wwPDB X-ray Structure Validation Summary Report (i)

Oct 3, 2023 – 08:40 AM EDT

PDB ID	:	6P3S
Title	:	Crystal structure of human Fab H5.28 in complex with influenza A H5N1 Vietnam hemagglutinin head domain
Authors	:	Dong, J.; Crowe, J.E.
Deposited on	:	2019-05-24
Resolution	:	4.00 Å(reported)

This is a wwPDB X-ray Structure 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/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 4.00 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 12 unique types of molecules in this entry. The entry contains 32097 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 Human Fab H5.28 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1472	932	258	275	7			
1	C	218	Total	C	N	O	S	0	0	0
			1301	803	237	257	4			
1	F	223	Total	C	N	O	S	0	0	0
			1436	902	258	269	7			
1	I	217	Total	C	N	O	S	0	0	0
			1364	850	248	260	6			
1	M	225	Total	C	N	O	S	0	0	0
			1432	908	260	257	7			
1	P	220	Total	C	N	O	S	0	0	0
			1313	820	241	246	6			
1	S	224	Total	C	N	O	S	0	0	0
			1393	875	256	255	7			
1	V	208	Total	C	N	O	S	0	0	0
			1236	773	225	232	6			

- Molecule 2 is a protein called Human Fab H5.28 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	215	Total	C	N	O	S	0	0	0
			1477	932	254	285	6			
2	D	203	Total	C	N	O	S	0	0	0
			1211	741	228	238	4			
2	G	214	Total	C	N	O	S	0	0	0
			1363	853	243	261	6			
2	J	187	Total	C	N	O	S	0	0	0
			1097	677	201	215	4			
2	N	214	Total	C	N	O	S	0	0	0
			1295	812	233	244	6			
2	Q	202	Total	C	N	O	S	0	0	0
			1179	731	224	219	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	214	Total	C	N	O	S	0	0	0
			1280	797	240	238	5			
2	W	198	Total	C	N	O	S	0	0	0
			1121	694	212	212	3			

- Molecule 3 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	196	Total	C	N	O	S	0	0	0
			1221	777	216	223	5			
3	H	202	Total	C	N	O	S	0	0	0
			1337	849	243	240	5			
3	K	206	Total	C	N	O	S	0	0	0
			1397	883	245	264	5			
3	L	185	Total	C	N	O	S	0	0	0
			1219	772	218	226	3			
3	O	209	Total	C	N	O	S	0	0	0
			1414	895	252	262	5			
3	R	194	Total	C	N	O	S	0	0	0
			1258	792	230	231	5			
3	U	196	Total	C	N	O	S	0	0	0
			1285	811	233	236	5			
3	X	196	Total	C	N	O	S	0	0	0
			1236	778	224	229	5			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	269	ALA	-	expression tag	UNP Q1KHK2
E	270	ALA	-	expression tag	UNP Q1KHK2
E	271	HIS	-	expression tag	UNP Q1KHK2
E	272	HIS	-	expression tag	UNP Q1KHK2
E	273	HIS	-	expression tag	UNP Q1KHK2
E	274	HIS	-	expression tag	UNP Q1KHK2
E	275	HIS	-	expression tag	UNP Q1KHK2
E	276	HIS	-	expression tag	UNP Q1KHK2
H	269	ALA	-	expression tag	UNP Q1KHK2
H	270	ALA	-	expression tag	UNP Q1KHK2
H	271	HIS	-	expression tag	UNP Q1KHK2
H	272	HIS	-	expression tag	UNP Q1KHK2
H	273	HIS	-	expression tag	UNP Q1KHK2
H	274	HIS	-	expression tag	UNP Q1KHK2

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Chain	Residue	Modelled	Actual	Comment	Reference
H	275	HIS	-	expression tag	UNP Q1KHK2
H	276	HIS	-	expression tag	UNP Q1KHK2
K	269	ALA	-	expression tag	UNP Q1KHK2
K	270	ALA	-	expression tag	UNP Q1KHK2
K	271	HIS	-	expression tag	UNP Q1KHK2
K	272	HIS	-	expression tag	UNP Q1KHK2
K	273	HIS	-	expression tag	UNP Q1KHK2
K	274	HIS	-	expression tag	UNP Q1KHK2
K	275	HIS	-	expression tag	UNP Q1KHK2
K	276	HIS	-	expression tag	UNP Q1KHK2
L	269	ALA	-	expression tag	UNP Q1KHK2
L	270	ALA	-	expression tag	UNP Q1KHK2
L	271	HIS	-	expression tag	UNP Q1KHK2
L	272	HIS	-	expression tag	UNP Q1KHK2
L	273	HIS	-	expression tag	UNP Q1KHK2
L	274	HIS	-	expression tag	UNP Q1KHK2
L	275	HIS	-	expression tag	UNP Q1KHK2
L	276	HIS	-	expression tag	UNP Q1KHK2
O	269	ALA	-	expression tag	UNP Q1KHK2
O	270	ALA	-	expression tag	UNP Q1KHK2
O	271	HIS	-	expression tag	UNP Q1KHK2
O	272	HIS	-	expression tag	UNP Q1KHK2
O	273	HIS	-	expression tag	UNP Q1KHK2
O	274	HIS	-	expression tag	UNP Q1KHK2
O	275	HIS	-	expression tag	UNP Q1KHK2
O	276	HIS	-	expression tag	UNP Q1KHK2
R	269	ALA	-	expression tag	UNP Q1KHK2
R	270	ALA	-	expression tag	UNP Q1KHK2
R	271	HIS	-	expression tag	UNP Q1KHK2
R	272	HIS	-	expression tag	UNP Q1KHK2
R	273	HIS	-	expression tag	UNP Q1KHK2
R	274	HIS	-	expression tag	UNP Q1KHK2
R	275	HIS	-	expression tag	UNP Q1KHK2
R	276	HIS	-	expression tag	UNP Q1KHK2
U	269	ALA	-	expression tag	UNP Q1KHK2
U	270	ALA	-	expression tag	UNP Q1KHK2
U	271	HIS	-	expression tag	UNP Q1KHK2
U	272	HIS	-	expression tag	UNP Q1KHK2
U	273	HIS	-	expression tag	UNP Q1KHK2
U	274	HIS	-	expression tag	UNP Q1KHK2
U	275	HIS	-	expression tag	UNP Q1KHK2
U	276	HIS	-	expression tag	UNP Q1KHK2

