wwPDB EM Validation Summary Report

Oct 7, 2024 – 02:34 PM JST

PDB ID	:	8WHU
EMDB ID	:	EMD-37548
Title	:	Spike Trimer of BA.2.86 in complex with two hACE2s
Authors	:	Yue, C.; Liu, P.
Deposited on	:	2023-09-23
Resolution	:	3.30 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

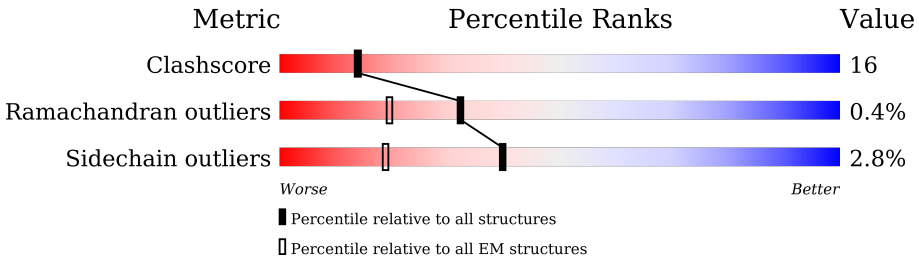
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	1206	61% 26% • 12%
1	B	1206	61% 26% • 12%
1	C	1206	57% 29% • 12%
2	D	597	69% 30% •
2	E	597	68% 30% •
3	F	2	50% 50%
3	G	2	100%
3	H	2	50% 50%
3	I	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	J	2	100%
3	K	2	50% 50%
3	L	2	100%
3	M	2	50% 50%
3	N	2	100%
3	O	2	100%
3	P	2	100%
3	Q	2	100%
3	R	2	50% 50%
3	S	2	100%
3	T	2	100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 35548 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1059	Total	C	N	O	S	0	0
			8285	5302	1376	1569	38		
1	B	1059	Total	C	N	O	S	0	0
			8285	5302	1376	1569	38		
1	C	1059	Total	C	N	O	S	0	0
			8285	5302	1376	1569	38		

There are 273 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ALA	-	expression tag	UNP P0DTC2
A	-1	THR	-	expression tag	UNP P0DTC2
A	0	MET	-	expression tag	UNP P0DTC2
A	1	PHE	-	expression tag	UNP P0DTC2
A	2	VAL	-	expression tag	UNP P0DTC2
A	3	PHE	-	expression tag	UNP P0DTC2
A	4	LEU	-	expression tag	UNP P0DTC2
A	5	VAL	-	expression tag	UNP P0DTC2
A	6	LEU	-	expression tag	UNP P0DTC2
A	7	LEU	-	expression tag	UNP P0DTC2
A	8	PRO	-	expression tag	UNP P0DTC2
A	9	LEU	-	expression tag	UNP P0DTC2
A	10	VAL	-	expression tag	UNP P0DTC2
A	11	SER	-	expression tag	UNP P0DTC2
A	12	SER	-	expression tag	UNP P0DTC2
A	13	GLN	-	expression tag	UNP P0DTC2
A	14	CYS	-	expression tag	UNP P0DTC2
A	15	VAL	-	expression tag	UNP P0DTC2
A	16	MET	-	expression tag	UNP P0DTC2
A	17	PRO	-	expression tag	UNP P0DTC2
A	18	LEU	-	expression tag	UNP P0DTC2
A	19	PHE	-	expression tag	UNP P0DTC2
A	20	ASN	-	expression tag	UNP P0DTC2
A	21	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ILE	-	expression tag	UNP P0DTC2
A	23	THR	-	expression tag	UNP P0DTC2
A	24	THR	-	expression tag	UNP P0DTC2
A	25	THR	-	expression tag	UNP P0DTC2
A	26	GLN	-	expression tag	UNP P0DTC2
A	27	SER	-	expression tag	UNP P0DTC2
A	50	LEU	SER	conflict	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	127	PHE	VAL	conflict	UNP P0DTC2
A	143	ASP	GLY	variant	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	157	SER	PHE	conflict	UNP P0DTC2
A	158	GLY	ARG	conflict	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	212	ILE	LEU	variant	UNP P0DTC2
A	213	GLY	VAL	variant	UNP P0DTC2
A	216	PHE	LEU	conflict	UNP P0DTC2
A	245	ASN	HIS	conflict	UNP P0DTC2
A	264	ASP	ALA	conflict	UNP P0DTC2
A	332	VAL	ILE	conflict	UNP P0DTC2
A	339	HIS	GLY	variant	UNP P0DTC2
A	356	THR	LYS	conflict	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	403	LYS	ARG	conflict	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	conflict	UNP P0DTC2
A	445	HIS	VAL	variant	UNP P0DTC2
A	446	SER	GLY	conflict	UNP P0DTC2
A	450	ASP	ASN	conflict	UNP P0DTC2
A	452	TRP	LEU	conflict	UNP P0DTC2
A	460	LYS	ASN	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	481	LYS	ASN	conflict	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	484	LYS	GLU	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	486	PRO	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	554	LYS	GLU	conflict	UNP P0DTC2
A	570	VAL	ALA	conflict	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	621	SER	PRO	conflict	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	ARG	PRO	variant	UNP P0DTC2
A	683	ALA	ARG	conflict	UNP P0DTC2
A	685	ALA	ARG	conflict	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	939	PHE	SER	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1143	LEU	PRO	conflict	UNP P0DTC2
B	-2	ALA	-	expression tag	UNP P0DTC2
B	-1	THR	-	expression tag	UNP P0DTC2
B	0	MET	-	expression tag	UNP P0DTC2
B	1	PHE	-	expression tag	UNP P0DTC2
B	2	VAL	-	expression tag	UNP P0DTC2
B	3	PHE	-	expression tag	UNP P0DTC2
B	4	LEU	-	expression tag	UNP P0DTC2
B	5	VAL	-	expression tag	UNP P0DTC2
B	6	LEU	-	expression tag	UNP P0DTC2
B	7	LEU	-	expression tag	UNP P0DTC2
B	8	PRO	-	expression tag	UNP P0DTC2
B	9	LEU	-	expression tag	UNP P0DTC2
B	10	VAL	-	expression tag	UNP P0DTC2
B	11	SER	-	expression tag	UNP P0DTC2
B	12	SER	-	expression tag	UNP P0DTC2
B	13	GLN	-	expression tag	UNP P0DTC2
B	14	CYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	15	VAL	-	expression tag	UNP P0DTC2
B	16	MET	-	expression tag	UNP P0DTC2
B	17	PRO	-	expression tag	UNP P0DTC2
B	18	LEU	-	expression tag	UNP P0DTC2
B	19	PHE	-	expression tag	UNP P0DTC2
B	20	ASN	-	expression tag	UNP P0DTC2
B	21	LEU	-	expression tag	UNP P0DTC2
B	22	ILE	-	expression tag	UNP P0DTC2
B	23	THR	-	expression tag	UNP P0DTC2
B	24	THR	-	expression tag	UNP P0DTC2
B	25	THR	-	expression tag	UNP P0DTC2
B	26	GLN	-	expression tag	UNP P0DTC2
B	27	SER	-	expression tag	UNP P0DTC2
B	50	LEU	SER	conflict	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	127	PHE	VAL	conflict	UNP P0DTC2
B	143	ASP	GLY	variant	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	157	SER	PHE	conflict	UNP P0DTC2
B	158	GLY	ARG	conflict	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	212	ILE	LEU	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	216	PHE	LEU	conflict	UNP P0DTC2
B	245	ASN	HIS	conflict	UNP P0DTC2
B	264	ASP	ALA	conflict	UNP P0DTC2
B	332	VAL	ILE	conflict	UNP P0DTC2
B	339	HIS	GLY	variant	UNP P0DTC2
B	356	THR	LYS	conflict	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	403	LYS	ARG	conflict	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	conflict	UNP P0DTC2
B	445	HIS	VAL	variant	UNP P0DTC2
B	446	SER	GLY	conflict	UNP P0DTC2
B	450	ASP	ASN	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	452	TRP	LEU	conflict	UNP P0DTC2
B	460	LYS	ASN	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	481	LYS	ASN	conflict	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	484	LYS	GLU	variant	UNP P0DTC2
B	486	PRO	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	554	LYS	GLU	conflict	UNP P0DTC2
B	570	VAL	ALA	conflict	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	621	SER	PRO	conflict	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	ARG	PRO	variant	UNP P0DTC2
B	683	ALA	ARG	conflict	UNP P0DTC2
B	685	ALA	ARG	conflict	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	939	PHE	SER	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1143	LEU	PRO	conflict	UNP P0DTC2
C	-2	ALA	-	expression tag	UNP P0DTC2
C	-1	THR	-	expression tag	UNP P0DTC2
C	0	MET	-	expression tag	UNP P0DTC2
C	1	PHE	-	expression tag	UNP P0DTC2
C	2	VAL	-	expression tag	UNP P0DTC2
C	3	PHE	-	expression tag	UNP P0DTC2
C	4	LEU	-	expression tag	UNP P0DTC2
C	5	VAL	-	expression tag	UNP P0DTC2
C	6	LEU	-	expression tag	UNP P0DTC2
C	7	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	8	PRO	-	expression tag	UNP P0DTC2
C	9	LEU	-	expression tag	UNP P0DTC2
C	10	VAL	-	expression tag	UNP P0DTC2
C	11	SER	-	expression tag	UNP P0DTC2
C	12	SER	-	expression tag	UNP P0DTC2
C	13	GLN	-	expression tag	UNP P0DTC2
C	14	CYS	-	expression tag	UNP P0DTC2
C	15	VAL	-	expression tag	UNP P0DTC2
C	16	MET	-	expression tag	UNP P0DTC2
C	17	PRO	-	expression tag	UNP P0DTC2
C	18	LEU	-	expression tag	UNP P0DTC2
C	19	PHE	-	expression tag	UNP P0DTC2
C	20	ASN	-	expression tag	UNP P0DTC2
C	21	LEU	-	expression tag	UNP P0DTC2
C	22	ILE	-	expression tag	UNP P0DTC2
C	23	THR	-	expression tag	UNP P0DTC2
C	24	THR	-	expression tag	UNP P0DTC2
C	25	THR	-	expression tag	UNP P0DTC2
C	26	GLN	-	expression tag	UNP P0DTC2
C	27	SER	-	expression tag	UNP P0DTC2
C	50	LEU	SER	conflict	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	127	PHE	VAL	conflict	UNP P0DTC2
C	143	ASP	GLY	variant	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	157	SER	PHE	conflict	UNP P0DTC2
C	158	GLY	ARG	conflict	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	212	ILE	LEU	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	216	PHE	LEU	conflict	UNP P0DTC2
C	245	ASN	HIS	conflict	UNP P0DTC2
C	264	ASP	ALA	conflict	UNP P0DTC2
C	332	VAL	ILE	conflict	UNP P0DTC2
C	339	HIS	GLY	variant	UNP P0DTC2
C	356	THR	LYS	conflict	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	403	LYS	ARG	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	conflict	UNP P0DTC2
C	445	HIS	VAL	variant	UNP P0DTC2
C	446	SER	GLY	conflict	UNP P0DTC2
C	450	ASP	ASN	conflict	UNP P0DTC2
C	452	TRP	LEU	conflict	UNP P0DTC2
C	460	LYS	ASN	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	481	LYS	ASN	conflict	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	484	LYS	GLU	variant	UNP P0DTC2
C	486	PRO	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	554	LYS	GLU	conflict	UNP P0DTC2
C	570	VAL	ALA	conflict	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	621	SER	PRO	conflict	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	ARG	PRO	variant	UNP P0DTC2
C	683	ALA	ARG	conflict	UNP P0DTC2
C	685	ALA	ARG	conflict	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	939	PHE	SER	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1143	LEU	PRO	conflict	UNP P0DTC2

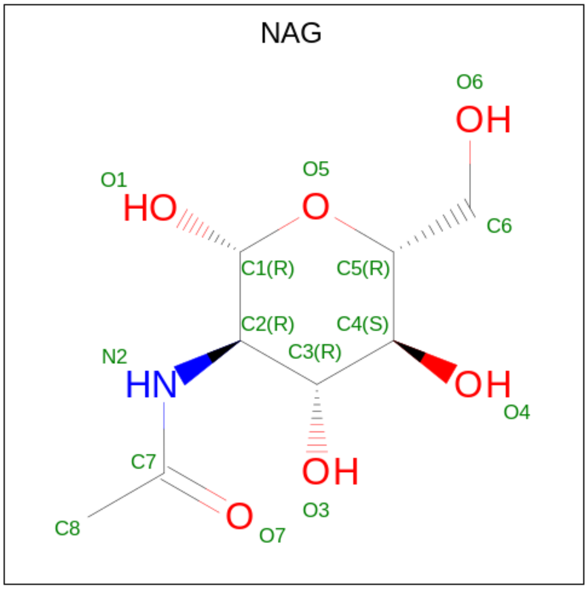
- Molecule 2 is a protein called Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	597	Total	C	N	O	S	0	0
			4870	3115	806	920	29		
2	E	597	Total	C	N	O	S	0	0
			4870	3115	806	920	29		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	2	Total	C	N	O	0	0
			25	14	1	10		
3	G	2	Total	C	N	O	0	0
			25	14	1	10		
3	H	2	Total	C	N	O	0	0
			25	14	1	10		
3	I	2	Total	C	N	O	0	0
			25	14	1	10		
3	J	2	Total	C	N	O	0	0
			25	14	1	10		
3	K	2	Total	C	N	O	0	0
			25	14	1	10		
3	L	2	Total	C	N	O	0	0
			25	14	1	10		
3	M	2	Total	C	N	O	0	0
			25	14	1	10		
3	N	2	Total	C	N	O	0	0
			25	14	1	10		
3	O	2	Total	C	N	O	0	0
			25	14	1	10		
3	P	2	Total	C	N	O	0	0
			25	14	1	10		
3	Q	2	Total	C	N	O	0	0
			25	14	1	10		
3	R	2	Total	C	N	O	0	0
			25	14	1	10		
3	S	2	Total	C	N	O	0	0
			25	14	1	10		
3	T	2	Total	C	N	O	0	0
			25	14	1	10		

- 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
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0

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

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Mol	Chain	Residues	Atoms				AltConf
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	D	1	Total	Zn	0
			1	1	
5	E	1	Total	Zn	0
			1	1	

