wwPDB EM Validation Summary Report (i)

Nov 5, 2022 – 05:52 PM EDT

PDB ID	:	5W9I
EMDB ID	:	EMD-8784
Title	:	MERS S ectodomain trimer in complex with variable domain of neutralizing antibody G4
Authors	:	Pallesen, J.; Ward, A.B.
Deposited on	:	2017-06-23
Resolution	:	3.60 Å(reported)

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

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

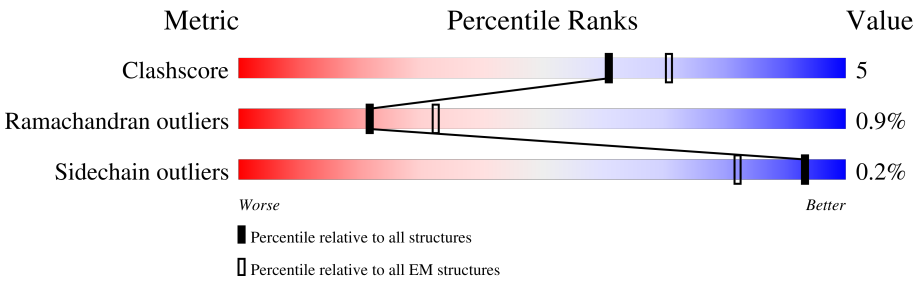
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.60 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1329	32% • 65%
1	B	1329	36% • 61%
1	E	1329	33% • 65%
1	F	1329	36% • 61%
1	I	1329	32% • 65%
1	J	1329	35% • 61%
2	C	233	50% • 49%
2	G	233	49% • 49%

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Mol	Chain	Length	Quality of chain
2	K	233	49% 49%
3	D	218	9% 50% 49%
3	H	218	10% 50% 49%
3	L	218	9% 50% 49%
4	M	2	50% 50%
4	N	2	50% 50%
4	O	2	50% 50%
4	P	2	100%
4	Q	2	100%
4	R	2	50% 50%
4	S	2	50% 50%
4	T	2	50% 50%
4	U	2	50% 50%
4	V	2	100%
4	W	2	50% 50%
4	X	2	50% 50%
4	Y	2	100%
4	Z	2	100%
4	a	2	100%
4	b	2	100%
4	c	2	100%
4	d	2	50% 50%
4	e	2	50% 100%
4	f	2	100%
4	g	2	100%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 28896 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	463	3545	2243	600	685	17	0	0
1	B	513	4010	2549	664	774	23	0	0
1	E	463	3545	2243	600	685	17	0	0
1	F	513	4010	2549	664	774	23	0	0
1	I	463	3545	2243	600	685	17	0	0
1	J	513	4010	2549	664	774	23	0	0

There are 258 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	506	PHE	LEU	conflict	UNP W5ZZF5
A	748	ALA	ARG	conflict	UNP W5ZZF5
A	751	GLY	ARG	conflict	UNP W5ZZF5
A	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
A	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
A	1292	GLY	-	expression tag	UNP W5ZZF5
A	1293	SER	-	expression tag	UNP W5ZZF5
A	1294	GLY	-	expression tag	UNP W5ZZF5
A	1295	TYR	-	expression tag	UNP W5ZZF5
A	1296	ILE	-	expression tag	UNP W5ZZF5
A	1297	PRO	-	expression tag	UNP W5ZZF5
A	1298	GLU	-	expression tag	UNP W5ZZF5
A	1299	ALA	-	expression tag	UNP W5ZZF5
A	1300	PRO	-	expression tag	UNP W5ZZF5
A	1301	ARG	-	expression tag	UNP W5ZZF5
A	1302	ASP	-	expression tag	UNP W5ZZF5
A	1303	GLY	-	expression tag	UNP W5ZZF5
A	1304	GLN	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1305	ALA	-	expression tag	UNP W5ZZF5
A	1306	TYR	-	expression tag	UNP W5ZZF5
A	1307	VAL	-	expression tag	UNP W5ZZF5
A	1308	ARG	-	expression tag	UNP W5ZZF5
A	1309	LYS	-	expression tag	UNP W5ZZF5
A	1310	ASP	-	expression tag	UNP W5ZZF5
A	1311	GLY	-	expression tag	UNP W5ZZF5
A	1312	GLU	-	expression tag	UNP W5ZZF5
A	1313	TRP	-	expression tag	UNP W5ZZF5
A	1314	VAL	-	expression tag	UNP W5ZZF5
A	1315	LEU	-	expression tag	UNP W5ZZF5
A	1316	LEU	-	expression tag	UNP W5ZZF5
A	1317	SER	-	expression tag	UNP W5ZZF5
A	1318	THR	-	expression tag	UNP W5ZZF5
A	1319	PHE	-	expression tag	UNP W5ZZF5
A	1320	LEU	-	expression tag	UNP W5ZZF5
A	1321	GLY	-	expression tag	UNP W5ZZF5
A	1322	ARG	-	expression tag	UNP W5ZZF5
A	1323	SER	-	expression tag	UNP W5ZZF5
A	1324	LEU	-	expression tag	UNP W5ZZF5
A	1325	GLU	-	expression tag	UNP W5ZZF5
A	1326	VAL	-	expression tag	UNP W5ZZF5
A	1327	LEU	-	expression tag	UNP W5ZZF5
A	1328	PHE	-	expression tag	UNP W5ZZF5
A	1329	GLN	-	expression tag	UNP W5ZZF5
B	506	PHE	LEU	conflict	UNP W5ZZF5
B	748	ALA	ARG	conflict	UNP W5ZZF5
B	751	GLY	ARG	conflict	UNP W5ZZF5
B	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
B	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
B	1292	GLY	-	expression tag	UNP W5ZZF5
B	1293	SER	-	expression tag	UNP W5ZZF5
B	1294	GLY	-	expression tag	UNP W5ZZF5
B	1295	TYR	-	expression tag	UNP W5ZZF5
B	1296	ILE	-	expression tag	UNP W5ZZF5
B	1297	PRO	-	expression tag	UNP W5ZZF5
B	1298	GLU	-	expression tag	UNP W5ZZF5
B	1299	ALA	-	expression tag	UNP W5ZZF5
B	1300	PRO	-	expression tag	UNP W5ZZF5
B	1301	ARG	-	expression tag	UNP W5ZZF5
B	1302	ASP	-	expression tag	UNP W5ZZF5
B	1303	GLY	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1304	GLN	-	expression tag	UNP W5ZZF5
B	1305	ALA	-	expression tag	UNP W5ZZF5
B	1306	TYR	-	expression tag	UNP W5ZZF5
B	1307	VAL	-	expression tag	UNP W5ZZF5
B	1308	ARG	-	expression tag	UNP W5ZZF5
B	1309	LYS	-	expression tag	UNP W5ZZF5
B	1310	ASP	-	expression tag	UNP W5ZZF5
B	1311	GLY	-	expression tag	UNP W5ZZF5
B	1312	GLU	-	expression tag	UNP W5ZZF5
B	1313	TRP	-	expression tag	UNP W5ZZF5
B	1314	VAL	-	expression tag	UNP W5ZZF5
B	1315	LEU	-	expression tag	UNP W5ZZF5
B	1316	LEU	-	expression tag	UNP W5ZZF5
B	1317	SER	-	expression tag	UNP W5ZZF5
B	1318	THR	-	expression tag	UNP W5ZZF5
B	1319	PHE	-	expression tag	UNP W5ZZF5
B	1320	LEU	-	expression tag	UNP W5ZZF5
B	1321	GLY	-	expression tag	UNP W5ZZF5
B	1322	ARG	-	expression tag	UNP W5ZZF5
B	1323	SER	-	expression tag	UNP W5ZZF5
B	1324	LEU	-	expression tag	UNP W5ZZF5
B	1325	GLU	-	expression tag	UNP W5ZZF5
B	1326	VAL	-	expression tag	UNP W5ZZF5
B	1327	LEU	-	expression tag	UNP W5ZZF5
B	1328	PHE	-	expression tag	UNP W5ZZF5
B	1329	GLN	-	expression tag	UNP W5ZZF5
E	506	PHE	LEU	conflict	UNP W5ZZF5
E	748	ALA	ARG	conflict	UNP W5ZZF5
E	751	GLY	ARG	conflict	UNP W5ZZF5
E	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
E	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
E	1292	GLY	-	expression tag	UNP W5ZZF5
E	1293	SER	-	expression tag	UNP W5ZZF5
E	1294	GLY	-	expression tag	UNP W5ZZF5
E	1295	TYR	-	expression tag	UNP W5ZZF5
E	1296	ILE	-	expression tag	UNP W5ZZF5
E	1297	PRO	-	expression tag	UNP W5ZZF5
E	1298	GLU	-	expression tag	UNP W5ZZF5
E	1299	ALA	-	expression tag	UNP W5ZZF5
E	1300	PRO	-	expression tag	UNP W5ZZF5
E	1301	ARG	-	expression tag	UNP W5ZZF5
E	1302	ASP	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1303	GLY	-	expression tag	UNP W5ZZF5
E	1304	GLN	-	expression tag	UNP W5ZZF5
E	1305	ALA	-	expression tag	UNP W5ZZF5
E	1306	TYR	-	expression tag	UNP W5ZZF5
E	1307	VAL	-	expression tag	UNP W5ZZF5
E	1308	ARG	-	expression tag	UNP W5ZZF5
E	1309	LYS	-	expression tag	UNP W5ZZF5
E	1310	ASP	-	expression tag	UNP W5ZZF5
E	1311	GLY	-	expression tag	UNP W5ZZF5
E	1312	GLU	-	expression tag	UNP W5ZZF5
E	1313	TRP	-	expression tag	UNP W5ZZF5
E	1314	VAL	-	expression tag	UNP W5ZZF5
E	1315	LEU	-	expression tag	UNP W5ZZF5
E	1316	LEU	-	expression tag	UNP W5ZZF5
E	1317	SER	-	expression tag	UNP W5ZZF5
E	1318	THR	-	expression tag	UNP W5ZZF5
E	1319	PHE	-	expression tag	UNP W5ZZF5
E	1320	LEU	-	expression tag	UNP W5ZZF5
E	1321	GLY	-	expression tag	UNP W5ZZF5
E	1322	ARG	-	expression tag	UNP W5ZZF5
E	1323	SER	-	expression tag	UNP W5ZZF5
E	1324	LEU	-	expression tag	UNP W5ZZF5
E	1325	GLU	-	expression tag	UNP W5ZZF5
E	1326	VAL	-	expression tag	UNP W5ZZF5
E	1327	LEU	-	expression tag	UNP W5ZZF5
E	1328	PHE	-	expression tag	UNP W5ZZF5
E	1329	GLN	-	expression tag	UNP W5ZZF5
F	506	PHE	LEU	conflict	UNP W5ZZF5
F	748	ALA	ARG	conflict	UNP W5ZZF5
F	751	GLY	ARG	conflict	UNP W5ZZF5
F	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
F	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
F	1292	GLY	-	expression tag	UNP W5ZZF5
F	1293	SER	-	expression tag	UNP W5ZZF5
F	1294	GLY	-	expression tag	UNP W5ZZF5
F	1295	TYR	-	expression tag	UNP W5ZZF5
F	1296	ILE	-	expression tag	UNP W5ZZF5
F	1297	PRO	-	expression tag	UNP W5ZZF5
F	1298	GLU	-	expression tag	UNP W5ZZF5
F	1299	ALA	-	expression tag	UNP W5ZZF5
F	1300	PRO	-	expression tag	UNP W5ZZF5
F	1301	ARG	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1302	ASP	-	expression tag	UNP W5ZZF5
F	1303	GLY	-	expression tag	UNP W5ZZF5
F	1304	GLN	-	expression tag	UNP W5ZZF5
F	1305	ALA	-	expression tag	UNP W5ZZF5
F	1306	TYR	-	expression tag	UNP W5ZZF5
F	1307	VAL	-	expression tag	UNP W5ZZF5
F	1308	ARG	-	expression tag	UNP W5ZZF5
F	1309	LYS	-	expression tag	UNP W5ZZF5
F	1310	ASP	-	expression tag	UNP W5ZZF5
F	1311	GLY	-	expression tag	UNP W5ZZF5
F	1312	GLU	-	expression tag	UNP W5ZZF5
F	1313	TRP	-	expression tag	UNP W5ZZF5
F	1314	VAL	-	expression tag	UNP W5ZZF5
F	1315	LEU	-	expression tag	UNP W5ZZF5
F	1316	LEU	-	expression tag	UNP W5ZZF5
F	1317	SER	-	expression tag	UNP W5ZZF5
F	1318	THR	-	expression tag	UNP W5ZZF5
F	1319	PHE	-	expression tag	UNP W5ZZF5
F	1320	LEU	-	expression tag	UNP W5ZZF5
F	1321	GLY	-	expression tag	UNP W5ZZF5
F	1322	ARG	-	expression tag	UNP W5ZZF5
F	1323	SER	-	expression tag	UNP W5ZZF5
F	1324	LEU	-	expression tag	UNP W5ZZF5
F	1325	GLU	-	expression tag	UNP W5ZZF5
F	1326	VAL	-	expression tag	UNP W5ZZF5
F	1327	LEU	-	expression tag	UNP W5ZZF5
F	1328	PHE	-	expression tag	UNP W5ZZF5
F	1329	GLN	-	expression tag	UNP W5ZZF5
I	506	PHE	LEU	conflict	UNP W5ZZF5
I	748	ALA	ARG	conflict	UNP W5ZZF5
I	751	GLY	ARG	conflict	UNP W5ZZF5
I	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
I	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
I	1292	GLY	-	expression tag	UNP W5ZZF5
I	1293	SER	-	expression tag	UNP W5ZZF5
I	1294	GLY	-	expression tag	UNP W5ZZF5
I	1295	TYR	-	expression tag	UNP W5ZZF5
I	1296	ILE	-	expression tag	UNP W5ZZF5
I	1297	PRO	-	expression tag	UNP W5ZZF5
I	1298	GLU	-	expression tag	UNP W5ZZF5
I	1299	ALA	-	expression tag	UNP W5ZZF5
I	1300	PRO	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
I	1301	ARG	-	expression tag	UNP W5ZZF5
I	1302	ASP	-	expression tag	UNP W5ZZF5
I	1303	GLY	-	expression tag	UNP W5ZZF5
I	1304	GLN	-	expression tag	UNP W5ZZF5
I	1305	ALA	-	expression tag	UNP W5ZZF5
I	1306	TYR	-	expression tag	UNP W5ZZF5
I	1307	VAL	-	expression tag	UNP W5ZZF5
I	1308	ARG	-	expression tag	UNP W5ZZF5
I	1309	LYS	-	expression tag	UNP W5ZZF5
I	1310	ASP	-	expression tag	UNP W5ZZF5
I	1311	GLY	-	expression tag	UNP W5ZZF5
I	1312	GLU	-	expression tag	UNP W5ZZF5
I	1313	TRP	-	expression tag	UNP W5ZZF5
I	1314	VAL	-	expression tag	UNP W5ZZF5
I	1315	LEU	-	expression tag	UNP W5ZZF5
I	1316	LEU	-	expression tag	UNP W5ZZF5
I	1317	SER	-	expression tag	UNP W5ZZF5
I	1318	THR	-	expression tag	UNP W5ZZF5
I	1319	PHE	-	expression tag	UNP W5ZZF5
I	1320	LEU	-	expression tag	UNP W5ZZF5
I	1321	GLY	-	expression tag	UNP W5ZZF5
I	1322	ARG	-	expression tag	UNP W5ZZF5
I	1323	SER	-	expression tag	UNP W5ZZF5
I	1324	LEU	-	expression tag	UNP W5ZZF5
I	1325	GLU	-	expression tag	UNP W5ZZF5
I	1326	VAL	-	expression tag	UNP W5ZZF5
I	1327	LEU	-	expression tag	UNP W5ZZF5
I	1328	PHE	-	expression tag	UNP W5ZZF5
I	1329	GLN	-	expression tag	UNP W5ZZF5
J	506	PHE	LEU	conflict	UNP W5ZZF5
J	748	ALA	ARG	conflict	UNP W5ZZF5
J	751	GLY	ARG	conflict	UNP W5ZZF5
J	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
J	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
J	1292	GLY	-	expression tag	UNP W5ZZF5
J	1293	SER	-	expression tag	UNP W5ZZF5
J	1294	GLY	-	expression tag	UNP W5ZZF5
J	1295	TYR	-	expression tag	UNP W5ZZF5
J	1296	ILE	-	expression tag	UNP W5ZZF5
J	1297	PRO	-	expression tag	UNP W5ZZF5
J	1298	GLU	-	expression tag	UNP W5ZZF5
J	1299	ALA	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
J	1300	PRO	-	expression tag	UNP W5ZZF5
J	1301	ARG	-	expression tag	UNP W5ZZF5
J	1302	ASP	-	expression tag	UNP W5ZZF5
J	1303	GLY	-	expression tag	UNP W5ZZF5
J	1304	GLN	-	expression tag	UNP W5ZZF5
J	1305	ALA	-	expression tag	UNP W5ZZF5
J	1306	TYR	-	expression tag	UNP W5ZZF5
J	1307	VAL	-	expression tag	UNP W5ZZF5
J	1308	ARG	-	expression tag	UNP W5ZZF5
J	1309	LYS	-	expression tag	UNP W5ZZF5
J	1310	ASP	-	expression tag	UNP W5ZZF5
J	1311	GLY	-	expression tag	UNP W5ZZF5
J	1312	GLU	-	expression tag	UNP W5ZZF5
J	1313	TRP	-	expression tag	UNP W5ZZF5
J	1314	VAL	-	expression tag	UNP W5ZZF5
J	1315	LEU	-	expression tag	UNP W5ZZF5
J	1316	LEU	-	expression tag	UNP W5ZZF5
J	1317	SER	-	expression tag	UNP W5ZZF5
J	1318	THR	-	expression tag	UNP W5ZZF5
J	1319	PHE	-	expression tag	UNP W5ZZF5
J	1320	LEU	-	expression tag	UNP W5ZZF5
J	1321	GLY	-	expression tag	UNP W5ZZF5
J	1322	ARG	-	expression tag	UNP W5ZZF5
J	1323	SER	-	expression tag	UNP W5ZZF5
J	1324	LEU	-	expression tag	UNP W5ZZF5
J	1325	GLU	-	expression tag	UNP W5ZZF5
J	1326	VAL	-	expression tag	UNP W5ZZF5
J	1327	LEU	-	expression tag	UNP W5ZZF5
J	1328	PHE	-	expression tag	UNP W5ZZF5
J	1329	GLN	-	expression tag	UNP W5ZZF5

- Molecule 2 is a protein called G4 VH.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	119	948	602	156	185	5	0	0
			Total	C	N	O	S		
2	G	119	948	602	156	185	5	0	0
			Total	C	N	O	S		
2	K	119	948	602	156	185	5	0	0

- Molecule 3 is a protein called G4 VL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	111	835	522	143	166	4	0	0
3	H	111	835	522	143	166	4	0	0
3	L	111	835	522	143	166	4	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	M	2	28	16	2	10	0	0
4	N	2	28	16	2	10	0	0
4	O	2	28	16	2	10	0	0
4	P	2	28	16	2	10	0	0
4	Q	2	28	16	2	10	0	0
4	R	2	28	16	2	10	0	0
4	S	2	28	16	2	10	0	0
4	T	2	28	16	2	10	0	0
4	U	2	28	16	2	10	0	0
4	V	2	28	16	2	10	0	0
4	W	2	28	16	2	10	0	0
4	X	2	28	16	2	10	0	0
4	Y	2	28	16	2	10	0	0
4	Z	2	28	16	2	10	0	0

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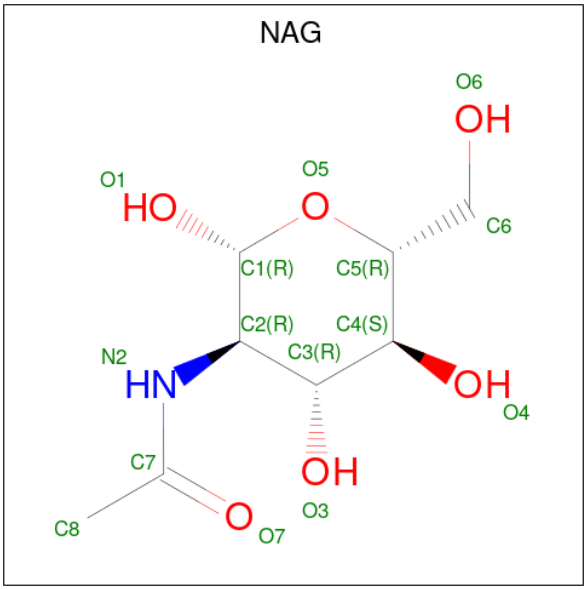
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	a	2	28	16	2	10	0	0
4	b	2	28	16	2	10	0	0
4	c	2	28	16	2	10	0	0
4	d	2	28	16	2	10	0	0
4	e	2	28	16	2	10	0	0
4	f	2	28	16	2	10	0	0
4	g	2	28	16	2	10	0	0

- Molecule 5 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	
5	A	1	14	8	1	5	0
5	B	1	84	48	6	30	0
5	B	1	84	48	6	30	0
5	B	1	84	48	6	30	0

Continued on next page...

Continued from previous page...