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Chain	Residue	Modelled	Actual	Comment	Reference
X	269	ALA	-	expression tag	UNP Q1KHK2
X	270	ALA	-	expression tag	UNP Q1KHK2
X	271	HIS	-	expression tag	UNP Q1KHK2
X	272	HIS	-	expression tag	UNP Q1KHK2
X	273	HIS	-	expression tag	UNP Q1KHK2
X	274	HIS	-	expression tag	UNP Q1KHK2
X	275	HIS	-	expression tag	UNP Q1KHK2
X	276	HIS	-	expression tag	UNP Q1KHK2

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-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
4	Y	7	Total	C	N	O	0	0	0
			95	53	4	38			

- Molecule 5 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-6)-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
5	Z	7	Total	C	N	O	0	0	0
			95	53	4	38			

- Molecule 6 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-alpha-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	a	6	Total	C	N	O	0	0	0
			81	45	3	33			

- Molecule 7 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-alpha-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-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
7	b	7	Total	C	N	O	0	0	0
			95	53	4	38			

- Molecule 8 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galacto pyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1 -6)-beta-D-mannopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	c	5	Total	C	N	O	0	0	0
			67	37	2	28			

- Molecule 9 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galacto pyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1 -6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-aceta mido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	d	7	Total	C	N	O	0	0	0
			95	53	4	38			

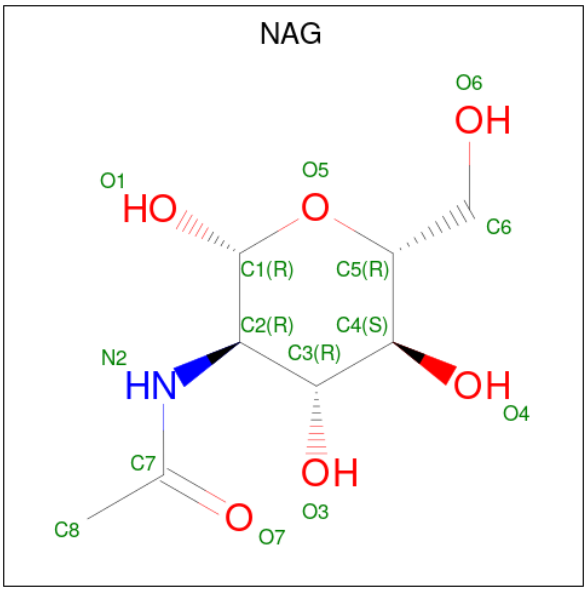
- Molecule 10 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galact opyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-6)-alpha-D-mannopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	e	5	Total	C	N	O	0	0	0
			67	37	2	28			

- Molecule 11 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galact opyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-alpha-D-mannopyranose -(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acet amido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	f	7	Total	C	N	O	0	0	0
			95	53	4	38			

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	L	1	Total C N O 14 8 1 5	0	0
12	O	1	Total C N O 14 8 1 5	0	0
12	R	1	Total C N O 14 8 1 5	0	0
12	U	1	Total C N O 14 8 1 5	0	0
12	X	1	Total C N O 14 8 1 5	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 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	135.48Å 187.22Å 342.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.46 – 4.00	Depositor
% Data completeness (in resolution range)	99.9 (49.46-4.00)	Depositor
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.18 (at 4.00Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, R_{free}	0.281 , 0.326	Depositor
Wilson B-factor (Å^2)	95.0	Xtriage
Anisotropy	0.456	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	32097	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.42% 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

