wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 02:55 PM JST

PDB ID	:	8ZHD
EMDB ID	:	EMD-60099
Title	:	SARS-CoV-2 spike trimer (6P) in complex with two R1-26 Fabs
Authors	:	Yan, Q.; Gao, X.; Liu, B.; Hou, R.; He, P.; Li, Z.; Chen, Q.; Wang, J.; He, J.; Chen, L.; Zhao, J.; Xiong, X.
Deposited on	:	2024-05-10
Resolution	:	3.41 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:

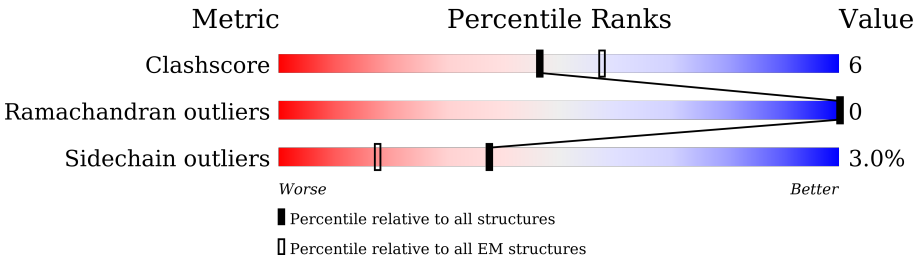
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.41 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	1278	72% 11% 17%
1	B	1278	68% 15% 17%
1	C	1278	68% 14% · 17%
2	F	243	40% 9% 51%
2	H	243	41% 8% 51%
3	G	240	36% 10% 54%
3	L	240	36% 8% · 54%
4	D	2	100%
4	E	2	100%

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Mol	Chain	Length	Quality of chain
4	I	2	100%
4	J	2	100%
4	K	2	100%
4	M	2	100%
4	N	2	100%
4	O	2	100%
4	P	2	100%
4	Q	2	100%
4	R	2	100%
4	S	2	50% 50%
4	T	2	100%
4	U	2	100%
4	V	2	100%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 29306 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,Fibritin,Expression Tag.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1066	Total	C	N	O	S	0	0
			8326	5312	1388	1588	38		
1	B	1066	Total	C	N	O	S	0	0
			8326	5312	1388	1588	38		
1	C	1066	Total	C	N	O	S	0	0
			8326	5312	1388	1588	38		

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1209	GLY	-	linker	UNP P0DTC2
A	1210	SER	-	linker	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1209	GLY	-	linker	UNP P0DTC2
B	1210	SER	-	linker	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	685	SER	ARG	conflict	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1209	GLY	-	linker	UNP P0DTC2
C	1210	SER	-	linker	UNP P0DTC2

- Molecule 2 is a protein called Heavy chain of R1-26 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	119	Total	C	N	O	S	0	0
			920	583	158	175	4		
2	F	119	Total	C	N	O	S	0	0
			920	583	158	175	4		

- Molecule 3 is a protein called Light chain of R1-26 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	110	Total	C	N	O	S	0	0
			824	506	136	179	3		
3	G	110	Total	C	N	O	S	0	0
			824	506	136	179	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	J	2	Total	C	N	O	0	0
			28	16	2	10		

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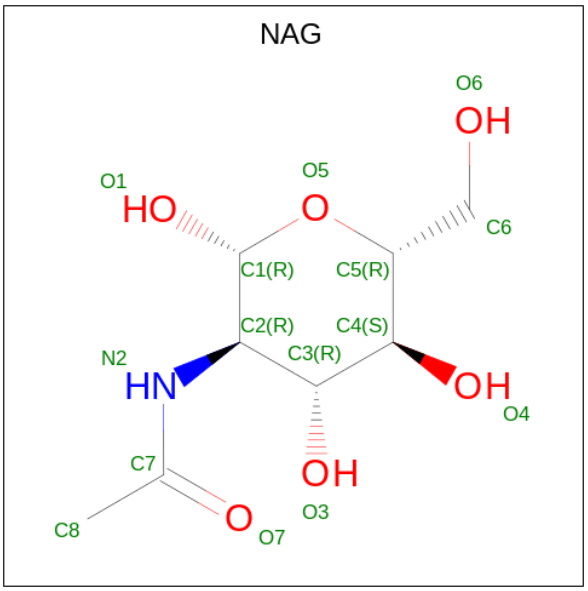
Mol	Chain	Residues	Atoms				AltConf	Trace
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16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

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

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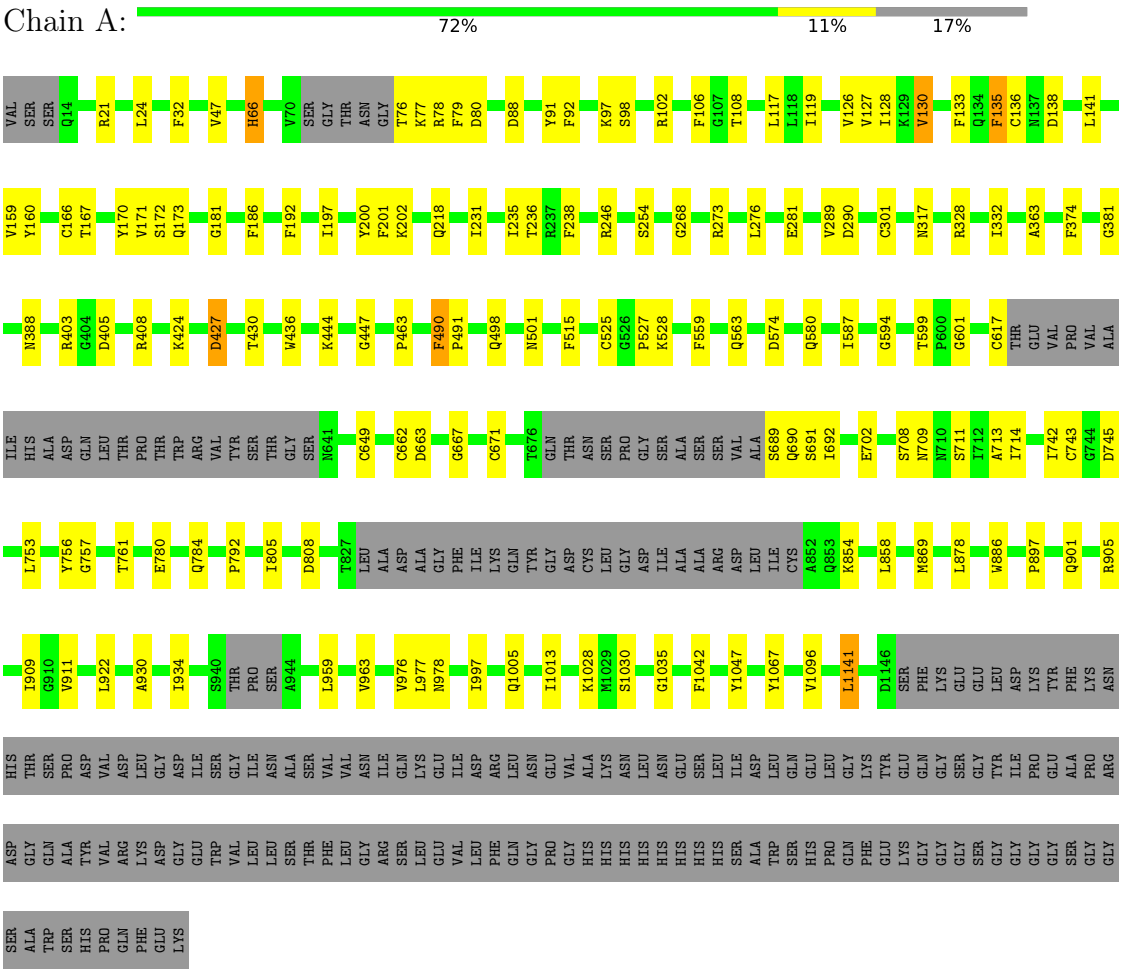
Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

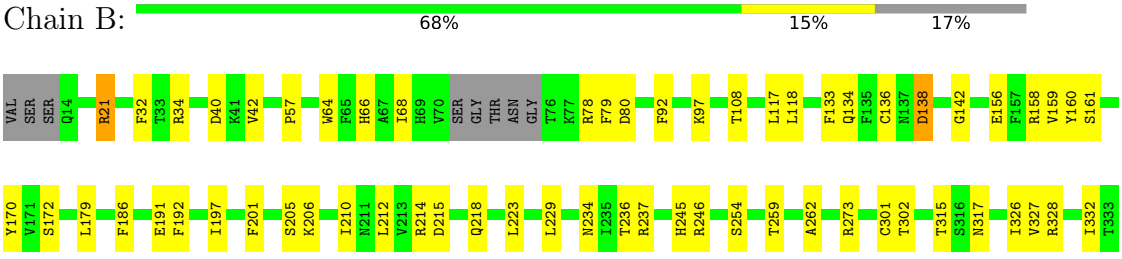
• Molecule 1: Spike glycoprotein,Fibritin,Expression Tag

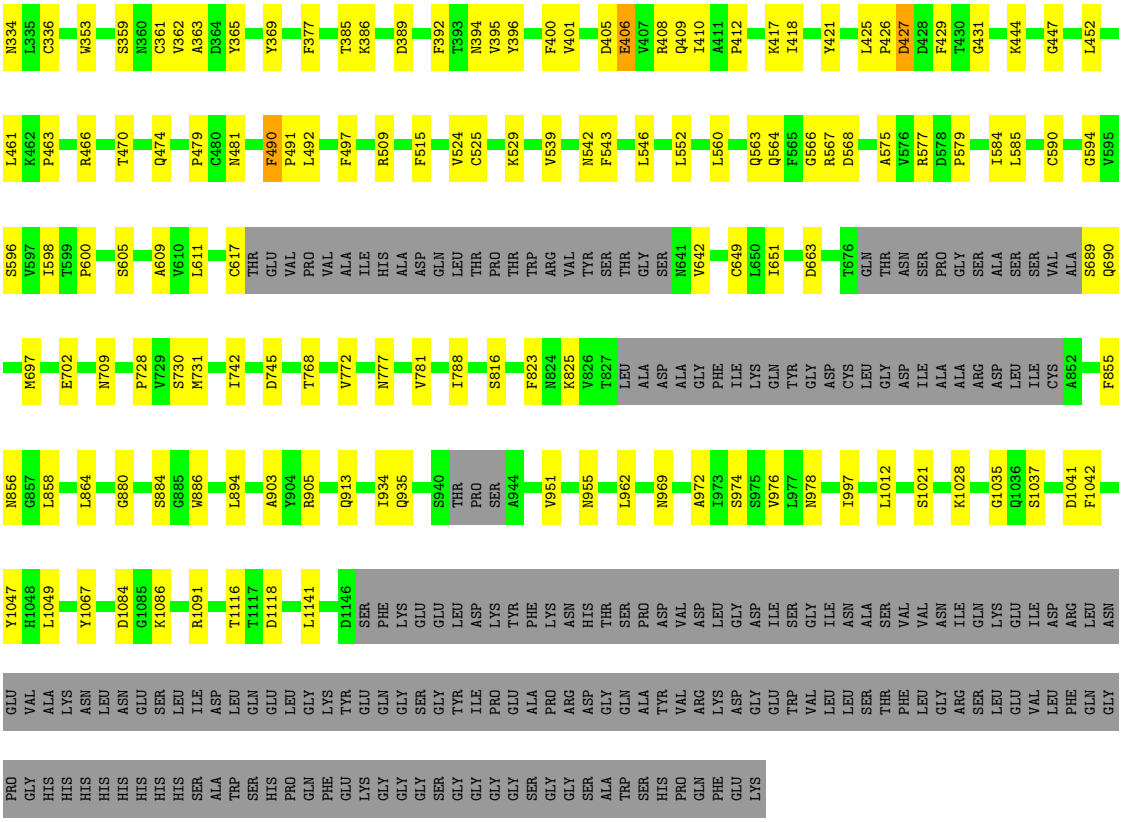
Chain A:



• Molecule 1: Spike glycoprotein,Fibritin,Expression Tag

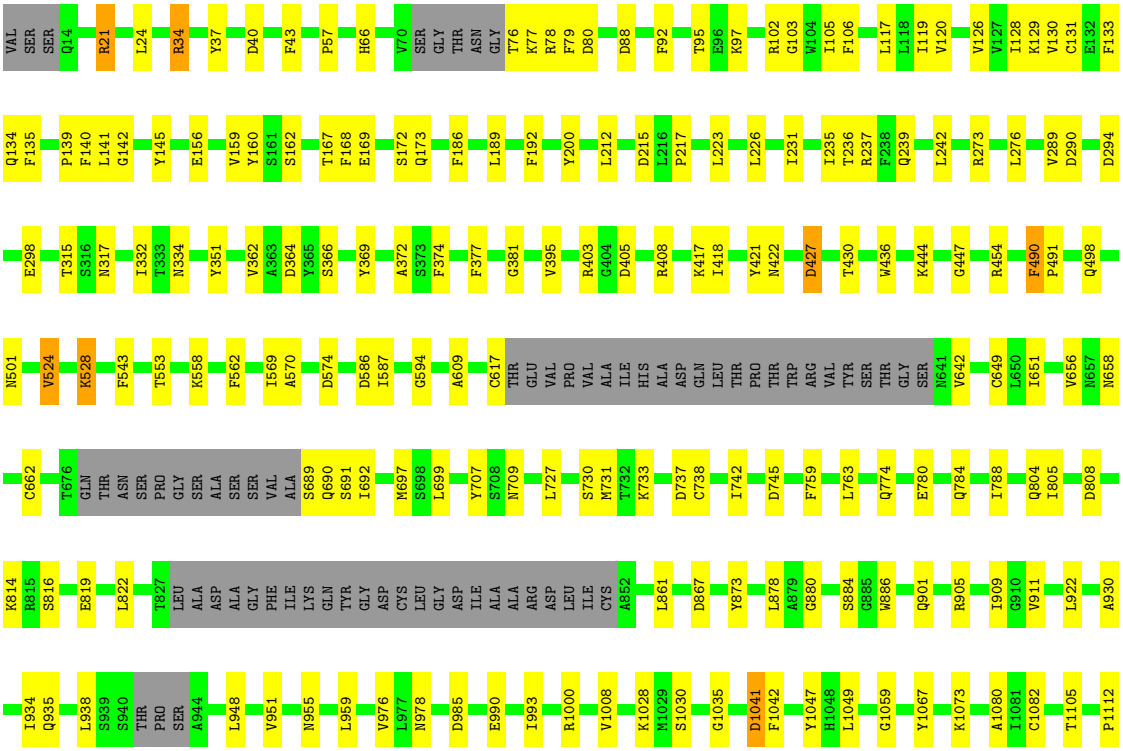
Chain B:

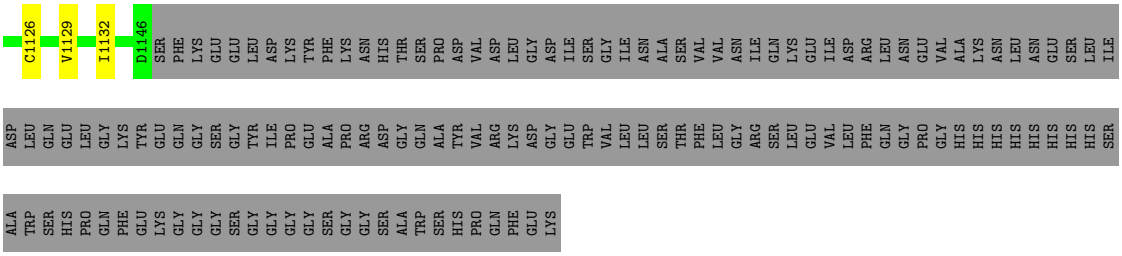




• Molecule 1: Spike glycoprotein,Fibritin,Expression Tag

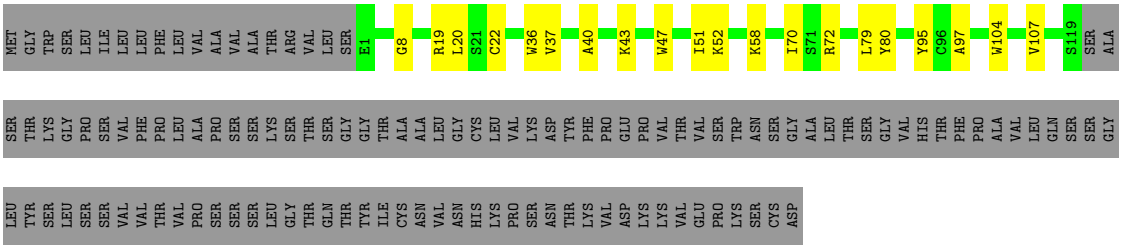
Chain C:





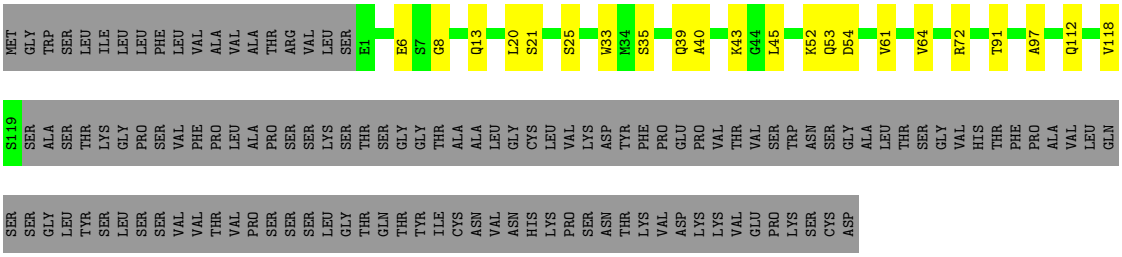
• Molecule 2: Heavy chain of R1-26 Fab

Chain H:



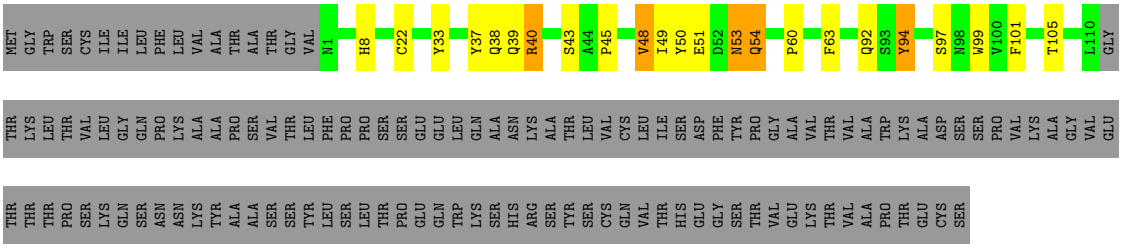
• Molecule 2: Heavy chain of R1-26 Fab

Chain F:



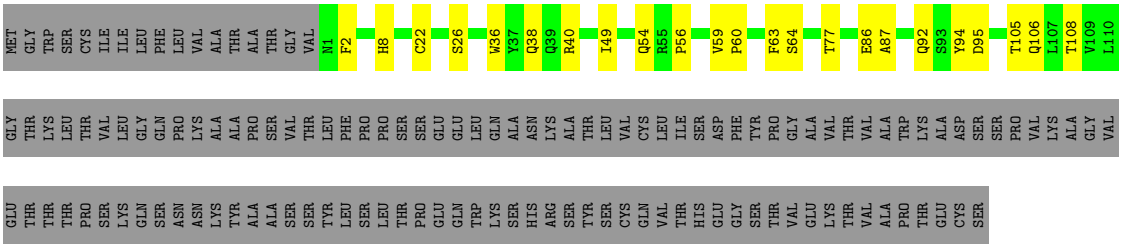
• Molecule 3: Light chain of R1-26 Fab

Chain L:



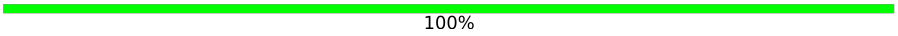
• Molecule 3: Light chain of R1-26 Fab

Chain G:



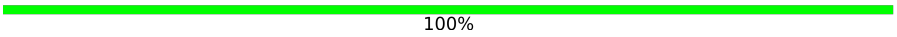
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



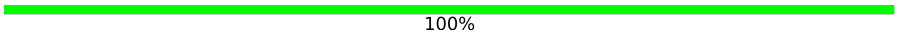
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



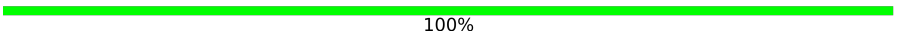
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



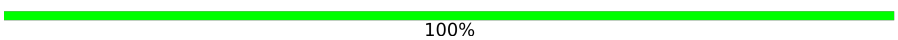
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



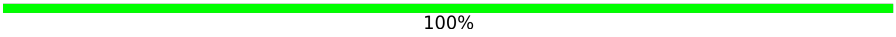
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



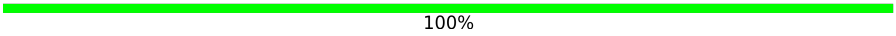
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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

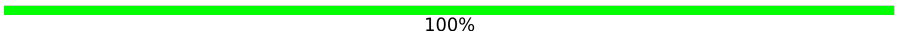
Chain O:

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

Chain P:

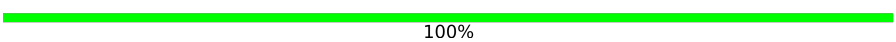
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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: 100%

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

Chain U: 100%

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

Chain V: 100%

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	110522	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (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: 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	0.27	0/8522	0.50	0/11605
1	B	0.29	0/8522	0.53	0/11605
1	C	0.26	0/8522	0.50	0/11605
2	F	0.25	0/942	0.57	0/1277
2	H	0.26	0/942	0.57	0/1277
3	G	0.26	0/843	0.51	0/1151
3	L	0.33	0/843	0.52	0/1151
All	All	0.27	0/29136	0.51	0/39671

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8326	0	8079	84	0
1	B	8326	0	8079	111	0
1	C	8326	0	8079	112	0
2	F	920	0	887	11	0
2	H	920	0	887	15	0
3	G	824	0	755	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	824	0	755	16	0
4	D	28	0	25	0	0
4	E	28	0	25	0	0
4	I	28	0	25	0	0
4	J	28	0	25	0	0
4	K	28	0	25	0	0
4	M	28	0	25	0	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	0	0
4	S	28	0	25	1	0
4	T	28	0	25	0	0
4	U	28	0	25	0	0
4	V	28	0	25	0	0
5	A	140	0	130	1	0
5	B	140	0	130	0	0
5	C	140	0	130	0	0
All	All	29306	0	28286	338	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 6.

