345 D355 F356 K363 V364 T365 M366 D367 D368 F369 L370 T371 H374 M383 A386 A387 Q388

P389 L392 R393 N394 G395 A396 G399 F400 H401 E402 L410 H417 L418 K419 S420 I421 G422 L423 L424 S425 P426 D427 F428 Q429 E430 D431 M432 E433 T434 E435 I436 N437 F438 L439 L440 K441 Q442 A443 L444 T445 I446 V447 G448 T449 L450 P451 F452 T453 Y454 M455 L456 E457 K458 W459 R460 W461

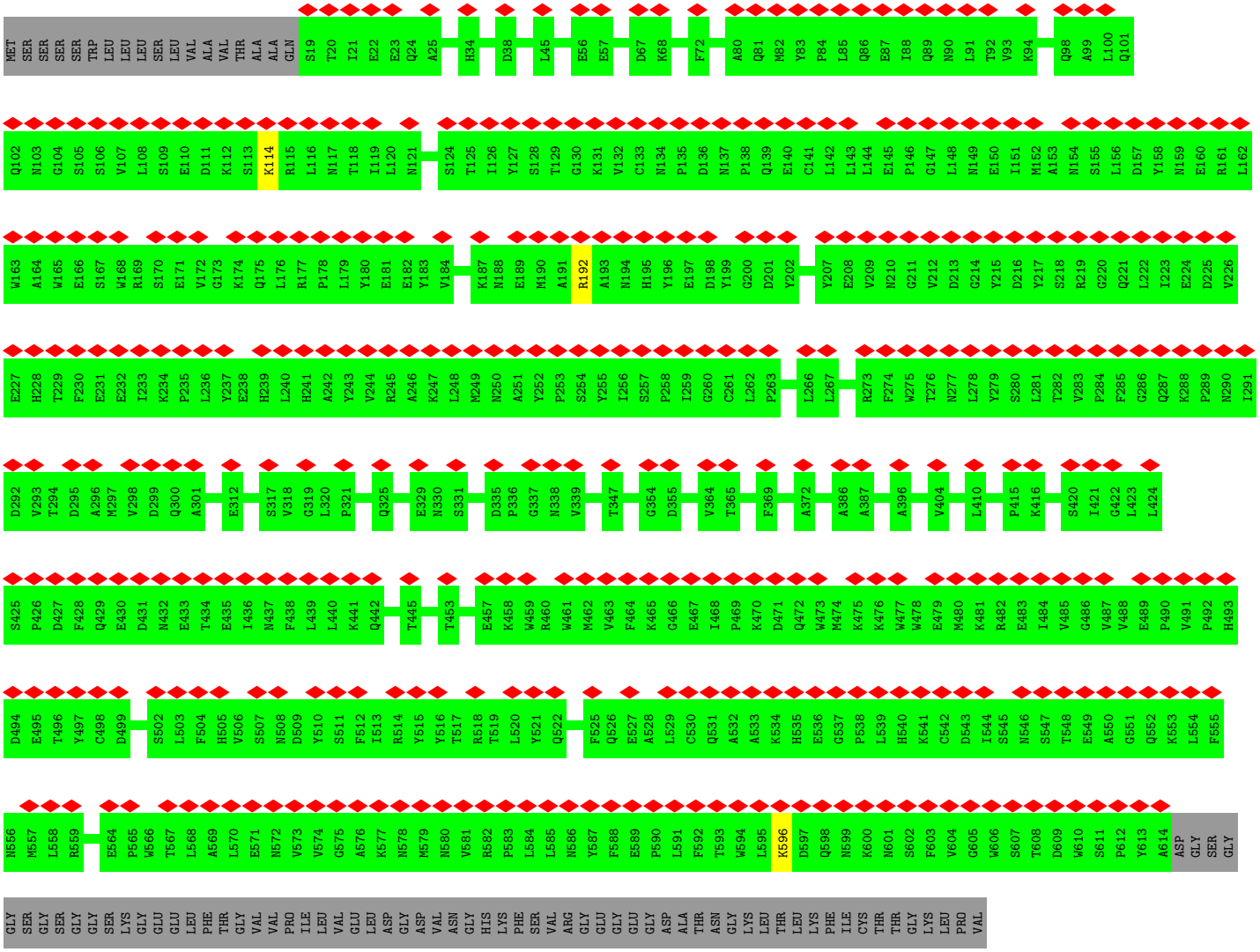
M462 V463 F464 K465 G466 E467 I468 P469 K470 D471 Q472 W473 M474 K475 K476 W477 W478 E479 M480 K481 R482 E483 I484 V485 G486 V487 V488 E489 P490 V491 P492 H493 D494 E495 T496 Y497 C498 D499 P500 A501 S502 L503 F504 H505 V506 S507 N508 D509 Y510 S511 F512 I513 R514 Y515 Y516 T517 R518 T519 L520 Y521

Q522 F523 Q524 F525 Q526 E527 A528 L529 C530 Q531 A532 A533 K534 H535 E536 G537 P538 L539 H540 K541 C542 D543 I544 S545 N546 S547 T548 E549 A550 G551 Q552 K553 L554 F555 N556 M557 L558 R559 L560 S563 E564 P565 W566 T567 L568 A569 L570 E571 N572 V573 V574 G575 A576 K577 N578 M579 N580 V581 R582



- Molecule 2: Angiotensin-converting enzyme 2 (ACE2) ectodomain

Chain K:



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

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

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

LEU TYR LYS

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

Chain D: 50% 100%

NAG1 NAG2

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

Chain E: 100%

NAG1 NAG2

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

Chain F: 100%

NAG1 NAG2

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

Chain G: 100%

NAG1 NAG2

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

Chain H: 50% 50%

NAG1 NAG2

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

Chain L: 100%

NAG1 NAG2

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

Chain M: 100%

NAG1 NAG2

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

Chain N: 50% 50% 50%

NAG1 NAG2

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

Chain O: 100%

NAG1 NAG2

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

Chain P: 50% 50%

NAG1 NAG2

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

Chain Q: 100%

NAG1 NAG2

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

Chain R: 100%

NAG1 NAG2

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

Chain S: 100%

NAG1 NAG2

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

Chain T: 50% 50%

NAG1 NAG2

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

Chain U: 50% 50%

NAG1 NAG2

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

Chain V: 100%

NAG1 NAG2

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

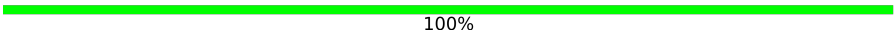
Chain W: 100%

NAG1 NAG2

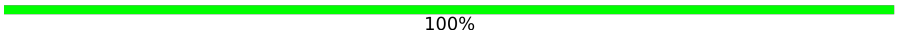
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X: 50% 100%

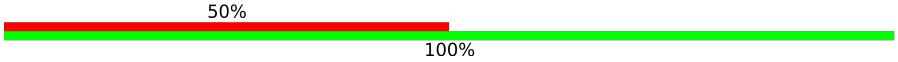
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y: 

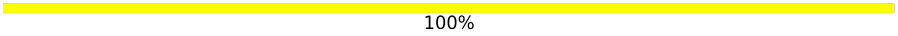
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z: 

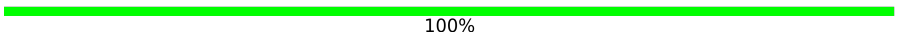
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 

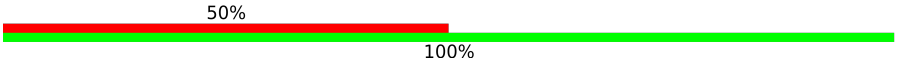
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b: 

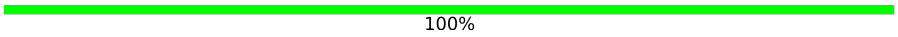
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c: 

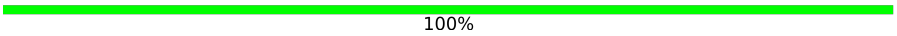
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d: 

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

Chain e: 

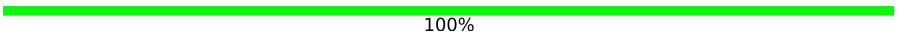
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f: 

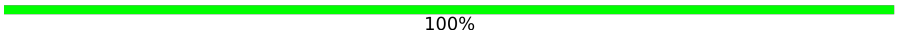
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:

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

Chain h: 

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

Chain i: 

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	460280	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 ($e^-/Å^2$)	1.0	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	3.115	Depositor
Minimum map value	-1.813	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.22	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.37	0/8172	0.53	0/11119
1	B	0.38	0/8113	0.52	0/11039
1	C	0.37	0/8057	0.52	0/10961
2	I	0.25	0/4999	0.45	0/6792
2	J	0.24	0/4999	0.44	0/6792
2	K	0.24	0/4999	0.45	0/6792
All	All	0.33	0/39339	0.50	0/53495

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	614	CYS	Peptide
1	C	658	GLU	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	1008/1286 (78%)	908 (90%)	98 (10%)	2 (0%)	47	77
1	B	1000/1286 (78%)	913 (91%)	84 (8%)	3 (0%)	41	71
1	C	990/1286 (77%)	898 (91%)	89 (9%)	3 (0%)	41	71
2	I	594/861 (69%)	556 (94%)	38 (6%)	0	100	100
2	J	594/861 (69%)	559 (94%)	35 (6%)	0	100	100
2	K	594/861 (69%)	558 (94%)	36 (6%)	0	100	100
All	All	4780/6441 (74%)	4392 (92%)	380 (8%)	8 (0%)	50	77

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	814	PHE
1	B	847	ILE
1	C	156	VAL
1	B	100	ARG
1	B	689	ILE
1	C	215	GLN
1	C	689	ILE
1	A	170	GLN

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	893/1115 (80%)	892 (100%)	1 (0%)	93	97
1	B	886/1115 (80%)	884 (100%)	2 (0%)	93	97
1	C	880/1115 (79%)	879 (100%)	1 (0%)	93	97
2	I	526/752 (70%)	525 (100%)	1 (0%)	93	97
2	J	526/752 (70%)	525 (100%)	1 (0%)	93	97
2	K	526/752 (70%)	523 (99%)	3 (1%)	86	91
All	All	4237/5601 (76%)	4228 (100%)	9 (0%)	93	97

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	LYS
1	B	851	LYS
1	B	961	LYS
1	C	383	LYS
2	I	596	LYS
2	J	596	LYS
2	K	114	LYS
2	K	192	ARG
2	K	596	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	419	ASN
1	B	419	ASN
1	C	52	GLN
2	I	24	GLN
2	J	380	GLN
2	K	374	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)

58 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	D	1	3,1	14,14,15	0.33	0	17,19,21	0.46	0
3	NAG	D	2	3	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	E	1	3,1	14,14,15	0.45	0	17,19,21	0.55	0
3	NAG	E	2	3	14,14,15	0.20	0	17,19,21	0.50	0
3	NAG	F	1	3,1	14,14,15	0.19	0	17,19,21	0.50	0
3	NAG	F	2	3	14,14,15	0.58	0	17,19,21	0.44	0
3	NAG	G	1	3,1	14,14,15	0.29	0	17,19,21	0.51	0
3	NAG	G	2	3	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	H	1	3,1	14,14,15	0.88	1 (7%)	17,19,21	1.45	2 (11%)
3	NAG	H	2	3	14,14,15	0.18	0	17,19,21	0.44	0
3	NAG	L	1	3,1	14,14,15	0.31	0	17,19,21	0.50	0
3	NAG	L	2	3	14,14,15	0.24	0	17,19,21	0.40	0
3	NAG	M	1	3,1	14,14,15	0.28	0	17,19,21	0.51	0
3	NAG	M	2	3	14,14,15	0.26	0	17,19,21	0.39	0
3	NAG	N	1	3,1	14,14,15	0.21	0	17,19,21	1.20	2 (11%)
3	NAG	N	2	3	14,14,15	0.41	0	17,19,21	0.50	0
3	NAG	O	1	3,1	14,14,15	0.22	0	17,19,21	0.39	0
3	NAG	O	2	3	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	P	1	3,1	14,14,15	0.39	0	17,19,21	1.26	1 (5%)
3	NAG	P	2	3	14,14,15	0.25	0	17,19,21	0.44	0
3	NAG	Q	1	3,1	14,14,15	0.34	0	17,19,21	0.50	0
3	NAG	Q	2	3	14,14,15	0.24	0	17,19,21	0.59	0
3	NAG	R	1	3,1	14,14,15	0.30	0	17,19,21	0.56	0
3	NAG	R	2	3	14,14,15	0.19	0	17,19,21	0.38	0
3	NAG	S	1	3,1	14,14,15	0.17	0	17,19,21	0.44	0
3	NAG	S	2	3	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	T	1	3,1	14,14,15	0.24	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	T	2	3	14,14,15	0.43	0	17,19,21	1.25	1 (5%)
3	NAG	U	1	3,1	14,14,15	0.74	1 (7%)	17,19,21	1.26	1 (5%)
3	NAG	U	2	3	14,14,15	0.20	0	17,19,21	0.49	0
3	NAG	V	1	3,1	14,14,15	0.30	0	17,19,21	0.52	0
3	NAG	V	2	3	14,14,15	0.20	0	17,19,21	0.38	0
3	NAG	W	1	3,1	14,14,15	0.25	0	17,19,21	0.42	0
3	NAG	W	2	3	14,14,15	0.35	0	17,19,21	0.56	0
3	NAG	X	1	3,1	14,14,15	0.27	0	17,19,21	0.42	0
3	NAG	X	2	3	14,14,15	0.27	0	17,19,21	0.39	0
3	NAG	Y	1	3,1	14,14,15	0.25	0	17,19,21	0.40	0
3	NAG	Y	2	3	14,14,15	0.17	0	17,19,21	0.41	0
3	NAG	Z	1	3,1	14,14,15	0.24	0	17,19,21	0.39	0
3	NAG	Z	2	3	14,14,15	0.28	0	17,19,21	0.51	0
3	NAG	a	1	3,1	14,14,15	0.36	0	17,19,21	0.45	0
3	NAG	a	2	3	14,14,15	0.25	0	17,19,21	0.38	0
3	NAG	b	1	3,1	14,14,15	0.28	0	17,19,21	1.18	2 (11%)
3	NAG	b	2	3	14,14,15	0.32	0	17,19,21	0.59	1 (5%)
3	NAG	c	1	3,1	14,14,15	0.25	0	17,19,21	0.53	0
3	NAG	c	2	3	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	d	1	3,1	14,14,15	0.25	0	17,19,21	0.42	0
3	NAG	d	2	3	14,14,15	0.22	0	17,19,21	0.45	0
3	NAG	e	1	3,1	14,14,15	0.26	0	17,19,21	0.42	0
3	NAG	e	2	3	14,14,15	0.23	0	17,19,21	0.47	0
3	NAG	f	1	3,1	14,14,15	0.28	0	17,19,21	0.43	0
3	NAG	f	2	3	14,14,15	0.21	0	17,19,21	0.48	0
3	NAG	g	1	3,1	14,14,15	0.46	0	17,19,21	0.78	1 (5%)
3	NAG	g	2	3	14,14,15	0.28	0	17,19,21	0.43	0
3	NAG	h	1	3,1	14,14,15	0.35	0	17,19,21	0.36	0
3	NAG	h	2	3	14,14,15	0.22	0	17,19,21	0.48	0
3	NAG	i	1	3,1	14,14,15	0.26	0	17,19,21	0.55	0
3	NAG	i	2	3	14,14,15	0.26	0	17,19,21	0.51	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
3	NAG	D	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	NAG	E	1	3,1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	L	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	1/6/23/26	0/1/1/1
3	NAG	M	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
3	NAG	N	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	N	2	3	-	4/6/23/26	0/1/1/1
3	NAG	O	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
3	NAG	P	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Q	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	3/6/23/26	0/1/1/1
3	NAG	R	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	R	2	3	-	0/6/23/26	0/1/1/1
3	NAG	S	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1
3	NAG	T	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	T	2	3	-	3/6/23/26	0/1/1/1
3	NAG	U	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
3	NAG	V	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	V	2	3	-	0/6/23/26	0/1/1/1
3	NAG	W	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	W	2	3	-	2/6/23/26	0/1/1/1
3	NAG	X	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	X	2	3	-	1/6/23/26	0/1/1/1
3	NAG	Y	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	2/6/23/26	0/1/1/1
3	NAG	Z	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	a	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	a	2	3	-	2/6/23/26	0/1/1/1
3	NAG	b	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	b	2	3	-	2/6/23/26	0/1/1/1
3	NAG	c	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	c	2	3	-	2/6/23/26	0/1/1/1
3	NAG	d	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	d	2	3	-	0/6/23/26	0/1/1/1
3	NAG	e	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	e	2	3	-	0/6/23/26	0/1/1/1
3	NAG	f	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	f	2	3	-	2/6/23/26	0/1/1/1
3	NAG	g	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	g	2	3	-	2/6/23/26	0/1/1/1
3	NAG	h	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	h	2	3	-	1/6/23/26	0/1/1/1
3	NAG	i	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	i	2	3	-	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1	NAG	C1-C2	2.84	1.56	1.52
3	U	1	NAG	O5-C1	2.38	1.47	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	U	1	NAG	C1-O5-C5	4.90	118.84	112.19
3	P	1	NAG	C1-O5-C5	4.70	118.56	112.19
3	H	1	NAG	C1-O5-C5	4.63	118.47	112.19
3	T	2	NAG	C2-N2-C7	4.31	129.04	122.90
3	N	1	NAG	C1-O5-C5	3.74	117.25	112.19
3	b	1	NAG	C1-O5-C5	3.49	116.92	112.19
3	b	1	NAG	O4-C4-C5	2.61	115.79	109.30
3	g	1	NAG	C1-O5-C5	2.59	115.70	112.19
3	N	1	NAG	O4-C4-C5	2.41	115.29	109.30
3	b	2	NAG	C1-O5-C5	2.01	114.92	112.19
3	H	1	NAG	C2-N2-C7	2.01	125.77	122.90

There are no chirality outliers.

All (97) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	N	2	NAG	O5-C5-C6-O6
3	c	2	NAG	O5-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6
3	a	2	NAG	O5-C5-C6-O6
3	e	1	NAG	O5-C5-C6-O6
3	i	2	NAG	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
3	g	1	NAG	O5-C5-C6-O6
3	i	1	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	g	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
3	S	2	NAG	O5-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
3	c	2	NAG	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	e	1	NAG	C4-C5-C6-O6
3	S	2	NAG	C4-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
3	i	2	NAG	C4-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	N	1	NAG	C4-C5-C6-O6
3	a	2	NAG	C4-C5-C6-O6
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	N	1	NAG	C8-C7-N2-C2
3	N	1	NAG	O7-C7-N2-C2
3	N	2	NAG	C8-C7-N2-C2
3	N	2	NAG	O7-C7-N2-C2
3	T	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	T	1	NAG	O7-C7-N2-C2
3	T	2	NAG	C8-C7-N2-C2
3	T	2	NAG	O7-C7-N2-C2
3	a	1	NAG	C8-C7-N2-C2
3	a	1	NAG	O7-C7-N2-C2
3	Q	2	NAG	O5-C5-C6-O6
3	V	1	NAG	O5-C5-C6-O6
3	S	1	NAG	O5-C5-C6-O6
3	g	1	NAG	C4-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
3	a	1	NAG	O5-C5-C6-O6
3	b	1	NAG	O5-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6
3	i	1	NAG	C4-C5-C6-O6
3	S	1	NAG	C4-C5-C6-O6
3	U	2	NAG	C4-C5-C6-O6
3	a	1	NAG	C4-C5-C6-O6
3	b	2	NAG	C4-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	f	1	NAG	C4-C5-C6-O6
3	Y	2	NAG	O5-C5-C6-O6
3	b	2	NAG	O5-C5-C6-O6
3	V	1	NAG	C4-C5-C6-O6
3	X	2	NAG	O5-C5-C6-O6
3	W	2	NAG	C4-C5-C6-O6
3	U	1	NAG	O5-C5-C6-O6
3	b	1	NAG	C4-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	W	1	NAG	O5-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	X	1	NAG	C4-C5-C6-O6
3	Z	2	NAG	C4-C5-C6-O6
3	g	2	NAG	C4-C5-C6-O6
3	H	1	NAG	C1-C2-N2-C7
3	f	1	NAG	O5-C5-C6-O6