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

51 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	Y	1	3,4	14,14,15	0.30	0	17,19,21	0.66	0
4	NAG	Y	2	4	14,14,15	0.29	0	17,19,21	1.37	2 (11%)
4	MAN	Y	3	4	11,11,12	0.23	0	15,15,17	0.73	1 (6%)
4	MAN	Y	4	4	11,11,12	0.66	0	15,15,17	1.55	1 (6%)
4	NDG	Y	5	4	14,14,15	0.38	0	17,19,21	1.84	4 (23%)
4	GAL	Y	6	4	11,11,12	0.30	0	15,15,17	0.78	0
4	SIA	Y	7	4	20,20,21	0.56	0	24,28,31	1.31	5 (20%)
5	NAG	Z	1	3,5	14,14,15	0.33	0	17,19,21	0.62	0
5	NAG	Z	2	5	14,14,15	0.27	0	17,19,21	1.31	2 (11%)
5	BMA	Z	3	5	11,11,12	0.30	0	15,15,17	1.09	1 (6%)
5	BMA	Z	4	5	11,11,12	0.34	0	15,15,17	1.64	2 (13%)
5	NAG	Z	5	5	14,14,15	0.32	0	17,19,21	1.22	2 (11%)
5	GAL	Z	6	5	11,11,12	0.36	0	15,15,17	1.46	2 (13%)
5	SIA	Z	7	5	20,20,21	0.60	0	24,28,31	0.94	0
6	NAG	a	1	6	14,14,15	0.35	0	17,19,21	0.80	0
6	MAN	a	2	6	11,11,12	0.28	0	15,15,17	0.96	2 (13%)
6	MAN	a	3	6	11,11,12	0.49	0	15,15,17	1.71	2 (13%)
6	NDG	a	4	6	14,14,15	0.37	0	17,19,21	1.15	2 (11%)
6	GLA	a	5	6	11,11,12	0.57	0	15,15,17	2.84	4 (26%)
6	SIA	a	6	6	20,20,21	0.62	0	24,28,31	1.08	2 (8%)
7	NAG	b	1	3,7	14,14,15	0.31	0	17,19,21	1.00	1 (5%)
7	NAG	b	2	7	14,14,15	0.46	0	17,19,21	1.64	2 (11%)
7	MAN	b	3	7	11,11,12	0.36	0	15,15,17	1.19	1 (6%)
7	MAN	b	4	7	11,11,12	0.25	0	15,15,17	0.96	1 (6%)
7	NAG	b	5	7	14,14,15	0.25	0	17,19,21	0.75	0
7	GLA	b	6	7	11,11,12	0.24	0	15,15,17	0.68	0
7	SIA	b	7	7	20,20,21	0.57	0	24,28,31	1.72	5 (20%)
8	BMA	c	1	8	11,11,12	0.25	0	15,15,17	0.68	0
8	BMA	c	2	8	11,11,12	0.37	0	15,15,17	1.64	2 (13%)
8	NDG	c	3	8	14,14,15	0.42	0	17,19,21	1.56	3 (17%)
8	GAL	c	4	8	11,11,12	0.40	0	15,15,17	1.76	2 (13%)
8	SIA	c	5	8	20,20,21	0.52	0	24,28,31	0.86	1 (4%)
9	NAG	d	1	9	14,14,15	0.29	0	17,19,21	0.76	1 (5%)
9	NAG	d	2	9	14,14,15	0.26	0	17,19,21	0.57	0
9	MAN	d	3	9	11,11,12	0.33	0	15,15,17	1.46	2 (13%)
9	BMA	d	4	9	11,11,12	0.26	0	15,15,17	0.60	0
9	NDG	d	5	9	14,14,15	0.29	0	17,19,21	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	GAL	d	6	9	11,11,12	0.28	0	15,15,17	1.41	1 (6%)
9	SIA	d	7	9	20,20,21	0.56	0	24,28,31	1.20	2 (8%)
10	MAN	e	1	10	11,11,12	0.31	0	15,15,17	1.20	2 (13%)
10	BMA	e	2	10	11,11,12	0.30	0	15,15,17	0.70	0
10	NDG	e	3	10	14,14,15	0.38	0	17,19,21	0.95	1 (5%)
10	GAL	e	4	10	11,11,12	0.38	0	15,15,17	1.31	2 (13%)
10	SIA	e	5	10	20,20,21	0.59	0	24,28,31	1.26	4 (16%)
11	NAG	f	1	11	14,14,15	0.41	0	17,19,21	0.95	1 (5%)
11	NAG	f	2	11	14,14,15	0.38	0	17,19,21	0.88	2 (11%)
11	BMA	f	3	11	11,11,12	0.27	0	15,15,17	0.80	0
11	MAN	f	4	11	11,11,12	0.24	0	15,15,17	0.77	0
11	NDG	f	5	11	14,14,15	0.33	0	17,19,21	0.88	0
11	GAL	f	6	11	11,11,12	0.30	0	15,15,17	1.67	3 (20%)
11	SIA	f	7	11	20,20,21	0.59	0	24,28,31	0.80	1 (4%)

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	Y	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	2/6/23/26	0/1/1/1
4	MAN	Y	3	4	-	2/2/19/22	0/1/1/1
4	MAN	Y	4	4	-	1/2/19/22	0/1/1/1
4	NDG	Y	5	4	-	3/6/23/26	0/1/1/1
4	GAL	Y	6	4	-	2/2/19/22	0/1/1/1
4	SIA	Y	7	4	-	9/18/34/38	0/1/1/1
5	NAG	Z	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	3/6/23/26	0/1/1/1
5	BMA	Z	3	5	-	1/2/19/22	1/1/1/1
5	BMA	Z	4	5	-	0/2/19/22	0/1/1/1
5	NAG	Z	5	5	-	3/6/23/26	0/1/1/1
5	GAL	Z	6	5	-	2/2/19/22	0/1/1/1
5	SIA	Z	7	5	-	7/18/34/38	0/1/1/1
6	NAG	a	1	6	-	2/6/23/26	0/1/1/1
6	MAN	a	2	6	-	0/2/19/22	1/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	a	3	6	-	0/2/19/22	0/1/1/1
6	NDG	a	4	6	-	1/6/23/26	0/1/1/1
6	GLA	a	5	6	-	2/2/19/22	0/1/1/1
6	SIA	a	6	6	-	8/18/34/38	0/1/1/1
7	NAG	b	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	b	2	7	-	1/6/23/26	0/1/1/1
7	MAN	b	3	7	-	1/2/19/22	0/1/1/1
7	MAN	b	4	7	-	1/2/19/22	1/1/1/1
7	NAG	b	5	7	-	4/6/23/26	0/1/1/1
7	GLA	b	6	7	-	2/2/19/22	0/1/1/1
7	SIA	b	7	7	-	10/18/34/38	0/1/1/1
8	BMA	c	1	8	-	2/2/19/22	0/1/1/1
8	BMA	c	2	8	-	0/2/19/22	1/1/1/1
8	NDG	c	3	8	-	4/6/23/26	0/1/1/1
8	GAL	c	4	8	-	1/2/19/22	0/1/1/1
8	SIA	c	5	8	-	2/18/34/38	0/1/1/1
9	NAG	d	1	9	-	2/6/23/26	0/1/1/1
9	NAG	d	2	9	-	4/6/23/26	0/1/1/1
9	MAN	d	3	9	-	2/2/19/22	0/1/1/1
9	BMA	d	4	9	-	1/2/19/22	0/1/1/1
9	NDG	d	5	9	-	3/6/23/26	0/1/1/1
9	GAL	d	6	9	-	1/2/19/22	0/1/1/1
9	SIA	d	7	9	-	8/18/34/38	0/1/1/1
10	MAN	e	1	10	-	2/2/19/22	1/1/1/1
10	BMA	e	2	10	-	0/2/19/22	0/1/1/1
10	NDG	e	3	10	-	0/6/23/26	0/1/1/1
10	GAL	e	4	10	-	0/2/19/22	0/1/1/1
10	SIA	e	5	10	-	7/18/34/38	0/1/1/1
11	NAG	f	1	11	-	0/6/23/26	0/1/1/1
11	NAG	f	2	11	-	4/6/23/26	0/1/1/1
11	BMA	f	3	11	-	0/2/19/22	0/1/1/1
11	MAN	f	4	11	-	0/2/19/22	1/1/1/1
11	NDG	f	5	11	-	2/6/23/26	0/1/1/1
11	GAL	f	6	11	-	1/2/19/22	0/1/1/1
11	SIA	f	7	11	-	3/18/34/38	0/1/1/1

