Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2023 – 02:41 AM EDT

PDB ID	:	6VEP
Title	:	Human insulin in complex with the human insulin microreceptor in turn in complex with Fv 83-7
Authors	:	Lawrence, M.C.; Menting, J.G.T.
Deposited on	:	2020-01-02
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

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

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

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 19318 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Insulin chain A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	21	163	99	25	35	4	0	0	0
1	G	21	163	99	25	35	4	0	0	0
1	M	21	163	99	25	35	4	0	0	0
1	S	21	163	99	25	35	4	0	0	0

- Molecule 2 is a protein called Insulin B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	27	212	137	36	37	2	0	0	0
2	H	25	200	129	34	35	2	0	0	0
2	N	26	207	134	35	36	2	0	0	0
2	T	26	207	134	35	36	2	0	0	0

- Molecule 3 is a protein called Fv 83-7 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	121	925	582	156	182	5	0	0	0
3	I	117	898	565	152	176	5	0	0	0
3	O	122	932	587	157	183	5	0	0	0
3	U	117	898	565	152	176	5	0	0	0

- Molecule 4 is a protein called Fv 83-7 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	116	897	567	148	178	4	0	0	0
4	J	113	881	559	145	173	4	0	0	0
4	P	114	887	562	146	175	4	0	0	0
4	V	114	881	558	145	174	4	0	0	0

- Molecule 5 is a protein called Insulin receptor subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	293	2332	1467	403	428	34	0	0	0
5	K	294	2339	1471	404	430	34	0	0	0
5	Q	302	2400	1506	422	438	34	0	0	0
5	W	296	2356	1481	408	433	34	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	144	HIS	TYR	conflict	UNP P06213
E	311	SER	-	expression tag	UNP P06213
E	312	SER	-	expression tag	UNP P06213
E	313	SER	-	expression tag	UNP P06213
E	314	LEU	-	expression tag	UNP P06213
E	315	VAL	-	expression tag	UNP P06213
E	316	PRO	-	expression tag	UNP P06213
E	317	ARG	-	expression tag	UNP P06213
K	144	HIS	TYR	conflict	UNP P06213
K	311	SER	-	expression tag	UNP P06213
K	312	SER	-	expression tag	UNP P06213
K	313	SER	-	expression tag	UNP P06213
K	314	LEU	-	expression tag	UNP P06213
K	315	VAL	-	expression tag	UNP P06213
K	316	PRO	-	expression tag	UNP P06213
K	317	ARG	-	expression tag	UNP P06213
Q	144	HIS	TYR	conflict	UNP P06213
Q	311	SER	-	expression tag	UNP P06213

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	312	SER	-	expression tag	UNP P06213
Q	313	SER	-	expression tag	UNP P06213
Q	314	LEU	-	expression tag	UNP P06213
Q	315	VAL	-	expression tag	UNP P06213
Q	316	PRO	-	expression tag	UNP P06213
Q	317	ARG	-	expression tag	UNP P06213
W	144	HIS	TYR	conflict	UNP P06213
W	311	SER	-	expression tag	UNP P06213
W	312	SER	-	expression tag	UNP P06213
W	313	SER	-	expression tag	UNP P06213
W	314	LEU	-	expression tag	UNP P06213
W	315	VAL	-	expression tag	UNP P06213
W	316	PRO	-	expression tag	UNP P06213
W	317	ARG	-	expression tag	UNP P06213

- Molecule 6 is a protein called Insulin receptor subunit beta.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	F	16	137	90	22	25	0	0	0
6	L	16	137	90	22	25	0	0	0
6	R	16	137	90	22	25	0	0	0
6	X	16	137	90	22	25	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	718	PRO	LYS	conflict	UNP P06213
F	719	SER	THR	conflict	UNP P06213
L	718	PRO	LYS	conflict	UNP P06213
L	719	SER	THR	conflict	UNP P06213
R	718	PRO	LYS	conflict	UNP P06213
R	719	SER	THR	conflict	UNP P06213
X	718	PRO	LYS	conflict	UNP P06213
X	719	SER	THR	conflict	UNP P06213

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
7	Y	3	38	22	2	14	0	0	0
7	c	3	38	22	2	14	0	0	0

- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
8	Z	4	49	28	2	19	0	0	0
8	a	4	49	28	2	19	0	0	0
8	f	4	49	28	2	19	0	0	0
8	g	4	49	28	2	19	0	0	0
8	j	4	49	28	2	19	0	0	0

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	b	2	28	16	2	10	0	0	0
9	h	2	28	16	2	10	0	0	0

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	d	5	60	34	2	24	0	0	0

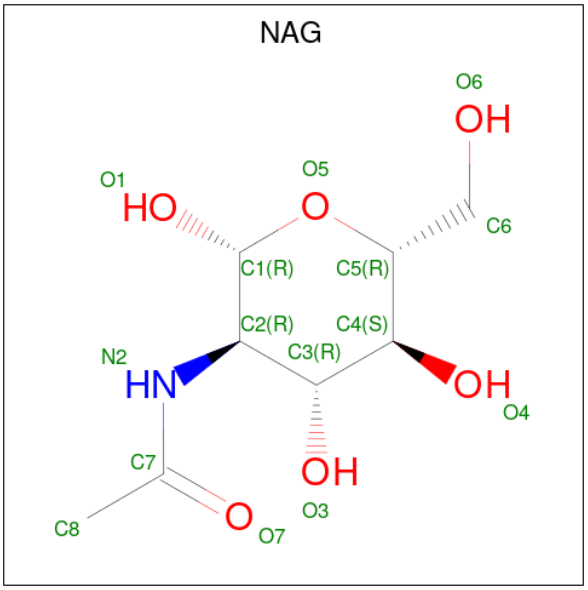
- Molecule 11 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
11	e	3	39	22	2	15	0	0	0

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
12	i	5	60	34	2	24	0	0	0

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
13	E	1	14	8	1	5	0	0
			Total	C	N	O		
13	E	1	14	8	1	5	0	0
			Total	C	N	O		
13	K	1	14	8	1	5	0	0
			Total	C	N	O		
13	K	1	14	8	1	5	0	0
			Total	C	N	O		
13	Q	1	14	8	1	5	0	0
			Total	C	N	O		
13	Q	1	14	8	1	5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
13	Q	1	14	8	1	5	0	0
13	W	1	14	8	1	5	0	0

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
14	C	4	4	4	0	0
14	E	3	3	3	0	0
14	I	1	1	1	0	0
14	J	1	1	1	0	0
14	K	1	1	1	0	0
14	O	2	2	2	0	0
14	P	1	1	1	0	0
14	Q	1	1	1	0	0
14	R	1	1	1	0	0
14	V	2	2	2	0	0
14	W	1	1	1	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	100.03Å 130.12Å 148.18Å 90.00° 90.27° 90.00°	Depositor
Resolution (Å)	48.89 – 2.90	Depositor
% Data completeness (in resolution range)	98.1 (48.89-2.90)	Depositor
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.06 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.193 , 0.225	Depositor
Wilson B-factor (Å^2)	68.1	Xtriage
Anisotropy	0.622	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.127 for h,-k,-l	Xtriage
Total number of atoms	19318	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates (i)