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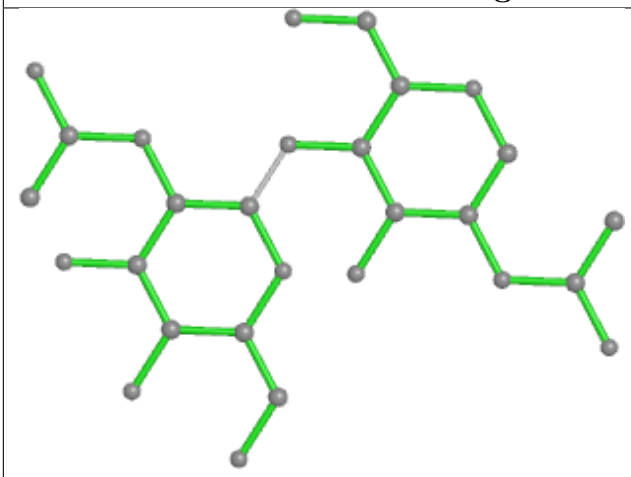
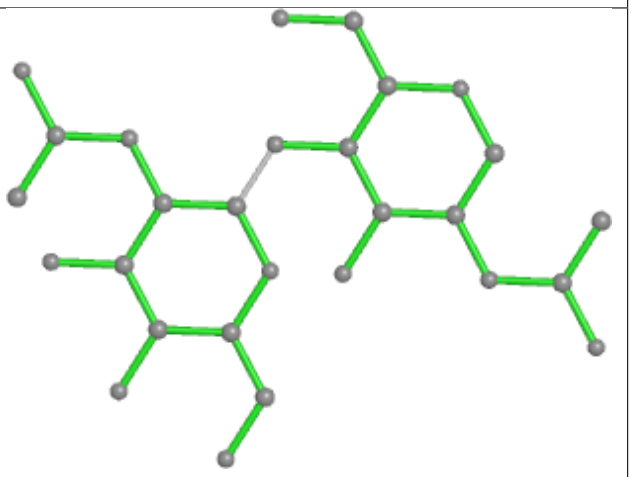
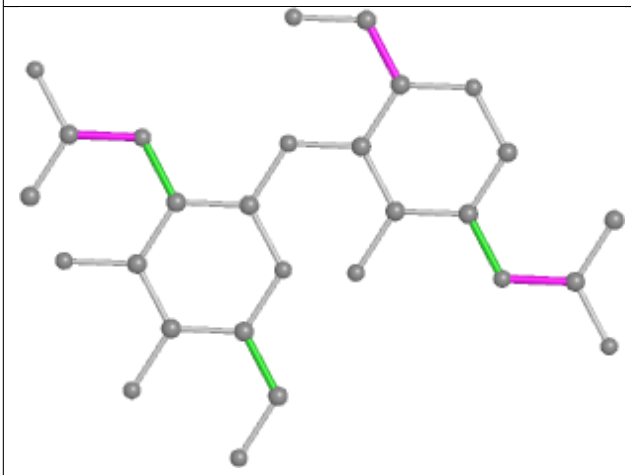
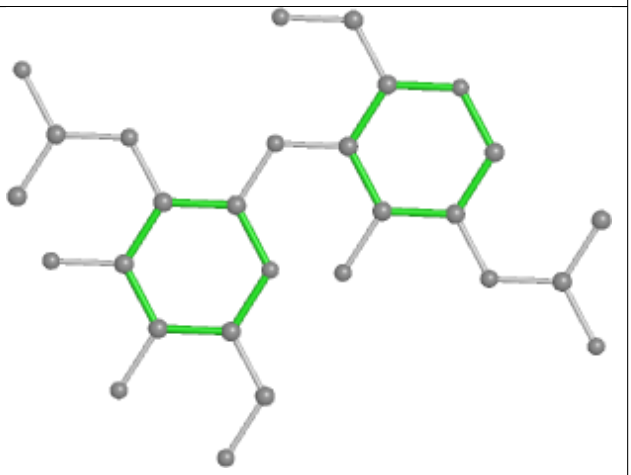
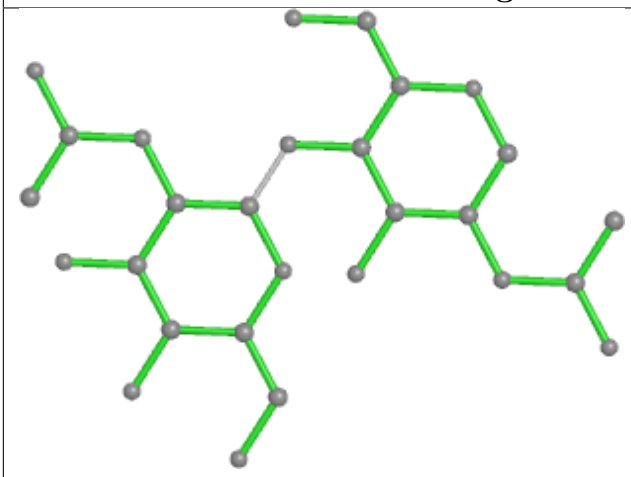
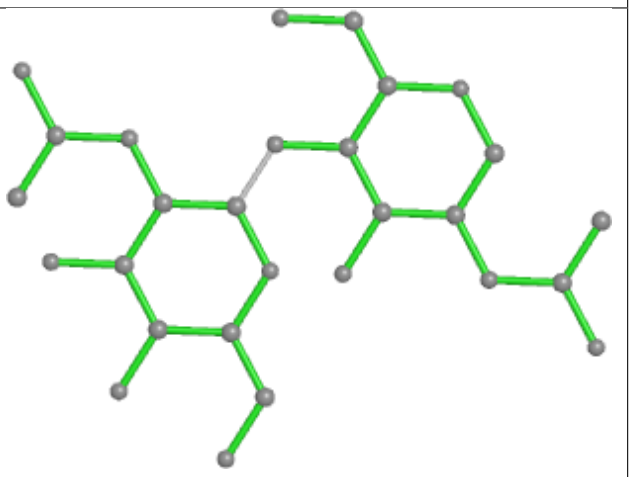
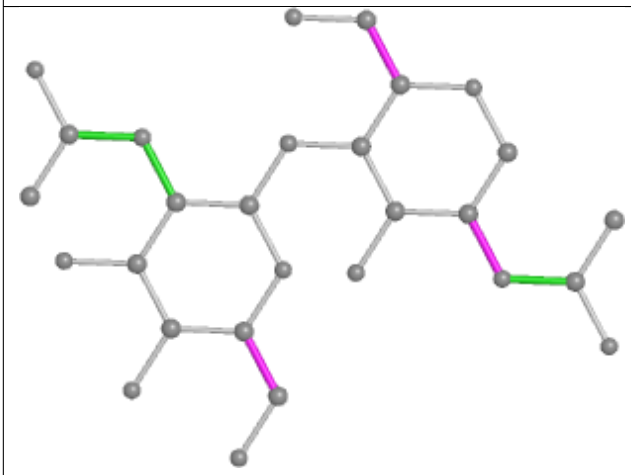
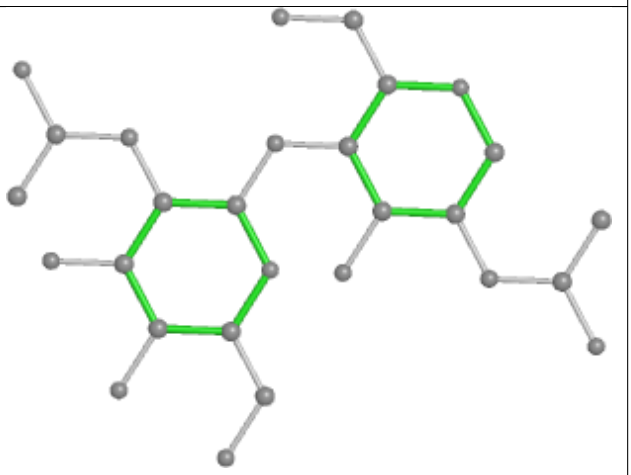
Mol	Chain	Res	Type	Atoms
3	X	1	NAG	O5-C5-C6-O6
3	W	2	NAG	O5-C5-C6-O6
3	Z	2	NAG	O5-C5-C6-O6
3	f	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C3-C2-N2-C7
3	Z	2	NAG	C3-C2-N2-C7
3	i	2	NAG	C3-C2-N2-C7
3	f	2	NAG	O5-C5-C6-O6
3	Q	2	NAG	C3-C2-N2-C7
3	R	1	NAG	C3-C2-N2-C7
3	T	2	NAG	C3-C2-N2-C7
3	h	2	NAG	C3-C2-N2-C7
3	i	1	NAG	C3-C2-N2-C7
3	L	2	NAG	C4-C5-C6-O6
3	Y	2	NAG	C4-C5-C6-O6

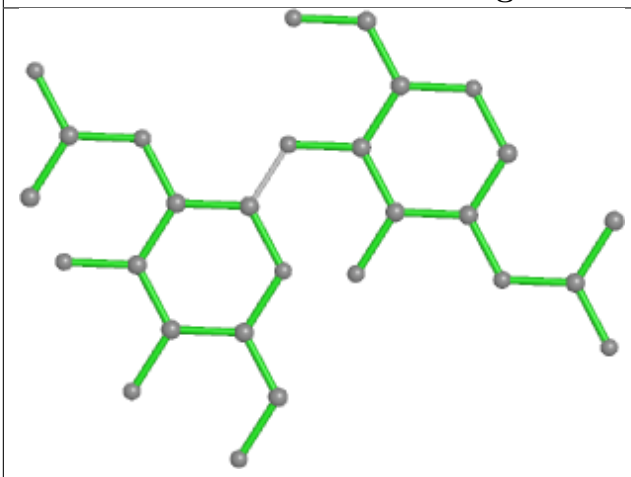
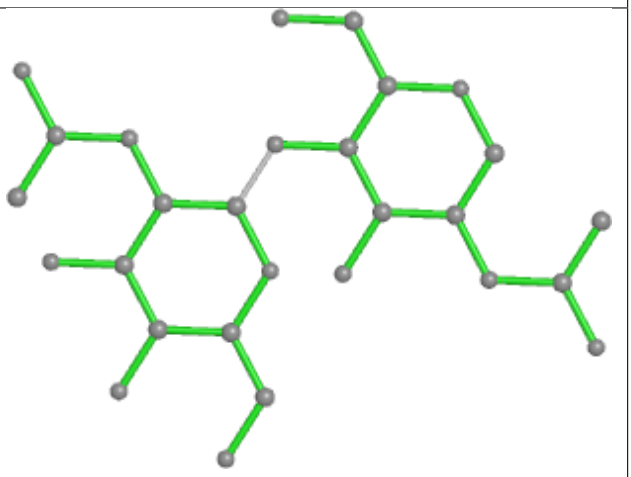
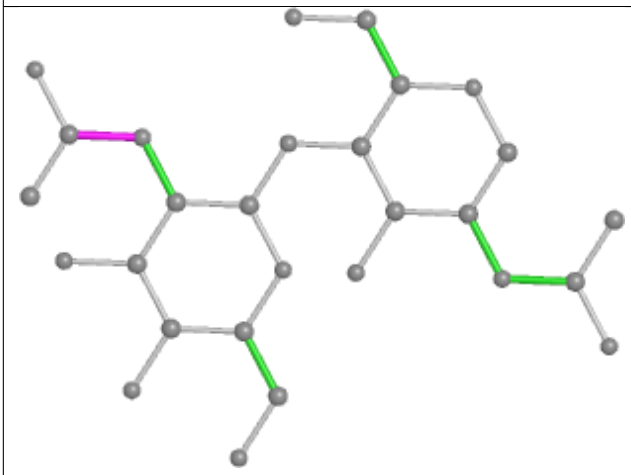
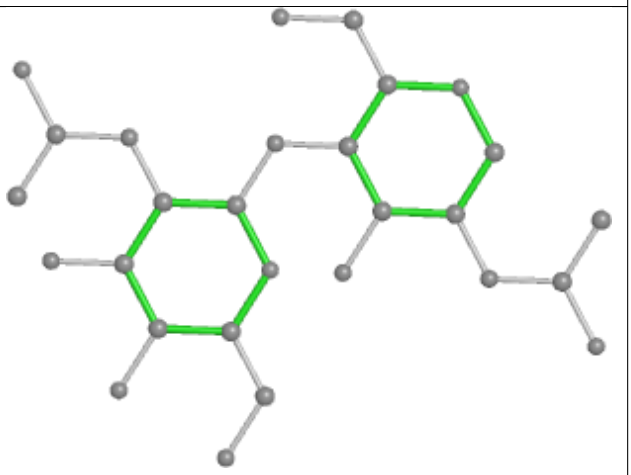
There are no ring outliers.

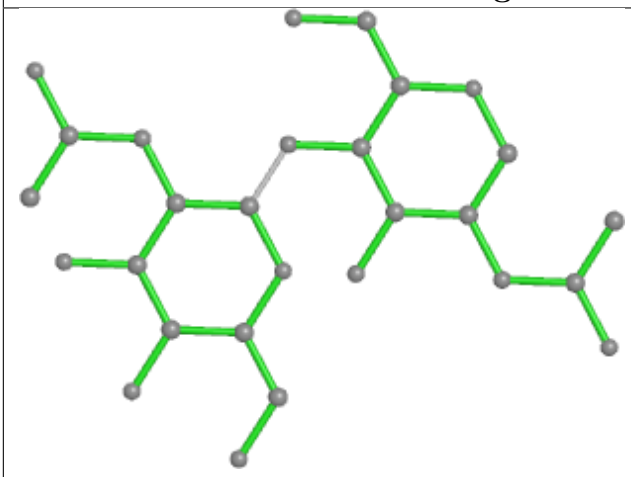
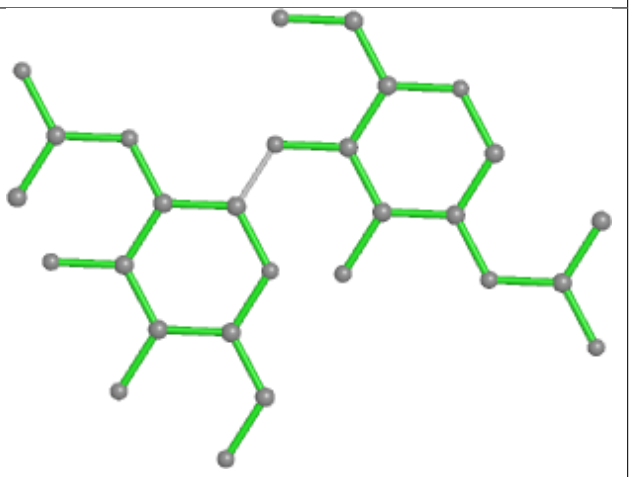
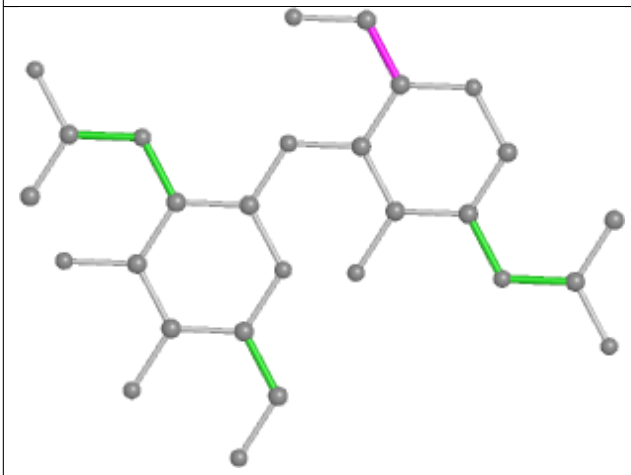
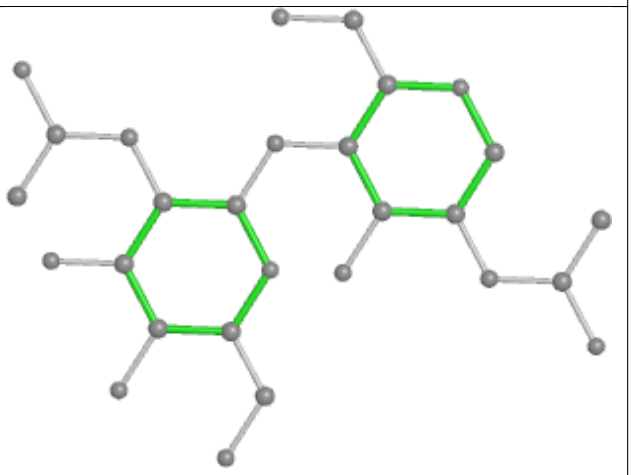
No monomer is involved in short contacts.

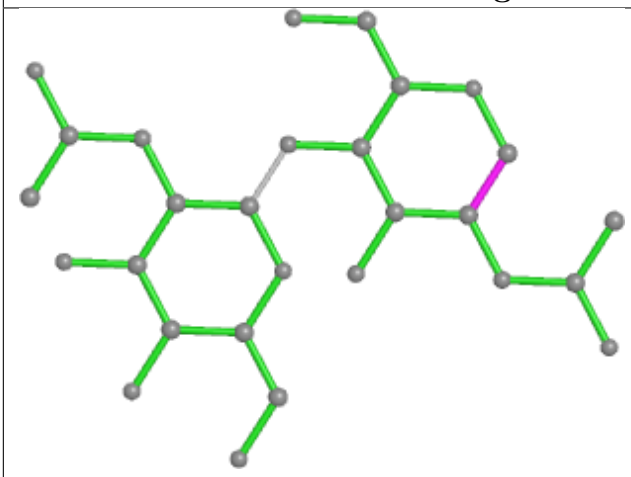
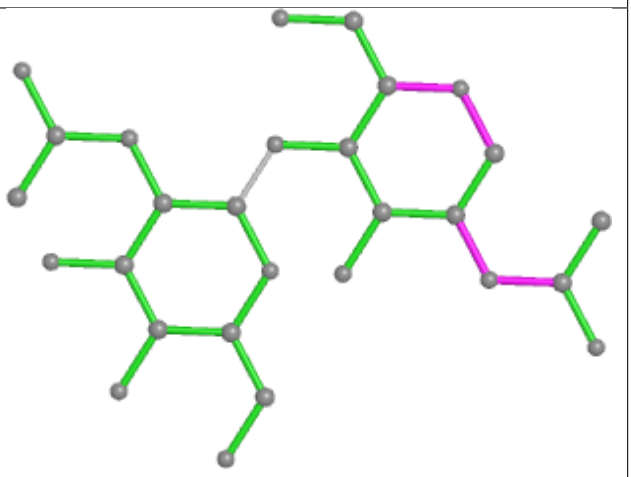
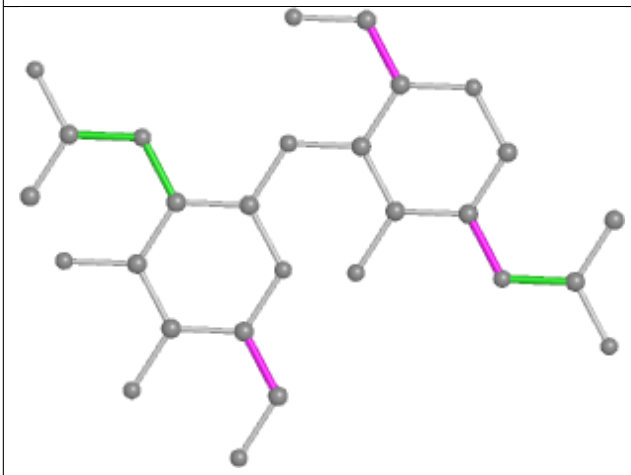
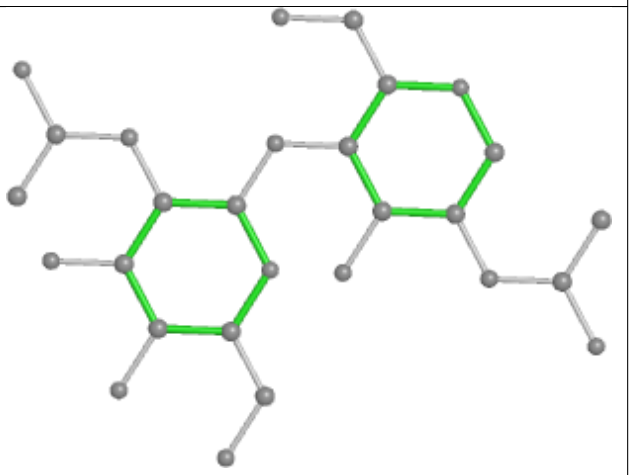
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

