Full wwPDB X-ray Structure Validation Report ⓘ

Sep 29, 2024 – 06:38 PM EDT

PDB ID	:	4LN8
Title	:	The crystal structure of hemagglutinin from a h7n9 influenza virus (a/shanghai/2/2013) in complex with lstb
Authors	:	Yang, H.; Carney, P.J.; Chang, J.C.; Villanueva, J.M.; Stevens, J.
Deposited on	:	2013-07-11
Resolution	:	2.50 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 ⓘ symbol.

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

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

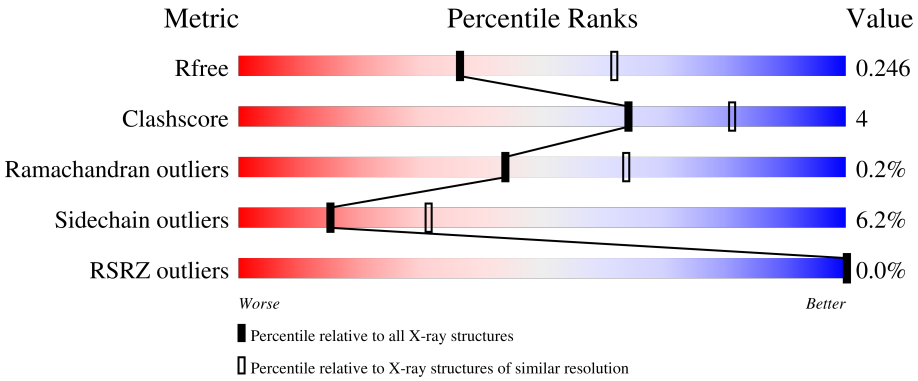
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	325	86% 10%
1	C	325	85% 12%
1	E	325	84% 12%
1	G	325	86% 10%
1	I	325	85% 12%

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Mol	Chain	Length	Quality of chain
1	K	325	85% 11%
2	B	181	81% 9% 8%
2	D	181	81% 9% 8%
2	F	181	79% 10% 8%
2	H	181	81% 9% 8%
2	J	181	81% 9% 8%
2	L	181	79% 12% 8%
3	M	4	75% 25%
3	P	4	75% 25%
3	S	4	75% 25%
4	N	3	100%
4	Q	3	33% 67%
4	T	3	100%
4	V	3	100%
4	X	3	100%
4	Z	3	33% 67%
5	O	4	25% 75%
5	W	4	100%
5	a	4	100%
6	R	3	33% 67%
6	Y	3	67% 33%
7	U	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FUC	M	4	X	-	-	-
3	FUC	S	4	X	-	-	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 23845 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.

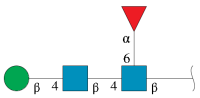
- Molecule 1 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	1	0	0
			2412	1498	436	463	15			
1	C	316	Total	C	N	O	S	1	0	0
			2412	1498	436	463	15			
1	E	316	Total	C	N	O	S	1	0	0
			2412	1498	436	463	15			
1	G	316	Total	C	N	O	S	1	0	0
			2412	1498	436	463	15			
1	I	316	Total	C	N	O	S	1	0	0
			2412	1498	436	463	15			
1	K	316	Total	C	N	O	S	1	0	0
			2412	1498	436	463	15			

- Molecule 2 is a protein called Hemagglutinin.

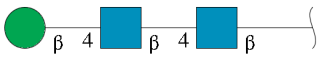
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	167	Total	C	N	O	S	0	0	0
			1360	838	238	277	7			
2	D	167	Total	C	N	O	S	0	0	0
			1360	838	238	277	7			
2	F	167	Total	C	N	O	S	0	0	0
			1360	838	238	277	7			
2	H	167	Total	C	N	O	S	0	0	0
			1360	838	238	277	7			
2	J	167	Total	C	N	O	S	0	0	0
			1360	838	238	277	7			
2	L	167	Total	C	N	O	S	0	0	0
			1360	838	238	277	7			

- Molecule 3 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.



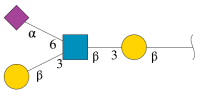
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	M	4	Total C N O 49 28 2 19	0	0	0
3	P	4	Total C N O 49 28 2 19	0	0	0
3	S	4	Total C N O 49 28 2 19	0	0	0

- Molecule 4 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
4	N	3	Total C N O 39 22 2 15	0	0	0
4	Q	3	Total C N O 39 22 2 15	0	0	0
4	T	3	Total C N O 39 22 2 15	0	0	0
4	V	3	Total C N O 39 22 2 15	0	0	0
4	X	3	Total C N O 39 22 2 15	0	0	0
4	Z	3	Total C N O 39 22 2 15	0	0	0

- Molecule 5 is an oligosaccharide called beta-D-galactopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	O	4	Total C N O 57 31 2 24	0	0	0

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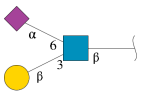
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	W	4	Total C N O 57 31 2 24	0	0	0
5	a	4	Total C N O 57 31 2 24	0	0	0

- Molecule 6 is an oligosaccharide called beta-D-galactopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	R	3	Total C N O 45 25 2 18	0	0	0
6	Y	3	Total C N O 45 25 2 18	0	0	0

- Molecule 7 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	U	2	Total C N O 33 19 2 12	0	0	0

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Ca 1 1	0	0
8	C	1	Total Ca 1 1	0	0
8	E	1	Total Ca 1 1	0	0
8	G	1	Total Ca 1 1	0	0

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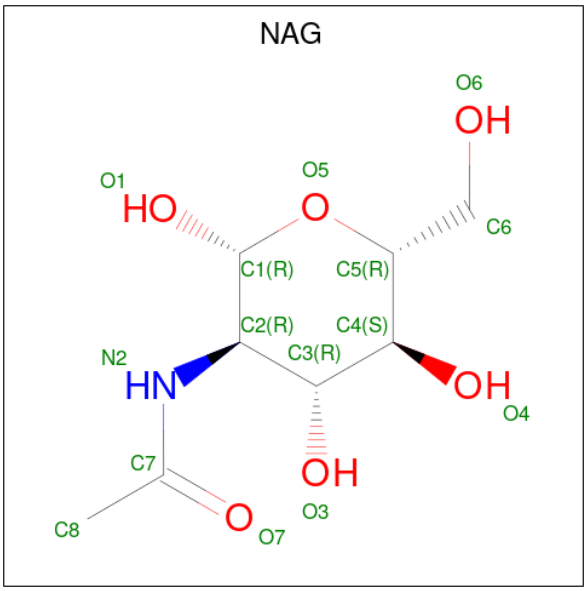
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	I	1	Total Ca 1 1	0	0
8	K	1	Total Ca 1 1	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C N O 14 8 1 5	0	0
9	D	1	Total C N O 14 8 1 5	0	0
9	F	1	Total C N O 14 8 1 5	0	0
9	H	1	Total C N O 14 8 1 5	0	0
9	J	1	Total C N O 14 8 1 5	0	0
9	L	1	Total C N O 14 8 1 5	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	48	Total O 48 48	0	0

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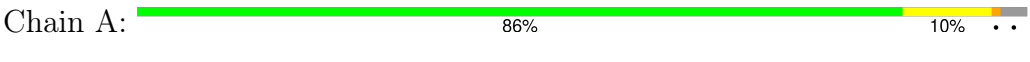
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	28	Total O 28 28	0	0
10	C	39	Total O 39 39	0	0
10	D	25	Total O 25 25	0	0
10	E	52	Total O 52 52	0	0
10	F	28	Total O 28 28	0	0
10	G	48	Total O 48 48	0	0
10	H	25	Total O 25 25	0	0
10	I	51	Total O 51 51	0	0
10	J	27	Total O 27 27	0	0
10	K	53	Total O 53 53	0	0
10	L	24	Total O 24 24	0	0

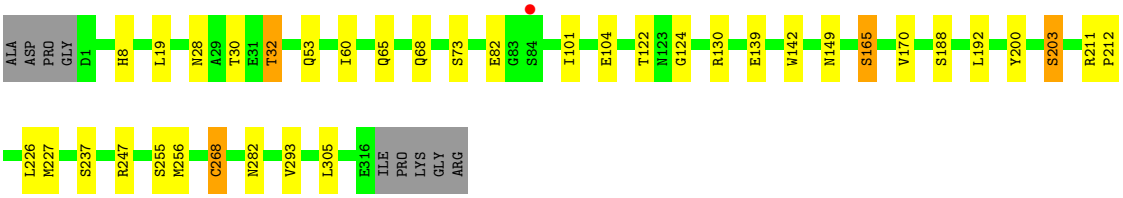
3 Residue-property plots (i)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: Hemagglutinin

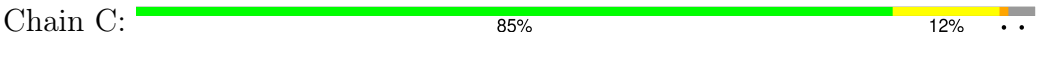
Chain A:

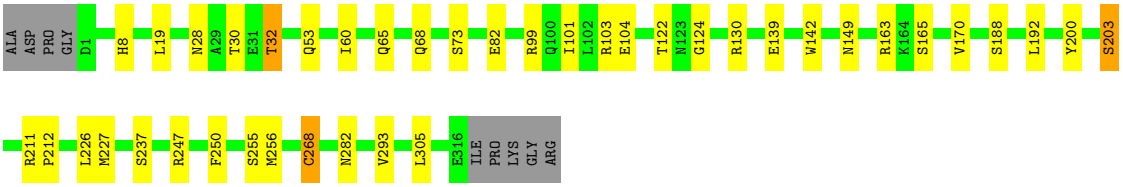




• Molecule 1: Hemagglutinin

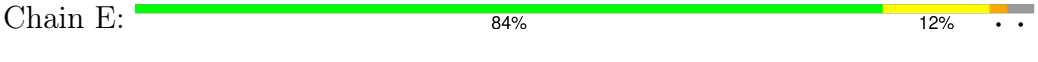
Chain C:

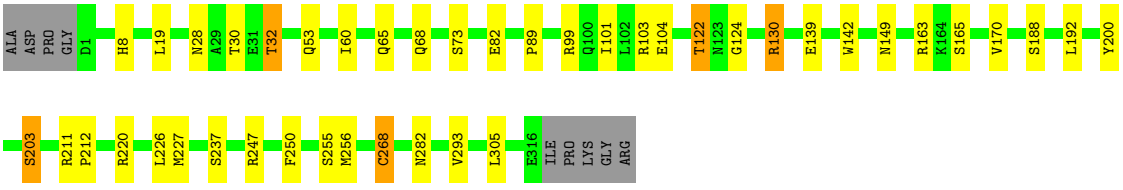




• Molecule 1: Hemagglutinin

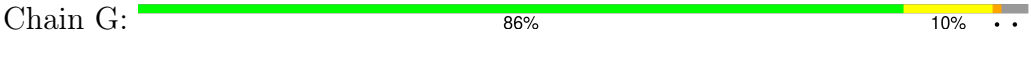
Chain E:

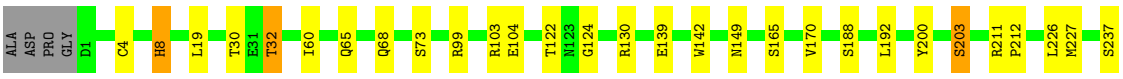


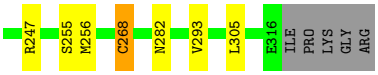


• Molecule 1: Hemagglutinin

Chain G:

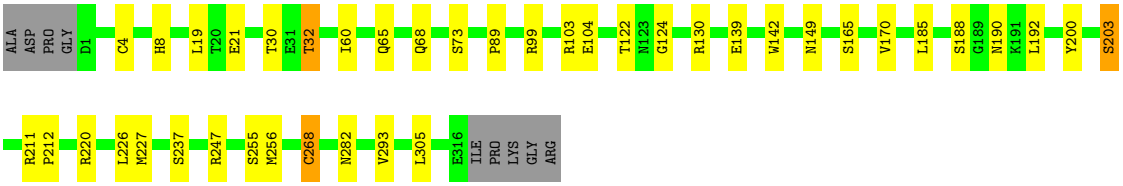






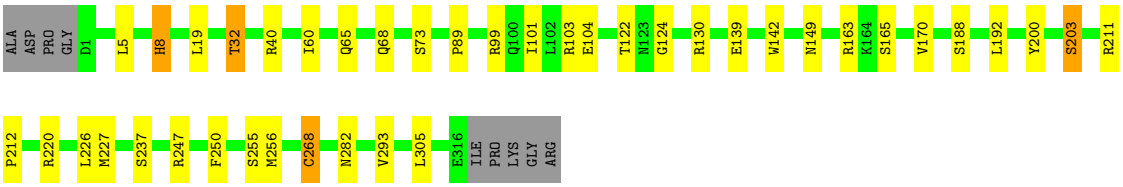
• Molecule 1: Hemagglutinin

Chain I:



• Molecule 1: Hemagglutinin

Chain K:



• Molecule 2: Hemagglutinin

Chain B:

• Molecule 2: Hemagglutinin

Chain D:

• Molecule 2: Hemagglutinin

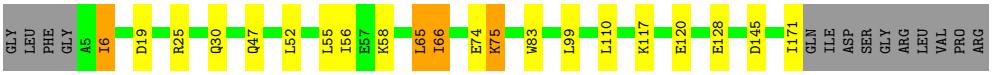
Chain F:

• Molecule 2: Hemagglutinin

Chain H:

• Molecule 2: Hemagglutinin

Chain J:

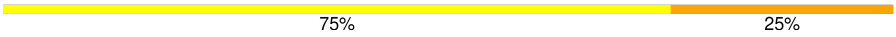


• Molecule 2: Hemagglutinin

Chain L:

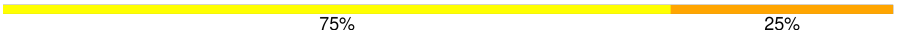
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



• Molecule 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

Chain P:

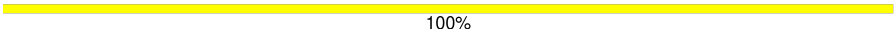


• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

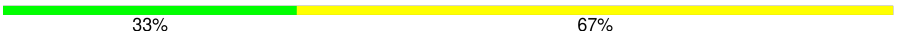
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



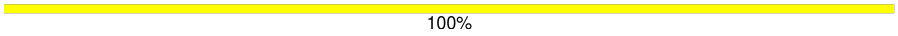
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



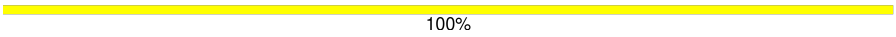
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



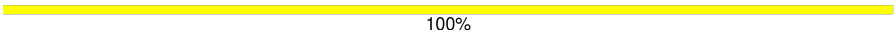
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



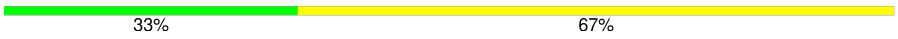
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



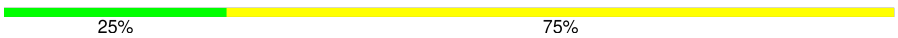
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:



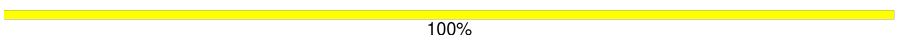
• Molecule 5: beta-D-galactopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain O:



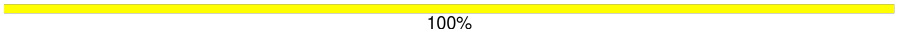
• Molecule 5: beta-D-galactopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain W:



• Molecule 5: beta-D-galactopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain a:



• Molecule 6: beta-D-galactopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

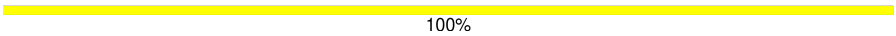
Chain R:

• Molecule 6: beta-D-galactopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:

• Molecule 7: N-acetyl-alpha-neuraminic acid-(2-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	154.36Å 154.44Å 154.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.62 – 2.50 38.62 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (38.62-2.50) 97.6 (38.62-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.217 , 0.246 0.217 , 0.246	Depositor DCC
R_{free} test set	6296 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	57.1	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 22.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.024 for k,h,-l 0.021 for -h,-l,-k 0.023 for l,-k,h 0.447 for k,l,h 0.447 for l,h,k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	23845	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.94% 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.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SIA, CA, NAG, FUC, BMA, GAL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.79	1/2458 (0.0%)	0.79	1/3322 (0.0%)
1	C	0.78	1/2458 (0.0%)	0.79	0/3322
1	E	0.78	1/2458 (0.0%)	0.79	1/3322 (0.0%)
1	G	0.86	1/2458 (0.0%)	0.80	1/3322 (0.0%)
1	I	0.82	1/2458 (0.0%)	0.80	1/3322 (0.0%)
1	K	0.83	1/2458 (0.0%)	0.80	1/3322 (0.0%)
2	B	0.73	1/1383 (0.1%)	0.77	1/1864 (0.1%)
2	D	0.74	1/1383 (0.1%)	0.77	2/1864 (0.1%)
2	F	0.75	1/1383 (0.1%)	0.78	2/1864 (0.1%)
2	H	0.75	1/1383 (0.1%)	0.78	0/1864
2	J	0.77	3/1383 (0.2%)	0.78	0/1864
2	L	0.78	3/1383 (0.2%)	0.78	0/1864
All	All	0.79	16/23046 (0.1%)	0.79	10/31116 (0.0%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	268	CYS	CB-SG	-25.39	1.39	1.82
1	K	268	CYS	CB-SG	-24.16	1.41	1.82
1	I	268	CYS	CB-SG	-22.43	1.44	1.82
1	A	268	CYS	CB-SG	-19.58	1.49	1.82
1	E	268	CYS	CB-SG	-18.99	1.50	1.82
1	C	268	CYS	CB-SG	-17.52	1.52	1.82
2	L	83	TRP	CB-CG	-6.55	1.38	1.50
2	L	74	GLU	CD-OE1	6.36	1.32	1.25
2	J	74	GLU	CD-OE1	5.74	1.31	1.25
2	H	74	GLU	CG-CD	5.59	1.60	1.51
2	L	74	GLU	CG-CD	5.51	1.60	1.51
2	J	74	GLU	CG-CD	5.46	1.60	1.51
2	F	74	GLU	CG-CD	5.42	1.60	1.51
2	J	83	TRP	CB-CG	-5.42	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	74	GLU	CG-CD	5.18	1.59	1.51
2	D	74	GLU	CG-CD	5.12	1.59	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	268	CYS	CA-CB-SG	7.30	127.14	114.00
1	K	268	CYS	CA-CB-SG	7.26	127.06	114.00
1	I	268	CYS	CA-CB-SG	7.12	126.81	114.00
2	D	85	ARG	NE-CZ-NH2	-5.51	117.55	120.30
2	B	85	ARG	NE-CZ-NH2	-5.47	117.56	120.30
2	D	65	LEU	CA-CB-CG	5.30	127.48	115.30
1	A	268	CYS	CA-CB-SG	5.29	123.52	114.00
1	E	268	CYS	CA-CB-SG	5.24	123.44	114.00
2	F	85	ARG	NE-CZ-NH2	-5.04	117.78	120.30
2	F	65	LEU	CA-CB-CG	5.02	126.84	115.30