43 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	$\#\|Z\| > 2$
7	NAG	Y	1	5,7	14,14,15	0.38	0	17,19,21	1.26	2 (11%)
7	NAG	Y	2	7	14,14,15	0.42	0	17,19,21	0.97	1 (5%)
7	FUC	Y	3	7	10,10,11	0.50	0	14,14,16	0.83	1 (7%)
8	NAG	Z	1	5,8	14,14,15	0.34	0	17,19,21	1.01	1 (5%)
8	NAG	Z	2	8	14,14,15	0.34	0	17,19,21	0.70	1 (5%)
8	BMA	Z	3	8	11,11,12	0.45	0	15,15,17	0.69	0
8	FUC	Z	4	8	10,10,11	0.51	0	14,14,16	0.80	0
8	NAG	a	1	5,8	14,14,15	0.33	0	17,19,21	0.64	0
8	NAG	a	2	8	14,14,15	0.27	0	17,19,21	1.04	2 (11%)
8	BMA	a	3	8	11,11,12	0.37	0	15,15,17	0.73	0
8	FUC	a	4	8	10,10,11	0.48	0	14,14,16	0.83	0
9	NAG	b	1	5,9	14,14,15	0.52	0	17,19,21	1.52	3 (17%)
9	NAG	b	2	9	14,14,15	0.32	0	17,19,21	0.90	1 (5%)
7	NAG	c	1	5,7	14,14,15	0.34	0	17,19,21	0.50	0
7	NAG	c	2	7	14,14,15	0.36	0	17,19,21	0.55	0
7	FUC	c	3	7	10,10,11	0.54	0	14,14,16	0.87	1 (7%)
10	NAG	d	1	5,10	14,14,15	0.41	0	17,19,21	0.70	0
10	NAG	d	2	10	14,14,15	0.30	0	17,19,21	0.90	1 (5%)
10	BMA	d	3	10	11,11,12	0.46	0	15,15,17	0.72	0
10	MAN	d	4	10	11,11,12	0.56	0	15,15,17	1.31	2 (13%)
10	FUC	d	5	10	10,10,11	0.45	0	14,14,16	0.91	1 (7%)
11	NAG	e	1	5,11	14,14,15	0.43	0	17,19,21	1.63	3 (17%)
11	NAG	e	2	11	14,14,15	0.41	0	17,19,21	1.39	4 (23%)
11	BMA	e	3	11	11,11,12	0.44	0	15,15,17	0.71	0
8	NAG	f	1	5,8	14,14,15	0.33	0	17,19,21	0.93	1 (5%)
8	NAG	f	2	8	14,14,15	0.32	0	17,19,21	1.02	2 (11%)
8	BMA	f	3	8	11,11,12	0.52	0	15,15,17	0.95	1 (6%)
8	FUC	f	4	8	10,10,11	0.40	0	14,14,16	0.73	0
8	NAG	g	1	5,8	14,14,15	0.32	0	17,19,21	0.65	0
8	NAG	g	2	8	14,14,15	0.36	0	17,19,21	0.64	1 (5%)
8	BMA	g	3	8	11,11,12	0.44	0	15,15,17	0.65	0
8	FUC	g	4	8	10,10,11	0.52	0	14,14,16	0.76	0
9	NAG	h	1	5,9	14,14,15	0.49	0	17,19,21	1.13	1 (5%)
9	NAG	h	2	9	14,14,15	0.37	0	17,19,21	1.06	3 (17%)
12	NAG	i	1	5,12	14,14,15	0.33	0	17,19,21	0.58	0
12	NAG	i	2	12	14,14,15	0.30	0	17,19,21	1.06	2 (11%)
12	BMA	i	3	12	11,11,12	0.44	0	15,15,17	0.73	0
12	MAN	i	4	12	11,11,12	0.51	0	15,15,17	0.77	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	FUC	i	5	12	10,10,11	0.39	0	14,14,16	0.83	1 (7%)
8	NAG	j	1	5,8	14,14,15	0.41	0	17,19,21	0.70	0
8	NAG	j	2	8	14,14,15	0.33	0	17,19,21	1.07	1 (5%)
8	BMA	j	3	8	11,11,12	0.38	0	15,15,17	0.74	0
8	FUC	j	4	8	10,10,11	0.53	0	14,14,16	1.25	1 (7%)

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
7	NAG	Y	1	5,7	-	2/6/23/26	0/1/1/1
7	NAG	Y	2	7	-	1/6/23/26	0/1/1/1
7	FUC	Y	3	7	-	-	0/1/1/1
8	NAG	Z	1	5,8	-	0/6/23/26	0/1/1/1
8	NAG	Z	2	8	-	0/6/23/26	0/1/1/1
8	BMA	Z	3	8	-	0/2/19/22	0/1/1/1
8	FUC	Z	4	8	-	-	0/1/1/1
8	NAG	a	1	5,8	-	0/6/23/26	0/1/1/1
8	NAG	a	2	8	-	1/6/23/26	0/1/1/1
8	BMA	a	3	8	-	0/2/19/22	0/1/1/1
8	FUC	a	4	8	-	-	0/1/1/1
9	NAG	b	1	5,9	-	0/6/23/26	0/1/1/1
9	NAG	b	2	9	-	0/6/23/26	0/1/1/1
7	NAG	c	1	5,7	-	0/6/23/26	0/1/1/1
7	NAG	c	2	7	-	0/6/23/26	0/1/1/1
7	FUC	c	3	7	-	-	0/1/1/1
10	NAG	d	1	5,10	-	0/6/23/26	0/1/1/1
10	NAG	d	2	10	-	0/6/23/26	0/1/1/1
10	BMA	d	3	10	-	0/2/19/22	0/1/1/1
10	MAN	d	4	10	-	0/2/19/22	0/1/1/1
10	FUC	d	5	10	-	-	0/1/1/1
11	NAG	e	1	5,11	-	1/6/23/26	0/1/1/1
11	NAG	e	2	11	-	1/6/23/26	0/1/1/1
11	BMA	e	3	11	-	0/2/19/22	0/1/1/1
8	NAG	f	1	5,8	-	0/6/23/26	0/1/1/1
8	NAG	f	2	8	-	0/6/23/26	0/1/1/1
8	BMA	f	3	8	-	0/2/19/22	0/1/1/1
8	FUC	f	4	8	-	-	0/1/1/1
8	NAG	g	1	5,8	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	g	2	8	-	0/6/23/26	0/1/1/1
8	BMA	g	3	8	-	0/2/19/22	0/1/1/1
8	FUC	g	4	8	-	-	0/1/1/1
9	NAG	h	1	5,9	-	2/6/23/26	0/1/1/1
9	NAG	h	2	9	-	1/6/23/26	0/1/1/1
12	NAG	i	1	5,12	-	0/6/23/26	0/1/1/1
12	NAG	i	2	12	-	0/6/23/26	0/1/1/1
12	BMA	i	3	12	-	0/2/19/22	0/1/1/1
12	MAN	i	4	12	-	0/2/19/22	0/1/1/1
12	FUC	i	5	12	-	-	0/1/1/1
8	NAG	j	1	5,8	-	2/6/23/26	0/1/1/1
8	NAG	j	2	8	-	0/6/23/26	0/1/1/1
8	BMA	j	3	8	-	1/2/19/22	0/1/1/1
8	FUC	j	4	8	-	-	0/1/1/1

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	e	1	NAG	C1-C2-N2	4.44	118.07	110.49
9	b	1	NAG	O5-C1-C2	-3.95	105.05	111.29
11	e	1	NAG	C2-N2-C7	3.88	128.43	122.90
10	d	4	MAN	C1-O5-C5	3.83	117.38	112.19
8	j	4	FUC	C1-C2-C3	3.53	114.00	109.67
7	Y	1	NAG	O5-C1-C2	-3.50	105.76	111.29
11	e	2	NAG	C2-N2-C7	3.38	127.72	122.90
9	h	1	NAG	C1-C2-N2	-3.35	104.77	110.49
8	Z	1	NAG	C1-O5-C5	3.31	116.67	112.19
7	Y	2	NAG	C2-N2-C7	3.29	127.58	122.90
8	j	2	NAG	C1-O5-C5	3.23	116.56	112.19
9	b	1	NAG	C1-O5-C5	3.01	116.27	112.19
11	e	2	NAG	C1-C2-N2	2.97	115.56	110.49
8	f	2	NAG	O5-C1-C2	-2.91	106.70	111.29
10	d	4	MAN	C1-C2-C3	2.82	113.14	109.67
9	b	1	NAG	C1-C2-N2	2.80	115.27	110.49
12	i	2	NAG	O5-C1-C2	-2.56	107.24	111.29
8	f	3	BMA	C1-O5-C5	2.55	115.65	112.19
12	i	2	NAG	C1-C2-N2	2.54	114.82	110.49
10	d	5	FUC	C1-C2-C3	2.52	112.77	109.67
8	f	1	NAG	C1-C2-N2	-2.51	106.20	110.49
8	f	2	NAG	C1-C2-N2	2.44	114.65	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	e	1	NAG	C1-O5-C5	2.43	115.48	112.19
7	Y	1	NAG	C1-C2-N2	2.43	114.63	110.49
10	d	2	NAG	O5-C1-C2	-2.40	107.49	111.29
11	e	2	NAG	C1-O5-C5	2.31	115.32	112.19
9	h	2	NAG	C2-N2-C7	2.27	126.13	122.90
8	a	2	NAG	O5-C1-C2	-2.24	107.75	111.29
8	a	2	NAG	C1-C2-N2	2.20	114.25	110.49
9	b	2	NAG	C1-C2-N2	-2.20	106.74	110.49
8	Z	2	NAG	C1-O5-C5	2.19	115.17	112.19
12	i	5	FUC	C1-C2-C3	2.14	112.29	109.67
11	e	2	NAG	O5-C1-C2	-2.13	107.93	111.29
12	i	4	MAN	C1-C2-C3	2.12	112.28	109.67
9	h	2	NAG	O5-C1-C2	-2.12	107.94	111.29
7	c	3	FUC	C1-C2-C3	2.11	112.26	109.67
8	g	2	NAG	C1-O5-C5	2.04	114.96	112.19
7	Y	3	FUC	C1-O5-C5	2.02	117.35	112.78
9	h	2	NAG	C1-C2-N2	2.01	113.93	110.49