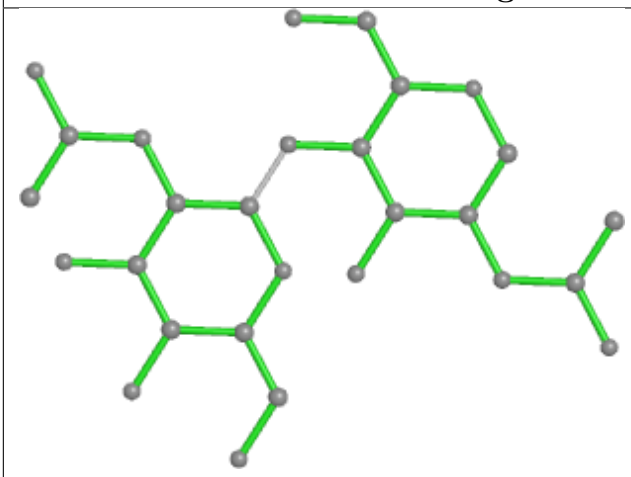
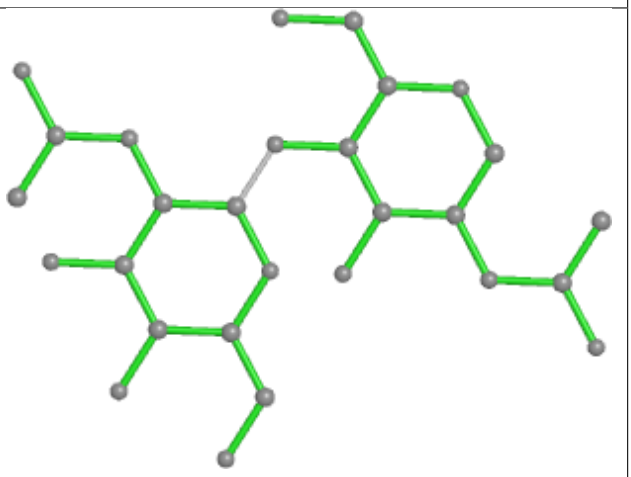
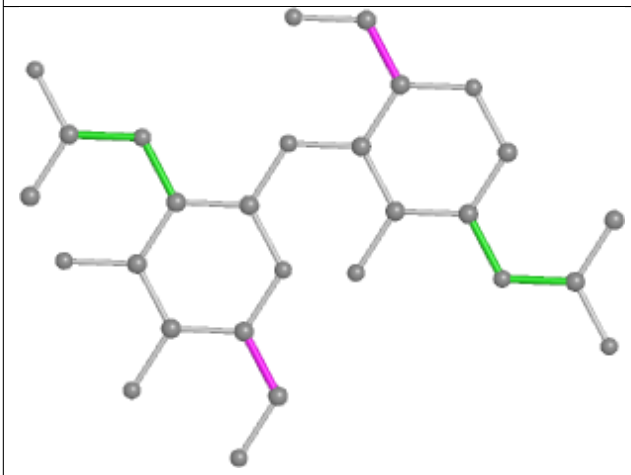
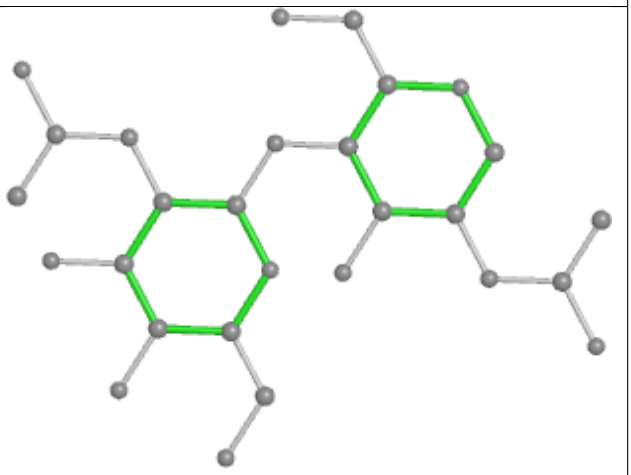
Oligosaccharide Chain D	
 Bond lengths	 Bond angles
 Torsions	 Rings

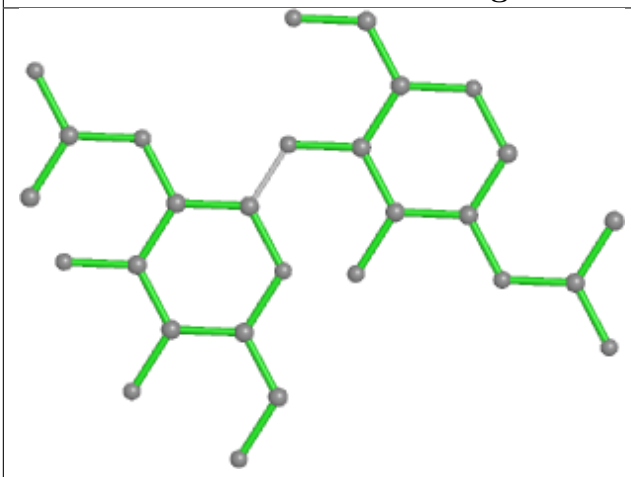
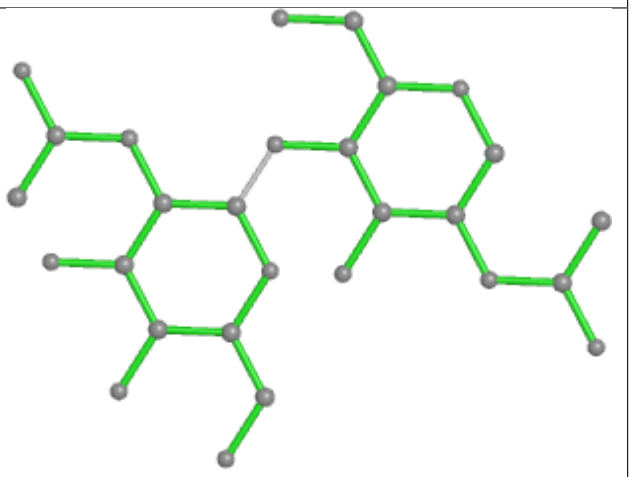
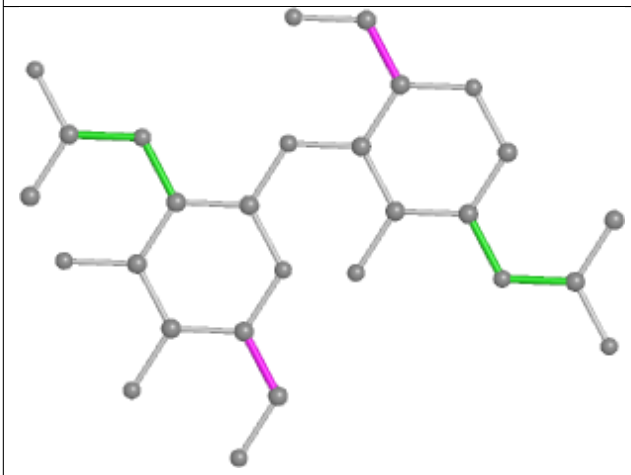
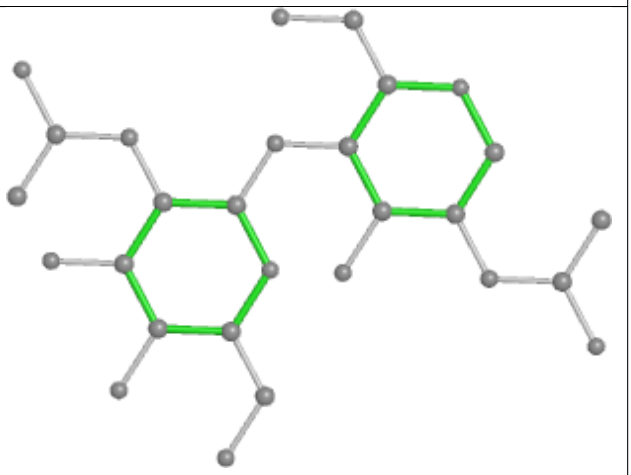
Oligosaccharide Chain E	
 Bond lengths	 Bond angles
 Torsions	 Rings

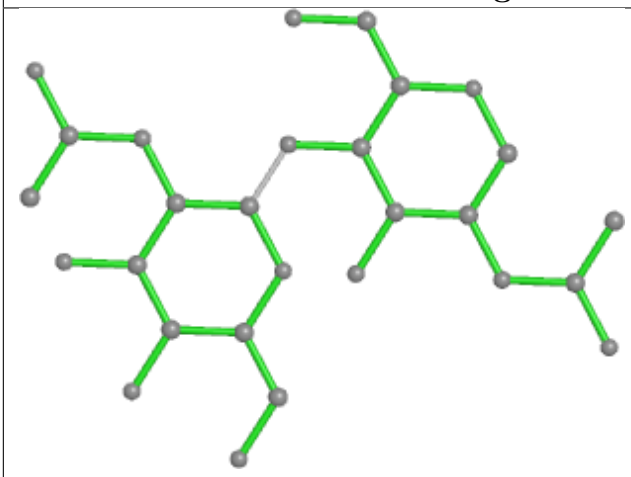
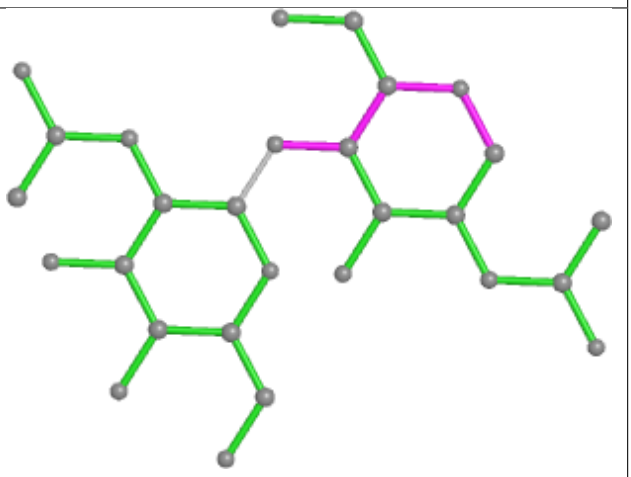
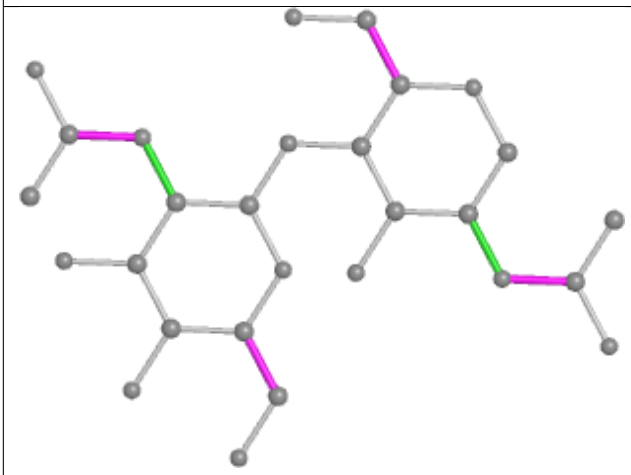
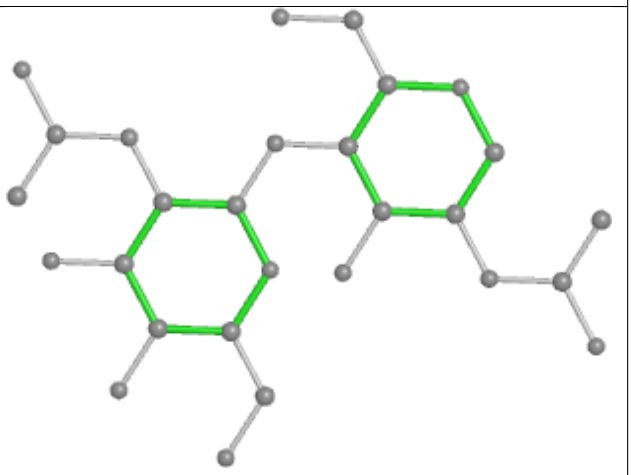
Oligosaccharide Chain F	
 Bond lengths	 Bond angles
 Torsions	 Rings

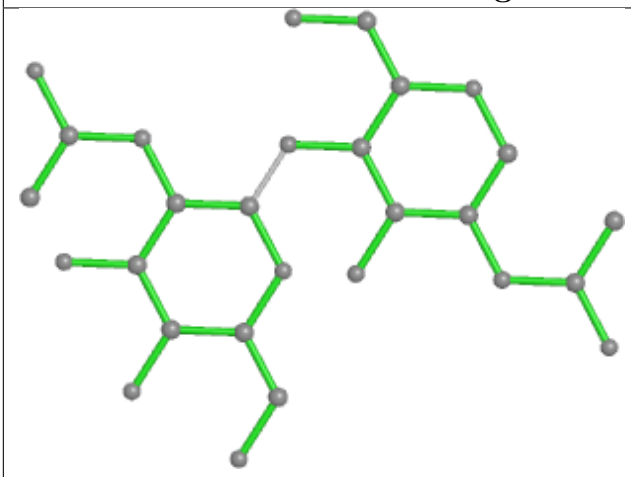
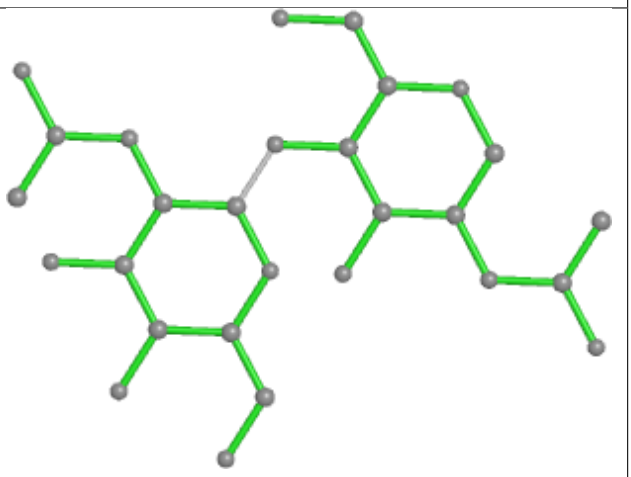
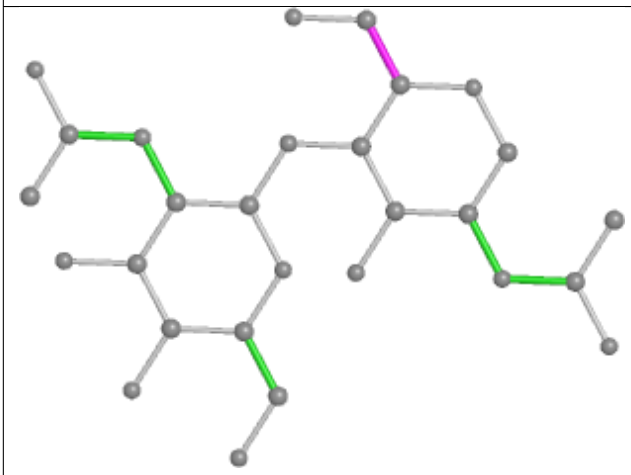
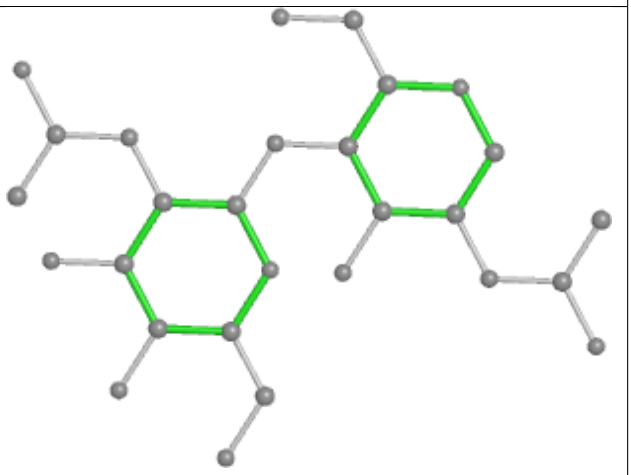
Oligosaccharide Chain G	
 Bond lengths	 Bond angles
 Torsions	 Rings

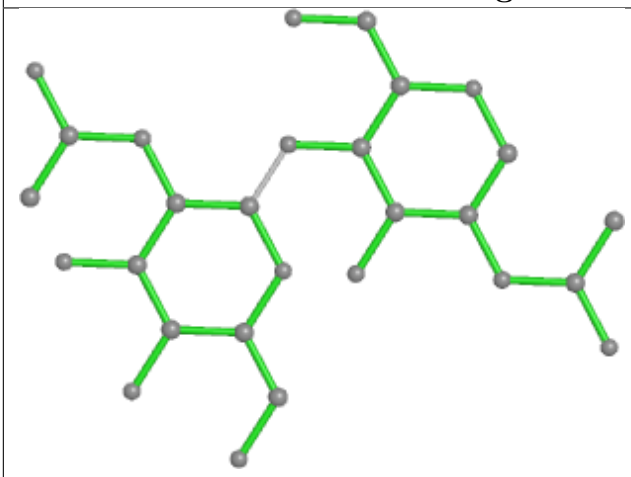
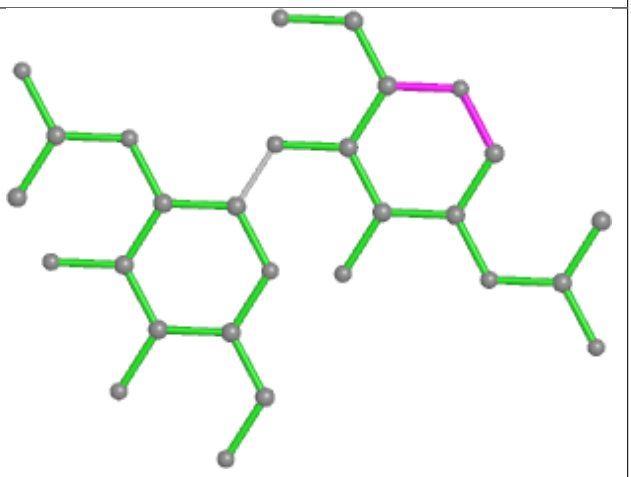
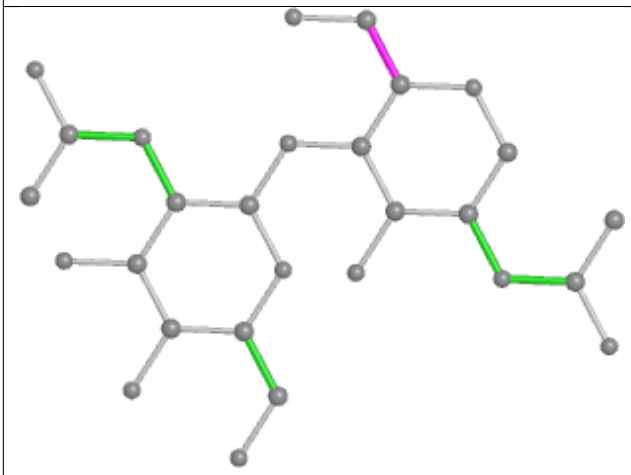
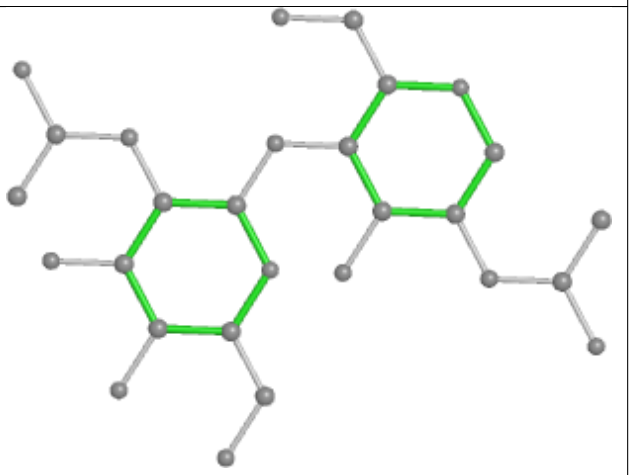
Oligosaccharide Chain H	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain L	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain M	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain N	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain O	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain P	
 Bond lengths	 Bond angles
 Torsions	 Rings