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

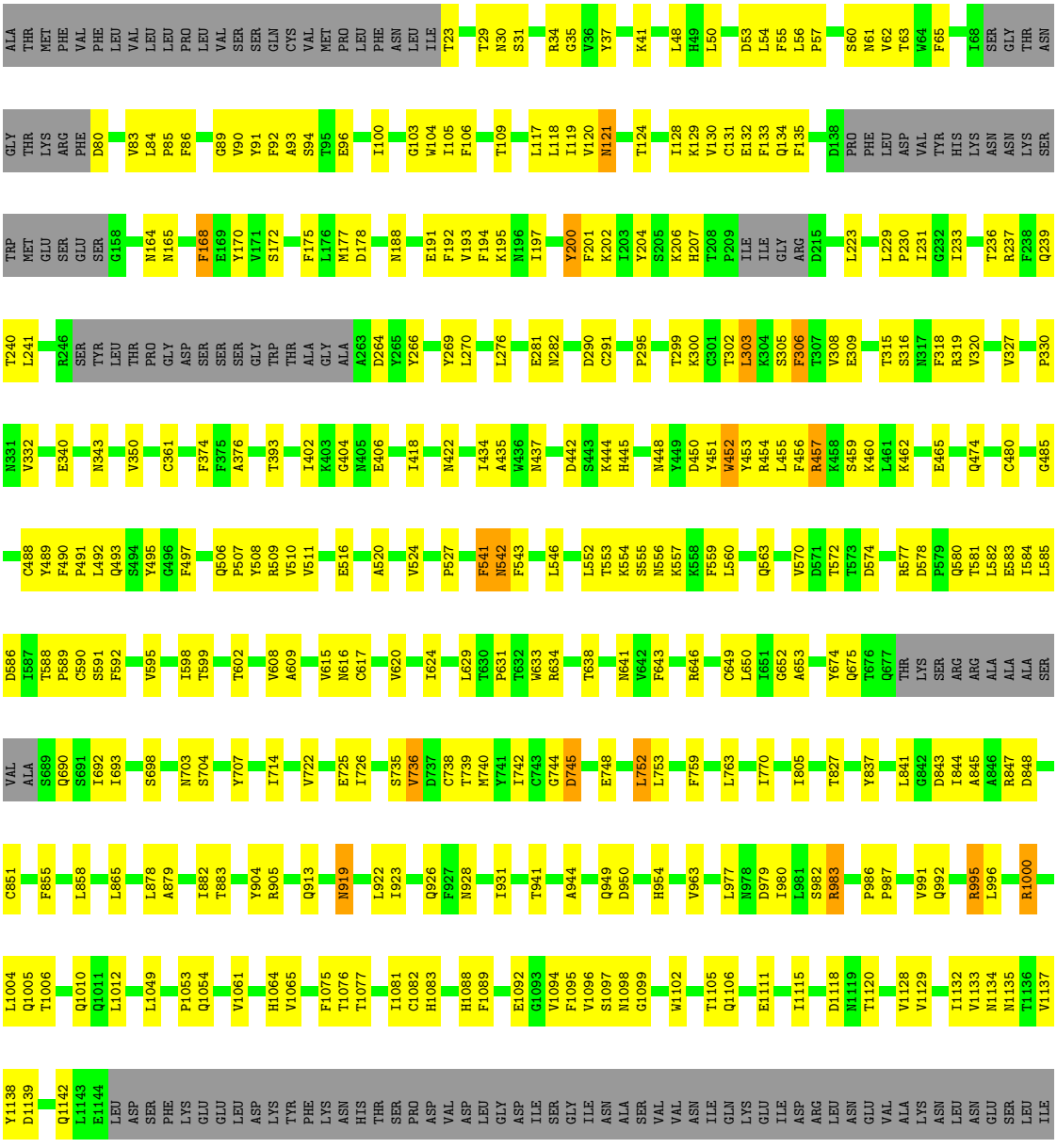
Mol	Chain	Residues	Atoms		AltConf
6	D	1	Total	Cl	0
			1	1	
6	E	1	Total	Cl	0
			1	1	

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. 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. 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.

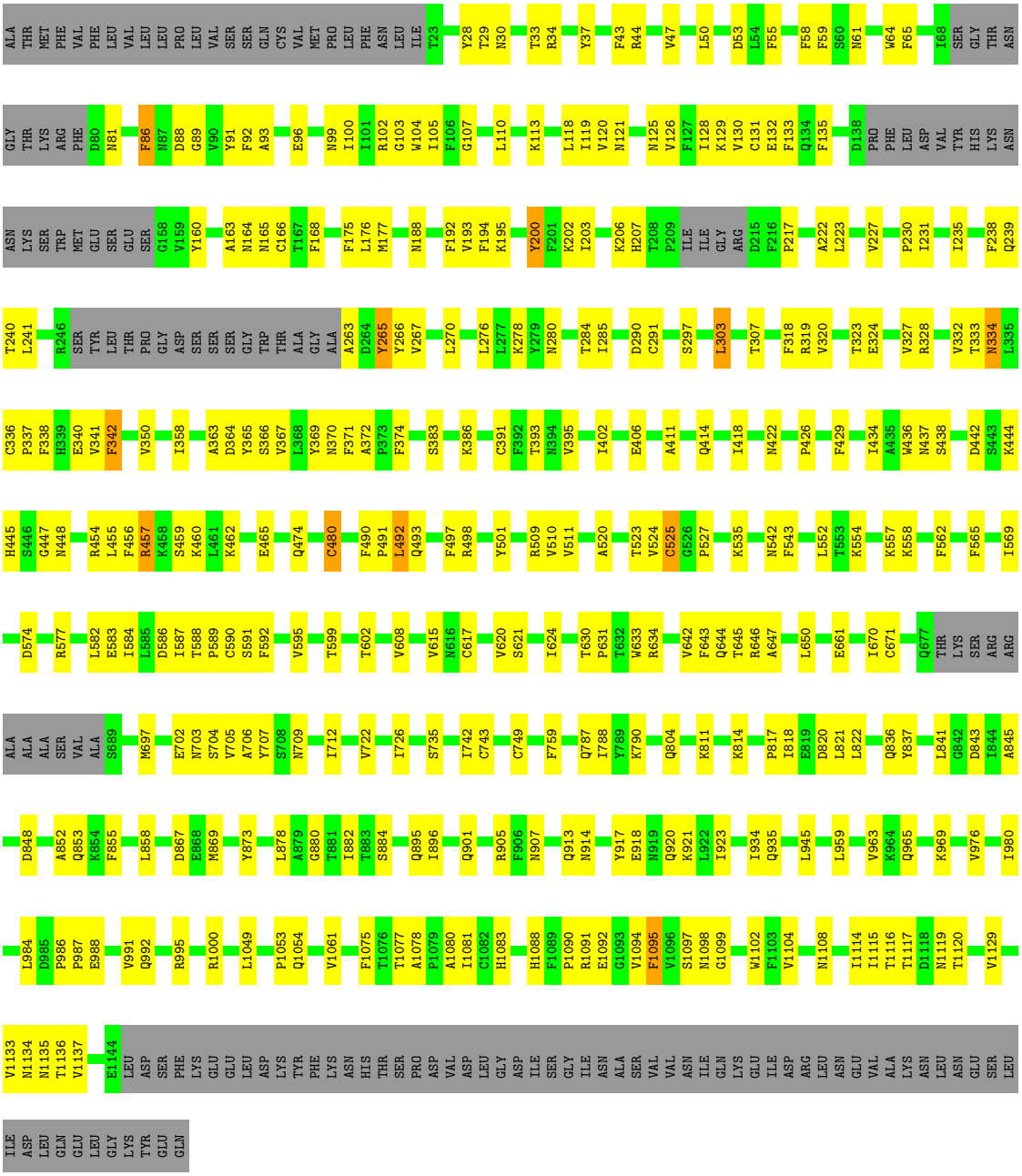
- Molecule 1: Spike glycoprotein

Chain A:



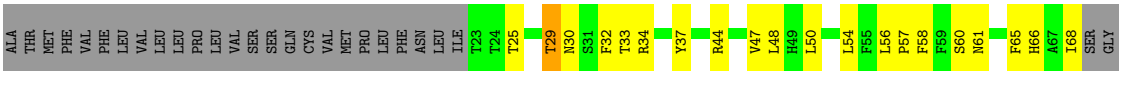
• Molecule 1: Spike glycoprotein

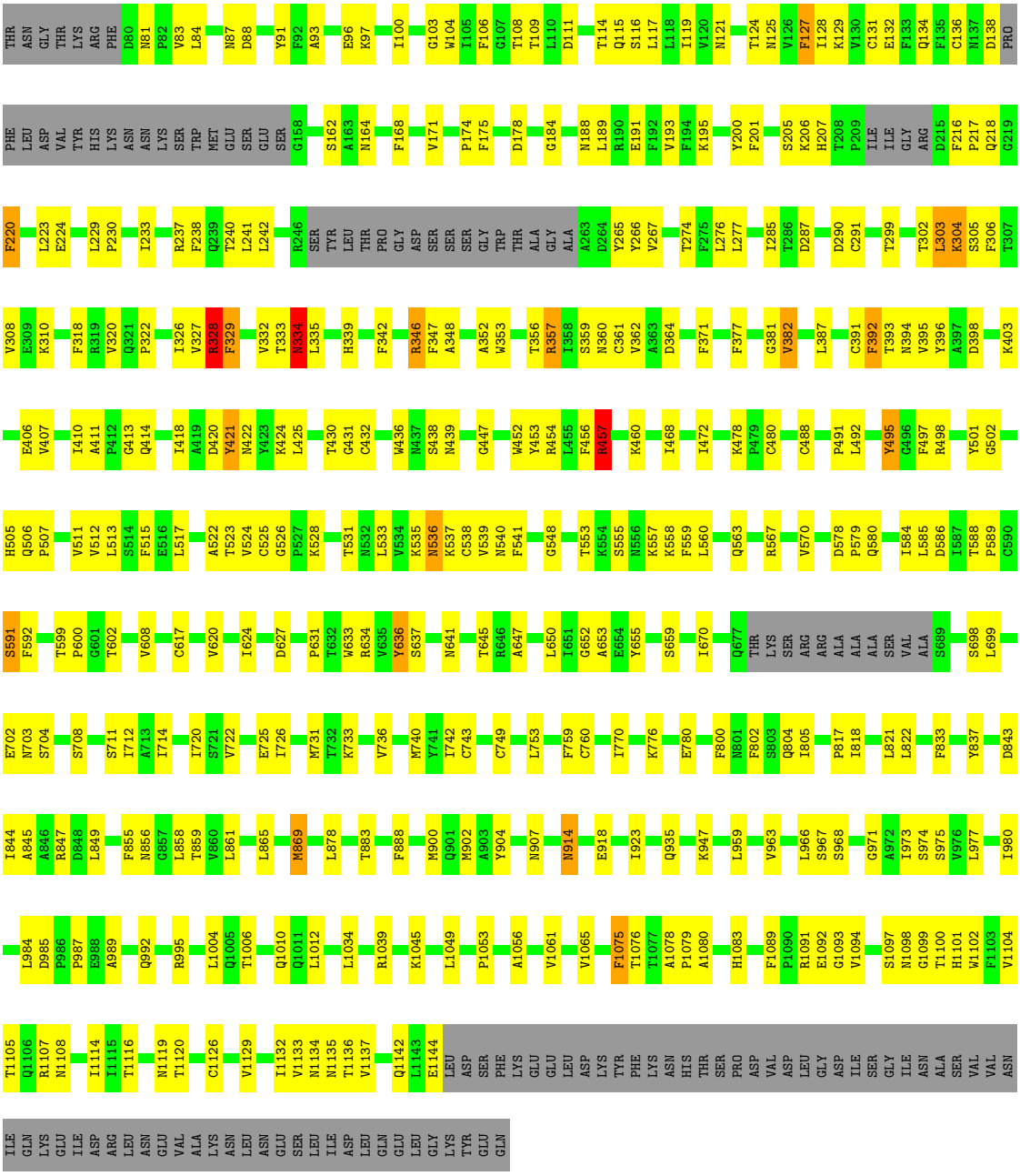
Chain B:



• Molecule 1: Spike glycoprotein

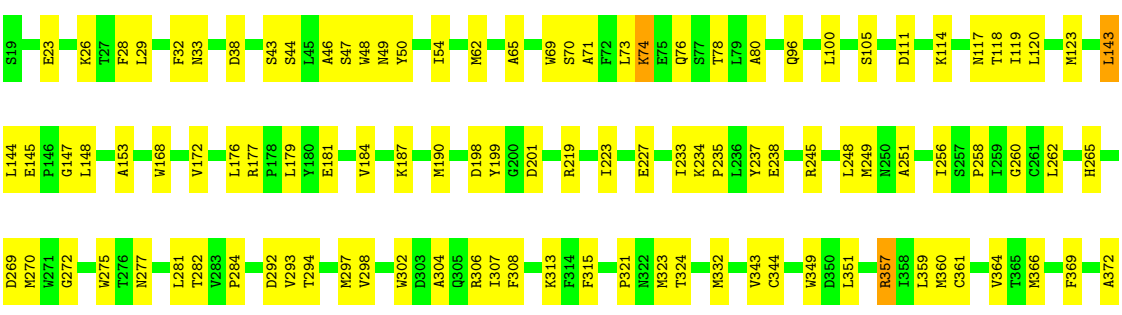
Chain C:

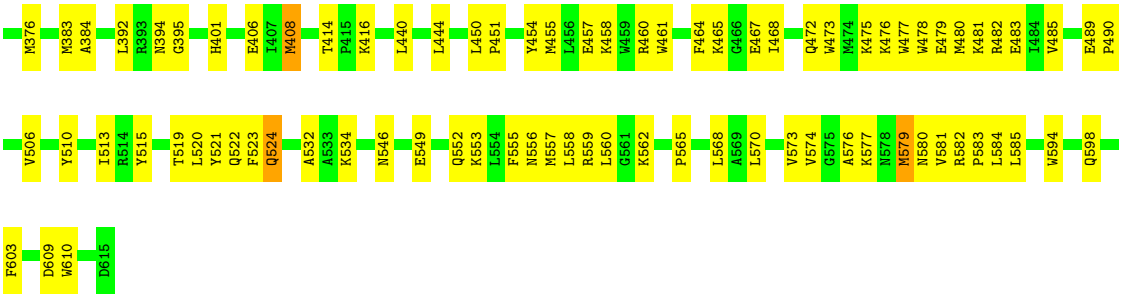




• Molecule 2: Processed angiotensin-converting enzyme 2

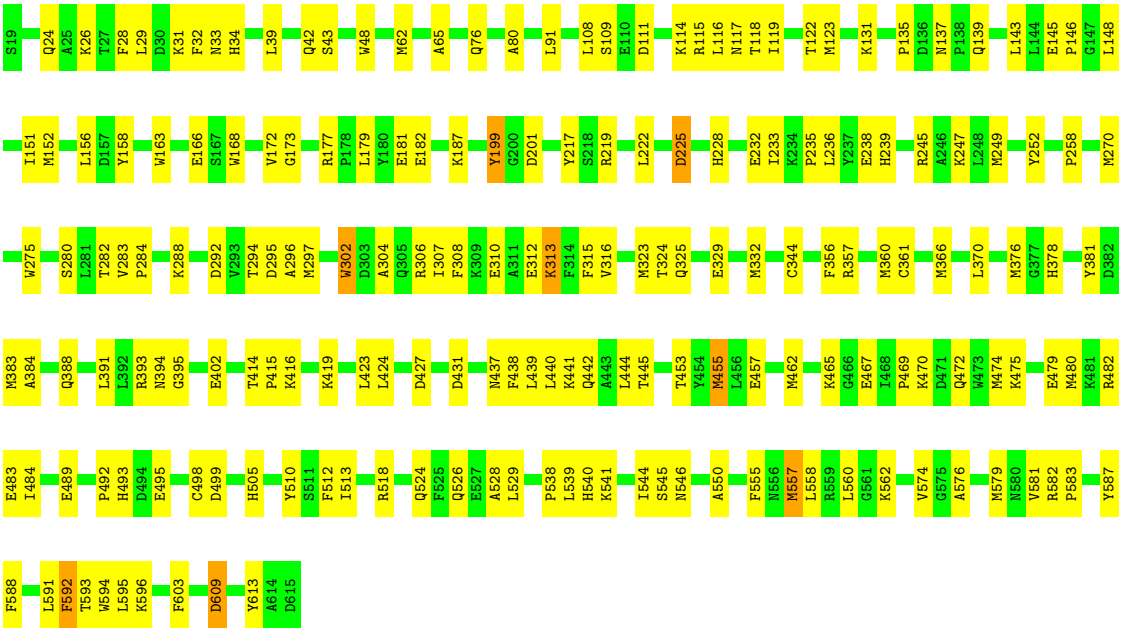
Chain D:





• Molecule 2: Processed angiotensin-converting enzyme 2

Chain E:

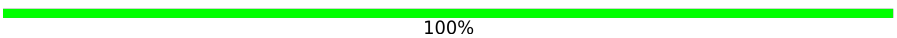


• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

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

Chain G:



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

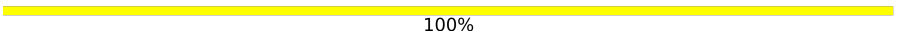
Chain H:

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

Chain I:

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

Chain J:

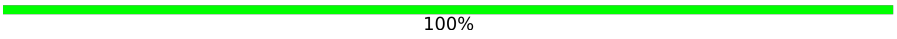


• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

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

Chain L:

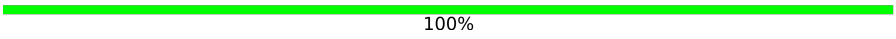


• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

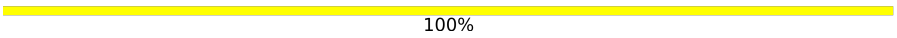
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



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

Chain O:

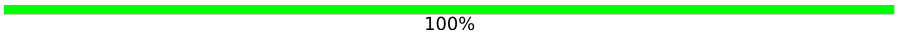


• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

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

Chain Q:

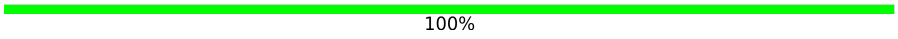


• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

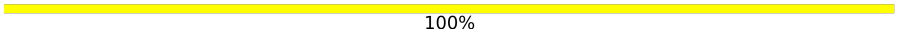
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



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

Chain T:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	284921	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.38	1/8484 (0.0%)	0.53	0/11547
1	B	0.36	0/8484	0.52	0/11547
1	C	0.39	0/8484	0.55	0/11547
2	D	0.31	0/5007	0.47	0/6803
2	E	0.32	0/5007	0.48	0/6803
All	All	0.36	1/35466 (0.0%)	0.52	0/48247

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	A	0	1
1	B	0	1
1	C	0	4
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	736	VAL	CB-CG2	-5.10	1.42	1.52

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	995	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	328	ARG	Sidechain
1	C	328	ARG	Sidechain
1	C	346	ARG	Sidechain
1	C	357	ARG	Sidechain

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	8285	0	8061	269	0
1	B	8285	0	8063	238	0
1	C	8285	0	8064	300	0
2	D	4870	0	4639	171	0
2	E	4870	0	4639	146	0
3	F	25	0	22	1	0
3	G	25	0	22	0	0
3	H	25	0	22	0	0
3	I	25	0	22	1	0
3	J	25	0	22	0	0
3	K	25	0	22	0	0
3	L	25	0	22	0	0
3	M	25	0	22	0	0
3	N	25	0	22	0	0
3	O	25	0	22	0	0
3	P	25	0	22	0	0
3	Q	25	0	22	0	0
3	R	25	0	22	1	0
3	S	25	0	22	0	0
3	T	25	0	22	0	0
4	A	154	0	143	6	0
4	B	154	0	143	4	0
4	C	154	0	143	3	0
4	D	56	0	52	0	0
4	E	56	0	52	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
6	D	1	0	0	1	0
6	E	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	35548	0	34329	1083	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 16.

The worst 5 of 1083 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)
2:D:476:LYS:HE3	2:D:480:MET:CE	1.72	1.19
1:B:586:ASP:O	1:B:587:ILE:HD13	1.43	1.16
2:E:302:TRP:CD1	2:E:306:ARG:HD3	1.86	1.09
1:C:726:ILE:HD12	1:C:1061:VAL:HG22	1.36	1.07
1:A:763:LEU:HD11	1:A:1005:GLN:HE22	0.99	1.07

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	1047/1206 (87%)	960 (92%)	83 (8%)	4 (0%)	30	61
1	B	1047/1206 (87%)	952 (91%)	91 (9%)	4 (0%)	30	61
1	C	1047/1206 (87%)	949 (91%)	90 (9%)	8 (1%)	16	46
2	D	595/597 (100%)	576 (97%)	18 (3%)	1 (0%)	44	71
2	E	595/597 (100%)	573 (96%)	22 (4%)	0	100	100
All	All	4331/4812 (90%)	4010 (93%)	304 (7%)	17 (0%)	32	61

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	591	SER
1	A	983	ARG
1	C	348	ALA
1	C	536	ASN
1	C	591	SER

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	922/1054 (88%)	902 (98%)	20 (2%)	47	69
1	B	922/1054 (88%)	894 (97%)	28 (3%)	36	62
1	C	922/1054 (88%)	885 (96%)	37 (4%)	27	55
2	D	527/527 (100%)	517 (98%)	10 (2%)	52	72
2	E	527/527 (100%)	514 (98%)	13 (2%)	42	67
All	All	3820/4216 (91%)	3712 (97%)	108 (3%)	40	64

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	306	PHE
1	C	495	TYR
2	E	302	TRP
1	C	328	ARG
1	C	356	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	334	ASN
1	C	1108	ASN
2	E	437	ASN
1	C	1083	HIS
1	C	1119	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)

30 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	F	1	3,1	14,14,15	0.49	0	17,19,21	0.97	1 (5%)
3	BMA	F	2	3	11,11,12	0.85	1 (9%)	15,15,17	0.84	0
3	NAG	G	1	3,1	14,14,15	0.20	0	17,19,21	0.40	0
3	BMA	G	2	3	11,11,12	0.66	0	15,15,17	0.71	0
3	NAG	H	1	3,1	14,14,15	0.38	0	17,19,21	0.96	2 (11%)
3	BMA	H	2	3	11,11,12	0.61	0	15,15,17	0.74	0
3	NAG	I	1	3,1	14,14,15	0.25	0	17,19,21	0.43	0
3	BMA	I	2	3	11,11,12	0.59	0	15,15,17	0.77	0
3	NAG	J	1	3,1	14,14,15	1.53	1 (7%)	17,19,21	1.31	1 (5%)
3	BMA	J	2	3	11,11,12	0.80	0	15,15,17	1.41	3 (20%)
3	NAG	K	1	3,1	14,14,15	0.21	0	17,19,21	0.38	0
3	BMA	K	2	3	11,11,12	0.83	1 (9%)	15,15,17	0.78	0
3	NAG	L	1	3,1	14,14,15	0.33	0	17,19,21	0.42	0
3	BMA	L	2	3	11,11,12	0.50	0	15,15,17	0.76	0
3	NAG	M	1	3,1	14,14,15	0.39	0	17,19,21	0.90	2 (11%)
3	BMA	M	2	3	11,11,12	0.72	0	15,15,17	0.70	0
3	NAG	N	1	3,1	14,14,15	0.24	0	17,19,21	0.43	0
3	BMA	N	2	3	11,11,12	0.66	0	15,15,17	0.74	0
3	NAG	O	1	3,1	14,14,15	1.51	1 (7%)	17,19,21	1.30	1 (5%)
3	BMA	O	2	3	11,11,12	1.00	2 (18%)	15,15,17	1.39	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	P	1	3,1	14,14,15	0.32	0	17,19,21	0.37	0
3	BMA	P	2	3	11,11,12	0.90	0	15,15,17	0.91	0
3	NAG	Q	1	3,1	14,14,15	0.27	0	17,19,21	0.52	0
3	BMA	Q	2	3	11,11,12	0.63	0	15,15,17	0.72	0
3	NAG	R	1	3,1	14,14,15	0.39	0	17,19,21	0.87	2 (11%)
3	BMA	R	2	3	11,11,12	0.83	0	15,15,17	0.64	0
3	NAG	S	1	3,1	14,14,15	0.29	0	17,19,21	0.47	0
3	BMA	S	2	3	11,11,12	0.66	0	15,15,17	0.76	0
3	NAG	T	1	3,1	14,14,15	1.58	1 (7%)	17,19,21	1.36	1 (5%)
3	BMA	T	2	3	11,11,12	0.91	1 (9%)	15,15,17	1.09	1 (6%)

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	F	1	3,1	-	2/6/23/26	0/1/1/1
3	BMA	F	2	3	-	0/2/19/22	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	BMA	G	2	3	-	0/2/19/22	0/1/1/1
3	NAG	H	1	3,1	-	5/6/23/26	0/1/1/1
3	BMA	H	2	3	-	2/2/19/22	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	BMA	I	2	3	-	0/2/19/22	0/1/1/1
3	NAG	J	1	3,1	-	2/6/23/26	0/1/1/1
3	BMA	J	2	3	-	2/2/19/22	0/1/1/1
3	NAG	K	1	3,1	-	4/6/23/26	0/1/1/1
3	BMA	K	2	3	-	0/2/19/22	0/1/1/1
3	NAG	L	1	3,1	-	0/6/23/26	0/1/1/1
3	BMA	L	2	3	-	0/2/19/22	0/1/1/1
3	NAG	M	1	3,1	-	5/6/23/26	0/1/1/1
3	BMA	M	2	3	-	2/2/19/22	0/1/1/1
3	NAG	N	1	3,1	-	1/6/23/26	0/1/1/1
3	BMA	N	2	3	-	0/2/19/22	0/1/1/1
3	NAG	O	1	3,1	-	2/6/23/26	0/1/1/1
3	BMA	O	2	3	-	2/2/19/22	0/1/1/1
3	NAG	P	1	3,1	-	4/6/23/26	0/1/1/1
3	BMA	P	2	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	Q	1	3,1	-	0/6/23/26	0/1/1/1
3	BMA	Q	2	3	-	0/2/19/22	0/1/1/1
3	NAG	R	1	3,1	-	5/6/23/26	0/1/1/1
3	BMA	R	2	3	-	1/2/19/22	0/1/1/1
3	NAG	S	1	3,1	-	2/6/23/26	0/1/1/1
3	BMA	S	2	3	-	0/2/19/22	0/1/1/1
3	NAG	T	1	3,1	-	2/6/23/26	0/1/1/1
3	BMA	T	2	3	-	1/2/19/22	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	1	NAG	O5-C1	-5.53	1.34	1.43
3	J	1	NAG	O5-C1	-5.32	1.35	1.43
3	O	1	NAG	O5-C1	-5.18	1.35	1.43
3	O	2	BMA	O5-C1	-2.37	1.39	1.43
3	K	2	BMA	C1-C2	2.13	1.57	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	T	1	NAG	C3-C4-C5	4.55	118.36	110.24
3	O	1	NAG	C3-C4-C5	4.15	117.65	110.24
3	J	1	NAG	C3-C4-C5	4.06	117.49	110.24
3	F	1	NAG	C1-O5-C5	3.37	116.76	112.19
3	J	2	BMA	C1-O5-C5	2.93	116.16	112.19

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	1	NAG	C3-C2-N2-C7
3	M	1	NAG	C3-C2-N2-C7
3	R	1	NAG	C3-C2-N2-C7
3	S	1	NAG	O5-C5-C6-O6
3	O	2	BMA	O5-C5-C6-O6

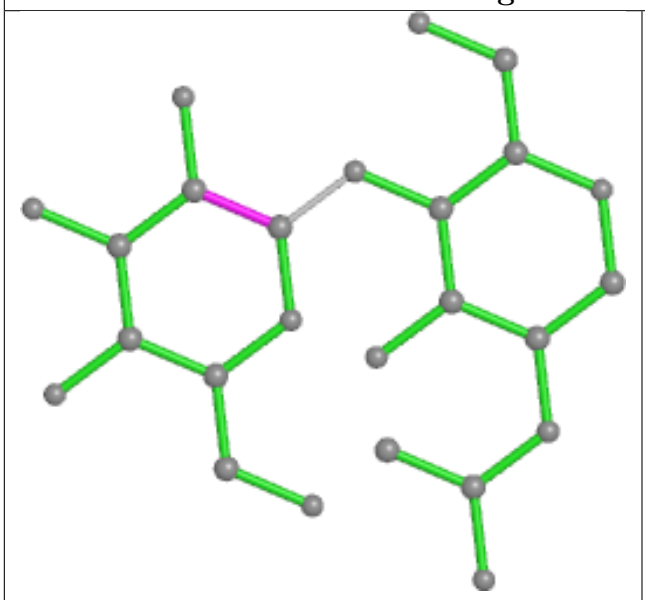
There are no ring outliers.

3 monomers are involved in 3 short contacts:

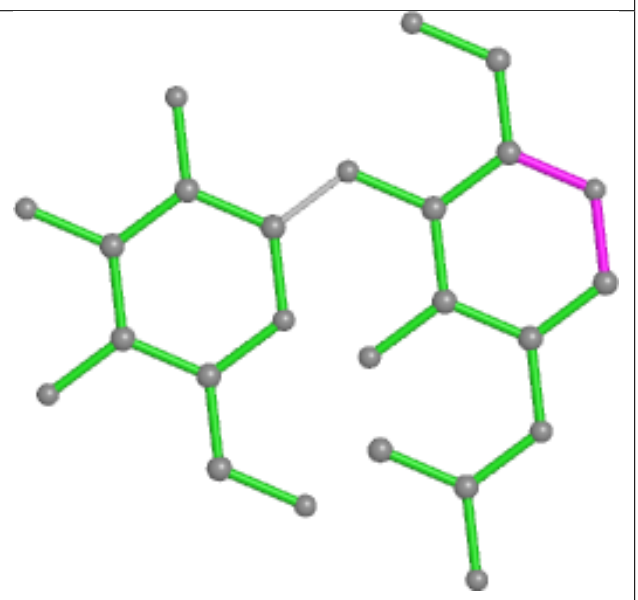
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	1	NAG	1	0
3	I	1	NAG	1	0
3	F	1	NAG	1	0