There are no chirality outliers.

All (14) torsion outliers are listed below:

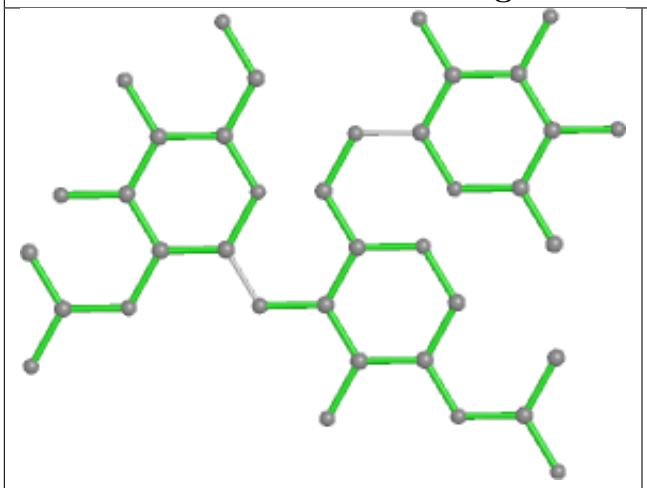
Mol	Chain	Res	Type	Atoms
7	Y	2	NAG	C3-C2-N2-C7
9	h	1	NAG	C1-C2-N2-C7
11	e	1	NAG	C1-C2-N2-C7
7	Y	1	NAG	O5-C5-C6-O6
8	j	1	NAG	O5-C5-C6-O6
8	j	1	NAG	C4-C5-C6-O6
7	Y	1	NAG	C4-C5-C6-O6
9	h	2	NAG	C1-C2-N2-C7
11	e	2	NAG	C1-C2-N2-C7
8	j	3	BMA	O5-C5-C6-O6
8	a	2	NAG	O5-C5-C6-O6
8	g	1	NAG	C4-C5-C6-O6
8	g	1	NAG	O5-C5-C6-O6
9	h	1	NAG	C3-C2-N2-C7

There are no ring outliers.

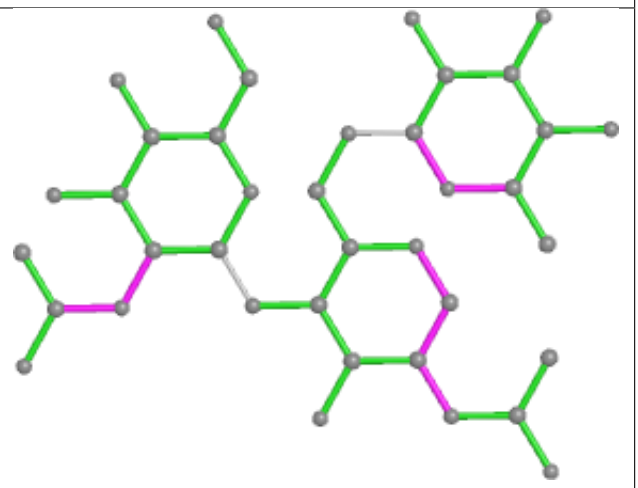
No monomer is involved in short contacts.