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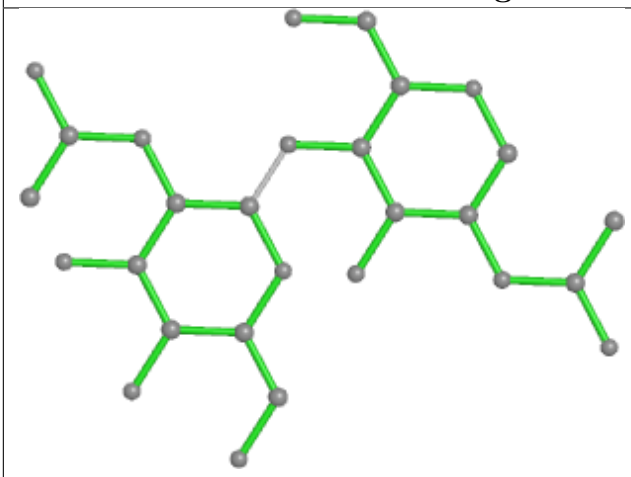
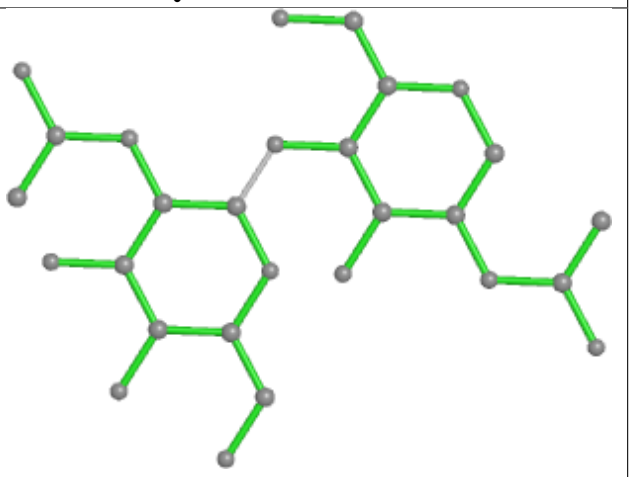
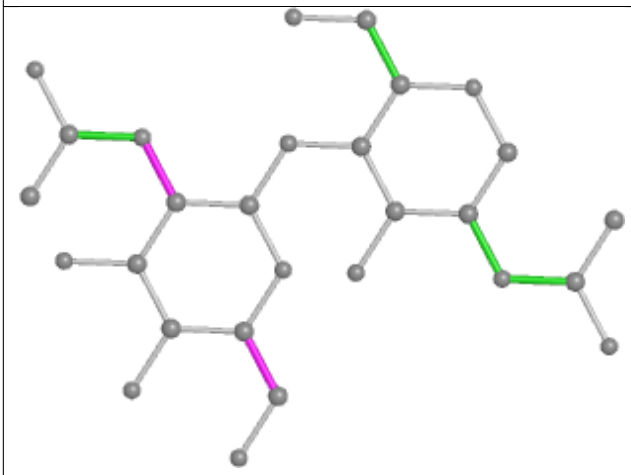
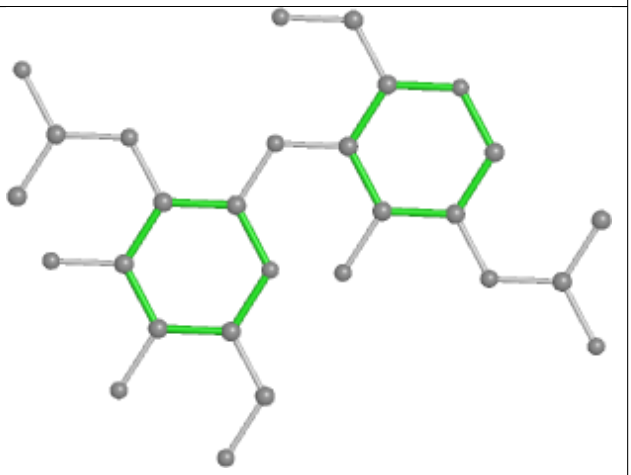
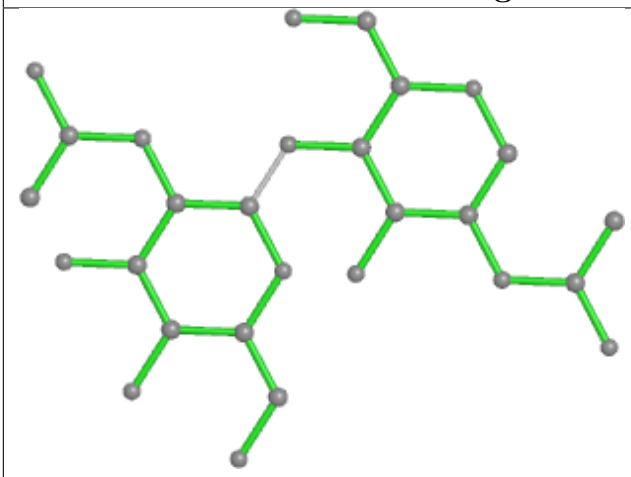
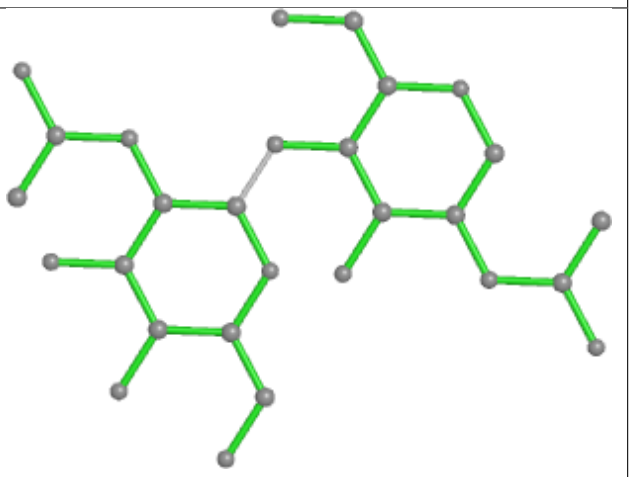
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain R



Bond lengths



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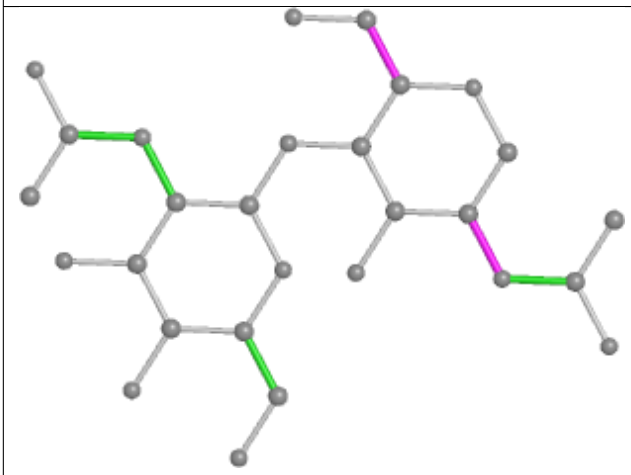

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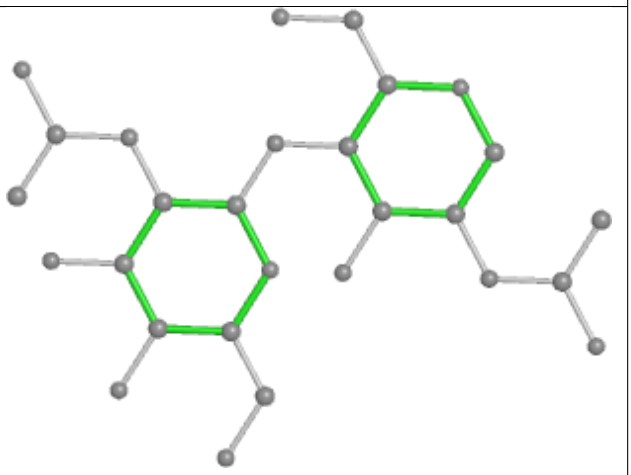
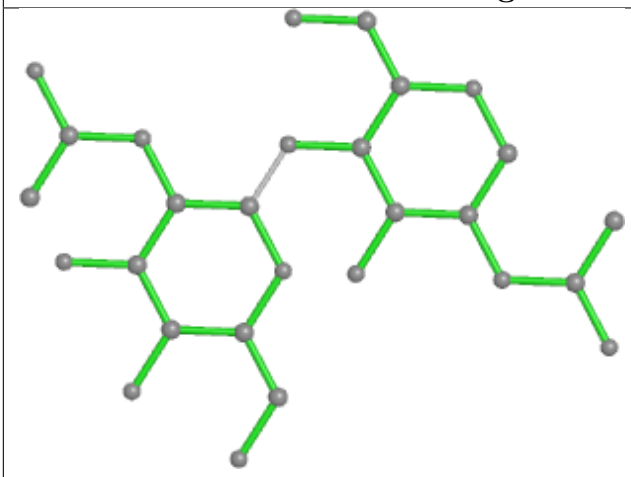
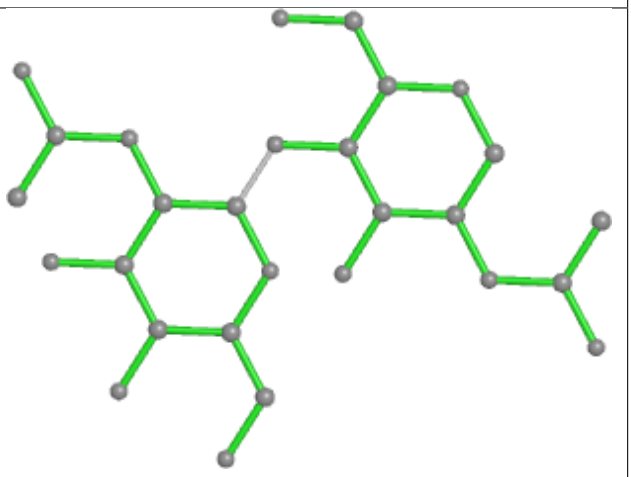
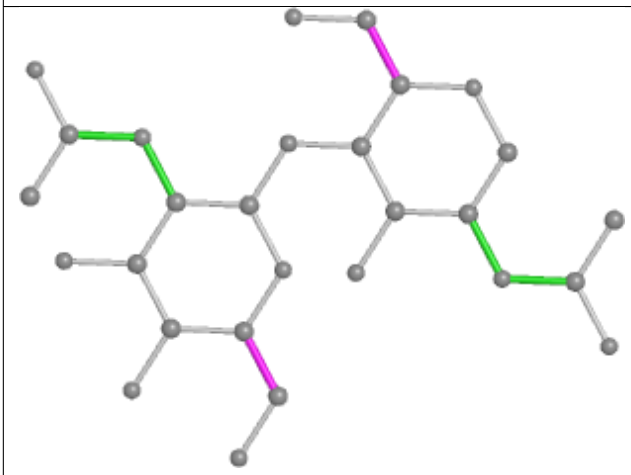
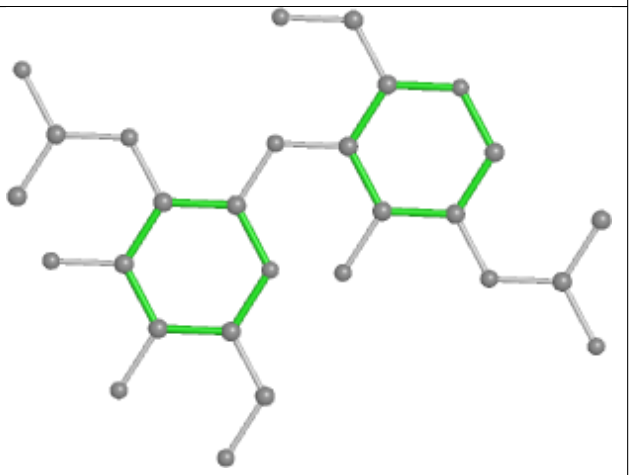
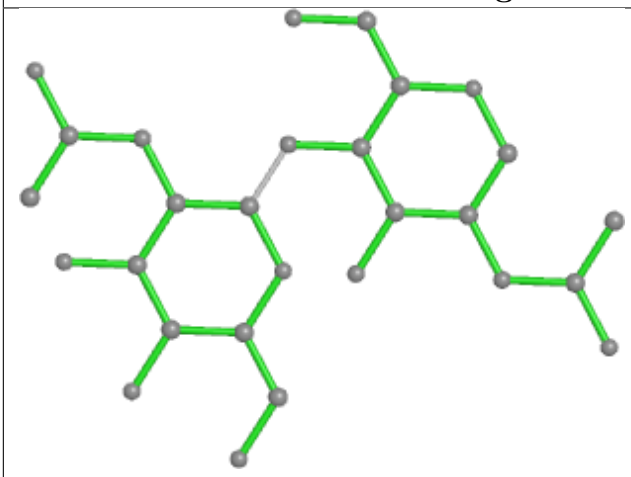


Rings

Oligosaccharide Chain S	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain T



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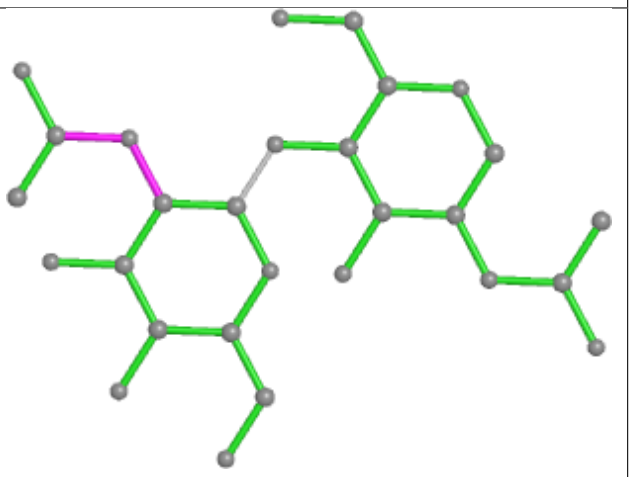

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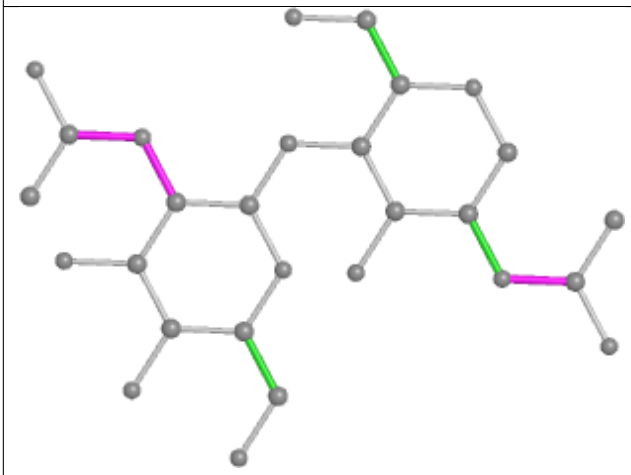

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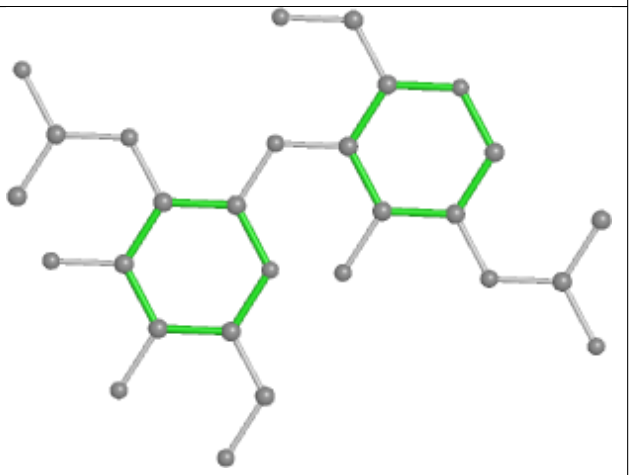
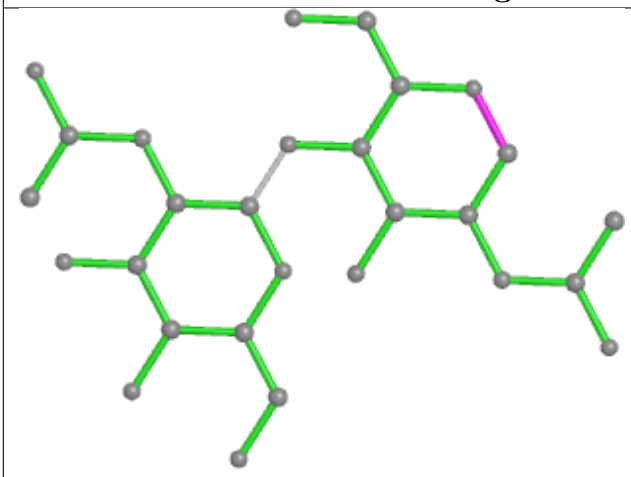
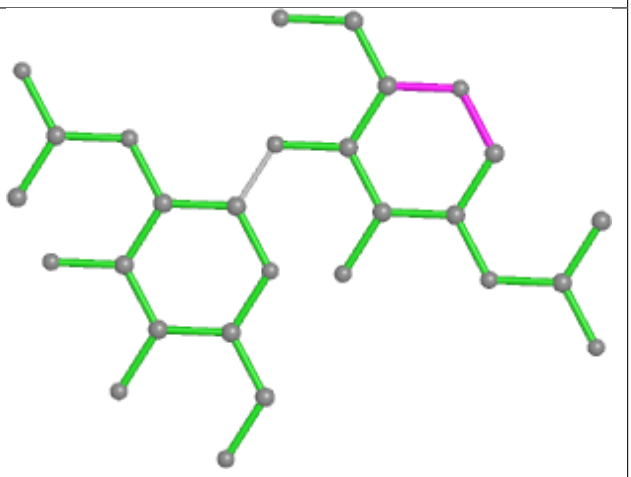
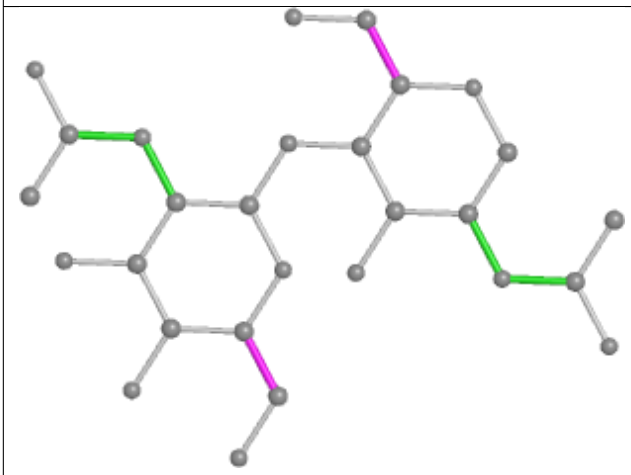
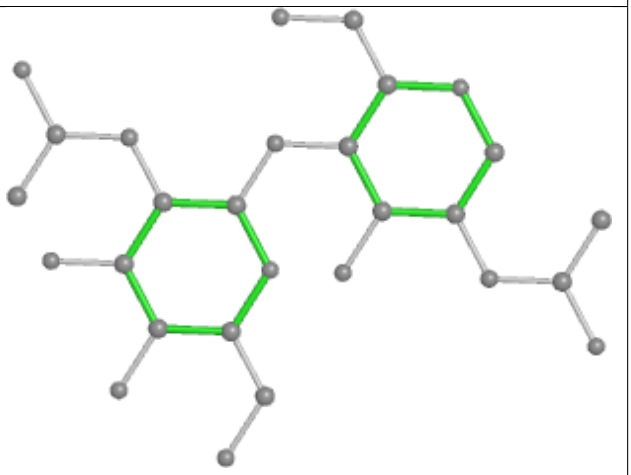


Rings

Oligosaccharide Chain U	
 Bond lengths	 Bond angles
 Torsions	 Rings

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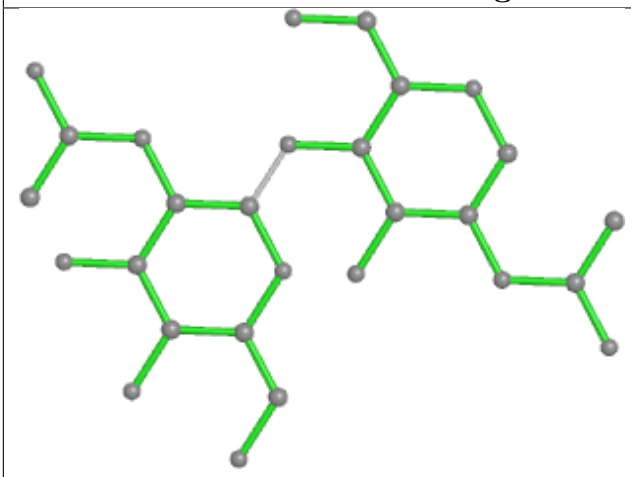
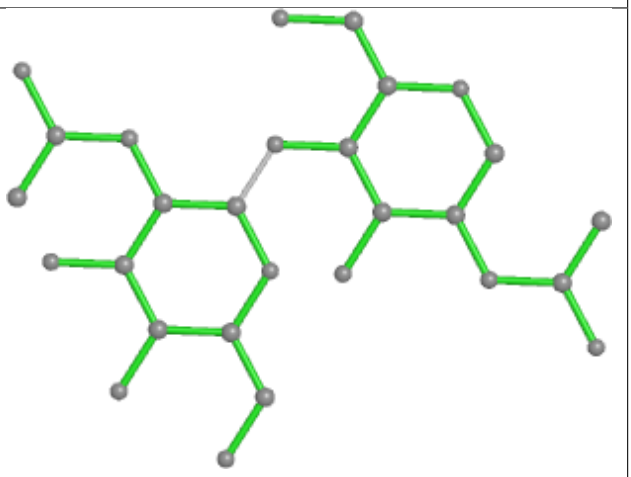
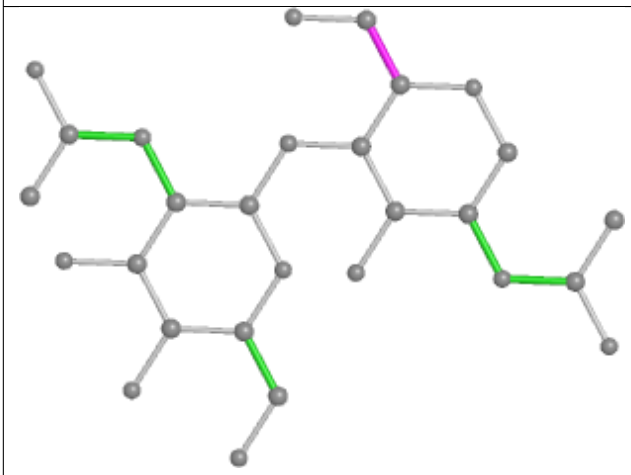
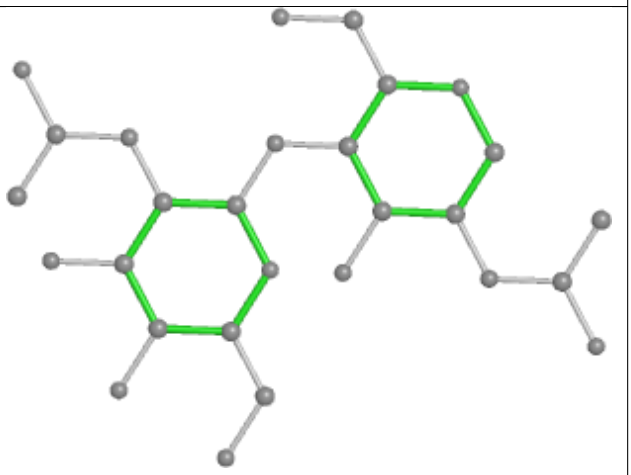
 Bond lengths	 Bond angles
 Torsions	 Rings