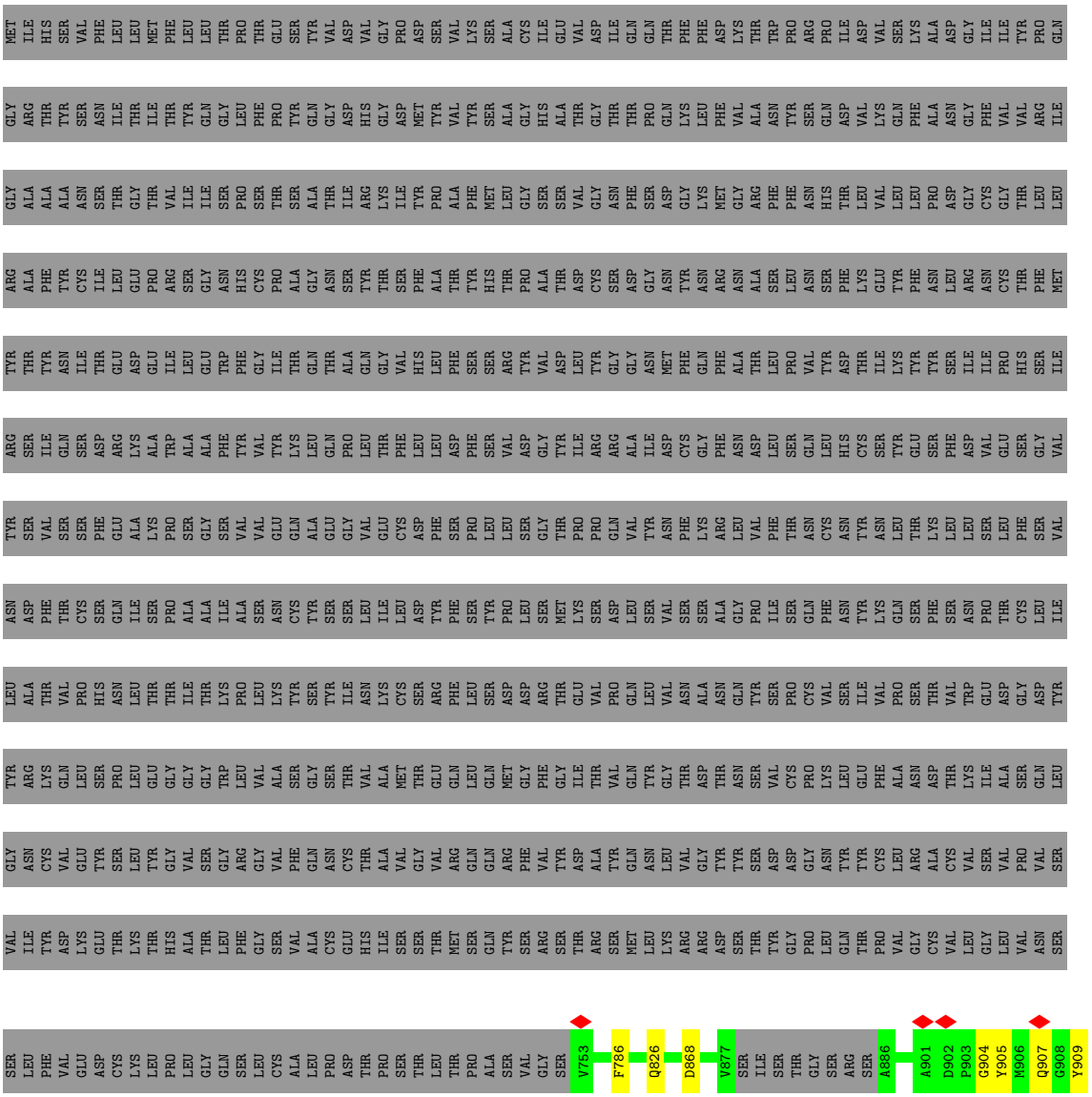
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	B	1	84	48	6	30	0
5	B	1	84	48	6	30	0
5	B	1	84	48	6	30	0
5	E	1	14	8	1	5	0
5	F	1	84	48	6	30	0
5	F	1	84	48	6	30	0
5	F	1	84	48	6	30	0
5	F	1	84	48	6	30	0
5	F	1	84	48	6	30	0
5	F	1	84	48	6	30	0
5	I	1	14	8	1	5	0
5	J	1	84	48	6	30	0
5	J	1	84	48	6	30	0
5	J	1	84	48	6	30	0
5	J	1	84	48	6	30	0
5	J	1	84	48	6	30	0
5	J	1	84	48	6	30	0

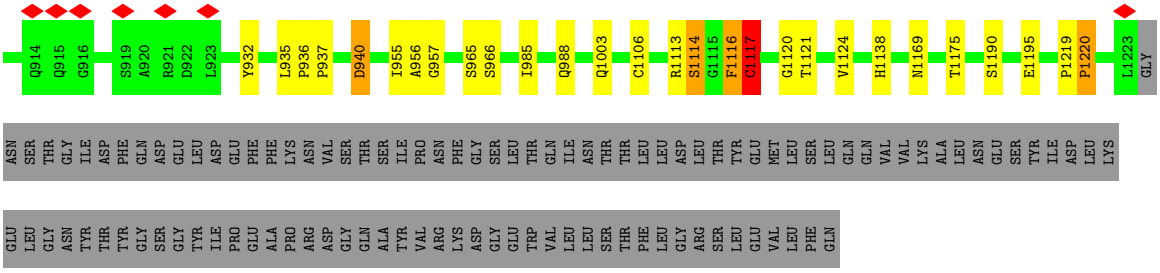
3 Residue-property plots (i)

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

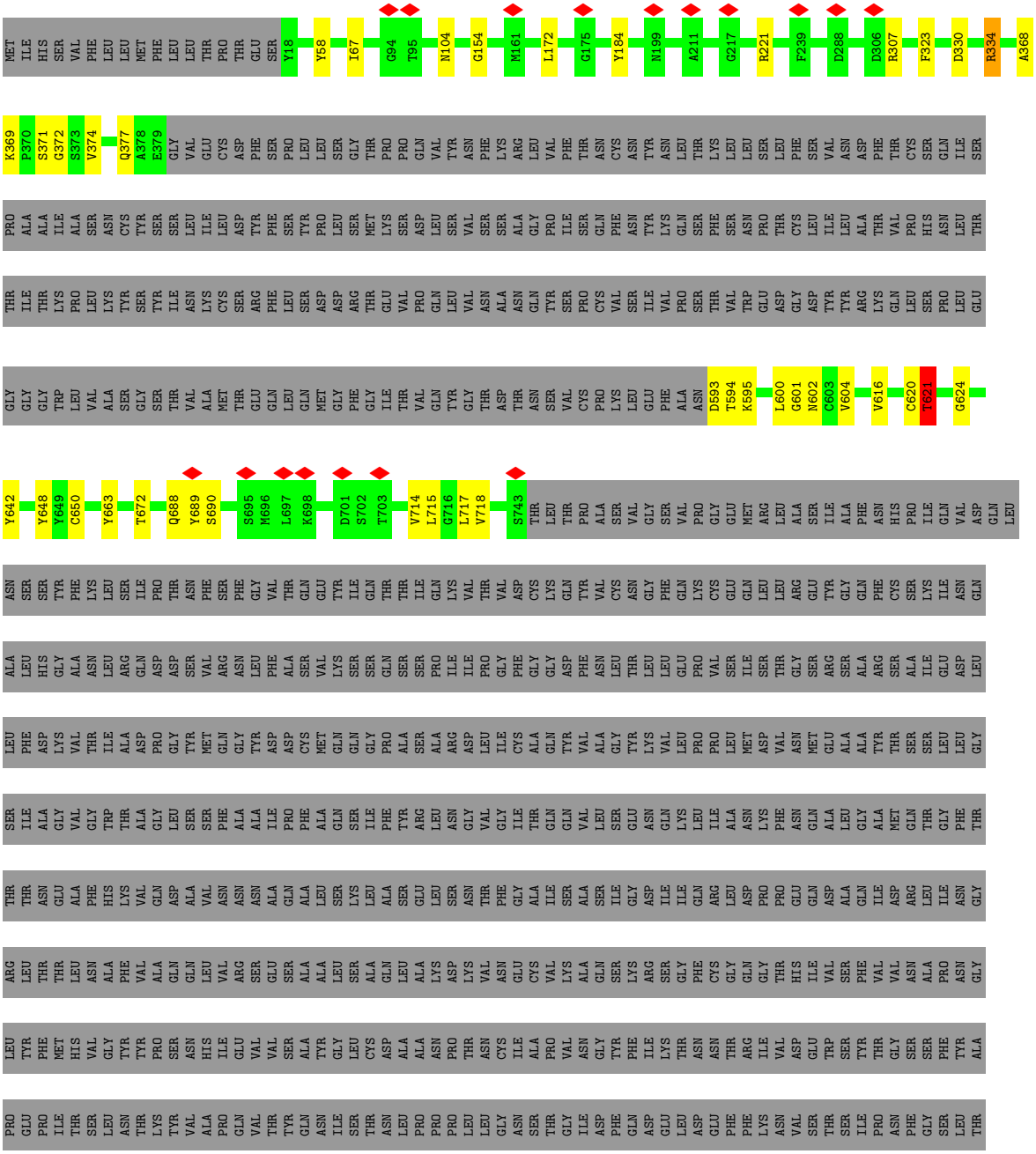
Chain A:

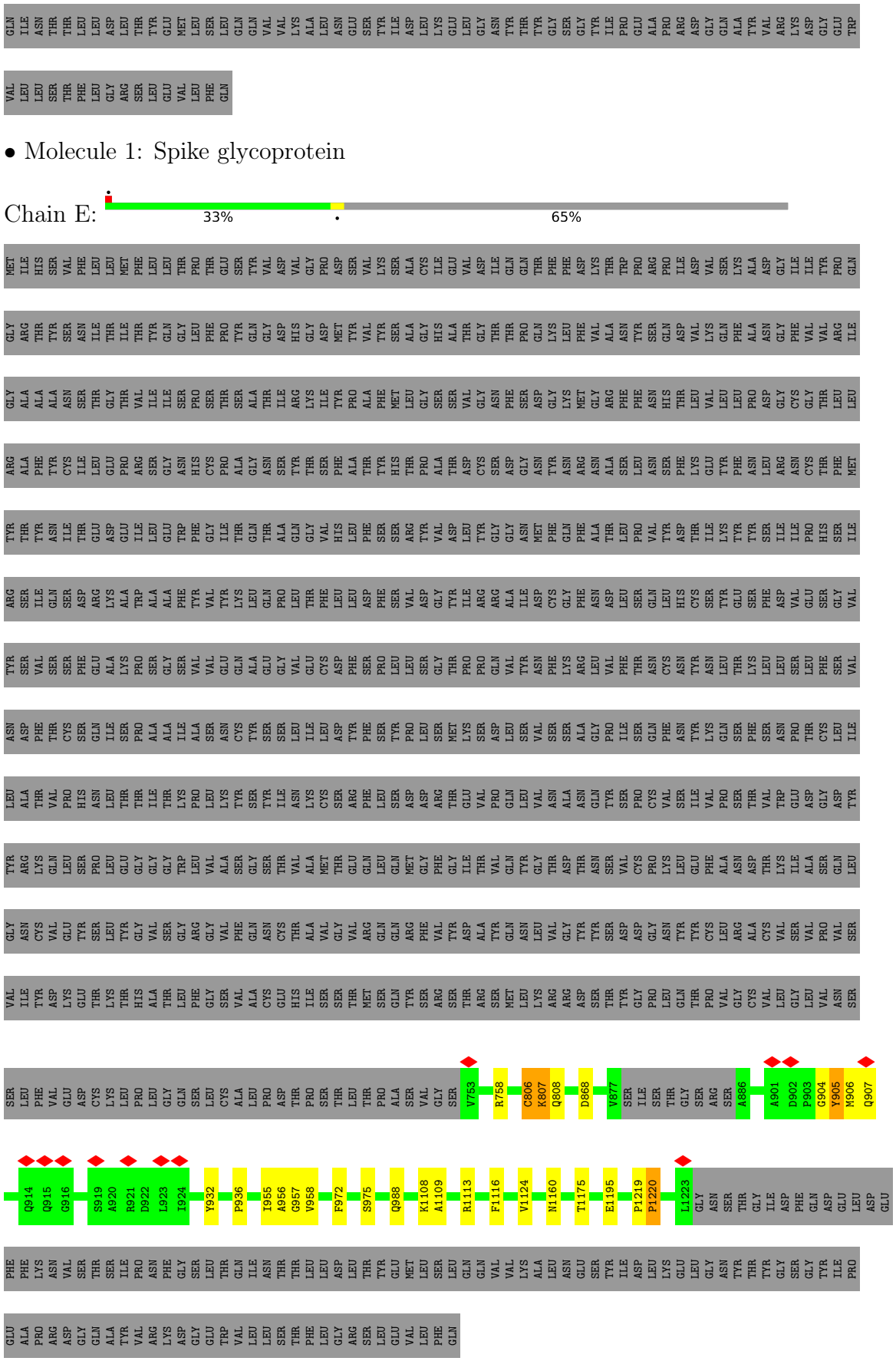




- Molecule 1: Spike glycoprotein

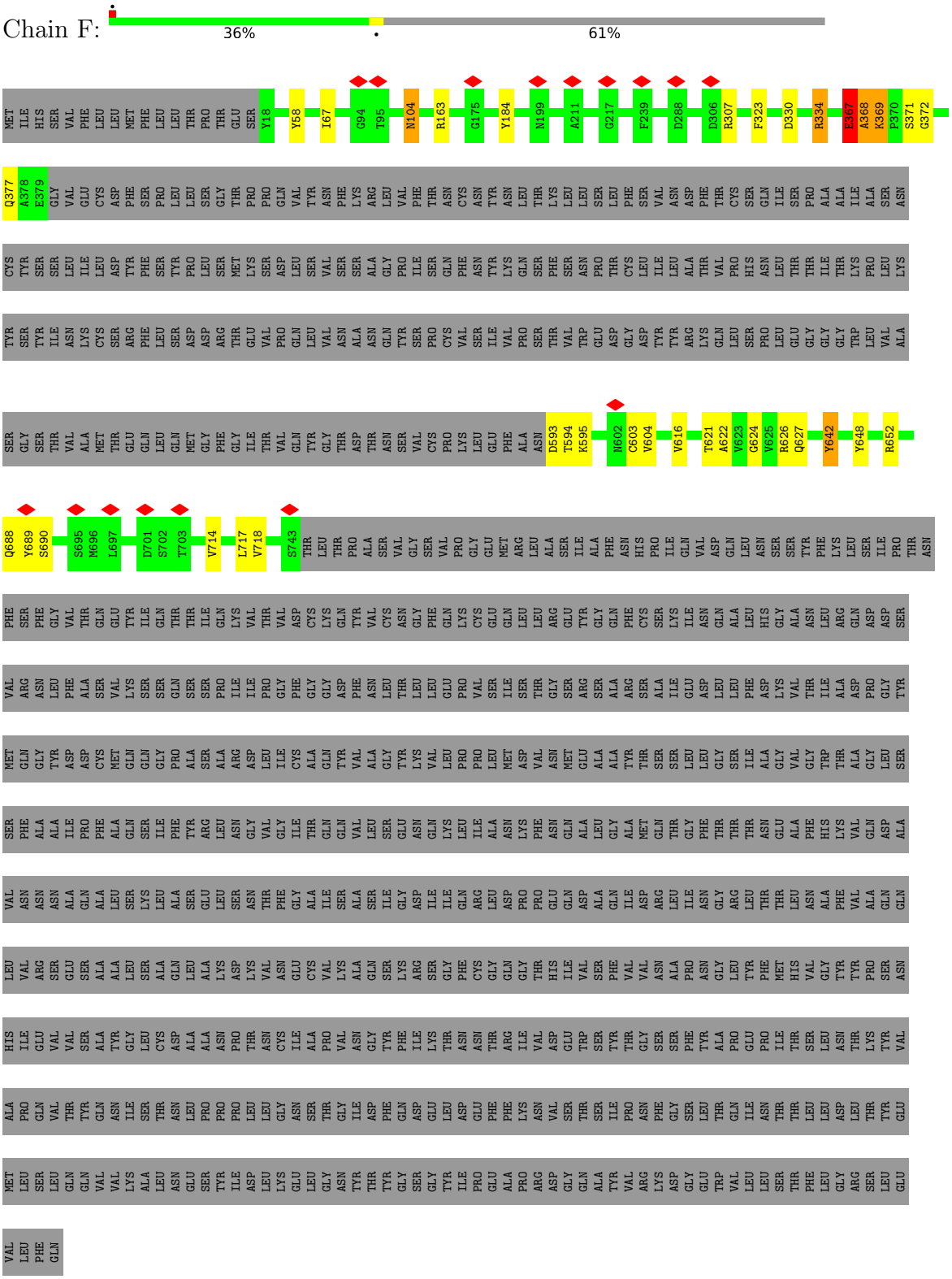
Chain B: 36% 61%




GLN ILE ASN THR THR LEU LEU ASP LEU THR TYR GLU MET LEU SER LEU GLN GLN VAL VAL LYS ALA LEU ASN GLU SER TYR ILE ASP LEU LYS GLU LEU GLY ASN TYR THR TYR GLY SER GLY TYR ILE PRO GLU ALA PRO ARG ASP GLY GLN ALA TYR VAL ARG LYS ASP GLY GLU TRP
VAL LEU LEU SER THR PHE LEU GLY ARG SER SER LEU GLU VAL LEU PHE GLN
• Molecule 1: Spike glycoprotein
Chain E:
33%
65%
MET ILE HIS SER VAL PHE LEU LEU LEU LEU THR PRO THR GLU SER SER TYR VAL ASP VAL GLY PRO ASP SER VAL LYS SER ALA CYS ILE GLU GLU VAL ASP ILE GLN GLN THR PHE PHE ASP LYS THR TRP PRO ARG PRO ILE ASP VAL SER LYS ALA ASP GLY ILE ILE TYR PRO GLN
GLY ARG THR TYR SER ASN ILE THR ILE THR TYR GLN GLY GLY LEU PHE PRO TYR GLN GLY ASP HIS GLY ASP MET TYR VAL TYR SER ALA GLY HIS ALA THR GLY THR THR PRO GLN LYS LEU PHE VAL ALA ASN TYR SER GLN ASP VAL LYS GLN PHE ALA ASN GLY PHE VAL VAL ARG ILE
GLY ALA ALA ASN SER THR GLY THR VAL ILE ILE SER PRO SER THR SER ALA THR ILE ARG LYS ILE TYR PRO ALA PHE MET LEU GLY SER SER VAL GLY ASN PHE SER ASP GLY LYS MET GLY ARG PHE PHE ASN HIS THR LEU VAL LEU LEU PRO ASP GLY CYS GLY THR LEU LEU
ARG ALA PHE TYR CYS ILE LEU GLU PRO ARG SER GLY ASN HIS CYS PRO ALA GLY ASN SER TYR THR SER PHE ALA THR TYR HIS THR PRO ALA THR ASP CYS SER ASP GLY ASN TYR ASN ARG ASN ALA SER LEU ASN SER PHE LYS GLU TYR PHE ASN LEU ARG ASN CYS THR PHE MET
TYR THR TYR ASN ILE THR GLU ASP GLU ILE LEU GLU TRP PHE GLY ILE THR GLN THR ALA GLN GLY VAL HIS LEU PHE SER SER ARG TYR VAL ASP LEU TYR GLY GLY GLY ASN MET PHE GLN PHE ALA THR LEU PRO VAL TYR ASP THR ILE LYS TYR TYR SER ILE ILE PRO HIS SER ILE
ARG SER ILE GLN SER ASP ARG LYS ALA TRP ALA ALA PHE TYR VAL TYR LYS LEU GLN PRO LEU THR PHE LEU LEU ASP PHE SER VAL ASP GLY TYR ILE ARG ARG ALA ILE ASP CYS GLY PHE ASN ASP LEU SER GLN LEU HIS CYS SER TYR GLU SER PHE ASP VAL GLU SER GLY VAL
TYR SER VAL SER SER PHE GLU ALA LYS PRO SER GLY SER VAL VAL GLU GLN ALA GLU GLY VAL GLU CYS ASP PHE SER PRO LEU LEU SER GLY THR PRO PRO GLN VAL TYR ASN PHE LYS ARG LEU VAL PHE THR ASN CYS ASN TYR ASN LEU THR LYS LEU LEU SER LEU PHE SER VAL
ASN ASP PHE THR CYS SER GLN ILE SER PRO ALA ALA ILE ALA SER ASN CYS TYR SER SER LEU ILE LEU ASP TYR PHE SER TYR PRO LEU SER MET LYS SER ASP LEU SER VAL SER SER ALA GLY PRO ILE SER GLN PHE ASN TYR LYS GLN SER PHE SER ASN PRO THR CYS LEU ILE
LEU ALA THR VAL PRO HIS ASN LEU THR THR ILE THR LYS PRO LEU LYS TYR SER TYR SER ILE ASN LYS CYS SER ARG PHE LEU SER ASP ASP ARG THR GLU VAL PRO GLN LEU VAL ASN ALA ASN GLN TYR SER PRO CYS VAL SER ILE ILE VAL PRO SER THR VAL TRP GLU ASP GLY ASP TYR
TYR ARG LYS GLN LEU SER PRO LEU GLU GLN GLY TRP TRP LEU VAL ALA SER GLY SER THR VAL ALA ALA MET THR GLU GLN LEU GLN MET GLY PHE GLY ILE THR VAL GLN TYR GLY THR ASP THR ASN SER VAL CYS PRO LYS LEU GLU PHE ALA ASN ASP THR LYS ILE ALA SER GLN LEU
GLY ASN CYS VAL GLU TYR SER LEU TYR GLY SER GLY ARG GLY VAL PHE GLN ASN CYS THR ALA VAL GLY VAL ARG GLN GLN ARG PHE VAL TYR ASP ALA TYR GLN ASN LEU VAL GLY TYR TYR SER ASP ASP GLY ASN TYR TYR CYS LEU ARG ALA CYS VAL LEU GLY LEU VAL SER VAL PRO VAL SER
VAL ILE TYR ASP LYS GLU THR LYS THR HIS ILE ALA THR LEU PHE GLY SER VAL ALA CYS GLU HIS ILE SER SER THR MET SER GLN SER ARG SER THR ARG SER MET LEU LYS ARG ARG ASP SER THR TYR GLY PRO LEU GLN THR PRO VAL GLY CYS VAL LEU ARG SER ILE ILE ALA ASN GLN GLU
SER LEU PHE VAL GLU ASP CYS LYS LEU PRO LEU GLY GLN SER LEU CYS ALA LEU PRO ASP THR PRO SER THR LEU THR PRO ALA SER VAL GLY SER V753 R758 C806 K807 Q808 D868 V877 SER ILE SER THR GLY SER ARG SER A886 A901 D902 P903 G904 Y905 M906 Q907
Q914 Q915 Q916 S919 A920 R921 D922 L923 I924 Y932 P936 I955 A956 G957 V958 F972 S975 Q988 K1108 A1109 R1113 F1116 V1124 N1160 T1175 E1195 P1219 P1220 L1223 GLY ASN SER THR GLY ILE ASP PHE GLN ASP GLU LEU ASP GLU
PHE LYS ASN VAL SER THR SER ILE PRO ASN PHE GLY SER LEU THR GLN ILE ASN THR THR LEU LEU ASP LEU THR TYR GLU MET LEU SER LEU GLN GLN VAL VAL LYS ALA LEU ASN GLU SER TYR ILE ASP LEU LYS GLU LEU GLY ASN TYR THR TYR GLY GLY SER GLY TYR ILE PRO
GLU ALA PRO ARG ASP GLY GLN ALA TYR VAL ARG LYS ASP GLY GLU TRP VAL LEU LEU SER THR PHE LEU GLY ARG SER LEU GLU VAL LEU PHE GLN

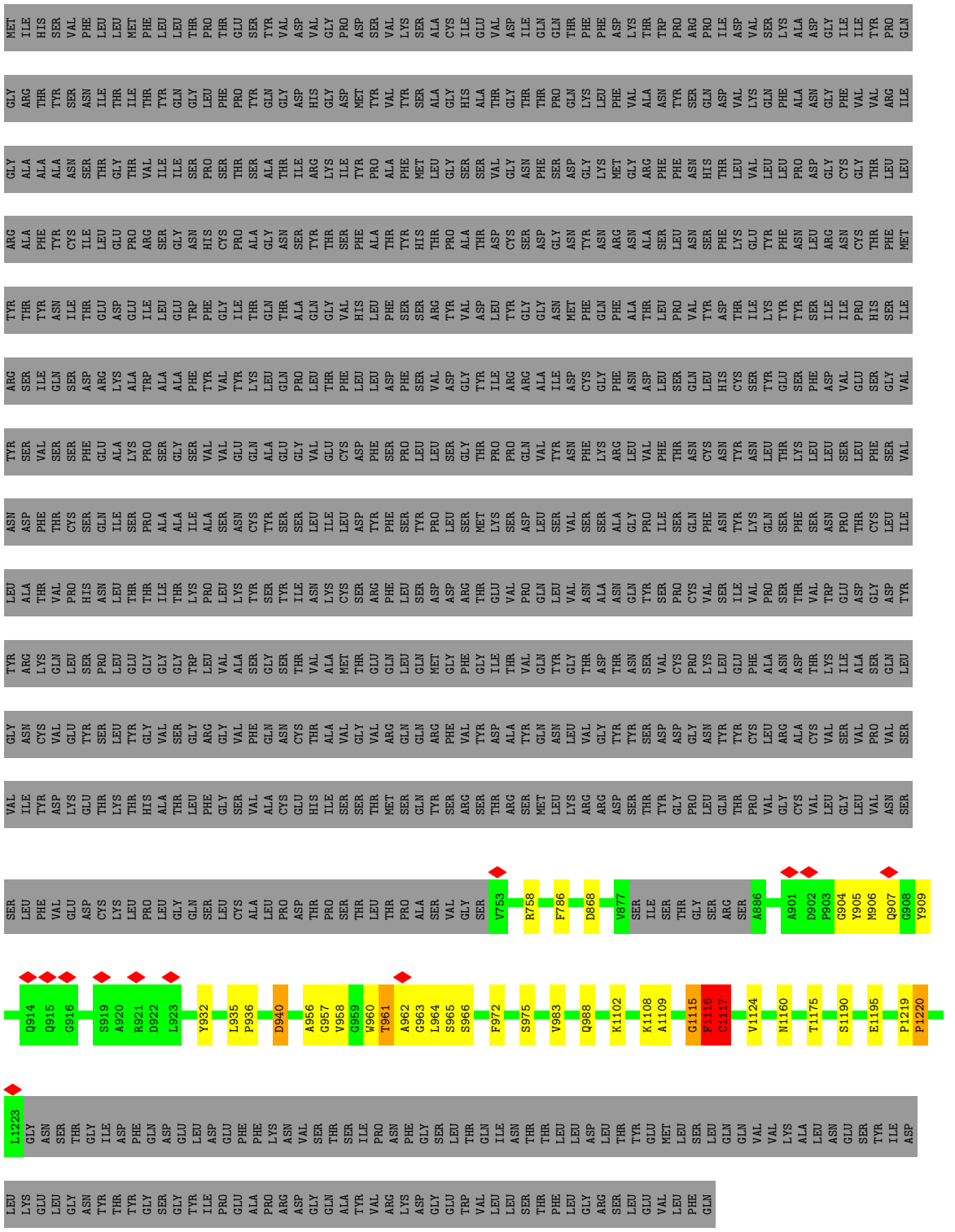
- Molecule 1: Spike glycoprotein

Chain F:



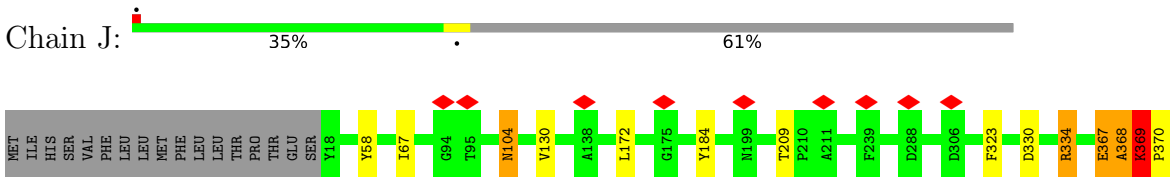
- Molecule 1: Spike glycoprotein

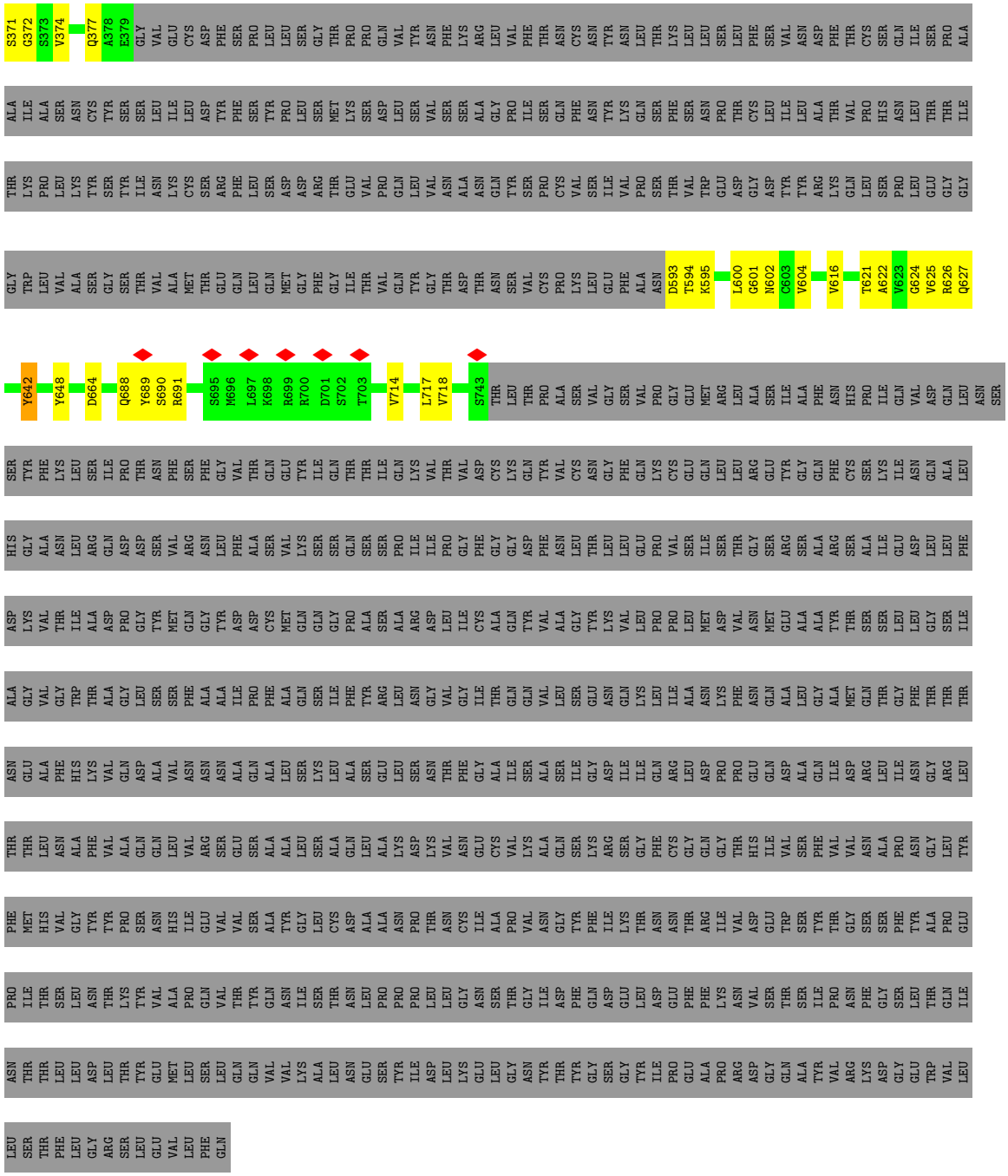
Chain I:



• Molecule 1: Spike glycoprotein

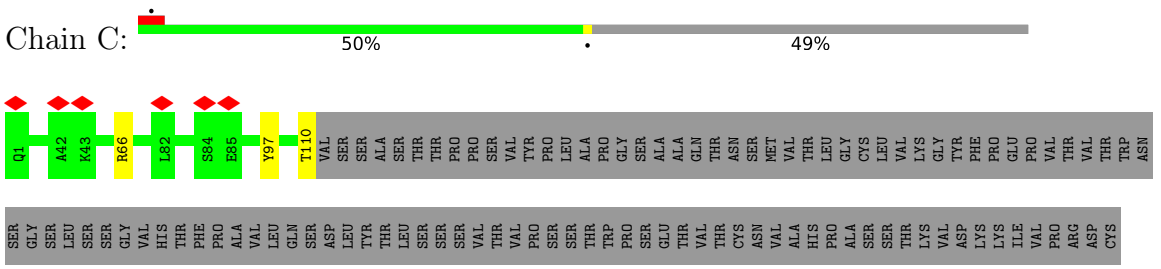
Chain J:





• Molecule 2: G4 VH

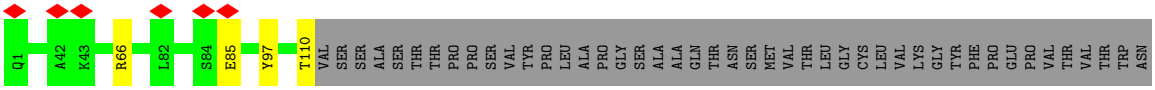
Chain C:



GLY LYS GLY LEU GLU VAL LEU PHE GLN

- Molecule 2: G4 VH

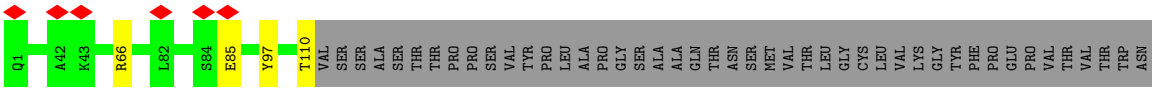
Chain G:



GLY LYS GLY LEU GLU VAL LEU PHE GLN

- Molecule 2: G4 VH

Chain K:



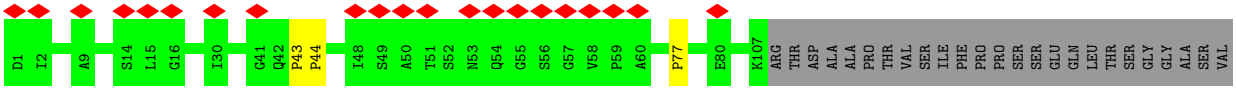
GLY LYS GLY LEU GLU VAL LEU PHE GLN

- Molecule 3: G4 VL

Chain D:

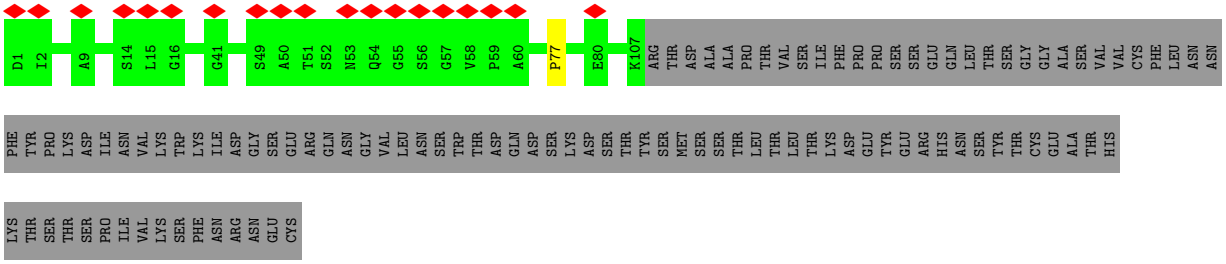
- Molecule 3: G4 VL

Chain H:



• Molecule 3: G4 VL

Chain L:



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

Chain M:

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

Chain N:

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

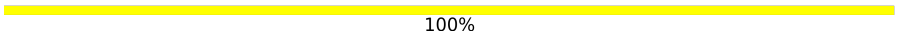
Chain O:

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

Chain P:

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

Chain Q:



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

Chain R:

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

Chain S:

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

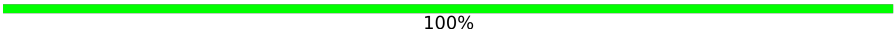
Chain T:

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

Chain U:

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

Chain V:



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

Chain W:

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

Chain X: 50% 50%

NAG1 NAG2

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

Chain Y: 100%

NAG1 NAG2

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

Chain Z: 100%

NAG1 NAG2

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

Chain a: 100%

NAG1 NAG2

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

Chain b: 100%

NAG1 NAG2

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

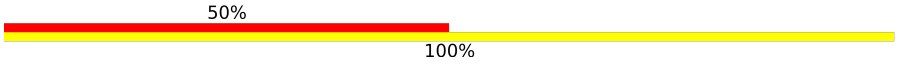
Chain c: 100%

NAG1 NAG2

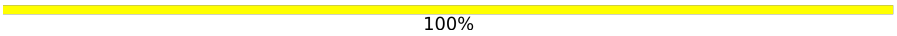
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d: 50% 50%

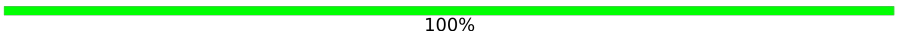
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e: 

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

Chain f: 

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

Chain g: 

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	37180	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 ($e^-/Å^2$)	1.89	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.124	Depositor
Minimum map value	-0.059	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	310.08, 310.08, 310.08	wwPDB
Map dimensions	304, 304, 304	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.02, 1.02, 1.02	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	0.75	0/3618	0.84	6/4921 (0.1%)
1	B	0.72	0/4112	0.90	9/5590 (0.2%)
1	E	0.75	0/3618	0.81	2/4921 (0.0%)
1	F	0.71	0/4112	0.90	10/5590 (0.2%)
1	I	0.76	0/3618	0.84	6/4921 (0.1%)
1	J	0.72	0/4112	0.89	8/5590 (0.1%)
2	C	0.72	0/972	0.88	2/1317 (0.2%)
2	G	0.71	0/972	0.87	2/1317 (0.2%)
2	K	0.71	0/972	0.87	2/1317 (0.2%)
3	D	0.73	0/852	0.88	1/1153 (0.1%)
3	H	0.74	0/852	0.87	0/1153
3	L	0.74	0/852	0.86	0/1153
All	All	0.73	0/28662	0.87	48/38943 (0.1%)

There are no bond length outliers.

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	642	TYR	CB-CG-CD1	-8.74	115.75	121.00
1	B	642	TYR	CB-CG-CD1	-8.61	115.83	121.00
1	J	334	ARG	NE-CZ-NH2	-8.57	116.02	120.30
1	F	334	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	B	334	ARG	NE-CZ-NH2	-8.18	116.21	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3545	0	3467	38	0
1	B	4010	0	3808	38	0
1	E	3545	0	3467	39	0
1	F	4010	0	3808	42	0
1	I	3545	0	3467	45	0
1	J	4010	0	3810	67	0
2	C	948	0	904	1	0
2	G	948	0	904	2	0
2	K	948	0	904	2	0
3	D	835	0	816	1	0
3	H	835	0	816	1	0
3	L	835	0	816	0	0
4	M	28	0	25	1	0
4	N	28	0	25	0	0
4	O	28	0	25	0	0
4	P	28	0	25	0	0
4	Q	28	0	25	0	0
4	R	28	0	25	1	0
4	S	28	0	25	0	0
4	T	28	0	25	0	0
4	U	28	0	25	0	0
4	V	28	0	25	0	0
4	W	28	0	25	0	0
4	X	28	0	25	0	0
4	Y	28	0	24	0	0
4	Z	28	0	25	0	0
4	a	28	0	25	0	0
4	b	28	0	25	0	0
4	c	28	0	25	0	0
4	d	28	0	25	0	0
4	e	28	0	25	0	0
4	f	28	0	25	0	0
4	g	28	0	25	0	0
5	A	14	0	13	0	0
5	B	84	0	78	1	0
5	E	14	0	13	0	0
5	F	84	0	78	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	14	0	13	0	0
5	J	84	0	75	0	0
All	All	28896	0	27781	259	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 259 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:905:TYR:OH	1:A:936:PRO:CA	1.68	1.41
1:E:905:TYR:OH	1:E:936:PRO:CA	1.70	1.39
1:I:905:TYR:OH	1:I:936:PRO:HA	1.26	1.34
1:I:905:TYR:OH	1:I:936:PRO:CA	1.75	1.32
1:A:905:TYR:OH	1:A:936:PRO:HA	1.13	1.24

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	459/1329 (34%)	441 (96%)	14 (3%)	4 (1%)	17	57
1	B	509/1329 (38%)	478 (94%)	27 (5%)	4 (1%)	19	59
1	E	459/1329 (34%)	435 (95%)	20 (4%)	4 (1%)	17	57
1	F	509/1329 (38%)	475 (93%)	29 (6%)	5 (1%)	15	55
1	I	459/1329 (34%)	438 (95%)	14 (3%)	7 (2%)	10	47
1	J	509/1329 (38%)	475 (93%)	30 (6%)	4 (1%)	19	59
2	C	117/233 (50%)	115 (98%)	2 (2%)	0	100	100
2	G	117/233 (50%)	115 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	117/233 (50%)	115 (98%)	2 (2%)	0	100	100
3	D	109/218 (50%)	105 (96%)	3 (3%)	1 (1%)	17	57
3	H	109/218 (50%)	105 (96%)	3 (3%)	1 (1%)	17	57
3	L	109/218 (50%)	105 (96%)	3 (3%)	1 (1%)	17	57
All	All	3582/9327 (38%)	3402 (95%)	149 (4%)	31 (1%)	21	57

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1114	SER
1	A	1117	CYS
1	E	806	CYS
1	E	807	LYS
1	F	367	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	388/1148 (34%)	387 (100%)	1 (0%)	92	97
1	B	442/1148 (38%)	441 (100%)	1 (0%)	93	98
1	E	388/1148 (34%)	388 (100%)	0	100	100
1	F	442/1148 (38%)	440 (100%)	2 (0%)	88	95
1	I	388/1148 (34%)	387 (100%)	1 (0%)	92	97
1	J	442/1148 (38%)	441 (100%)	1 (0%)	93	98
2	C	102/202 (50%)	102 (100%)	0	100	100
2	G	102/202 (50%)	102 (100%)	0	100	100
2	K	102/202 (50%)	102 (100%)	0	100	100
3	D	93/192 (48%)	93 (100%)	0	100	100
3	H	93/192 (48%)	93 (100%)	0	100	100
3	L	93/192 (48%)	93 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3075/8070 (38%)	3069 (100%)	6 (0%)	93 98

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	367	GLU
1	I	1116	PHE
1	J	104	ASN
1	B	621	THR
1	A	1116	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1003	GLN
1	I	1169	ASN

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)

42 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	$\#\|Z\| > 2$
4	NAG	M	1	4,1	14,14,15	0.47	0	17,19,21	0.87	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	M	2	4	14,14,15	0.63	0	17,19,21	0.88	1 (5%)
4	NAG	N	1	4,1	14,14,15	0.80	1 (7%)	17,19,21	0.50	0
4	NAG	N	2	4	14,14,15	0.25	0	17,19,21	0.56	0
4	NAG	O	1	4,1	14,14,15	0.32	0	17,19,21	0.47	0
4	NAG	O	2	4	14,14,15	0.33	0	17,19,21	0.62	1 (5%)
4	NAG	P	1	4,1	14,14,15	0.41	0	17,19,21	0.58	0
4	NAG	P	2	4	14,14,15	0.29	0	17,19,21	0.42	0
4	NAG	Q	1	4,1	14,14,15	0.96	1 (7%)	17,19,21	0.70	0
4	NAG	Q	2	4	14,14,15	0.19	0	17,19,21	0.68	1 (5%)
4	NAG	R	1	4,1	14,14,15	1.36	1 (7%)	17,19,21	1.24	2 (11%)
4	NAG	R	2	4	14,14,15	0.67	1 (7%)	17,19,21	0.48	0
4	NAG	S	1	4,1	14,14,15	1.44	3 (21%)	17,19,21	1.46	2 (11%)
4	NAG	S	2	4	14,14,15	0.59	0	17,19,21	0.70	0
4	NAG	T	1	4,1	14,14,15	0.60	0	17,19,21	0.81	0
4	NAG	T	2	4	14,14,15	0.78	1 (7%)	17,19,21	2.24	3 (17%)
4	NAG	U	1	4,1	14,14,15	0.53	0	17,19,21	1.07	1 (5%)
4	NAG	U	2	4	14,14,15	0.20	0	17,19,21	0.49	0
4	NAG	V	1	4,1	14,14,15	0.46	0	17,19,21	0.68	0
4	NAG	V	2	4	14,14,15	0.27	0	17,19,21	0.51	0
4	NAG	W	1	4,1	14,14,15	0.33	0	17,19,21	0.88	0
4	NAG	W	2	4	14,14,15	0.61	1 (7%)	17,19,21	0.64	1 (5%)
4	NAG	X	1	4,1	14,14,15	0.43	0	17,19,21	1.40	3 (17%)
4	NAG	X	2	4	14,14,15	0.27	0	17,19,21	0.59	0
4	NAG	Y	1	4,1	14,14,15	0.73	1 (7%)	17,19,21	1.04	1 (5%)
4	NAG	Y	2	4	14,14,15	0.63	0	17,19,21	0.94	1 (5%)
4	NAG	Z	1	4,1	14,14,15	0.30	0	17,19,21	0.59	0
4	NAG	Z	2	4	14,14,15	0.37	0	17,19,21	0.53	0
4	NAG	a	1	4,1	14,14,15	0.30	0	17,19,21	0.65	0
4	NAG	a	2	4	14,14,15	0.48	0	17,19,21	0.56	0
4	NAG	b	1	4,1	14,14,15	1.13	1 (7%)	17,19,21	0.67	1 (5%)
4	NAG	b	2	4	14,14,15	0.41	0	17,19,21	0.73	1 (5%)
4	NAG	c	1	4,1	14,14,15	0.21	0	17,19,21	1.12	2 (11%)
4	NAG	c	2	4	14,14,15	0.41	0	17,19,21	1.03	1 (5%)
4	NAG	d	1	4,1	14,14,15	0.57	1 (7%)	17,19,21	0.72	1 (5%)
4	NAG	d	2	4	14,14,15	0.25	0	17,19,21	0.55	0
4	NAG	e	1	4,1	14,14,15	0.81	1 (7%)	17,19,21	1.21	2 (11%)
4	NAG	e	2	4	14,14,15	0.71	0	17,19,21	0.92	1 (5%)
4	NAG	f	1	4,1	14,14,15	0.73	1 (7%)	17,19,21	1.15	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	f	2	4	14,14,15	1.77	2 (14%)	17,19,21	1.35	1 (5%)
4	NAG	g	1	4,1	14,14,15	0.19	0	17,19,21	0.59	0
4	NAG	g	2	4	14,14,15	0.29	0	17,19,21	0.43	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	M	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	NAG	N	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	0/6/23/26	0/1/1/1
4	NAG	O	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	NAG	P	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Q	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	4/6/23/26	0/1/1/1
4	NAG	R	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	R	2	4	-	1/6/23/26	0/1/1/1
4	NAG	S	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	S	2	4	-	3/6/23/26	0/1/1/1
4	NAG	T	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	4/6/23/26	0/1/1/1
4	NAG	U	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	U	2	4	-	2/6/23/26	0/1/1/1
4	NAG	V	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	V	2	4	-	2/6/23/26	0/1/1/1
4	NAG	W	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	W	2	4	-	2/6/23/26	0/1/1/1
4	NAG	X	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	X	2	4	-	3/6/23/26	0/1/1/1
4	NAG	Y	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Z	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	2/6/23/26	0/1/1/1

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	f	2	NAG	O5-C1	5.52	1.52	1.43
4	R	1	NAG	O5-C1	-4.88	1.35	1.43
4	b	1	NAG	O5-C1	-3.90	1.37	1.43
4	S	1	NAG	O5-C1	-3.83	1.37	1.43
4	f	2	NAG	C1-C2	3.37	1.57	1.52

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	T	2	NAG	C2-N2-C7	7.85	134.07	122.90
4	f	2	NAG	C1-O5-C5	5.03	119.01	112.19
4	S	1	NAG	C4-C3-C2	4.36	117.41	111.02
4	X	1	NAG	C1-O5-C5	3.81	117.35	112.19
4	T	2	NAG	C1-C2-N2	3.57	116.58	110.49

There are no chirality outliers.

5 of 83 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	X	1	NAG	O5-C5-C6-O6
4	c	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	O	1	NAG	O5-C5-C6-O6
4	Z	2	NAG	O5-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6

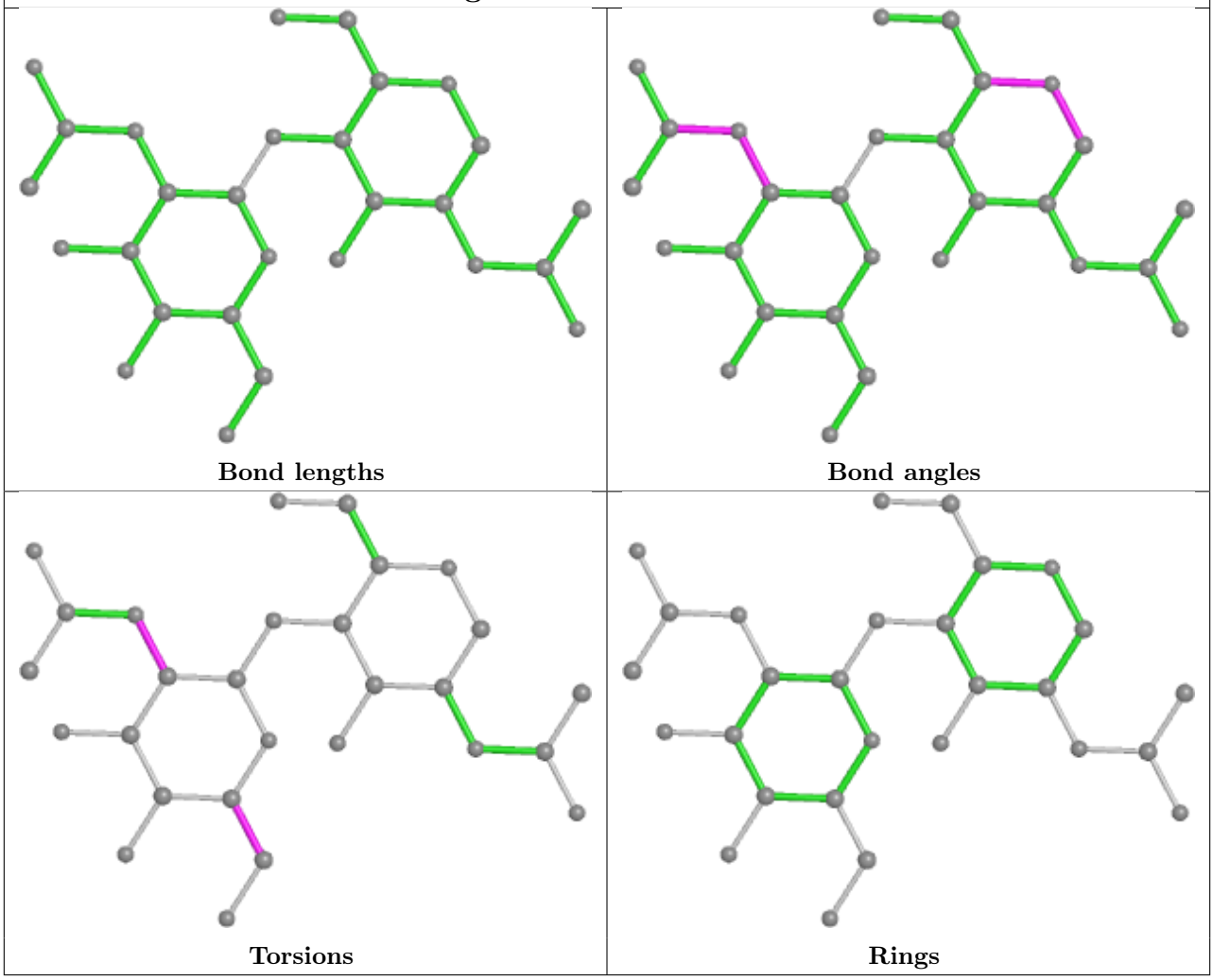
There are no ring outliers.