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	2412	0	2374	15	1
1	C	2412	0	2374	17	1
1	E	2412	0	2374	20	1
1	G	2412	0	2375	15	1
1	I	2412	0	2375	17	1
1	K	2412	0	2375	18	1
2	B	1360	0	1262	13	0
2	D	1360	0	1262	18	0
2	F	1360	0	1262	18	0
2	H	1360	0	1262	14	0
2	J	1360	0	1262	13	0
2	L	1360	0	1262	14	0
3	M	49	0	43	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	49	0	43	1	0
3	S	49	0	43	1	0
4	N	39	0	34	0	0
4	Q	39	0	34	0	0
4	T	39	0	34	0	0
4	V	39	0	34	0	0
4	X	39	0	34	0	0
4	Z	39	0	34	0	0
5	O	57	0	49	0	0
5	W	57	0	48	0	0
5	a	57	0	48	0	0
6	R	45	0	37	0	0
6	Y	45	0	37	2	0
7	U	33	0	27	0	0
8	A	1	0	0	0	0
8	C	1	0	0	0	0
8	E	1	0	0	0	0
8	G	1	0	0	0	0
8	I	1	0	0	0	0
8	K	1	0	0	0	0
9	B	14	0	13	0	0
9	D	14	0	13	0	0
9	F	14	0	13	1	0
9	H	14	0	13	0	0
9	J	14	0	13	0	0
9	L	14	0	13	0	0
10	A	48	0	0	2	0
10	B	28	0	0	0	0
10	C	39	0	0	0	0
10	D	25	0	0	3	0
10	E	52	0	0	2	0
10	F	28	0	0	3	0
10	G	48	0	0	0	0
10	H	25	0	0	2	0
10	I	51	0	0	2	0
10	J	27	0	0	0	0
10	K	53	0	0	1	0
10	L	24	0	0	2	0
All	All	23845	0	22476	172	3

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 4.

All (172) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:58:LYS:HA	10:D:612:HOH:O	1.80	0.80
1:I:139:GLU:OE1	1:I:247:ARG:HD3	1.82	0.79
1:G:139:GLU:OE1	1:G:247:ARG:HD3	1.83	0.78
1:K:139:GLU:OE1	1:K:247:ARG:HD3	1.83	0.77
1:C:139:GLU:OE1	1:C:247:ARG:HD3	1.84	0.77
1:A:139:GLU:OE1	1:A:247:ARG:HD3	1.84	0.77
1:E:139:GLU:OE1	1:E:247:ARG:HD3	1.84	0.77
1:I:282:ASN:OD1	2:J:58:LYS:NZ	2.18	0.75
2:L:66:ILE:HD13	2:L:66:ILE:H	1.55	0.72
1:G:282:ASN:OD1	2:H:58:LYS:NZ	2.22	0.70
1:C:282:ASN:OD1	2:D:58:LYS:NZ	2.23	0.70
2:H:66:ILE:HD13	2:H:66:ILE:H	1.56	0.70
2:J:66:ILE:H	2:J:66:ILE:HD13	1.57	0.69
2:F:66:ILE:H	2:F:66:ILE:HD13	1.58	0.68
1:G:8:HIS:HD2	10:H:607:HOH:O	1.76	0.68
1:E:282:ASN:OD1	2:F:58:LYS:NZ	2.24	0.67
2:D:66:ILE:HD13	2:D:66:ILE:H	1.59	0.67
2:B:66:ILE:H	2:B:66:ILE:HD13	1.60	0.67
1:C:293:VAL:HG11	2:D:65:LEU:HD13	1.78	0.65
1:E:122:THR:HG22	10:E:503:HOH:O	1.95	0.65
1:E:293:VAL:HG11	2:F:65:LEU:HD13	1.78	0.65
2:L:55:LEU:HD22	2:L:99:LEU:HD21	1.80	0.64
1:K:282:ASN:OD1	2:L:58:LYS:NZ	2.29	0.64
1:G:293:VAL:HG11	2:H:65:LEU:HD13	1.80	0.63
1:A:282:ASN:OD1	2:B:58:LYS:NZ	2.28	0.63
2:H:55:LEU:HD22	2:H:99:LEU:HD21	1.80	0.63
2:F:55:LEU:HD22	2:F:99:LEU:HD21	1.80	0.62
2:J:55:LEU:HD22	2:J:99:LEU:HD21	1.79	0.62
1:C:28:ASN:OD1	3:P:1:NAG:H83	2.00	0.61
1:A:293:VAL:HG11	2:B:65:LEU:HD13	1.82	0.61
2:B:55:LEU:HD22	2:B:99:LEU:HD21	1.81	0.61
2:D:55:LEU:HD22	2:D:99:LEU:HD21	1.82	0.61
1:K:293:VAL:HG11	2:L:65:LEU:HD13	1.82	0.60
2:J:75:LYS:HD2	1:K:101:ILE:HD11	1.83	0.59
2:F:47:GLN:OE1	2:F:110:LEU:HD11	2.02	0.59
2:B:47:GLN:OE1	2:B:110:LEU:HD11	2.01	0.59
2:D:47:GLN:OE1	2:D:110:LEU:HD11	2.02	0.59
2:H:47:GLN:OE1	2:H:110:LEU:HD11	2.03	0.59
1:A:28:ASN:OD1	3:M:1:NAG:H83	2.03	0.59
1:I:293:VAL:HG11	2:J:65:LEU:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:47:GLN:OE1	2:L:110:LEU:HD11	2.03	0.58
2:B:6:ILE:HD11	2:B:25:ARG:HG2	1.86	0.58
2:H:6:ILE:HD11	2:H:25:ARG:HG2	1.86	0.58
2:J:47:GLN:OE1	2:J:110:LEU:HD11	2.03	0.57
2:F:6:ILE:HD11	2:F:25:ARG:HG2	1.86	0.57
2:D:6:ILE:HD11	2:D:25:ARG:HG2	1.85	0.57
2:J:6:ILE:HD11	2:J:25:ARG:HG2	1.87	0.57
1:K:32:THR:HG22	1:K:305:LEU:HB2	1.87	0.56
1:I:60:ILE:HG21	1:I:170:VAL:HG21	1.88	0.56
1:A:60:ILE:HG21	1:A:170:VAL:HG21	1.87	0.56
1:C:32:THR:HG22	1:C:305:LEU:HB2	1.88	0.55
1:E:60:ILE:HG21	1:E:170:VAL:HG21	1.88	0.55
2:L:6:ILE:HD11	2:L:25:ARG:HG2	1.87	0.55
1:A:32:THR:HG22	1:A:305:LEU:HB2	1.89	0.54
1:E:32:THR:HG22	1:E:305:LEU:HB2	1.89	0.54
1:G:60:ILE:HG21	1:G:170:VAL:HG21	1.88	0.54
1:G:32:THR:HG22	1:G:305:LEU:HB2	1.89	0.54
1:K:60:ILE:HG21	1:K:170:VAL:HG21	1.89	0.54
2:D:117:LYS:NZ	10:D:614:HOH:O	2.40	0.54
1:C:60:ILE:HG21	1:C:170:VAL:HG21	1.88	0.54
2:F:56:ILE:O	2:F:56:ILE:HG23	2.09	0.53
2:L:67:ASP:HB2	10:L:605:HOH:O	2.08	0.53
2:D:56:ILE:O	2:D:56:ILE:CG2	2.57	0.52
1:I:32:THR:HG22	1:I:305:LEU:HB2	1.89	0.52
2:B:56:ILE:O	2:B:56:ILE:HG23	2.09	0.52
2:D:56:ILE:O	2:D:56:ILE:HG23	2.10	0.52
2:F:56:ILE:O	2:F:56:ILE:CG2	2.57	0.52
1:K:8:HIS:HE1	10:K:504:HOH:O	1.91	0.52
2:B:56:ILE:O	2:B:56:ILE:CG2	2.57	0.52
1:A:226:LEU:HD12	1:A:226:LEU:C	2.30	0.52
1:A:101:ILE:HD11	2:F:75:LYS:HD2	1.92	0.51
1:E:226:LEU:HD12	1:E:226:LEU:C	2.30	0.51
2:L:66:ILE:HD13	2:L:66:ILE:N	2.25	0.51
2:J:56:ILE:O	2:J:56:ILE:HG23	2.10	0.51
2:H:56:ILE:HG23	2:H:56:ILE:O	2.11	0.51
2:L:56:ILE:HG23	2:L:56:ILE:O	2.11	0.51
2:L:56:ILE:O	2:L:56:ILE:CG2	2.59	0.51
1:G:226:LEU:C	1:G:226:LEU:HD12	2.31	0.50
2:J:56:ILE:O	2:J:56:ILE:CG2	2.58	0.50
1:C:226:LEU:C	1:C:226:LEU:HD12	2.32	0.50
1:E:130:ARG:CZ	10:E:512:HOH:O	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:56:ILE:O	2:H:56:ILE:CG2	2.59	0.49
1:K:226:LEU:C	1:K:226:LEU:HD12	2.33	0.49
2:F:79:ASN:OD1	9:F:500:NAG:H82	2.12	0.49
1:A:192:LEU:HD11	1:A:203:SER:OG	2.13	0.49
1:C:192:LEU:HD11	1:C:203:SER:OG	2.13	0.48
2:F:67:ASP:HB2	10:F:611:HOH:O	2.13	0.48
1:G:192:LEU:HD11	1:G:203:SER:OG	2.13	0.48
1:I:192:LEU:HD11	1:I:203:SER:OG	2.14	0.48
1:K:192:LEU:HD11	1:K:203:SER:OG	2.13	0.48
1:E:192:LEU:HD11	1:E:203:SER:OG	2.12	0.48
2:J:66:ILE:HD13	2:J:66:ILE:N	2.26	0.48
1:I:226:LEU:HD12	1:I:226:LEU:C	2.34	0.48
2:F:66:ILE:HD13	2:F:66:ILE:N	2.27	0.48
1:I:21:GLU:HG2	10:I:521:HOH:O	2.14	0.47
2:B:75:LYS:HD2	1:C:101:ILE:HD11	1.96	0.47
2:J:6:ILE:CG2	2:J:6:ILE:O	2.63	0.47
1:K:211:ARG:HB2	1:K:212:PRO:CD	2.45	0.47
2:B:66:ILE:HD13	2:B:66:ILE:N	2.27	0.47
2:D:66:ILE:HD13	2:D:66:ILE:N	2.27	0.47
2:F:125:GLN:HG2	10:F:615:HOH:O	2.15	0.46
2:J:30:GLN:HE22	2:J:145:ASP:HB2	1.80	0.46
2:F:117:LYS:HD2	10:F:617:HOH:O	2.16	0.46
2:D:75:LYS:HD2	1:E:101:ILE:HD11	1.97	0.45
1:E:28:ASN:OD1	3:S:1:NAG:H83	2.16	0.45
2:F:6:ILE:O	2:F:6:ILE:CG2	2.65	0.45
2:H:161:LYS:CE	10:H:621:HOH:O	2.64	0.45
2:D:6:ILE:O	2:D:6:ILE:CG2	2.65	0.45
1:A:211:ARG:HB2	1:A:212:PRO:HD2	1.99	0.45
1:K:211:ARG:HB2	1:K:212:PRO:HD2	1.99	0.45
2:H:66:ILE:HD13	2:H:66:ILE:N	2.25	0.45
2:H:6:ILE:O	2:H:6:ILE:CG2	2.64	0.45
1:I:190:ASN:HB2	10:I:508:HOH:O	2.17	0.45
2:L:6:ILE:O	2:L:6:ILE:CG2	2.64	0.44
1:C:124:GLY:HA3	1:C:142:TRP:HB3	2.00	0.44
1:A:211:ARG:HB2	1:A:212:PRO:CD	2.47	0.44
1:E:104:GLU:HA	1:E:255:SER:O	2.18	0.44
1:C:211:ARG:HB2	1:C:212:PRO:CD	2.48	0.44
1:G:211:ARG:HB2	1:G:212:PRO:CD	2.46	0.44
2:D:30:GLN:HE22	2:D:145:ASP:HB2	1.82	0.44
1:I:211:ARG:HB2	1:I:212:PRO:CD	2.47	0.44
1:E:211:ARG:HB2	1:E:212:PRO:CD	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:GLN:HE22	2:B:145:ASP:HB2	1.83	0.44
2:F:30:GLN:HE22	2:F:145:ASP:HB2	1.83	0.44
1:G:211:ARG:HB2	1:G:212:PRO:HD2	2.00	0.44
1:G:104:GLU:HA	1:G:255:SER:O	2.18	0.44
2:H:30:GLN:HE22	2:H:145:ASP:HB2	1.83	0.43
2:B:94:TYR:CD2	2:B:94:TYR:C	2.92	0.43
1:I:104:GLU:HA	1:I:255:SER:O	2.18	0.43
2:L:30:GLN:HE22	2:L:145:ASP:HB2	1.81	0.43
2:B:6:ILE:O	2:B:6:ILE:CG2	2.65	0.43
2:D:94:TYR:CD2	2:D:94:TYR:C	2.91	0.43
1:I:185:LEU:HD22	6:Y:3:SIA:H111	2.01	0.43
1:C:211:ARG:HB2	1:C:212:PRO:HD2	2.00	0.43
1:A:104:GLU:HA	1:A:255:SER:O	2.19	0.43
1:E:211:ARG:HB2	1:E:212:PRO:HD2	2.00	0.43
1:K:104:GLU:HA	1:K:255:SER:O	2.19	0.42
1:C:99:ARG:O	1:C:103:ARG:HG3	2.19	0.42
1:E:124:GLY:HA3	1:E:142:TRP:HB3	2.00	0.42
1:I:211:ARG:HB2	1:I:212:PRO:HD2	2.02	0.42
1:A:165:SER:HB2	10:A:542:HOH:O	2.18	0.42
1:C:104:GLU:HA	1:C:255:SER:O	2.18	0.42
1:C:293:VAL:CG1	2:D:65:LEU:HD13	2.46	0.42
1:G:4:CYS:SG	2:H:6:ILE:HG23	2.60	0.42
1:K:124:GLY:HA3	1:K:142:TRP:HB3	2.02	0.42
1:E:293:VAL:CG1	2:F:65:LEU:HD13	2.46	0.42
10:A:516:HOH:O	1:K:40:ARG:HD2	2.19	0.42
1:C:53:GLN:NE2	1:C:82:GLU:HB2	2.34	0.42
1:I:124:GLY:HA3	1:I:142:TRP:HB3	2.01	0.41
1:K:99:ARG:O	1:K:103:ARG:HG3	2.20	0.41
1:E:99:ARG:O	1:E:103:ARG:HG3	2.20	0.41
1:A:124:GLY:HA3	1:A:142:TRP:HB3	2.00	0.41
1:E:89:PRO:HB2	1:E:220:ARG:HD3	2.03	0.41
1:G:293:VAL:CG1	2:H:65:LEU:HD13	2.49	0.41
6:Y:3:SIA:O7	6:Y:3:SIA:H113	2.20	0.41
1:I:4:CYS:SG	2:J:6:ILE:HG23	2.61	0.41
1:E:163:ARG:HD3	1:E:250:PHE:CZ	2.56	0.41
1:I:99:ARG:O	1:I:103:ARG:HG3	2.21	0.41
1:K:89:PRO:HB2	1:K:220:ARG:HD3	2.02	0.41
1:K:163:ARG:HD3	1:K:250:PHE:CZ	2.56	0.41
2:F:94:TYR:CD2	2:F:94:TYR:C	2.94	0.41
1:G:124:GLY:HA3	1:G:142:TRP:HB3	2.02	0.41
1:I:89:PRO:HB2	1:I:220:ARG:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:122:VAL:O	2:L:123:LYS:C	2.58	0.41
2:D:117:LYS:HD2	10:D:614:HOH:O	2.21	0.41
1:A:53:GLN:NE2	1:A:82:GLU:HB2	2.36	0.40
2:L:66:ILE:HD13	10:L:605:HOH:O	2.19	0.40
1:E:53:GLN:NE2	1:E:82:GLU:HB2	2.37	0.40
1:G:99:ARG:O	1:G:103:ARG:HG3	2.21	0.40
1:C:163:ARG:HD3	1:C:250:PHE:CZ	2.55	0.40
2:D:6:ILE:HD13	2:D:6:ILE:HG21	1.83	0.40
1:K:5:LEU:HD13	1:K:5:LEU:HA	1.93	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:ASN:OD1	1:I:149:ASN:OD1[4_445]	2.00	0.20
1:A:149:ASN:OD1	1:K:149:ASN:OD1[4_445]	2.03	0.17
1:E:149:ASN:OD1	1:G:149:ASN:OD1[2_444]	2.03	0.17