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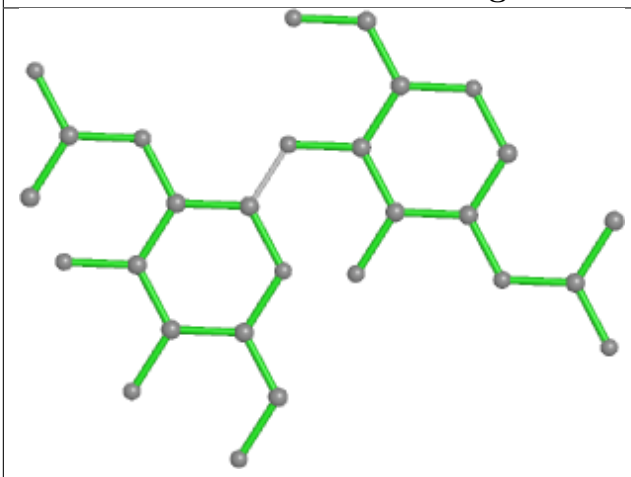
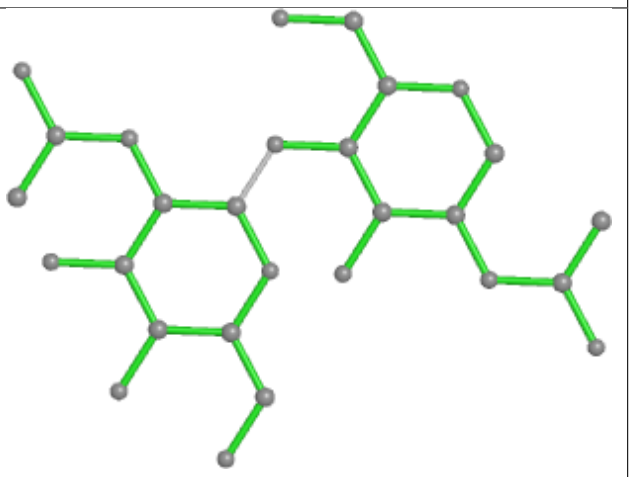
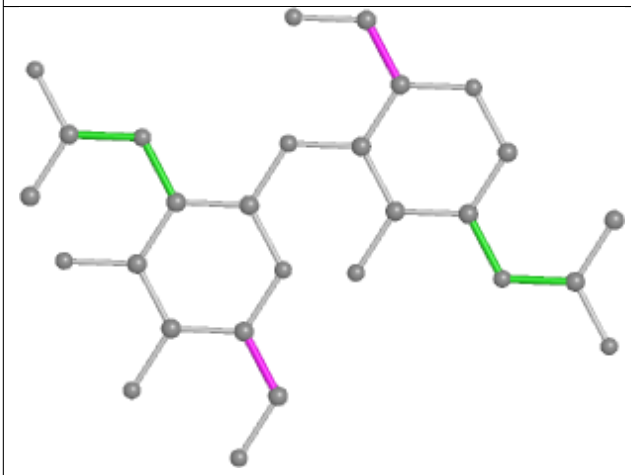
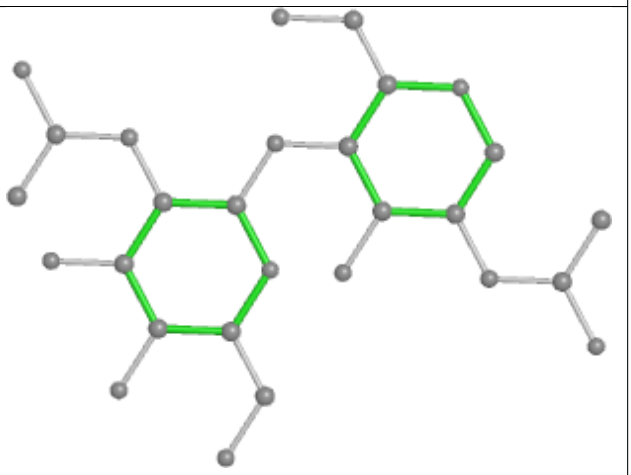
 Bond lengths	 Bond angles
 Torsions	 Rings

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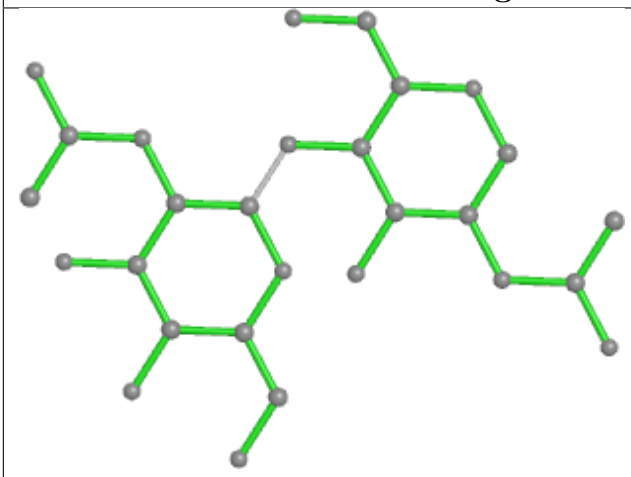
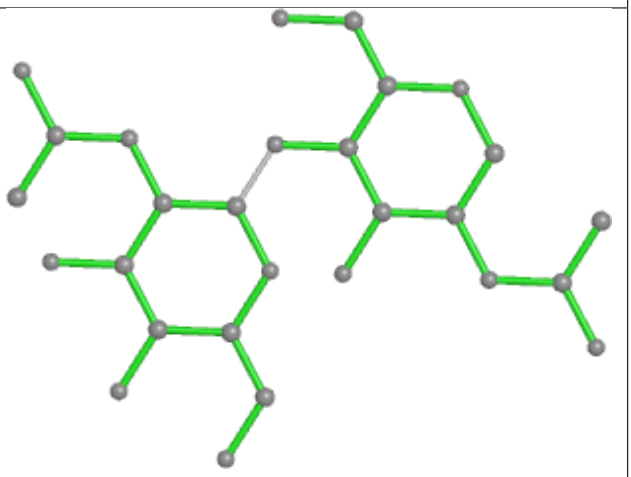
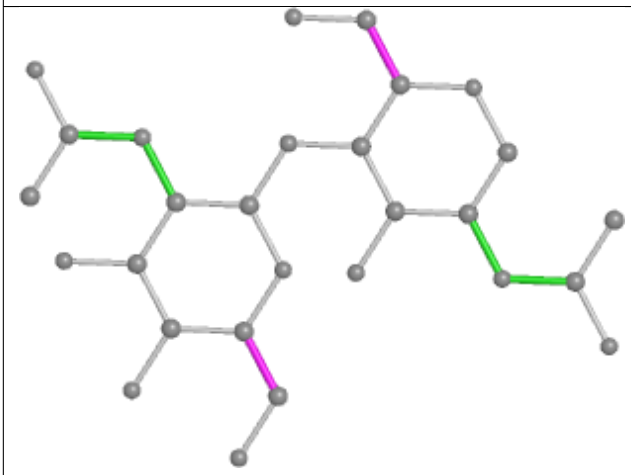
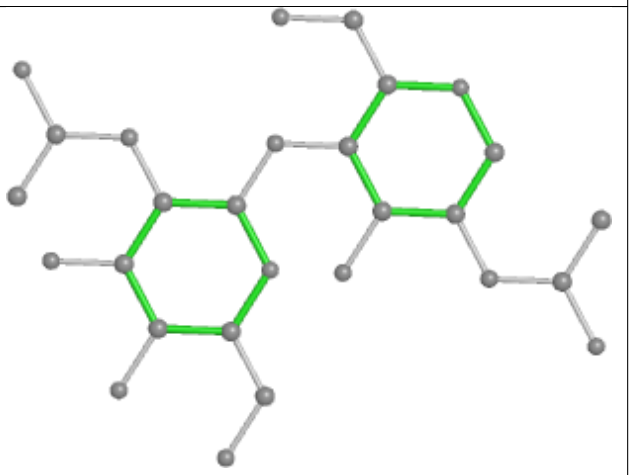
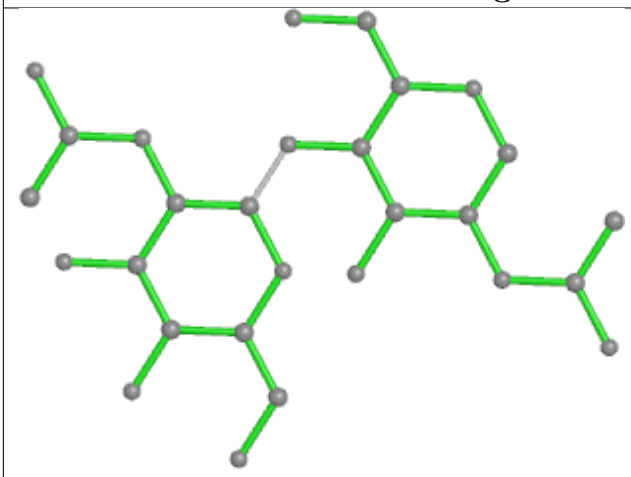
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain Y



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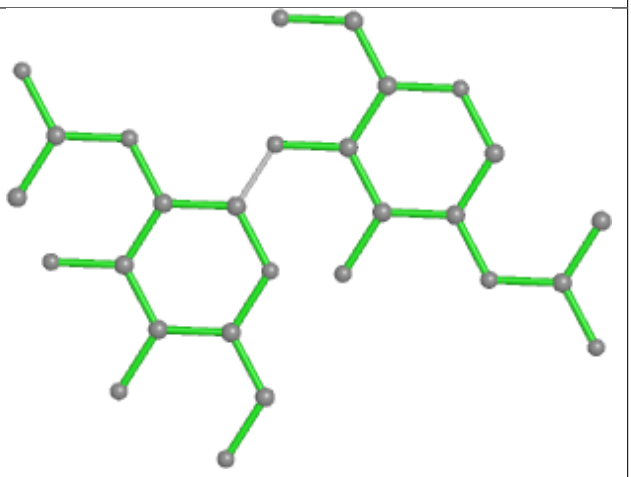

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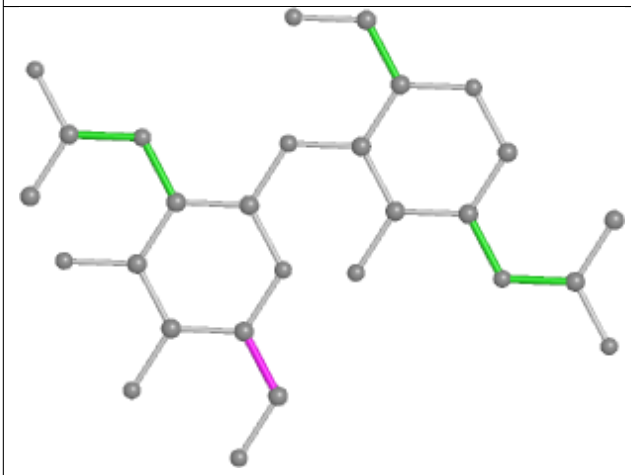

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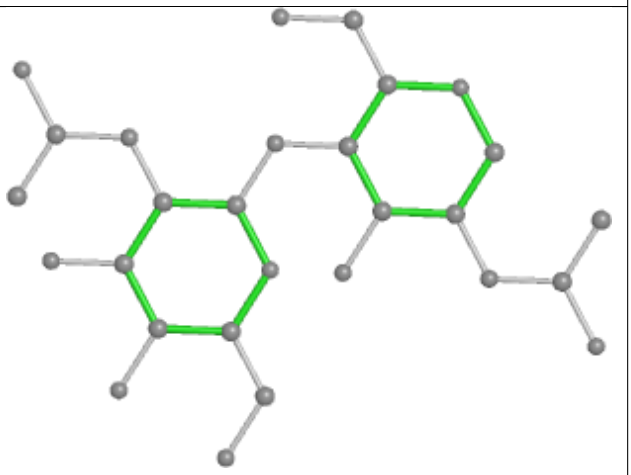

Rings

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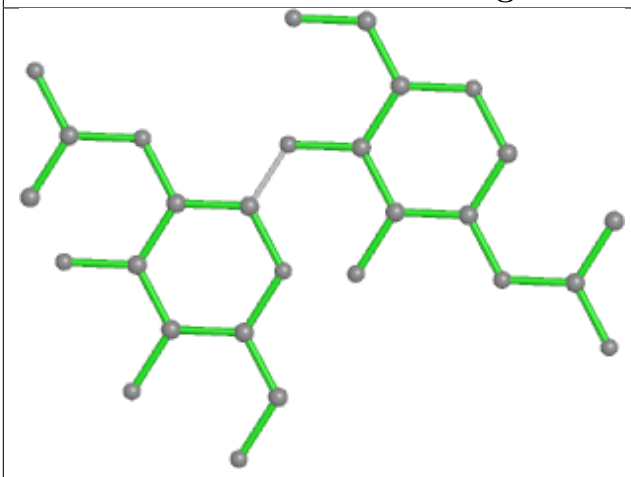
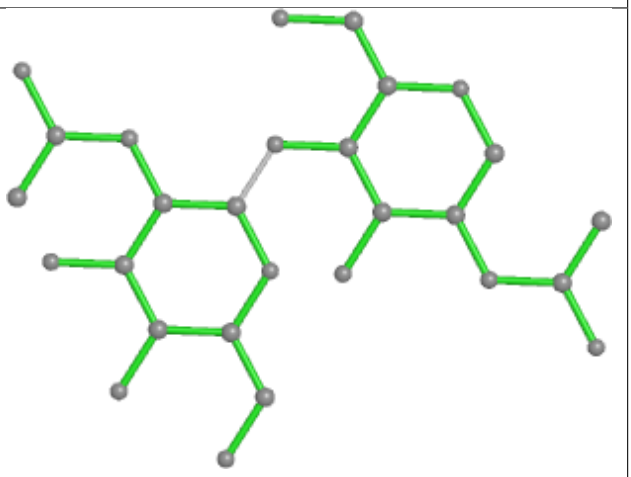
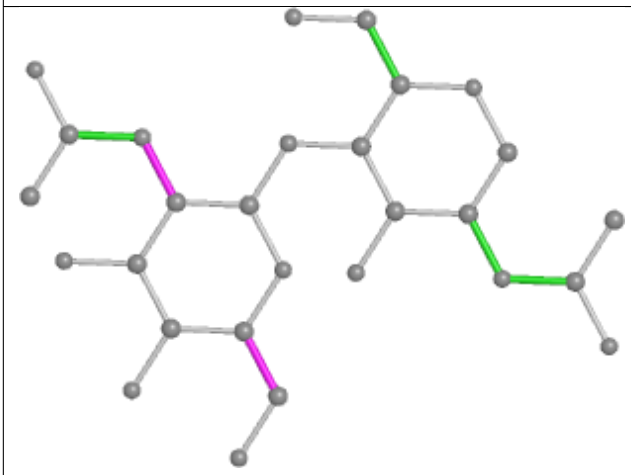
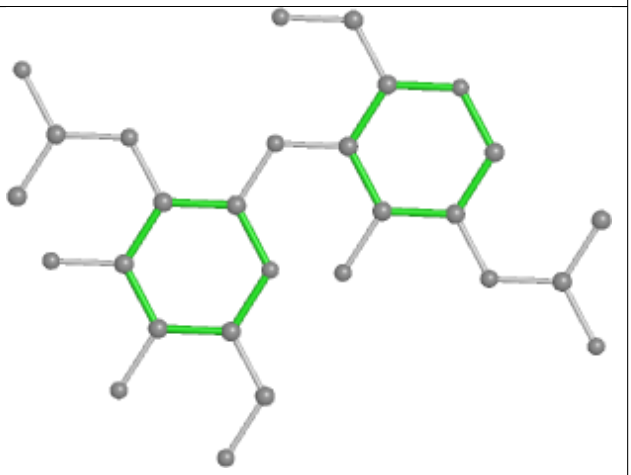
 Bond lengths	 Bond angles
 Torsions	 Rings

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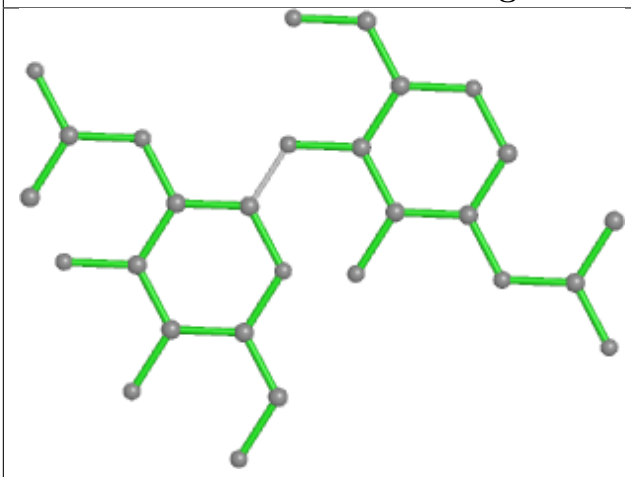
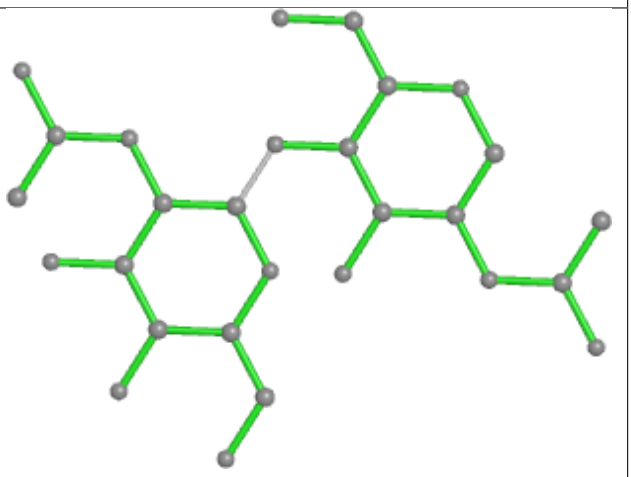
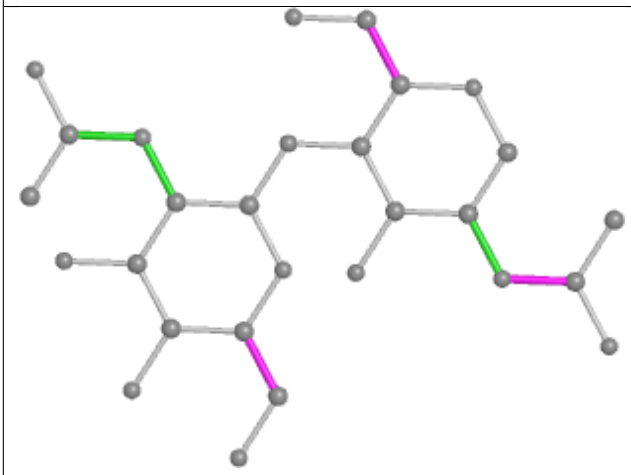
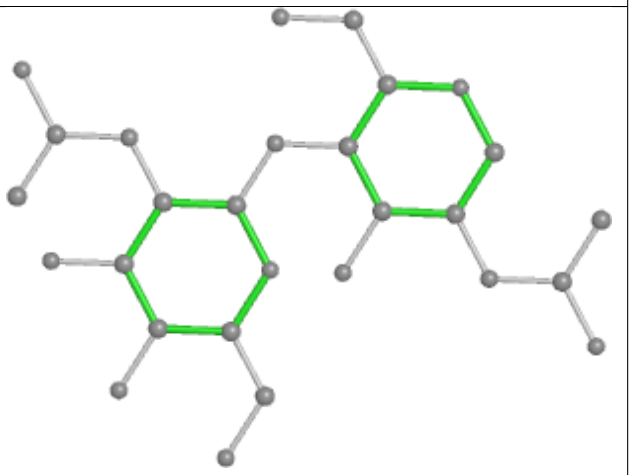
 Bond lengths	 Bond angles
 Torsions	 Rings