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

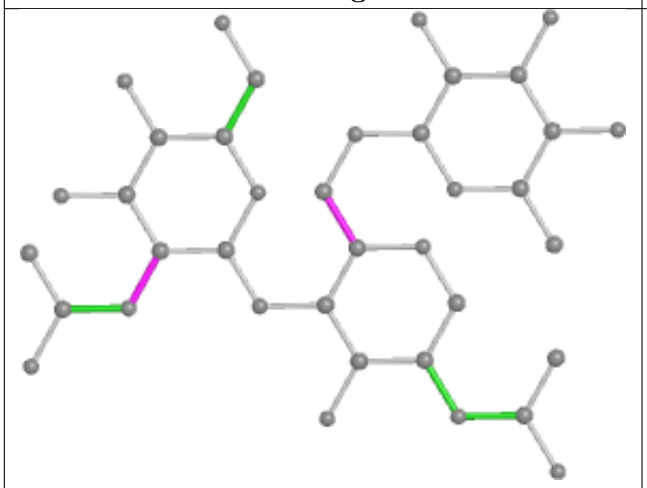
Oligosaccharide Chain Y



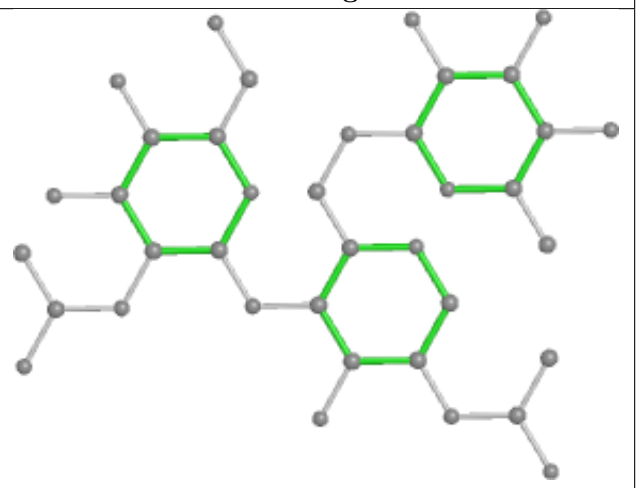
Bond lengths



Bond angles

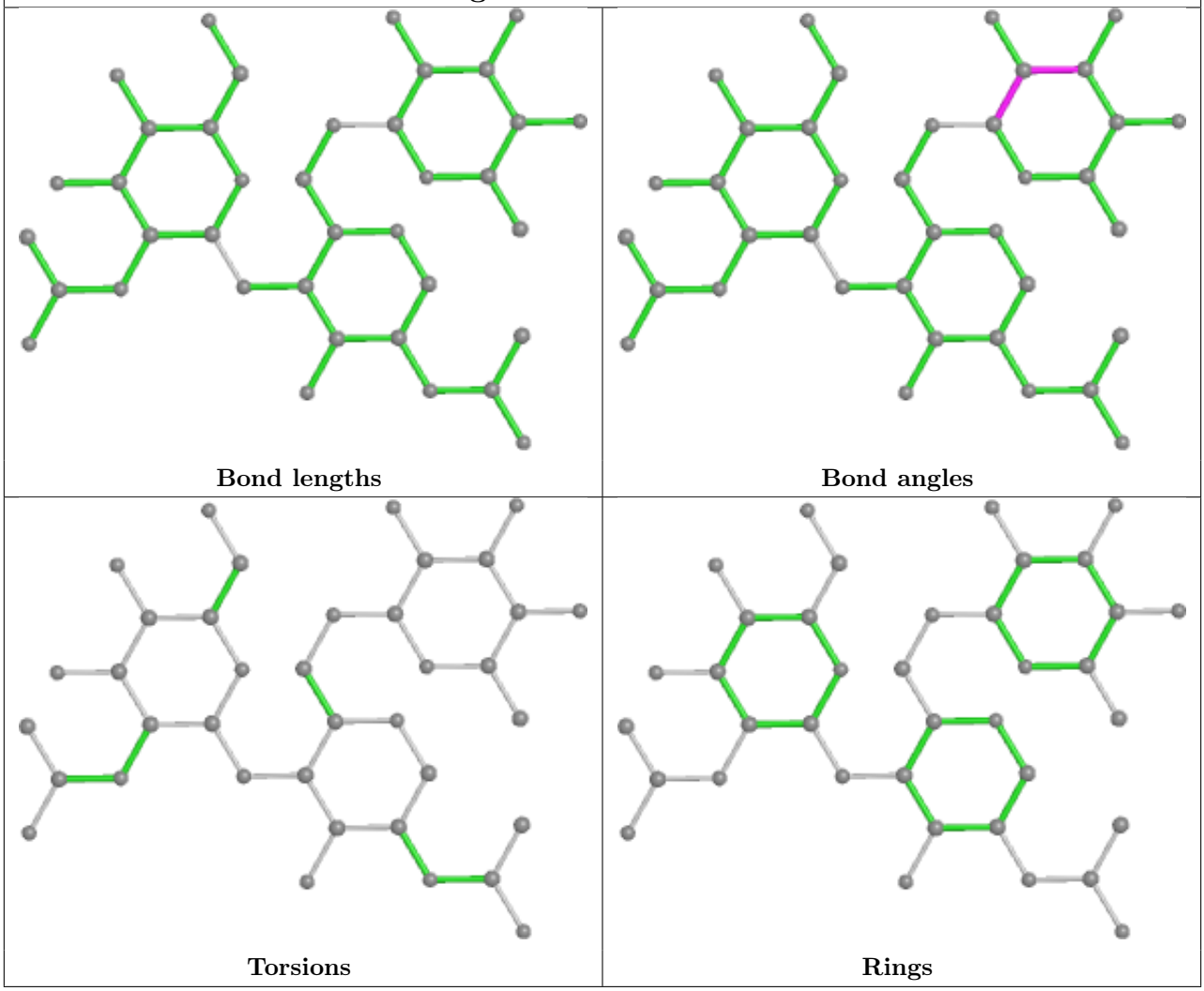


Torsions

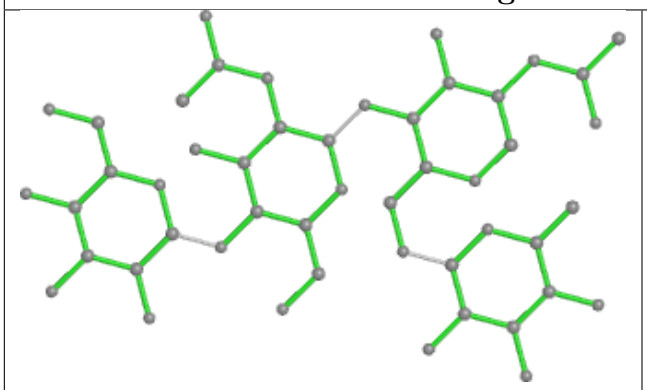


Rings

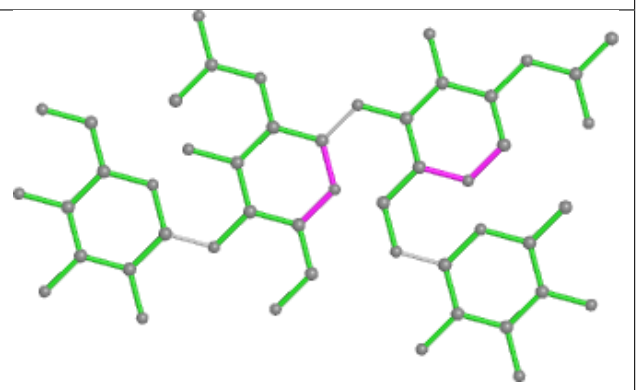
Oligosaccharide Chain c



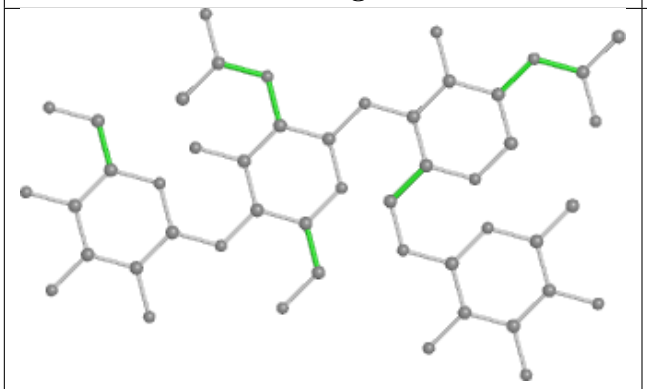
Oligosaccharide Chain Z



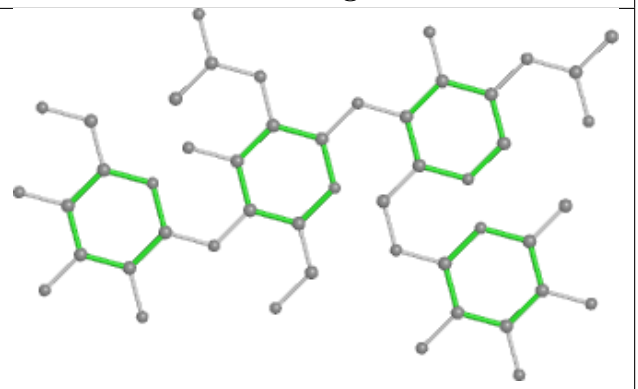
Bond lengths



Bond angles

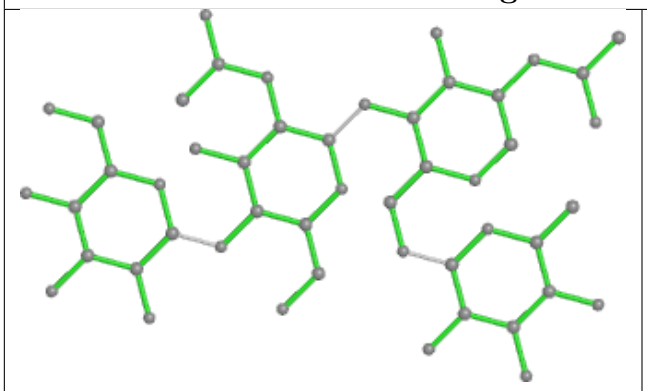


Torsions

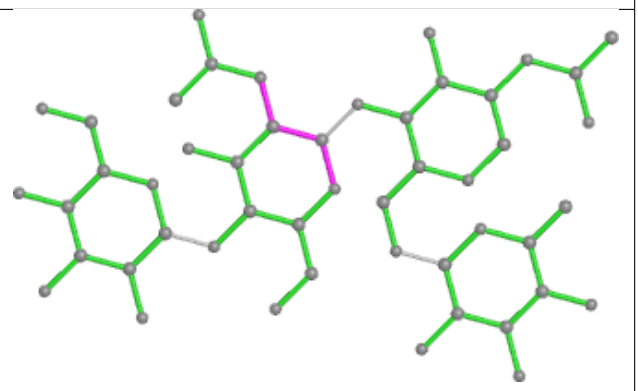


Rings

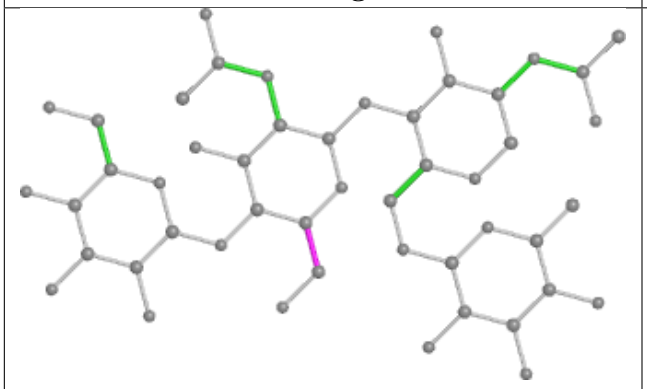
Oligosaccharide Chain a



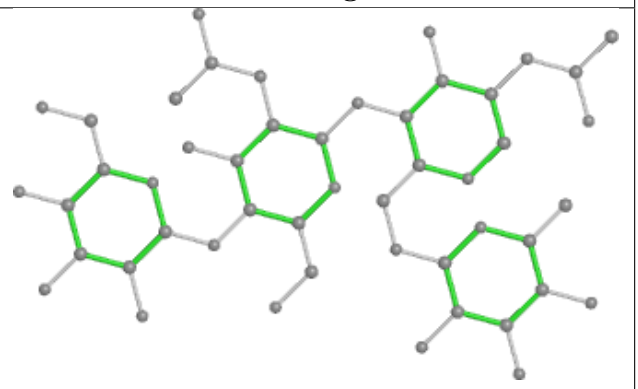
Bond lengths