There are no bond length outliers.

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	a	5	GLA	C1-O5-C5	6.57	121.09	112.19
6	a	5	GLA	C1-C2-C3	6.35	117.47	109.67
7	b	2	NAG	C1-O5-C5	5.96	120.26	112.19
8	c	4	GAL	C1-O5-C5	5.04	119.02	112.19
4	Y	4	MAN	O2-C2-C3	5.04	120.23	110.14

There are no chirality outliers.

5 of 122 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Y	1	NAG	C8-C7-N2-C2
4	Y	1	NAG	O7-C7-N2-C2
4	Y	5	NDG	C1-C2-N2-C7
4	Y	5	NDG	C8-C7-N2-C2
4	Y	5	NDG	O7-C7-N2-C2

5 of 6 ring outliers are listed below:

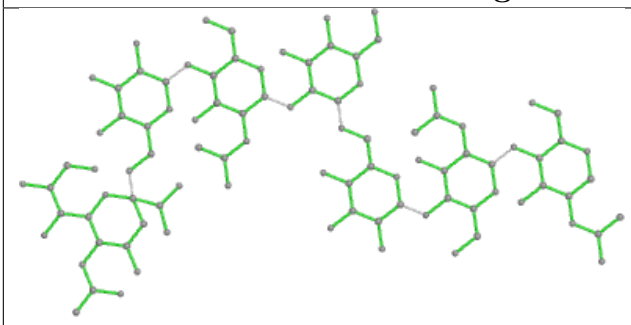
Mol	Chain	Res	Type	Atoms
5	Z	3	BMA	C1-C2-C3-C4-C5-O5
11	f	4	MAN	C1-C2-C3-C4-C5-O5
8	c	2	BMA	C1-C2-C3-C4-C5-O5
10	e	1	MAN	C1-C2-C3-C4-C5-O5
6	a	2	MAN	C1-C2-C3-C4-C5-O5

7 monomers are involved in 14 short contacts:

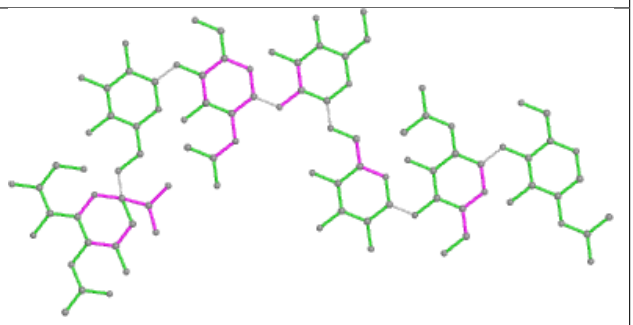
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Y	6	GAL	0	1
8	c	5	SIA	0	2
7	b	7	SIA	0	1
10	e	5	SIA	0	2
11	f	7	SIA	0	1
9	d	7	SIA	0	4
4	Y	7	SIA	0	3