The worst 5 of 338 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)
3:L:92:GLN:HE22	3:L:99:TRP:HB3	1.47	0.80
1:A:200:TYR:HB3	1:A:202:LYS:HE3	1.70	0.73
1:C:273:ARG:NH2	1:C:290:ASP:OD2	2.26	0.68
1:B:577:ARG:HG3	1:B:584:ILE:HD13	1.76	0.67
1:B:206:LYS:HG2	1:B:223:LEU:HD12	1.77	0.67

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	1054/1278 (82%)	1020 (97%)	34 (3%)	0	100	100
1	B	1054/1278 (82%)	1019 (97%)	35 (3%)	0	100	100
1	C	1054/1278 (82%)	1016 (96%)	38 (4%)	0	100	100
2	F	117/243 (48%)	110 (94%)	7 (6%)	0	100	100
2	H	117/243 (48%)	109 (93%)	8 (7%)	0	100	100
3	G	108/240 (45%)	98 (91%)	10 (9%)	0	100	100
3	L	108/240 (45%)	100 (93%)	8 (7%)	0	100	100
All	All	3612/4800 (75%)	3472 (96%)	140 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	930/1106 (84%)	909 (98%)	21 (2%)	45	67
1	B	930/1106 (84%)	893 (96%)	37 (4%)	27	52
1	C	930/1106 (84%)	906 (97%)	24 (3%)	41	64
2	F	96/203 (47%)	93 (97%)	3 (3%)	35	60
2	H	96/203 (47%)	96 (100%)	0	100	100
3	G	95/206 (46%)	92 (97%)	3 (3%)	34	59
3	L	95/206 (46%)	88 (93%)	7 (7%)	11	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3172/4136 (77%)	3077 (97%)	95 (3%)	37 61

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1037	SER
1	C	528	LYS
1	C	34	ARG
1	C	242	LEU
1	C	662	CYS

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	804	GLN
1	A	935	GLN

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	$\#\|Z\| > 2$
4	NAG	D	1	1,4	14,14,15	0.41	0	17,19,21	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	D	2	4	14,14,15	0.23	0	17,19,21	0.48	0
4	NAG	E	1	1,4	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	E	2	4	14,14,15	0.24	0	17,19,21	0.43	0
4	NAG	I	1	1,4	14,14,15	0.24	0	17,19,21	0.44	0
4	NAG	I	2	4	14,14,15	0.25	0	17,19,21	0.42	0
4	NAG	J	1	1,4	14,14,15	0.21	0	17,19,21	0.45	0
4	NAG	J	2	4	14,14,15	0.29	0	17,19,21	0.41	0
4	NAG	K	1	1,4	14,14,15	0.23	0	17,19,21	0.45	0
4	NAG	K	2	4	14,14,15	0.27	0	17,19,21	0.44	0
4	NAG	M	1	1,4	14,14,15	0.29	0	17,19,21	0.48	0
4	NAG	M	2	4	14,14,15	0.28	0	17,19,21	0.45	0
4	NAG	N	1	1,4	14,14,15	0.23	0	17,19,21	0.44	0
4	NAG	N	2	4	14,14,15	0.26	0	17,19,21	0.43	0
4	NAG	O	1	1,4	14,14,15	0.25	0	17,19,21	0.51	0
4	NAG	O	2	4	14,14,15	0.26	0	17,19,21	0.42	0
4	NAG	P	1	1,4	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	P	2	4	14,14,15	0.27	0	17,19,21	0.42	0
4	NAG	Q	1	1,4	14,14,15	0.23	0	17,19,21	0.45	0
4	NAG	Q	2	4	14,14,15	0.26	0	17,19,21	0.41	0
4	NAG	R	1	1,4	14,14,15	0.24	0	17,19,21	0.43	0
4	NAG	R	2	4	14,14,15	0.30	0	17,19,21	0.44	0
4	NAG	S	1	1,4	14,14,15	0.23	0	17,19,21	0.44	0
4	NAG	S	2	4	14,14,15	0.27	0	17,19,21	0.42	0
4	NAG	T	1	1,4	14,14,15	0.23	0	17,19,21	0.44	0
4	NAG	T	2	4	14,14,15	0.27	0	17,19,21	0.42	0
4	NAG	U	1	1,4	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	U	2	4	14,14,15	0.26	0	17,19,21	0.43	0
4	NAG	V	1	1,4	14,14,15	0.22	0	17,19,21	0.46	0
4	NAG	V	2	4	14,14,15	0.25	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	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	1/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	J	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	NAG	M	1	1,4	-	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	1,4	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	NAG	O	1	1,4	-	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	1,4	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Q	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
4	NAG	R	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	2/6/23/26	0/1/1/1
4	NAG	S	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	2/6/23/26	0/1/1/1
4	NAG	T	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	2/6/23/26	0/1/1/1
4	NAG	U	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	U	2	4	-	2/6/23/26	0/1/1/1
4	NAG	V	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	V	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

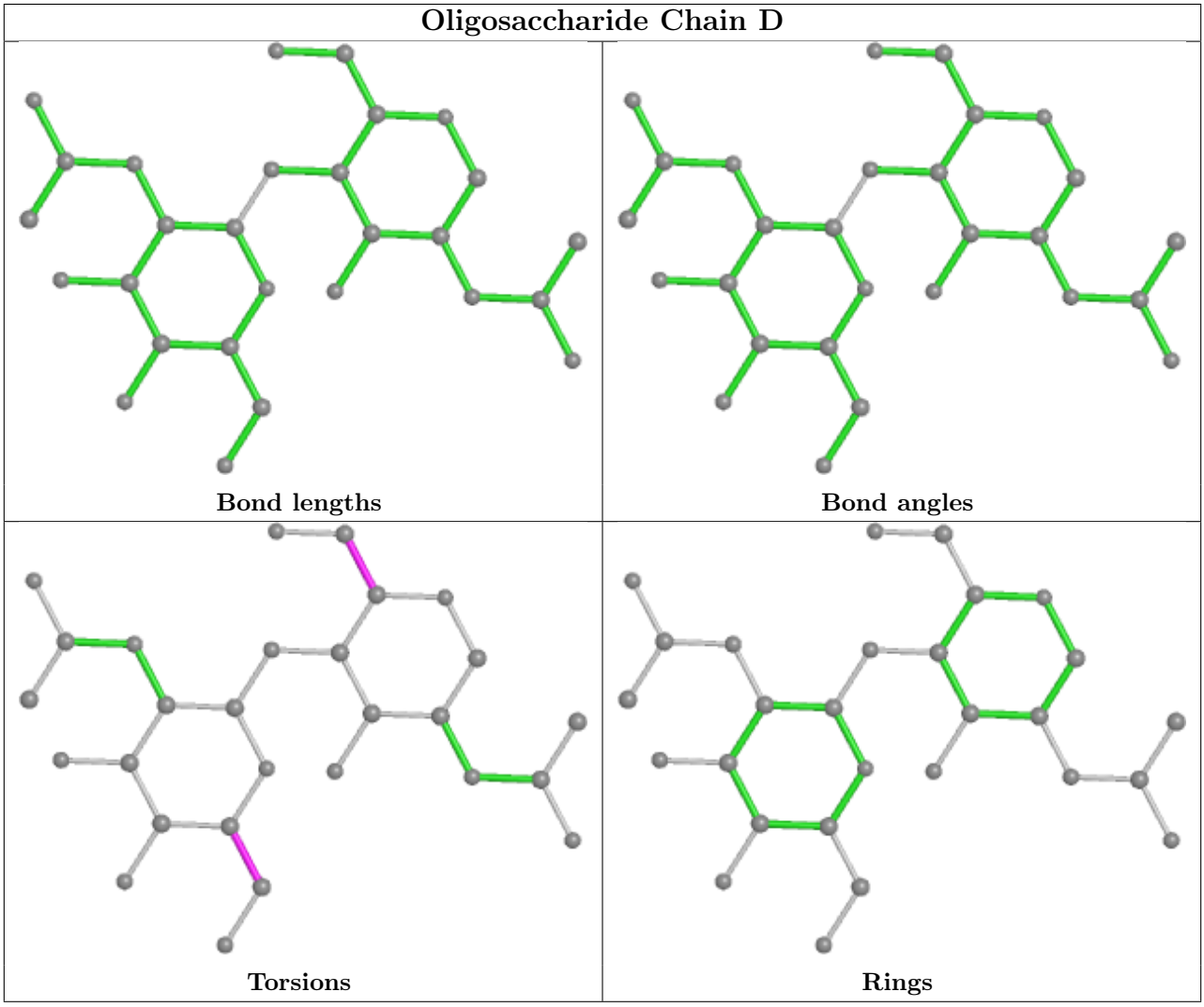
Mol	Chain	Res	Type	Atoms
4	O	1	NAG	O5-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
4	V	1	NAG	O5-C5-C6-O6

There are no ring outliers.

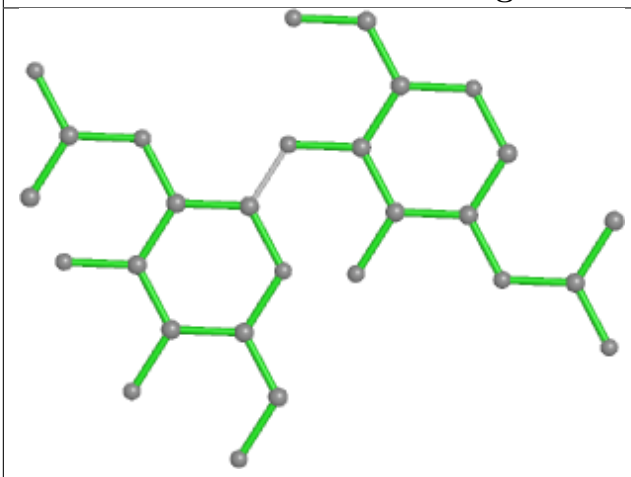
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	S	1	NAG	1	0

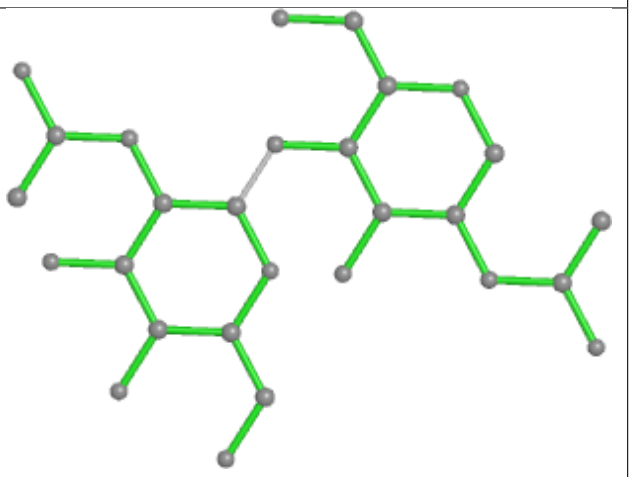
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