Bond angles

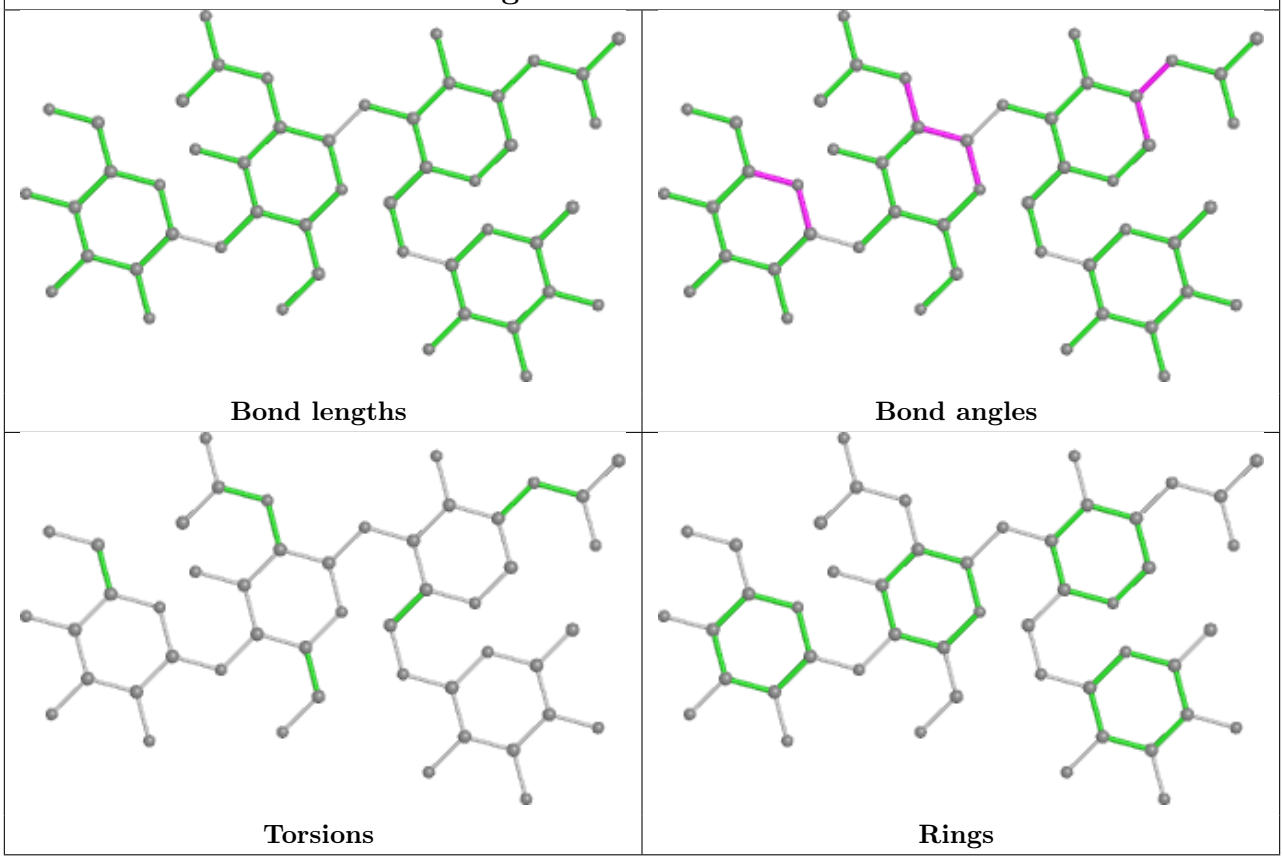


Torsions

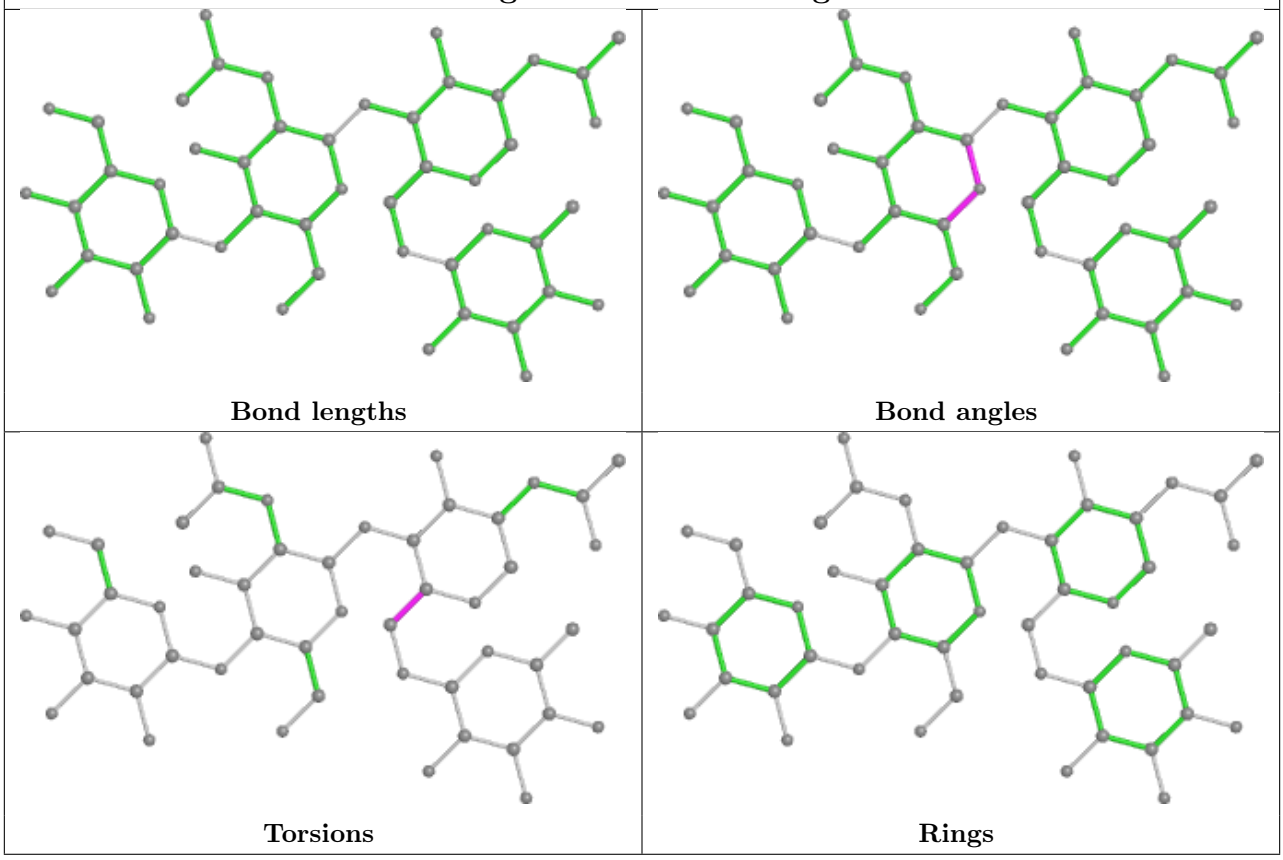


Rings

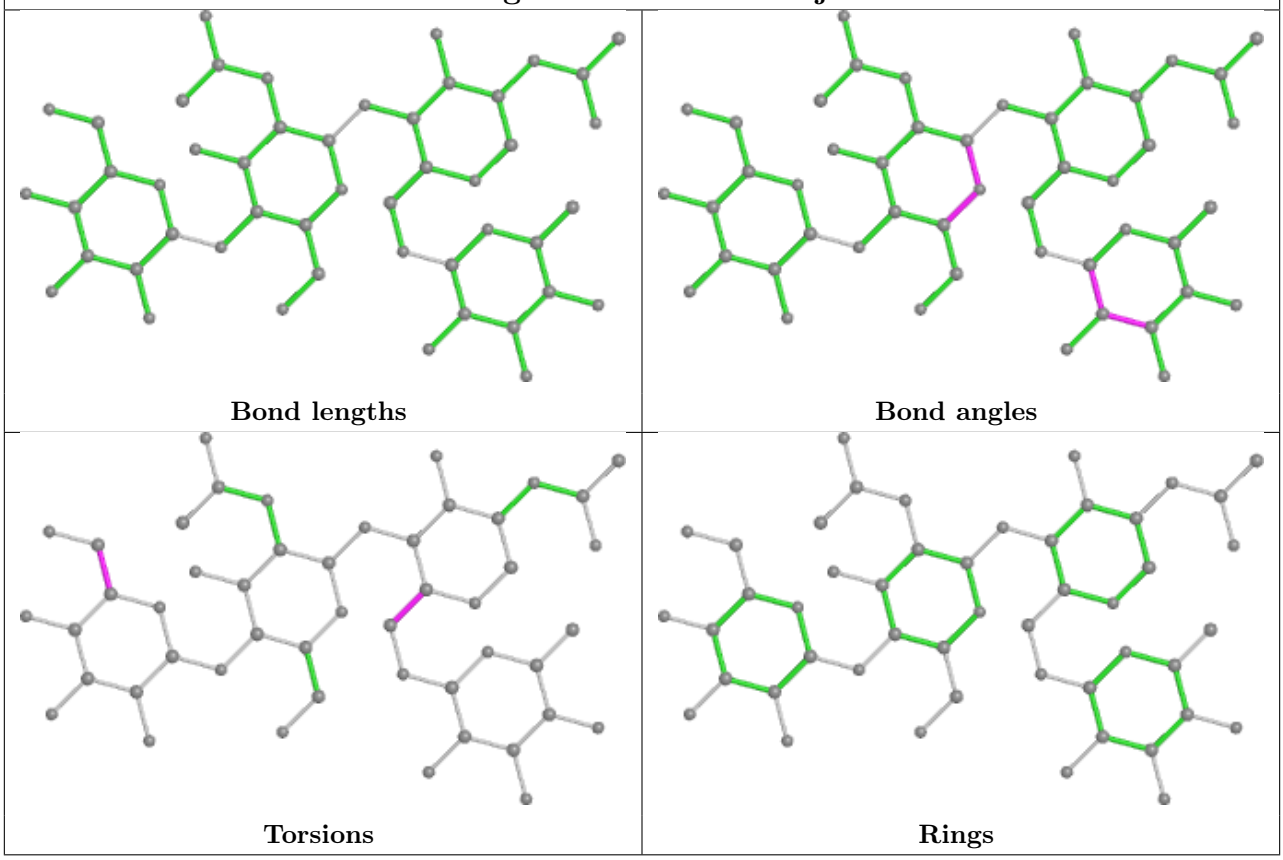
Oligosaccharide Chain f



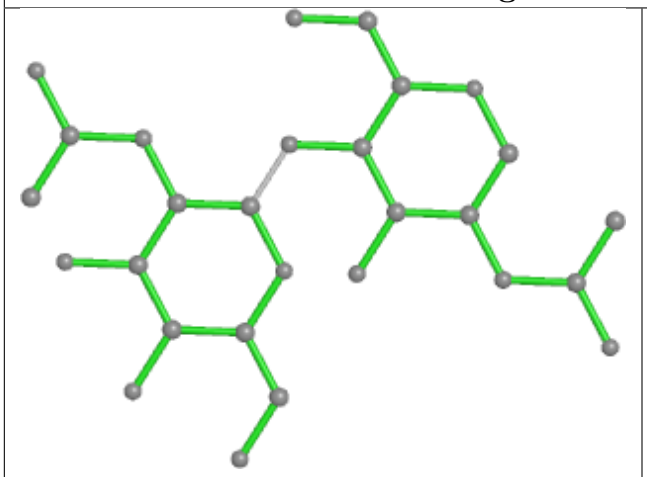
Oligosaccharide Chain g



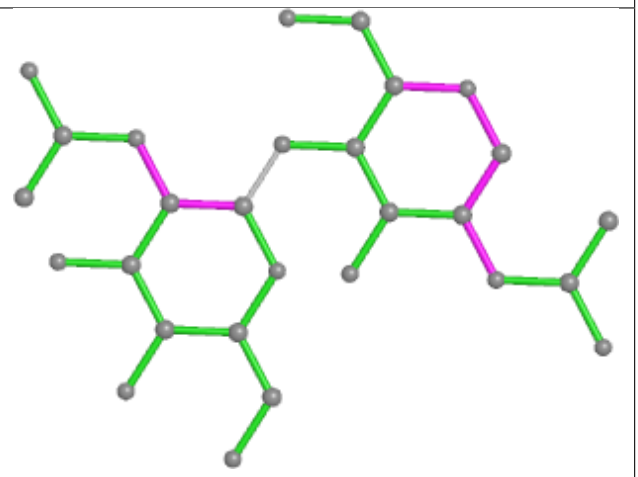
Oligosaccharide Chain j



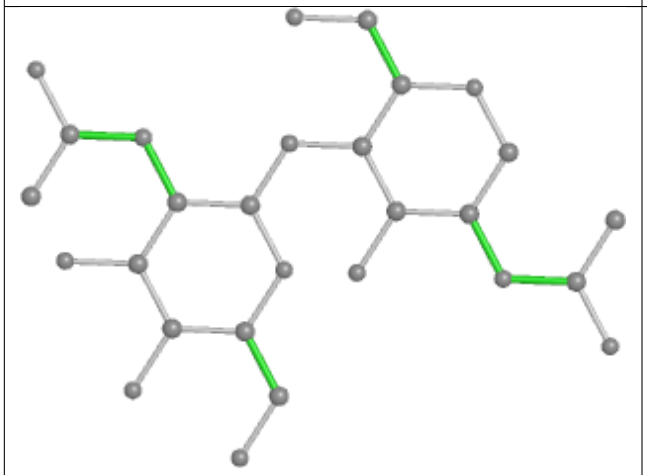
Oligosaccharide Chain b



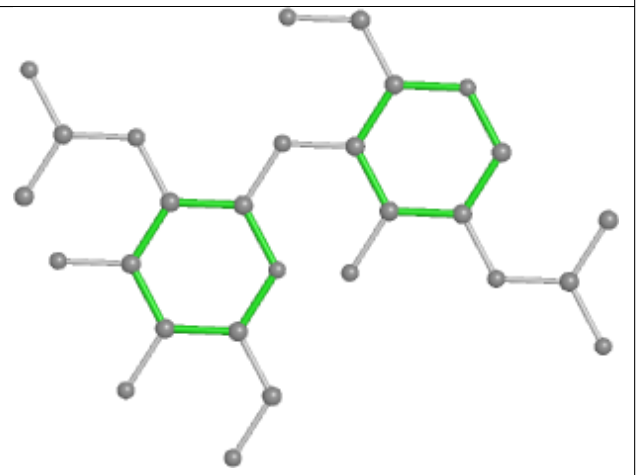
Bond lengths



Bond angles

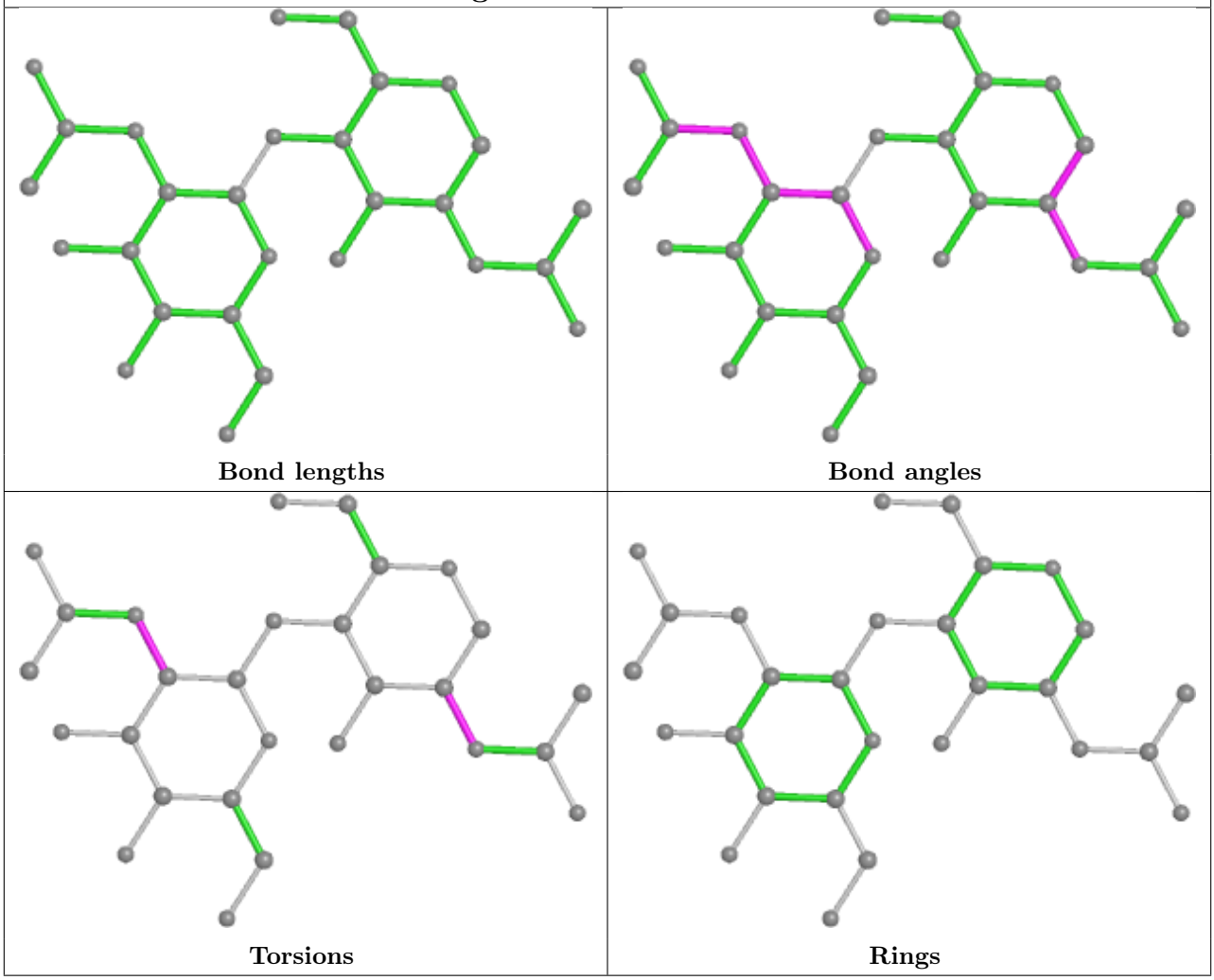


Torsions

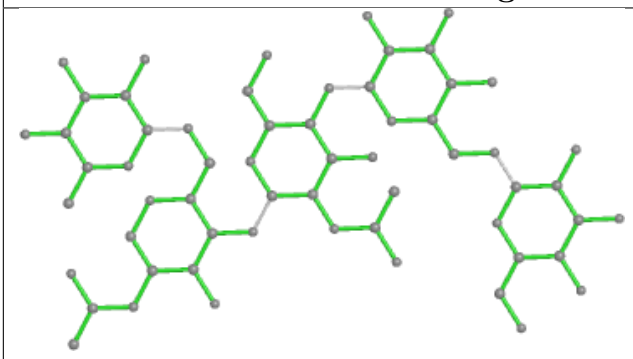


Rings

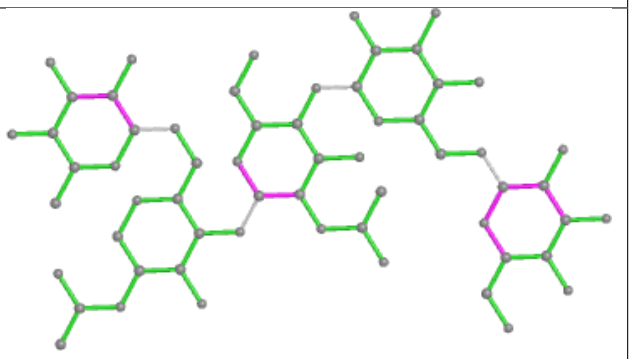
Oligosaccharide Chain h



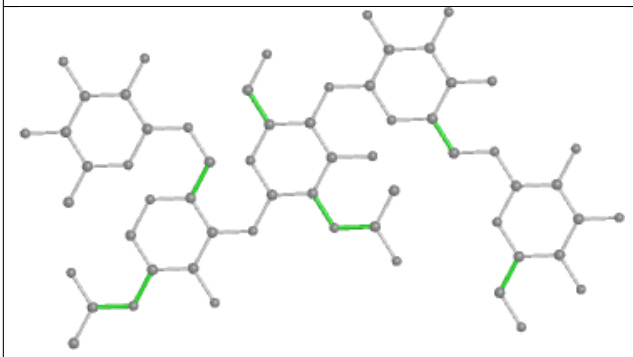
Oligosaccharide Chain d



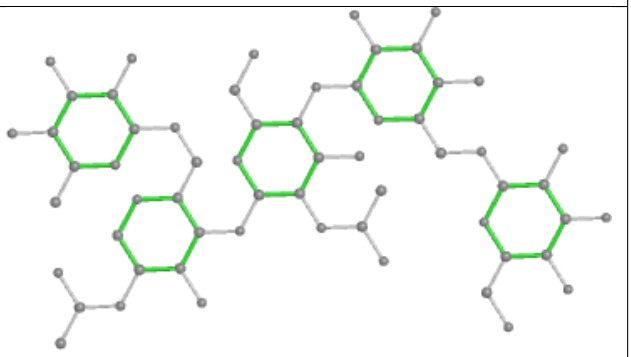