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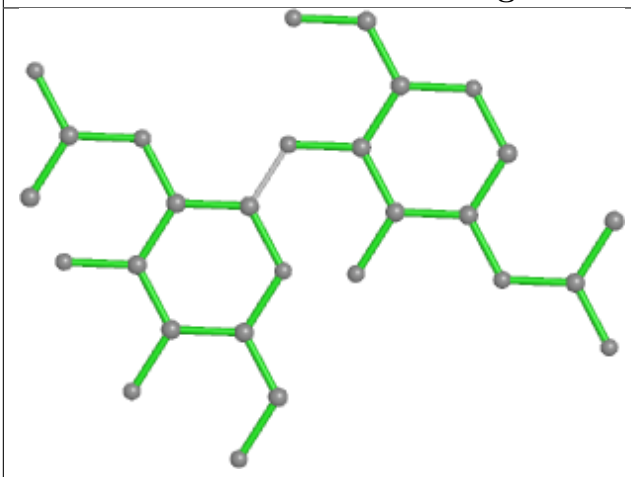
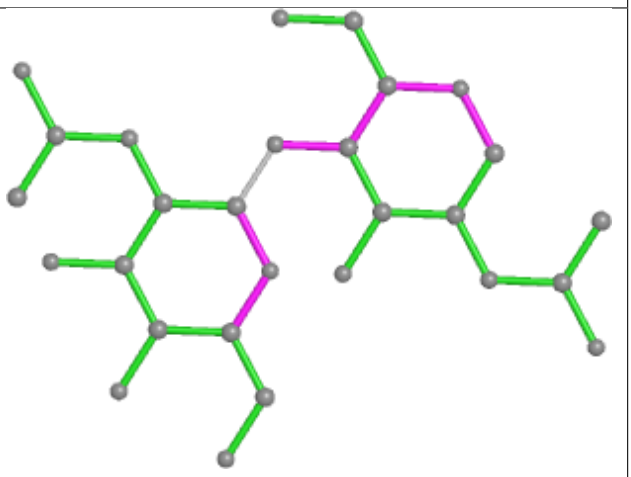
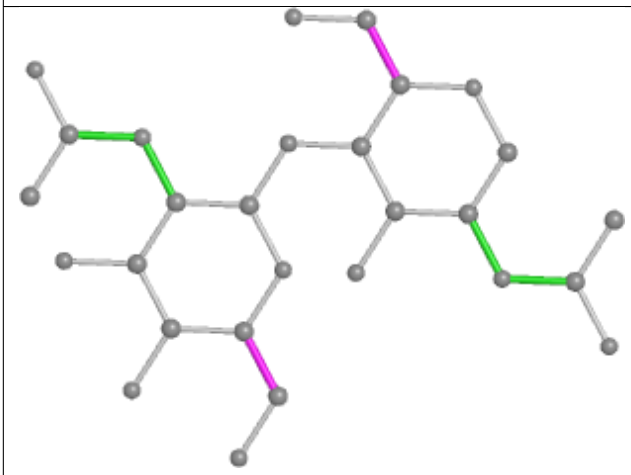
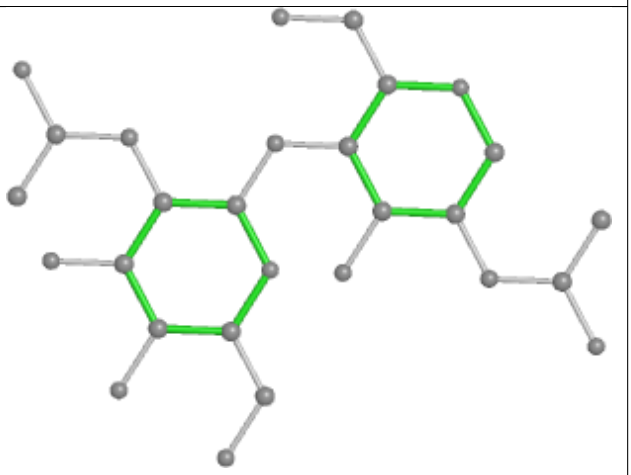
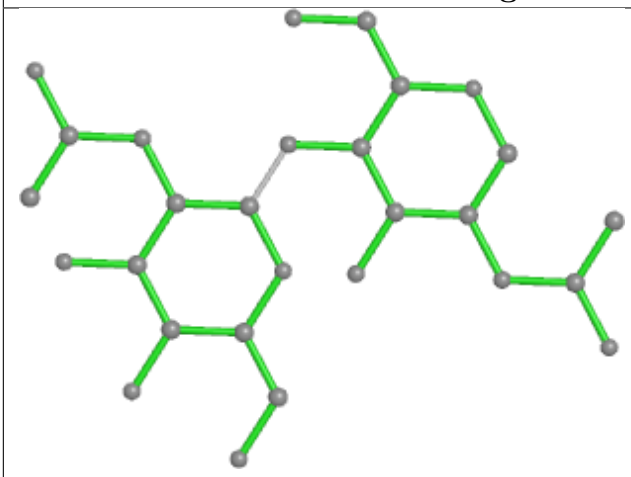
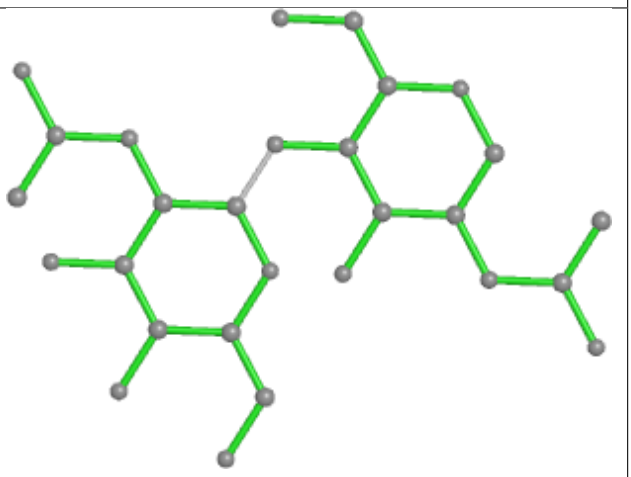
 Bond lengths	 Bond angles
 Torsions	 Rings

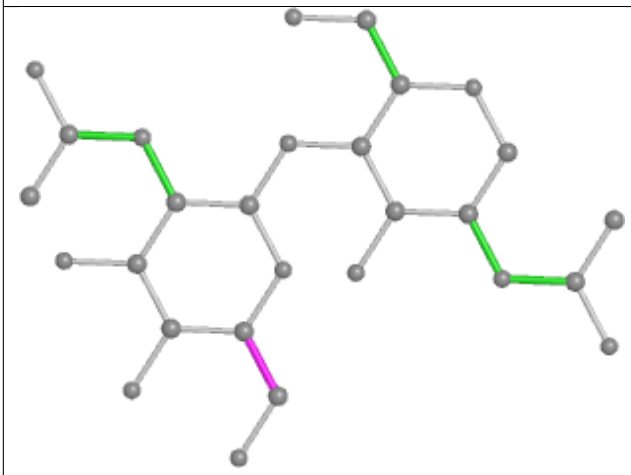
Oligosaccharide Chain c



Bond lengths



Bond angles



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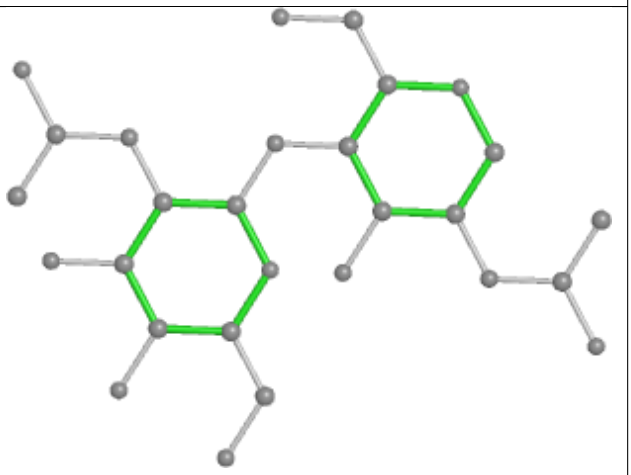
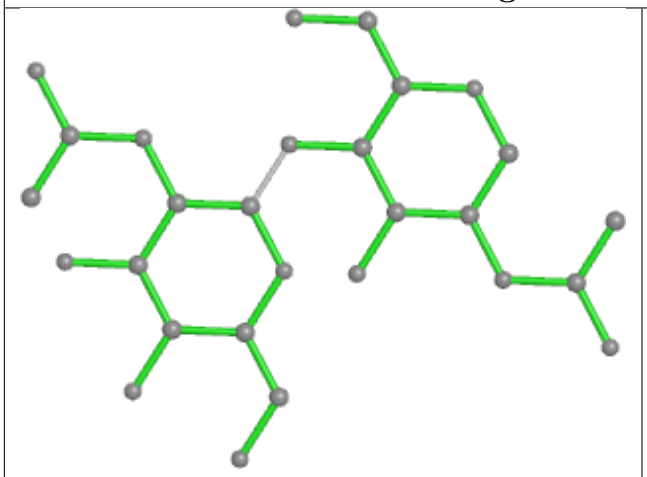


Rings

Oligosaccharide Chain d



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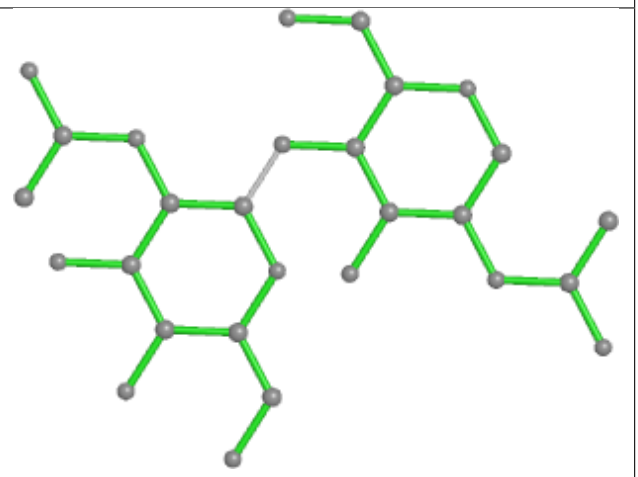

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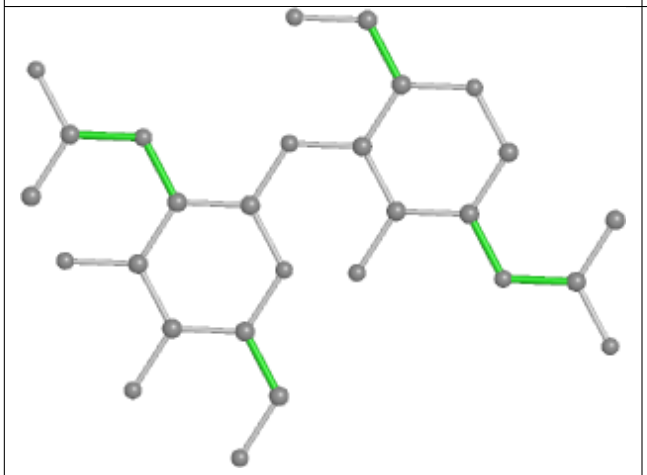
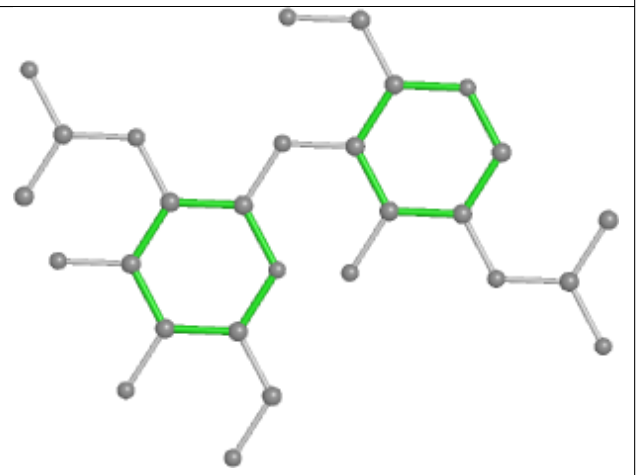
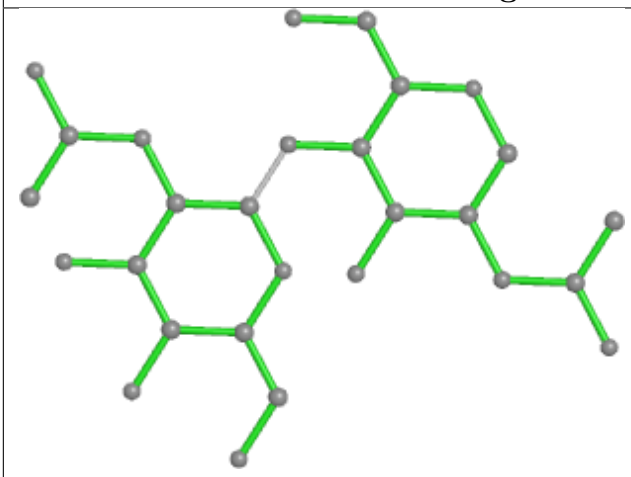
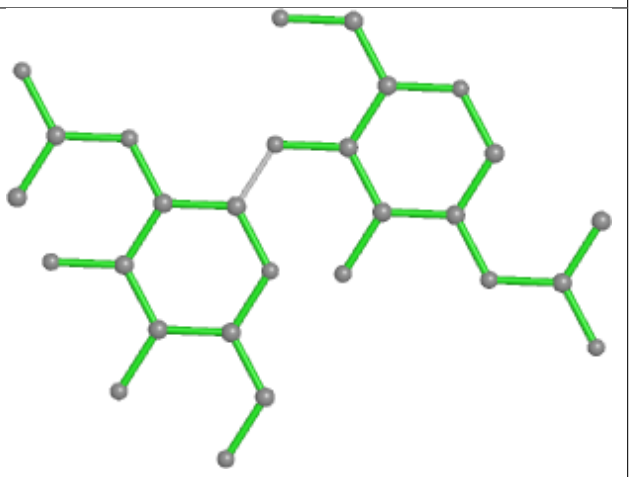
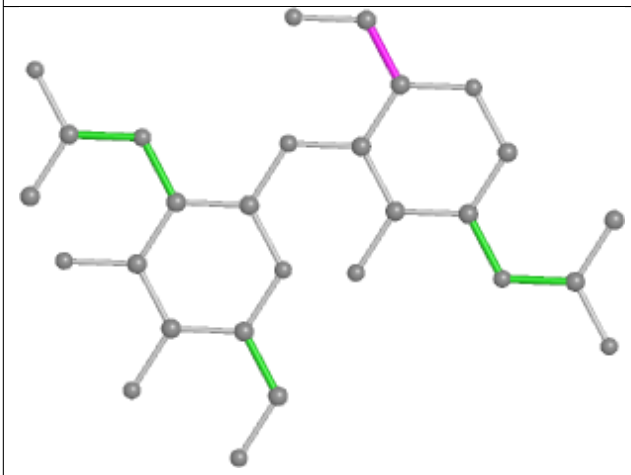
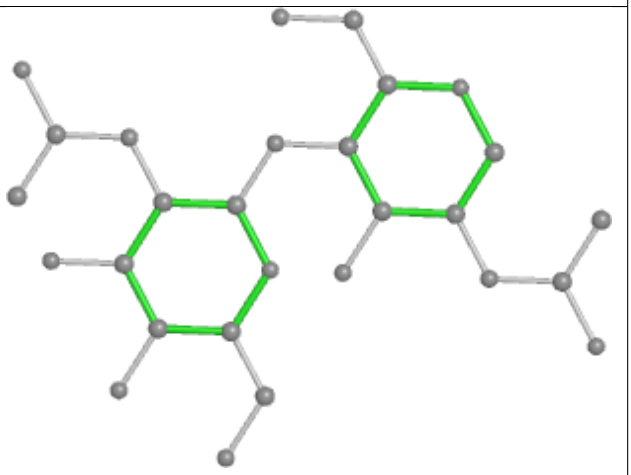


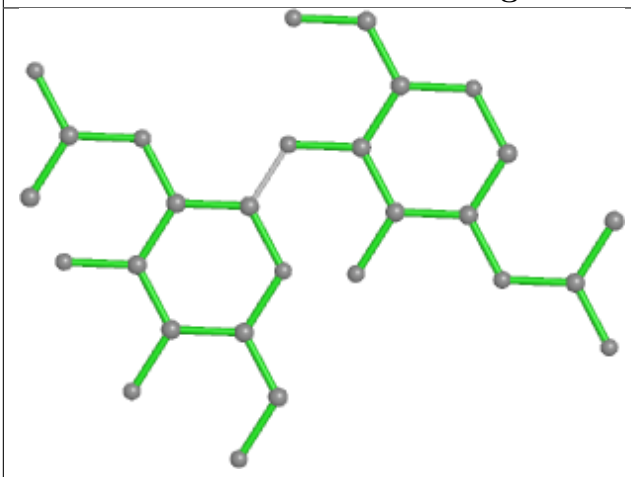
Torsions



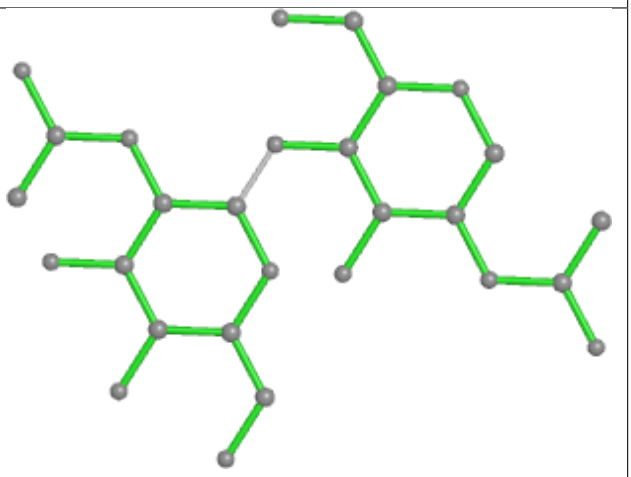
Rings

Oligosaccharide Chain e	
 Bond lengths	 Bond angles
 Torsions	 Rings

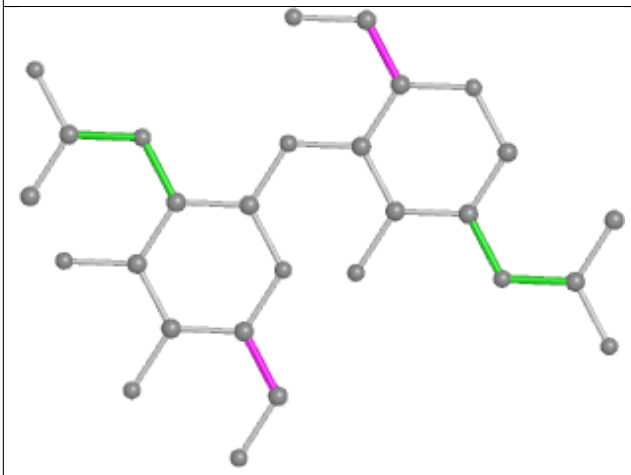
Oligosaccharide Chain f



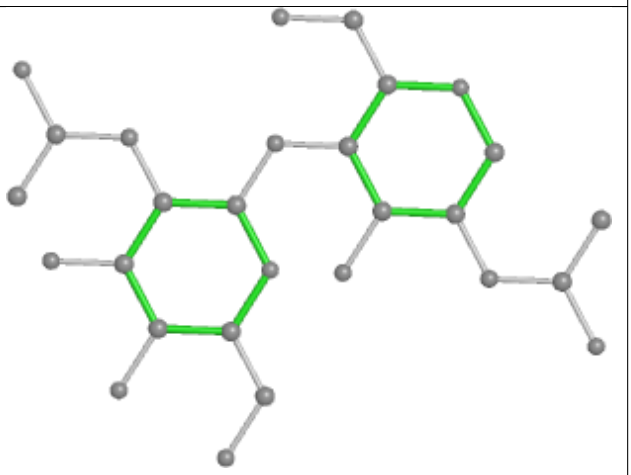
Bond lengths



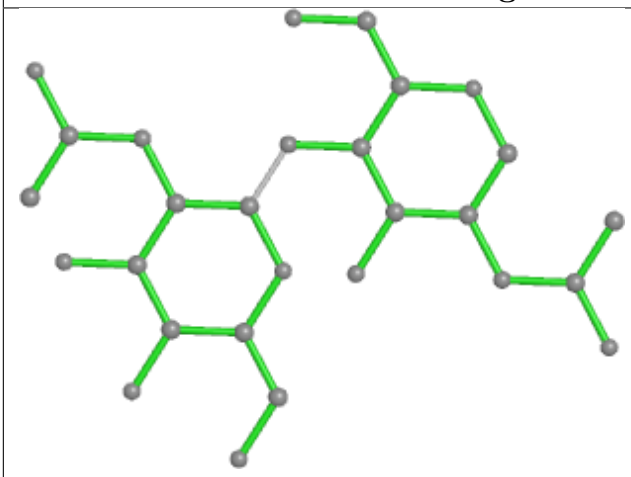
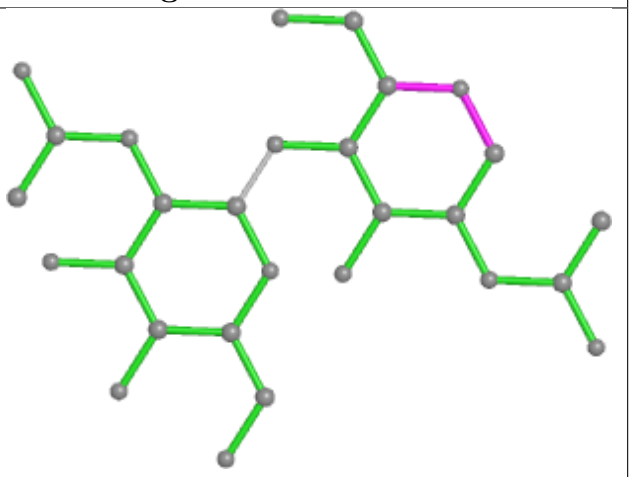
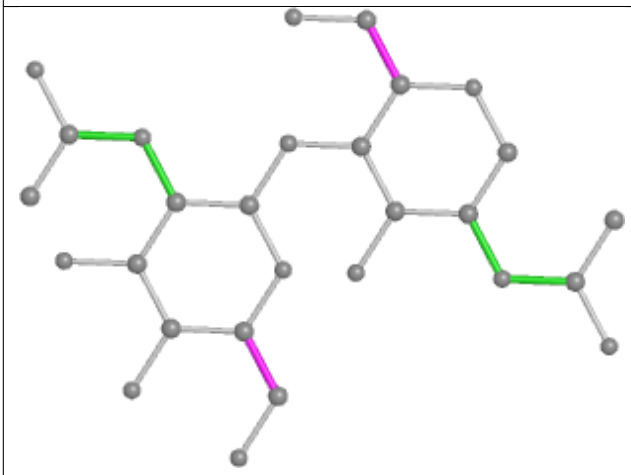
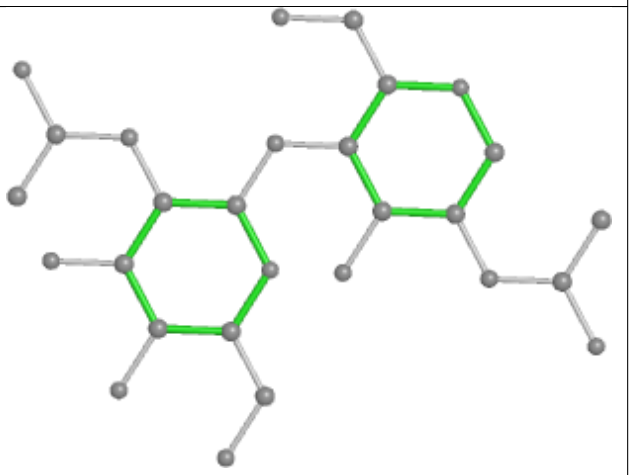
Bond angles