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

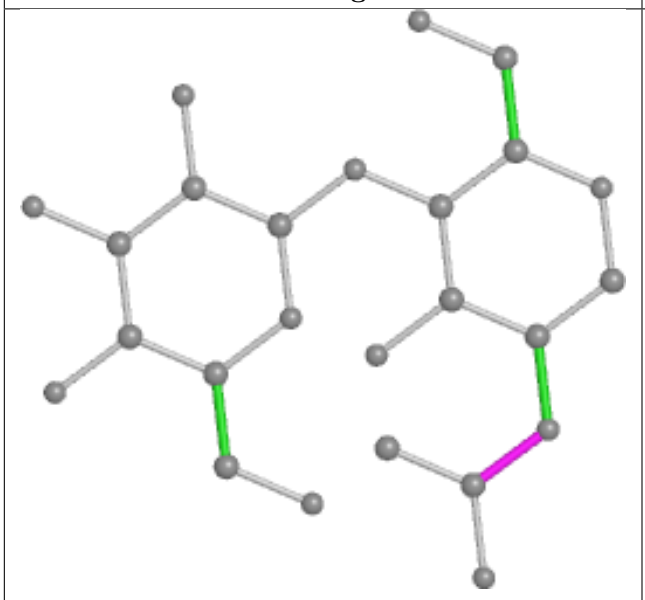
Oligosaccharide Chain F



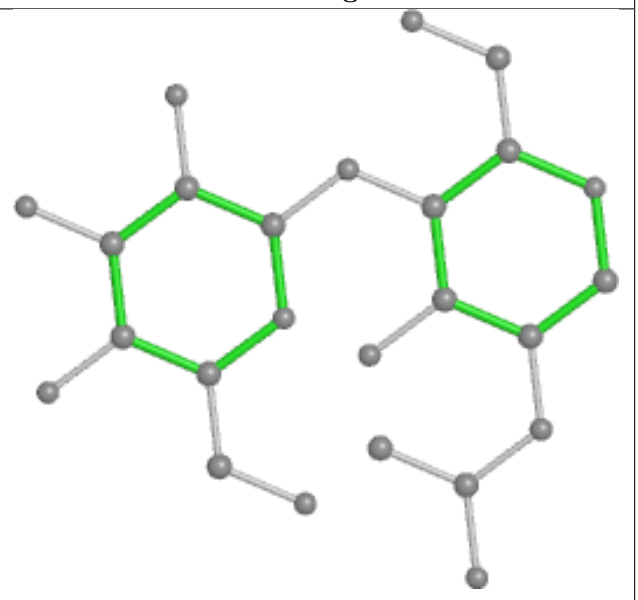
Bond lengths



Bond angles

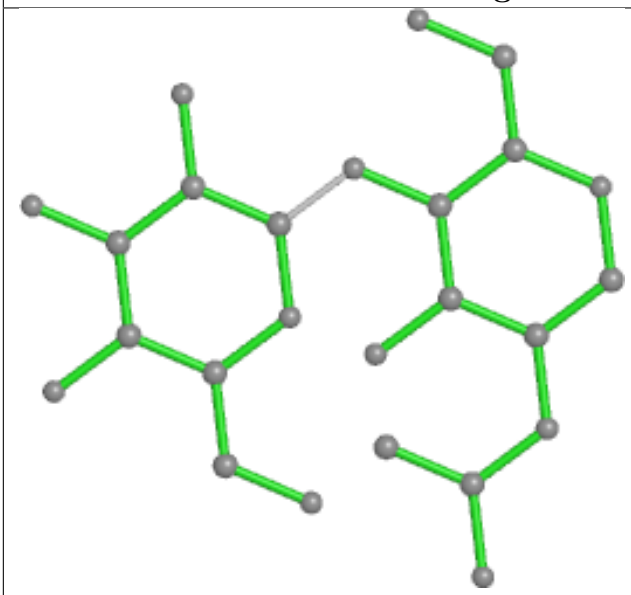


Torsions

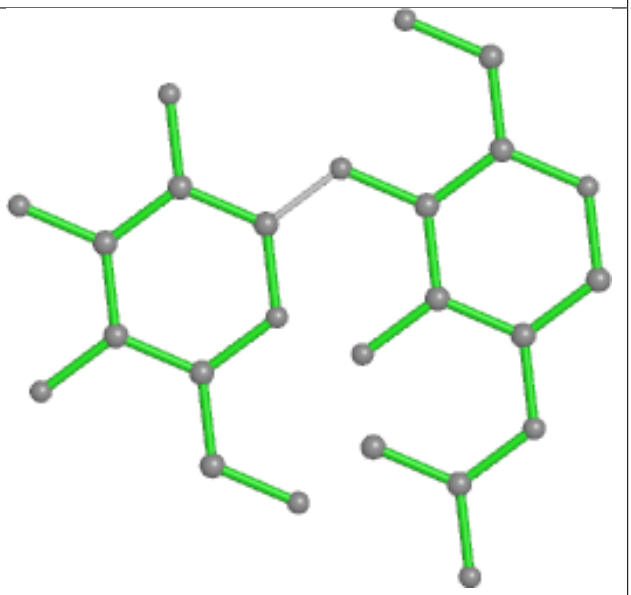


Rings

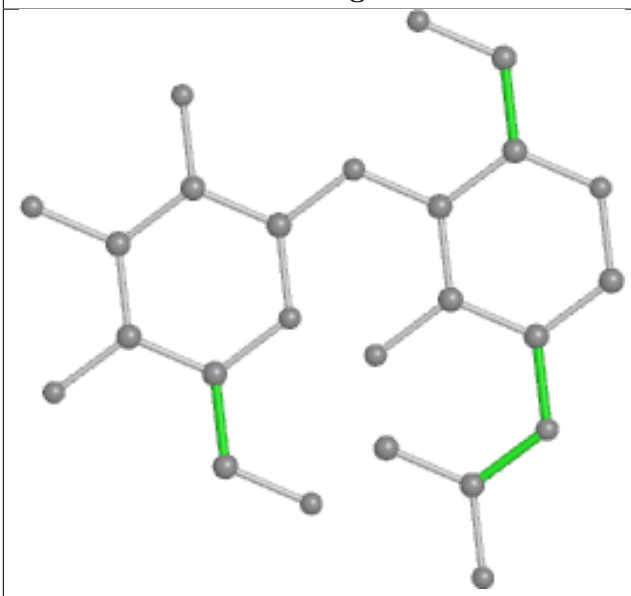
Oligosaccharide Chain G



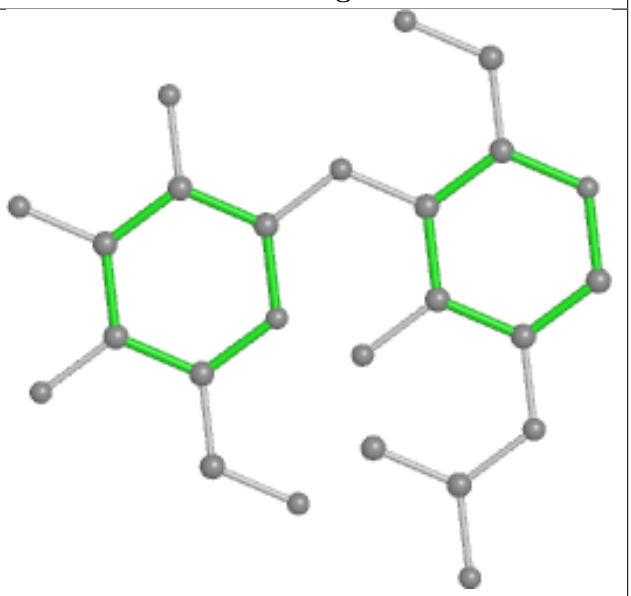
Bond lengths



Bond angles

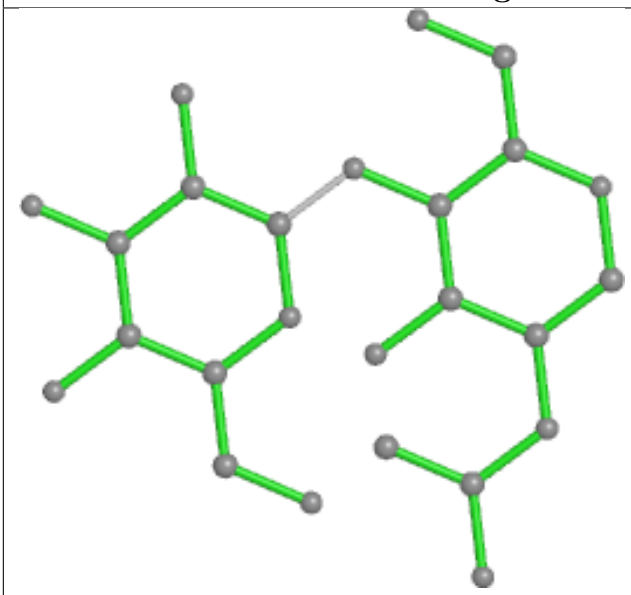


Torsions

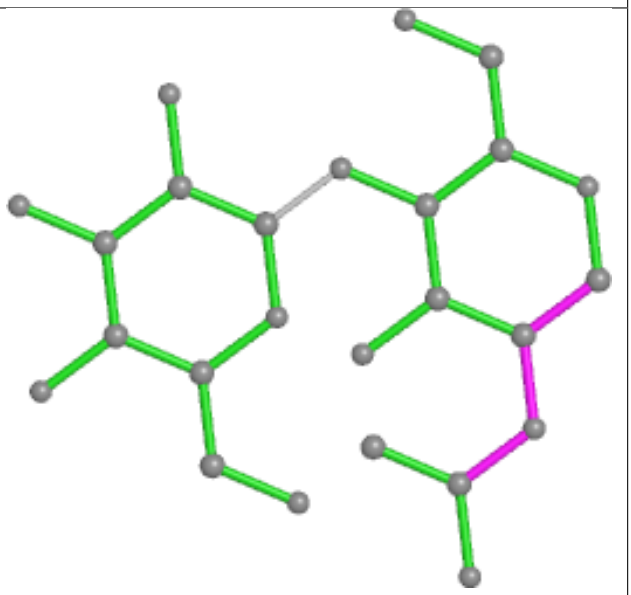


Rings

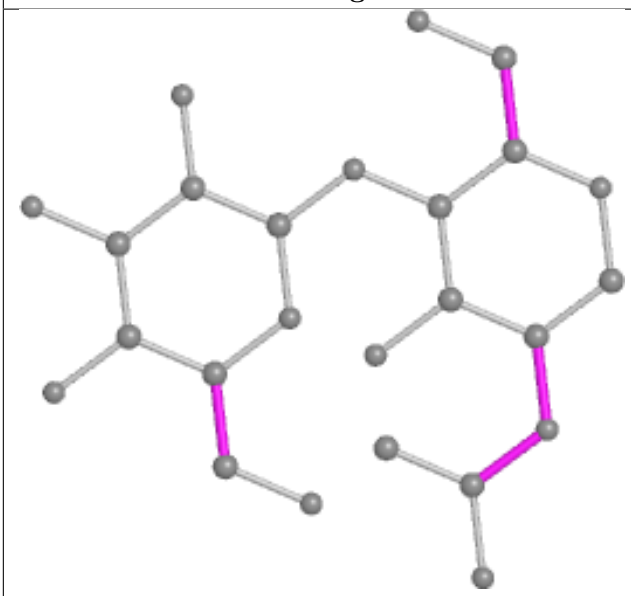
Oligosaccharide Chain H



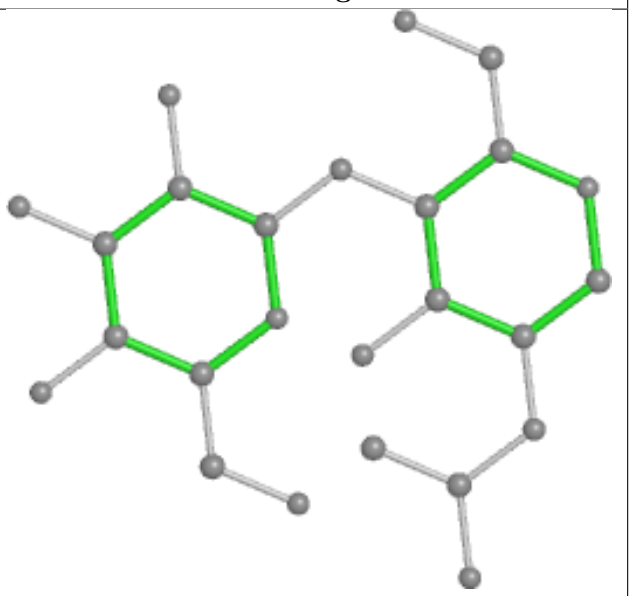
Bond lengths



Bond angles

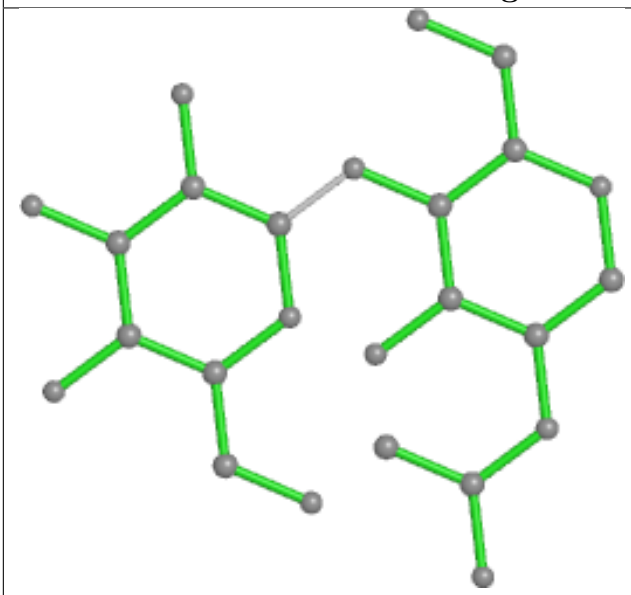


Torsions

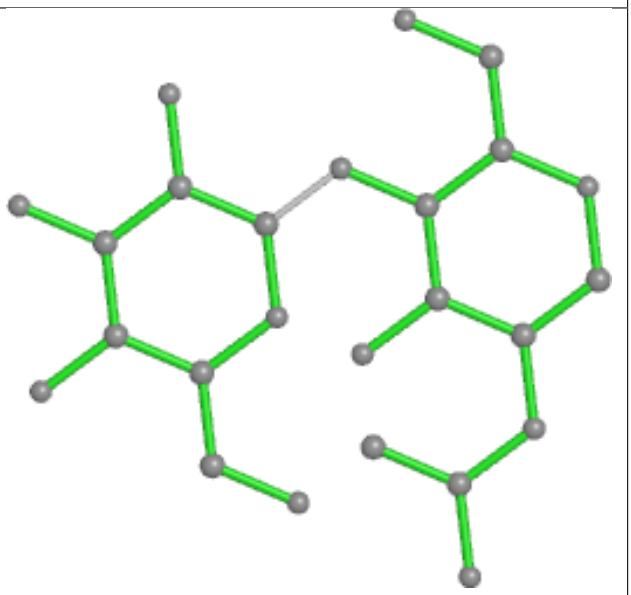


Rings

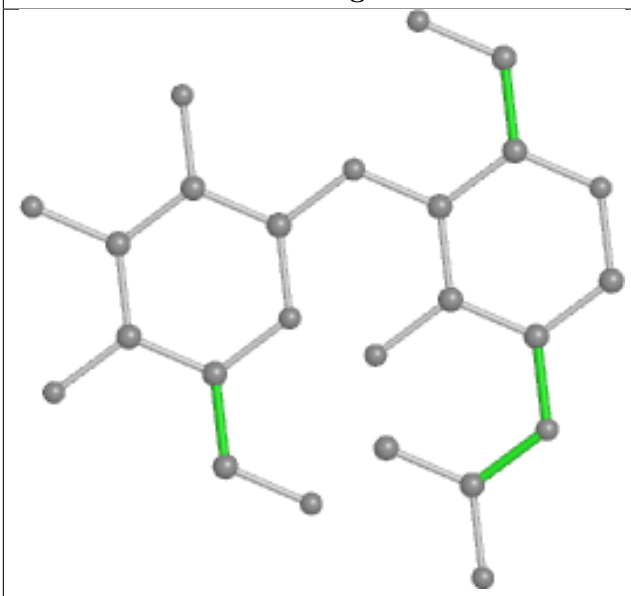