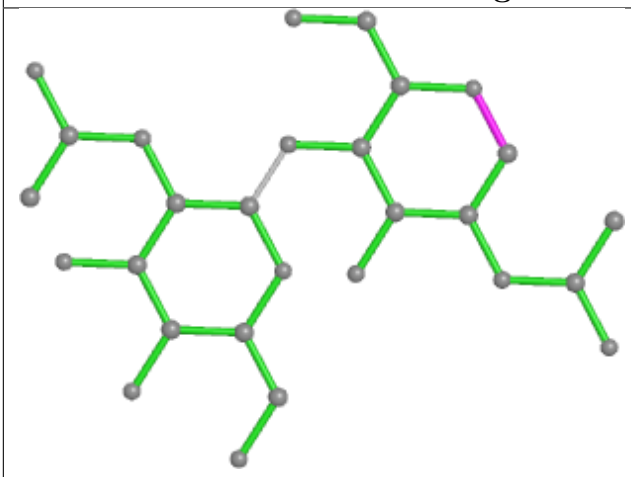
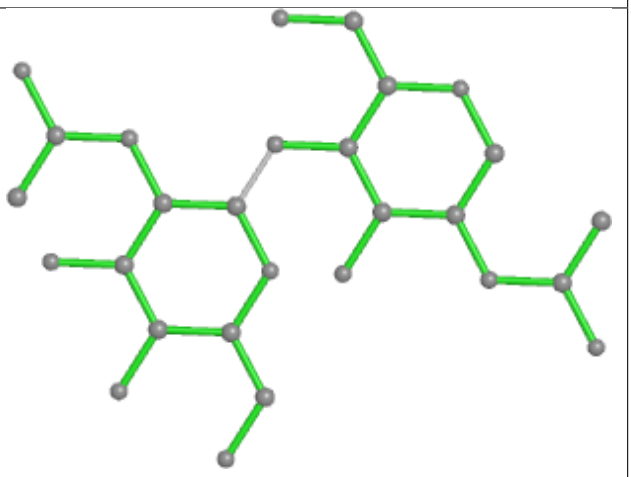
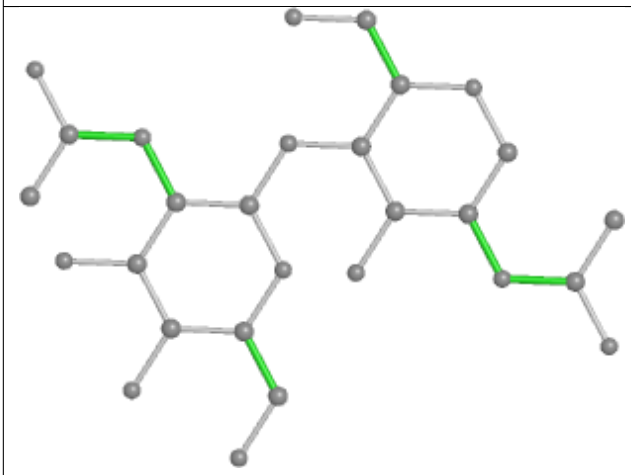
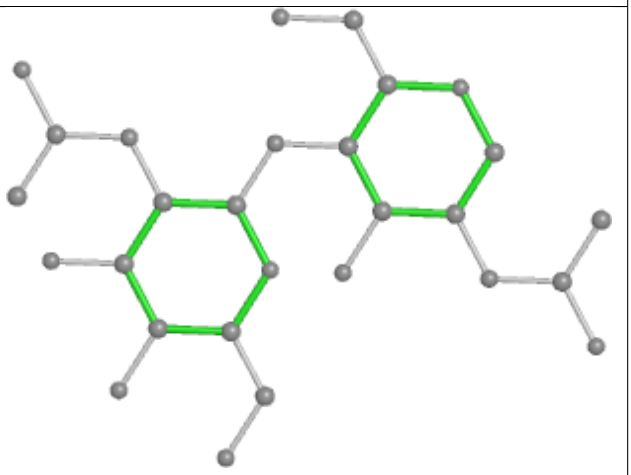
2 monomers are involved in 2 short contacts:

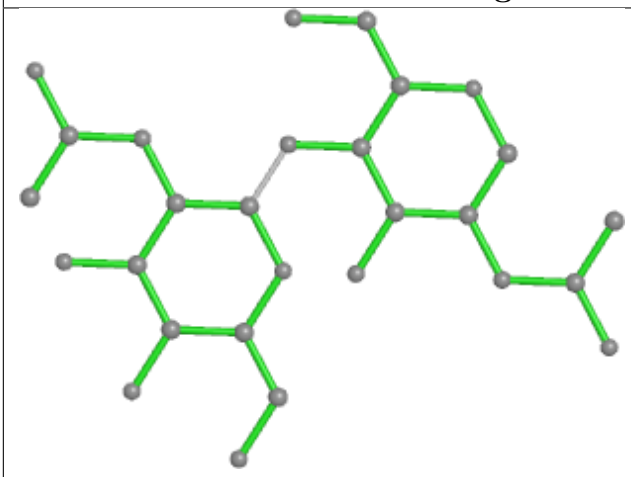
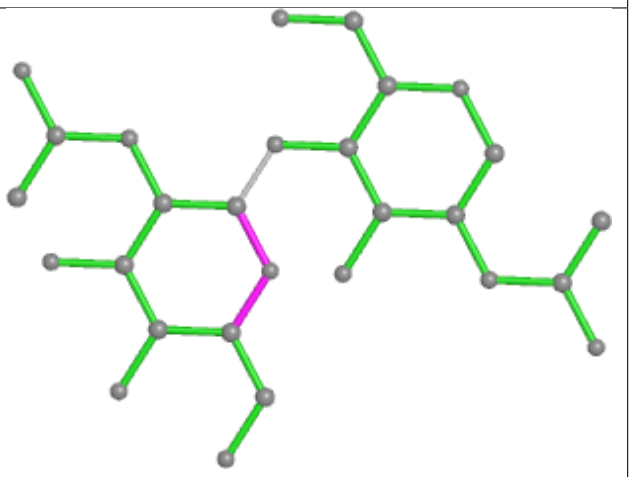
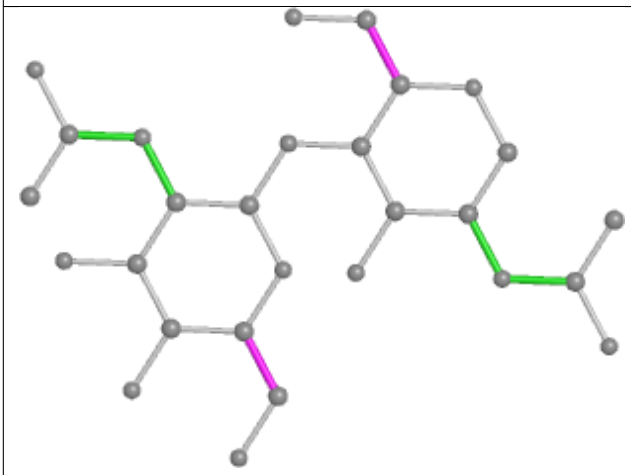
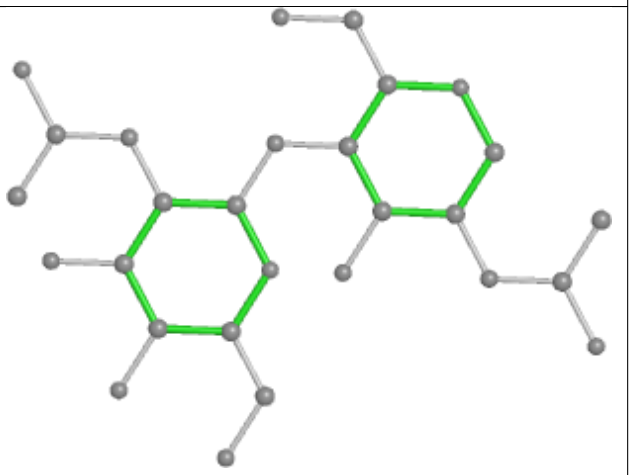
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	R	1	NAG	1	0
4	M	2	NAG	1	0

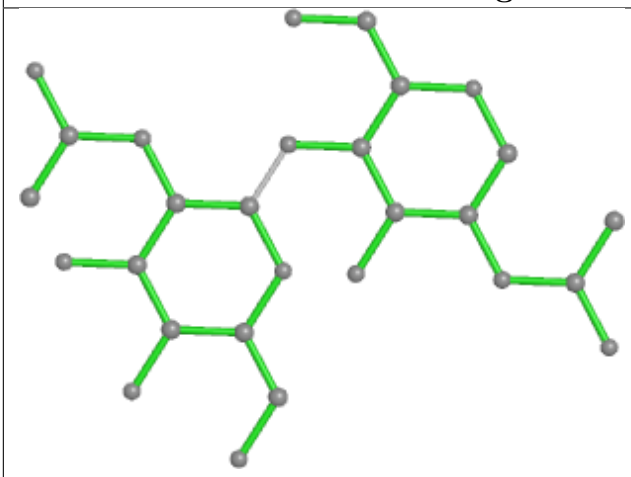
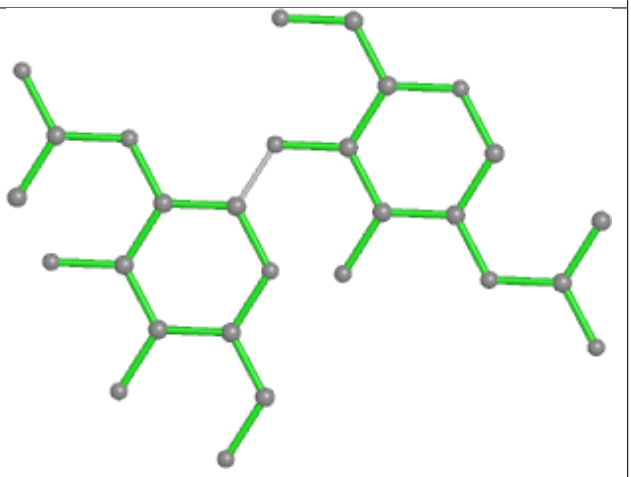
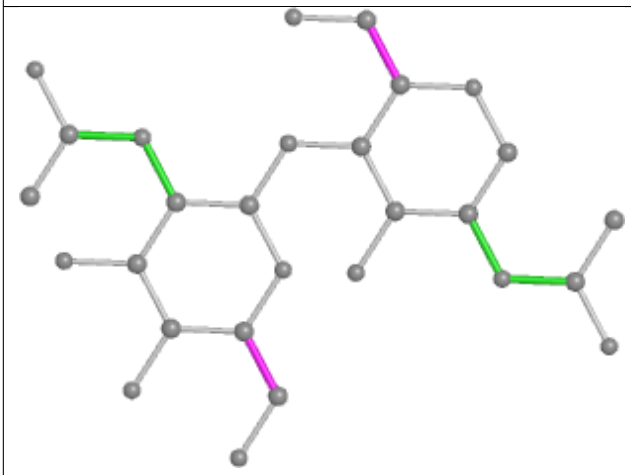
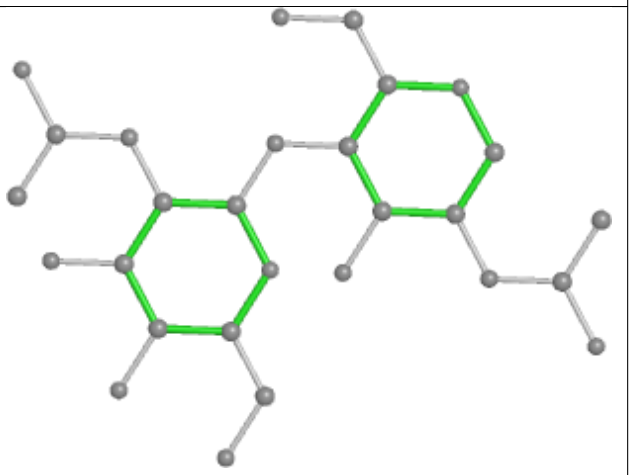
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

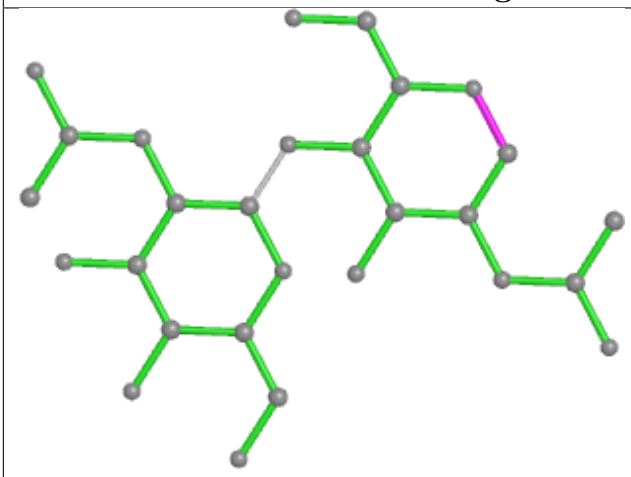
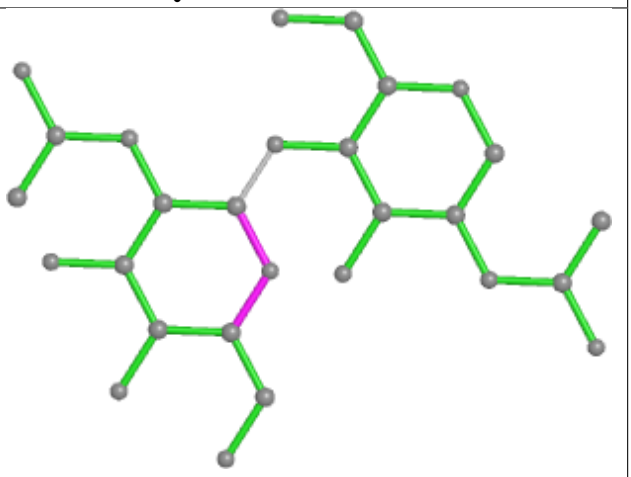
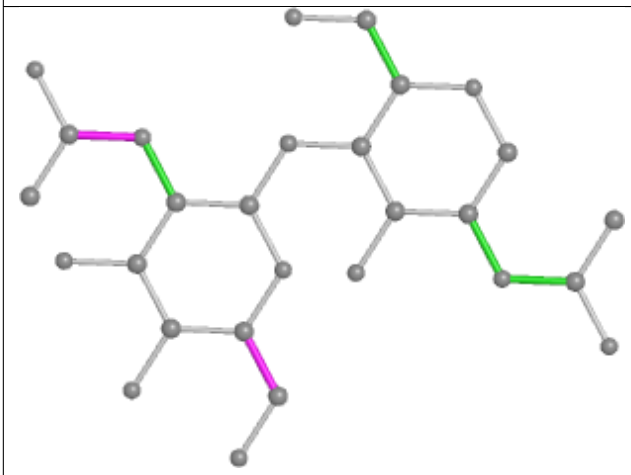
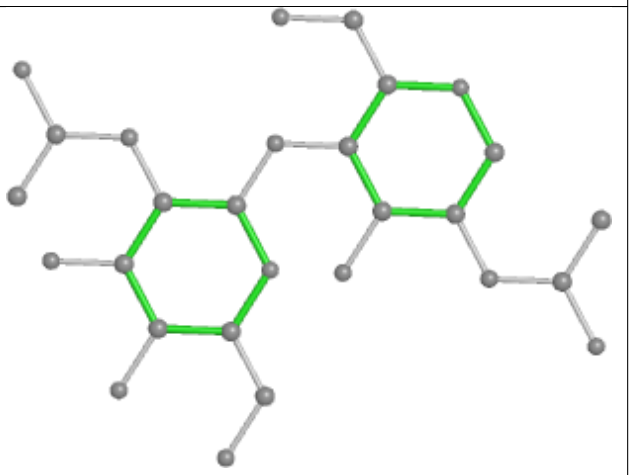
Oligosaccharide Chain M



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

Oligosaccharide Chain Q	
 Bond lengths	 Bond angles
 Torsions	 Rings

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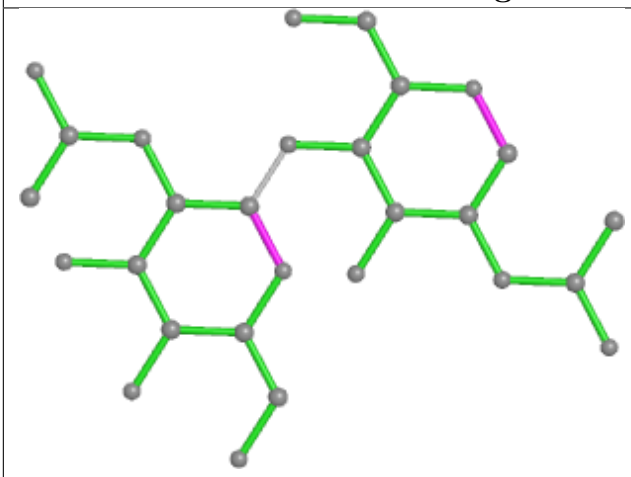
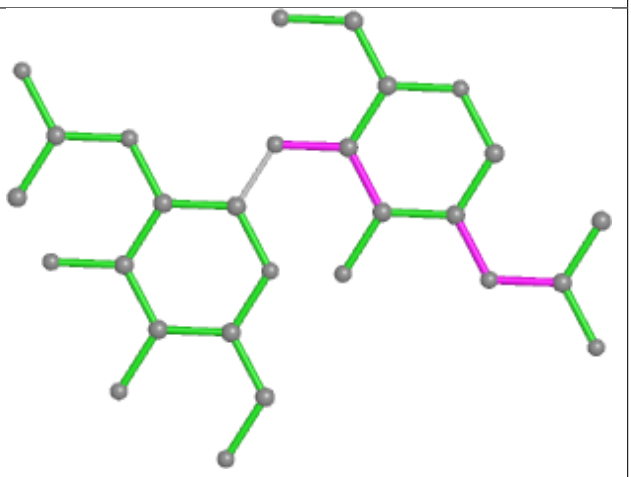
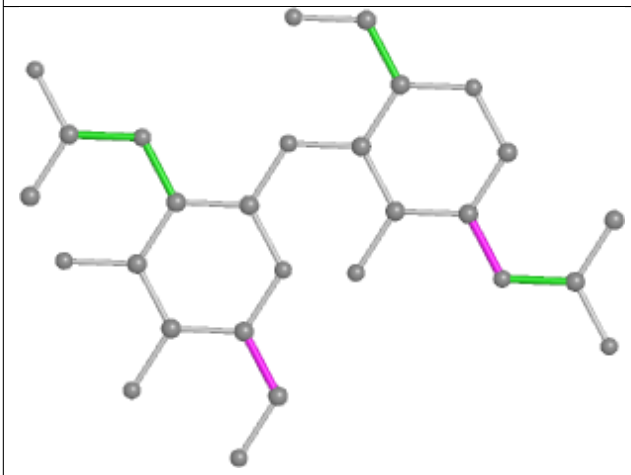
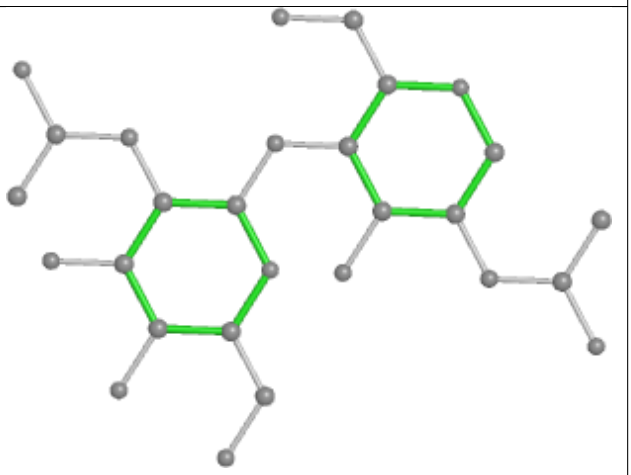
 Bond lengths	 Bond angles
 Torsions	 Rings

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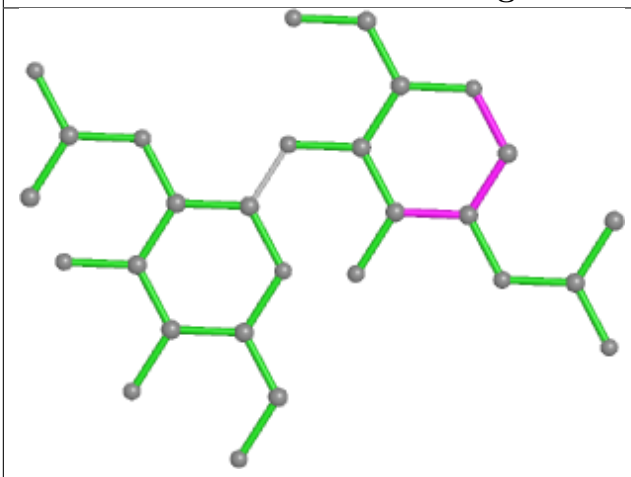
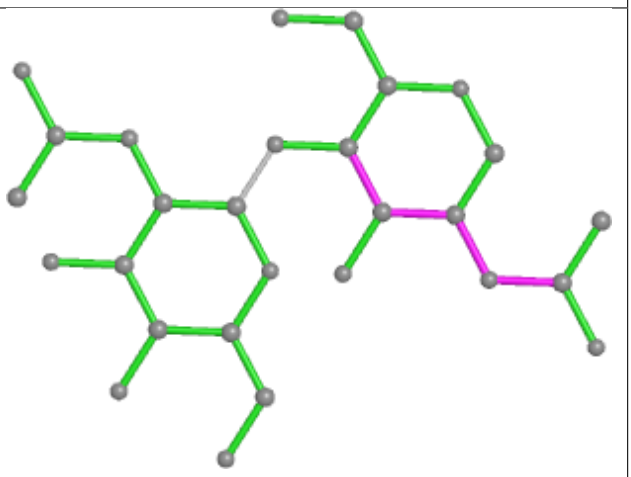


Bond lengths



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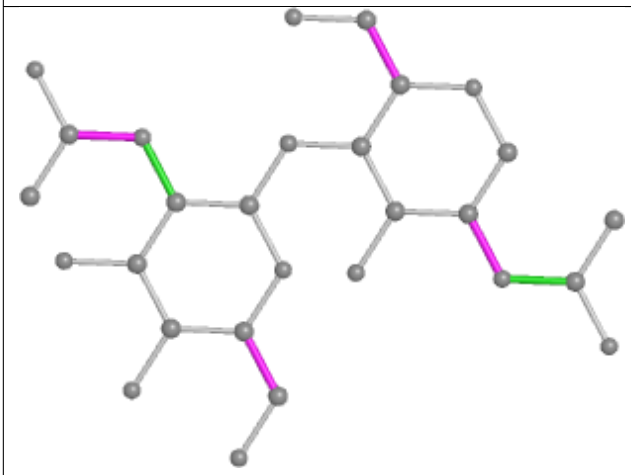