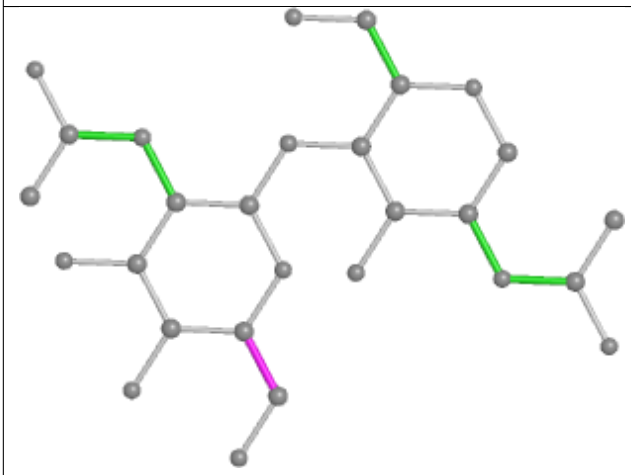
Oligosaccharide Chain E



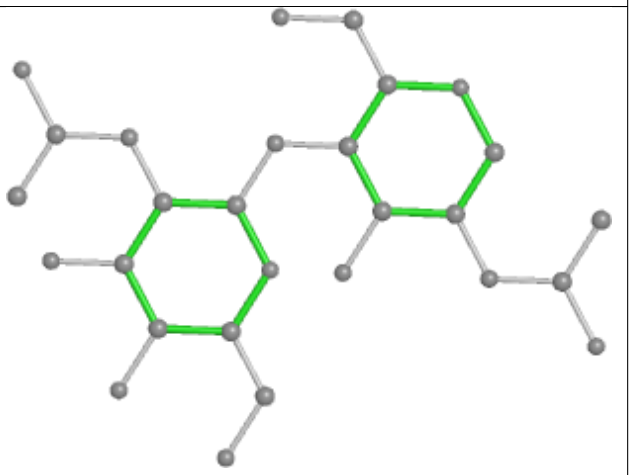
Bond lengths



Bond angles

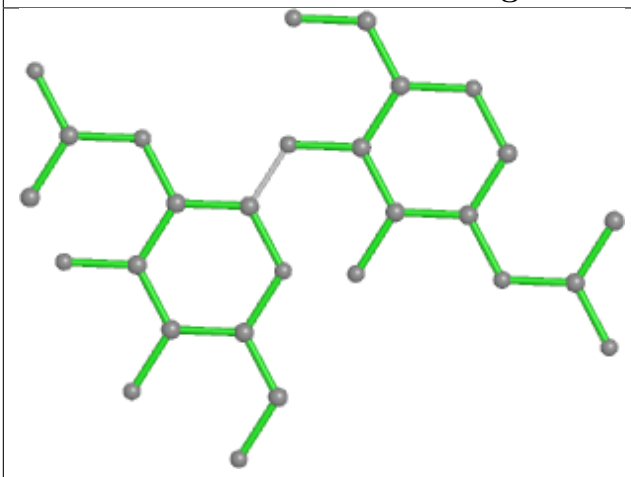


Torsions

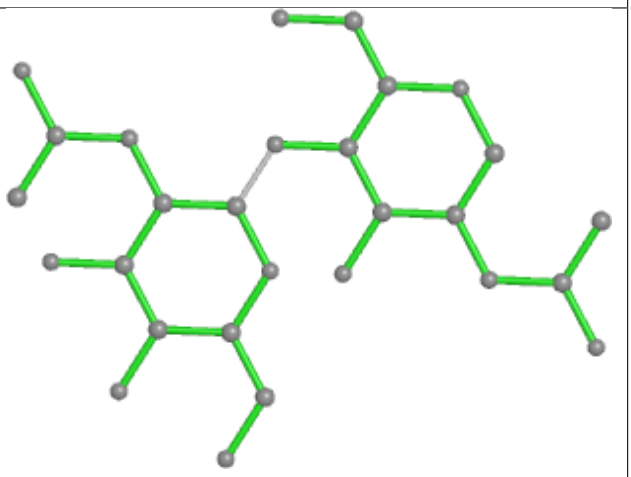


Rings

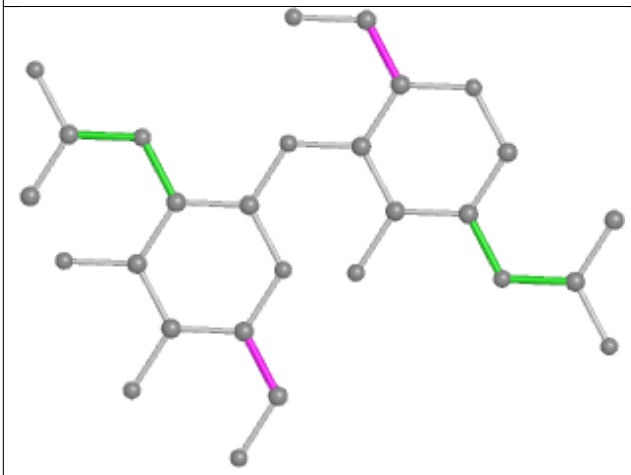
Oligosaccharide Chain I



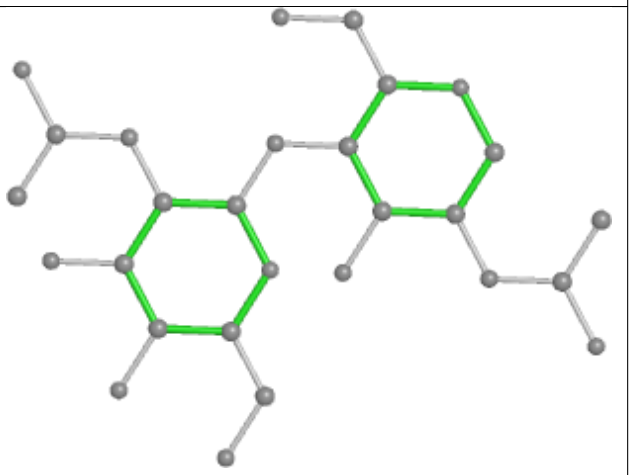
Bond lengths



Bond angles

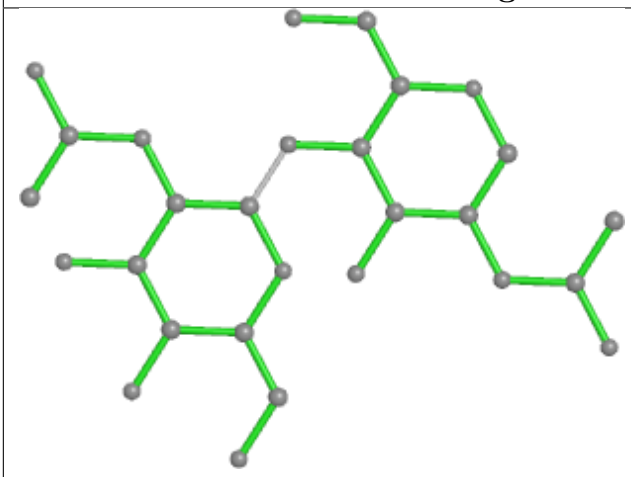


Torsions

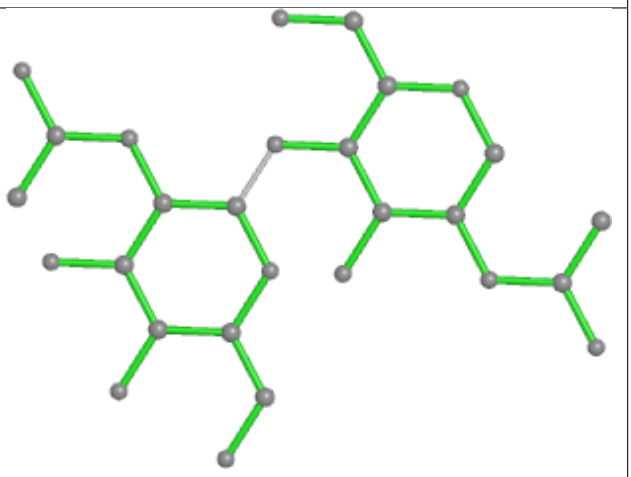


Rings

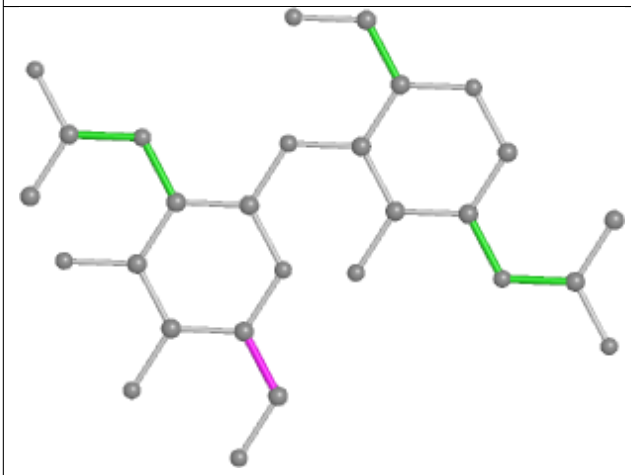
Oligosaccharide Chain J



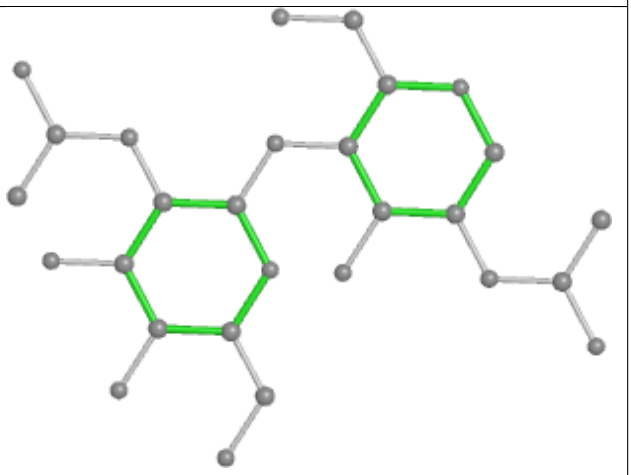
Bond lengths



Bond angles

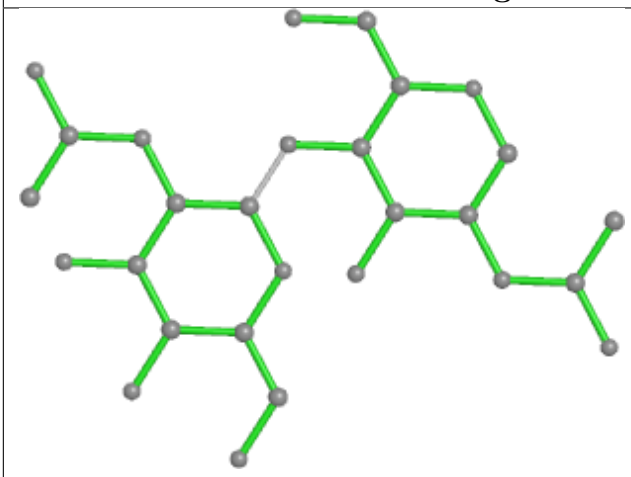