Oligosaccharide Chain I



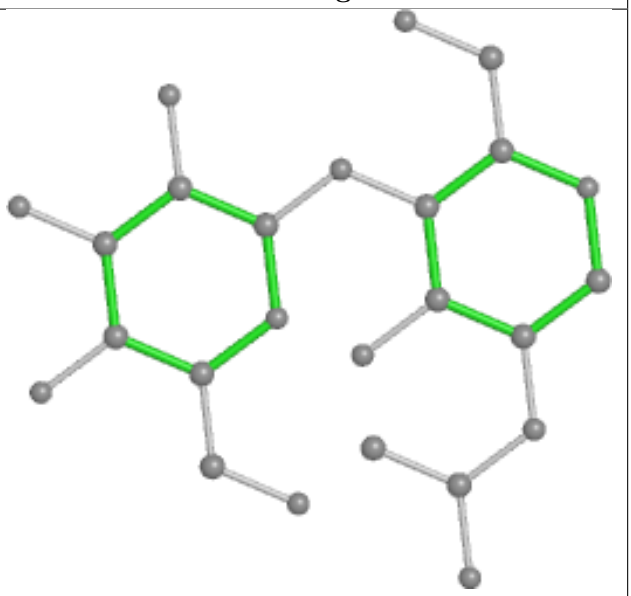
Bond lengths



Bond angles

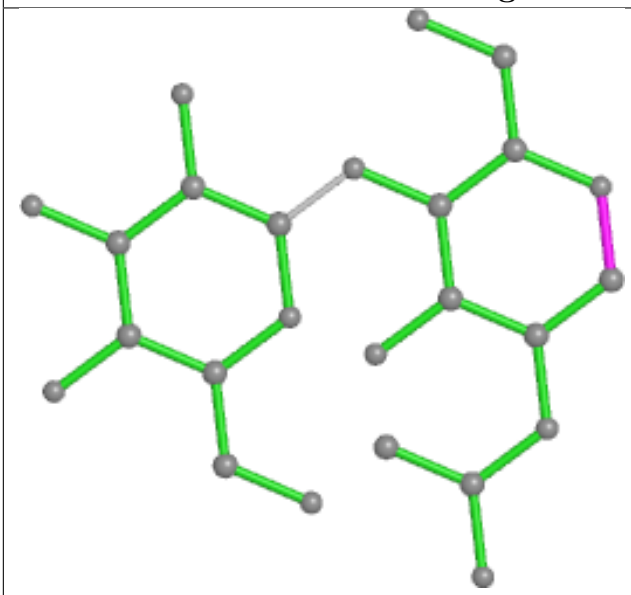


Torsions

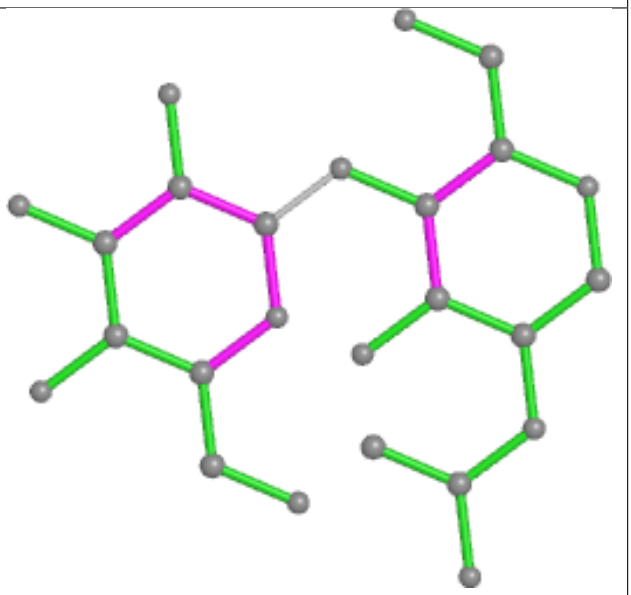


Rings

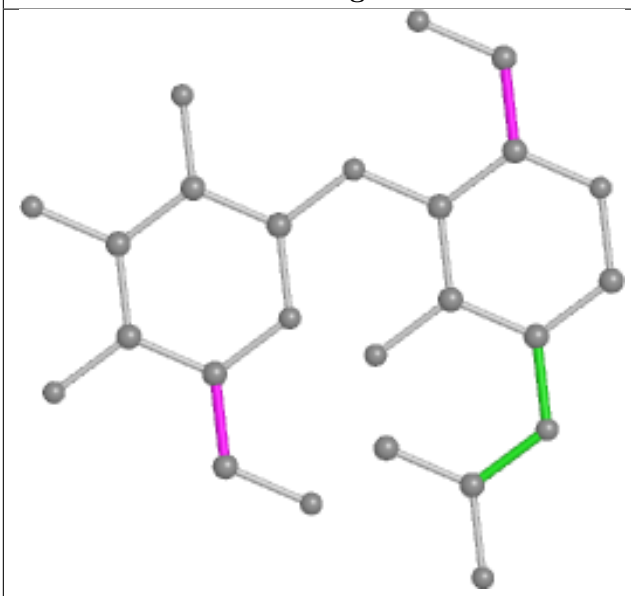
Oligosaccharide Chain J



Bond lengths



Bond angles



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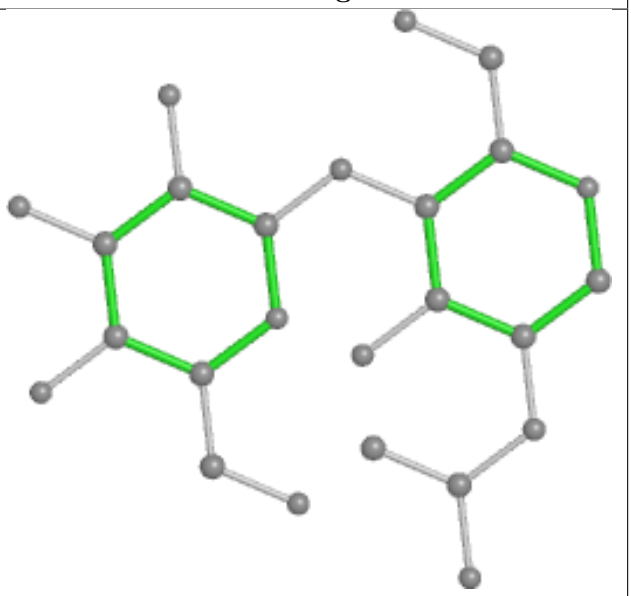
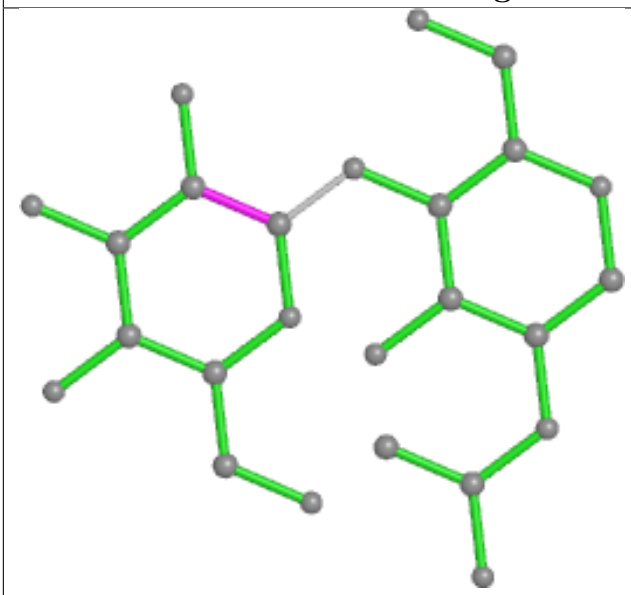


Rings

Oligosaccharide Chain K



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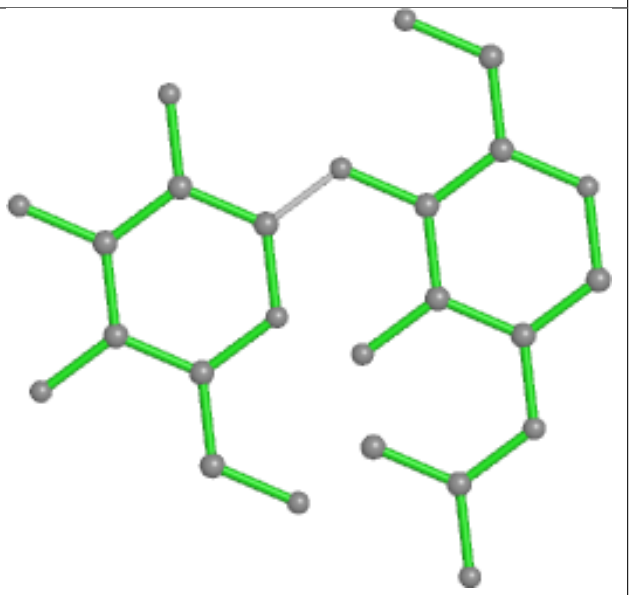

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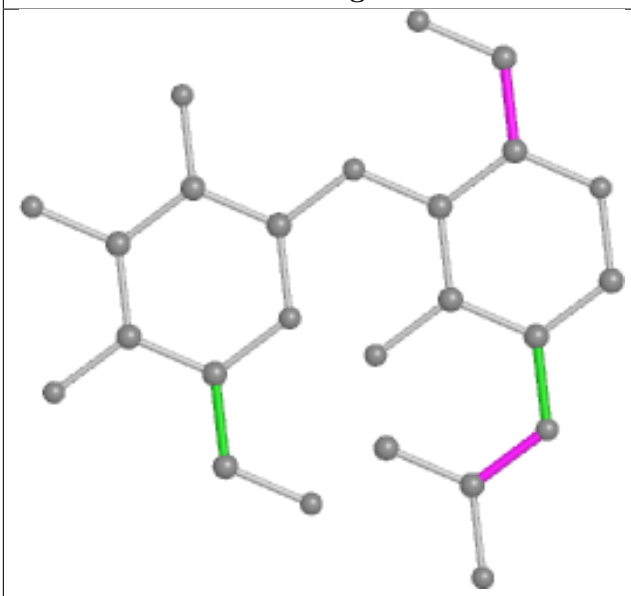

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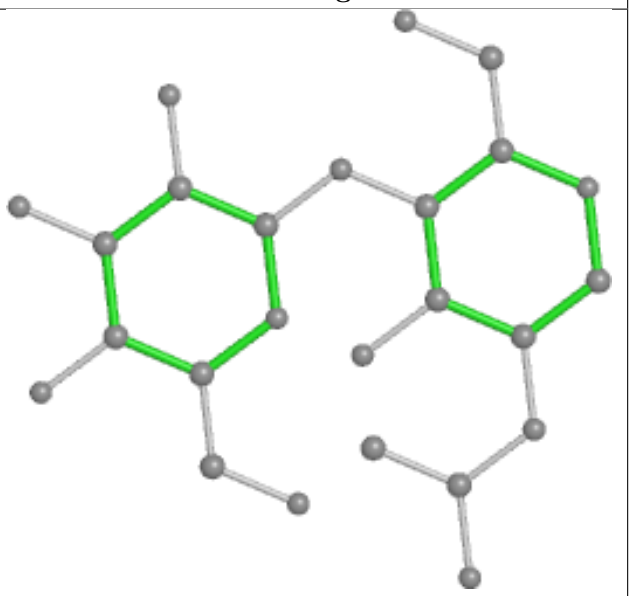
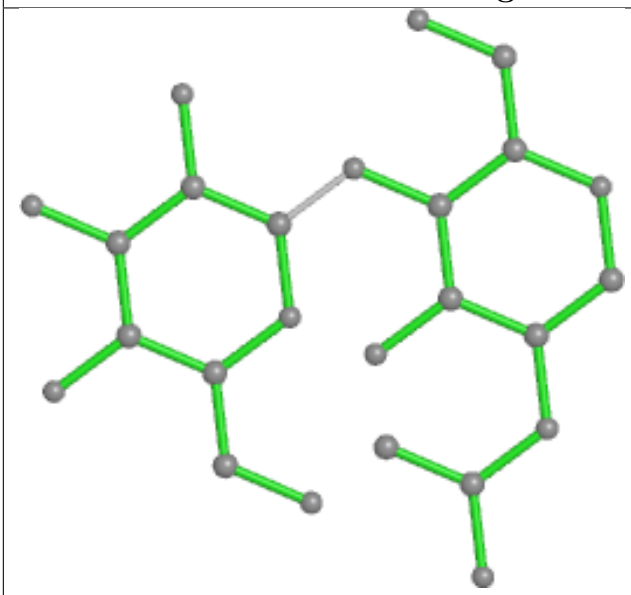
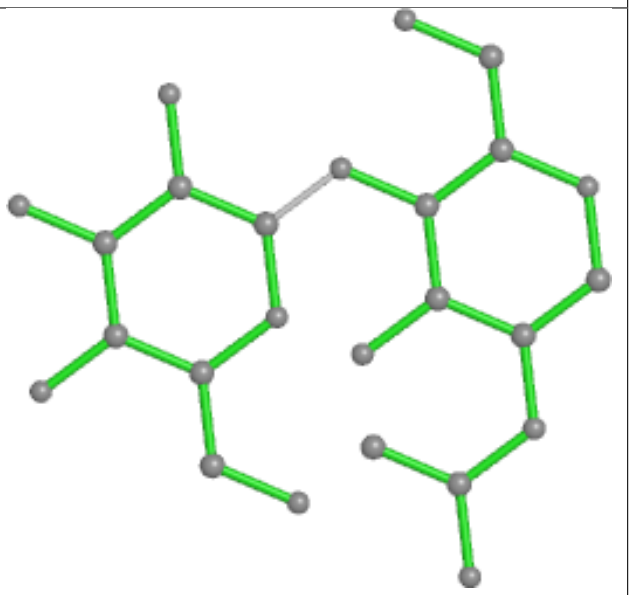