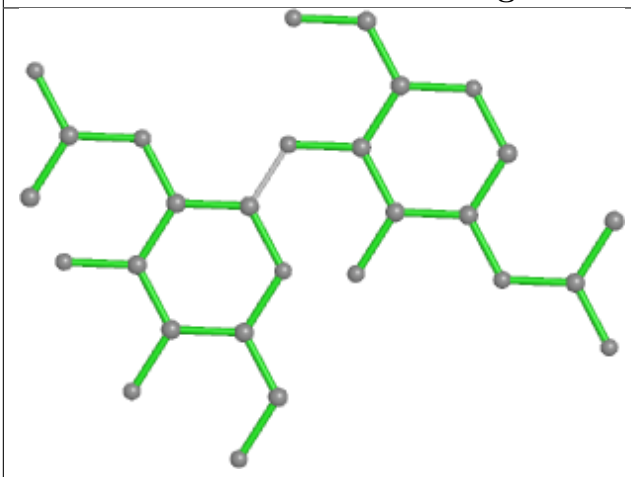
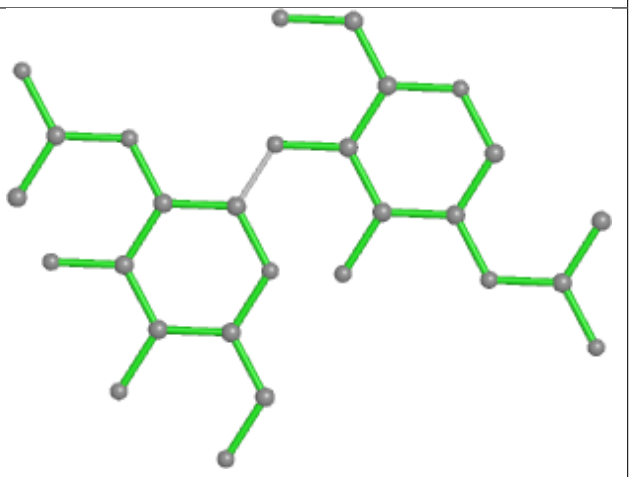
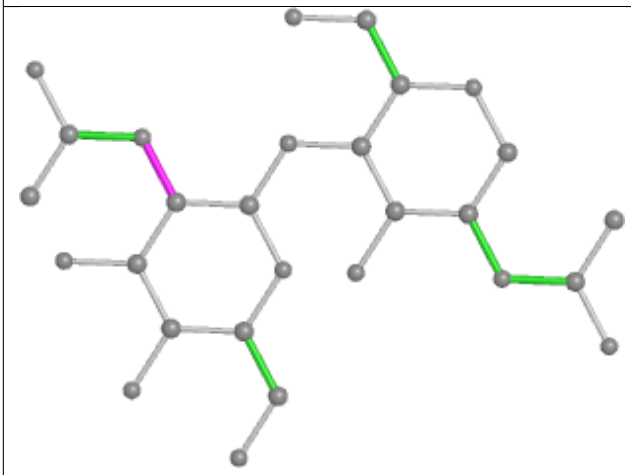
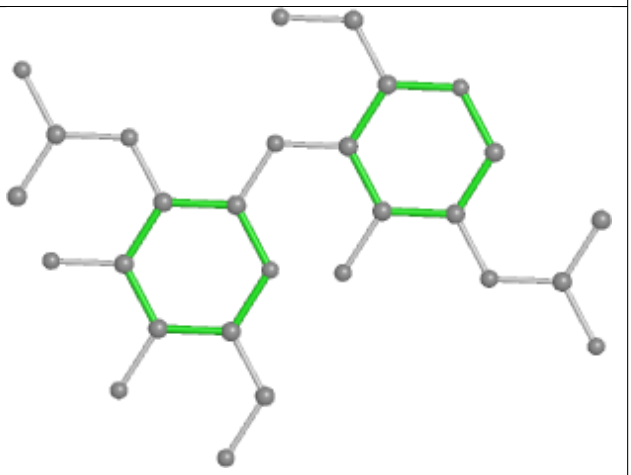


Torsions

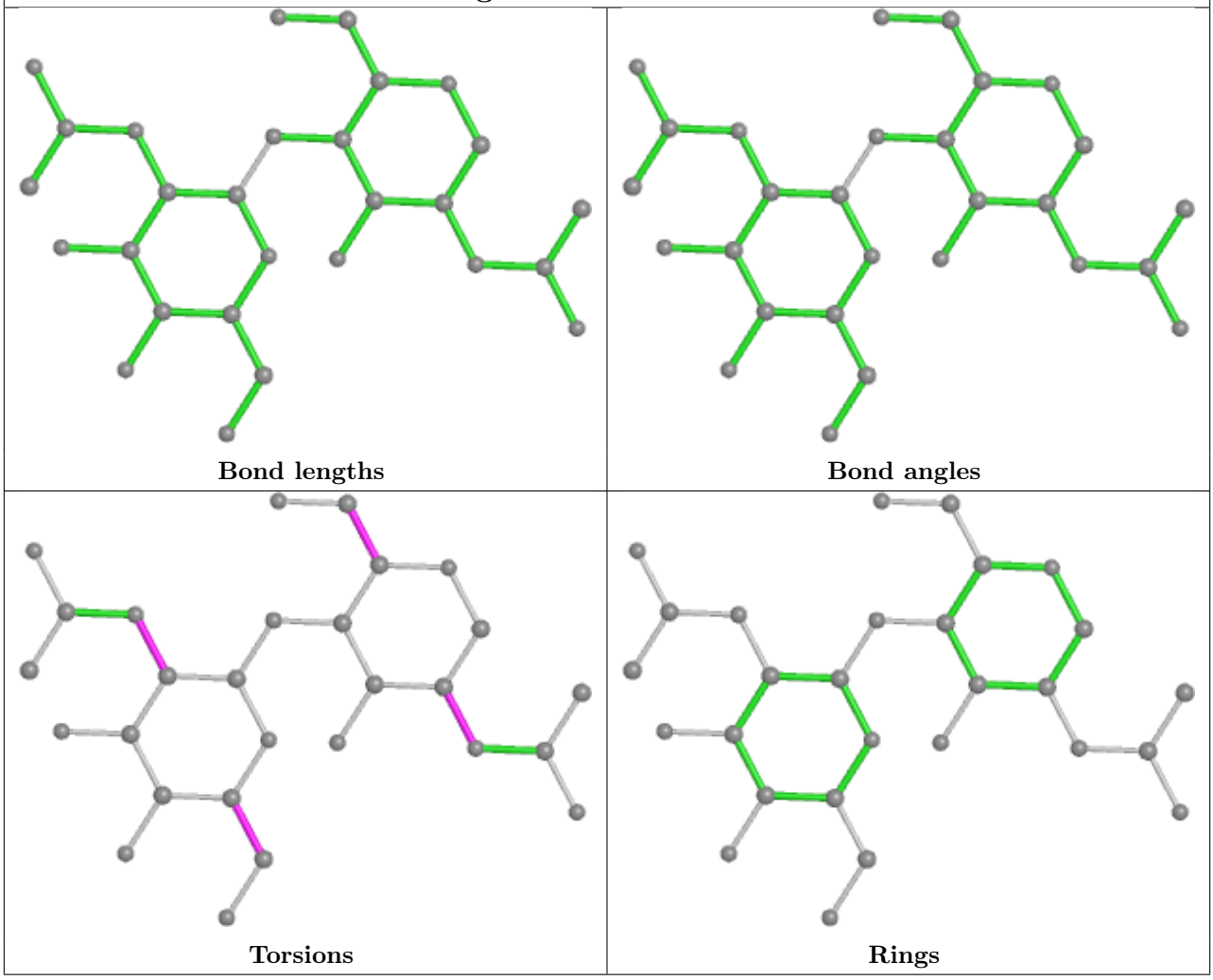


Rings

Oligosaccharide Chain g	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain h	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain i



5.6 Ligand geometry (i)

26 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	$\#\|Z\| > 2$
4	NAG	C	2007	1	14,14,15	0.28	0	17,19,21	0.47	0
4	NAG	I	1003	2	14,14,15	0.19	0	17,19,21	0.37	0
4	NAG	C	2006	1	14,14,15	0.21	0	17,19,21	0.38	0
4	NAG	I	1004	2	14,14,15	0.23	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	B	2005	1	14,14,15	0.25	0	17,19,21	0.50	0
4	NAG	B	2001	1	14,14,15	0.46	0	17,19,21	0.62	0
4	NAG	B	2002	1	14,14,15	0.44	0	17,19,21	0.69	1 (5%)
4	NAG	A	2003	-	14,14,15	0.24	0	17,19,21	0.38	0
4	NAG	I	1006	2	14,14,15	0.18	0	17,19,21	0.47	0
4	NAG	I	1002	2	14,14,15	0.18	0	17,19,21	0.45	0
4	NAG	A	2002	1	14,14,15	0.24	0	17,19,21	0.40	0
4	NAG	C	2003	1	14,14,15	0.46	0	17,19,21	1.22	1 (5%)
4	NAG	C	2002	1	14,14,15	0.18	0	17,19,21	0.60	0
4	NAG	C	2004	1	14,14,15	0.25	0	17,19,21	0.45	0
4	NAG	A	2004	1	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	A	2006	1	14,14,15	0.30	0	17,19,21	0.51	0
4	NAG	B	2006	1	14,14,15	0.23	0	17,19,21	0.50	0
4	NAG	I	1005	2	14,14,15	0.22	0	17,19,21	0.50	0
4	NAG	J	1001	2	14,14,15	0.20	0	17,19,21	0.49	0
4	NAG	I	1001	2	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	B	2003	1	14,14,15	0.16	0	17,19,21	0.48	0
4	NAG	C	2005	1	14,14,15	0.29	0	17,19,21	0.36	0
4	NAG	C	2001	1	14,14,15	0.28	0	17,19,21	0.44	0
4	NAG	A	2005	1	14,14,15	0.19	0	17,19,21	0.40	0
4	NAG	B	2004	1	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	A	2001	1	14,14,15	0.52	0	17,19,21	0.63	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
4	NAG	C	2007	1	-	2/6/23/26	0/1/1/1
4	NAG	I	1003	2	-	2/6/23/26	0/1/1/1
4	NAG	C	2006	1	-	2/6/23/26	0/1/1/1
4	NAG	I	1004	2	-	2/6/23/26	0/1/1/1
4	NAG	B	2005	1	-	1/6/23/26	0/1/1/1
4	NAG	B	2001	1	-	4/6/23/26	0/1/1/1
4	NAG	B	2002	1	-	3/6/23/26	0/1/1/1
4	NAG	A	2003	-	-	1/6/23/26	0/1/1/1
4	NAG	I	1006	2	-	0/6/23/26	0/1/1/1
4	NAG	I	1002	2	-	2/6/23/26	0/1/1/1
4	NAG	A	2002	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	2003	1	-	4/6/23/26	0/1/1/1
4	NAG	C	2002	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2004	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2004	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2006	1	-	3/6/23/26	0/1/1/1
4	NAG	B	2006	1	-	2/6/23/26	0/1/1/1
4	NAG	I	1005	2	-	0/6/23/26	0/1/1/1
4	NAG	J	1001	2	-	1/6/23/26	0/1/1/1
4	NAG	I	1001	2	-	0/6/23/26	0/1/1/1
4	NAG	B	2003	1	-	4/6/23/26	0/1/1/1
4	NAG	C	2005	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2001	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2005	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2004	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2001	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	2003	NAG	C2-N2-C7	4.27	128.98	122.90
4	B	2002	NAG	C1-O5-C5	2.28	115.28	112.19

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	2001	NAG	O5-C5-C6-O6
4	B	2002	NAG	C4-C5-C6-O6
4	I	1004	NAG	C4-C5-C6-O6
4	B	2001	NAG	O5-C5-C6-O6
4	C	2001	NAG	C4-C5-C6-O6
4	C	2005	NAG	O5-C5-C6-O6
4	C	2007	NAG	O5-C5-C6-O6
4	A	2001	NAG	O5-C5-C6-O6
4	B	2002	NAG	O5-C5-C6-O6
4	A	2001	NAG	C4-C5-C6-O6
4	C	2007	NAG	C4-C5-C6-O6
4	B	2003	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	B	2006	NAG	O5-C5-C6-O6
4	B	2001	NAG	C8-C7-N2-C2
4	B	2001	NAG	O7-C7-N2-C2
4	B	2003	NAG	C8-C7-N2-C2
4	B	2003	NAG	O7-C7-N2-C2
4	C	2003	NAG	C8-C7-N2-C2
4	C	2003	NAG	O7-C7-N2-C2
4	I	1003	NAG	C8-C7-N2-C2
4	I	1003	NAG	O7-C7-N2-C2
4	B	2001	NAG	C4-C5-C6-O6
4	I	1004	NAG	O5-C5-C6-O6
4	B	2003	NAG	C4-C5-C6-O6
4	B	2006	NAG	C4-C5-C6-O6
4	B	2005	NAG	O5-C5-C6-O6
4	C	2005	NAG	C4-C5-C6-O6
4	C	2002	NAG	O5-C5-C6-O6
4	C	2002	NAG	C4-C5-C6-O6
4	A	2006	NAG	O5-C5-C6-O6
4	A	2005	NAG	C4-C5-C6-O6
4	C	2006	NAG	C4-C5-C6-O6
4	A	2003	NAG	O5-C5-C6-O6
4	C	2006	NAG	O5-C5-C6-O6
4	C	2003	NAG	O5-C5-C6-O6
4	A	2005	NAG	O5-C5-C6-O6
4	I	1002	NAG	C4-C5-C6-O6
4	B	2002	NAG	C3-C2-N2-C7
4	A	2006	NAG	C4-C5-C6-O6
4	I	1002	NAG	O5-C5-C6-O6
4	A	2006	NAG	C3-C2-N2-C7
4	C	2003	NAG	C3-C2-N2-C7
4	J	1001	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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.

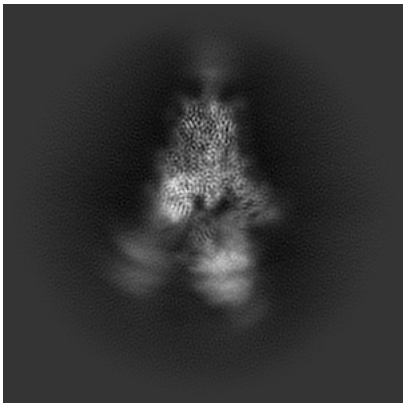
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-31073. These allow visual inspection of the internal detail of the map and identification of artifacts.

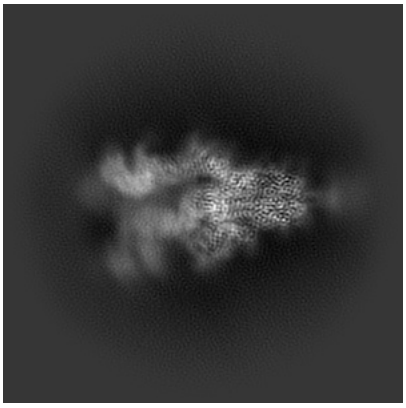
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

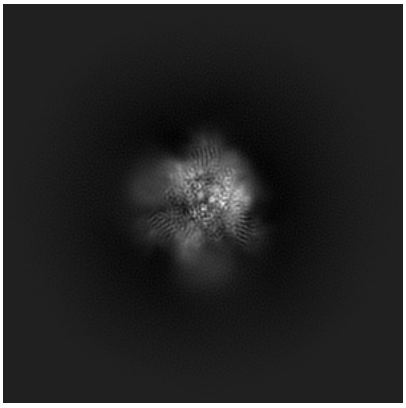
6.1.1 Primary map



X



Y

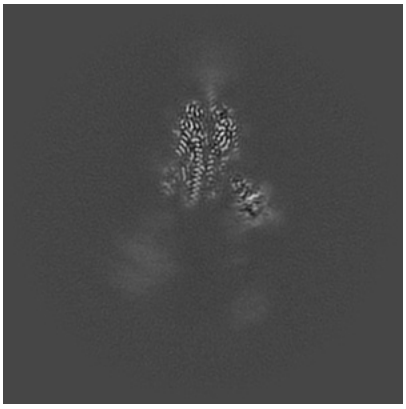


Z

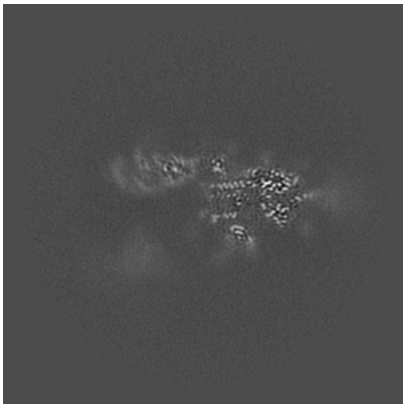
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

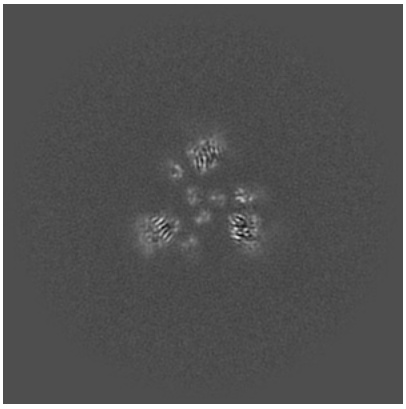
6.2.1 Primary map



X Index: 192



Y Index: 192

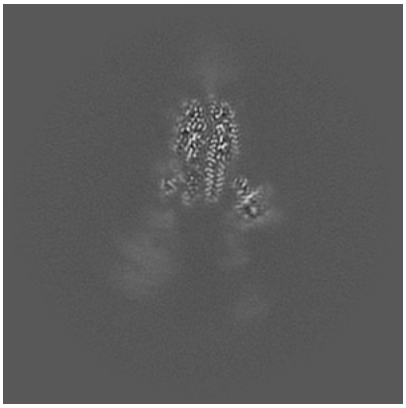


Z Index: 192

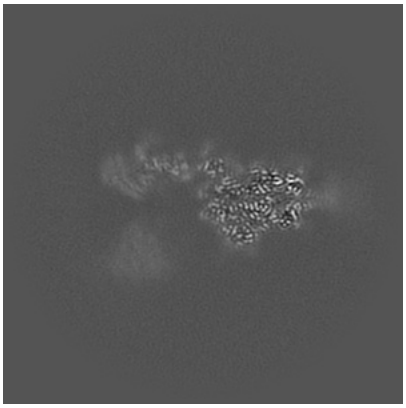
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

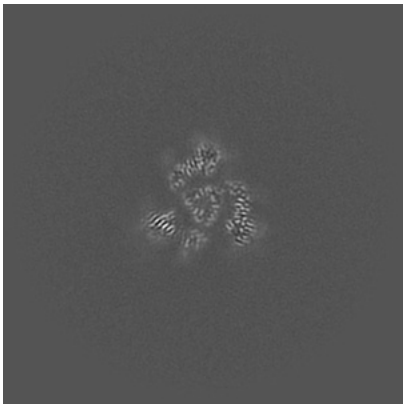
6.3.1 Primary map



X Index: 188



Y Index: 201

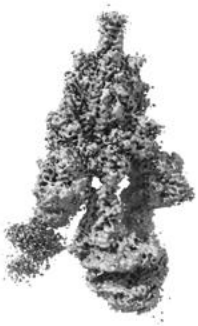


Z Index: 203

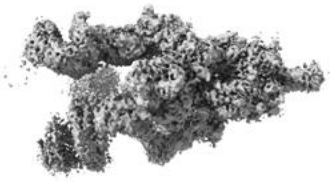
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.22. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

