wwPDB EM Validation Summary Report (i)

Nov 21, 2022 – 12:23 pm GMT

PDB ID	:	7ZLK
EMDB ID	:	EMD-14783
Title	:	AMC009 SOSIPv5.2 in complex with Fabs ACS101 and ACS124
Authors	:	van Schooten, J.; Ozorowski, G.; Ward, A.
Deposited on	:	2022-04-15
Resolution	:	3.99 Å(reported)

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

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

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

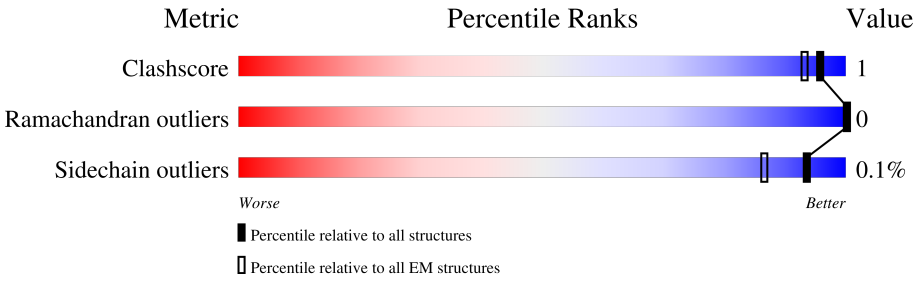
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.99 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	482	85% 6% 10%
1	C	482	87% • 10%
1	D	482	87% • 10%
2	B	154	73% 5% • 22%
2	E	154	80% 20%
2	F	154	80% 6% 14%
3	H	120	96% •
3	O	120	96% •
3	Q	120	95% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	L	112	97%
4	P	112	96%
4	R	112	95% 5%
5	M	124	94% 5%
5	S	124	83% 12%
6	N	108	93% 6%
6	T	108	93% 6%
7	G	2	100%
7	V	2	100%
7	e	2	100%
8	I	5	100%
8	U	5	100%
8	W	5	100%
8	Y	5	100%
8	Z	5	80% 20%
8	b	5	100%
8	f	5	100%
9	J	7	100%
9	X	7	100%
9	c	7	100%
10	K	4	25% 75%
11	a	3	100%
12	d	8	100%

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 23518 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 AMC009 SOSIPv5.2 envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	436	Total	C	N	O	S	0	0
			3460	2185	606	642	27		
1	C	436	Total	C	N	O	S	0	0
			3460	2185	606	642	27		
1	D	436	Total	C	N	O	S	0	0
			3460	2185	606	642	27		

- Molecule 2 is a protein called AMC009 SOSIPv5.2 envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	120	Total	C	N	O	S	0	0
			954	601	170	176	7		
2	E	123	Total	C	N	O	S	0	0
			982	616	176	183	7		
2	F	132	Total	C	N	O	S	0	0
			1058	662	187	202	7		

- Molecule 3 is a protein called ACS114 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	120	Total	C	N	O	S	0	0
			934	594	163	171	6		
3	O	120	Total	C	N	O	S	0	0
			934	594	163	171	6		
3	Q	120	Total	C	N	O	S	0	0
			934	594	163	171	6		

- Molecule 4 is a protein called ACS114 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	112	Total	C	N	O	S	0	0
			856	538	147	168	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	112	Total 856	C 538	N 147	O 168	S 3	0	0
4	R	112	Total 856	C 538	N 147	O 168	S 3	0	0

- Molecule 5 is a protein called ACS122 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	124	Total 971	C 618	N 165	O 185	S 3	0	0
5	S	119	Total 938	C 598	N 160	O 177	S 3	0	0

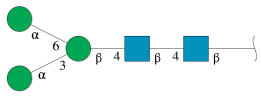
- Molecule 6 is a protein called ACS122 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	107	Total 814	C 509	N 141	O 161	S 3	0	0
6	T	107	Total 814	C 509	N 141	O 161	S 3	0	0

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

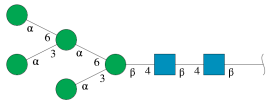
Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	2	Total 28	C 16	N 2	O 10	0	0
7	V	2	Total 28	C 16	N 2	O 10	0	0
7	e	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-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				AltConf	Trace
8	I	5	Total	C	N	O	0	0
			61	34	2	25		
8	U	5	Total	C	N	O	0	0
			61	34	2	25		
8	W	5	Total	C	N	O	0	0
			61	34	2	25		
8	Y	5	Total	C	N	O	0	0
			61	34	2	25		
8	Z	5	Total	C	N	O	0	0
			61	34	2	25		
8	b	5	Total	C	N	O	0	0
			61	34	2	25		
8	f	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

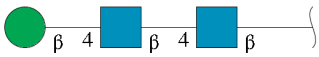


Mol	Chain	Residues	Atoms				AltConf	Trace
9	J	7	Total	C	N	O	0	0
			83	46	2	35		
9	X	7	Total	C	N	O	0	0
			83	46	2	35		
9	c	7	Total	C	N	O	0	0
			83	46	2	35		

- 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)-2-acetamido-2-deoxy-beta-D-glucopyranose.

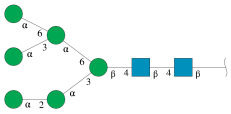
Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	4	Total	C	N	O	0	0
			50	28	2	20		

- 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.



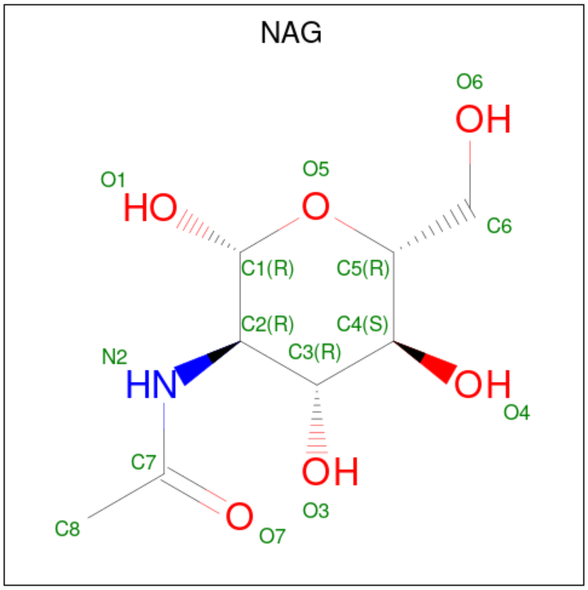
Mol	Chain	Residues	Atoms				AltConf	Trace
11	a	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-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				AltConf	Trace
12	d	8	Total	C	N	O	0	0
			94	52	2	40		

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



Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total 70	C 40	N 5	O 25	0
13	A	1	Total 70	C 40	N 5	O 25	0
13	A	1	Total 70	C 40	N 5	O 25	0
13	A	1	Total 70	C 40	N 5	O 25	0
13	A	1	Total 70	C 40	N 5	O 25	0
13	C	1	Total 112	C 64	N 8	O 40	0
13	C	1	Total 112	C 64	N 8	O 40	0
13	C	1	Total 112	C 64	N 8	O 40	0
13	C	1	Total 112	C 64	N 8	O 40	0
13	C	1	Total 112	C 64	N 8	O 40	0
13	C	1	Total 112	C 64	N 8	O 40	0
13	C	1	Total 112	C 64	N 8	O 40	0
13	C	1	Total 112	C 64	N 8	O 40	0
13	D	1	Total 112	C 64	N 8	O 40	0

Continued on next page...

Continued from previous page...

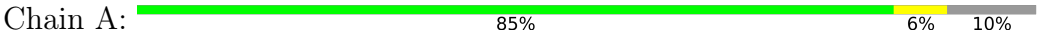
Mol	Chain	Residues	Atoms				AltConf
13	D	1	Total 112	C 64	N 8	O 40	0
13	D	1	Total 112	C 64	N 8	O 40	0
13	D	1	Total 112	C 64	N 8	O 40	0
13	D	1	Total 112	C 64	N 8	O 40	0
13	D	1	Total 112	C 64	N 8	O 40	0
13	D	1	Total 112	C 64	N 8	O 40	0
13	D	1	Total 112	C 64	N 8	O 40	0

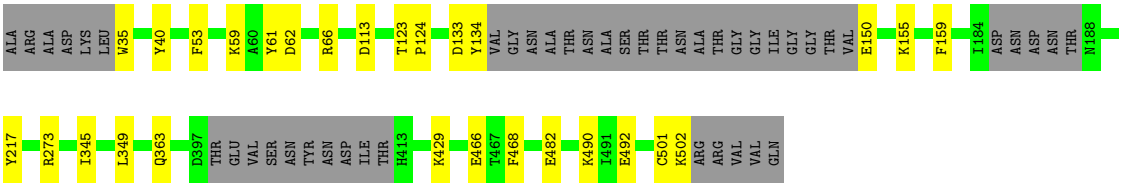
3 Residue-property plots (i)

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: AMC009 SOSIPv5.2 envelope glycoprotein gp120

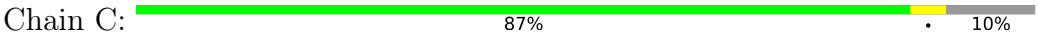
Chain A:

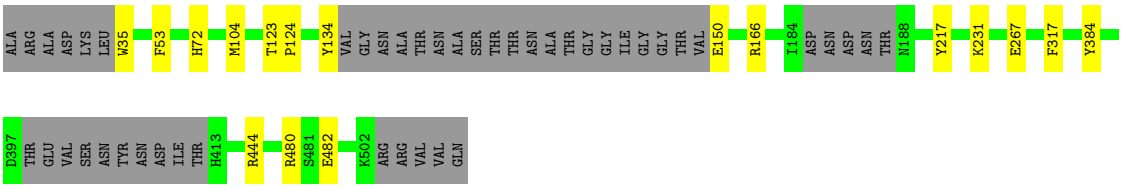




• Molecule 1: AMC009 SOSIPv5.2 envelope glycoprotein gp120

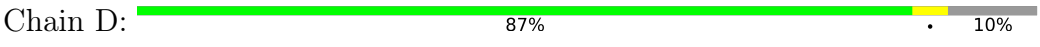
Chain C:

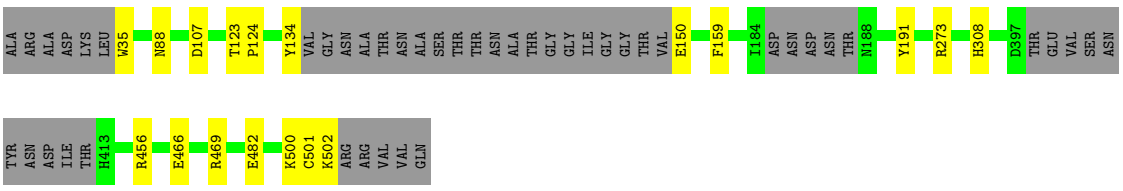




• Molecule 1: AMC009 SOSIPv5.2 envelope glycoprotein gp120

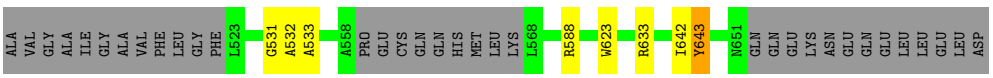
Chain D:





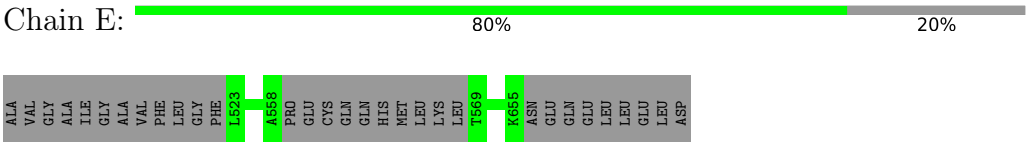
• Molecule 2: AMC009 SOSIPv5.2 envelope glycoprotein gp41

Chain B:



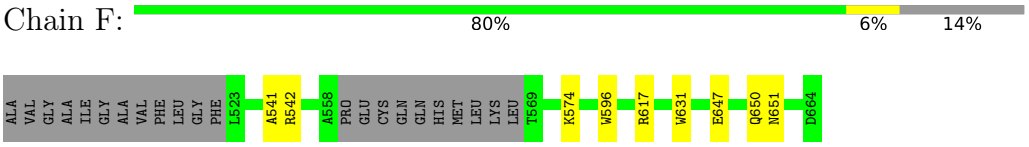
• Molecule 2: AMC009 SOSIPv5.2 envelope glycoprotein gp41

Chain E:



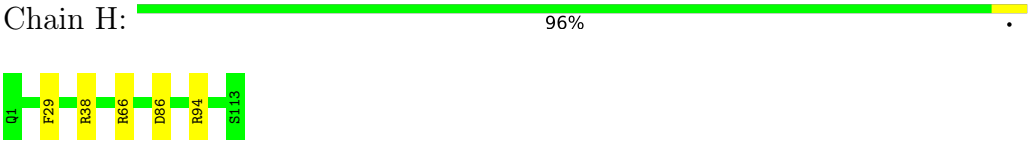
• Molecule 2: AMC009 SOSIPv5.2 envelope glycoprotein gp41

Chain F:



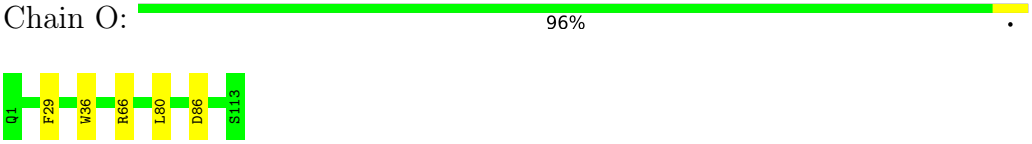
• Molecule 3: ACS114 heavy chain

Chain H:



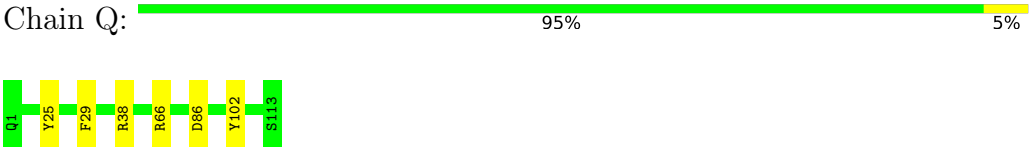
• Molecule 3: ACS114 heavy chain

Chain O:



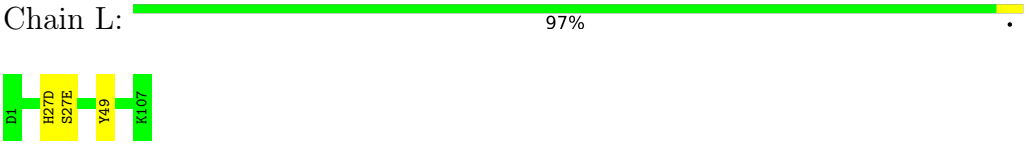
• Molecule 3: ACS114 heavy chain

Chain Q:



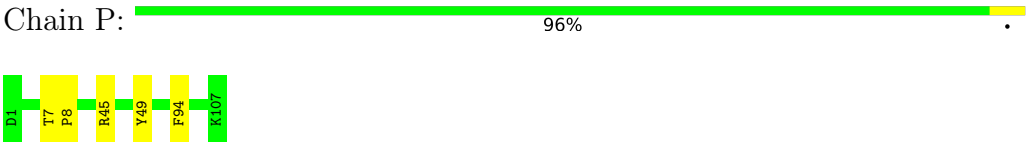
• Molecule 4: ACS114 light chain

Chain L:



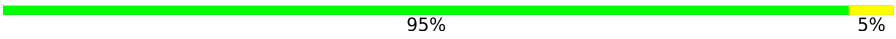
• Molecule 4: ACS114 light chain

Chain P:



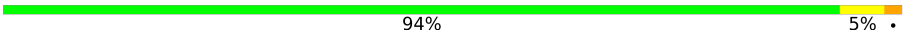
• Molecule 4: ACS114 light chain

Chain R:



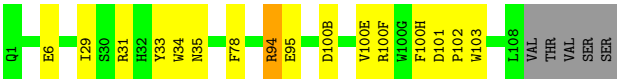
• Molecule 5: ACS122 heavy chain

Chain M:



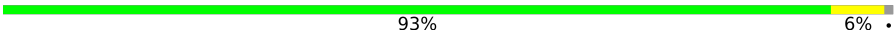
• Molecule 5: ACS122 heavy chain

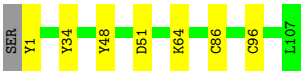
Chain S:



• Molecule 6: ACS122 light chain

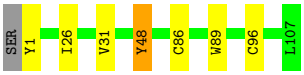
Chain N:





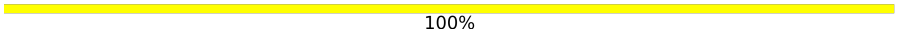
• Molecule 6: ACS122 light chain

Chain T:



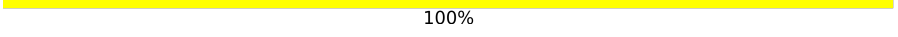
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



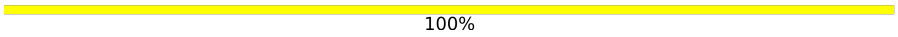
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



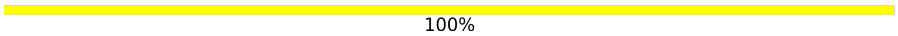
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:



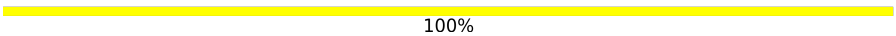
• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



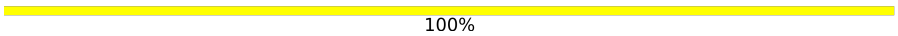
• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



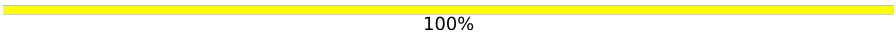
• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



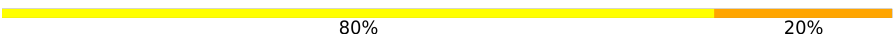
• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:



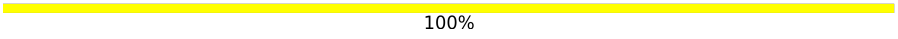
• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:



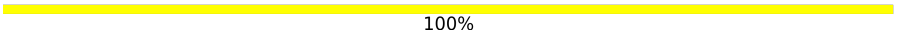
• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



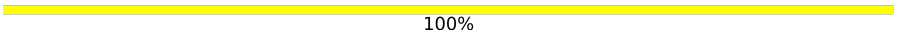
• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:



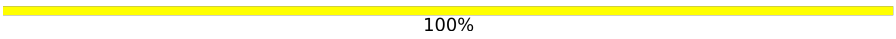
• Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



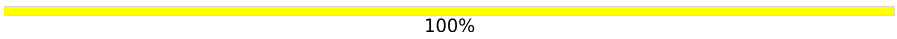
• Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



• Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

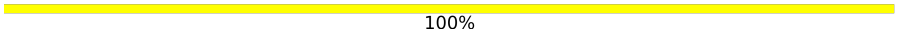
Chain c:



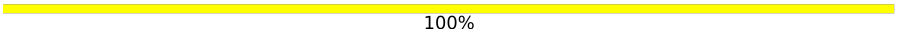
• Molecule 10: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

• Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 

• Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-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

Chain d: 

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	159597	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	49.3	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k 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, MAN, BMA

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	1.11	13/3535 (0.4%)	0.92	4/4800 (0.1%)
1	C	1.08	12/3535 (0.3%)	0.89	5/4800 (0.1%)
1	D	1.06	13/3535 (0.4%)	0.92	6/4800 (0.1%)
2	B	1.06	1/970 (0.1%)	1.01	2/1317 (0.2%)
2	E	1.08	0/998	0.87	0/1353
2	F	1.16	3/1074 (0.3%)	0.88	1/1456 (0.1%)
3	H	1.03	1/963 (0.1%)	1.02	7/1314 (0.5%)
3	O	1.01	1/963 (0.1%)	0.94	3/1314 (0.2%)
3	Q	1.11	2/963 (0.2%)	1.02	6/1314 (0.5%)
4	L	0.98	1/875 (0.1%)	1.01	1/1190 (0.1%)
4	P	1.02	1/875 (0.1%)	1.01	2/1190 (0.2%)
4	R	0.98	1/875 (0.1%)	0.99	2/1190 (0.2%)
5	M	1.16	6/997 (0.6%)	0.93	1/1361 (0.1%)
5	S	1.15	6/964 (0.6%)	1.04	4/1315 (0.3%)
6	N	1.15	8/834 (1.0%)	0.92	1/1136 (0.1%)
6	T	1.12	6/834 (0.7%)	0.97	2/1136 (0.2%)
All	All	1.08	75/22790 (0.3%)	0.94	47/30986 (0.2%)

The worst 5 of 75 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	102	PRO	N-CD	10.08	1.61	1.47
3	Q	29	PHE	CB-CG	-8.49	1.36	1.51
6	N	1	TYR	CG-CD2	8.02	1.49	1.39
6	T	1	TYR	CG-CD2	8.01	1.49	1.39
1	C	482	GLU	CG-CD	-7.81	1.40	1.51

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	T	48	TYR	CB-CG-CD1	-11.38	114.17	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	S	101	ASP	N-CA-C	10.86	140.32	111.00
3	H	66	ARG	NE-CZ-NH2	-10.20	115.20	120.30
3	Q	66	ARG	NE-CZ-NH2	-9.00	115.80	120.30
3	O	66	ARG	NE-CZ-NH2	-8.89	115.85	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3460	0	3412	9	0
1	C	3460	0	3410	4	0
1	D	3460	0	3410	4	0
2	B	954	0	945	3	0
2	E	982	0	969	0	0
2	F	1058	0	1038	3	0
3	H	934	0	900	0	0
3	O	934	0	900	1	0
3	Q	934	0	900	0	0
4	L	856	0	848	1	0
4	P	856	0	848	1	0
4	R	856	0	848	2	0
5	M	971	0	948	3	0
5	S	938	0	913	6	0
6	N	814	0	785	3	0
6	T	814	0	785	3	0
7	G	28	0	25	0	0
7	V	28	0	25	0	0
7	e	28	0	25	0	0
8	I	61	0	52	0	0
8	U	61	0	52	0	0
8	W	61	0	52	0	0
8	Y	61	0	52	0	0
8	Z	61	0	52	1	0
8	b	61	0	52	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	f	61	0	52	0	0
9	J	83	0	70	0	0
9	X	83	0	70	0	0
9	c	83	0	70	0	0
10	K	50	0	43	0	0
11	a	39	0	34	0	0
12	d	94	0	79	0	0
13	A	70	0	65	1	0
13	C	112	0	104	0	0
13	D	112	0	104	0	0
All	All	23518	0	22937	38	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 1.

The worst 5 of 38 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:444:ARG:HH12	8:Z:1:NAG:H81	1.65	0.62
5:M:100(G):TRP:HE1	6:N:48:TYR:H	1.48	0.62
5:S:100(H):PHE:O	5:S:103:TRP:NE1	2.35	0.60
5:S:35:ASN:ND2	5:S:95:GLU:HB2	2.20	0.57
1:A:113:ASP:OD1	1:A:429:LYS:NZ	2.38	0.56

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	428/482 (89%)	413 (96%)	15 (4%)	0	100	100
1	C	428/482 (89%)	422 (99%)	6 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	428/482 (89%)	414 (97%)	14 (3%)	0	100	100
2	B	116/154 (75%)	110 (95%)	6 (5%)	0	100	100
2	E	119/154 (77%)	116 (98%)	3 (2%)	0	100	100
2	F	128/154 (83%)	122 (95%)	6 (5%)	0	100	100
3	H	118/120 (98%)	116 (98%)	2 (2%)	0	100	100
3	O	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
3	Q	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
4	L	110/112 (98%)	107 (97%)	3 (3%)	0	100	100
4	P	110/112 (98%)	108 (98%)	2 (2%)	0	100	100
4	R	110/112 (98%)	107 (97%)	3 (3%)	0	100	100
5	M	122/124 (98%)	117 (96%)	5 (4%)	0	100	100
5	S	117/124 (94%)	113 (97%)	4 (3%)	0	100	100
6	N	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
6	T	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
All	All	2780/3068 (91%)	2699 (97%)	81 (3%)	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	393/429 (92%)	393 (100%)	0	100	100
1	C	393/429 (92%)	393 (100%)	0	100	100
1	D	393/429 (92%)	392 (100%)	1 (0%)	92	95
2	B	102/130 (78%)	102 (100%)	0	100	100
2	E	105/130 (81%)	105 (100%)	0	100	100
2	F	114/130 (88%)	114 (100%)	0	100	100
3	H	101/101 (100%)	101 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	O	101/101 (100%)	101 (100%)	0	100 100
3	Q	101/101 (100%)	101 (100%)	0	100 100
4	L	98/98 (100%)	98 (100%)	0	100 100
4	P	98/98 (100%)	98 (100%)	0	100 100
4	R	98/98 (100%)	98 (100%)	0	100 100
5	M	109/109 (100%)	109 (100%)	0	100 100
5	S	104/109 (95%)	103 (99%)	1 (1%)	76 86
6	N	90/91 (99%)	90 (100%)	0	100 100
6	T	90/91 (99%)	90 (100%)	0	100 100
All	All	2490/2674 (93%)	2488 (100%)	2 (0%)	93 97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	88	ASN
5	S	94	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