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

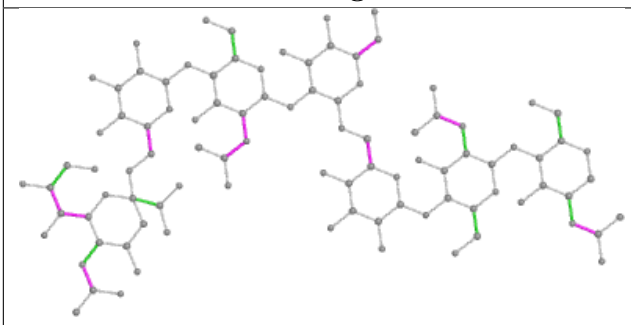
Oligosaccharide Chain Y



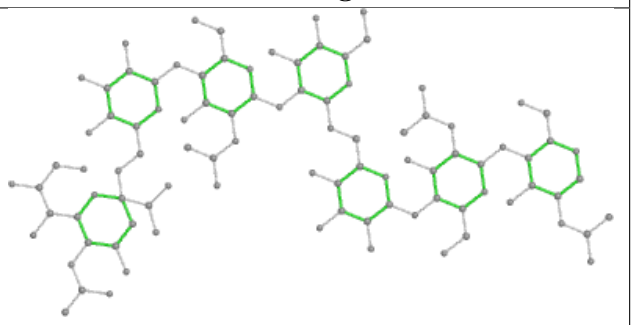
Bond lengths



Bond angles

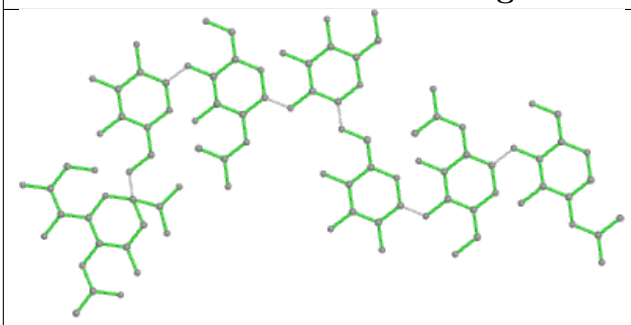


Torsions

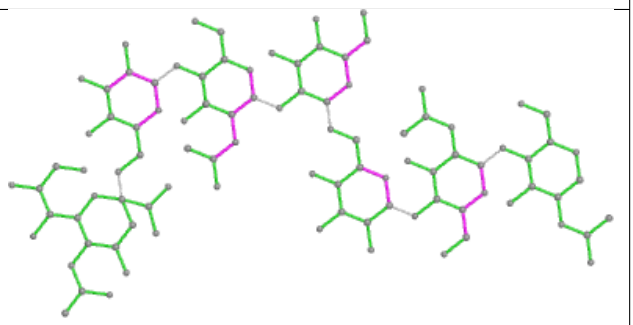


Rings

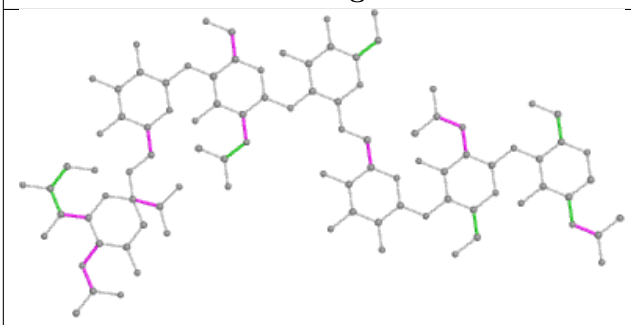
Oligosaccharide Chain Z



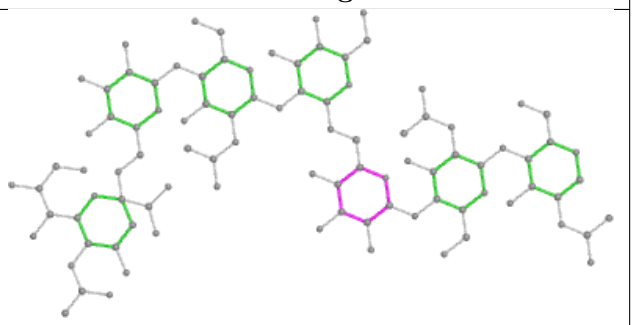
Bond lengths



Bond angles

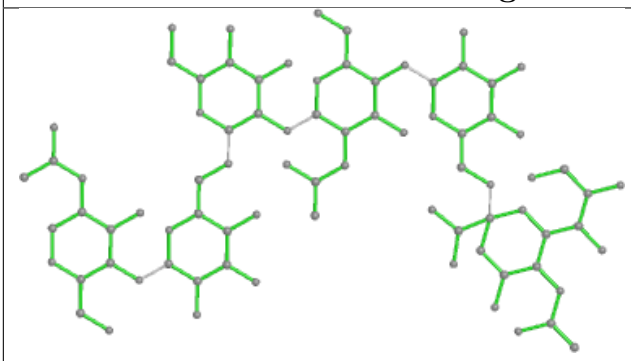


Torsions

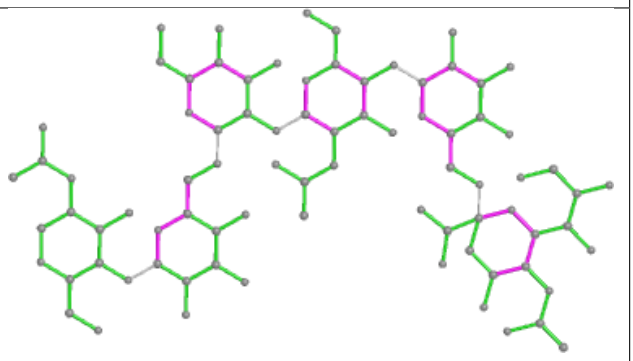


Rings

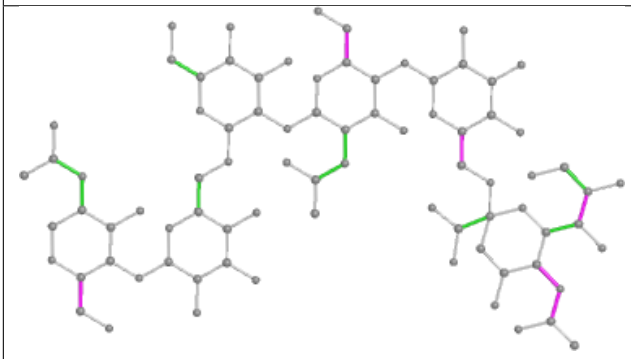
Oligosaccharide Chain a



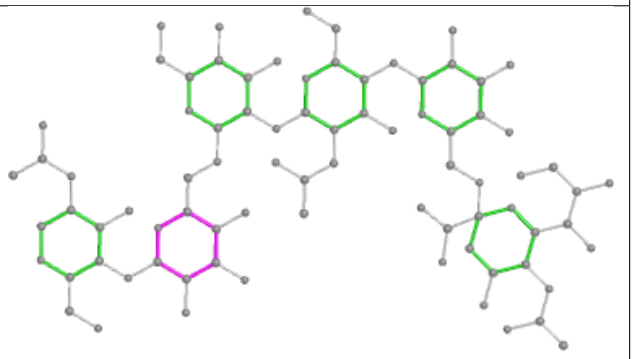
Bond lengths



Bond angles

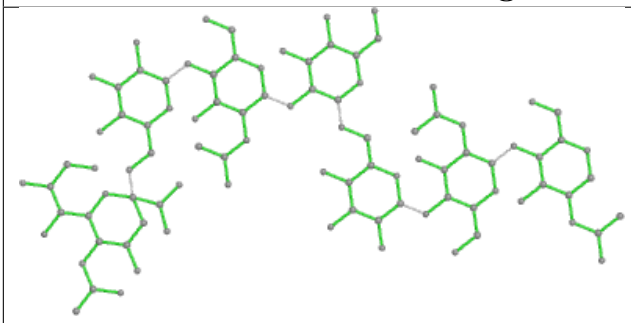


Torsions