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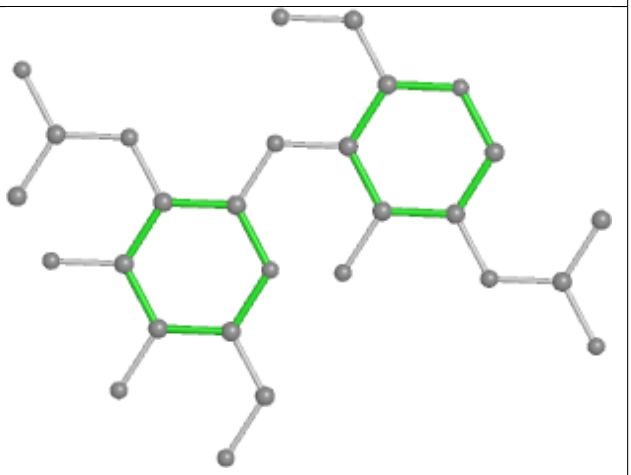
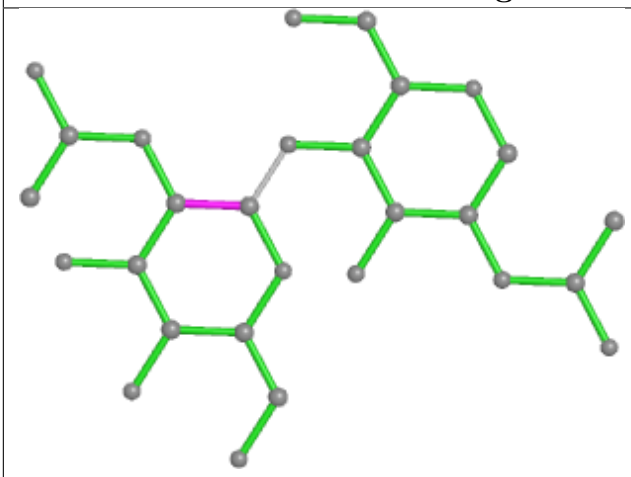
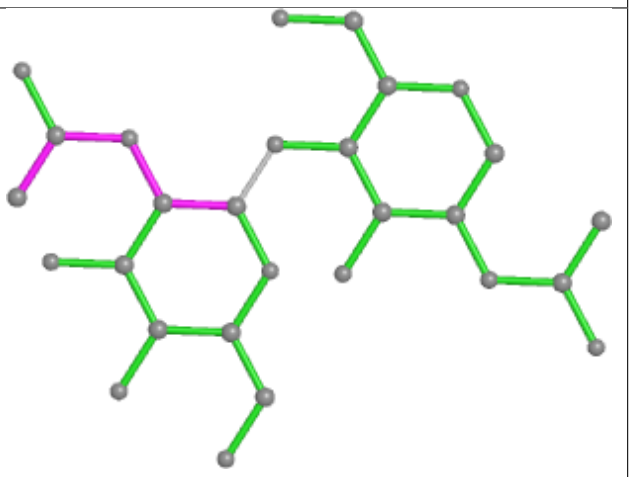
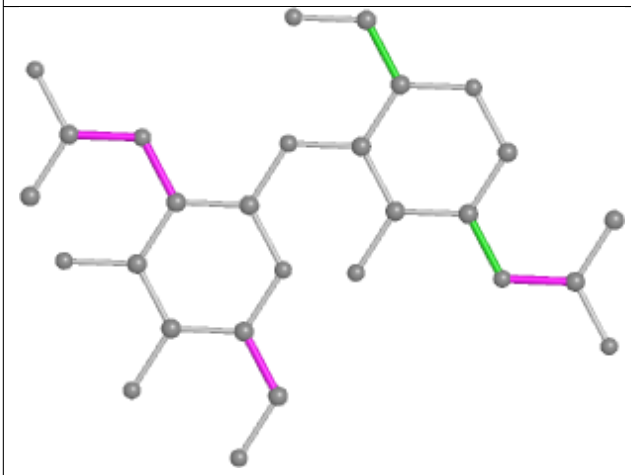
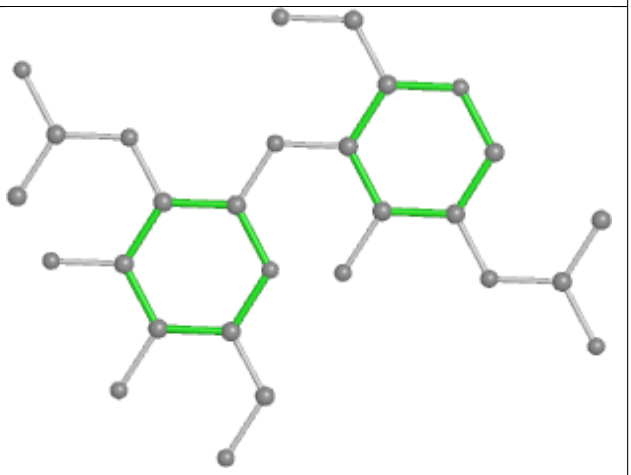
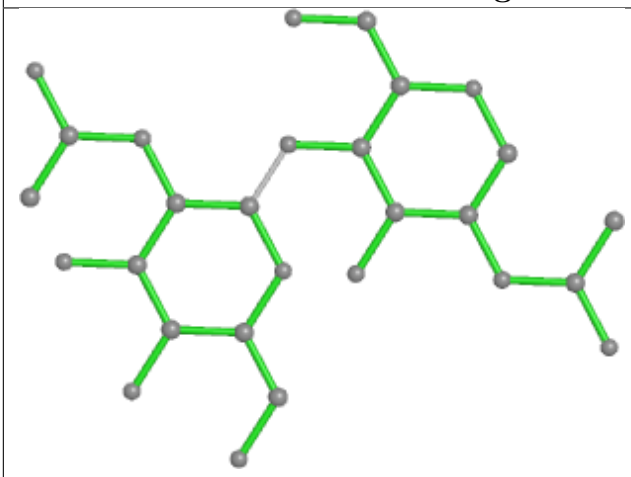


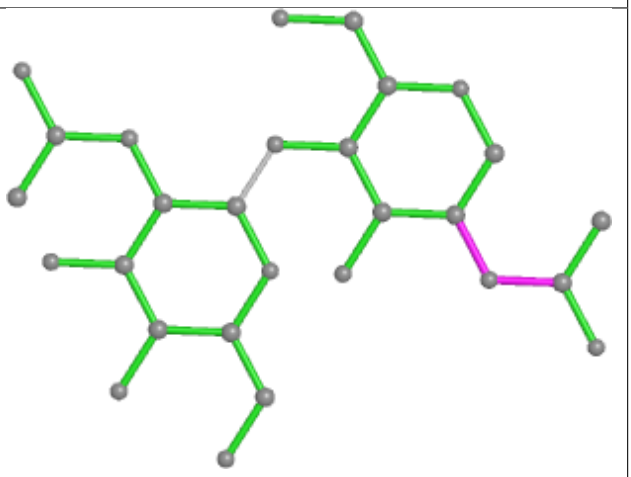
Rings

Oligosaccharide Chain T	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain U



Bond lengths



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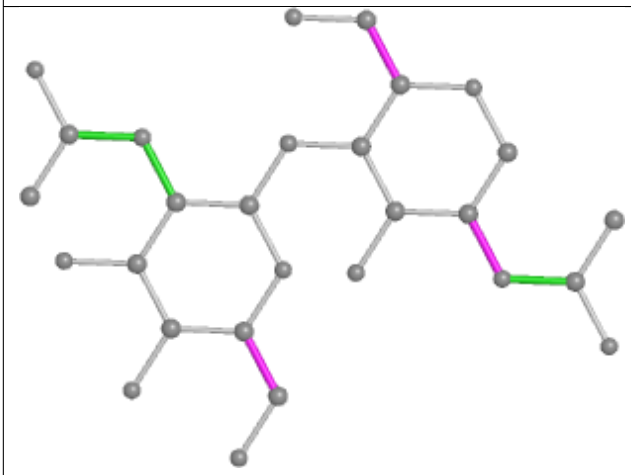

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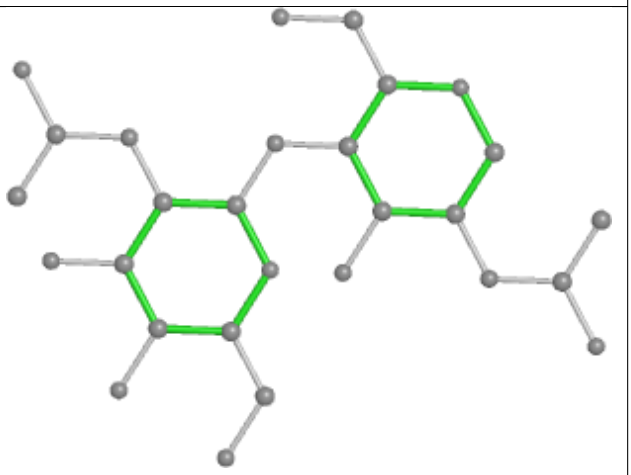
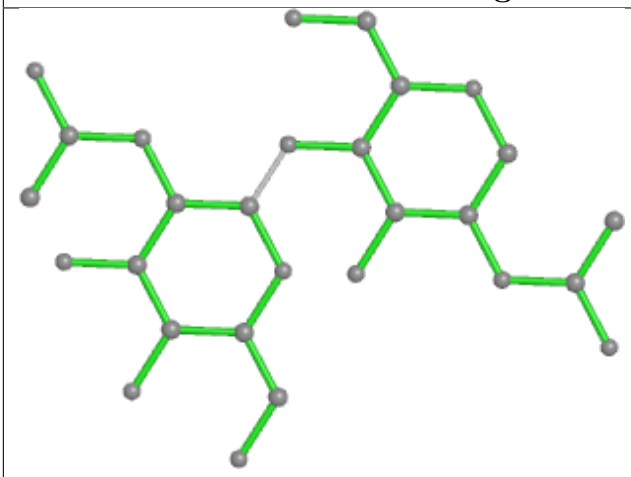
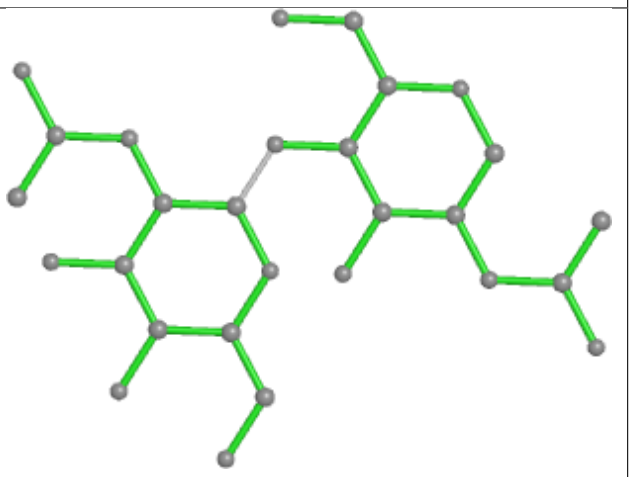
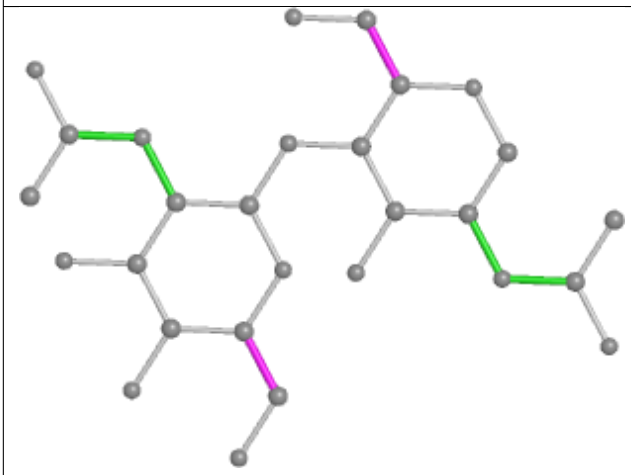
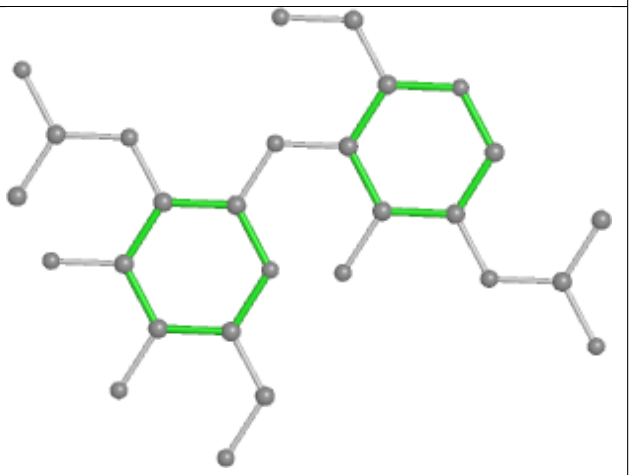


Rings

Oligosaccharide Chain V	
 Bond lengths	 Bond angles
 Torsions	 Rings

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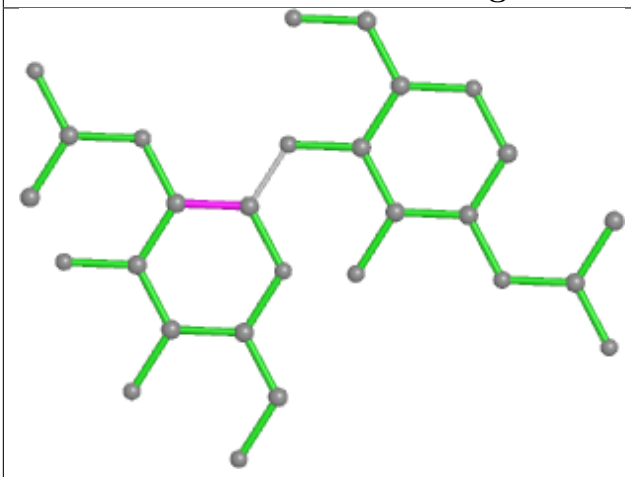
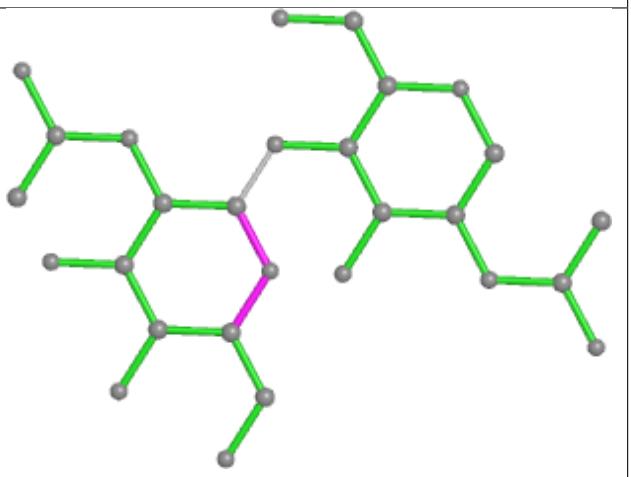
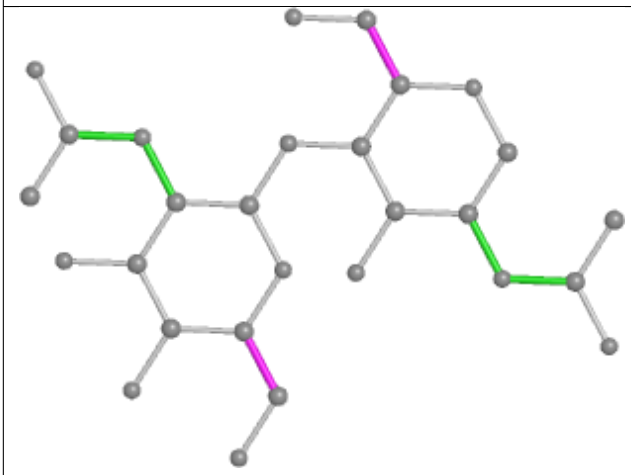
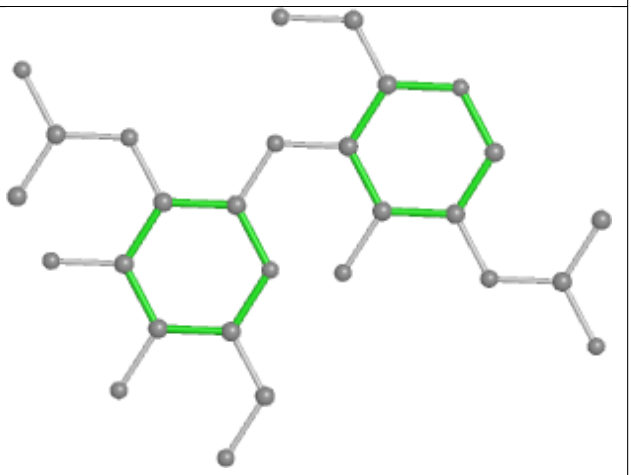
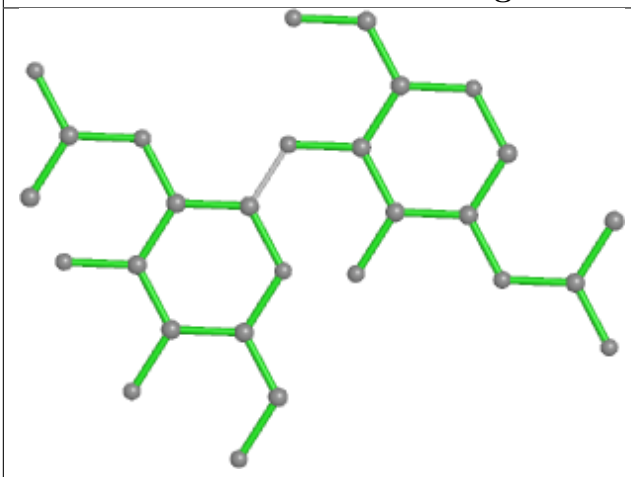
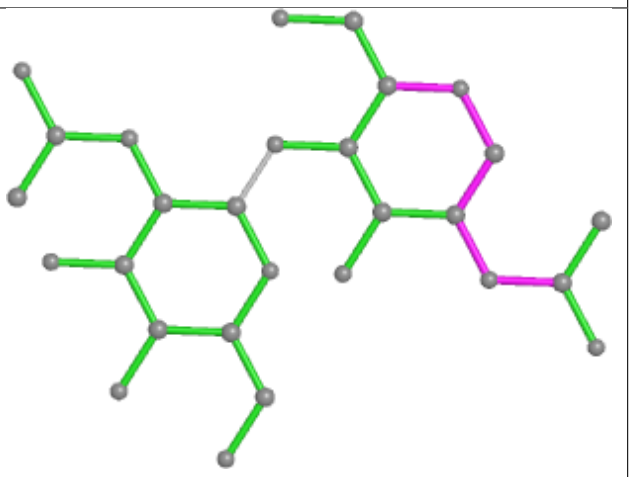
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain X



Bond lengths



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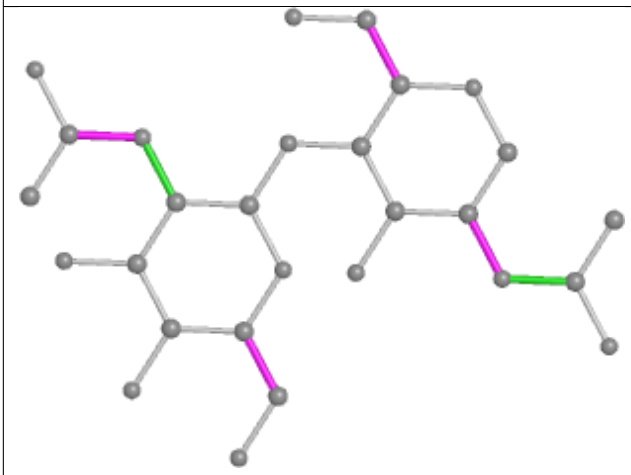

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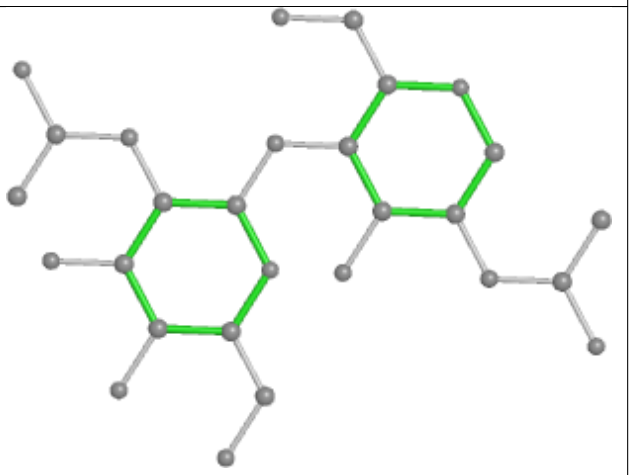
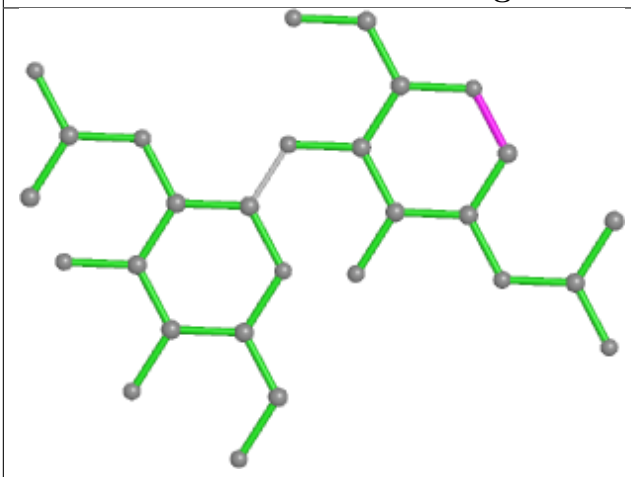


Rings

Oligosaccharide Chain Y



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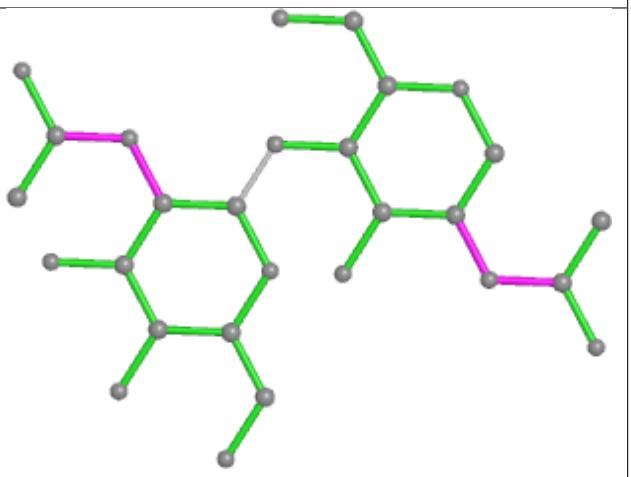

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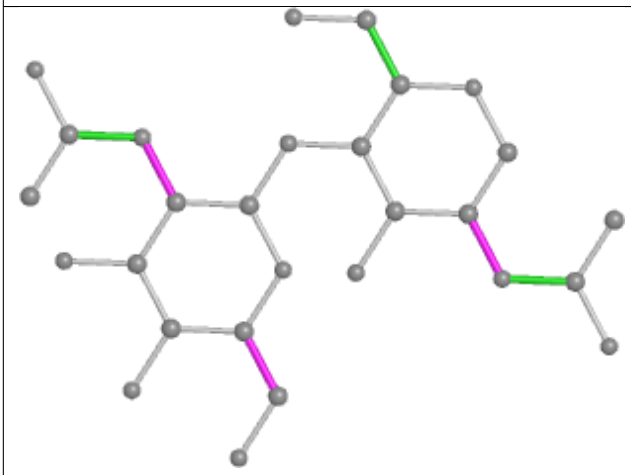