77 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	G	1	7,1	14,14,15	2.28	7 (50%)	17,19,21	1.08	2 (11%)
7	NAG	G	2	7	14,14,15	2.00	4 (28%)	17,19,21	0.92	1 (5%)
8	NAG	I	1	8,1	14,14,15	2.14	6 (42%)	17,19,21	1.56	3 (17%)
8	NAG	I	2	8	14,14,15	2.15	6 (42%)	17,19,21	1.32	3 (17%)
8	BMA	I	3	8	11,11,12	1.48	3 (27%)	15,15,17	0.70	0
8	MAN	I	4	8	11,11,12	1.99	5 (45%)	15,15,17	0.63	0
8	MAN	I	5	8	11,11,12	1.95	6 (54%)	15,15,17	0.73	0
9	NAG	J	1	9,1	14,14,15	1.88	4 (28%)	17,19,21	1.19	1 (5%)
9	NAG	J	2	9	14,14,15	2.04	6 (42%)	17,19,21	1.22	2 (11%)
9	BMA	J	3	9	11,11,12	1.43	3 (27%)	15,15,17	0.66	0
9	MAN	J	4	9	11,11,12	1.40	2 (18%)	15,15,17	0.64	0
9	MAN	J	5	9	11,11,12	1.92	5 (45%)	15,15,17	0.82	0
9	MAN	J	6	9	11,11,12	1.83	4 (36%)	15,15,17	0.81	0
9	MAN	J	7	9	11,11,12	1.94	6 (54%)	15,15,17	0.77	0
10	NAG	K	1	10,1	14,14,15	2.06	7 (50%)	17,19,21	2.55	5 (29%)
10	NAG	K	2	10	14,14,15	1.97	5 (35%)	17,19,21	1.33	2 (11%)
10	BMA	K	3	10	11,11,12	0.75	0	15,15,17	0.94	0
10	MAN	K	4	10	11,11,12	2.00	6 (54%)	15,15,17	0.76	0
8	NAG	U	1	8,1	14,14,15	2.02	7 (50%)	17,19,21	1.26	2 (11%)
8	NAG	U	2	8	14,14,15	2.05	4 (28%)	17,19,21	1.14	3 (17%)
8	BMA	U	3	8	11,11,12	1.45	2 (18%)	15,15,17	0.68	0
8	MAN	U	4	8	11,11,12	2.00	6 (54%)	15,15,17	0.93	1 (6%)
8	MAN	U	5	8	11,11,12	1.90	6 (54%)	15,15,17	0.78	0
7	NAG	V	1	7,1	14,14,15	2.23	7 (50%)	17,19,21	1.29	2 (11%)
7	NAG	V	2	7	14,14,15	1.98	6 (42%)	17,19,21	0.91	1 (5%)
8	NAG	W	1	8,1	14,14,15	1.72	2 (14%)	17,19,21	1.11	1 (5%)
8	NAG	W	2	8	14,14,15	1.74	5 (35%)	17,19,21	0.99	1 (5%)
8	BMA	W	3	8	11,11,12	1.41	3 (27%)	15,15,17	0.68	0
8	MAN	W	4	8	11,11,12	1.86	4 (36%)	15,15,17	0.77	0
8	MAN	W	5	8	11,11,12	1.99	5 (45%)	15,15,17	0.72	0
9	NAG	X	1	9,1	14,14,15	1.70	2 (14%)	17,19,21	1.17	2 (11%)
9	NAG	X	2	9	14,14,15	1.76	4 (28%)	17,19,21	1.01	1 (5%)
9	BMA	X	3	9	11,11,12	1.38	3 (27%)	15,15,17	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	MAN	X	4	9	11,11,12	1.36	1 (9%)	15,15,17	0.70	0
9	MAN	X	5	9	11,11,12	1.90	5 (45%)	15,15,17	0.78	0
9	MAN	X	6	9	11,11,12	1.76	5 (45%)	15,15,17	0.85	0
9	MAN	X	7	9	11,11,12	1.98	5 (45%)	15,15,17	0.69	0
8	NAG	Y	1	8,1	14,14,15	1.92	6 (42%)	17,19,21	1.06	1 (5%)
8	NAG	Y	2	8	14,14,15	1.80	5 (35%)	17,19,21	1.02	1 (5%)
8	BMA	Y	3	8	11,11,12	1.38	3 (27%)	15,15,17	0.63	0
8	MAN	Y	4	8	11,11,12	1.97	6 (54%)	15,15,17	0.74	0
8	MAN	Y	5	8	11,11,12	1.90	6 (54%)	15,15,17	0.73	0
8	NAG	Z	1	8,1	14,14,15	1.99	4 (28%)	17,19,21	1.15	3 (17%)
8	NAG	Z	2	8	14,14,15	1.91	4 (28%)	17,19,21	0.88	0
8	BMA	Z	3	8	11,11,12	1.56	3 (27%)	15,15,17	0.77	0
8	MAN	Z	4	8	11,11,12	2.07	5 (45%)	15,15,17	0.75	0
8	MAN	Z	5	8	11,11,12	1.92	5 (45%)	15,15,17	0.75	0
11	NAG	a	1	11,1	14,14,15	2.03	6 (42%)	17,19,21	1.01	0
11	NAG	a	2	11	14,14,15	2.00	5 (35%)	17,19,21	0.93	1 (5%)
11	BMA	a	3	11	11,11,12	2.02	6 (54%)	15,15,17	0.69	0
8	NAG	b	1	8,1	14,14,15	1.96	3 (21%)	17,19,21	0.98	1 (5%)
8	NAG	b	2	8	14,14,15	0.52	0	17,19,21	1.08	1 (5%)
8	BMA	b	3	8	11,11,12	1.44	3 (27%)	15,15,17	0.62	0
8	MAN	b	4	8	11,11,12	1.93	5 (45%)	15,15,17	0.77	0
8	MAN	b	5	8	11,11,12	2.00	6 (54%)	15,15,17	0.74	0
9	NAG	c	1	9,1	14,14,15	1.85	5 (35%)	17,19,21	1.17	1 (5%)
9	NAG	c	2	9	14,14,15	1.87	5 (35%)	17,19,21	1.02	1 (5%)
9	BMA	c	3	9	11,11,12	1.45	3 (27%)	15,15,17	0.66	0
9	MAN	c	4	9	11,11,12	1.54	2 (18%)	15,15,17	1.02	0
9	MAN	c	5	9	11,11,12	1.92	5 (45%)	15,15,17	0.73	0
9	MAN	c	6	9	11,11,12	1.94	5 (45%)	15,15,17	0.86	0
9	MAN	c	7	9	11,11,12	2.00	6 (54%)	15,15,17	0.72	0
12	NAG	d	1	12,1	14,14,15	1.90	7 (50%)	17,19,21	1.31	2 (11%)
12	NAG	d	2	12	14,14,15	1.92	5 (35%)	17,19,21	0.92	0
12	BMA	d	3	12	11,11,12	1.41	3 (27%)	15,15,17	0.72	0
12	MAN	d	4	12	11,11,12	1.03	2 (18%)	15,15,17	1.72	2 (13%)
12	MAN	d	5	12	11,11,12	1.99	5 (45%)	15,15,17	0.83	1 (6%)
12	MAN	d	6	12	11,11,12	1.44	2 (18%)	15,15,17	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	MAN	d	7	12	11,11,12	2.01	6 (54%)	15,15,17	0.62	0
12	MAN	d	8	12	11,11,12	1.97	6 (54%)	15,15,17	0.73	0
7	NAG	e	1	7,1	14,14,15	1.99	5 (35%)	17,19,21	0.99	0
7	NAG	e	2	7	14,14,15	1.94	6 (42%)	17,19,21	0.98	1 (5%)
8	NAG	f	1	8,1	14,14,15	2.03	6 (42%)	17,19,21	1.09	1 (5%)
8	NAG	f	2	8	14,14,15	1.83	5 (35%)	17,19,21	0.91	1 (5%)
8	BMA	f	3	8	11,11,12	1.45	3 (27%)	15,15,17	0.63	0
8	MAN	f	4	8	11,11,12	2.02	5 (45%)	15,15,17	0.69	0
8	MAN	f	5	8	11,11,12	1.90	5 (45%)	15,15,17	0.74	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
7	NAG	G	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	G	2	7	-	0/6/23/26	0/1/1/1
8	NAG	I	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	I	2	8	-	0/6/23/26	0/1/1/1
8	BMA	I	3	8	-	0/2/19/22	0/1/1/1
8	MAN	I	4	8	-	2/2/19/22	0/1/1/1
8	MAN	I	5	8	-	1/2/19/22	0/1/1/1
9	NAG	J	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	J	2	9	-	1/6/23/26	0/1/1/1
9	BMA	J	3	9	-	0/2/19/22	0/1/1/1
9	MAN	J	4	9	-	0/2/19/22	0/1/1/1
9	MAN	J	5	9	-	1/2/19/22	0/1/1/1
9	MAN	J	6	9	-	1/2/19/22	0/1/1/1
9	MAN	J	7	9	-	1/2/19/22	0/1/1/1
10	NAG	K	1	10,1	-	3/6/23/26	0/1/1/1
10	NAG	K	2	10	-	1/6/23/26	0/1/1/1
10	BMA	K	3	10	-	2/2/19/22	0/1/1/1
10	MAN	K	4	10	-	0/2/19/22	0/1/1/1
8	NAG	U	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	U	2	8	-	0/6/23/26	0/1/1/1
8	BMA	U	3	8	-	2/2/19/22	0/1/1/1
8	MAN	U	4	8	-	1/2/19/22	0/1/1/1
8	MAN	U	5	8	-	0/2/19/22	0/1/1/1
7	NAG	V	1	7,1	-	1/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	V	2	7	-	0/6/23/26	0/1/1/1
8	NAG	W	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	W	2	8	-	0/6/23/26	0/1/1/1
8	BMA	W	3	8	-	0/2/19/22	0/1/1/1
8	MAN	W	4	8	-	1/2/19/22	0/1/1/1
8	MAN	W	5	8	-	1/2/19/22	0/1/1/1
9	NAG	X	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	X	2	9	-	0/6/23/26	0/1/1/1
9	BMA	X	3	9	-	0/2/19/22	0/1/1/1
9	MAN	X	4	9	-	2/2/19/22	0/1/1/1
9	MAN	X	5	9	-	0/2/19/22	0/1/1/1
9	MAN	X	6	9	-	0/2/19/22	0/1/1/1
9	MAN	X	7	9	-	0/2/19/22	0/1/1/1
8	NAG	Y	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	1/6/23/26	0/1/1/1
8	BMA	Y	3	8	-	0/2/19/22	0/1/1/1
8	MAN	Y	4	8	-	0/2/19/22	0/1/1/1
8	MAN	Y	5	8	-	0/2/19/22	0/1/1/1
8	NAG	Z	1	8,1	-	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	MAN	Z	4	8	-	1/2/19/22	0/1/1/1
8	MAN	Z	5	8	-	1/2/19/22	0/1/1/1
11	NAG	a	1	11,1	-	0/6/23/26	0/1/1/1
11	NAG	a	2	11	-	0/6/23/26	0/1/1/1
11	BMA	a	3	11	-	0/2/19/22	0/1/1/1
8	NAG	b	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	b	2	8	-	2/6/23/26	0/1/1/1
8	BMA	b	3	8	-	0/2/19/22	0/1/1/1
8	MAN	b	4	8	-	1/2/19/22	0/1/1/1
8	MAN	b	5	8	-	1/2/19/22	0/1/1/1
9	NAG	c	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	c	2	9	-	0/6/23/26	0/1/1/1
9	BMA	c	3	9	-	0/2/19/22	0/1/1/1
9	MAN	c	4	9	-	1/2/19/22	0/1/1/1
9	MAN	c	5	9	-	1/2/19/22	0/1/1/1
9	MAN	c	6	9	-	0/2/19/22	0/1/1/1
9	MAN	c	7	9	-	1/2/19/22	0/1/1/1
12	NAG	d	1	12,1	-	0/6/23/26	0/1/1/1
12	NAG	d	2	12	-	0/6/23/26	0/1/1/1
12	BMA	d	3	12	-	1/2/19/22	0/1/1/1
12	MAN	d	4	12	-	2/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	MAN	d	5	12	-	0/2/19/22	0/1/1/1
12	MAN	d	6	12	-	2/2/19/22	0/1/1/1
12	MAN	d	7	12	-	0/2/19/22	0/1/1/1
12	MAN	d	8	12	-	0/2/19/22	0/1/1/1
7	NAG	e	1	7,1	-	1/6/23/26	0/1/1/1
7	NAG	e	2	7	-	0/6/23/26	0/1/1/1
8	NAG	f	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	f	2	8	-	2/6/23/26	0/1/1/1
8	BMA	f	3	8	-	0/2/19/22	0/1/1/1
8	MAN	f	4	8	-	0/2/19/22	0/1/1/1
8	MAN	f	5	8	-	0/2/19/22	0/1/1/1

The worst 5 of 350 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	1	NAG	C1-C2	5.64	1.60	1.52
11	a	1	NAG	C1-C2	4.99	1.59	1.52
7	V	1	NAG	C1-C2	4.98	1.59	1.52
8	Z	1	NAG	C1-C2	4.93	1.59	1.52
8	U	2	NAG	C1-C2	4.91	1.59	1.52

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	K	1	NAG	C8-C7-N2	7.47	128.75	116.10
12	d	4	MAN	O2-C2-C1	5.22	119.84	109.15
10	K	1	NAG	O7-C7-N2	-4.54	113.60	121.95
8	I	1	NAG	O4-C4-C3	4.25	120.18	110.35
10	K	1	NAG	C2-N2-C7	4.13	128.79	122.90

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	b	2	NAG	C8-C7-N2-C2
8	b	2	NAG	O7-C7-N2-C2
9	X	4	MAN	C4-C5-C6-O6
9	X	4	MAN	O5-C5-C6-O6
8	U	3	BMA	C4-C5-C6-O6

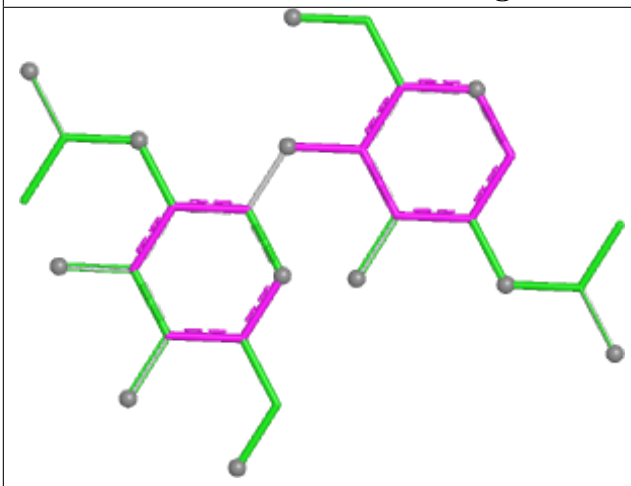
There are no ring outliers.