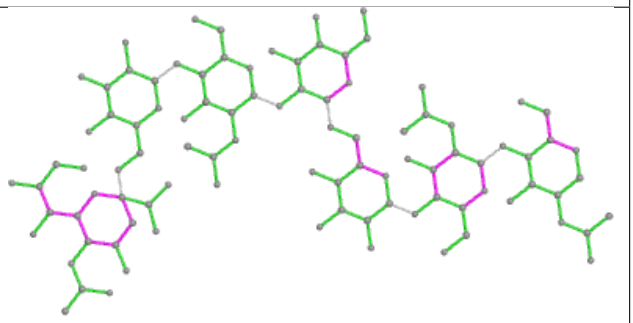


Rings

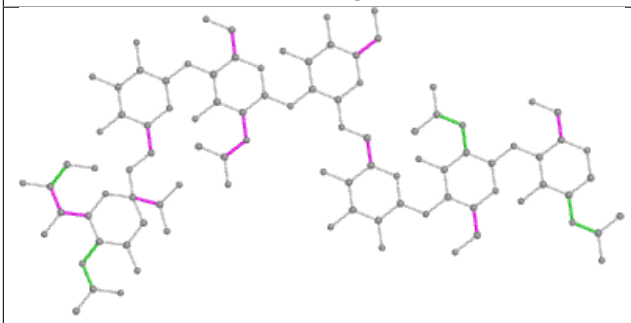
Oligosaccharide Chain b



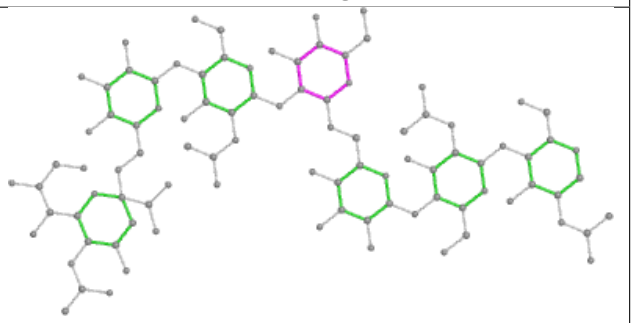
Bond lengths



Bond angles

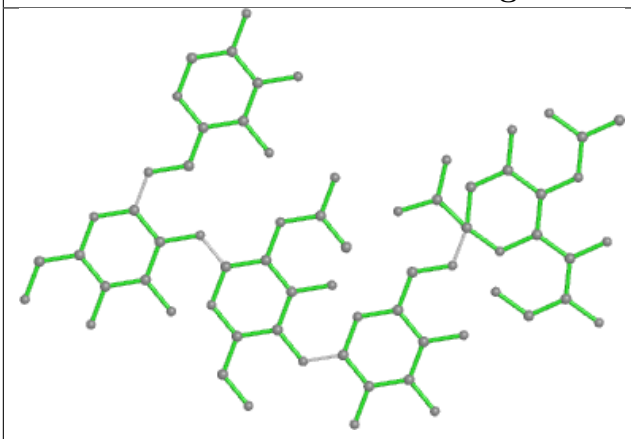


Torsions

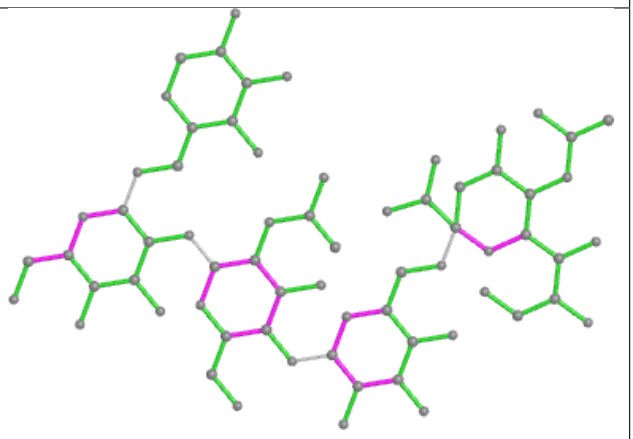


Rings

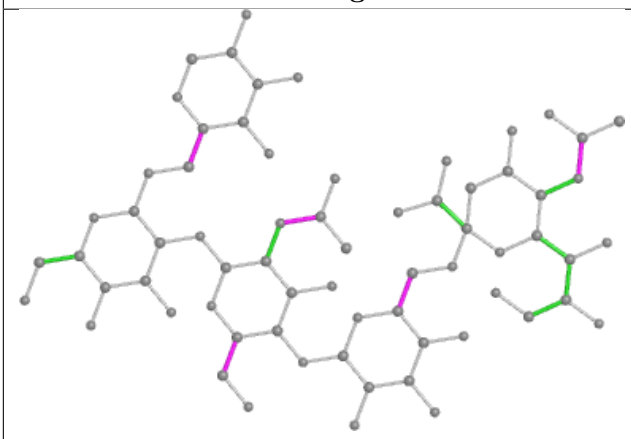
Oligosaccharide Chain c



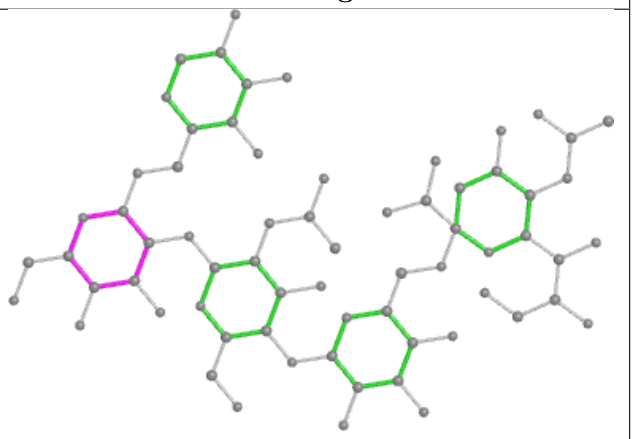
Bond lengths



Bond angles

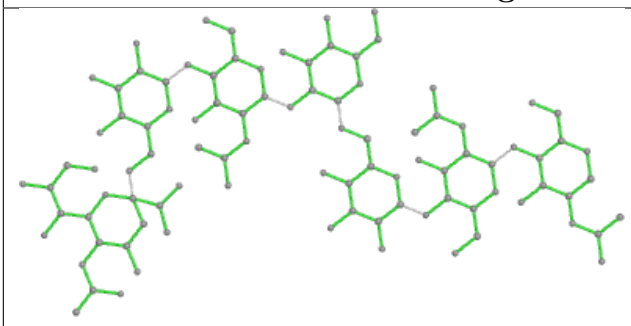


Torsions

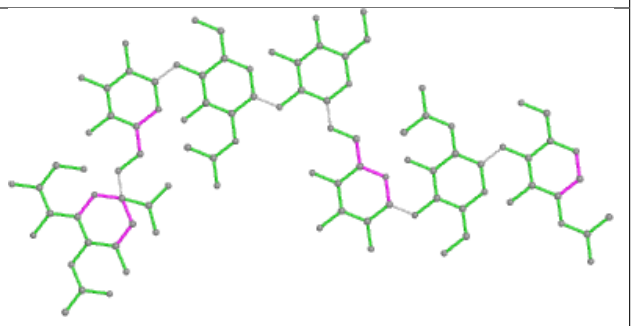


Rings

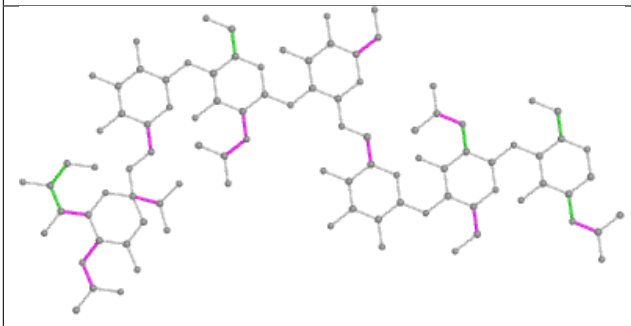
Oligosaccharide Chain d



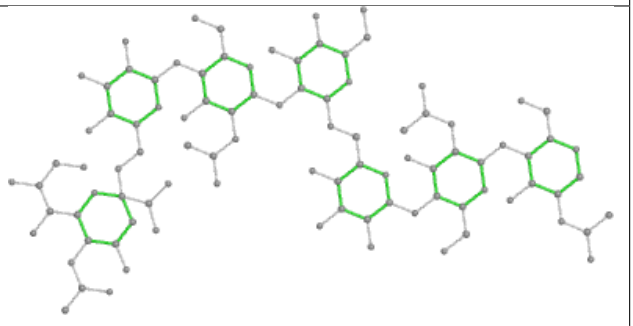
Bond lengths



Bond angles

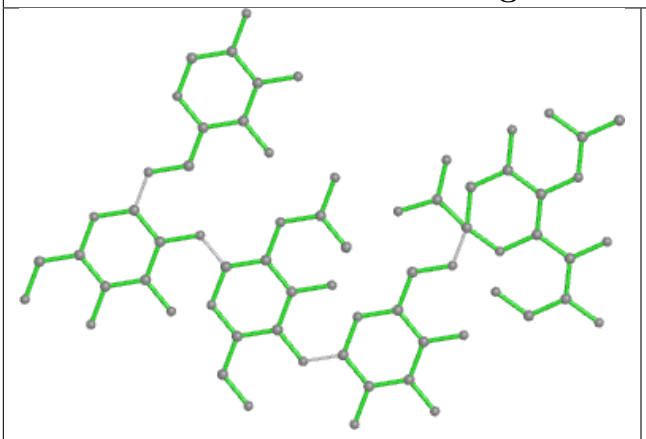


Torsions