Torsions

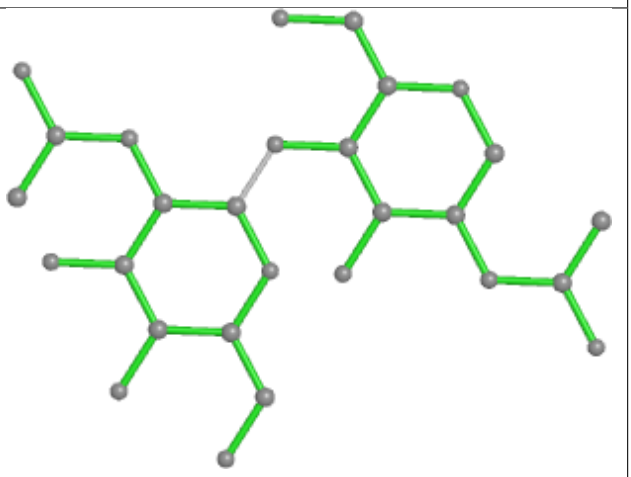


Rings

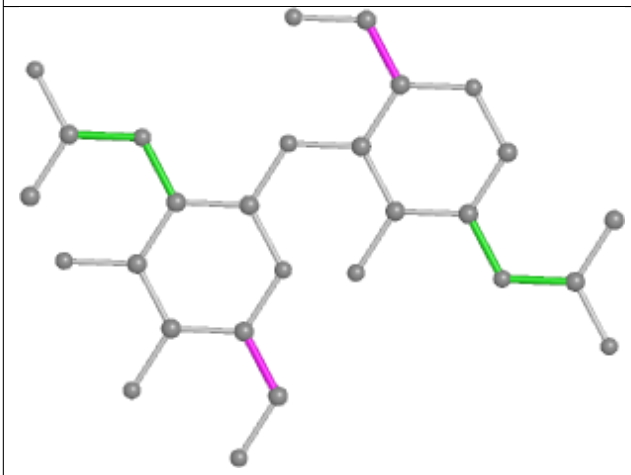
Oligosaccharide Chain K



Bond lengths



Bond angles



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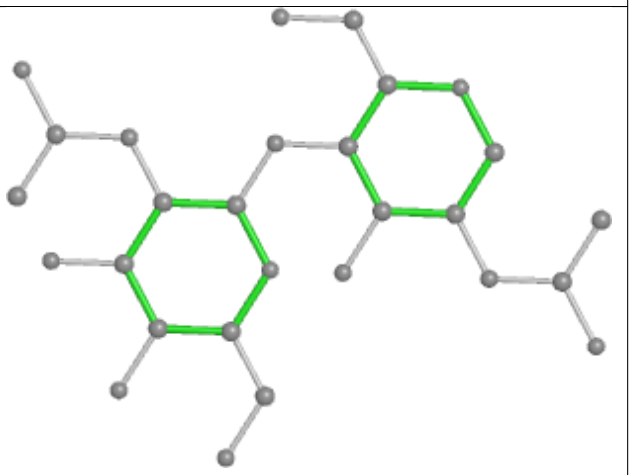
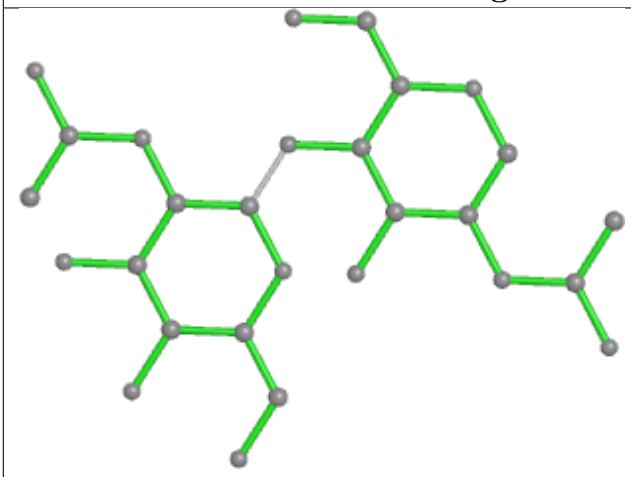
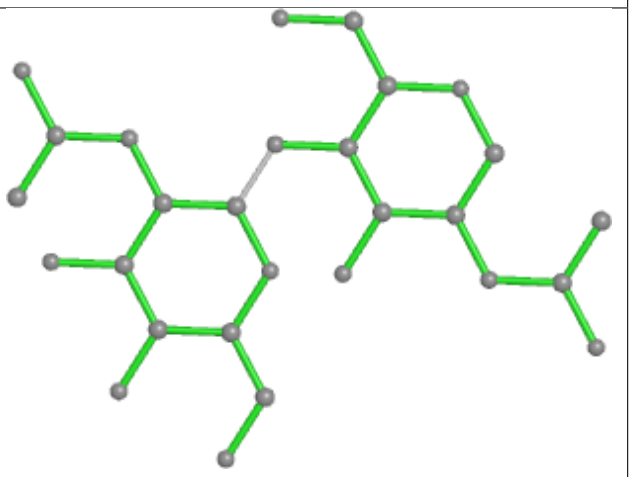


Rings

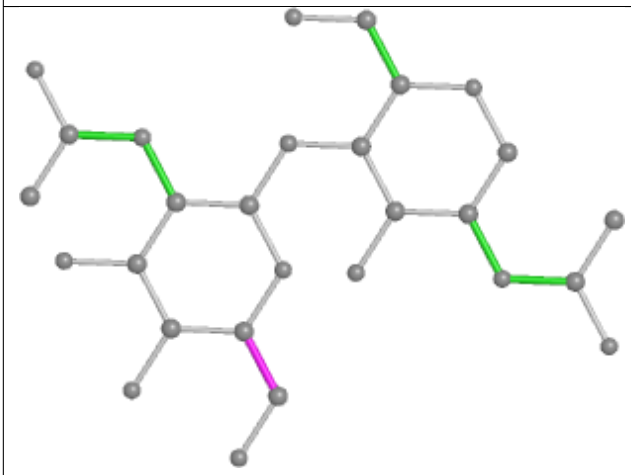
Oligosaccharide Chain M



Bond lengths



Bond angles



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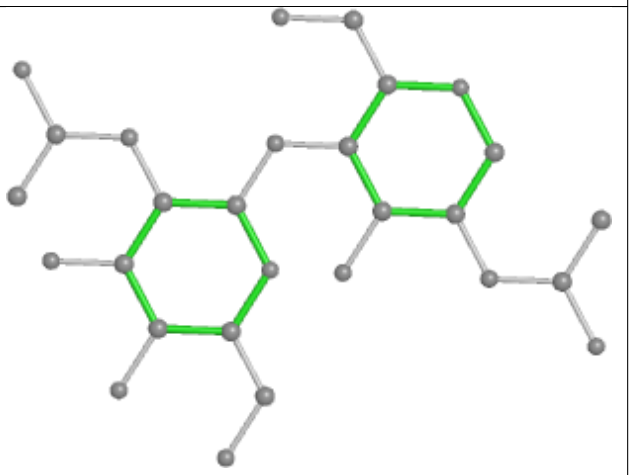
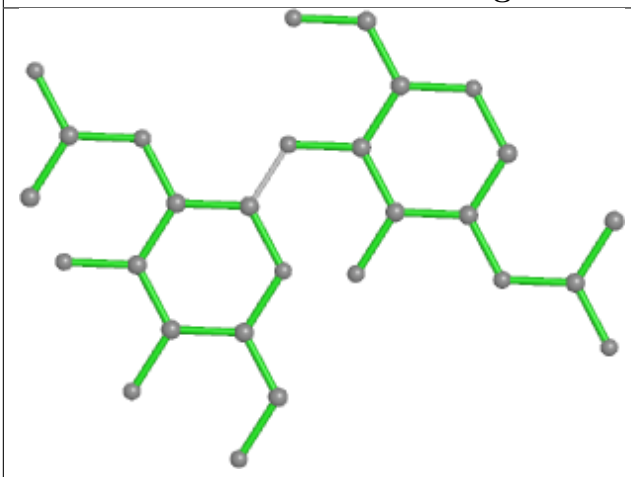
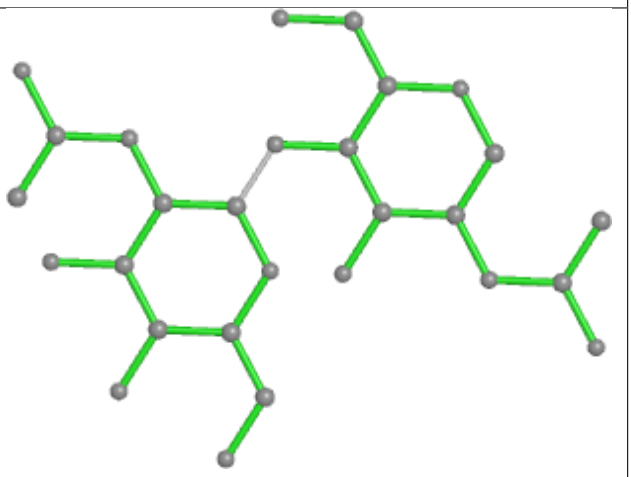