1 monomer is involved in 1 short contact:

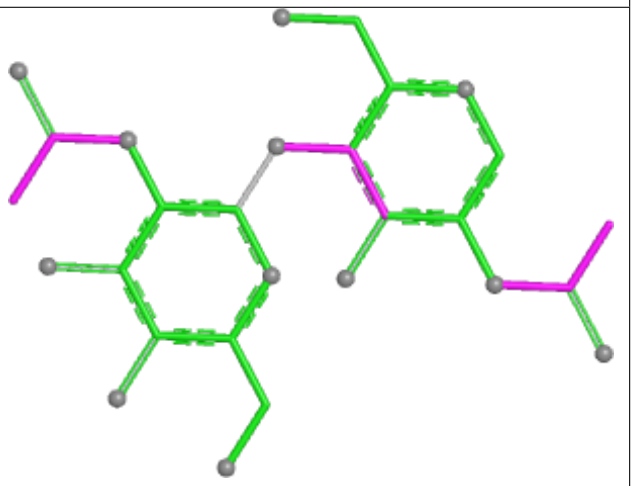
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	Z	1	NAG	1	0

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

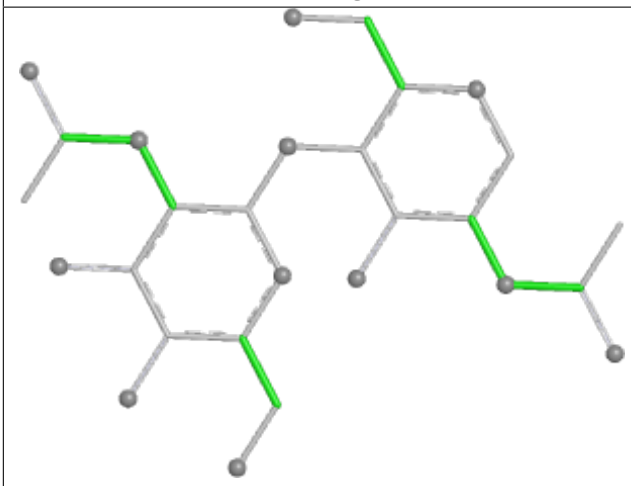
Oligosaccharide Chain G



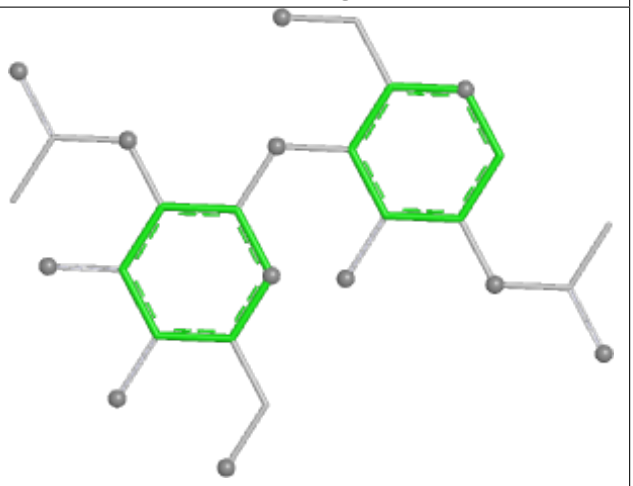
Bond lengths



Bond angles

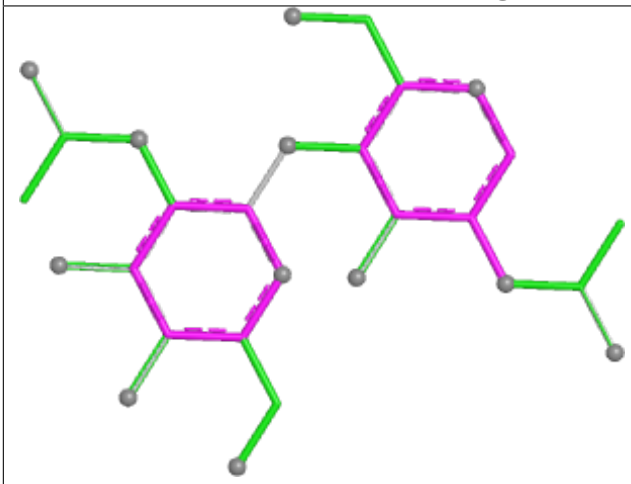


Torsions

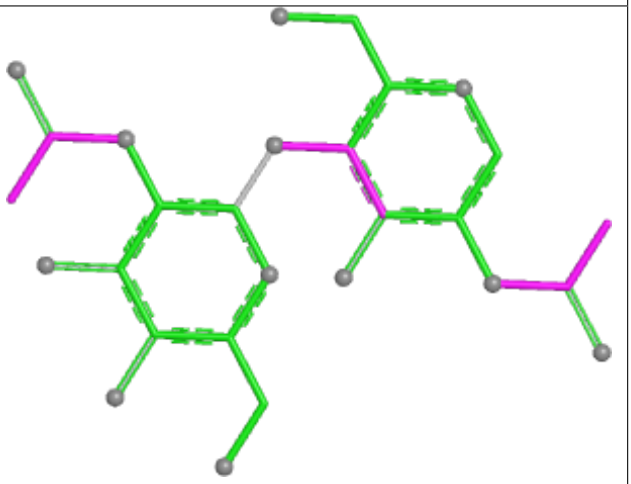


Rings

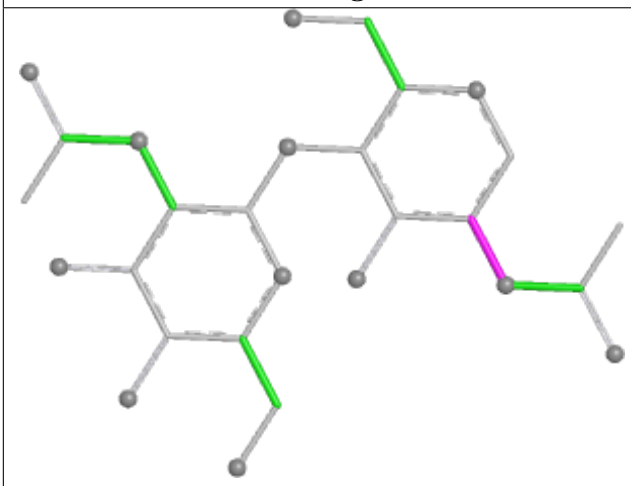
Oligosaccharide Chain V



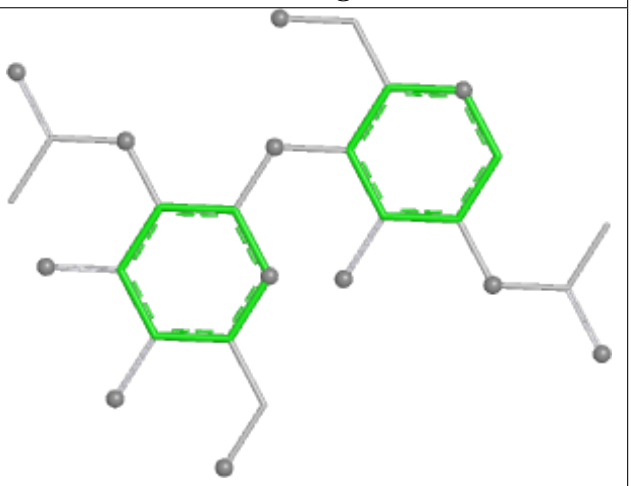
Bond lengths



Bond angles

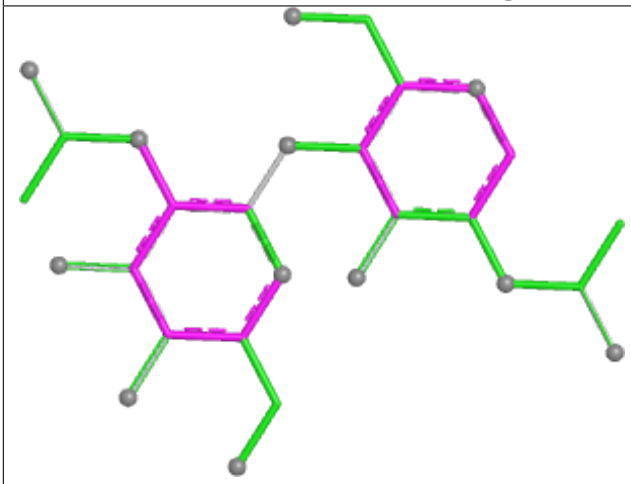


Torsions

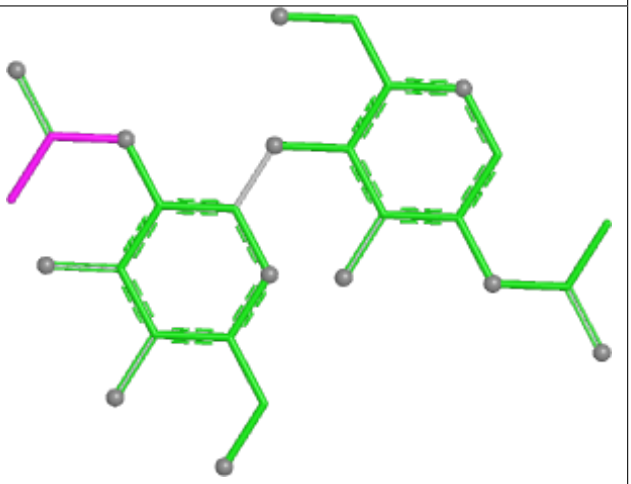


Rings

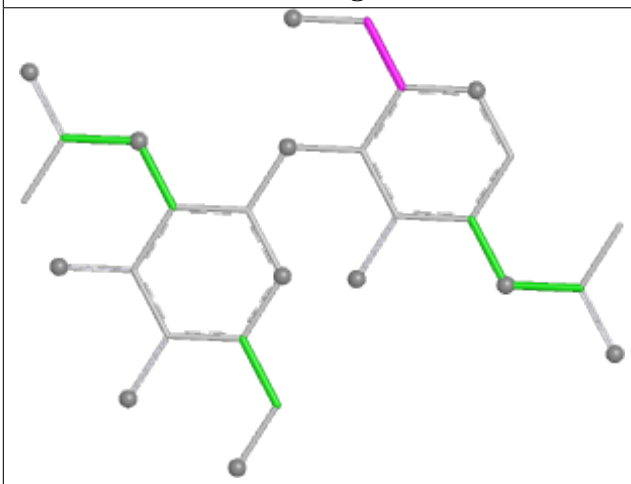
Oligosaccharide Chain e



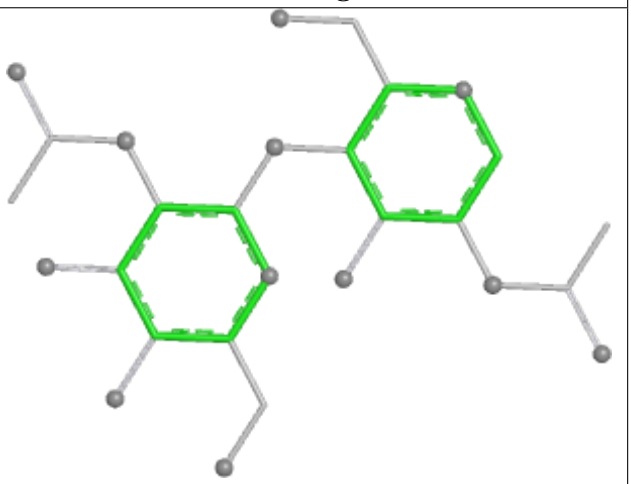
Bond lengths



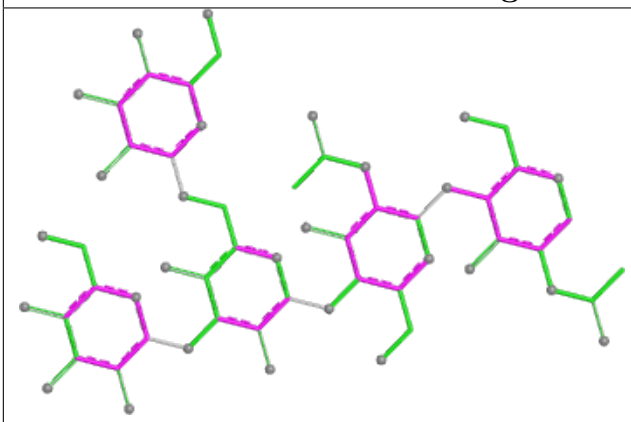