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 X-ray entries followed by that with respect to entries of similar resolution.

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	314/325 (97%)	305 (97%)	8 (2%)	1 (0%)	37	56
1	C	314/325 (97%)	306 (98%)	7 (2%)	1 (0%)	37	56
1	E	314/325 (97%)	304 (97%)	9 (3%)	1 (0%)	37	56
1	G	314/325 (97%)	306 (98%)	7 (2%)	1 (0%)	37	56
1	I	314/325 (97%)	304 (97%)	9 (3%)	1 (0%)	37	56
1	K	314/325 (97%)	304 (97%)	9 (3%)	1 (0%)	37	56
2	B	165/181 (91%)	158 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	165/181 (91%)	158 (96%)	7 (4%)	0	100	100
2	F	165/181 (91%)	158 (96%)	7 (4%)	0	100	100
2	H	165/181 (91%)	157 (95%)	8 (5%)	0	100	100
2	J	165/181 (91%)	157 (95%)	8 (5%)	0	100	100
2	L	165/181 (91%)	158 (96%)	7 (4%)	0	100	100
All	All	2874/3036 (95%)	2775 (97%)	93 (3%)	6 (0%)	44	64

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	200	TYR
1	A	200	TYR
1	C	200	TYR
1	E	200	TYR
1	G	200	TYR
1	I	200	TYR

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 X-ray entries followed by that with respect to entries of similar resolution.