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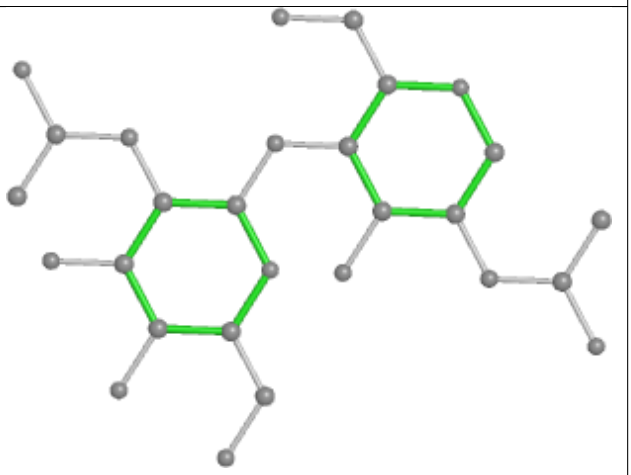
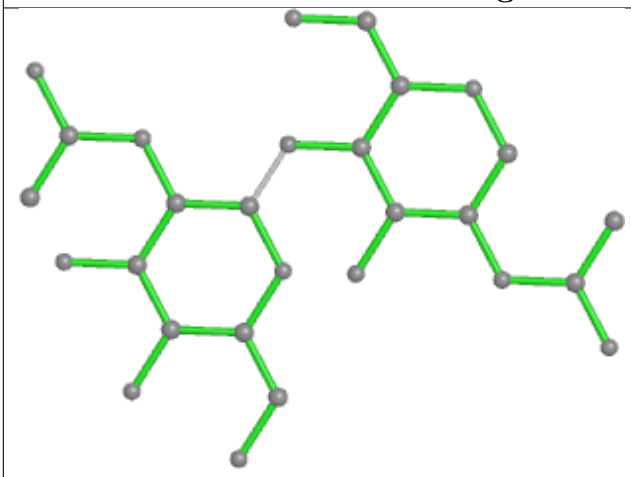
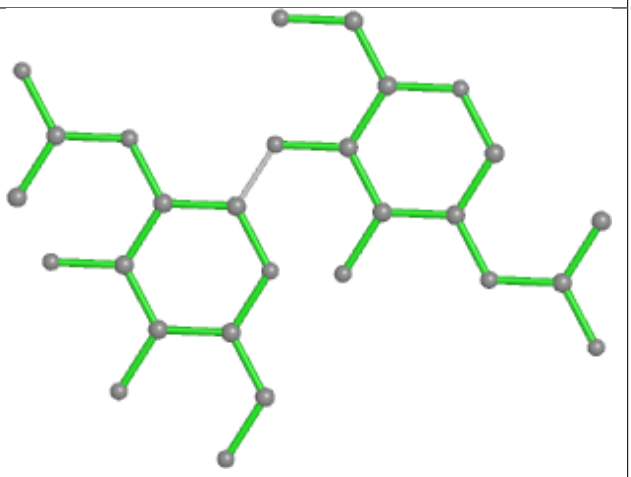
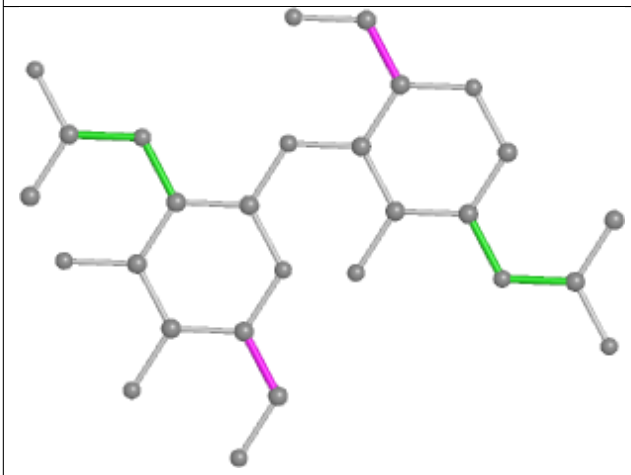
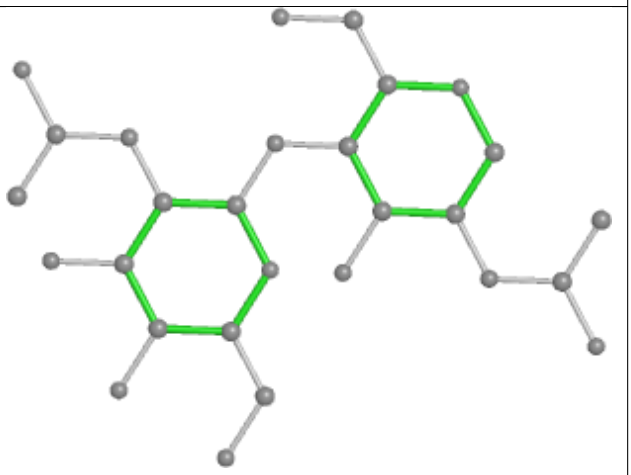
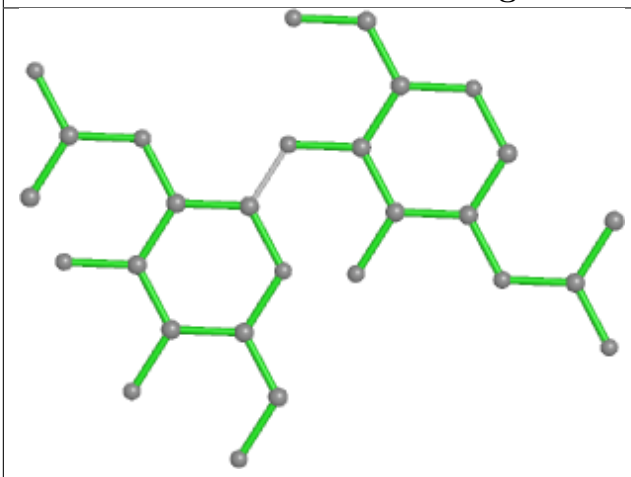


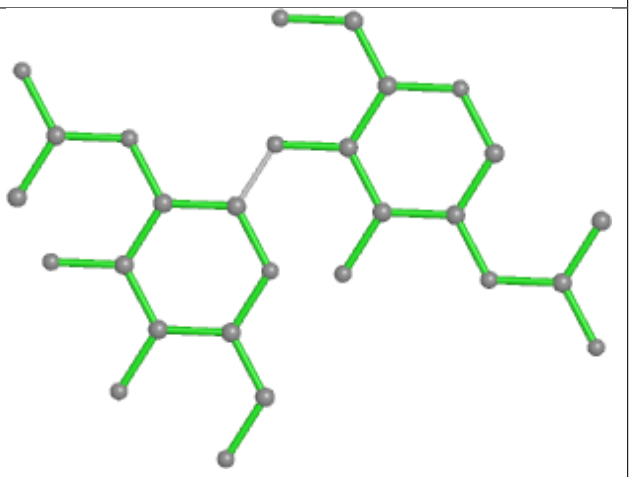
Rings

Oligosaccharide Chain Z	
 Bond lengths	 Bond angles
 Torsions	 Rings

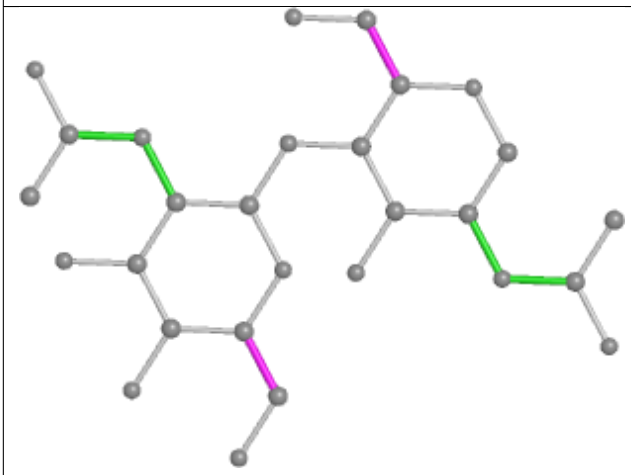
Oligosaccharide Chain a



Bond lengths



Bond angles



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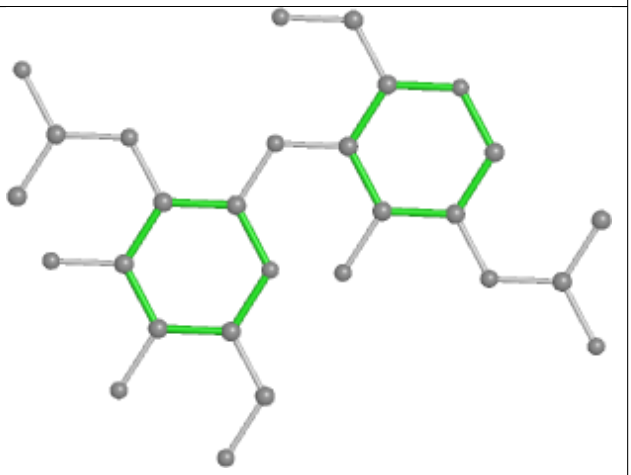
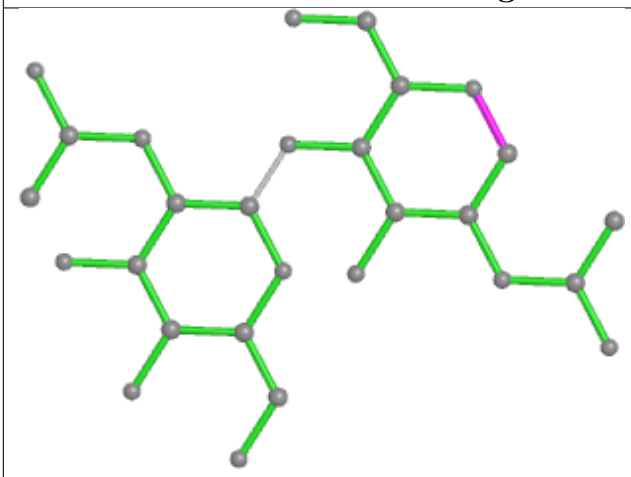


Rings

Oligosaccharide Chain b



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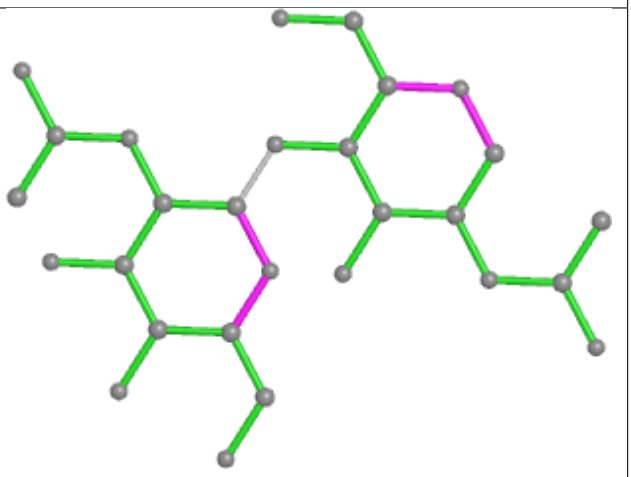
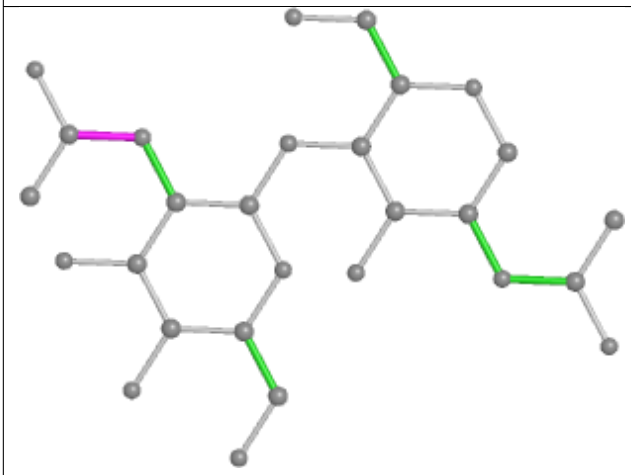


Bond angles



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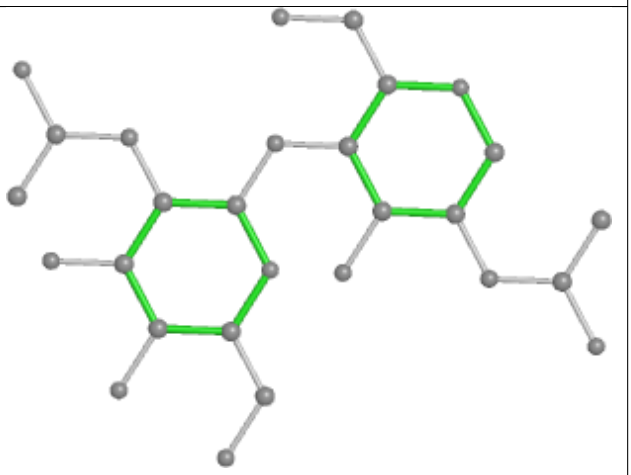
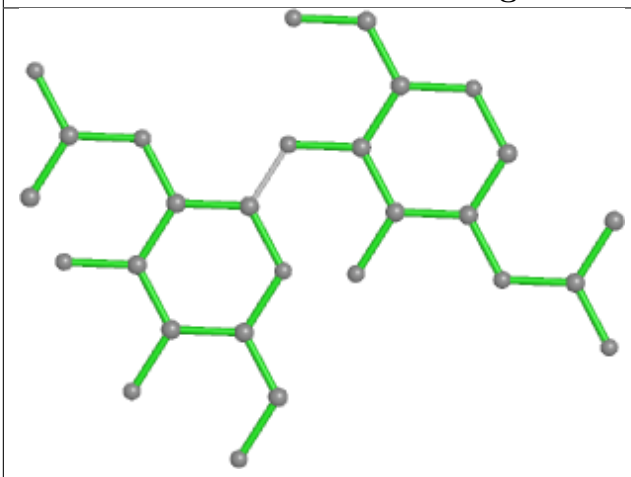


Rings

Oligosaccharide Chain c



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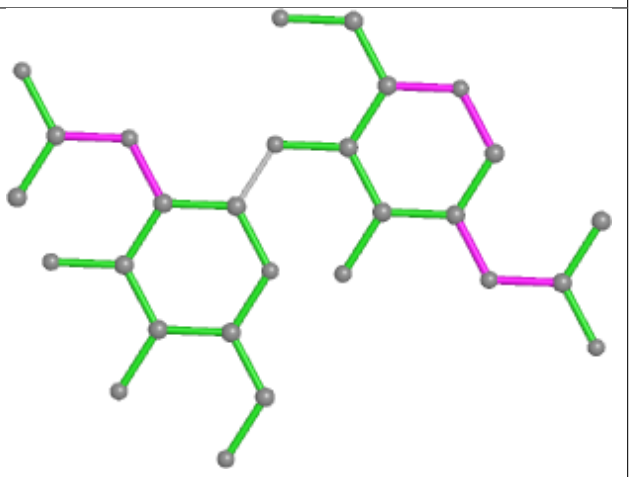
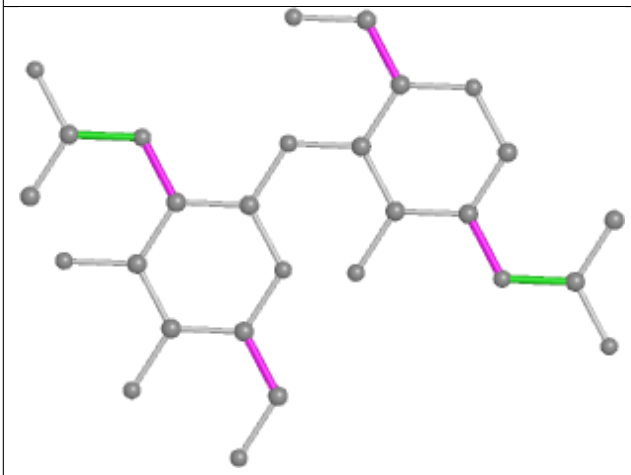
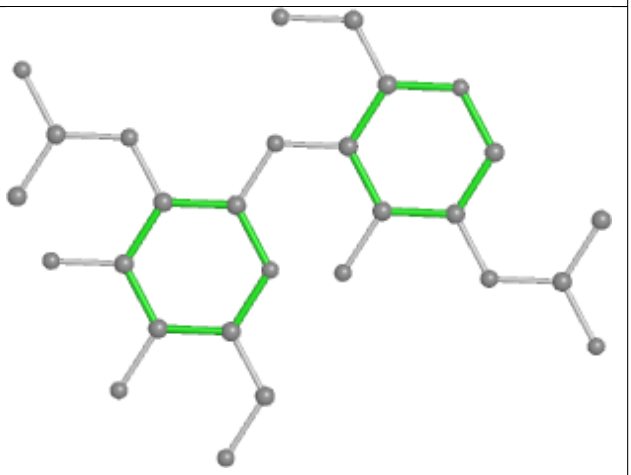


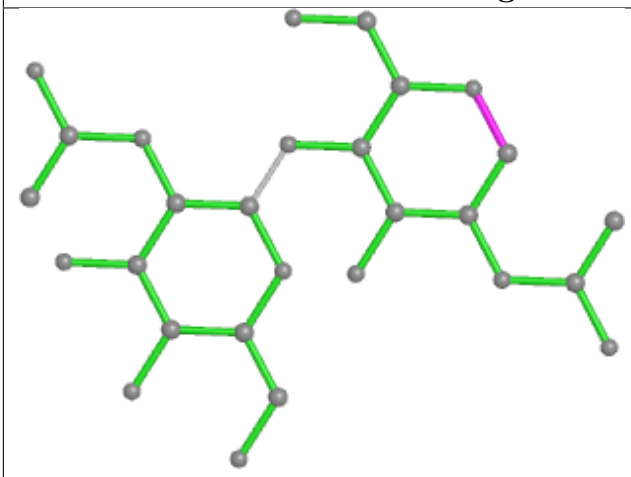
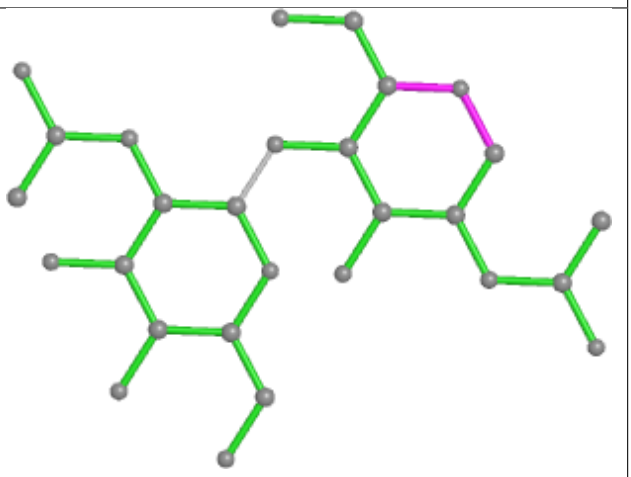
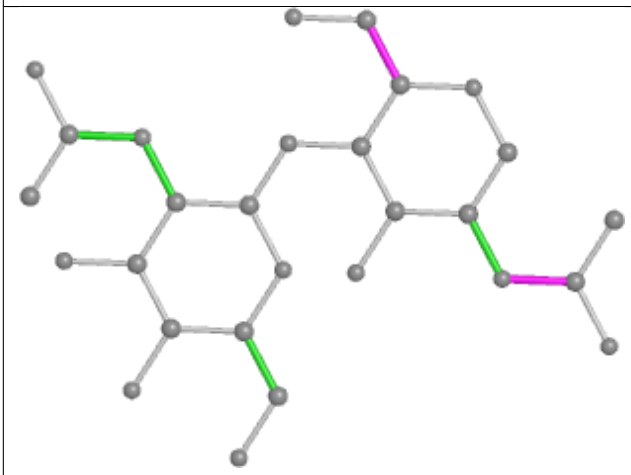
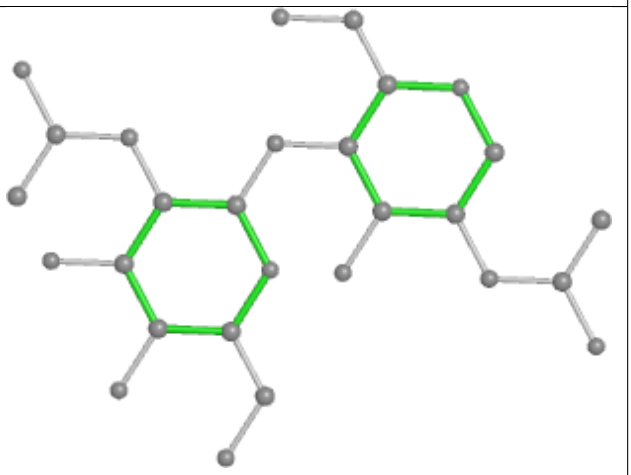
Bond angles

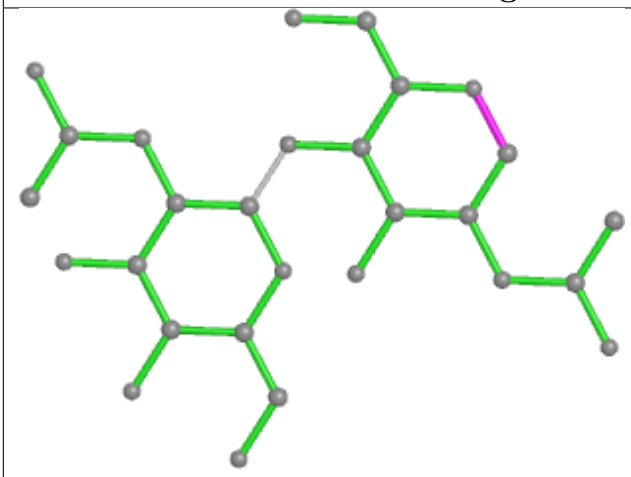
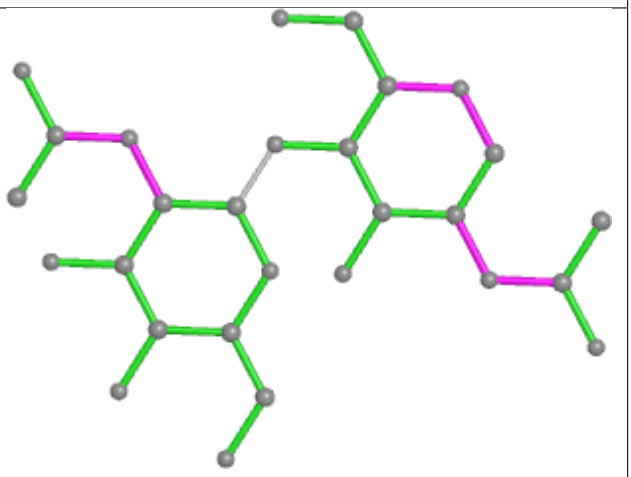
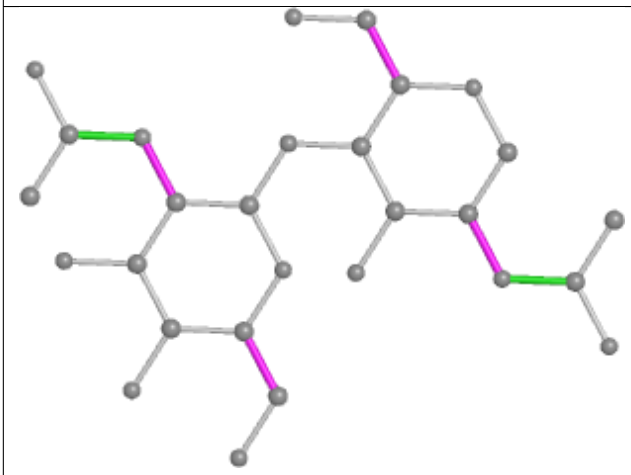
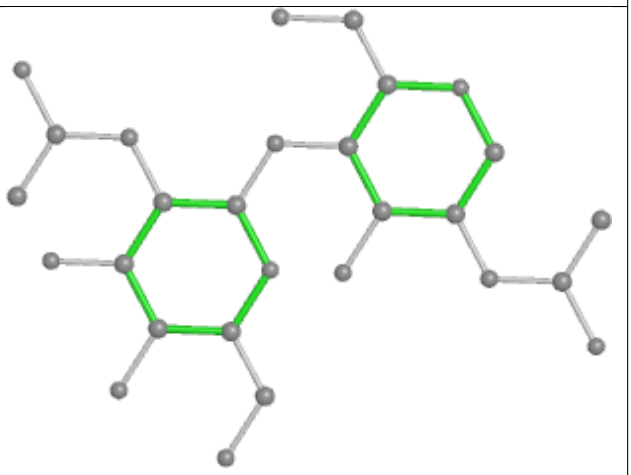