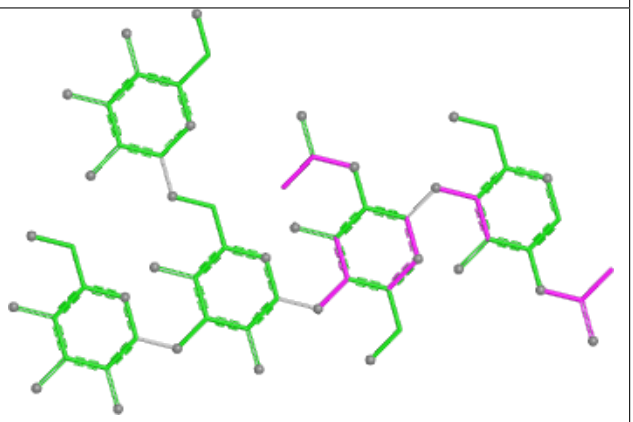
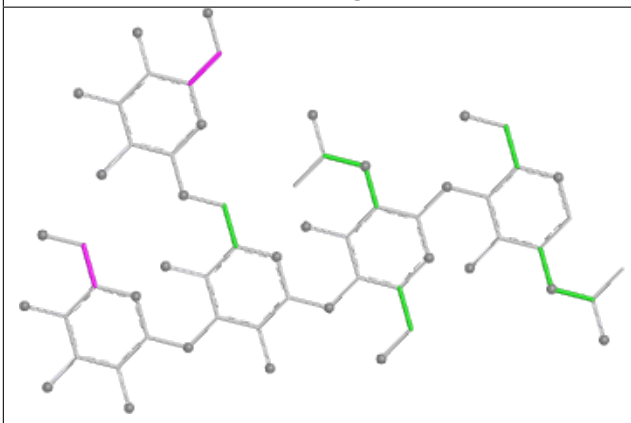
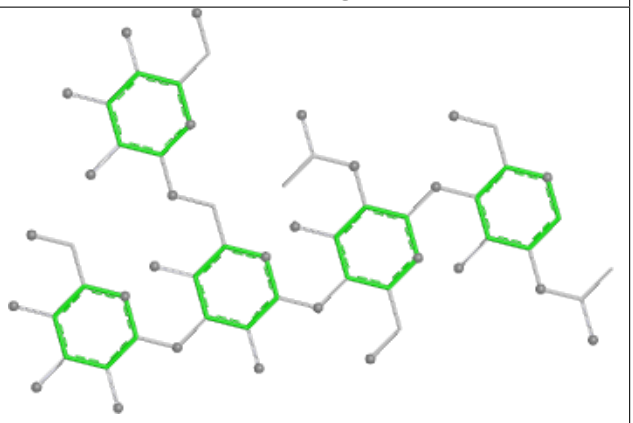
Bond angles

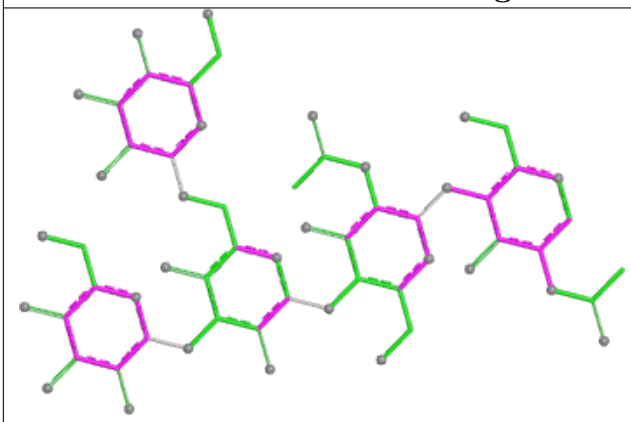
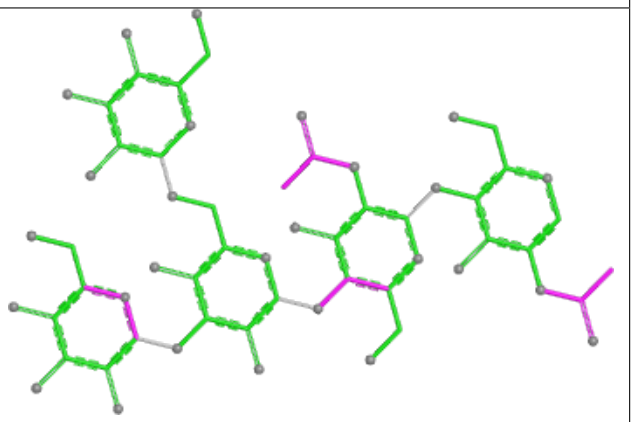
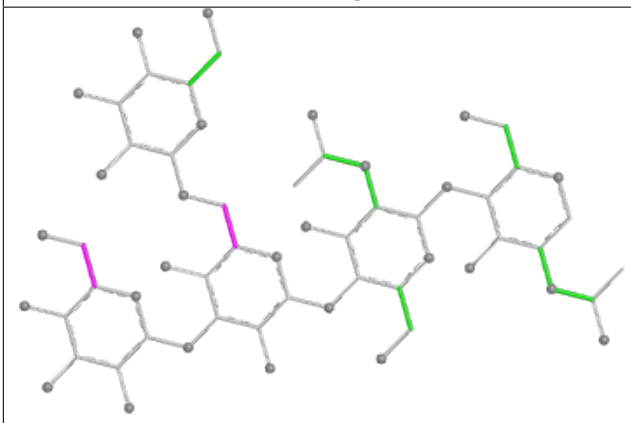
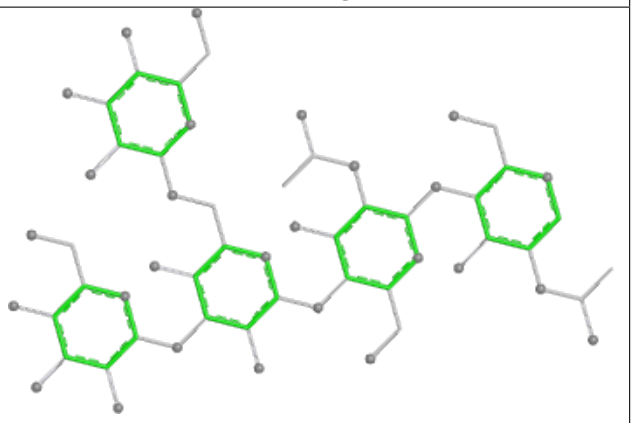


Torsions

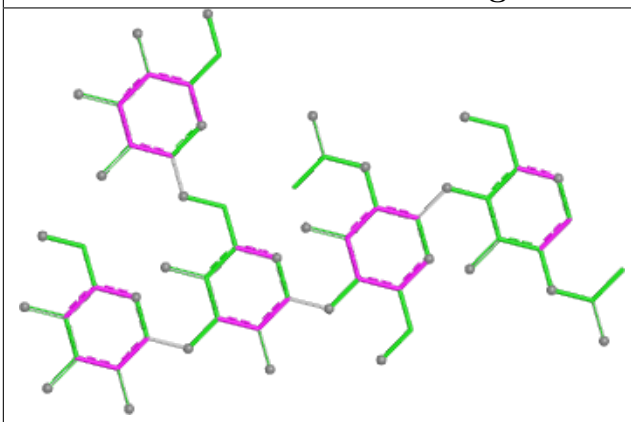


Rings

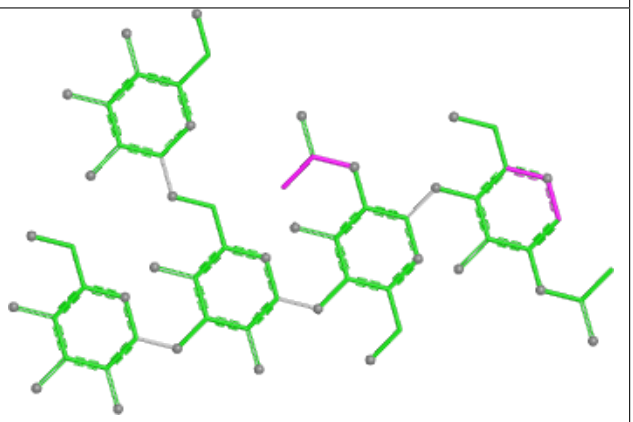
Oligosaccharide Chain I	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain U	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

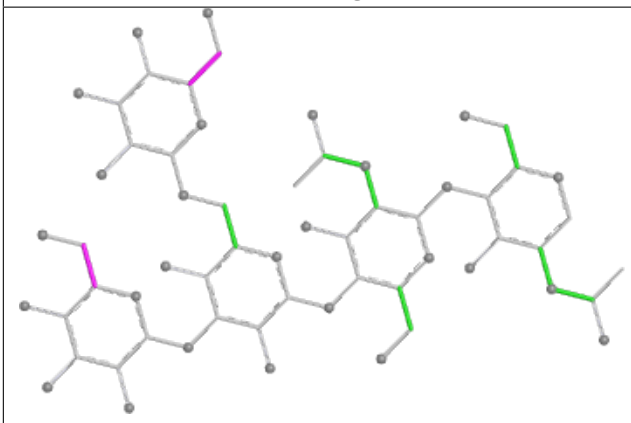
Oligosaccharide Chain W



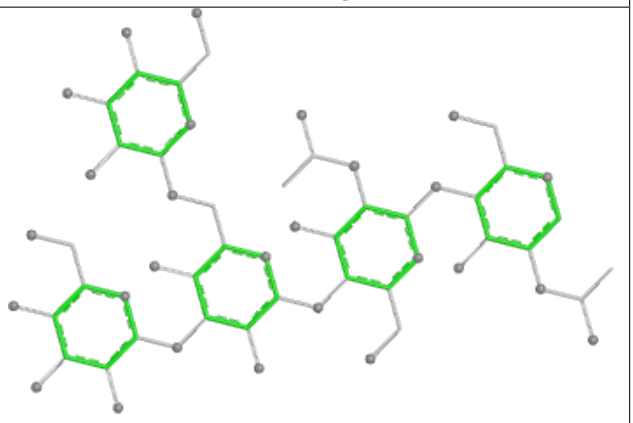
Bond lengths



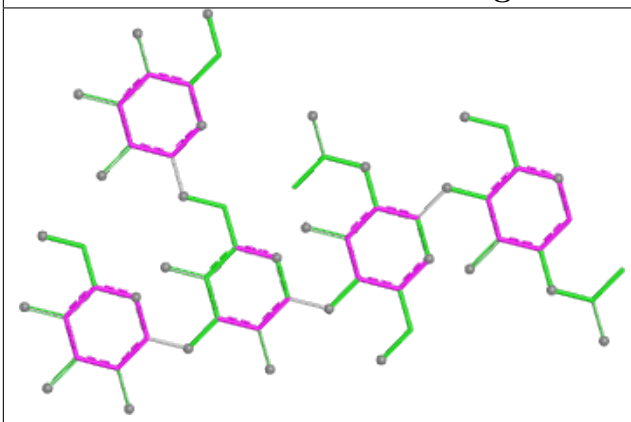
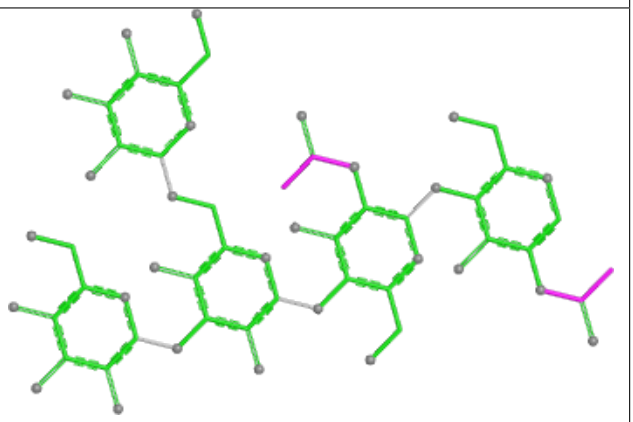
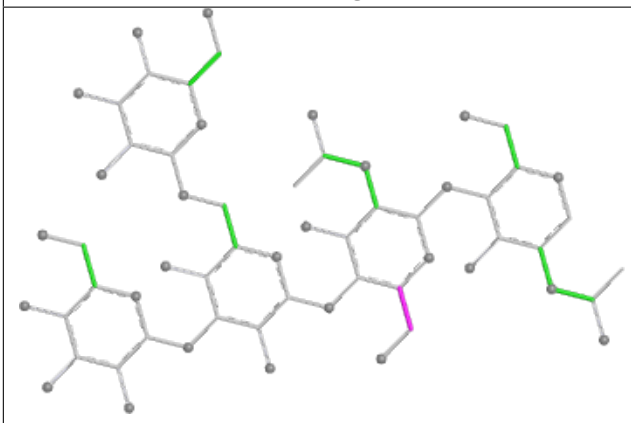
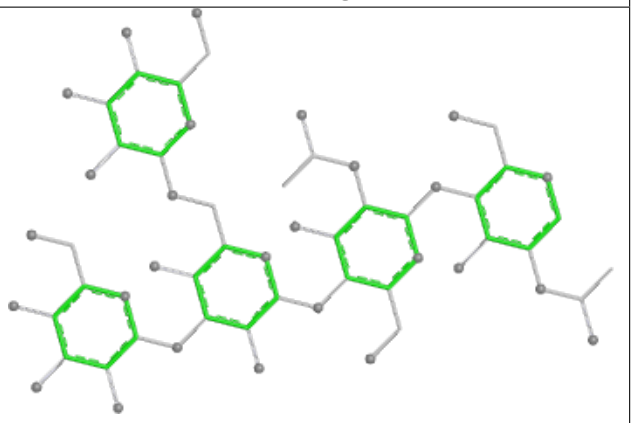
Bond angles