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	265/271 (98%)	249 (94%)	16 (6%)	16	33
1	C	265/271 (98%)	249 (94%)	16 (6%)	16	33
1	E	265/271 (98%)	249 (94%)	16 (6%)	16	33
1	G	265/271 (98%)	249 (94%)	16 (6%)	16	33
1	I	265/271 (98%)	249 (94%)	16 (6%)	16	33
1	K	265/271 (98%)	250 (94%)	15 (6%)	17	35
2	B	144/155 (93%)	135 (94%)	9 (6%)	15	30
2	D	144/155 (93%)	135 (94%)	9 (6%)	15	30
2	F	144/155 (93%)	135 (94%)	9 (6%)	15	30
2	H	144/155 (93%)	135 (94%)	9 (6%)	15	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	J	144/155 (93%)	134 (93%)	10 (7%)	13 26
2	L	144/155 (93%)	134 (93%)	10 (7%)	13 26
All	All	2454/2556 (96%)	2303 (94%)	151 (6%)	15 31

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	19	LEU
1	A	30	THR
1	A	32	THR
1	A	65	GLN
1	A	68	GLN
1	A	73	SER
1	A	122	THR
1	A	130	ARG
1	A	165	SER
1	A	188	SER
1	A	203	SER
1	A	227	MET
1	A	237	SER
1	A	256	MET
1	A	268	CYS
2	B	6	ILE
2	B	52	LEU
2	B	65	LEU
2	B	66	ILE
2	B	75	LYS
2	B	117	LYS
2	B	120	GLU
2	B	128	GLU
2	B	171	ILE
1	C	8	HIS
1	C	19	LEU
1	C	30	THR
1	C	32	THR
1	C	65	GLN
1	C	68	GLN
1	C	73	SER
1	C	122	THR
1	C	130	ARG

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Mol	Chain	Res	Type
1	C	165	SER
1	C	188	SER
1	C	203	SER
1	C	227	MET
1	C	237	SER
1	C	256	MET
1	C	268	CYS
2	D	6	ILE
2	D	52	LEU
2	D	65	LEU
2	D	66	ILE
2	D	75	LYS
2	D	117	LYS
2	D	120	GLU
2	D	128	GLU
2	D	171	ILE
1	E	8	HIS
1	E	19	LEU
1	E	30	THR
1	E	32	THR
1	E	65	GLN
1	E	68	GLN
1	E	73	SER
1	E	122	THR
1	E	130	ARG
1	E	165	SER
1	E	188	SER
1	E	203	SER
1	E	227	MET
1	E	237	SER
1	E	256	MET
1	E	268	CYS
2	F	6	ILE
2	F	52	LEU
2	F	65	LEU
2	F	66	ILE
2	F	75	LYS
2	F	117	LYS
2	F	120	GLU
2	F	128	GLU
2	F	171	ILE
1	G	8	HIS

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Mol	Chain	Res	Type
1	G	19	LEU
1	G	30	THR
1	G	32	THR
1	G	65	GLN
1	G	68	GLN
1	G	73	SER
1	G	122	THR
1	G	130	ARG
1	G	165	SER
1	G	188	SER
1	G	203	SER
1	G	227	MET
1	G	237	SER
1	G	256	MET
1	G	268	CYS
2	H	6	ILE
2	H	52	LEU
2	H	65	LEU
2	H	66	ILE
2	H	75	LYS
2	H	117	LYS
2	H	120	GLU
2	H	128	GLU
2	H	171	ILE
1	I	8	HIS
1	I	19	LEU
1	I	30	THR
1	I	32	THR
1	I	65	GLN
1	I	68	GLN
1	I	73	SER
1	I	122	THR
1	I	130	ARG
1	I	165	SER
1	I	188	SER
1	I	203	SER
1	I	227	MET
1	I	237	SER
1	I	256	MET
1	I	268	CYS
2	J	6	ILE
2	J	19	ASP

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Mol	Chain	Res	Type
2	J	52	LEU
2	J	65	LEU
2	J	66	ILE
2	J	75	LYS
2	J	117	LYS
2	J	120	GLU
2	J	128	GLU
2	J	171	ILE
1	K	8	HIS
1	K	19	LEU
1	K	32	THR
1	K	65	GLN
1	K	68	GLN
1	K	73	SER
1	K	122	THR
1	K	130	ARG
1	K	165	SER
1	K	188	SER
1	K	203	SER
1	K	227	MET
1	K	237	SER
1	K	256	MET
1	K	268	CYS
2	L	6	ILE
2	L	19	ASP
2	L	52	LEU
2	L	65	LEU
2	L	66	ILE
2	L	75	LYS
2	L	117	LYS
2	L	120	GLU
2	L	128	GLU
2	L	171	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	J	76	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

50 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	M	1	1,3	14,14,15	1.04	1 (7%)	17,19,21	2.61	1 (5%)
3	NAG	M	2	3	14,14,15	0.88	1 (7%)	17,19,21	1.30	2 (11%)
3	BMA	M	3	3	11,11,12	0.85	0	15,15,17	2.31	2 (13%)
3	FUC	M	4	3	10,10,11	1.00	0	14,14,16	1.57	2 (14%)
4	NAG	N	1	1,4	14,14,15	0.90	0	17,19,21	1.12	1 (5%)
4	NAG	N	2	4	14,14,15	0.50	0	17,19,21	1.16	1 (5%)
4	BMA	N	3	4	11,11,12	0.79	0	15,15,17	1.72	4 (26%)
5	GAL	O	1	5	12,12,12	0.90	1 (8%)	17,17,17	1.84	4 (23%)
5	NAG	O	2	5	14,14,15	0.60	0	17,19,21	1.55	3 (17%)
5	GAL	O	3	5	11,11,12	0.67	0	15,15,17	0.81	0
5	SIA	O	4	5	20,20,21	0.84	1 (5%)	21,28,31	1.57	4 (19%)
3	NAG	P	1	1,3	14,14,15	0.99	1 (7%)	17,19,21	2.50	5 (29%)
3	NAG	P	2	3	14,14,15	0.93	1 (7%)	17,19,21	1.43	1 (5%)
3	BMA	P	3	3	11,11,12	0.58	0	15,15,17	1.77	1 (6%)
3	FUC	P	4	3	10,10,11	0.68	0	14,14,16	1.56	4 (28%)
4	NAG	Q	1	1,4	14,14,15	0.75	0	17,19,21	1.67	3 (17%)
4	NAG	Q	2	4	14,14,15	0.48	0	17,19,21	1.11	2 (11%)
4	BMA	Q	3	4	11,11,12	0.65	0	15,15,17	1.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	R	1	6	14,14,15	0.60	0	17,19,21	5.80	3 (17%)
6	GAL	R	2	6	11,11,12	0.62	0	15,15,17	0.93	0
6	SIA	R	3	6	20,20,21	0.89	0	21,28,31	1.61	3 (14%)
3	NAG	S	1	1,3	14,14,15	0.97	1 (7%)	17,19,21	2.43	4 (23%)
3	NAG	S	2	3	14,14,15	0.81	0	17,19,21	1.21	1 (5%)
3	BMA	S	3	3	11,11,12	0.49	0	15,15,17	2.25	1 (6%)
3	FUC	S	4	3	10,10,11	0.91	0	14,14,16	1.77	5 (35%)
4	NAG	T	1	1,4	14,14,15	0.82	0	17,19,21	1.04	1 (5%)
4	NAG	T	2	4	14,14,15	0.58	0	17,19,21	1.44	2 (11%)
4	BMA	T	3	4	11,11,12	0.68	0	15,15,17	2.28	3 (20%)
7	NAG	U	1	7	13,13,15	1.11	1 (7%)	15,17,21	2.21	4 (26%)
7	SIA	U	2	7	20,20,21	1.09	1 (5%)	21,28,31	1.44	3 (14%)
4	NAG	V	1	1,4	14,14,15	0.58	0	17,19,21	1.13	1 (5%)
4	NAG	V	2	4	14,14,15	0.64	0	17,19,21	1.23	2 (11%)
4	BMA	V	3	4	11,11,12	0.70	0	15,15,17	1.29	2 (13%)
5	GAL	W	1	5	12,12,12	0.60	0	17,17,17	1.20	2 (11%)
5	NAG	W	2	5	14,14,15	0.54	0	17,19,21	2.79	5 (29%)
5	GAL	W	3	5	11,11,12	0.63	0	15,15,17	1.27	1 (6%)
5	SIA	W	4	5	20,20,21	0.87	1 (5%)	21,28,31	1.51	4 (19%)
4	NAG	X	1	1,4	14,14,15	0.65	0	17,19,21	1.01	1 (5%)
4	NAG	X	2	4	14,14,15	0.72	0	17,19,21	1.25	2 (11%)
4	BMA	X	3	4	11,11,12	0.61	0	15,15,17	1.44	2 (13%)
6	NAG	Y	1	6	14,14,15	0.63	0	17,19,21	4.94	8 (47%)
6	GAL	Y	2	6	11,11,12	0.73	0	15,15,17	1.19	2 (13%)
6	SIA	Y	3	6	20,20,21	0.90	1 (5%)	21,28,31	1.95	6 (28%)
4	NAG	Z	1	1,4	14,14,15	0.60	0	17,19,21	0.95	0
4	NAG	Z	2	4	14,14,15	0.72	0	17,19,21	1.52	4 (23%)
4	BMA	Z	3	4	11,11,12	0.70	0	15,15,17	1.34	2 (13%)
5	GAL	a	1	5	12,12,12	0.79	0	17,17,17	1.70	4 (23%)
5	NAG	a	2	5	14,14,15	0.64	0	17,19,21	4.35	4 (23%)
5	GAL	a	3	5	11,11,12	0.70	0	15,15,17	1.23	2 (13%)
5	SIA	a	4	5	20,20,21	0.84	2 (10%)	21,28,31	1.27	2 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	M	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
3	BMA	M	3	3	-	2/2/19/22	0/1/1/1
3	FUC	M	4	3	1/1/4/5	-	0/1/1/1
4	NAG	N	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	0/6/23/26	0/1/1/1
4	BMA	N	3	4	-	2/2/19/22	0/1/1/1
5	GAL	O	1	5	-	2/2/22/22	0/1/1/1
5	NAG	O	2	5	-	2/6/23/26	0/1/1/1
5	GAL	O	3	5	-	2/2/19/22	0/1/1/1
5	SIA	O	4	5	-	3/18/34/38	0/1/1/1
3	NAG	P	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1
3	BMA	P	3	3	-	2/2/19/22	0/1/1/1
3	FUC	P	4	3	-	-	0/1/1/1
4	NAG	Q	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	0/6/23/26	0/1/1/1
4	BMA	Q	3	4	-	2/2/19/22	0/1/1/1
6	NAG	R	1	6	-	2/6/23/26	0/1/1/1
6	GAL	R	2	6	-	2/2/19/22	0/1/1/1
6	SIA	R	3	6	-	2/18/34/38	0/1/1/1
3	NAG	S	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	S	2	3	-	0/6/23/26	0/1/1/1
3	BMA	S	3	3	-	2/2/19/22	0/1/1/1
3	FUC	S	4	3	1/1/4/5	-	0/1/1/1
4	NAG	T	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	T	2	4	-	0/6/23/26	0/1/1/1
4	BMA	T	3	4	-	0/2/19/22	0/1/1/1
7	NAG	U	1	7	-	0/6/19/26	0/1/1/1
7	SIA	U	2	7	-	2/18/34/38	0/1/1/1
4	NAG	V	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	V	2	4	-	0/6/23/26	0/1/1/1
4	BMA	V	3	4	-	2/2/19/22	0/1/1/1
5	GAL	W	1	5	-	1/2/22/22	0/1/1/1
5	NAG	W	2	5	-	2/6/23/26	0/1/1/1
5	GAL	W	3	5	-	2/2/19/22	0/1/1/1
5	SIA	W	4	5	-	2/18/34/38	0/1/1/1
4	NAG	X	1	1,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	X	2	4	-	0/6/23/26	0/1/1/1
4	BMA	X	3	4	-	0/2/19/22	0/1/1/1
6	NAG	Y	1	6	-	2/6/23/26	0/1/1/1
6	GAL	Y	2	6	-	2/2/19/22	0/1/1/1
6	SIA	Y	3	6	-	2/18/34/38	0/1/1/1
4	NAG	Z	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	0/6/23/26	0/1/1/1
4	BMA	Z	3	4	-	1/2/19/22	0/1/1/1
5	GAL	a	1	5	-	1/2/22/22	0/1/1/1
5	NAG	a	2	5	-	4/6/23/26	0/1/1/1
5	GAL	a	3	5	-	2/2/19/22	0/1/1/1
5	SIA	a	4	5	-	5/18/34/38	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	U	1	NAG	C1-C2	3.29	1.55	1.51
7	U	2	SIA	C2-C1	3.22	1.56	1.52
3	M	1	NAG	C1-C2	2.91	1.56	1.52
3	S	1	NAG	C1-C2	2.59	1.55	1.52
3	P	1	NAG	C1-C2	2.52	1.55	1.52
3	P	2	NAG	C1-C2	2.33	1.55	1.52
6	Y	3	SIA	C2-C1	2.32	1.55	1.52
5	a	4	SIA	O1A-C1	2.24	1.28	1.22
5	O	4	SIA	C2-C1	2.22	1.55	1.52
3	M	2	NAG	C1-C2	2.21	1.55	1.52
5	O	1	GAL	C4-C5	2.07	1.57	1.53
5	a	4	SIA	C2-C1	2.02	1.54	1.52
5	W	4	SIA	C2-C1	2.01	1.54	1.52