Bond lengths



Bond angles

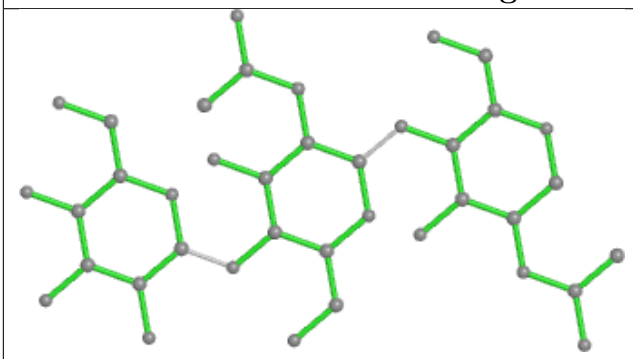


Torsions

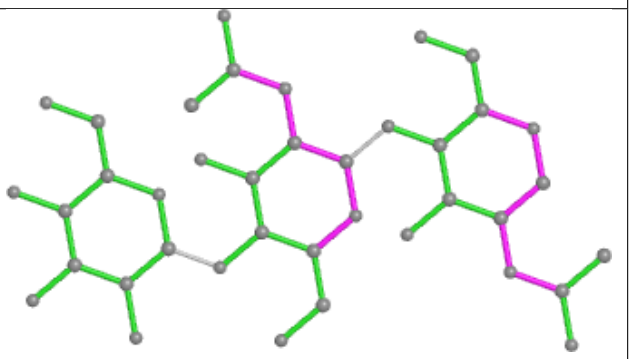


Rings

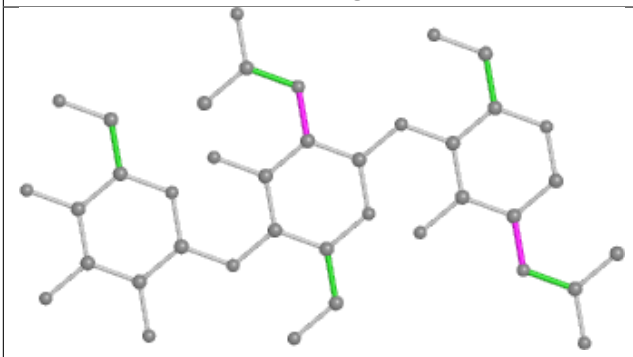
Oligosaccharide Chain e



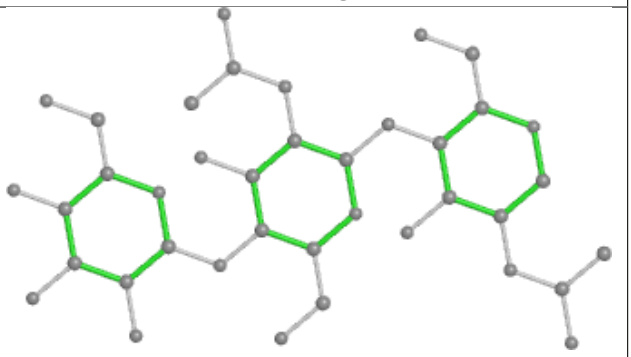
Bond lengths



Bond angles

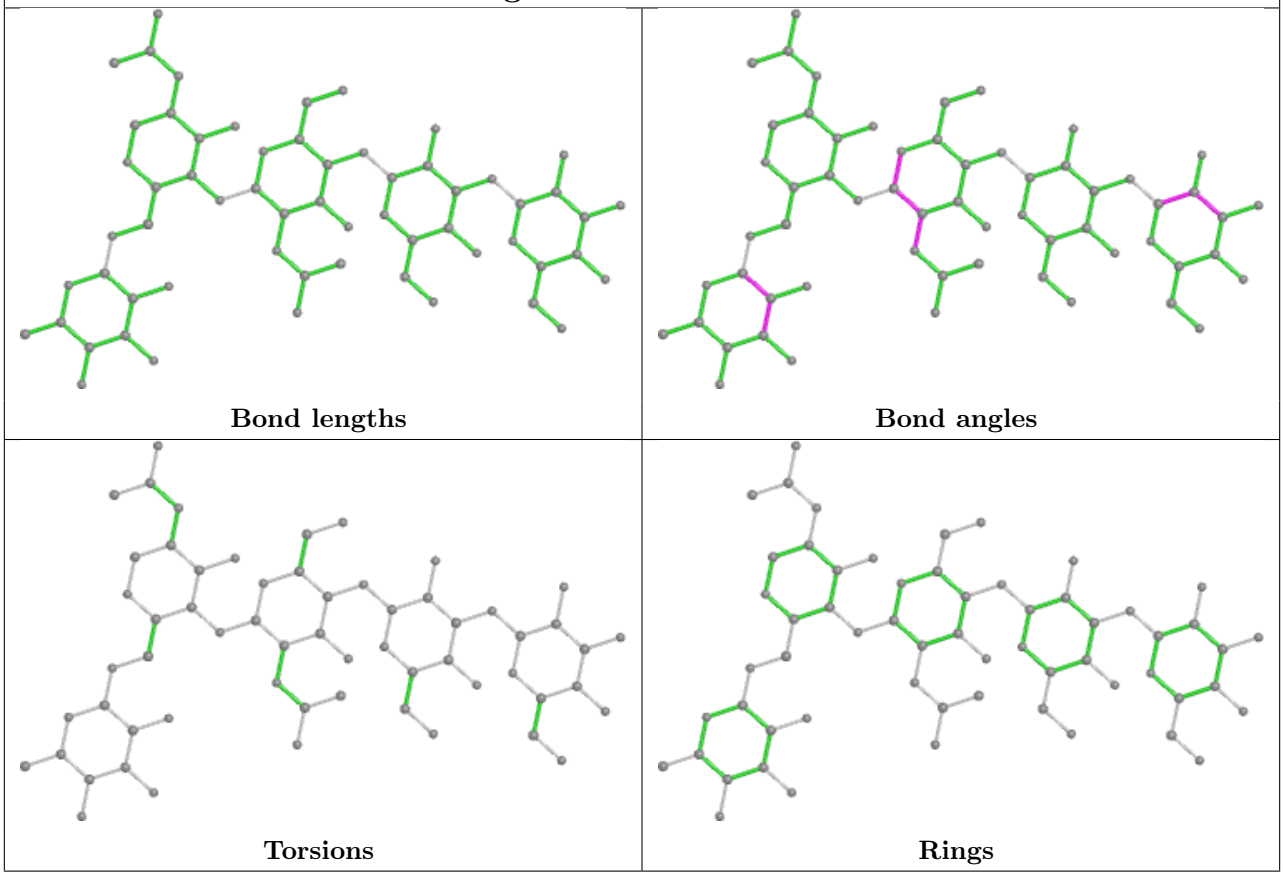


Torsions



Rings

Oligosaccharide Chain i



4.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
13	NAG	Q	405	5	14,14,15	0.40	0	17,19,21	1.09	2 (11%)
13	NAG	K	407	5	14,14,15	0.30	0	17,19,21	0.97	1 (5%)
13	NAG	E	409	5	14,14,15	0.36	0	17,19,21	0.74	1 (5%)
13	NAG	Q	401	5	14,14,15	0.42	0	17,19,21	1.58	3 (17%)
13	NAG	W	416	5	14,14,15	0.46	0	17,19,21	1.49	2 (11%)