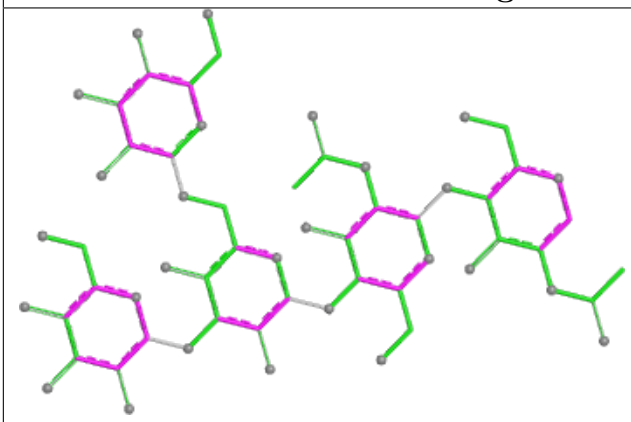
Torsions



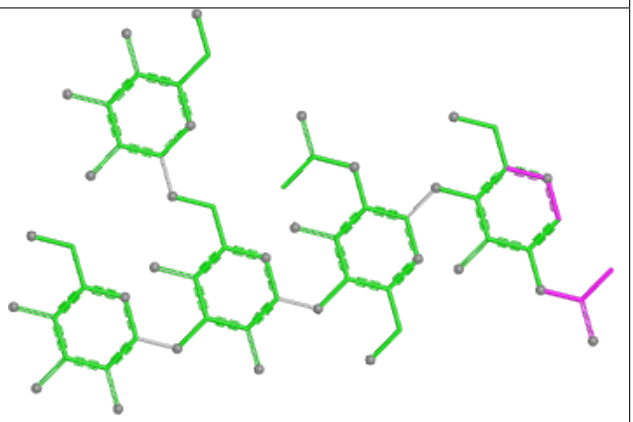
Rings

Oligosaccharide Chain Y	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

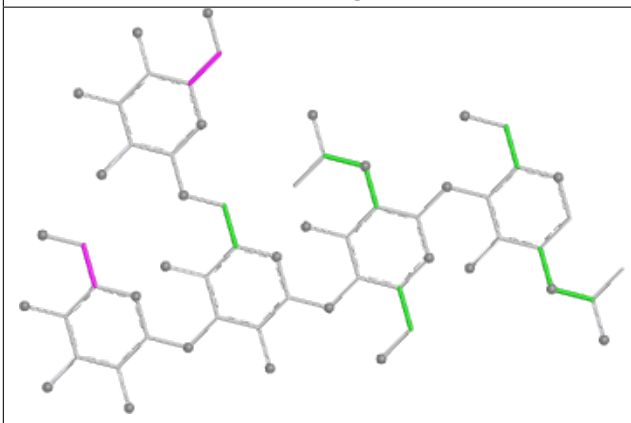
Oligosaccharide Chain Z



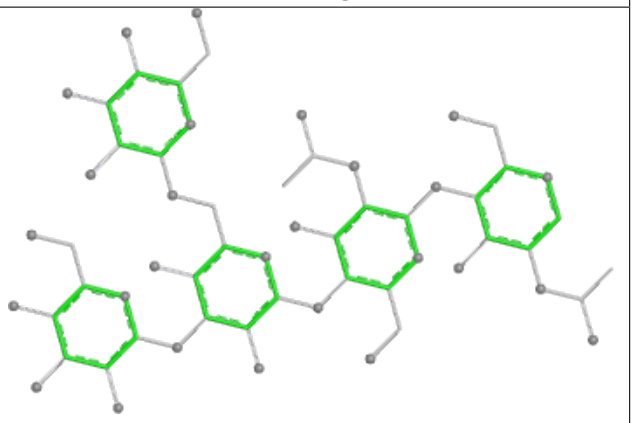
Bond lengths



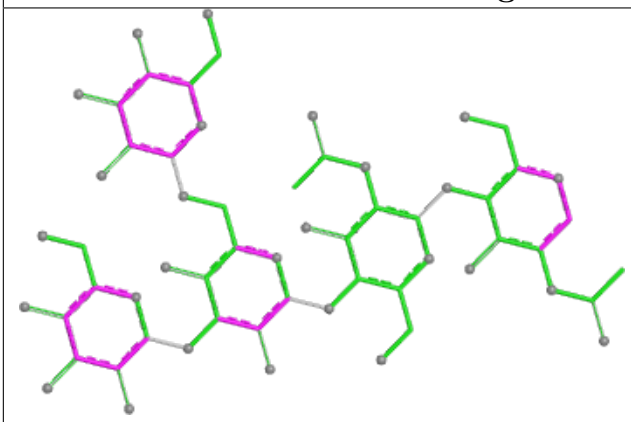
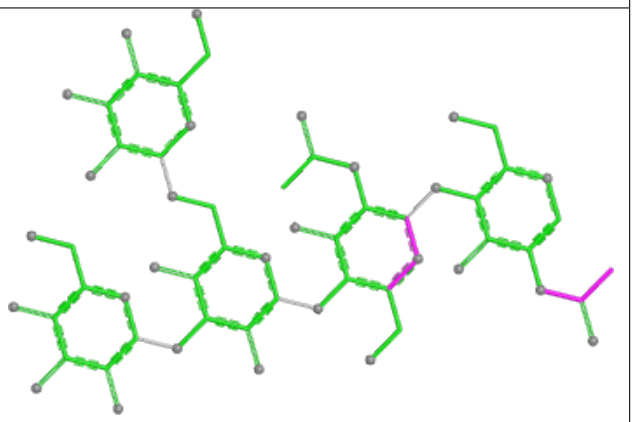
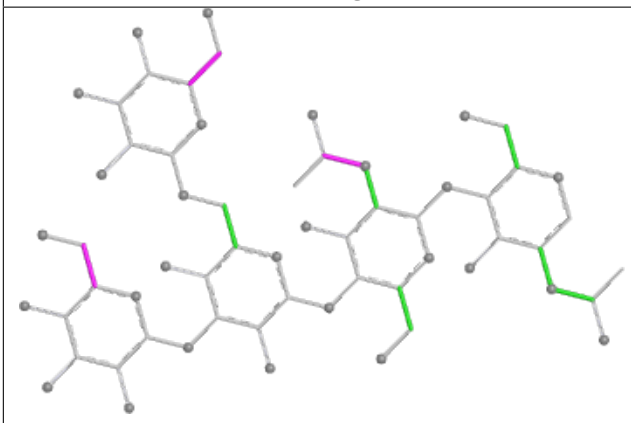
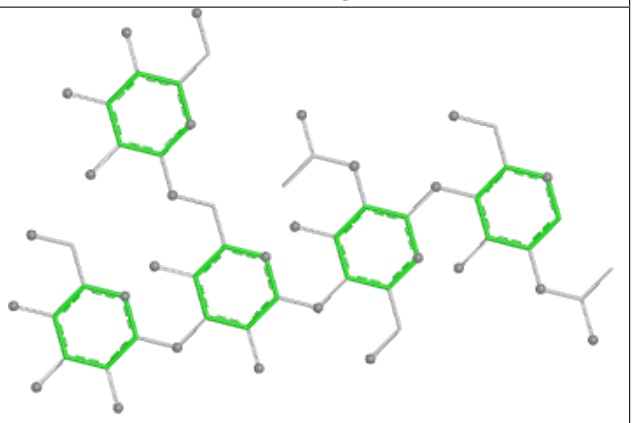
Bond angles