Rings

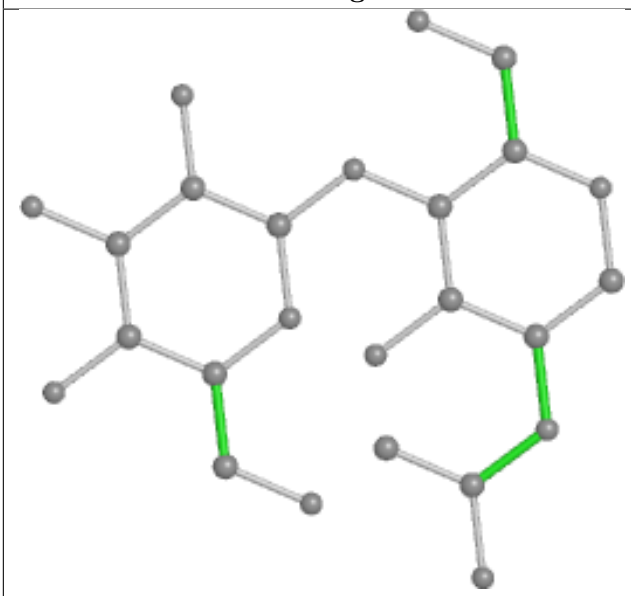
Oligosaccharide Chain L



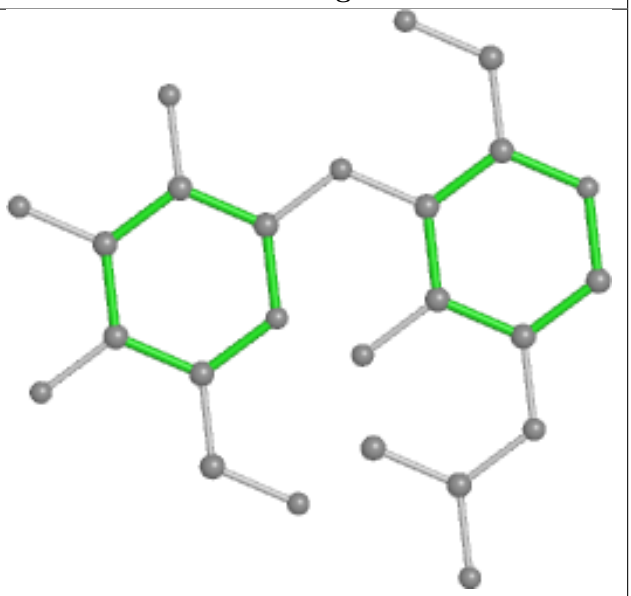
Bond lengths



Bond angles

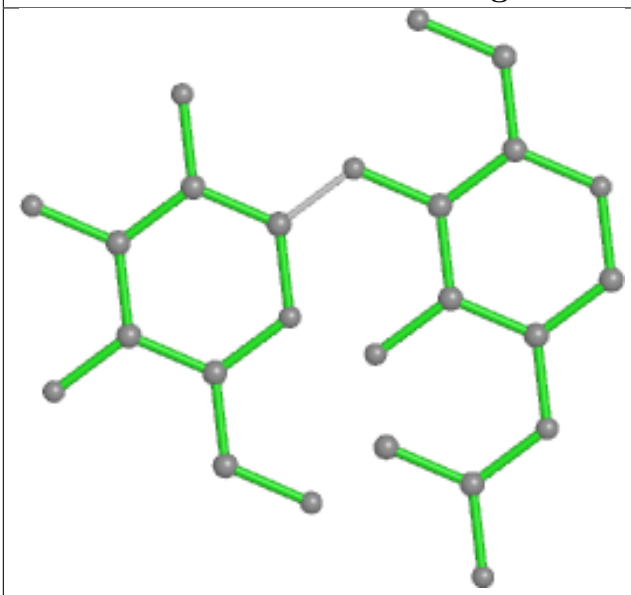


Torsions



Rings

Oligosaccharide Chain M



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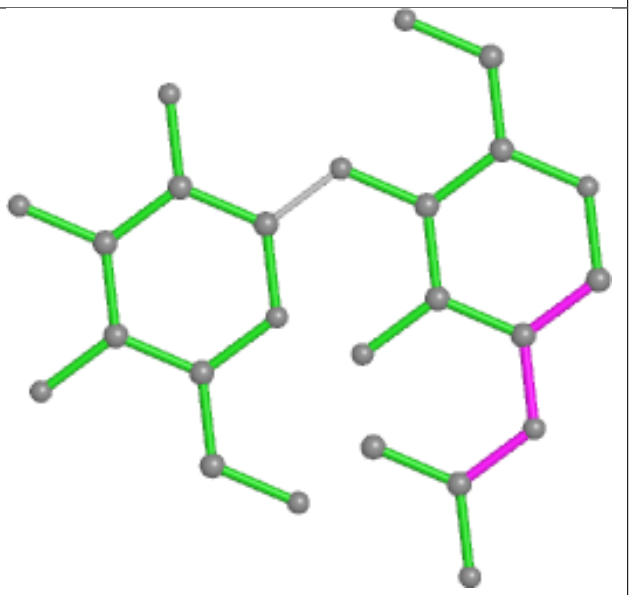
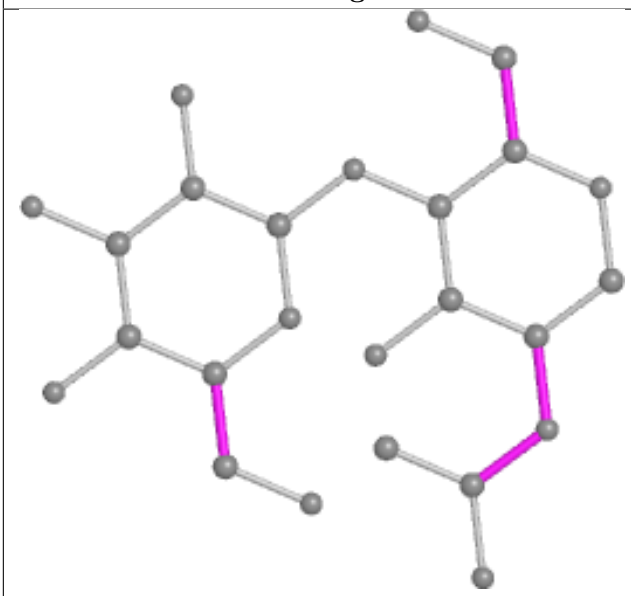
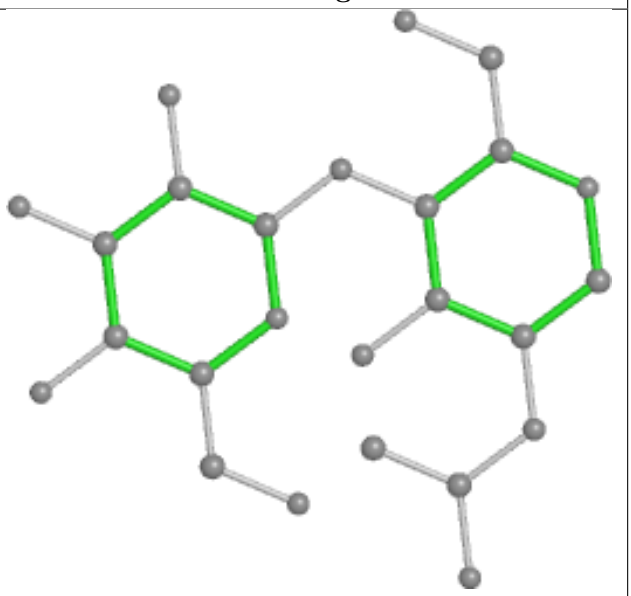