Rings

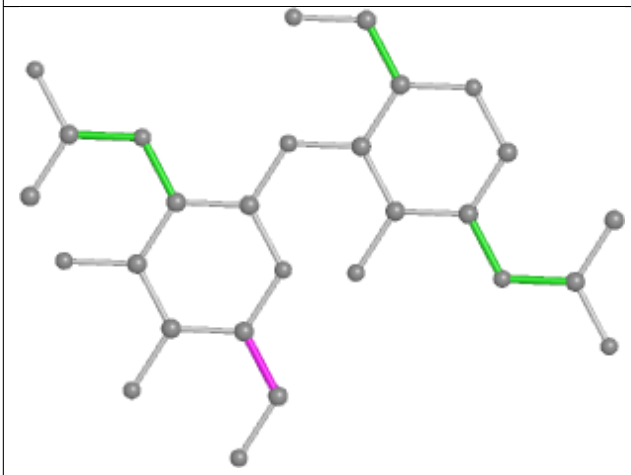
Oligosaccharide Chain N



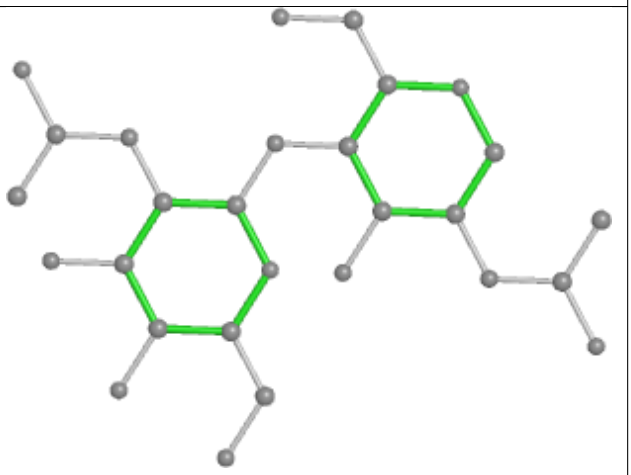
Bond lengths



Bond angles

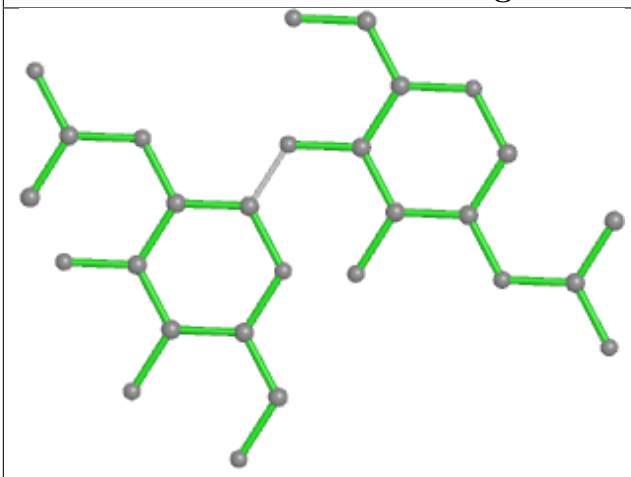


Torsions

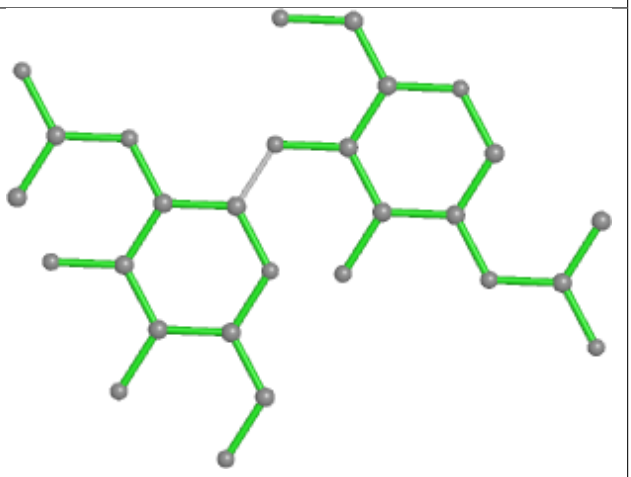


Rings

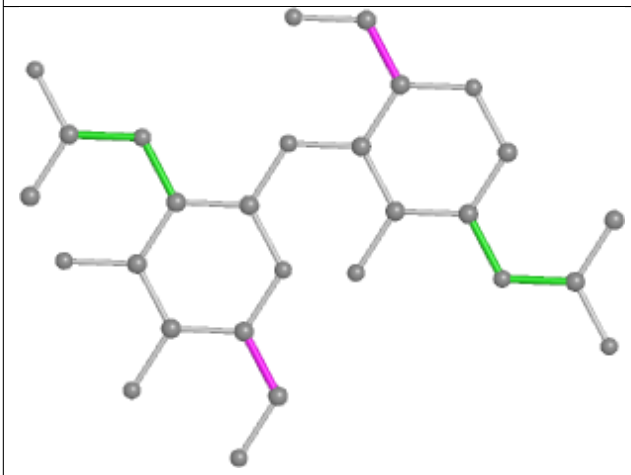
Oligosaccharide Chain O



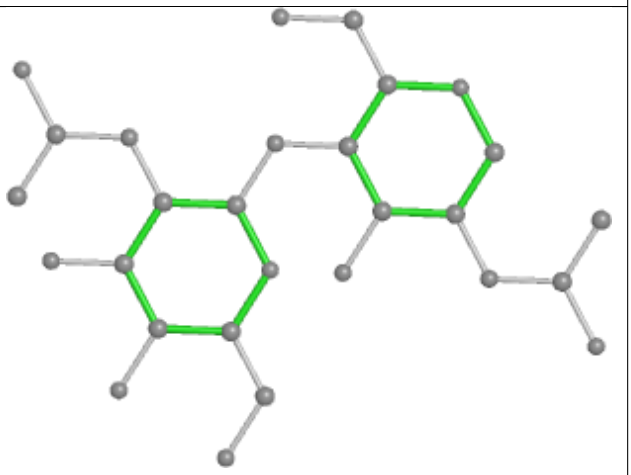
Bond lengths



Bond angles

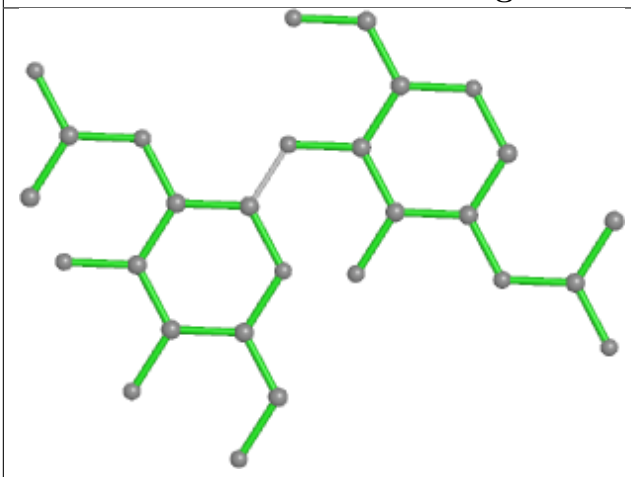


Torsions

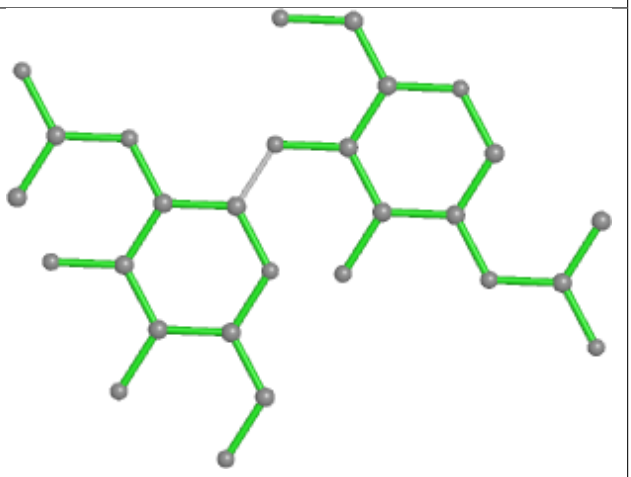


Rings

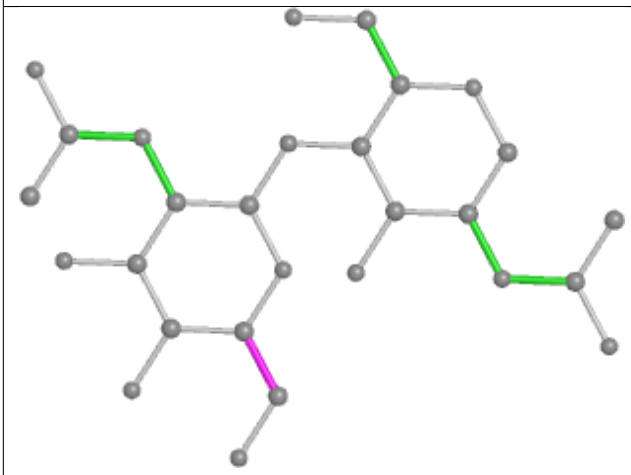
Oligosaccharide Chain P



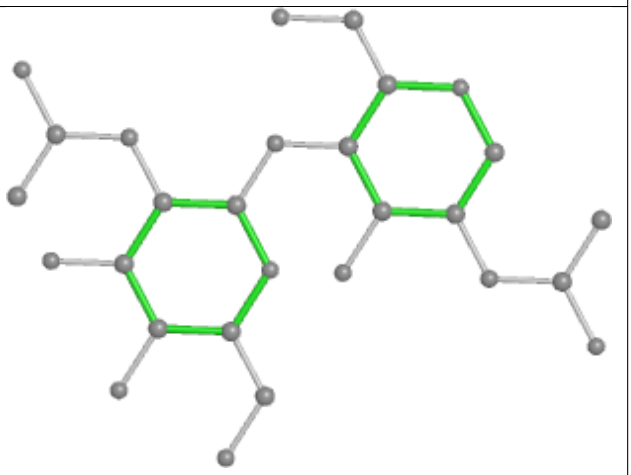
Bond lengths



Bond angles

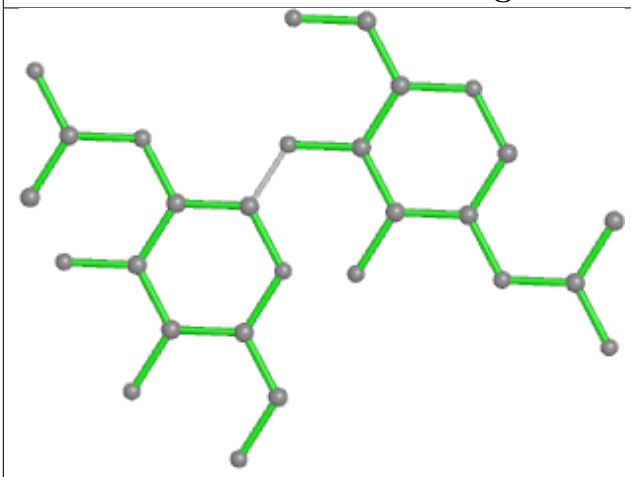


Torsions

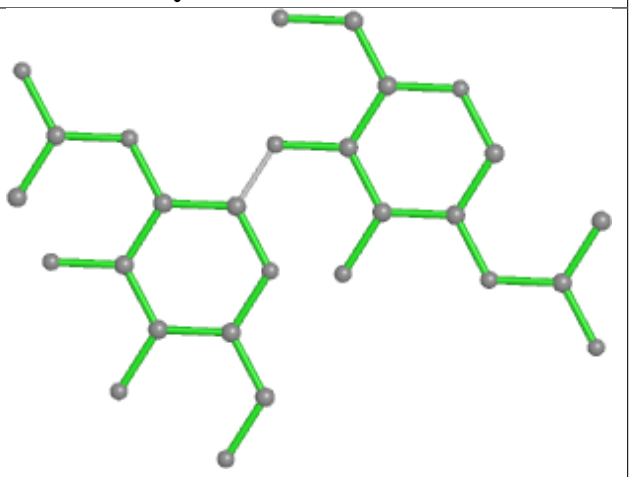


Rings

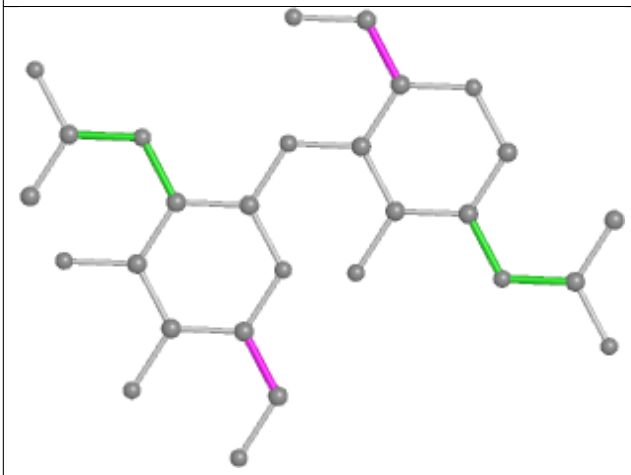
Oligosaccharide Chain Q



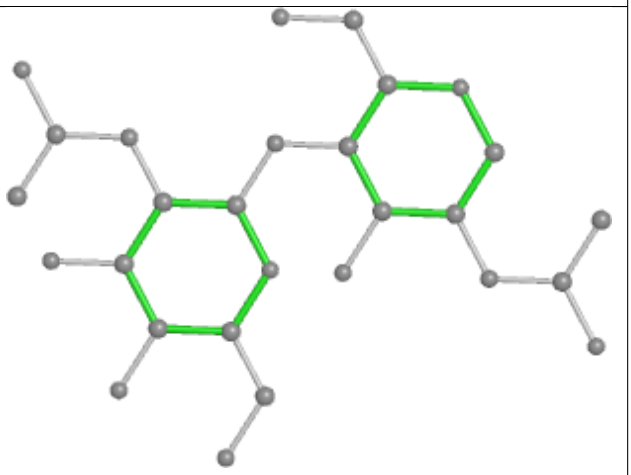
Bond lengths



Bond angles

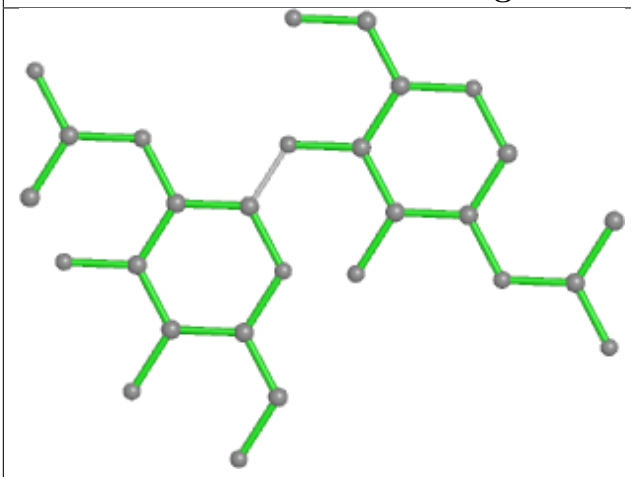


Torsions

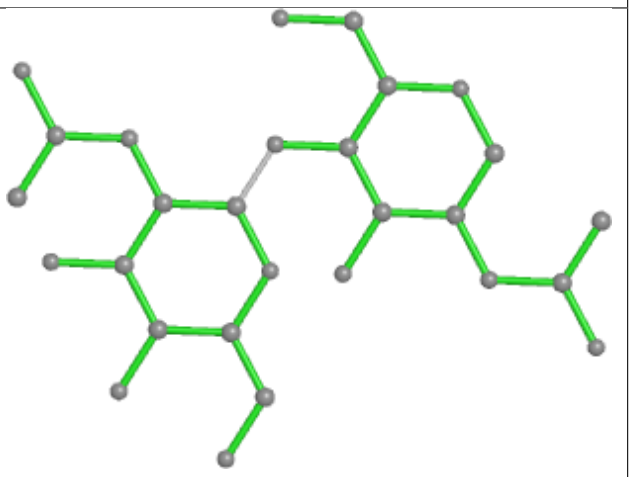


Rings

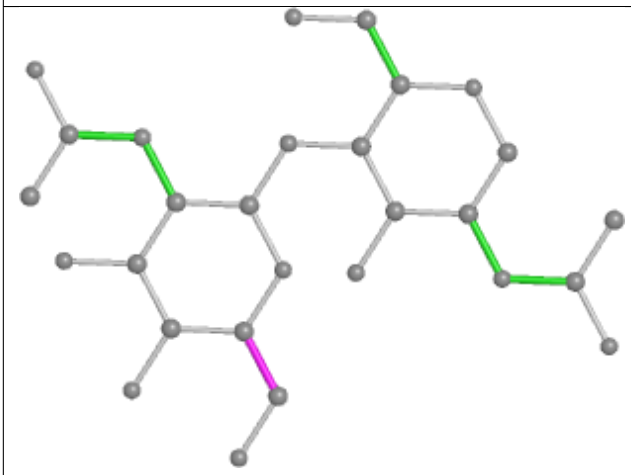
Oligosaccharide Chain R



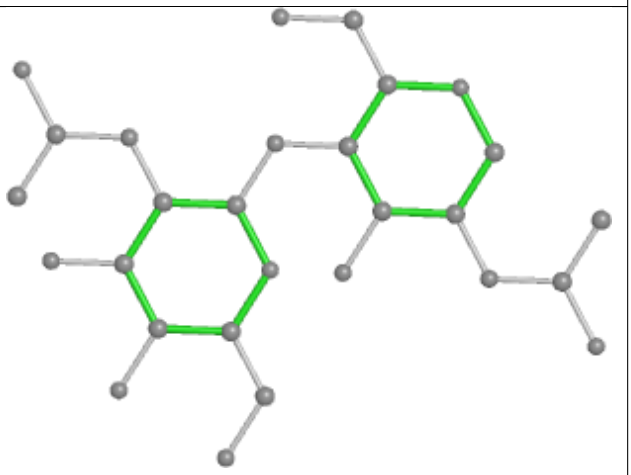
Bond lengths



Bond angles

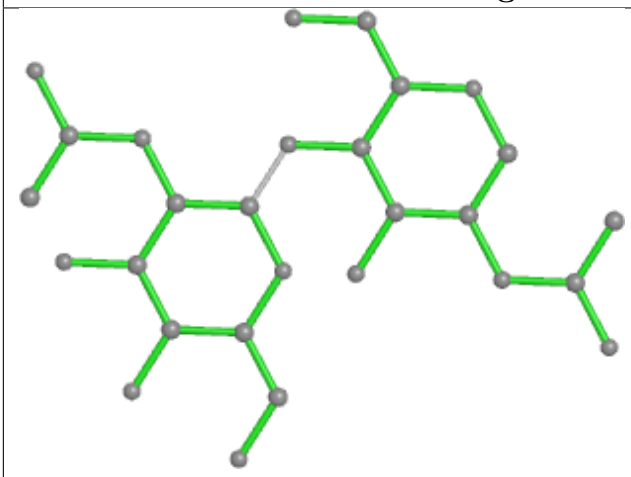


Torsions

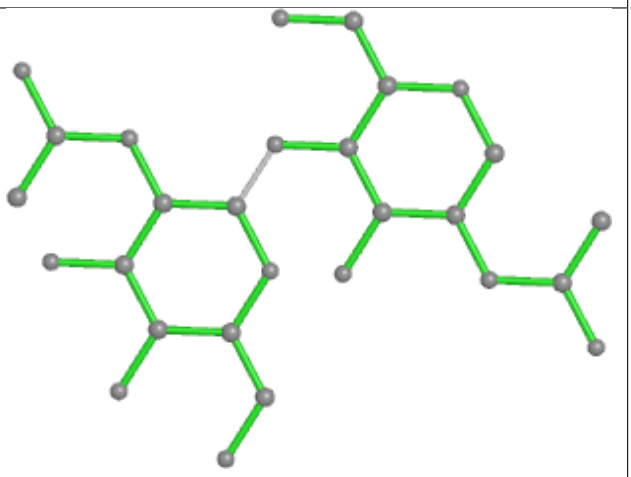


Rings

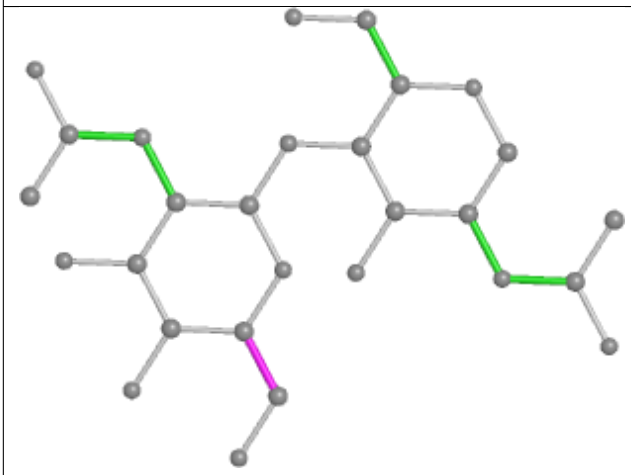
Oligosaccharide Chain S



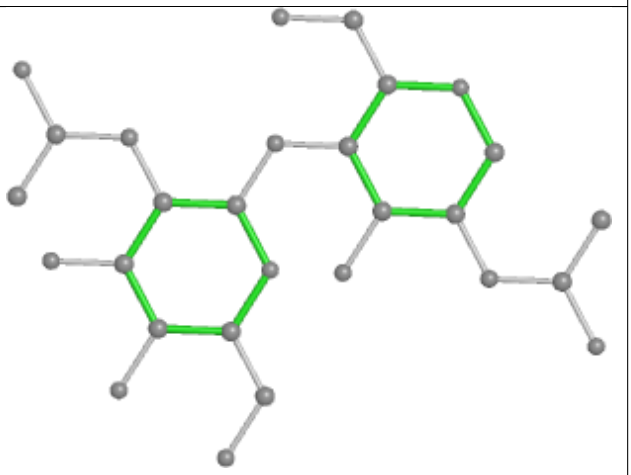
Bond lengths



Bond angles

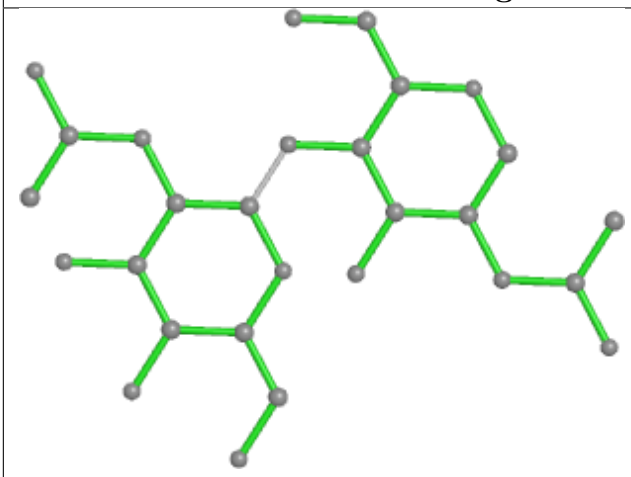


Torsions

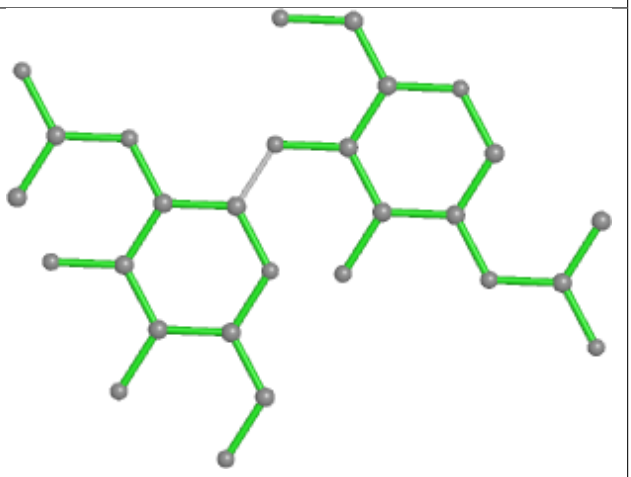