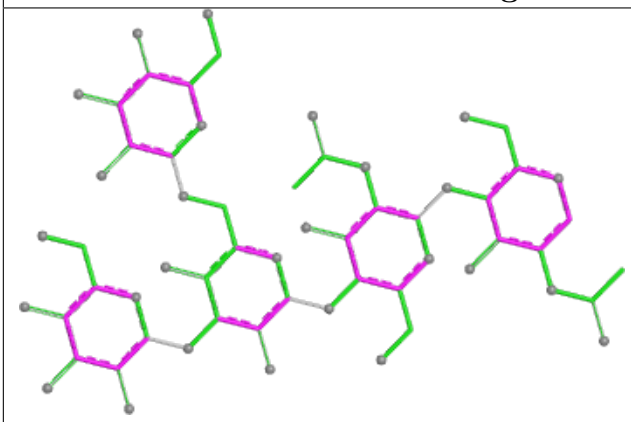
Torsions



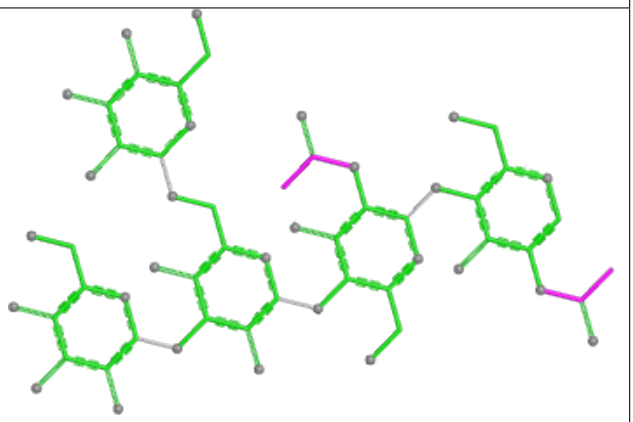
Rings

Oligosaccharide Chain b	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

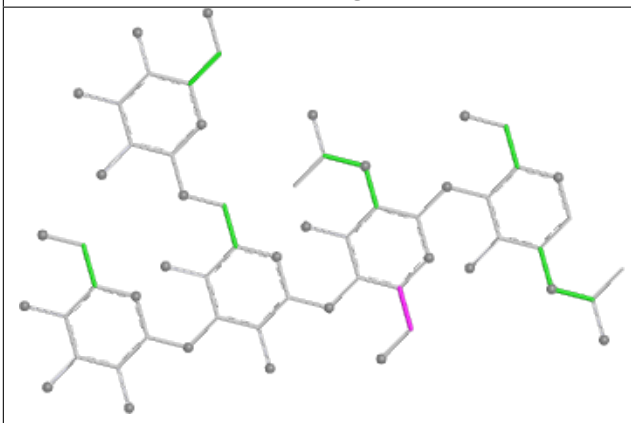
Oligosaccharide Chain f



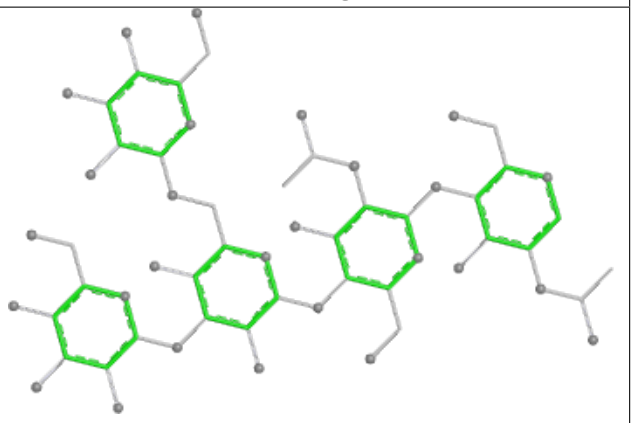
Bond lengths



Bond angles

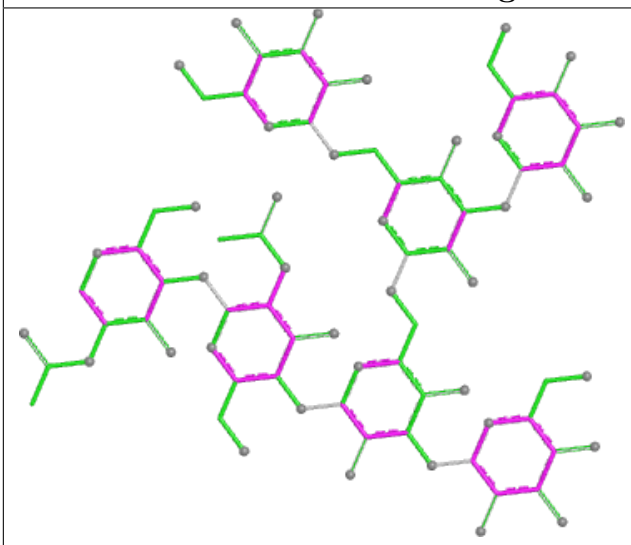


Torsions

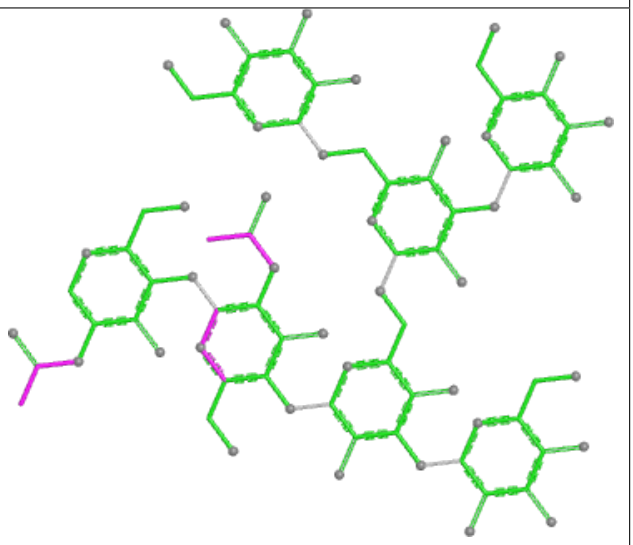


Rings

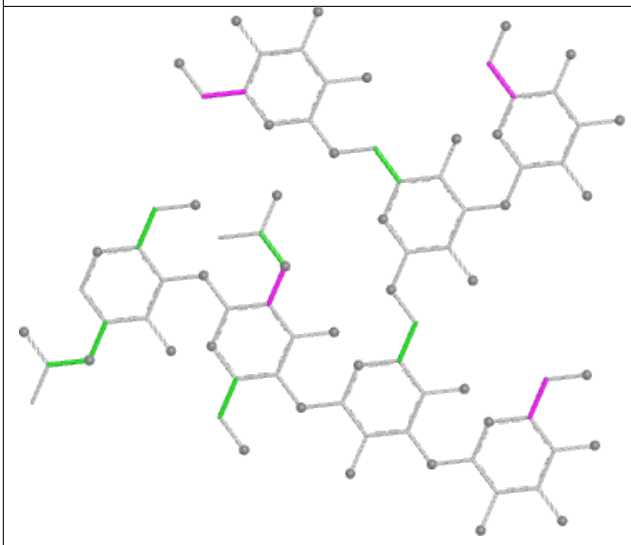
Oligosaccharide Chain J



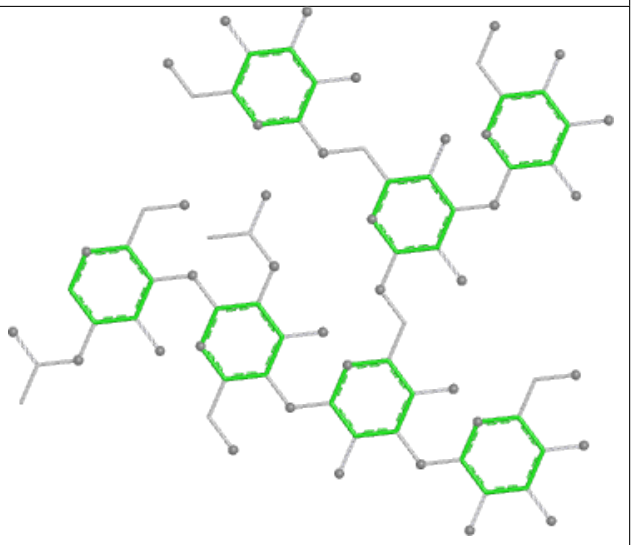
Bond lengths



Bond angles

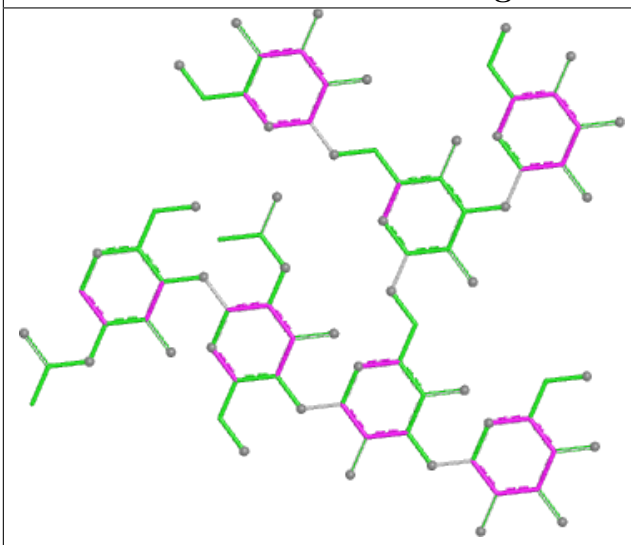


Torsions

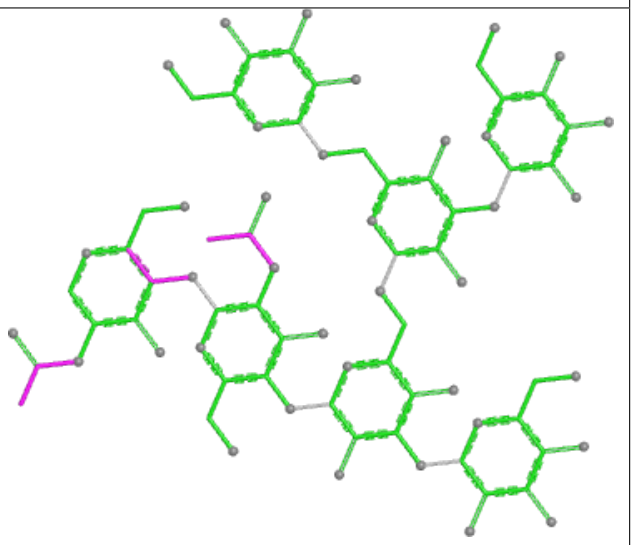


Rings

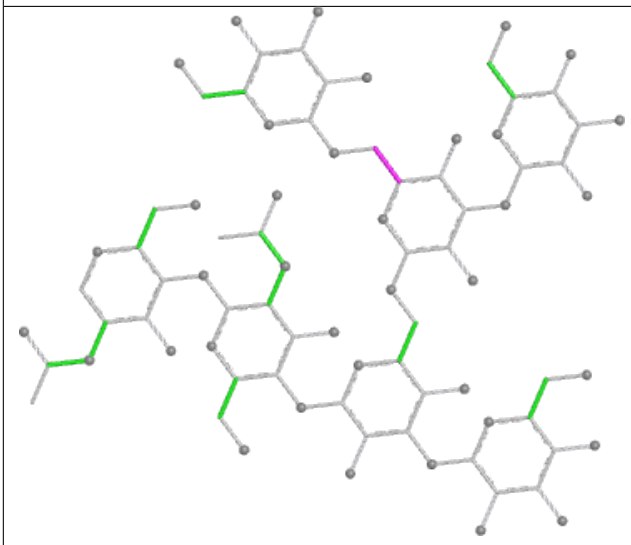
Oligosaccharide Chain X



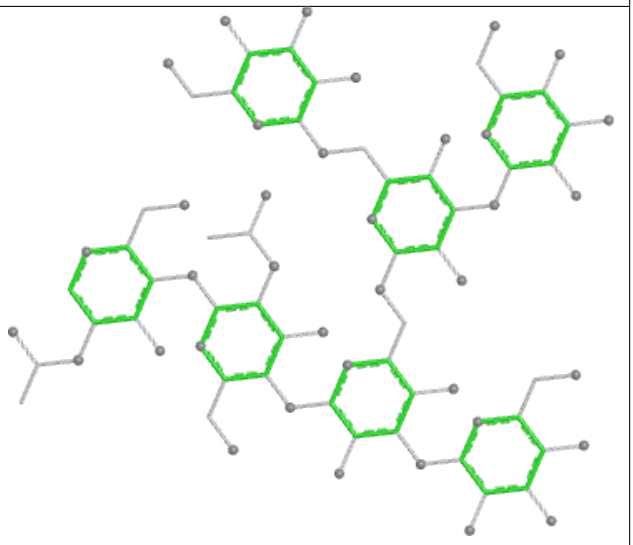
Bond lengths



Bond angles

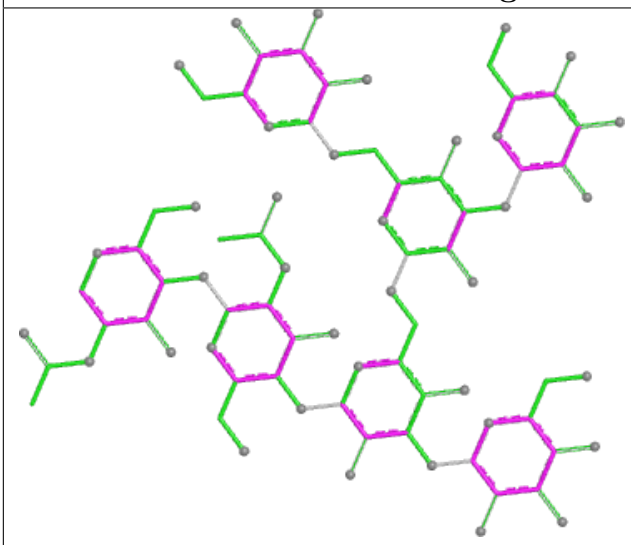


Torsions

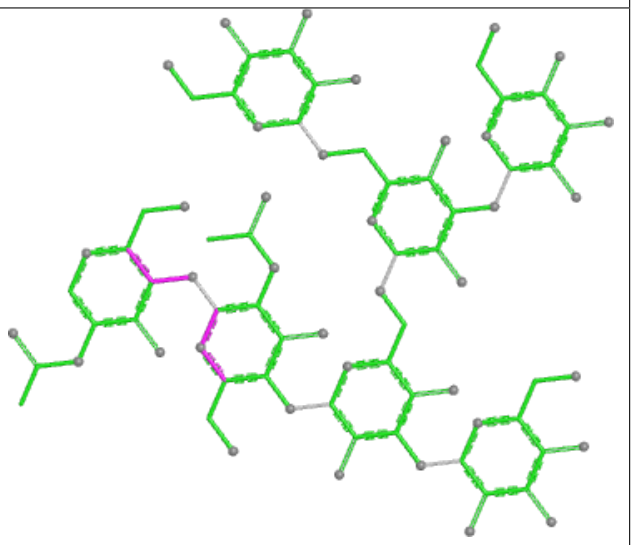


Rings

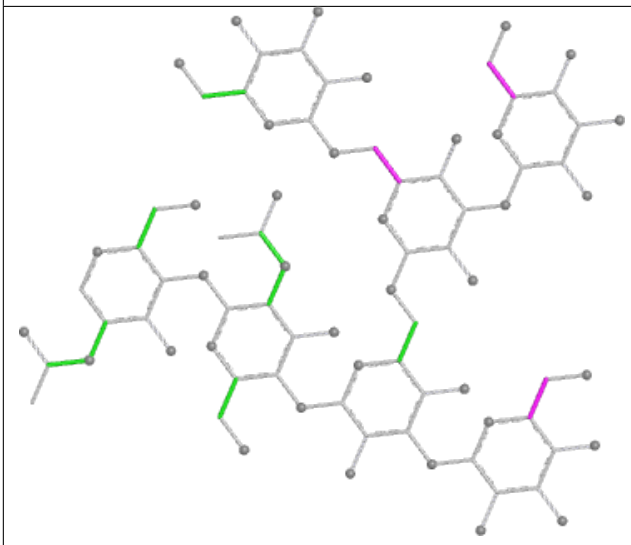
Oligosaccharide Chain c



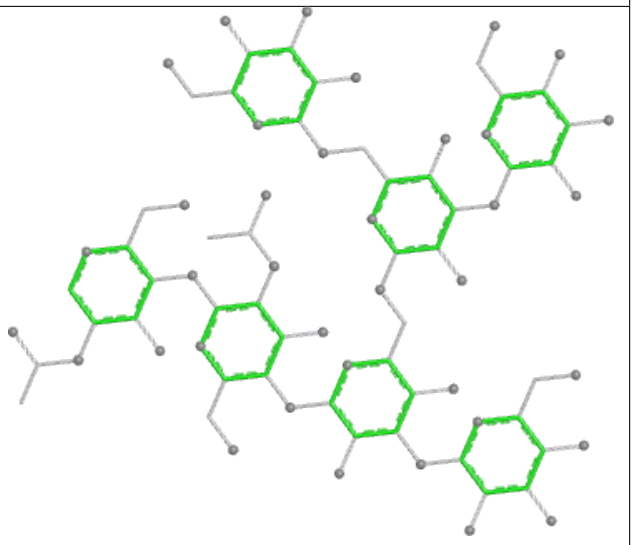
Bond lengths



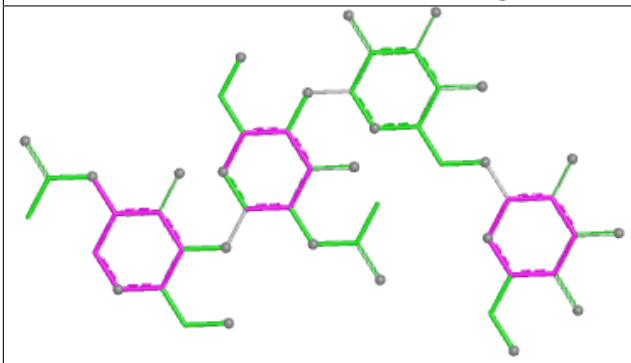
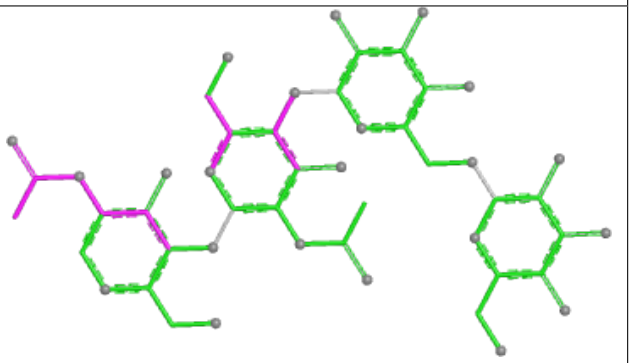
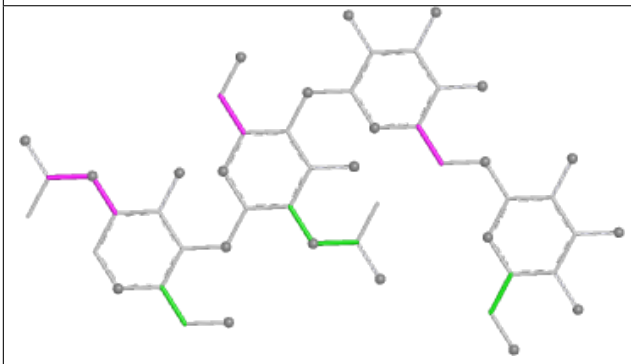
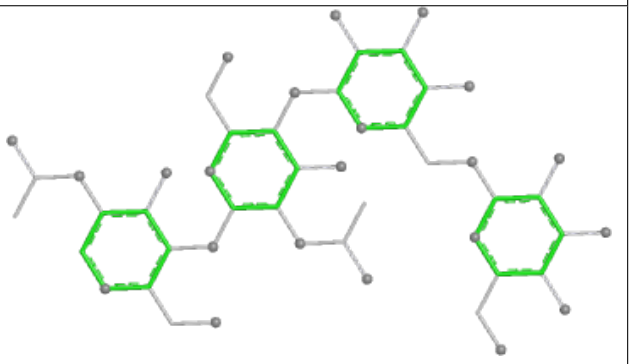
Bond angles