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	R	1	NAG	O3-C3-C2	21.86	154.81	109.40
5	a	2	NAG	O3-C3-C2	16.71	144.10	109.40
6	Y	1	NAG	O3-C3-C2	16.28	143.22	109.40
3	M	1	NAG	C1-O5-C5	9.83	125.36	112.19
6	Y	1	NAG	O3-C3-C4	-9.40	88.21	110.38
3	P	1	NAG	C1-O5-C5	8.74	123.89	112.19
3	S	1	NAG	C1-O5-C5	8.70	123.84	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	S	3	BMA	C1-O5-C5	8.10	123.04	112.19
6	R	1	NAG	O3-C3-C4	-8.06	91.38	110.38
5	W	2	NAG	O3-C3-C4	7.35	127.71	110.38
4	T	3	BMA	C1-O5-C5	7.33	122.01	112.19
3	M	3	BMA	C1-O5-C5	6.47	120.85	112.19
5	W	2	NAG	O3-C3-C2	6.02	121.91	109.40
3	P	3	BMA	C1-O5-C5	5.96	120.17	112.19
7	U	1	NAG	C3-C2-C1	5.14	114.23	109.50
4	Q	1	NAG	C1-O5-C5	5.05	118.95	112.19
5	a	2	NAG	O3-C3-C4	-4.91	98.81	110.38
7	U	1	NAG	C4-C3-C2	-4.71	106.70	112.50
5	W	2	NAG	C1-O5-C5	4.65	118.42	112.19
5	O	1	GAL	O3-C3-C4	4.64	121.31	110.38
3	M	3	BMA	C1-C2-C3	4.50	116.20	109.64
5	a	1	GAL	O5-C5-C4	4.45	117.72	109.70
5	O	2	NAG	O3-C3-C2	4.41	118.56	109.40
6	Y	3	SIA	O6-C2-C3	-4.35	104.71	110.56
3	P	2	NAG	C4-C3-C2	4.29	117.30	111.02
6	Y	3	SIA	O6-C2-C1	4.15	115.56	107.72
6	R	3	SIA	C6-C5-N5	-4.15	104.29	110.91
4	N	3	BMA	O5-C5-C6	4.11	115.65	107.66
4	X	3	BMA	C1-O5-C5	3.99	117.53	112.19
5	W	4	SIA	O6-C2-C1	3.98	115.23	107.72
6	R	3	SIA	O6-C2-C1	3.75	114.80	107.72
5	a	4	SIA	O6-C2-C1	3.74	114.78	107.72
5	O	4	SIA	O6-C2-C1	3.73	114.76	107.72
6	Y	1	NAG	C4-C3-C2	-3.71	105.58	111.02
3	S	2	NAG	C4-C3-C2	3.65	116.37	111.02
6	Y	1	NAG	O5-C1-C2	-3.54	105.81	111.29
3	M	4	FUC	C3-C4-C5	3.52	115.17	109.81
3	P	4	FUC	C1-O5-C5	3.50	121.22	112.97
5	O	1	GAL	O5-C5-C4	3.48	115.97	109.70
6	Y	3	SIA	O1B-C1-C2	3.42	121.61	112.71
4	T	2	NAG	O4-C4-C5	3.34	117.54	109.32
7	U	2	SIA	O6-C2-C1	3.22	113.80	107.72
3	S	4	FUC	C3-C4-C5	3.21	114.69	109.81
4	Z	3	BMA	C3-C4-C5	3.21	116.05	110.23
6	R	3	SIA	C4-C5-N5	3.17	116.69	110.44
4	V	3	BMA	C3-C4-C5	3.10	115.86	110.23
6	Y	3	SIA	O1A-C1-C2	-3.08	116.20	122.85
5	O	4	SIA	C6-C5-N5	-3.07	106.00	110.91
7	U	1	NAG	O5-C5-C6	3.06	113.62	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	W	1	GAL	C1-O5-C5	3.05	119.56	113.65
5	a	3	GAL	O5-C1-C2	-3.00	103.62	110.79
5	a	1	GAL	C1-O5-C5	2.99	119.44	113.65
5	O	4	SIA	O1B-C1-C2	2.97	120.44	112.71
6	R	1	NAG	O5-C5-C6	2.89	113.30	107.66
4	Q	1	NAG	C3-C4-C5	2.86	115.42	110.23
3	M	2	NAG	C4-C3-C2	2.86	115.21	111.02
4	V	2	NAG	O5-C1-C2	-2.83	106.92	111.29
3	S	4	FUC	O5-C1-C2	2.82	117.52	110.79
4	Z	2	NAG	C1-C2-N2	2.79	114.83	110.43
4	T	3	BMA	O5-C5-C4	2.78	117.58	110.83
4	N	3	BMA	C1-O5-C5	-2.76	108.49	112.19
5	W	4	SIA	C6-C5-N5	-2.73	106.55	110.91
6	Y	3	SIA	C6-C5-N5	-2.69	106.62	110.91
5	a	1	GAL	C3-C4-C5	2.69	115.11	110.23
6	Y	2	GAL	C1-O5-C5	2.67	115.77	112.19
6	Y	1	NAG	O5-C5-C4	2.65	117.29	110.83
5	W	3	GAL	O5-C5-C6	2.64	112.81	107.66
4	T	3	BMA	C3-C4-C5	2.63	115.00	110.23
5	O	1	GAL	O5-C1-C2	-2.58	105.76	110.30
4	Q	1	NAG	O5-C5-C6	-2.50	102.80	107.66
4	Z	2	NAG	C2-N2-C7	2.50	126.25	122.90
5	O	2	NAG	O3-C3-C4	2.49	116.24	110.38
5	a	2	NAG	C4-C3-C2	-2.47	107.40	111.02
6	Y	1	NAG	C1-O5-C5	2.47	115.50	112.19
3	S	4	FUC	C6-C5-C4	2.47	117.60	113.08
3	M	2	NAG	C1-O5-C5	2.45	115.47	112.19
3	P	4	FUC	C1-C2-C3	2.45	113.21	109.64
5	W	4	SIA	O6-C2-C3	-2.45	107.26	110.56
5	a	3	GAL	C3-C4-C5	2.43	114.64	110.23
5	a	2	NAG	O5-C5-C6	2.41	112.36	107.66
4	X	1	NAG	C1-C2-N2	-2.40	106.65	110.43
3	P	1	NAG	O5-C1-C2	-2.40	107.58	111.29
4	N	1	NAG	C4-C3-C2	2.39	114.52	111.02
6	Y	1	NAG	C3-C4-C5	2.37	114.54	110.23
7	U	2	SIA	O1B-C1-C2	2.36	118.85	112.71
4	Q	2	NAG	O4-C4-C5	2.34	115.10	109.32
5	O	2	NAG	O5-C5-C6	2.32	112.19	107.66
5	W	2	NAG	C1-C2-N2	2.32	114.09	110.43
3	P	4	FUC	O5-C5-C6	2.31	112.42	107.40
4	Z	3	BMA	C2-C3-C4	2.31	114.92	110.86
4	V	2	NAG	C1-C2-N2	2.30	114.06	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	X	2	NAG	C1-C2-N2	2.30	114.06	110.43
4	X	2	NAG	O5-C1-C2	-2.30	107.74	111.29
4	V	3	BMA	C2-C3-C4	2.27	114.85	110.86
6	Y	2	GAL	O5-C1-C2	-2.26	105.39	110.79
3	P	1	NAG	O3-C3-C2	2.26	114.09	109.40
3	S	1	NAG	O3-C3-C2	2.26	114.09	109.40
4	V	1	NAG	O3-C3-C2	-2.25	104.72	109.40
6	Y	1	NAG	C6-C5-C4	-2.25	107.50	113.02
4	Z	2	NAG	C1-O5-C5	2.25	115.20	112.19
5	a	1	GAL	O4-C4-C5	2.25	114.86	109.32
5	W	1	GAL	O5-C5-C4	2.24	113.74	109.70
6	Y	3	SIA	C11-C10-N5	2.23	119.82	116.12
4	X	3	BMA	C3-C4-C5	2.23	114.27	110.23
5	O	1	GAL	C3-C4-C5	2.22	114.26	110.23
3	S	4	FUC	O4-C4-C5	2.22	114.63	109.74
7	U	2	SIA	C6-C5-N5	-2.21	107.38	110.91
4	T	2	NAG	C6-C5-C4	2.20	118.42	113.02
4	N	3	BMA	C1-C2-C3	-2.20	106.45	109.64
5	W	4	SIA	O1B-C1-C2	2.17	118.35	112.71
5	O	4	SIA	O1A-C1-C2	-2.17	118.17	122.85
3	P	4	FUC	C3-C4-C5	2.17	113.11	109.81
4	Z	2	NAG	O4-C4-C3	2.16	115.46	110.38
5	a	4	SIA	O6-C2-C3	-2.15	107.66	110.56
7	U	1	NAG	O7-C7-C8	-2.15	118.23	122.05
4	T	1	NAG	C1-O5-C5	-2.12	109.34	112.19
5	W	2	NAG	C4-C3-C2	-2.11	107.92	111.02
3	S	1	NAG	O4-C4-C5	2.08	114.44	109.32
3	P	1	NAG	O7-C7-C8	-2.07	118.37	122.05
3	S	1	NAG	C4-C3-C2	-2.07	107.99	111.02
3	S	4	FUC	C1-O5-C5	2.03	117.75	112.97
4	Q	2	NAG	C2-N2-C7	2.03	125.62	122.90
4	N	3	BMA	O2-C2-C3	2.01	114.31	110.15
3	P	1	NAG	O4-C4-C5	2.01	114.27	109.32
3	M	4	FUC	O5-C1-C2	2.01	115.58	110.79
4	N	2	NAG	O7-C7-C8	-2.00	118.49	122.05