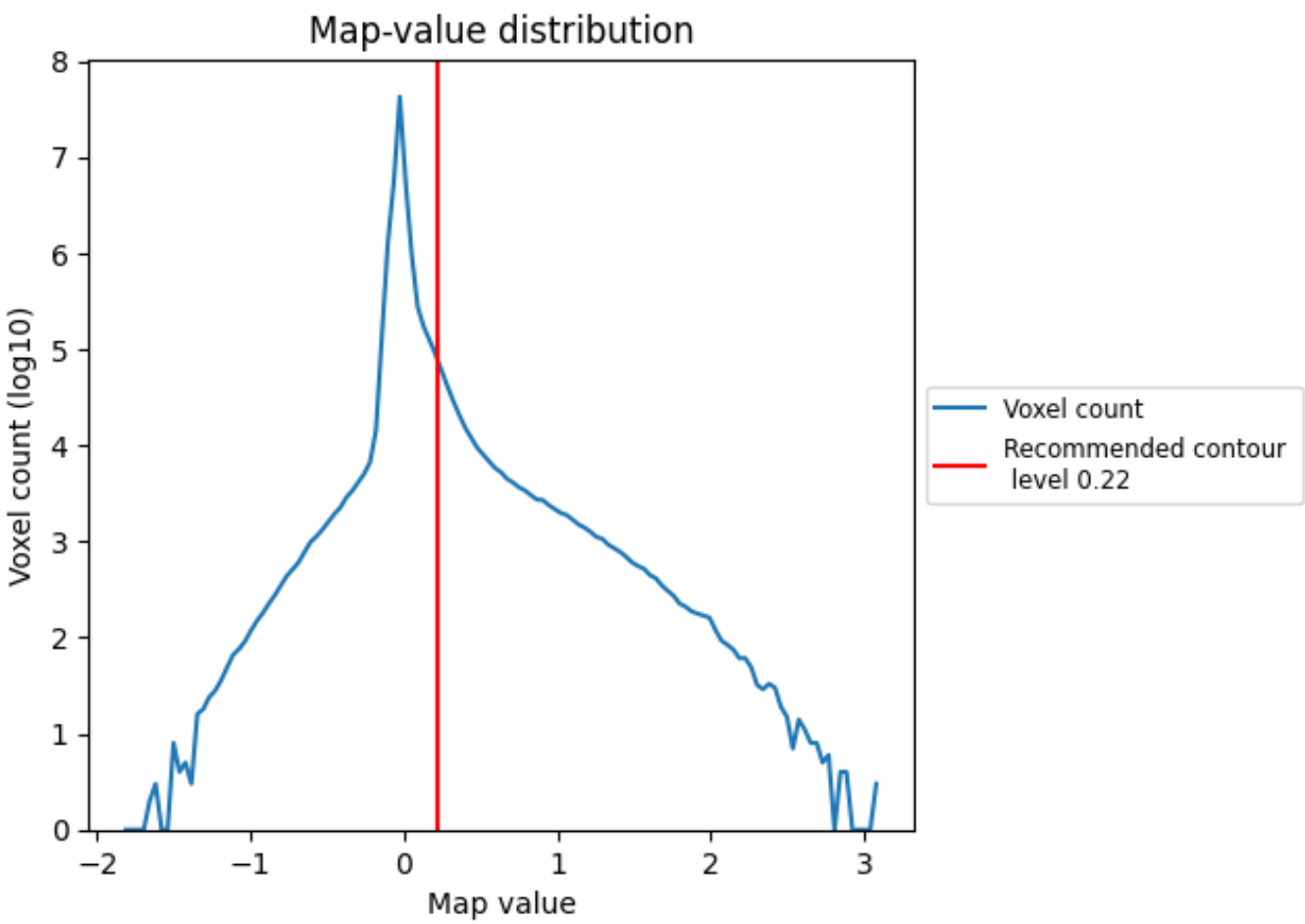
6.5 Mask visualisation (i)

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

7 Map analysis (i)

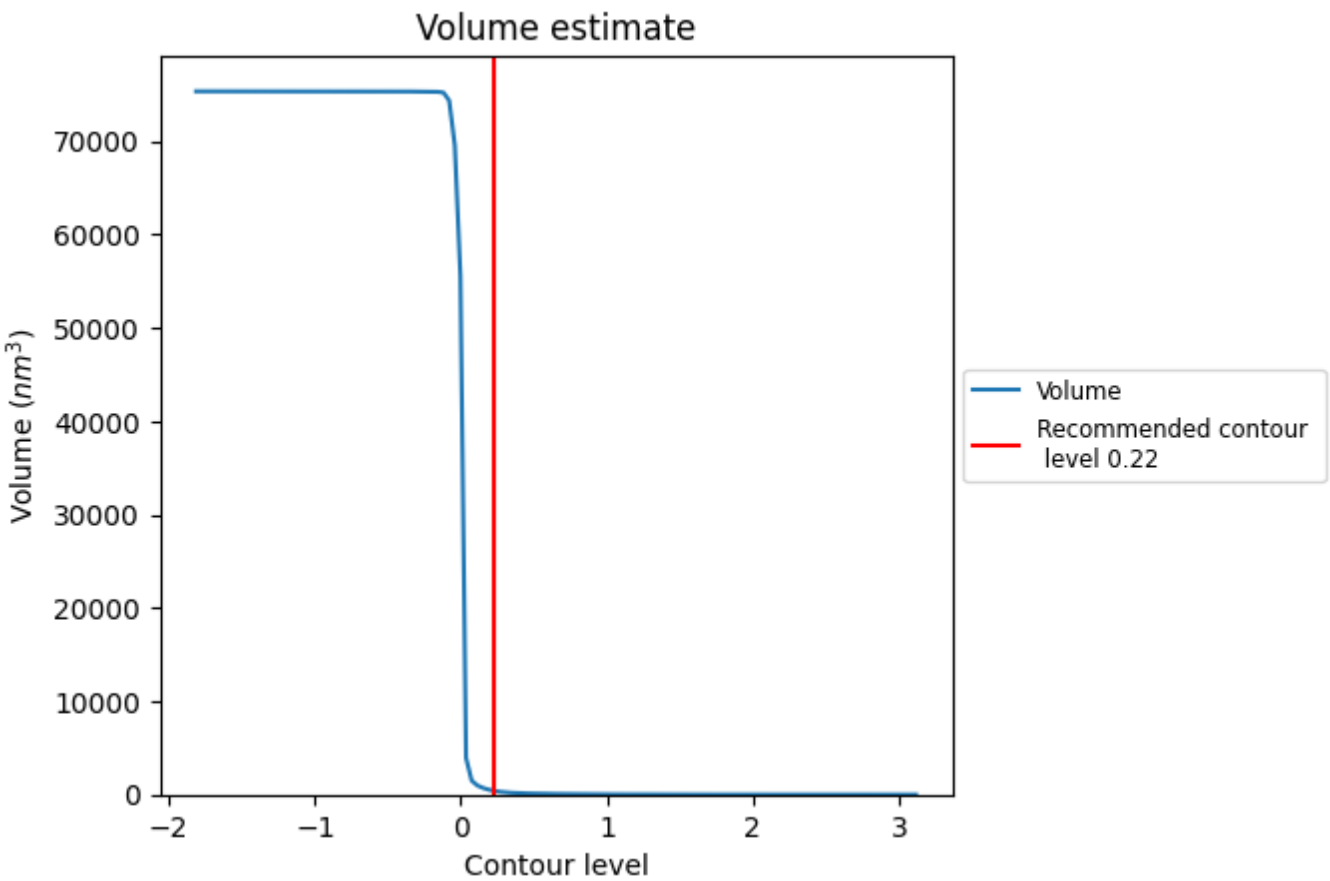
This section contains the results of statistical analysis of the map.

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.

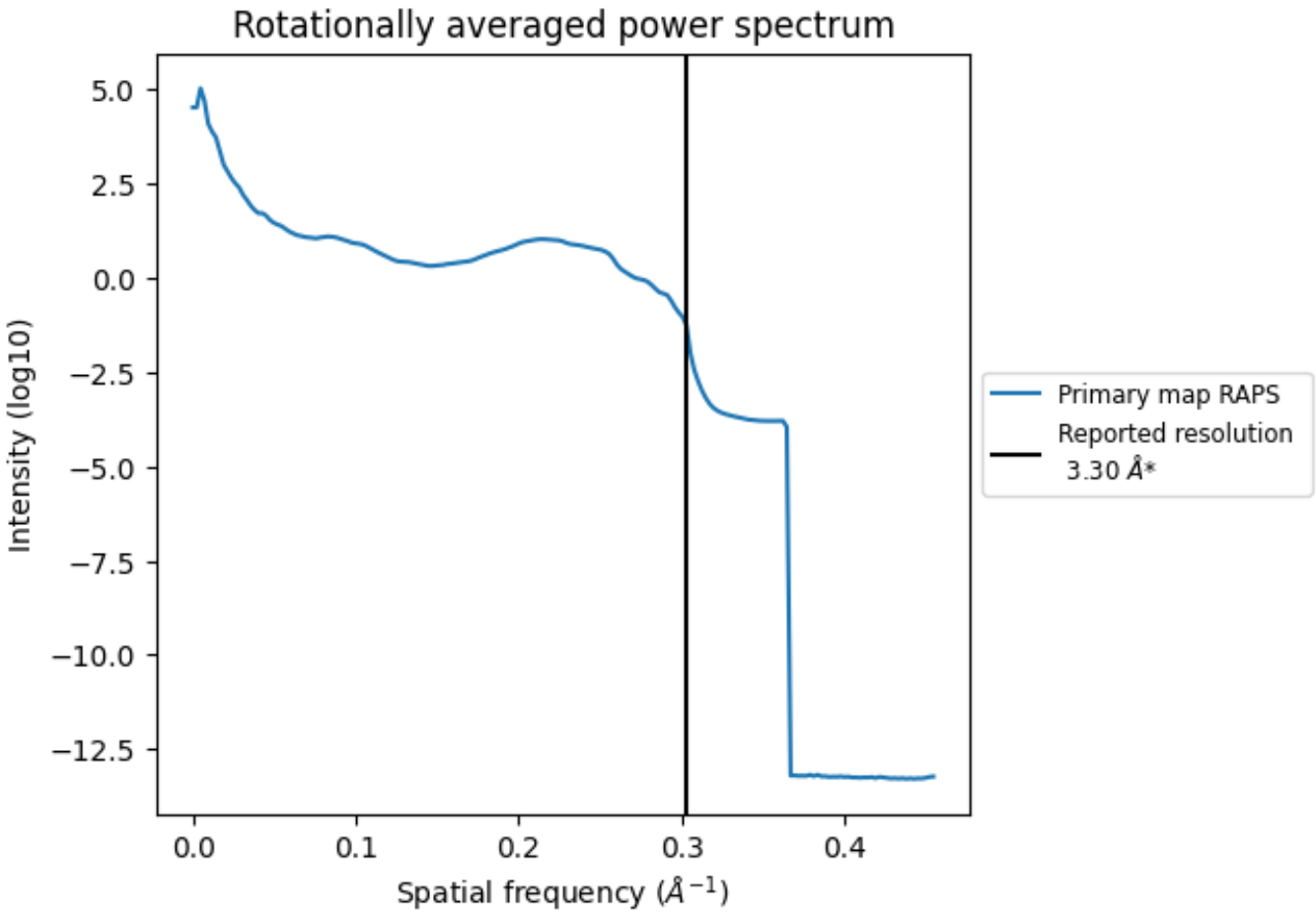
7.2 Volume estimate (i)



The volume at the recommended contour level is 420 nm^3; this corresponds to an approximate mass of 379 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

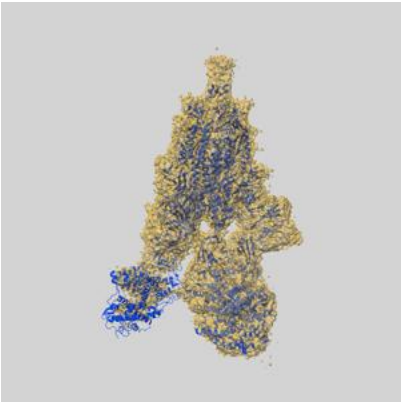
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

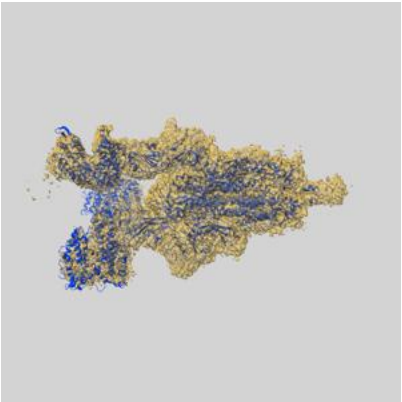
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-31073 and PDB model 7EDJ. Per-residue inclusion information can be found in section 3 on page 17.

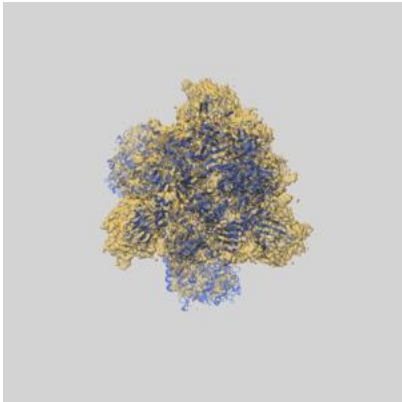
9.1 Map-model overlay (i)



X



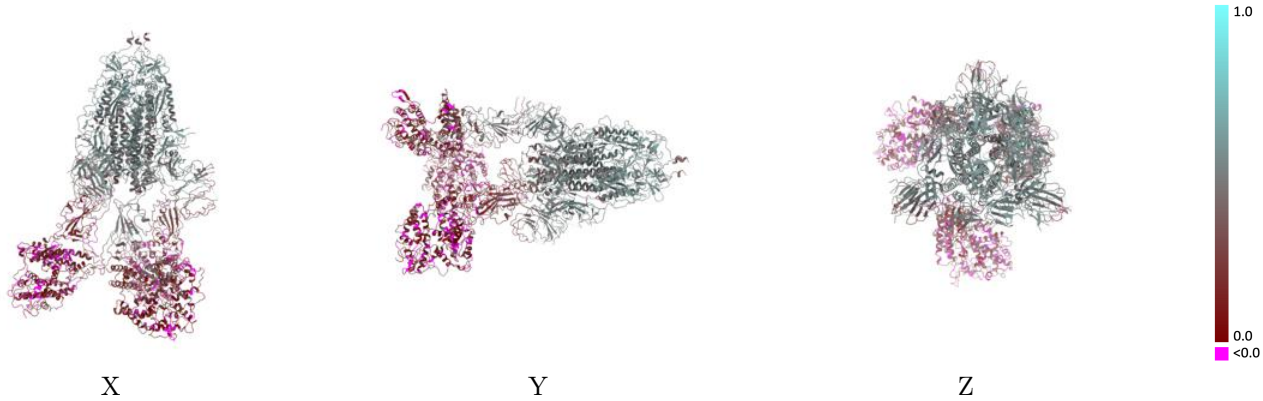
Y



Z

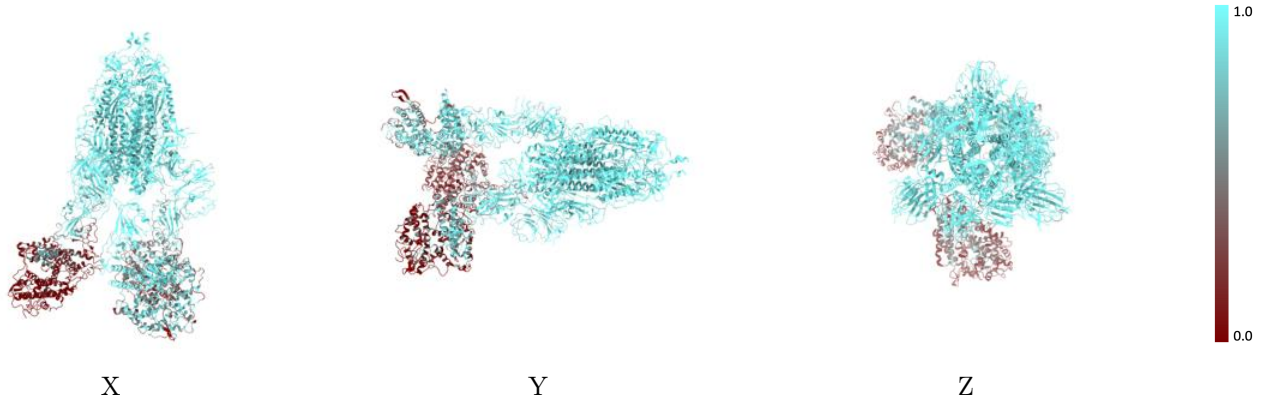
The images above show the 3D surface view of the map at the recommended contour level 0.22 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



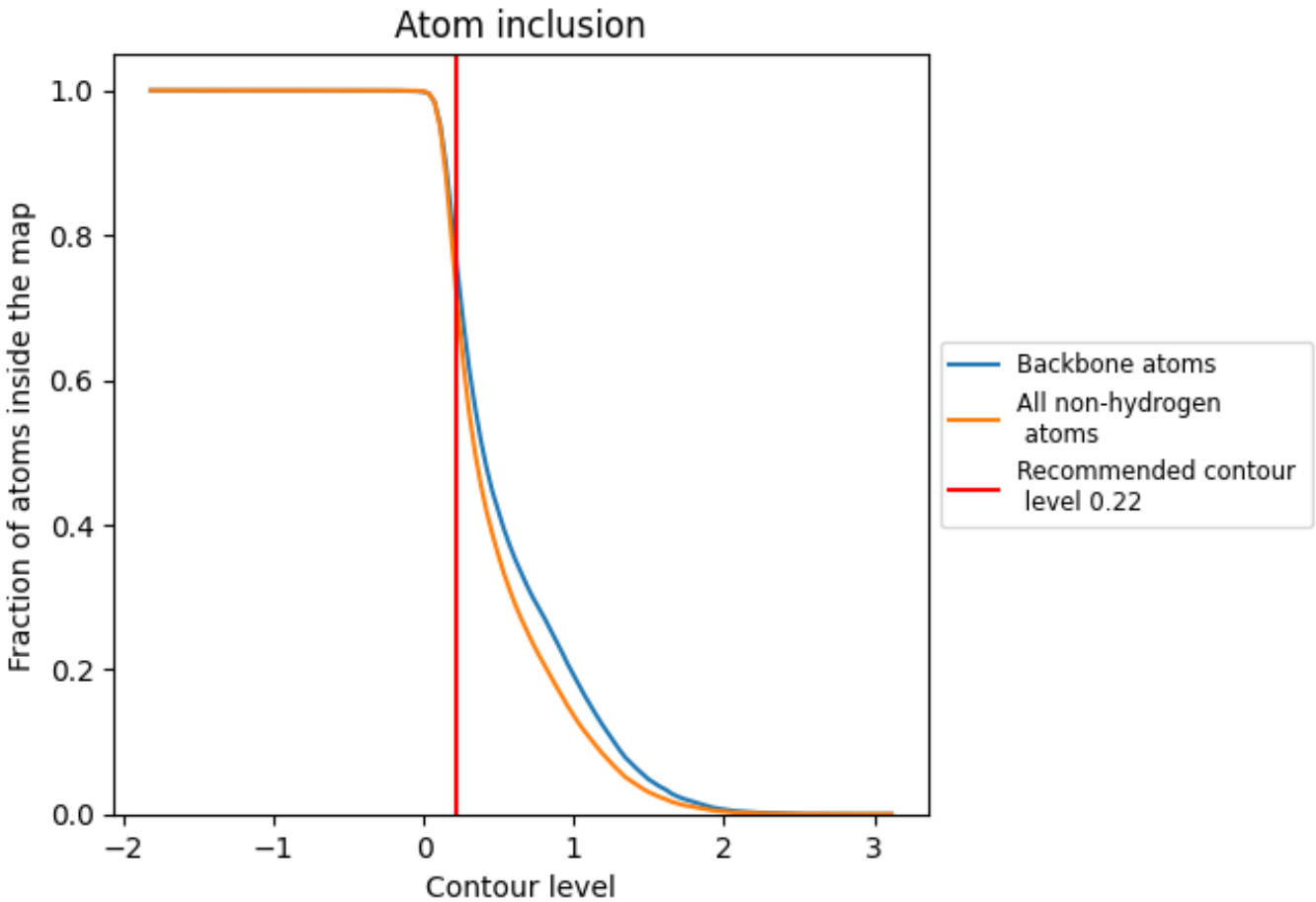
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.22).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 72% 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 (0.22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7195	0.3340
A	0.9482	0.4750
B	0.8831	0.4290
C	0.9088	0.4360
D	0.6429	0.2970
E	0.8571	0.3910
F	0.9286	0.3900
G	0.8571	0.3710
H	0.7857	0.3540
I	0.7320	0.2030
J	0.1336	0.1140
K	0.3188	0.1180
L	0.9286	0.5060
M	0.8571	0.4040
N	0.6071	0.3450
O	0.9643	0.5090
P	0.8571	0.3030
Q	0.7857	0.2250
R	0.6429	0.3740
S	0.8214	0.4320
T	0.9286	0.4350
U	0.6786	0.3880
V	0.8571	0.4750
W	0.9286	0.3960
X	0.5714	0.3960
Y	0.9286	0.4360
Z	0.8571	0.4680
a	0.5357	0.2540
b	0.7500	0.2650
c	0.8571	0.3790
d	0.6071	0.3770
e	0.7143	0.4620
f	0.9286	0.4480
g	0.6786	0.3890
h	0.8929	0.4510
i	0.8214	0.3870