13	NAG	Q	406	5	14,14,15	0.34	0	17,19,21	0.76	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	NAG	K	406	5	14,14,15	0.39	0	17,19,21	1.12	2 (11%)
13	NAG	E	408	5	14,14,15	0.34	0	17,19,21	0.99	2 (11%)

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
13	NAG	Q	405	5	-	0/6/23/26	0/1/1/1
13	NAG	K	407	5	-	2/6/23/26	0/1/1/1
13	NAG	E	409	5	-	2/6/23/26	0/1/1/1
13	NAG	Q	401	5	-	0/6/23/26	0/1/1/1
13	NAG	W	416	5	-	2/6/23/26	0/1/1/1
13	NAG	Q	406	5	-	3/6/23/26	0/1/1/1
13	NAG	K	406	5	-	0/6/23/26	0/1/1/1
13	NAG	E	408	5	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	W	416	NAG	O5-C1-C2	-4.97	103.44	111.29
13	Q	401	NAG	O5-C1-C2	-4.58	104.05	111.29
13	Q	401	NAG	C1-C2-N2	3.59	116.61	110.49
13	Q	405	NAG	O5-C1-C2	-3.47	105.81	111.29
13	K	407	NAG	C1-O5-C5	3.32	116.69	112.19
13	K	406	NAG	C1-O5-C5	3.10	116.39	112.19
13	W	416	NAG	C1-O5-C5	2.87	116.08	112.19
13	K	406	NAG	O5-C1-C2	-2.55	107.25	111.29
13	E	408	NAG	C1-O5-C5	2.44	115.50	112.19
13	Q	405	NAG	C1-O5-C5	2.36	115.39	112.19
13	Q	406	NAG	C1-O5-C5	2.32	115.33	112.19
13	E	409	NAG	C1-O5-C5	2.28	115.28	112.19
13	E	408	NAG	C1-C2-N2	2.27	114.36	110.49
13	Q	401	NAG	C1-O5-C5	2.06	114.99	112.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	W	416	NAG	C8-C7-N2-C2
13	W	416	NAG	O7-C7-N2-C2
13	K	407	NAG	O5-C5-C6-O6
13	Q	406	NAG	O5-C5-C6-O6
13	K	407	NAG	C4-C5-C6-O6
13	E	409	NAG	O5-C5-C6-O6
13	E	408	NAG	C8-C7-N2-C2
13	Q	406	NAG	C1-C2-N2-C7
13	E	409	NAG	C1-C2-N2-C7
13	E	408	NAG	O7-C7-N2-C2
13	Q	406	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.