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	M	4	FUC	C1
3	S	4	FUC	C1

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	R	3	SIA	O10-C10-N5-C5
6	R	1	NAG	C4-C5-C6-O6
3	M	3	BMA	C4-C5-C6-O6
3	M	3	BMA	O5-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
6	R	1	NAG	O5-C5-C6-O6
6	R	2	GAL	O5-C5-C6-O6
6	Y	2	GAL	O5-C5-C6-O6
6	R	3	SIA	C11-C10-N5-C5
4	N	3	BMA	O5-C5-C6-O6
5	W	3	GAL	O5-C5-C6-O6
5	O	2	NAG	C4-C5-C6-O6
4	Q	1	NAG	C4-C5-C6-O6
5	O	1	GAL	O5-C5-C6-O6
5	a	3	GAL	O5-C5-C6-O6
4	N	3	BMA	C4-C5-C6-O6
6	Y	2	GAL	C4-C5-C6-O6
5	a	2	NAG	C4-C5-C6-O6
6	R	2	GAL	C4-C5-C6-O6
5	O	4	SIA	O10-C10-N5-C5
5	O	1	GAL	C4-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
5	a	2	NAG	O5-C5-C6-O6
5	O	4	SIA	C11-C10-N5-C5
5	W	4	SIA	C11-C10-N5-C5
5	W	4	SIA	O10-C10-N5-C5
5	a	4	SIA	C11-C10-N5-C5
5	a	4	SIA	O10-C10-N5-C5
6	Y	3	SIA	C11-C10-N5-C5
6	Y	3	SIA	O10-C10-N5-C5
7	U	2	SIA	C11-C10-N5-C5
7	U	2	SIA	O10-C10-N5-C5
3	S	3	BMA	C4-C5-C6-O6
5	O	3	GAL	C4-C5-C6-O6
3	P	3	BMA	C4-C5-C6-O6
6	Y	1	NAG	O5-C5-C6-O6
5	W	2	NAG	C4-C5-C6-O6
5	W	3	GAL	C4-C5-C6-O6
5	a	3	GAL	C4-C5-C6-O6
4	Q	3	BMA	C4-C5-C6-O6
5	W	2	NAG	O5-C5-C6-O6
4	Q	3	BMA	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	a	1	GAL	O5-C5-C6-O6
4	V	3	BMA	C4-C5-C6-O6
5	O	3	GAL	O5-C5-C6-O6
4	Z	1	NAG	C4-C5-C6-O6
4	Z	3	BMA	O5-C5-C6-O6
3	S	3	BMA	O5-C5-C6-O6
4	Z	1	NAG	O5-C5-C6-O6
5	W	1	GAL	O5-C5-C6-O6
3	P	3	BMA	O5-C5-C6-O6
6	Y	1	NAG	C4-C5-C6-O6
5	a	4	SIA	C6-C7-C8-O8
4	V	3	BMA	O5-C5-C6-O6
5	a	2	NAG	C3-C2-N2-C7
5	O	4	SIA	C6-C7-C8-O8
5	a	2	NAG	C1-C2-N2-C7
5	a	4	SIA	O7-C7-C8-C9
5	a	4	SIA	O7-C7-C8-O8
3	M	1	NAG	C4-C5-C6-O6

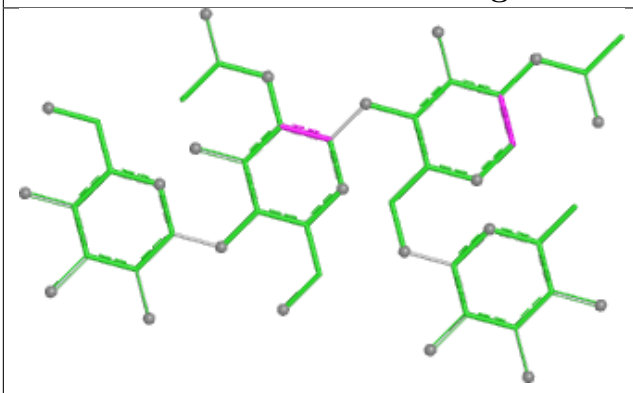
There are no ring outliers.

4 monomers are involved in 5 short contacts:

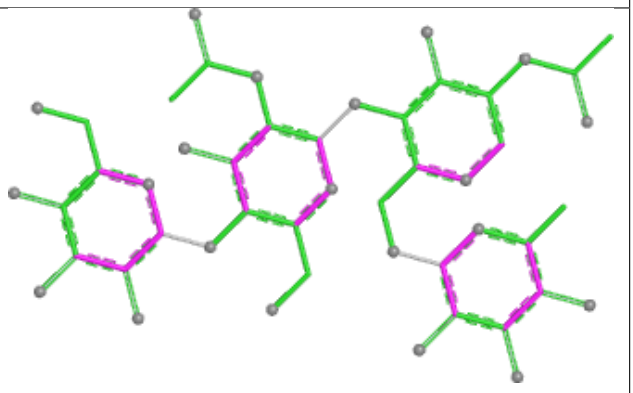
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	1	NAG	1	0
3	P	1	NAG	1	0
3	S	1	NAG	1	0
6	Y	3	SIA	2	0