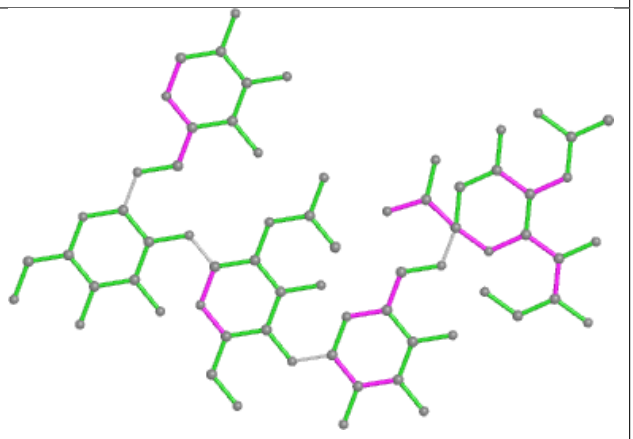


Rings

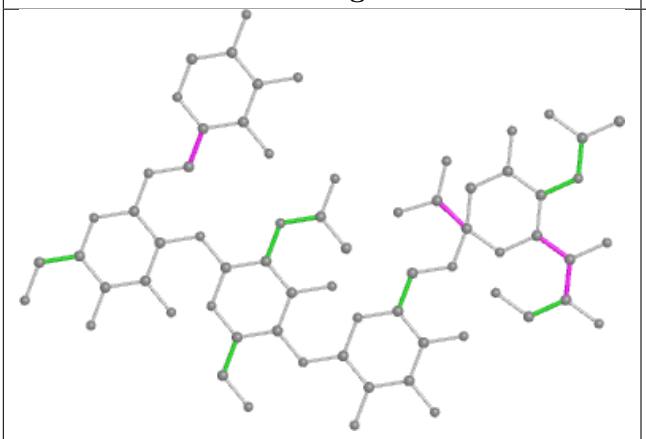
Oligosaccharide Chain e



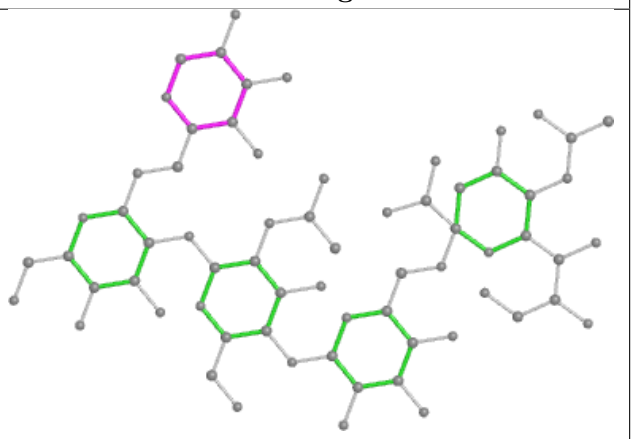
Bond lengths



Bond angles

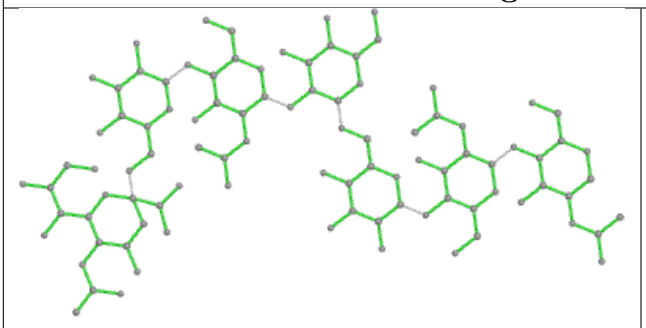


Torsions

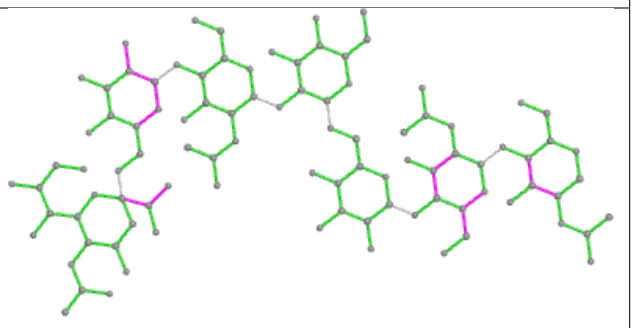


Rings

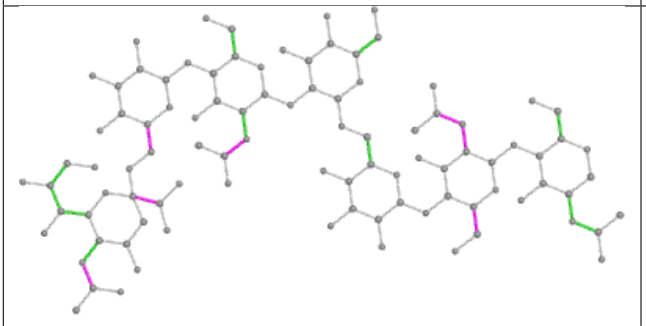
Oligosaccharide Chain f



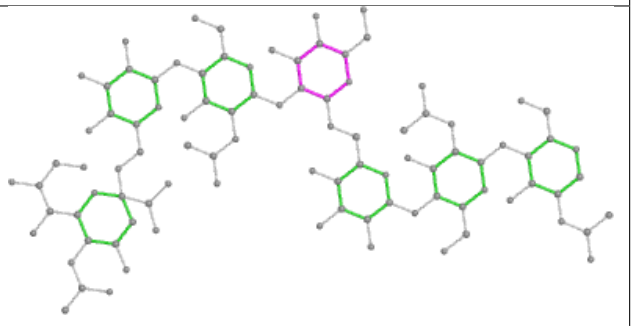
Bond lengths



Bond angles



Torsions



Rings

4.6 Ligand geometry (i)

5 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	$\#\|Z\| > 2$
12	NAG	O	301	3	14,14,15	0.30	0	17,19,21	0.58	0
12	NAG	R	301	3	14,14,15	0.35	0	17,19,21	0.44	0
12	NAG	L	306	-	14,14,15	0.26	0	17,19,21	0.96	0
12	NAG	X	301	3	14,14,15	0.22	0	17,19,21	0.44	0
12	NAG	U	301	3	14,14,15	0.39	0	17,19,21	0.42	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
12	NAG	O	301	3	-	0/6/23/26	0/1/1/1
12	NAG	R	301	3	-	4/6/23/26	0/1/1/1
12	NAG	L	306	-	-	0/6/23/26	0/1/1/1
12	NAG	X	301	3	-	2/6/23/26	0/1/1/1
12	NAG	U	301	3	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	U	301	NAG	C4-C5-C6-O6
12	U	301	NAG	O5-C5-C6-O6
12	R	301	NAG	C1-C2-N2-C7
12	U	301	NAG	C1-C2-N2-C7
12	X	301	NAG	O5-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

5.1 Protein, DNA and RNA chains

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

5.2 Non-standard residues in protein, DNA, RNA chains

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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