Bond angles

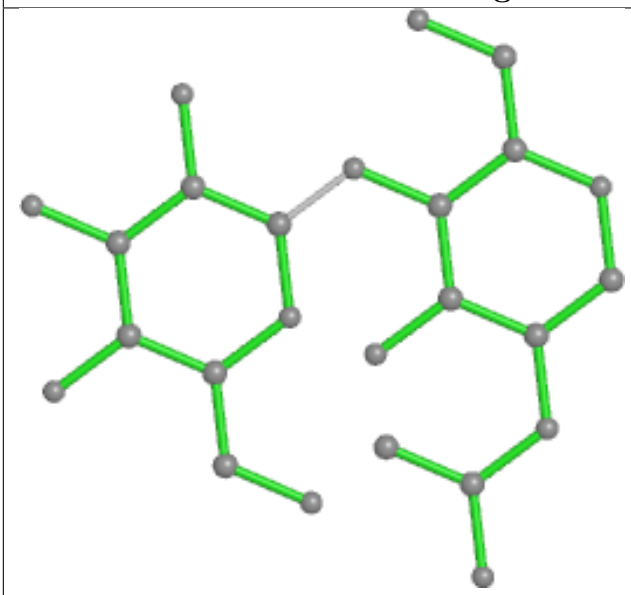


Torsions

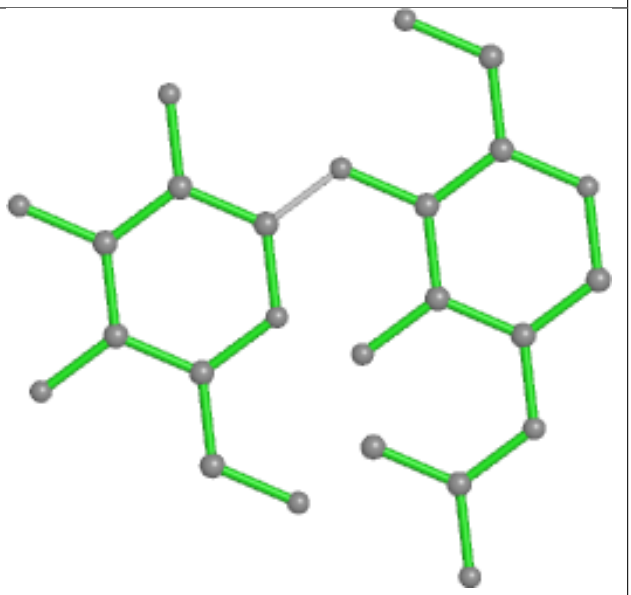


Rings

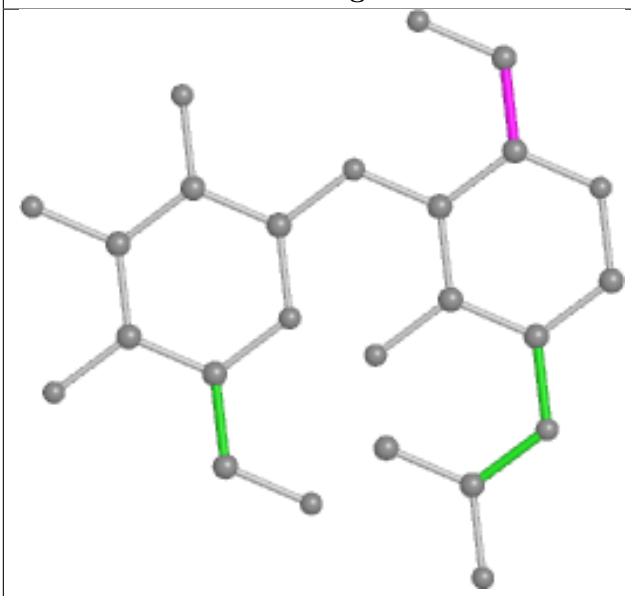
Oligosaccharide Chain N



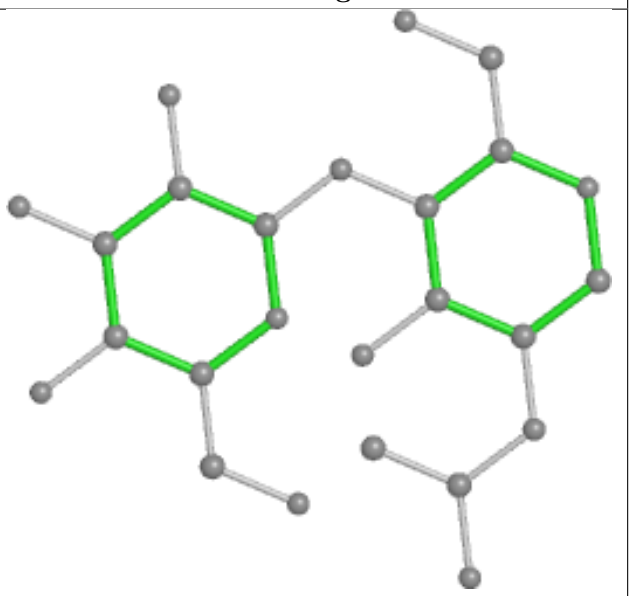
Bond lengths



Bond angles

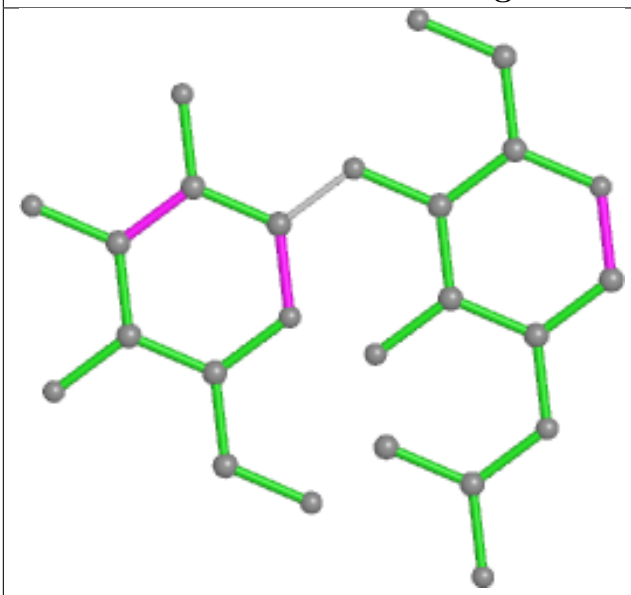


Torsions

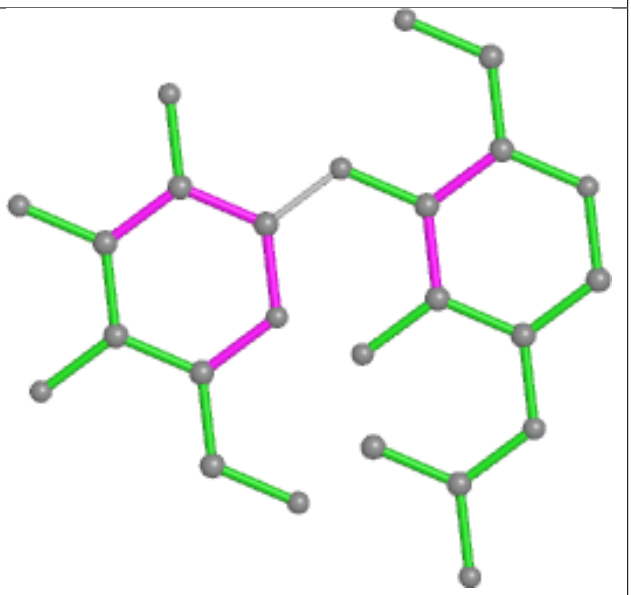


Rings

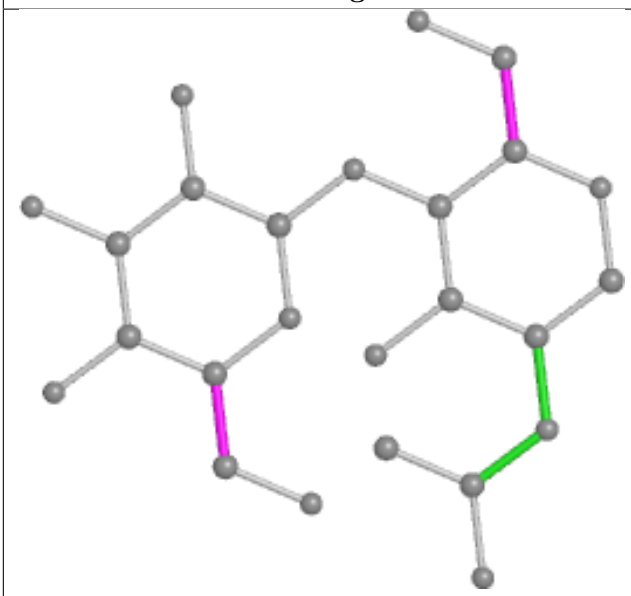
Oligosaccharide Chain O



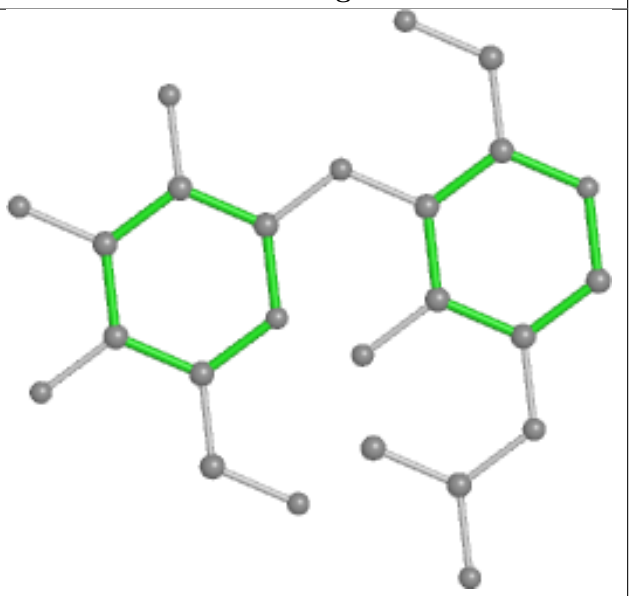
Bond lengths



Bond angles

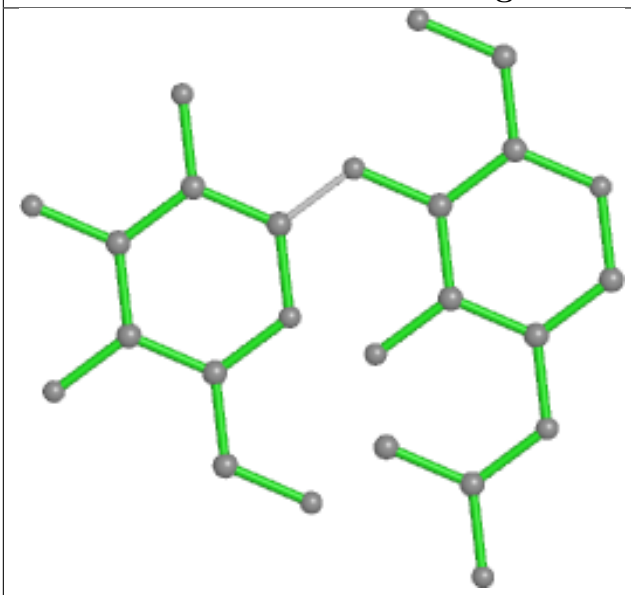


Torsions

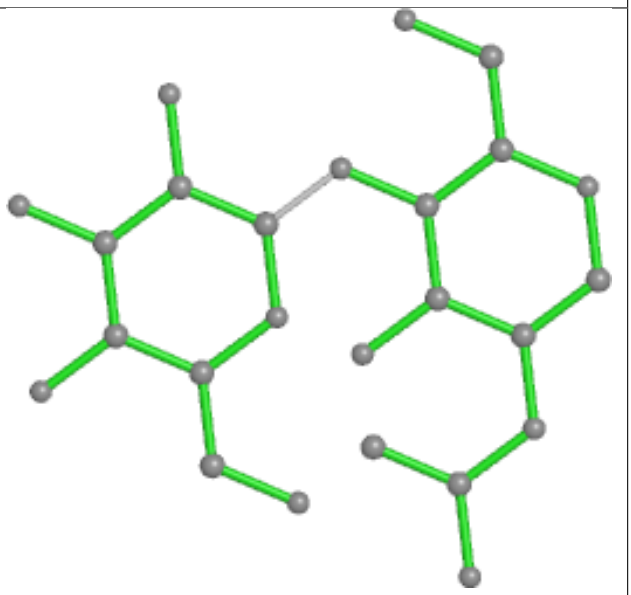


Rings

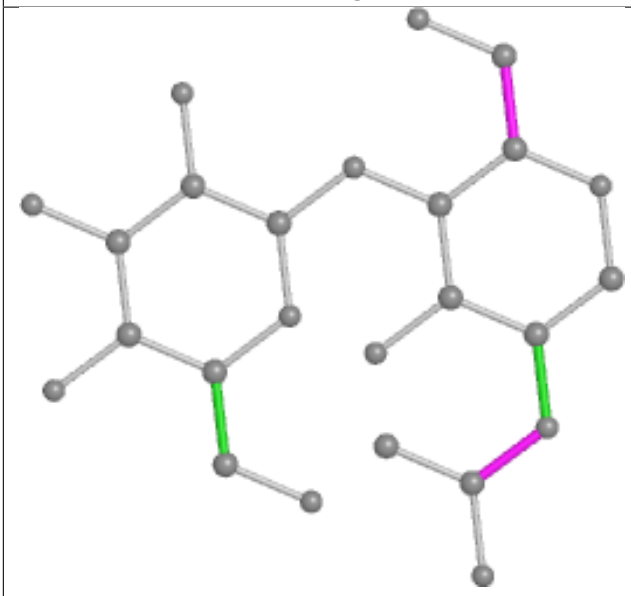
Oligosaccharide Chain P



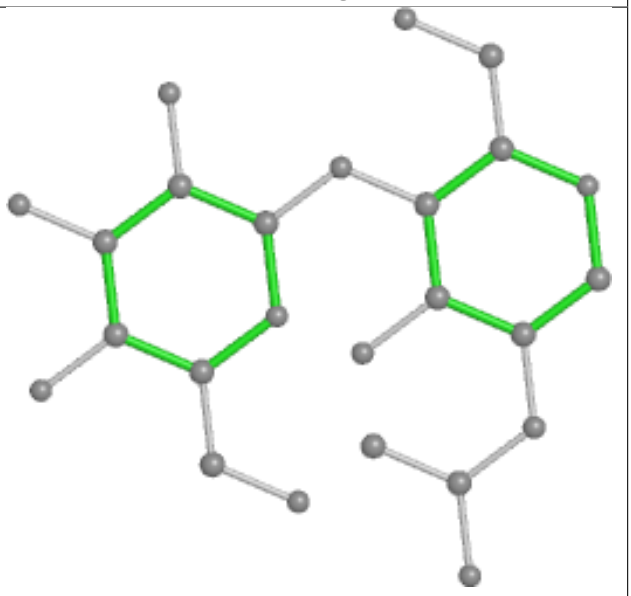
Bond lengths



Bond angles

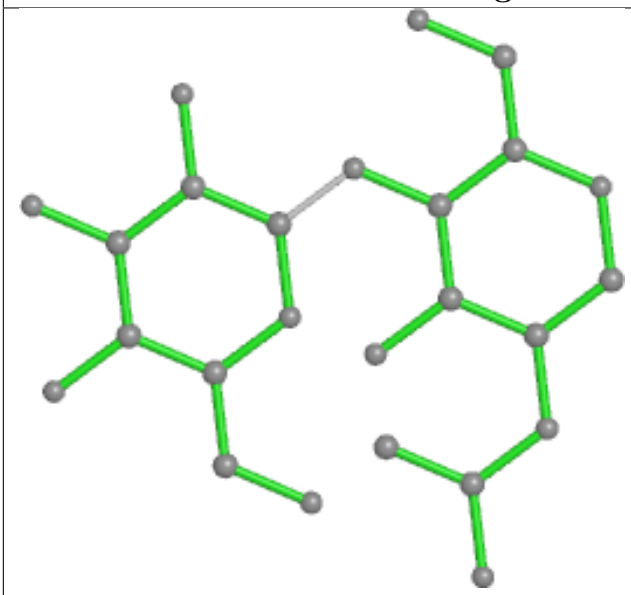


Torsions

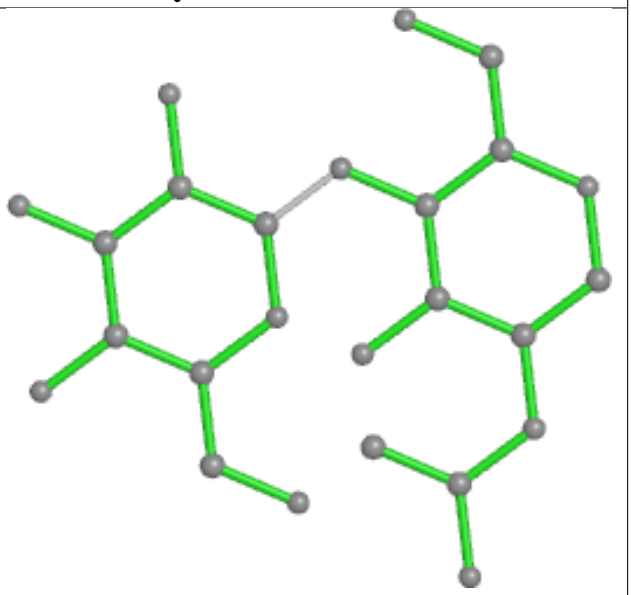


Rings

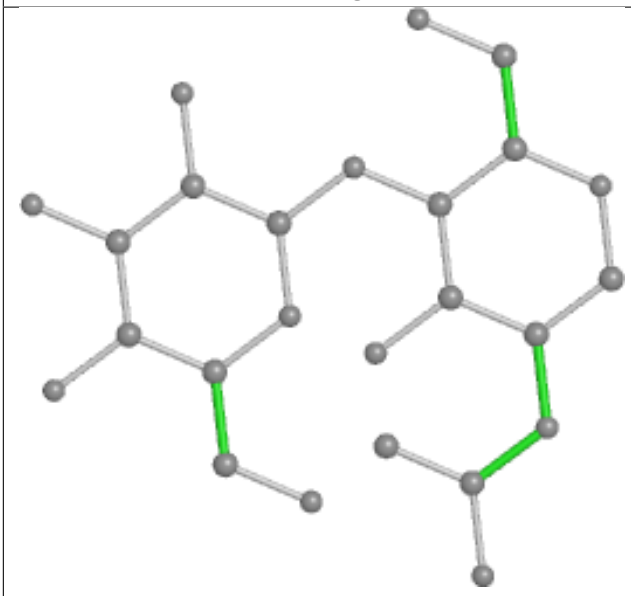
Oligosaccharide Chain Q



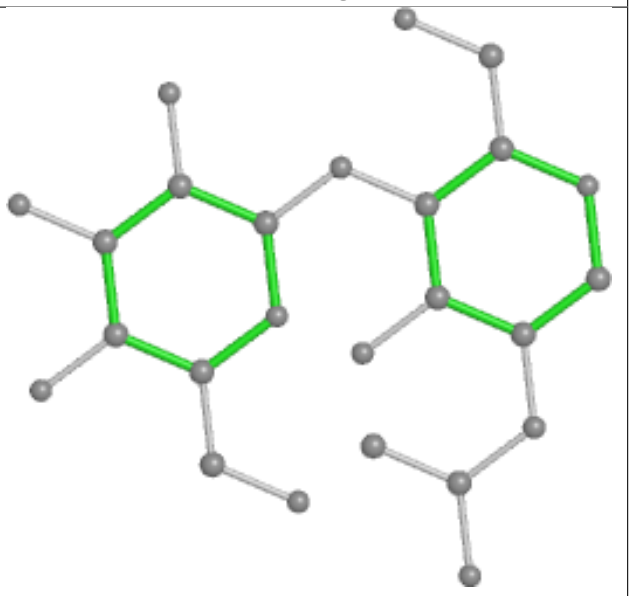
Bond lengths



Bond angles

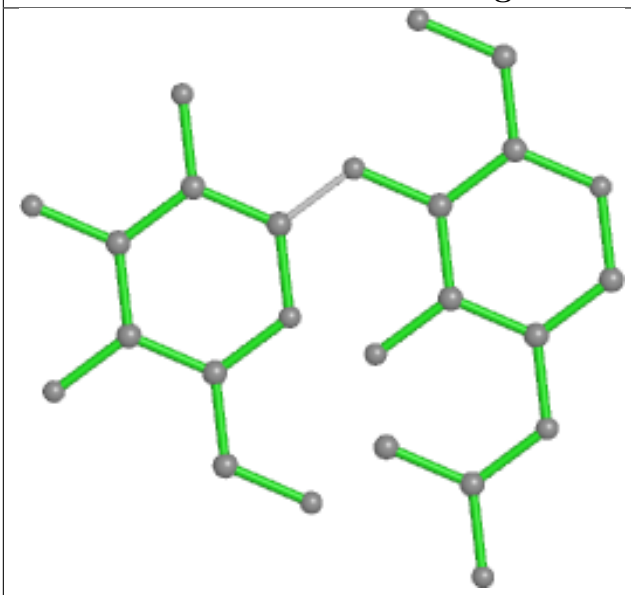


Torsions

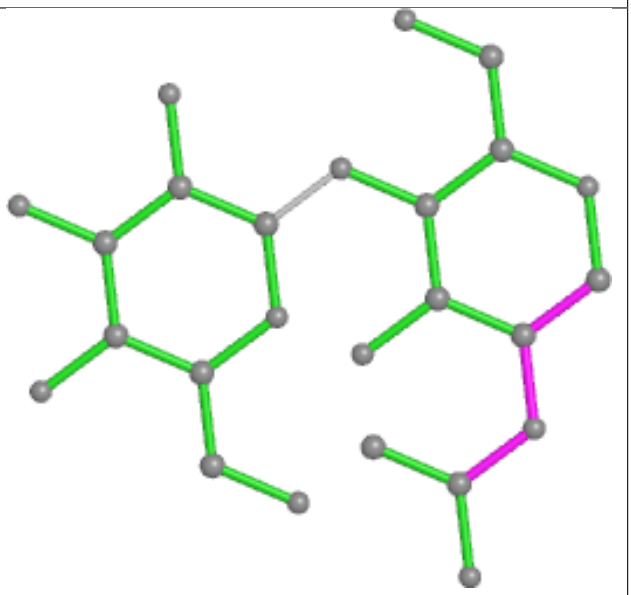


Rings

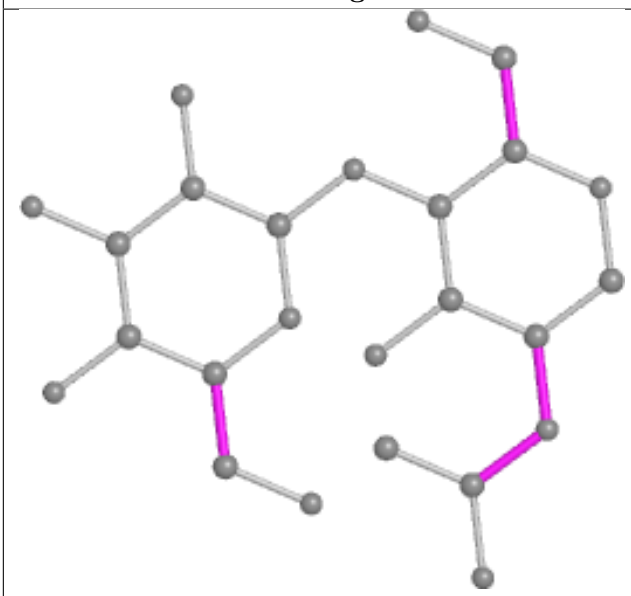
Oligosaccharide Chain R



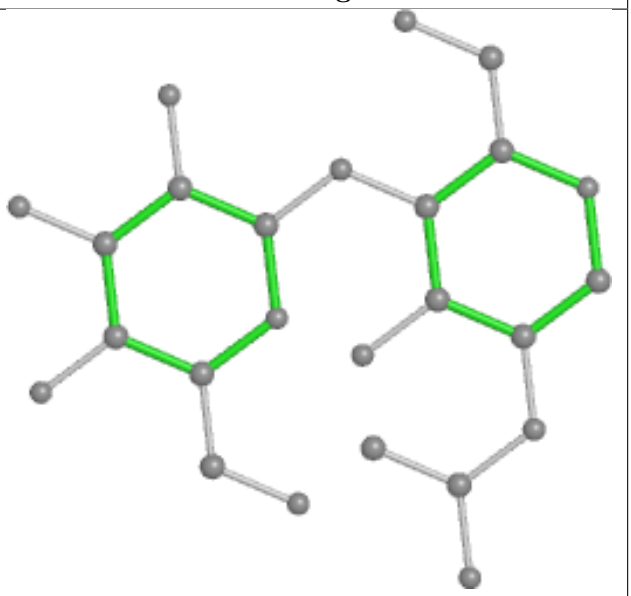
Bond lengths



Bond angles

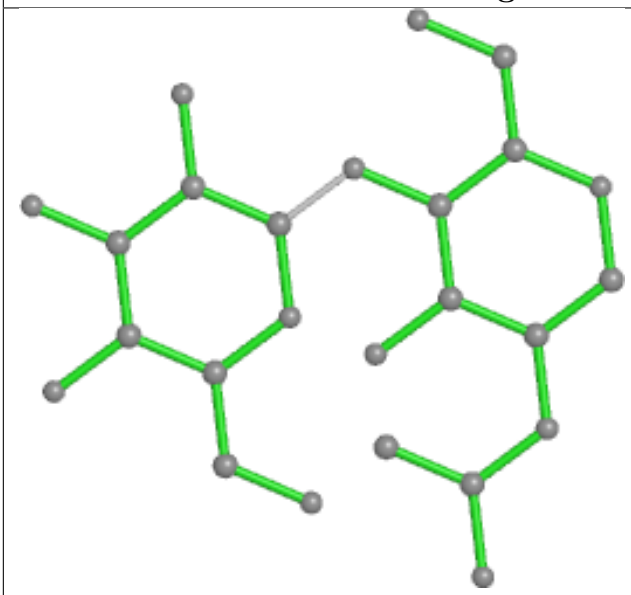


Torsions

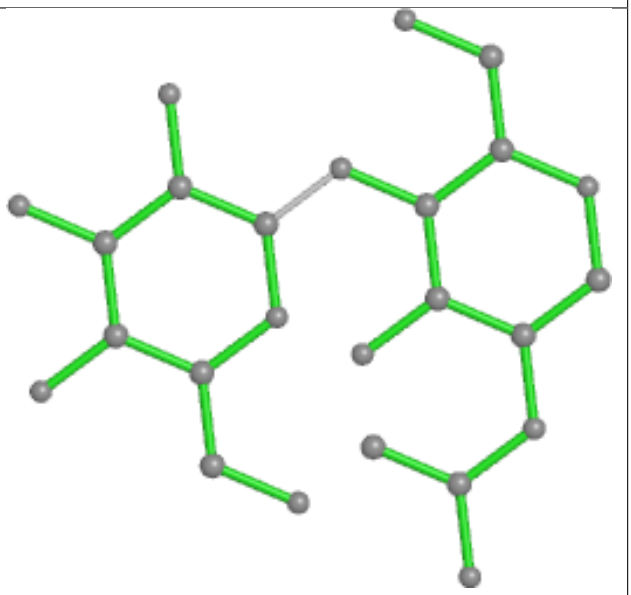


Rings

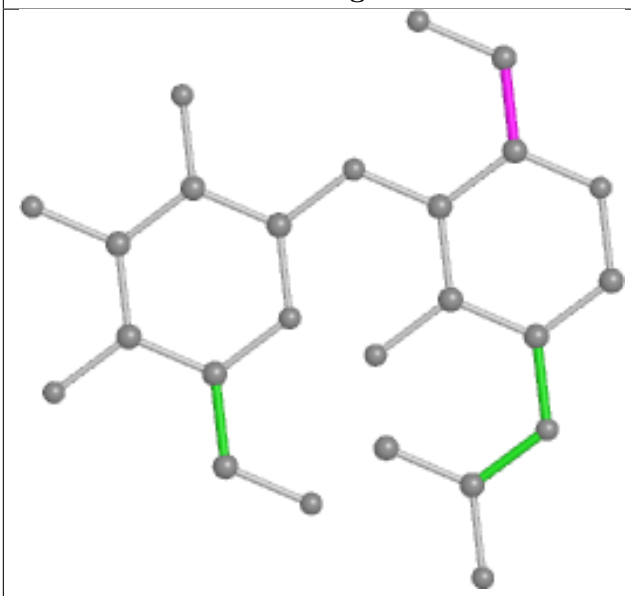
Oligosaccharide Chain S



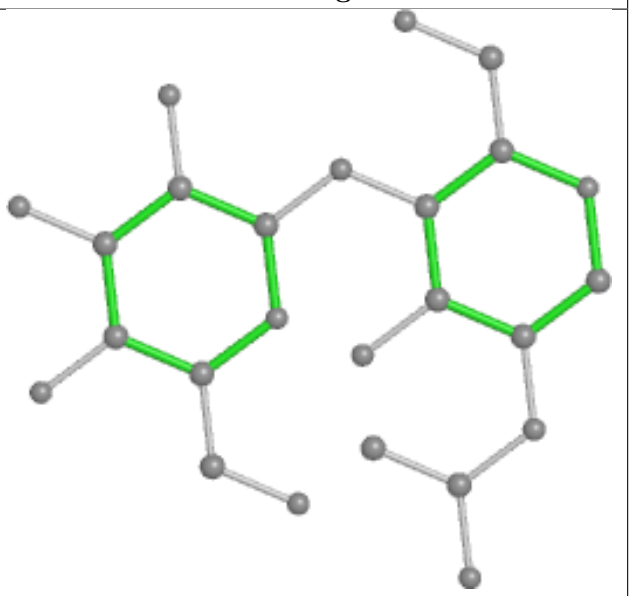
Bond lengths



Bond angles

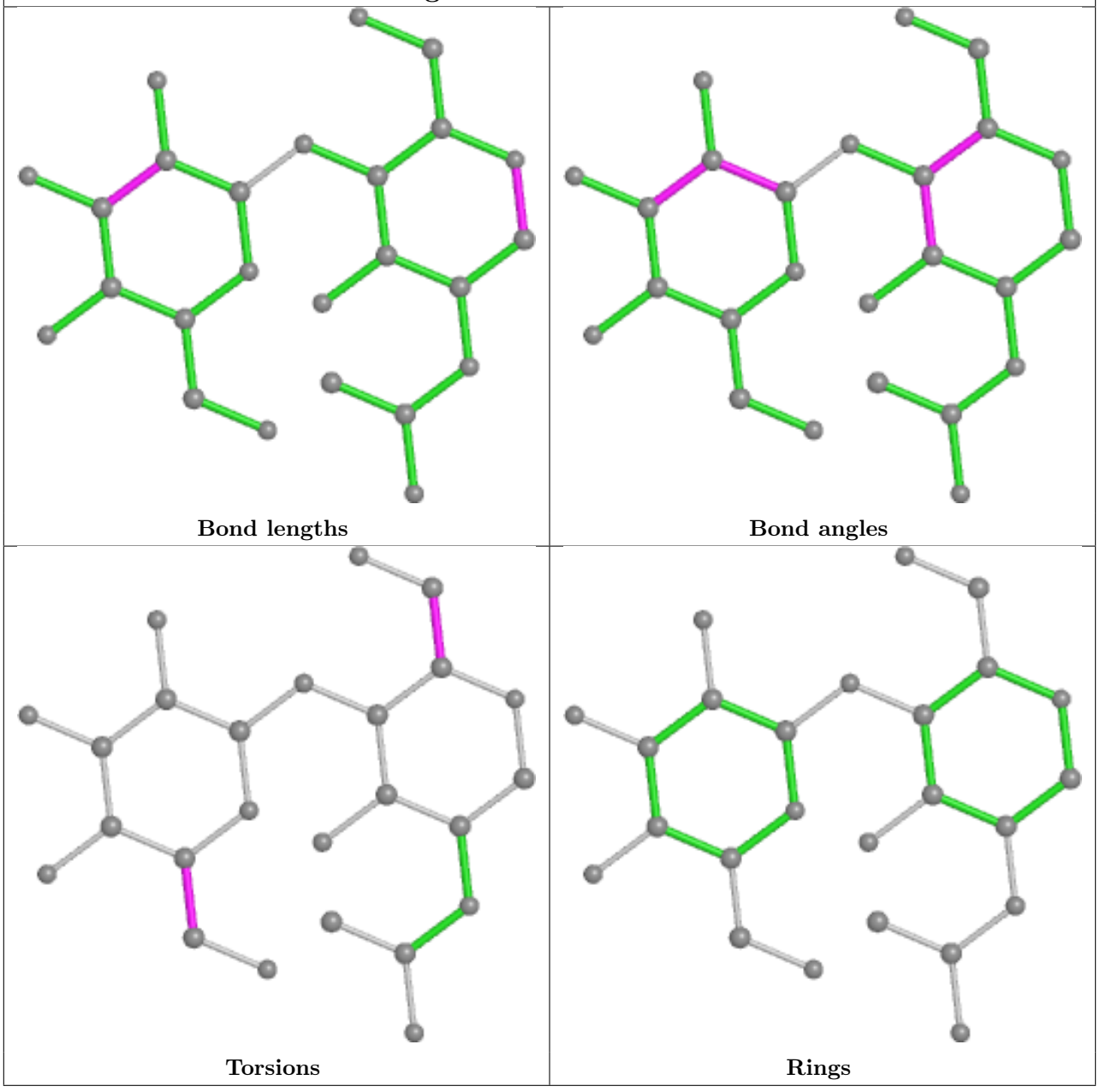


Torsions



Rings

Oligosaccharide Chain T



5.6 Ligand geometry (i)

Of 45 ligands modelled in this entry, 4 are monoatomic - leaving 41 for Mogul analysis.

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	A	1304	1	14,14,15	0.42	0	17,19,21	0.53	0
4	NAG	B	1309	1	14,14,15	0.41	0	17,19,21	0.65	1 (5%)
4	NAG	B	1307	1	14,14,15	0.29	0	17,19,21	0.37	0
4	NAG	C	1302	1	14,14,15	0.71	1 (7%)	17,19,21	0.65	1 (5%)
4	NAG	C	1307	1	14,14,15	0.38	0	17,19,21	0.56	0
4	NAG	C	1301	1	14,14,15	0.22	0	17,19,21	0.55	0
4	NAG	C	1309	1	14,14,15	0.40	0	17,19,21	0.53	0
4	NAG	B	1306	1	14,14,15	0.67	1 (7%)	17,19,21	0.69	0
4	NAG	E	903	2	14,14,15	0.79	1 (7%)	17,19,21	1.58	2 (11%)
4	NAG	A	1306	1	14,14,15	0.19	0	17,19,21	0.45	0
4	NAG	A	1305	1	14,14,15	0.37	0	17,19,21	0.48	0
4	NAG	B	1305	1	14,14,15	0.30	0	17,19,21	0.46	0
4	NAG	E	906	2	14,14,15	0.40	0	17,19,21	0.81	0
4	NAG	A	1309	1	14,14,15	0.36	0	17,19,21	0.40	0
4	NAG	C	1311	1	14,14,15	0.38	0	17,19,21	0.56	0
4	NAG	E	904	2	14,14,15	0.62	1 (7%)	17,19,21	0.52	0
4	NAG	B	1304	1	14,14,15	0.41	0	17,19,21	0.83	1 (5%)
4	NAG	B	1302	1	14,14,15	0.38	0	17,19,21	0.48	0
4	NAG	B	1310	1	14,14,15	0.37	0	17,19,21	0.46	0
4	NAG	B	1301	1	14,14,15	0.38	0	17,19,21	0.77	1 (5%)
4	NAG	E	905	2	14,14,15	0.36	0	17,19,21	0.42	0
4	NAG	D	905	2	14,14,15	0.57	0	17,19,21	0.53	0
4	NAG	A	1307	1	14,14,15	0.37	0	17,19,21	0.52	0
4	NAG	D	903	2	14,14,15	0.39	0	17,19,21	0.47	0