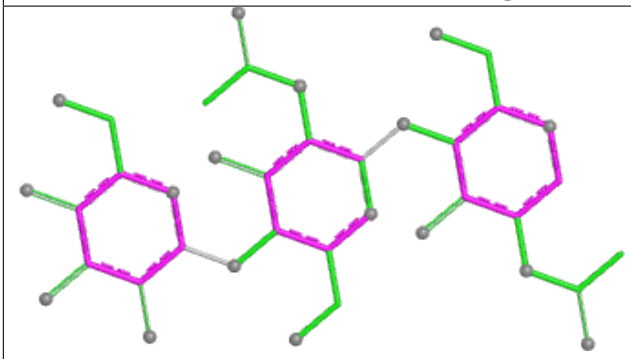
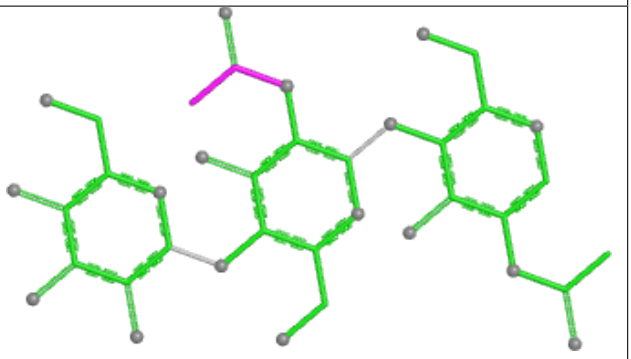
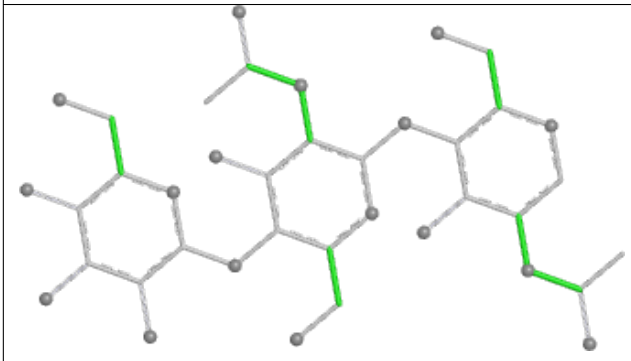
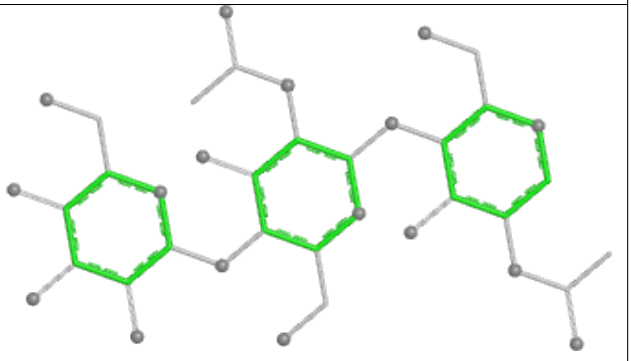


Torsions

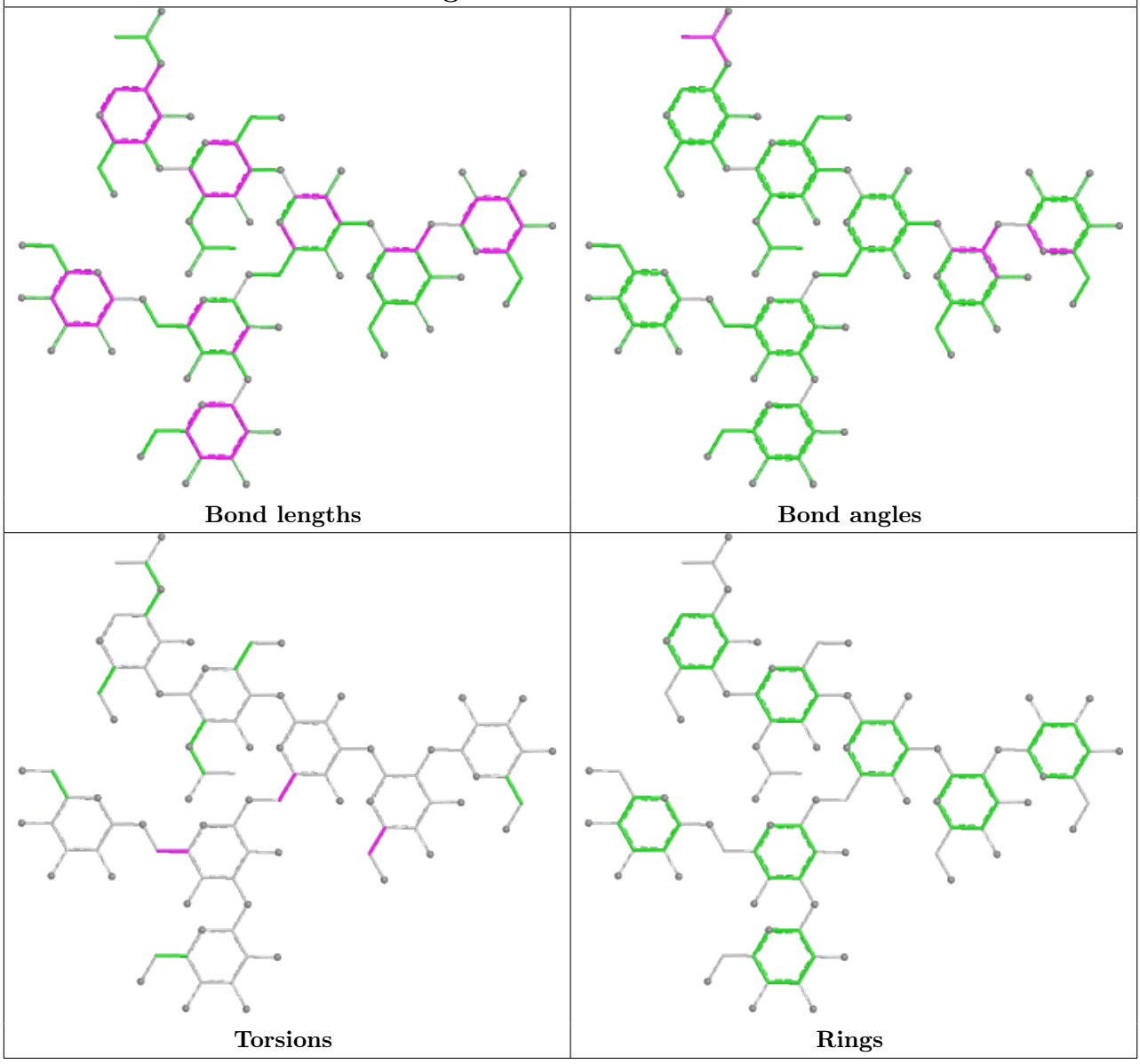


Rings

Oligosaccharide Chain K	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain a	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain d



5.6 Ligand geometry (i)

21 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	NAG	A	602	1	14,14,15	2.08	5 (35%)	17,19,21	0.93	0
13	NAG	C	605	1	14,14,15	2.07	6 (42%)	17,19,21	0.98	1 (5%)
13	NAG	A	604	1	14,14,15	2.18	6 (42%)	17,19,21	0.94	1 (5%)
13	NAG	D	604	1	14,14,15	1.99	5 (35%)	17,19,21	1.09	1 (5%)
13	NAG	C	606	1	14,14,15	2.02	5 (35%)	17,19,21	0.91	1 (5%)
13	NAG	D	607	1	14,14,15	2.01	6 (42%)	17,19,21	1.03	1 (5%)
13	NAG	C	601	1	14,14,15	2.09	5 (35%)	17,19,21	0.95	1 (5%)
13	NAG	C	604	1	14,14,15	2.17	6 (42%)	17,19,21	1.02	1 (5%)
13	NAG	C	602	1	14,14,15	2.03	4 (28%)	17,19,21	0.91	0
13	NAG	D	603	1	14,14,15	0.46	0	17,19,21	0.76	0
13	NAG	C	607	1	14,14,15	1.99	5 (35%)	17,19,21	1.05	1 (5%)
13	NAG	D	606	1	14,14,15	2.09	7 (50%)	17,19,21	0.92	1 (5%)
13	NAG	D	602	1	14,14,15	2.09	6 (42%)	17,19,21	0.98	1 (5%)
13	NAG	D	608	1	14,14,15	0.40	0	17,19,21	0.81	1 (5%)
13	NAG	A	603	1	14,14,15	2.06	4 (28%)	17,19,21	1.05	0
13	NAG	C	603	1	14,14,15	2.08	5 (35%)	17,19,21	0.99	1 (5%)
13	NAG	A	605	1	14,14,15	2.09	6 (42%)	17,19,21	1.12	2 (11%)
13	NAG	A	601	1	14,14,15	2.12	5 (35%)	17,19,21	0.96	0
13	NAG	D	605	1	14,14,15	2.29	7 (50%)	17,19,21	1.13	1 (5%)
13	NAG	C	608	1	14,14,15	2.14	5 (35%)	17,19,21	0.98	1 (5%)
13	NAG	D	601	1	14,14,15	2.02	5 (35%)	17,19,21	0.93	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	A	602	1	-	0/6/23/26	0/1/1/1
13	NAG	C	605	1	-	1/6/23/26	0/1/1/1
13	NAG	A	604	1	-	0/6/23/26	0/1/1/1
13	NAG	D	604	1	-	1/6/23/26	0/1/1/1
13	NAG	C	606	1	-	1/6/23/26	0/1/1/1
13	NAG	D	607	1	-	1/6/23/26	0/1/1/1
13	NAG	C	601	1	-	0/6/23/26	0/1/1/1
13	NAG	C	604	1	-	0/6/23/26	0/1/1/1
13	NAG	C	602	1	-	0/6/23/26	0/1/1/1
13	NAG	D	603	1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	C	607	1	-	0/6/23/26	0/1/1/1
13	NAG	D	606	1	-	0/6/23/26	0/1/1/1
13	NAG	D	602	1	-	0/6/23/26	0/1/1/1
13	NAG	D	608	1	-	3/6/23/26	0/1/1/1
13	NAG	A	603	1	-	0/6/23/26	0/1/1/1
13	NAG	C	603	1	-	1/6/23/26	0/1/1/1
13	NAG	A	605	1	-	0/6/23/26	0/1/1/1
13	NAG	A	601	1	-	1/6/23/26	0/1/1/1
13	NAG	D	605	1	-	1/6/23/26	0/1/1/1
13	NAG	C	608	1	-	0/6/23/26	0/1/1/1
13	NAG	D	601	1	-	0/6/23/26	0/1/1/1

The worst 5 of 103 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	605	NAG	C1-C2	5.56	1.60	1.52
13	A	604	NAG	C1-C2	5.37	1.60	1.52
13	A	601	NAG	C1-C2	5.36	1.60	1.52
13	A	602	NAG	C1-C2	5.34	1.60	1.52
13	C	601	NAG	C1-C2	5.30	1.60	1.52

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	605	NAG	C8-C7-N2	2.80	120.83	116.10
13	D	602	NAG	C8-C7-N2	2.57	120.45	116.10
13	C	605	NAG	C8-C7-N2	2.46	120.26	116.10
13	C	607	NAG	C1-C2-N2	-2.45	106.30	110.49
13	A	605	NAG	O7-C7-C8	-2.45	117.52	122.06

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	D	603	NAG	C8-C7-N2-C2
13	D	603	NAG	O7-C7-N2-C2
13	D	608	NAG	C8-C7-N2-C2
13	D	608	NAG	O7-C7-N2-C2
13	C	605	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
13	A	605	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14783. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

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

7 Map analysis

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

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.