Rings

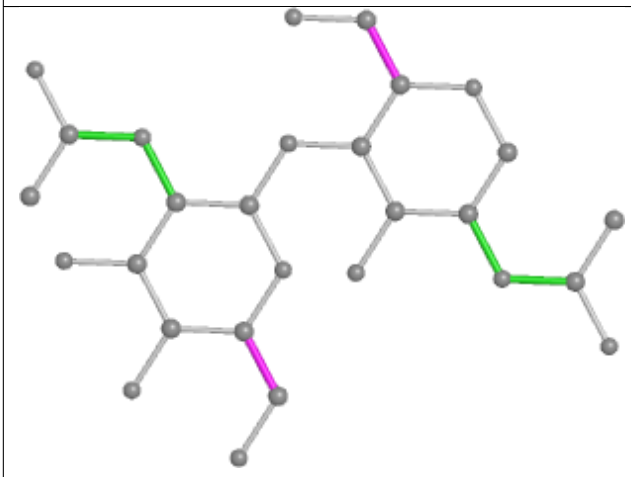
Oligosaccharide Chain T



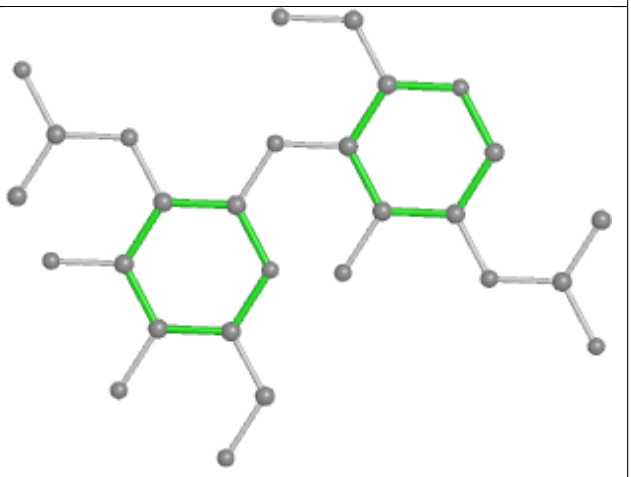
Bond lengths



Bond angles

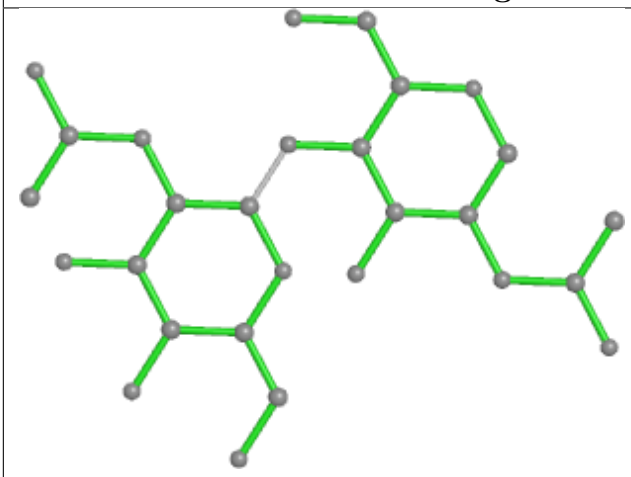


Torsions

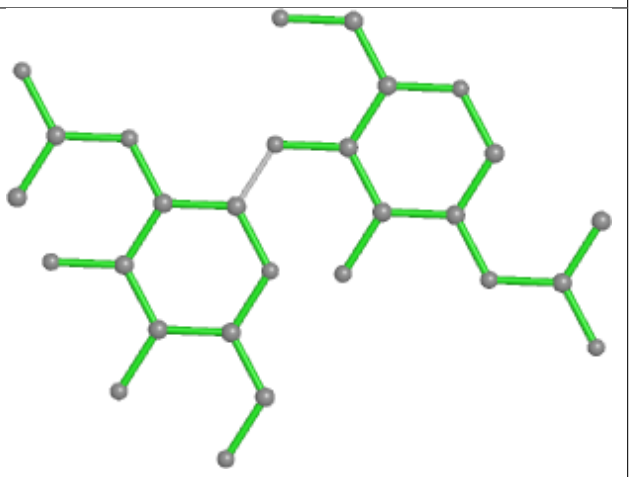


Rings

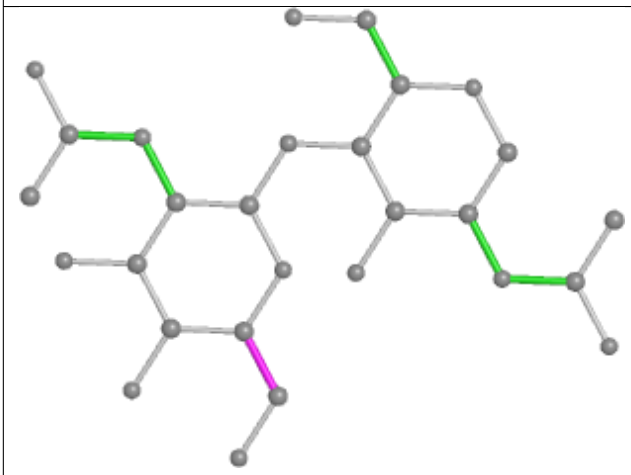
Oligosaccharide Chain U



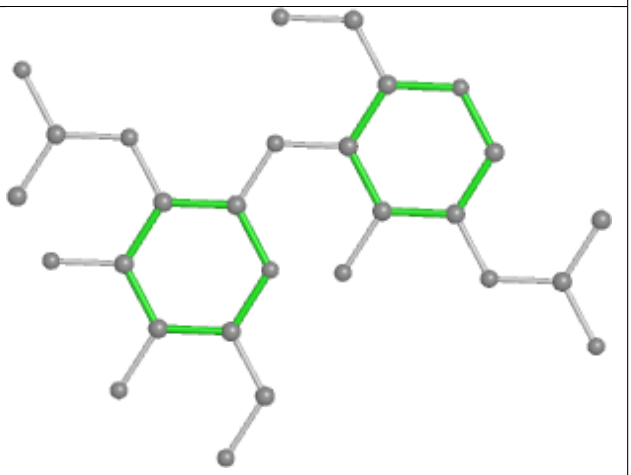
Bond lengths



Bond angles

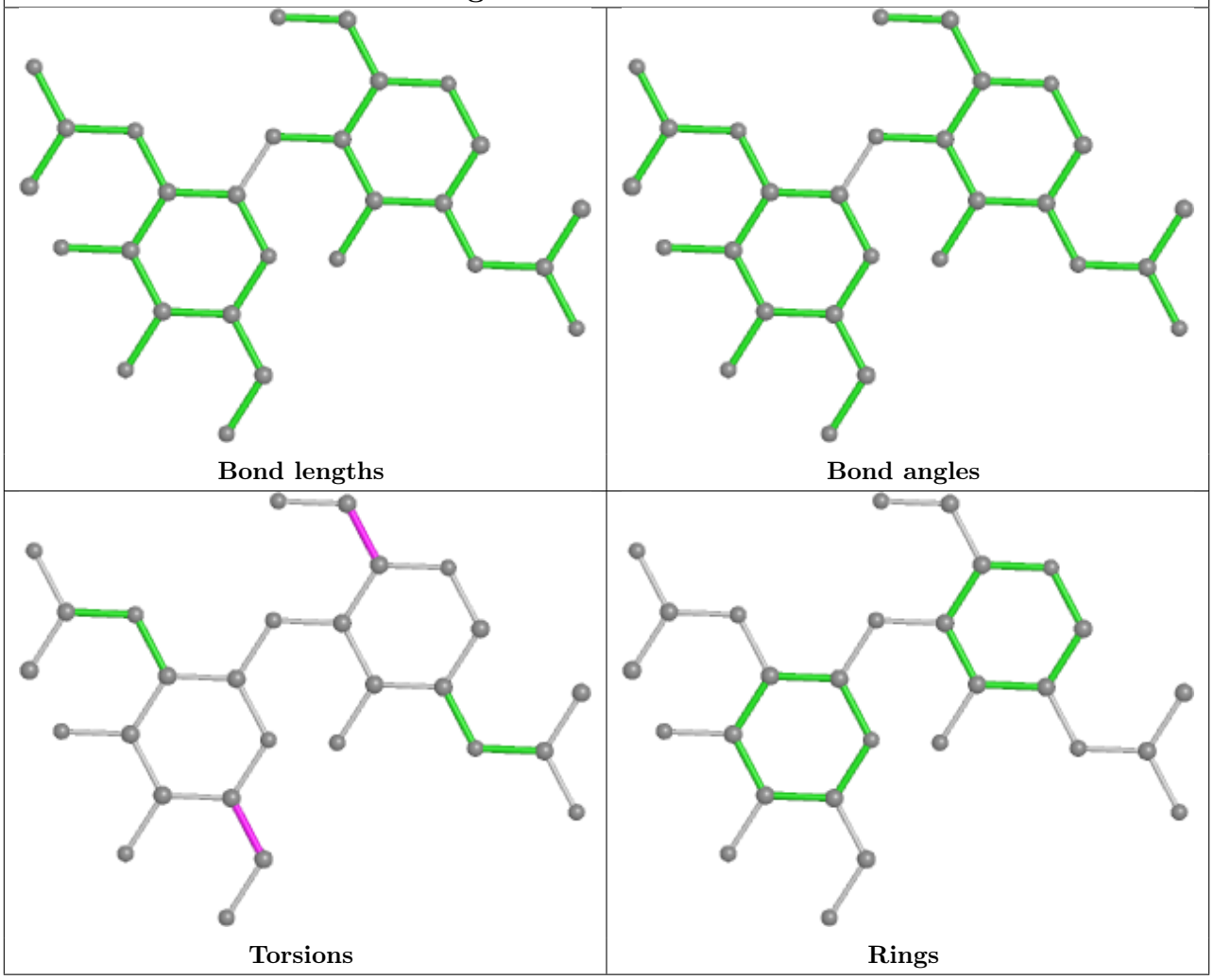


Torsions



Rings

Oligosaccharide Chain V



5.6 Ligand geometry (i)

30 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	C	1307	1	14,14,15	0.24	0	17,19,21	0.44	0
5	NAG	B	1301	1	14,14,15	0.45	0	17,19,21	0.44	0
5	NAG	A	1305	1	14,14,15	0.19	0	17,19,21	0.37	0
5	NAG	B	1303	1	14,14,15	0.26	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	A	1301	1	14,14,15	0.28	0	17,19,21	0.45	0
5	NAG	A	1310	1	14,14,15	0.24	0	17,19,21	0.46	0
5	NAG	B	1310	1	14,14,15	0.27	0	17,19,21	0.47	0
5	NAG	B	1309	1	14,14,15	0.24	0	17,19,21	0.44	0
5	NAG	A	1303	1	14,14,15	0.45	0	17,19,21	0.46	0
5	NAG	C	1305	1	14,14,15	0.30	0	17,19,21	0.48	0
5	NAG	C	1309	1	14,14,15	0.24	0	17,19,21	0.43	0
5	NAG	B	1302	1	14,14,15	0.25	0	17,19,21	0.49	0
5	NAG	B	1304	1	14,14,15	0.26	0	17,19,21	0.43	0
5	NAG	C	1302	1	14,14,15	0.54	0	17,19,21	0.42	0
5	NAG	A	1302	1	14,14,15	0.21	0	17,19,21	0.50	0
5	NAG	B	1308	1	14,14,15	0.56	0	17,19,21	0.51	0
5	NAG	C	1303	1	14,14,15	0.26	0	17,19,21	0.44	0
5	NAG	C	1301	1	14,14,15	0.38	0	17,19,21	0.44	0