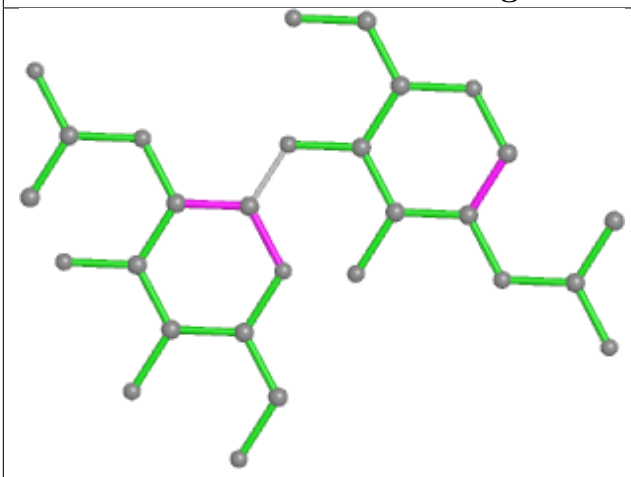
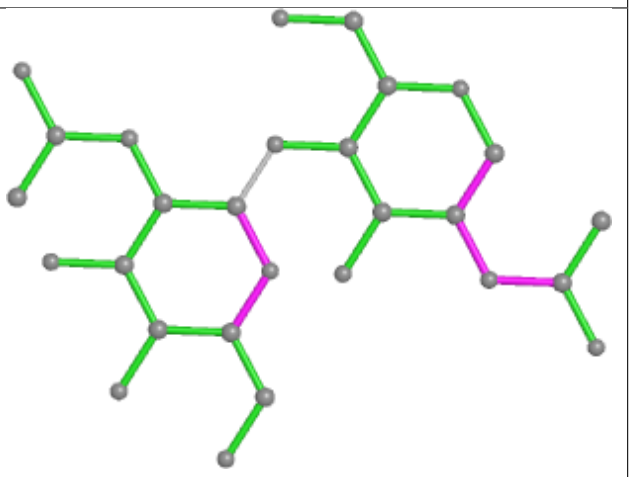
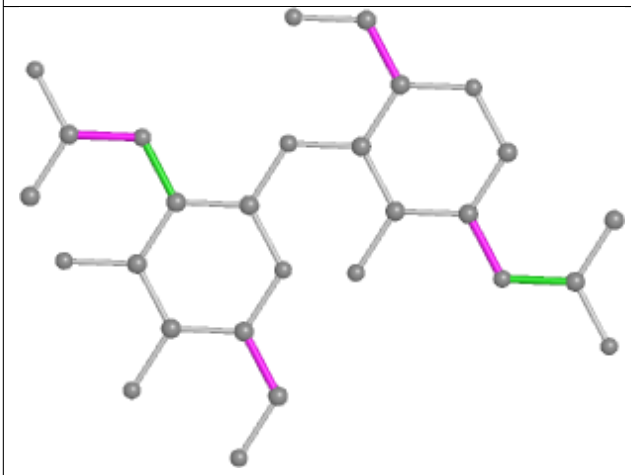
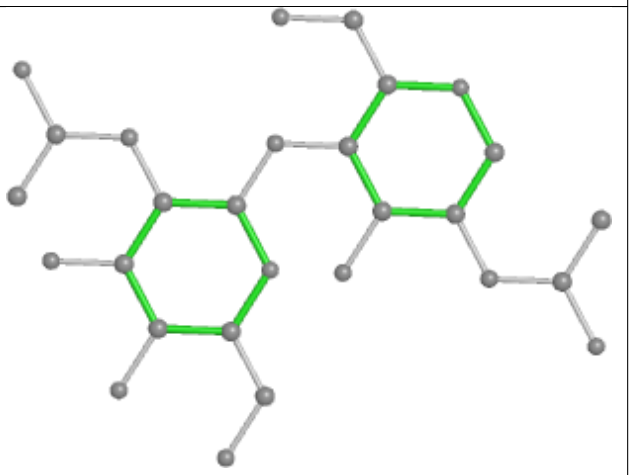
Torsions



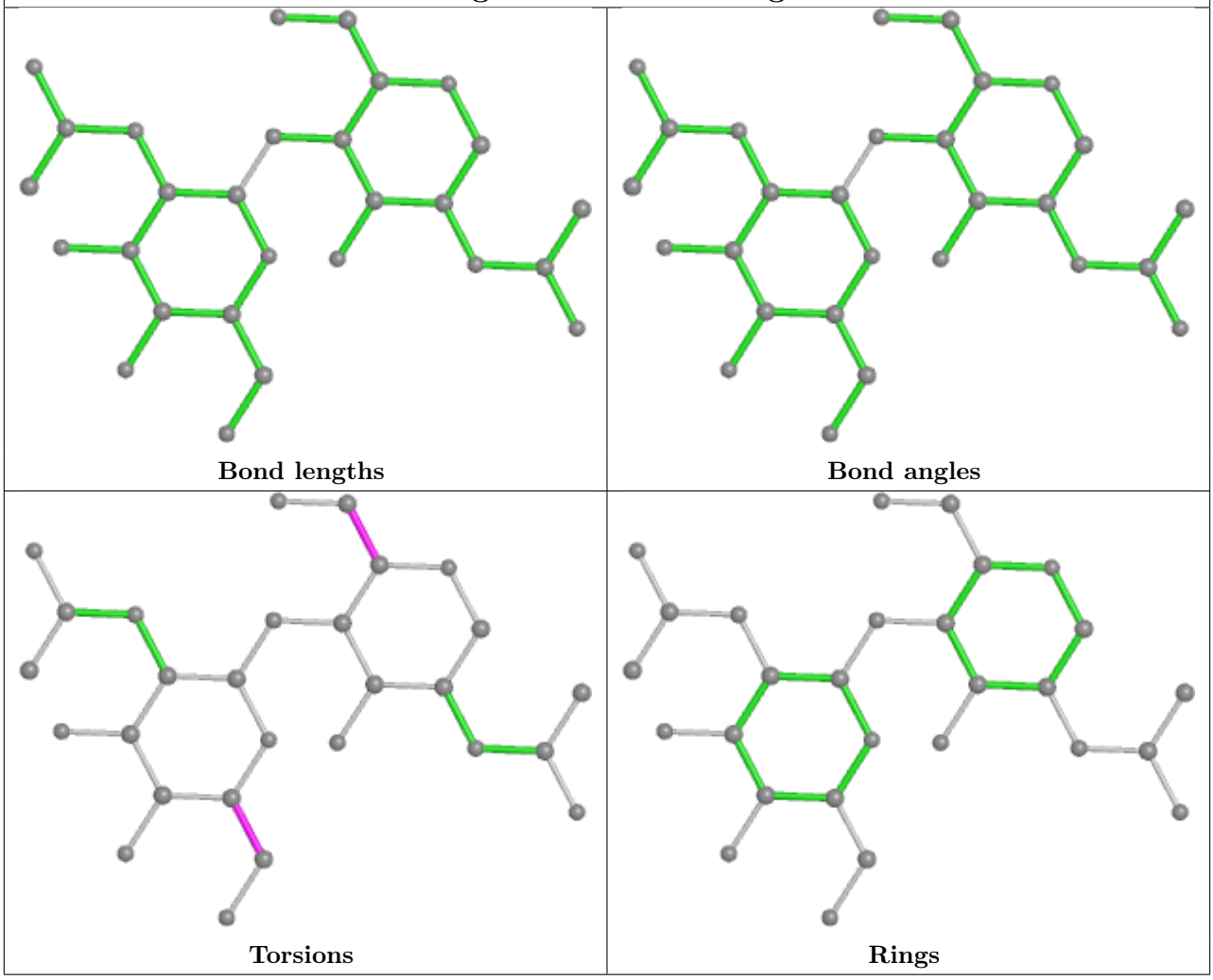
Rings

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



5.6 Ligand geometry (i)

21 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	A	1401	1	14,14,15	0.58	0	17,19,21	1.04	1 (5%)
5	NAG	J	1412	1	14,14,15	0.60	0	17,19,21	0.62	0
5	NAG	I	1401	1	14,14,15	0.30	0	17,19,21	0.78	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	B	1404	1	14,14,15	0.75	1 (7%)	17,19,21	1.12	3 (17%)
5	NAG	J	1401	1	14,14,15	0.69	0	17,19,21	0.77	1 (5%)
5	NAG	F	1401	1	14,14,15	0.48	0	17,19,21	0.99	1 (5%)
5	NAG	F	1403	1	14,14,15	1.19	1 (7%)	17,19,21	2.19	3 (17%)
5	NAG	J	1403	1	14,14,15	0.43	0	17,19,21	0.55	0
5	NAG	B	1403	1	14,14,15	0.73	1 (7%)	17,19,21	0.97	1 (5%)
5	NAG	F	1402	1	14,14,15	0.28	0	17,19,21	0.65	1 (5%)
5	NAG	B	1401	1	14,14,15	1.83	1 (7%)	17,19,21	1.89	3 (17%)
5	NAG	B	1405	1	14,14,15	0.67	0	17,19,21	0.63	0
5	NAG	F	1405	1	14,14,15	0.69	0	17,19,21	0.62	0
5	NAG	E	1401	1	14,14,15	0.35	0	17,19,21	0.90	1 (5%)
5	NAG	F	1404	1	14,14,15	0.52	0	17,19,21	0.73	0
5	NAG	B	1402	1	14,14,15	0.44	0	17,19,21	0.64	1 (5%)
5	NAG	B	1406	1	14,14,15	0.50	0	17,19,21	0.67	0
5	NAG	J	1402	1	14,14,15	0.33	0	17,19,21	0.78	1 (5%)
5	NAG	F	1406	1	14,14,15	0.62	0	17,19,21	0.74	1 (5%)
5	NAG	J	1410	1	14,14,15	0.45	0	17,19,21	0.42	0
5	NAG	J	1411	1	14,14,15	0.22	0	17,19,21	0.56	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
5	NAG	A	1401	1	-	4/6/23/26	0/1/1/1
5	NAG	J	1412	1	-	2/6/23/26	0/1/1/1
5	NAG	I	1401	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1404	1	-	2/6/23/26	0/1/1/1
5	NAG	J	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	F	1401	1	-	1/6/23/26	0/1/1/1
5	NAG	F	1403	1	-	5/6/23/26	0/1/1/1
5	NAG	J	1403	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1403	1	-	3/6/23/26	0/1/1/1
5	NAG	F	1402	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1401	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1405	1	-	2/6/23/26	0/1/1/1
5	NAG	F	1405	1	-	3/6/23/26	0/1/1/1

Continued on next page...

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	F	1404	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1402	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1406	1	-	3/6/23/26	0/1/1/1
5	NAG	J	1402	1	-	4/6/23/26	0/1/1/1
5	NAG	F	1406	1	-	1/6/23/26	0/1/1/1
5	NAG	J	1410	1	-	2/6/23/26	0/1/1/1
5	NAG	J	1411	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1401	NAG	C1-C2	6.53	1.62	1.52
5	F	1403	NAG	C1-C2	3.76	1.58	1.52
5	B	1404	NAG	O5-C1	2.36	1.47	1.43
5	B	1403	NAG	C1-C2	2.21	1.55	1.52

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	1403	NAG	C2-N2-C7	7.71	133.88	122.90
5	B	1401	NAG	C2-N2-C7	5.89	131.29	122.90
5	E	1401	NAG	C1-O5-C5	3.38	116.78	112.19
5	A	1401	NAG	C2-N2-C7	3.10	127.32	122.90
5	F	1401	NAG	C2-N2-C7	3.07	127.28	122.90

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	J	1402	NAG	O5-C5-C6-O6
5	B	1403	NAG	O5-C5-C6-O6
5	A	1401	NAG	C4-C5-C6-O6
5	J	1401	NAG	O5-C5-C6-O6
5	J	1410	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1402	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

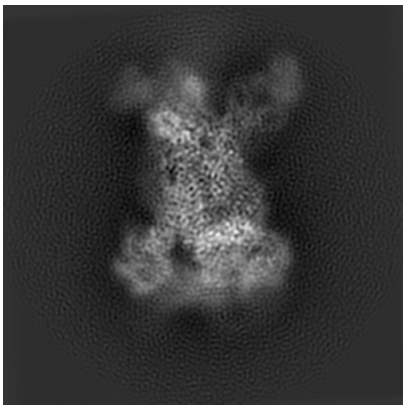
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-8784. These allow visual inspection of the internal detail of the map and identification of artifacts.

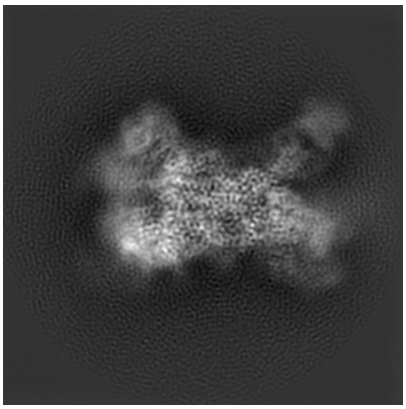
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

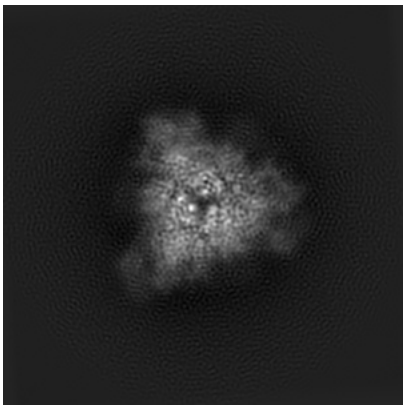
6.1.1 Primary map



X

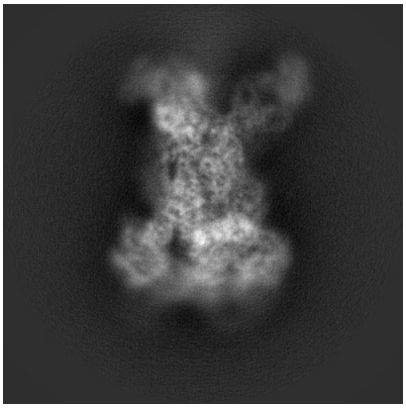


Y

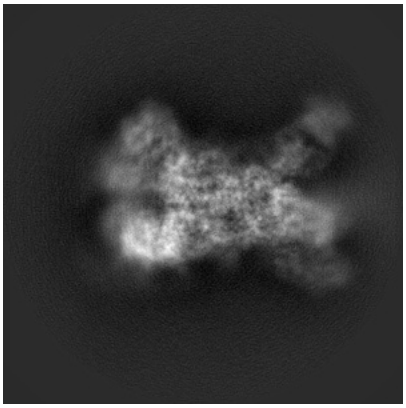


Z

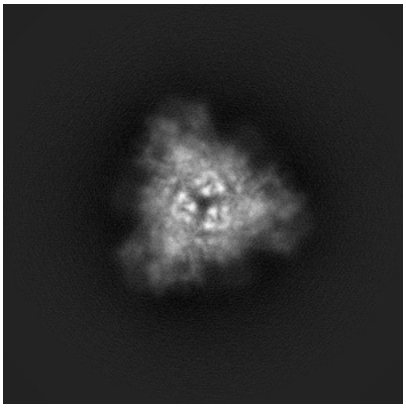
6.1.2 Raw map



X



Y

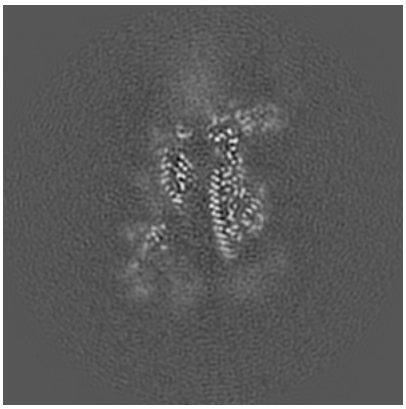


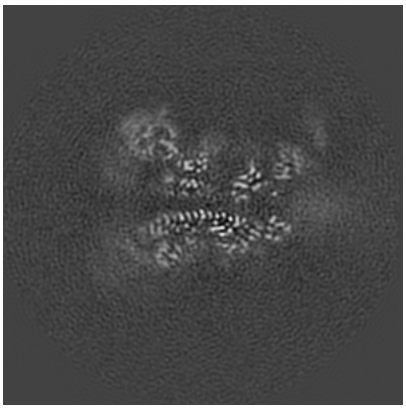
Z

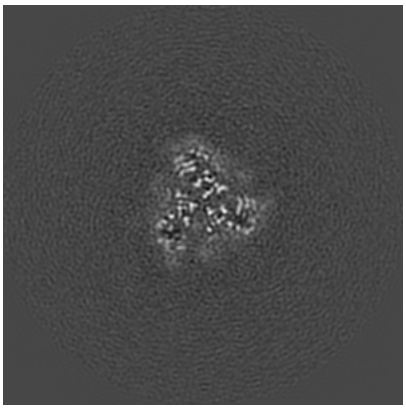
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

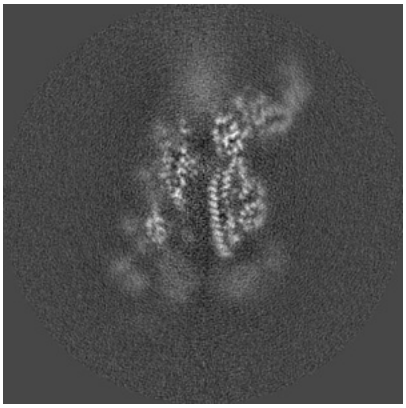
6.2.1 Primary map

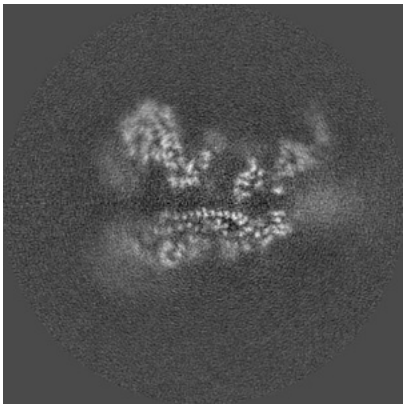

X Index: 152

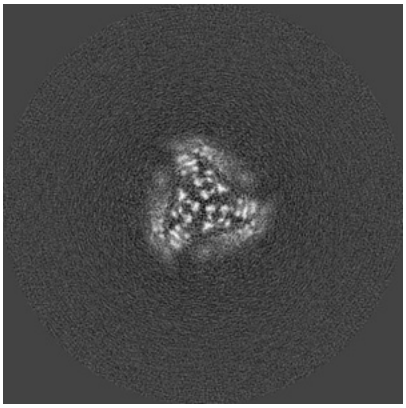

Y Index: 152


Z Index: 152

6.2.2 Raw map


X Index: 152

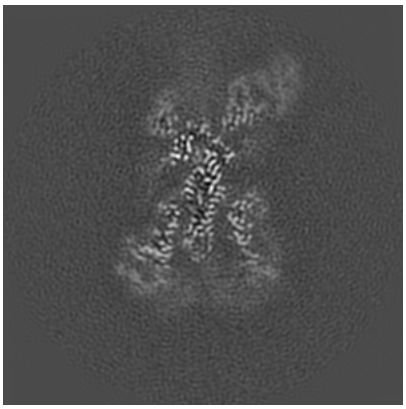

Y Index: 152

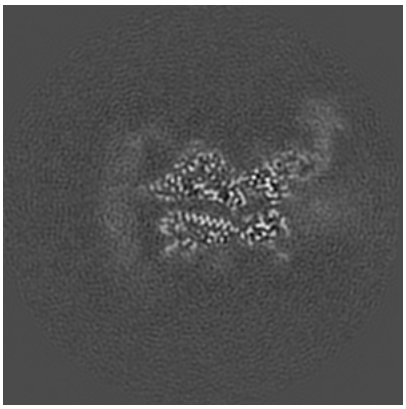

Z Index: 152

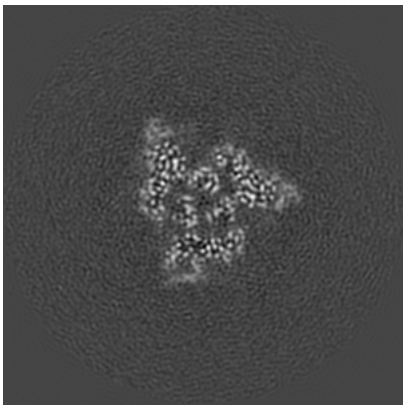
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

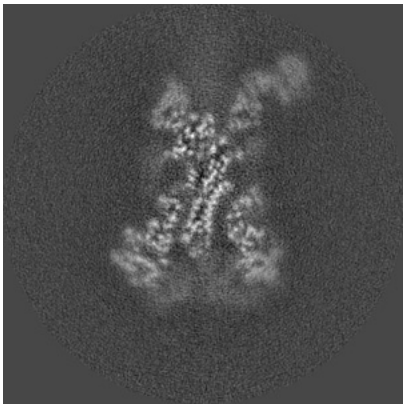
6.3.1 Primary map

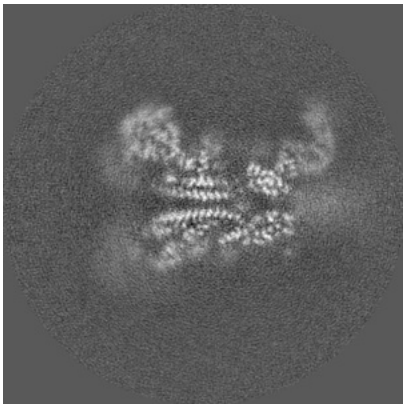

X Index: 136

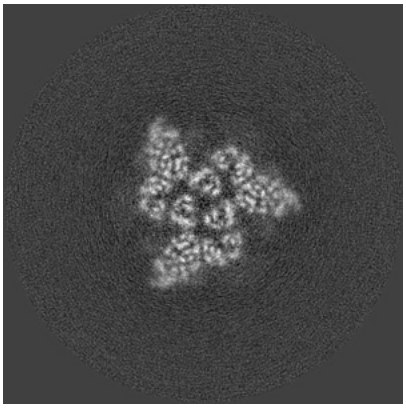

Y Index: 141


Z Index: 126

6.3.2 Raw map


X Index: 135

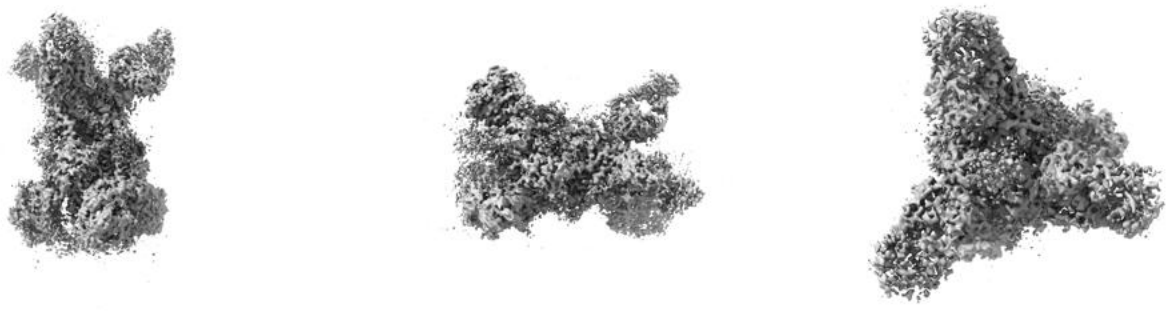

Y Index: 148


Z Index: 127

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

6.4 Orthogonal surface views (i)

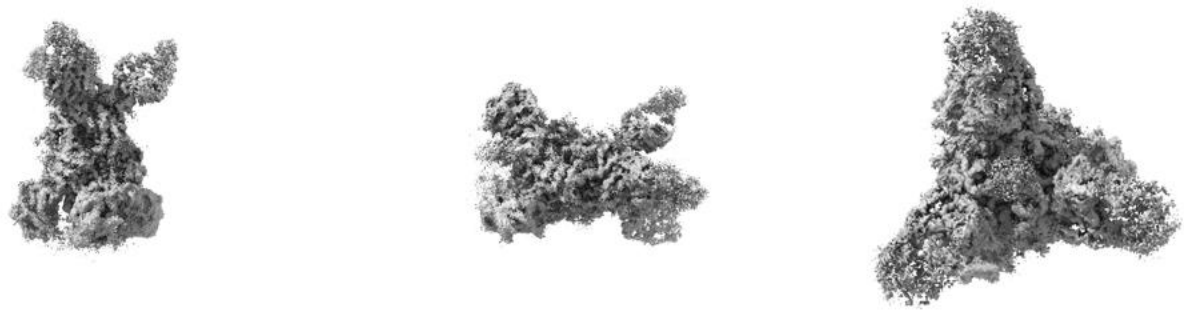
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