4	NAG	C	1304	1	14,14,15	0.20	0	17,19,21	0.52	0
4	NAG	C	1306	1	14,14,15	0.28	0	17,19,21	0.31	0
4	NAG	C	1308	1	14,14,15	0.54	0	17,19,21	0.83	1 (5%)
4	NAG	D	906	2	14,14,15	0.28	0	17,19,21	0.37	0
4	NAG	A	1310	1	14,14,15	0.36	0	17,19,21	0.61	1 (5%)
4	NAG	B	1303	1	14,14,15	0.27	0	17,19,21	0.45	0
4	NAG	D	904	2	14,14,15	0.27	0	17,19,21	0.66	1 (5%)
4	NAG	C	1303	1	14,14,15	0.24	0	17,19,21	0.54	0
4	NAG	A	1311	1	14,14,15	0.26	0	17,19,21	0.52	0
4	NAG	A	1302	1	14,14,15	0.35	0	17,19,21	0.41	0
4	NAG	B	1311	1	14,14,15	0.39	0	17,19,21	0.54	0
4	NAG	A	1301	1	14,14,15	0.22	0	17,19,21	0.58	0
4	NAG	A	1308	1	14,14,15	0.57	0	17,19,21	1.52	3 (17%)
4	NAG	C	1310	1	14,14,15	0.40	0	17,19,21	0.59	1 (5%)
4	NAG	C	1305	1	14,14,15	0.43	0	17,19,21	1.26	2 (11%)
4	NAG	A	1303	1	14,14,15	0.36	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	1308	1	14,14,15	0.58	1 (7%)	17,19,21	0.64	1 (5%)

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	A	1304	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	E	903	2	-	1/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	E	906	2	-	0/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1311	1	-	0/6/23/26	0/1/1/1
4	NAG	E	904	2	-	0/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1310	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	1/6/23/26	0/1/1/1
4	NAG	E	905	2	-	4/6/23/26	0/1/1/1
4	NAG	D	905	2	-	2/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	D	903	2	-	1/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	3/6/23/26	0/1/1/1
4	NAG	D	906	2	-	4/6/23/26	0/1/1/1
4	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	904	2	-	1/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1311	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1311	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1310	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	3/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	903	NAG	O5-C1	-2.84	1.39	1.43
4	C	1302	NAG	C1-C2	2.34	1.55	1.52
4	B	1306	NAG	C1-C2	2.30	1.55	1.52
4	E	904	NAG	O5-C1	-2.09	1.40	1.43
4	B	1308	NAG	C1-C2	2.01	1.55	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	903	NAG	C1-O5-C5	5.11	119.12	112.19
4	A	1308	NAG	C1-O5-C5	4.46	118.24	112.19
4	A	1308	NAG	C3-C4-C5	3.24	116.01	110.24
4	C	1305	NAG	O5-C1-C2	3.04	116.08	111.29
4	C	1305	NAG	C1-O5-C5	2.98	116.23	112.19

There are no chirality outliers.

5 of 75 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1311	NAG	C8-C7-N2-C2
4	B	1311	NAG	O7-C7-N2-C2
4	B	1306	NAG	C4-C5-C6-O6
4	B	1306	NAG	O5-C5-C6-O6
4	A	1308	NAG	O5-C5-C6-O6

There are no ring outliers.

13 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1304	NAG	1	0
4	C	1302	NAG	1	0
4	C	1301	NAG	1	0
4	B	1306	NAG	1	0
4	A	1305	NAG	1	0
4	B	1302	NAG	1	0
4	B	1301	NAG	1	0
4	A	1307	NAG	1	0
4	C	1306	NAG	1	0
4	A	1302	NAG	1	0
4	A	1301	NAG	1	0
4	A	1308	NAG	1	0
4	B	1308	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.