5	NAG	A	1308	1	14,14,15	0.23	0	17,19,21	0.38	0
5	NAG	B	1306	1	14,14,15	0.41	0	17,19,21	0.63	1 (5%)
5	NAG	A	1309	1	14,14,15	0.24	0	17,19,21	0.45	0
5	NAG	C	1306	1	14,14,15	0.27	0	17,19,21	0.42	0
5	NAG	A	1306	1	14,14,15	0.23	0	17,19,21	0.46	0
5	NAG	B	1305	1	14,14,15	0.25	0	17,19,21	0.41	0
5	NAG	C	1304	1	14,14,15	0.29	0	17,19,21	0.43	0
5	NAG	A	1304	1	14,14,15	0.21	0	17,19,21	0.43	0
5	NAG	C	1310	1	14,14,15	0.45	0	17,19,21	0.40	0
5	NAG	C	1308	1	14,14,15	0.26	0	17,19,21	0.43	0
5	NAG	A	1307	1	14,14,15	0.27	0	17,19,21	0.44	0
5	NAG	B	1307	1	14,14,15	0.25	0	17,19,21	0.44	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	C	1307	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1301	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1309	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1302	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1308	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1306	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1310	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1308	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1307	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1306	NAG	C1-O5-C5	2.08	115.01	112.19

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1302	NAG	C4-C5-C6-O6
5	A	1301	NAG	O5-C5-C6-O6
5	A	1305	NAG	C4-C5-C6-O6
5	B	1310	NAG	O5-C5-C6-O6
5	A	1307	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	A	1305	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.