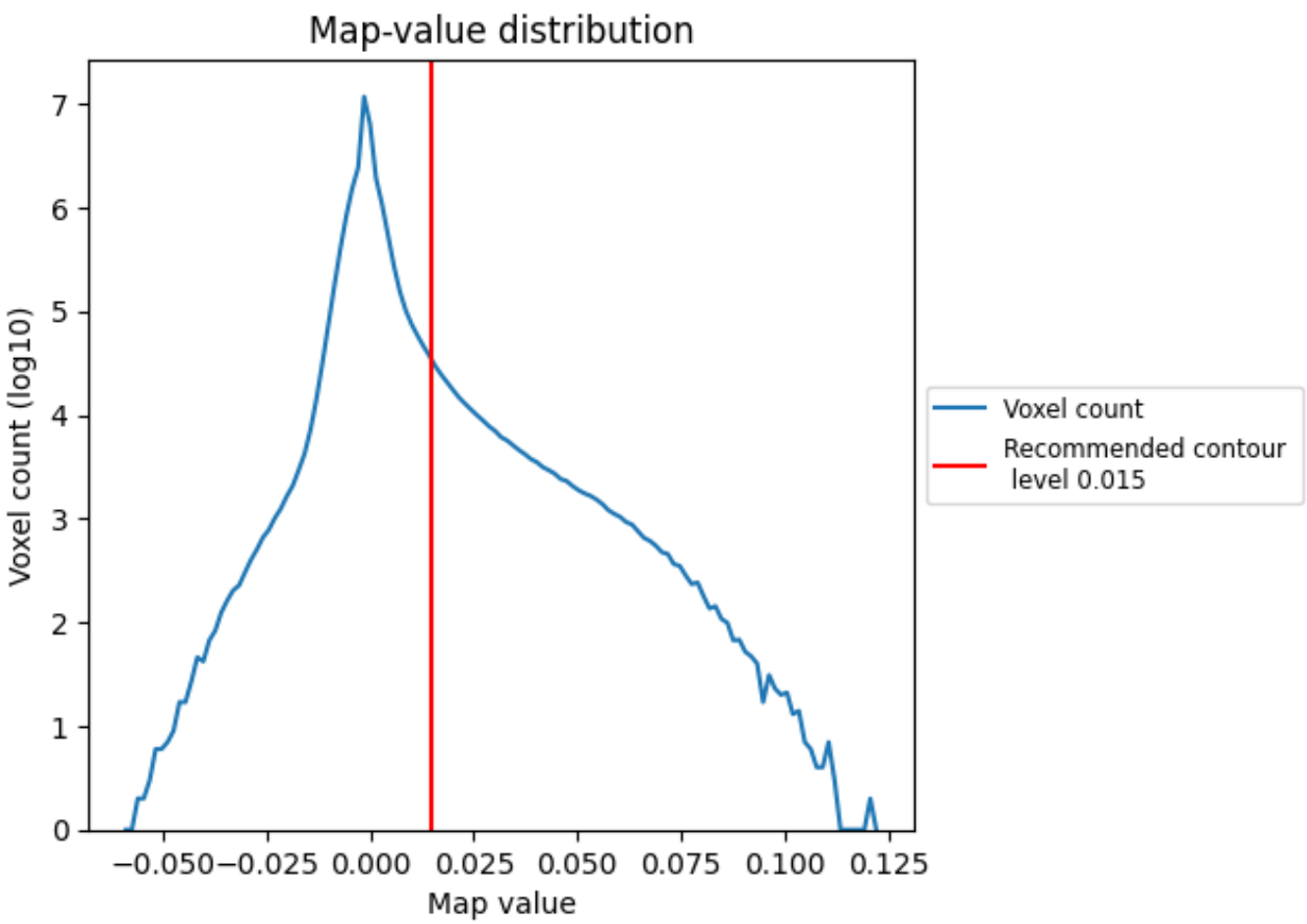
6.5 Mask visualisation (i)

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

7 Map analysis (i)

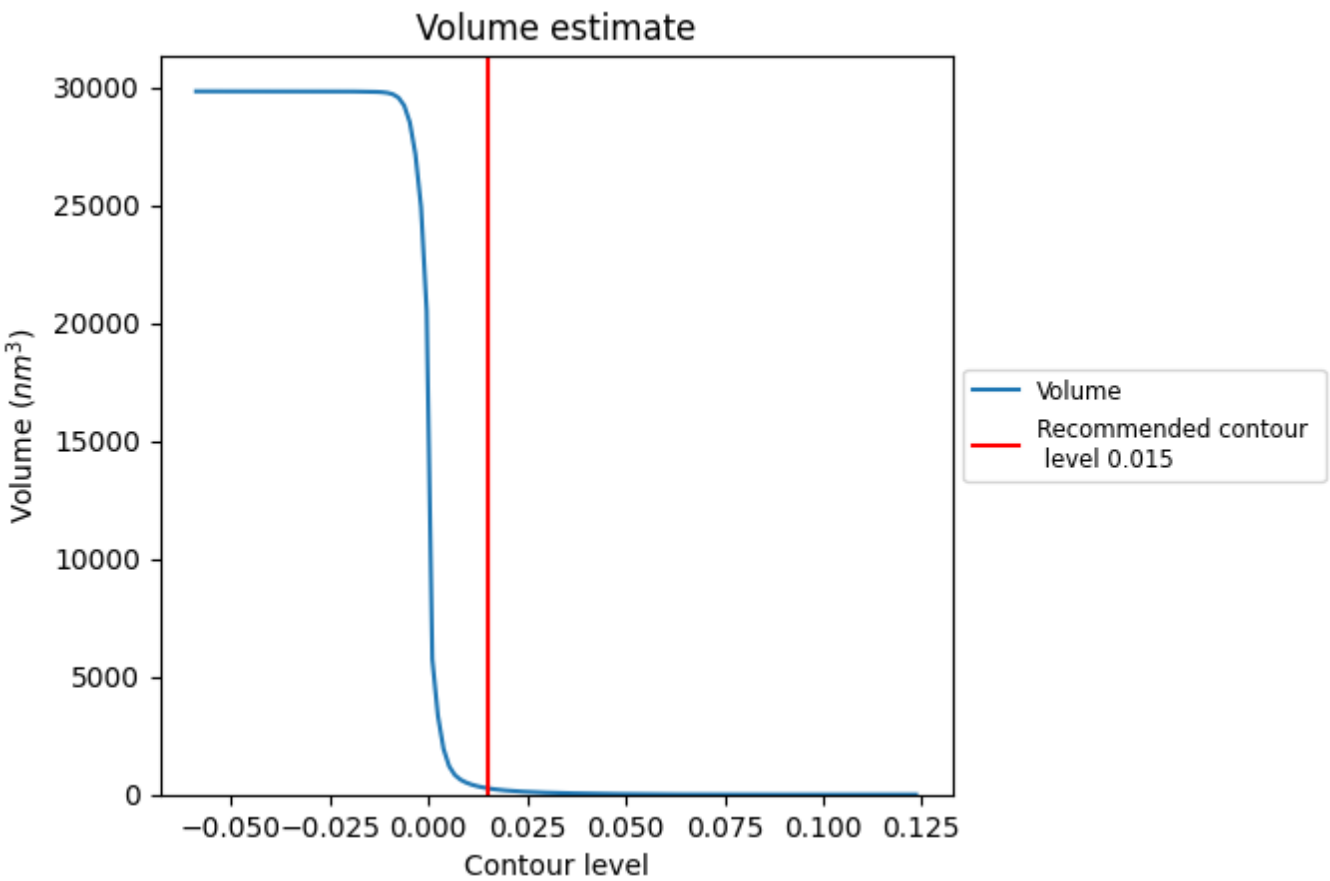
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

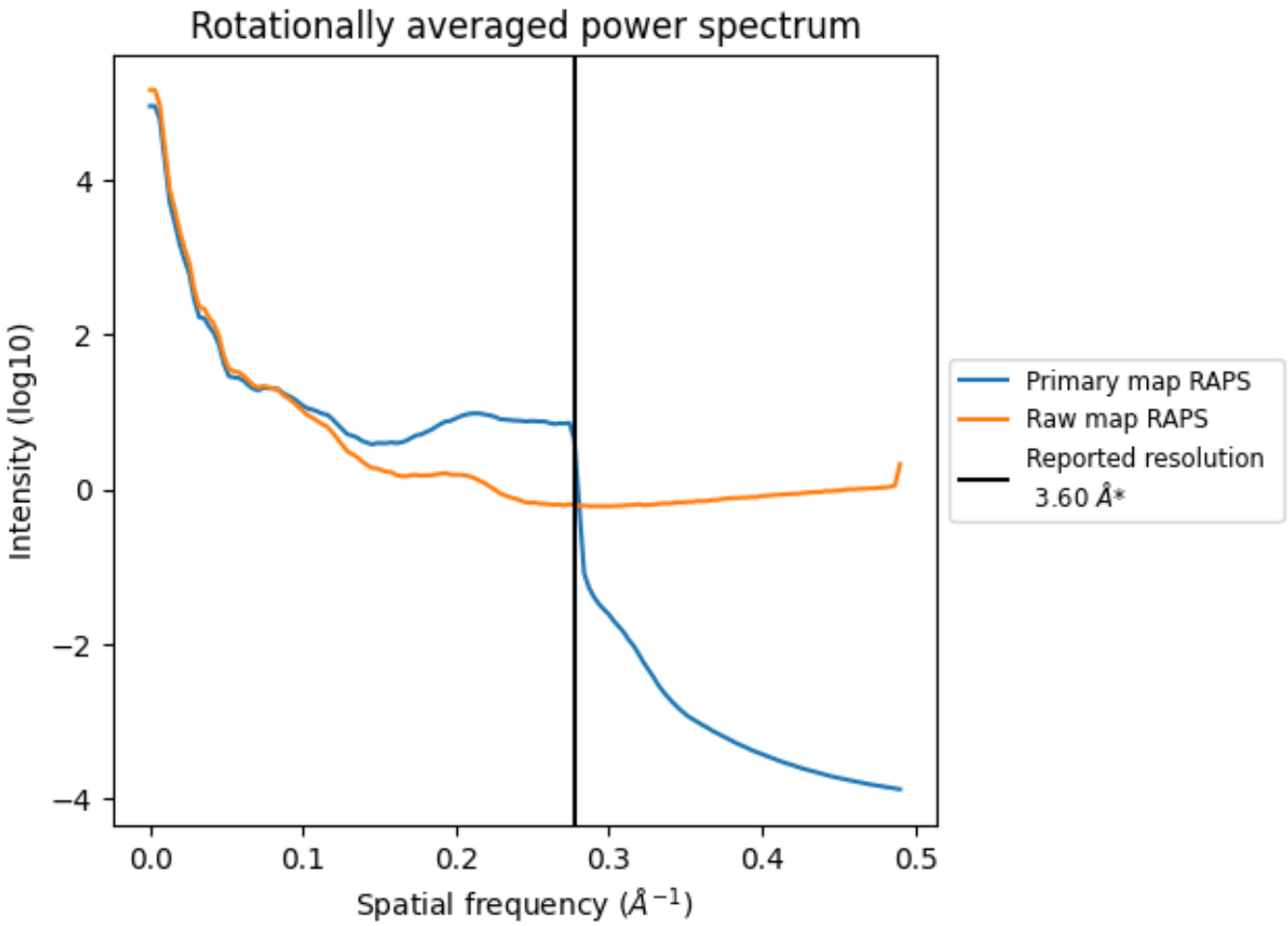
7.2 Volume estimate (i)



The volume at the recommended contour level is 266 nm^3; this corresponds to an approximate mass of 241 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)

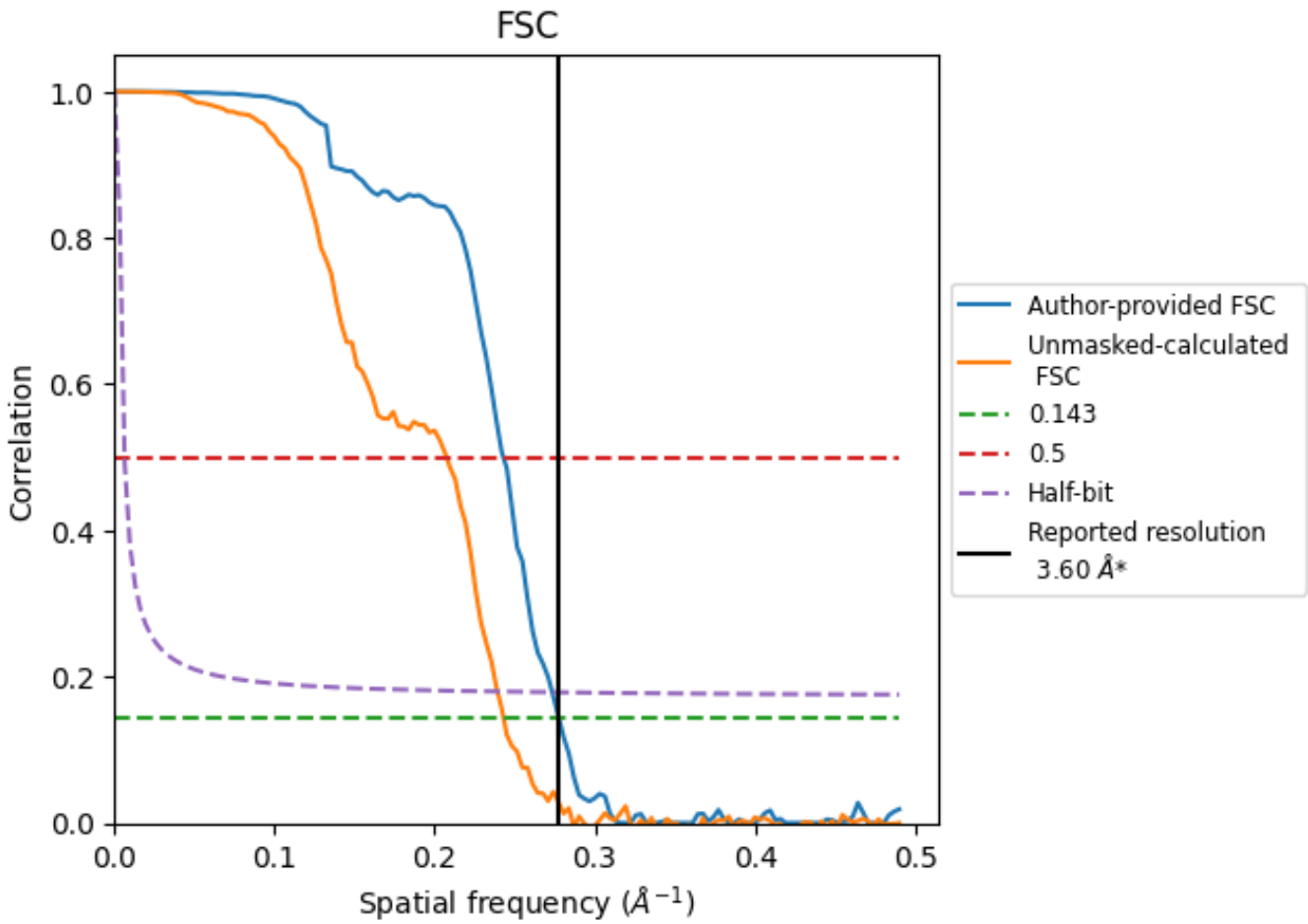


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

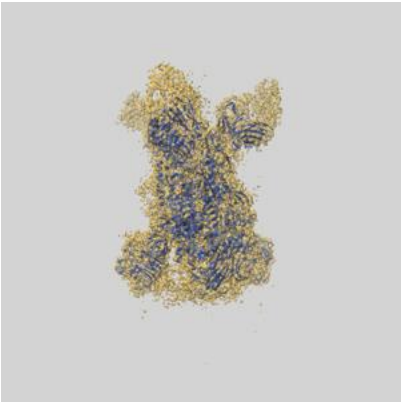
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.60	4.12	3.66
Unmasked-calculated*	4.11	4.82	4.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.11 differs from the reported value 3.6 by more than 10 %

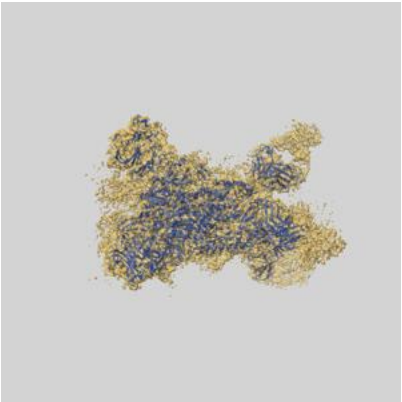
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-8784 and PDB model 5W9I. Per-residue inclusion information can be found in section 3 on page 14.

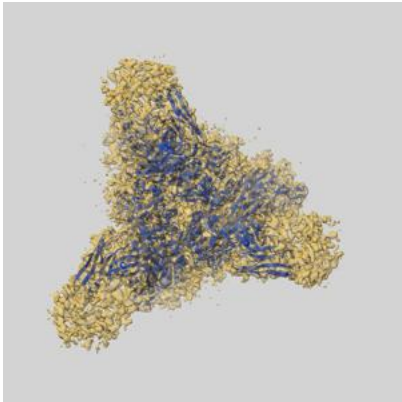
9.1 Map-model overlay (i)



X



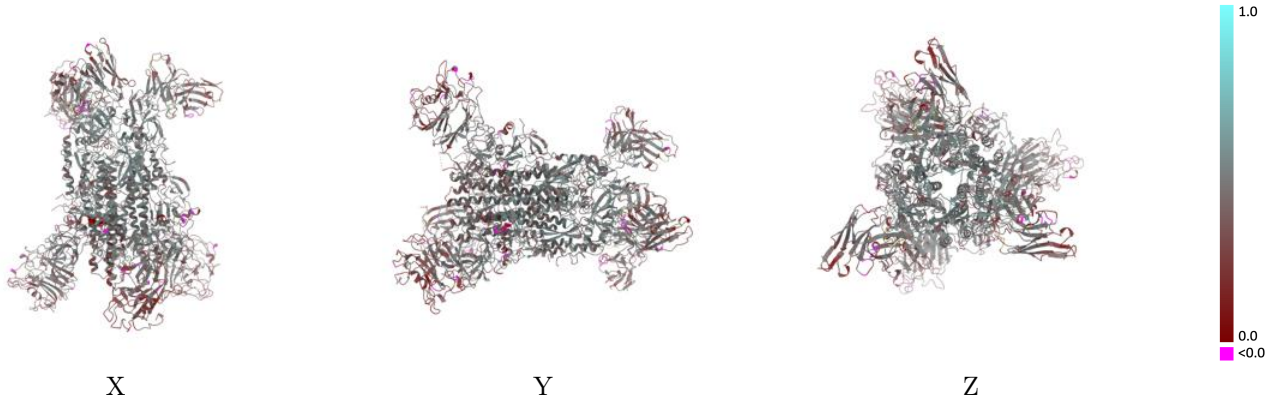
Y



Z

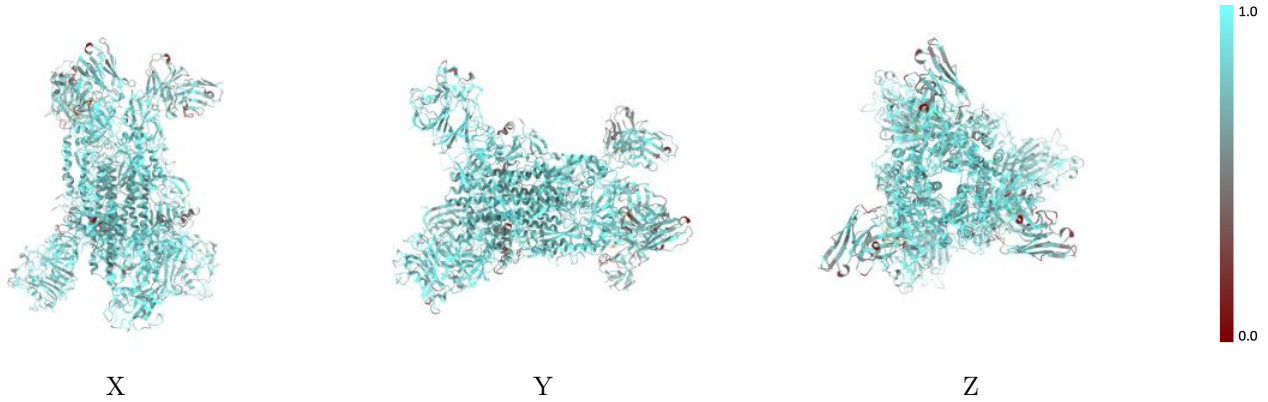
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



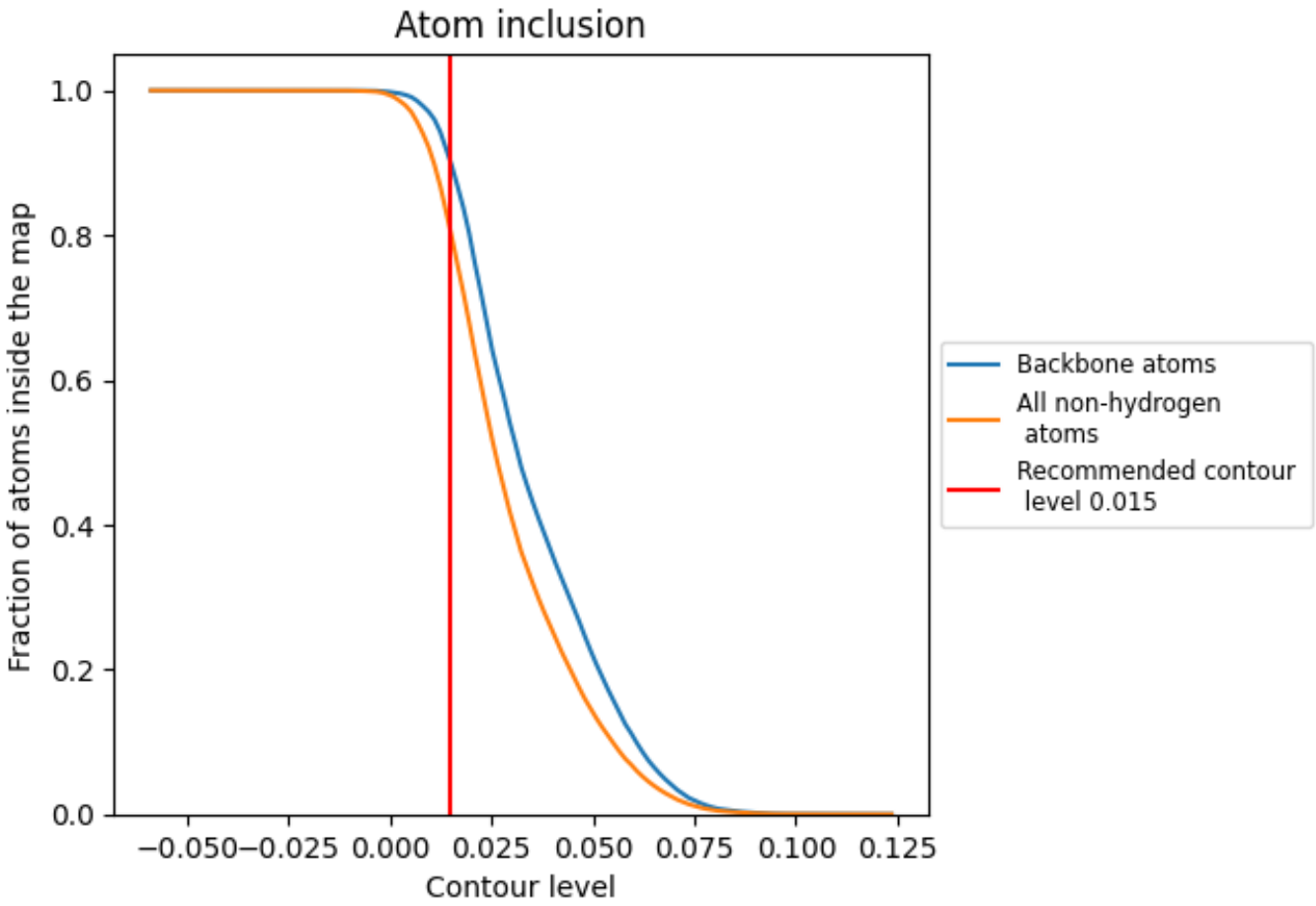
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 80% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8028	0.4140
A	0.8448	0.4580
B	0.8229	0.3930
C	0.7449	0.4070
D	0.6299	0.3480
E	0.8437	0.4600
F	0.8244	0.3950
G	0.7395	0.4010
H	0.6262	0.3460
I	0.8437	0.4620
J	0.8232	0.3930
K	0.7384	0.4090
L	0.6323	0.3490
M	0.6429	0.3210
N	0.6071	0.3020
O	0.7857	0.4420
P	0.7857	0.4600
Q	0.6071	0.3100
R	0.6429	0.3240
S	0.8571	0.3380
T	0.5714	0.2840
U	0.7857	0.3840
V	0.6429	0.3240
W	0.6786	0.3760
X	0.5714	0.3490
Y	0.5357	0.2730
Z	0.7143	0.3030
a	0.7143	0.4280
b	0.6071	0.2610
c	0.6071	0.3170
d	0.7857	0.4620
e	0.3214	0.2230
f	0.5714	0.3510
g	0.8214	0.3460