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

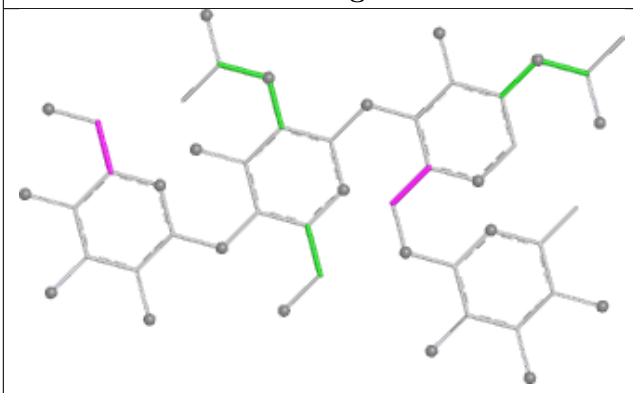
Oligosaccharide Chain M



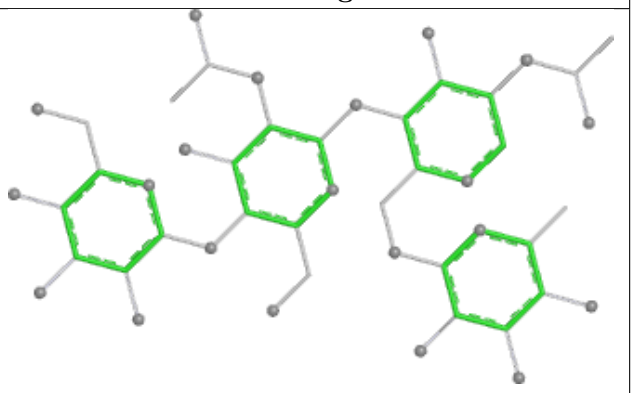
Bond lengths



Bond angles

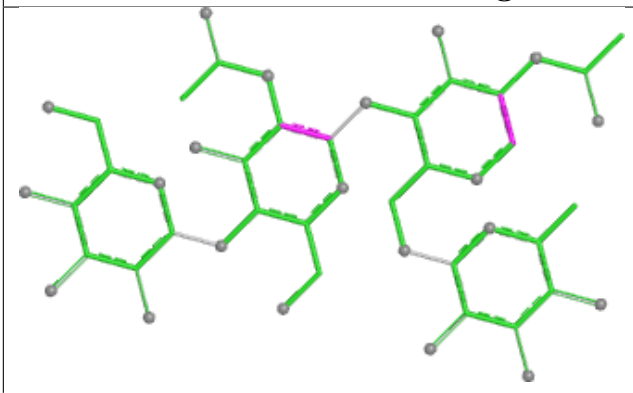


Torsions

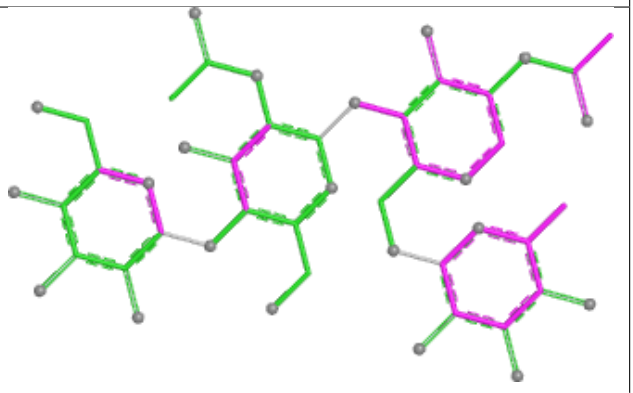


Rings

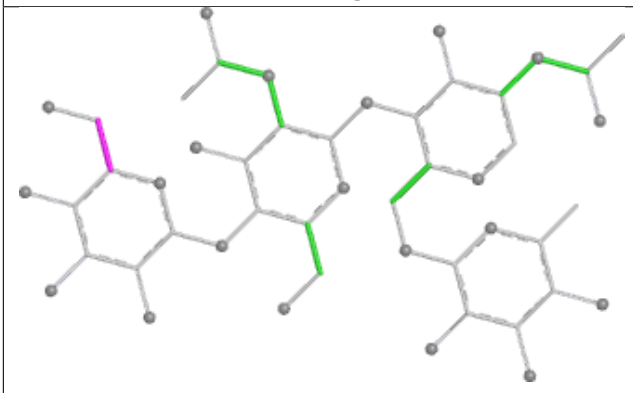
Oligosaccharide Chain P



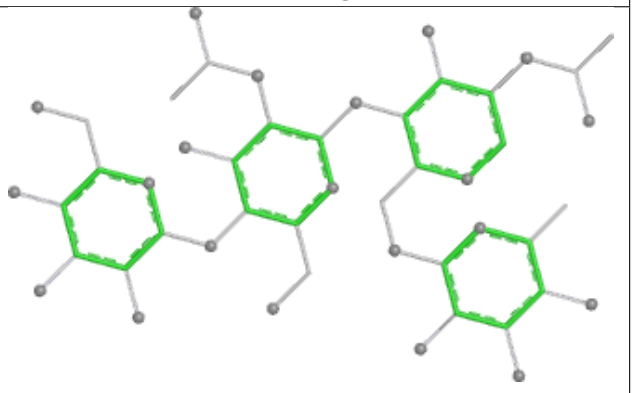
Bond lengths



Bond angles

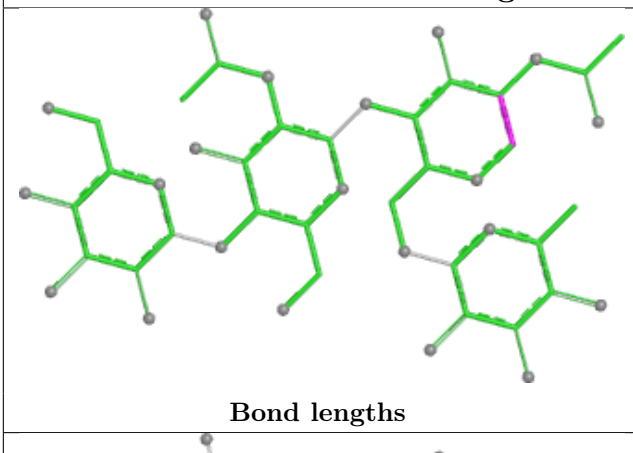


Torsions

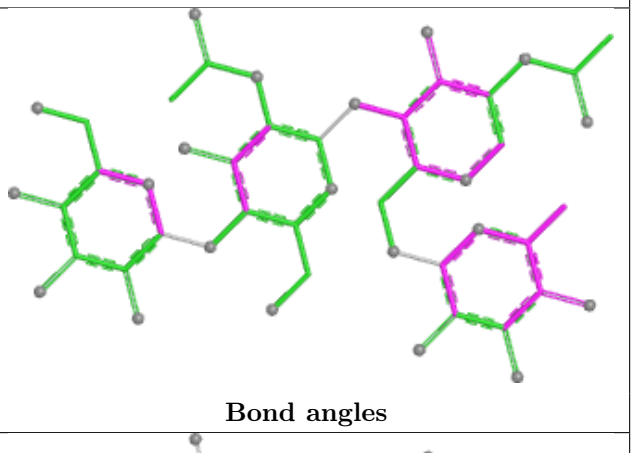


Rings

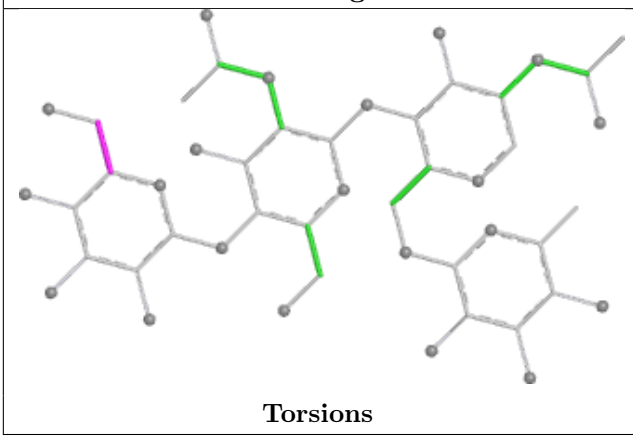
Oligosaccharide Chain S



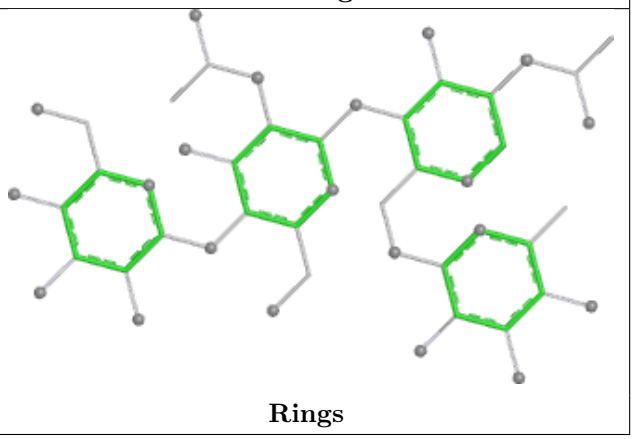
Bond lengths



Bond angles

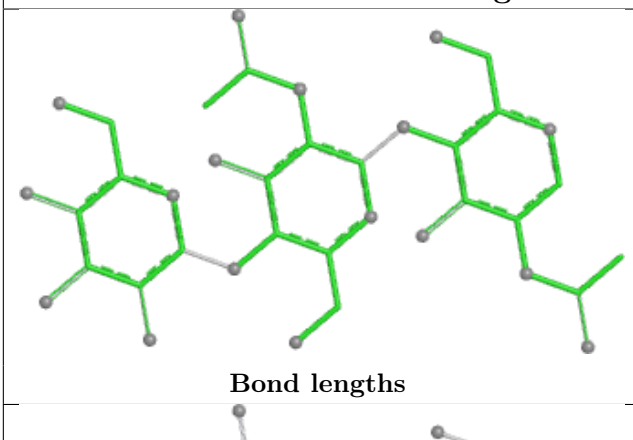


Torsions

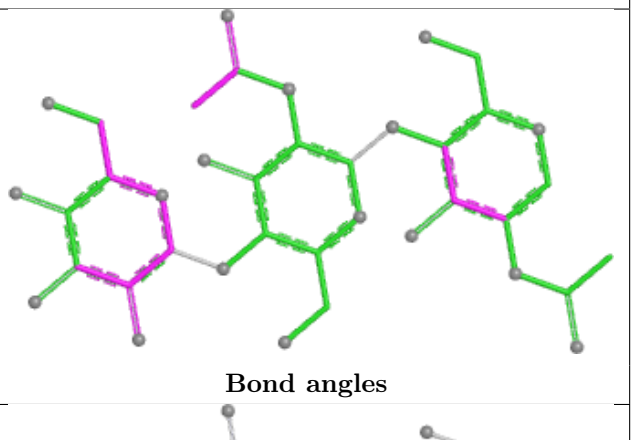


Rings

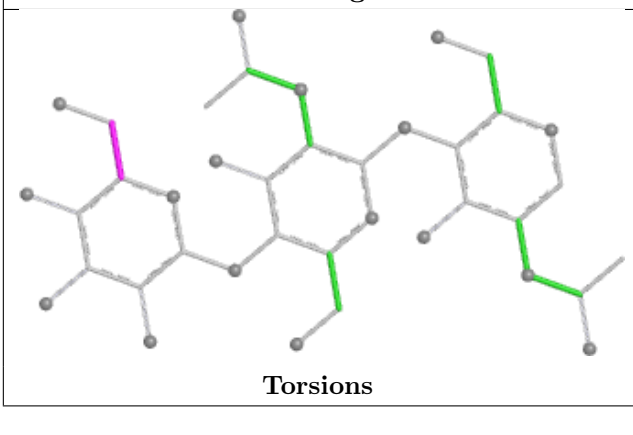
Oligosaccharide Chain N



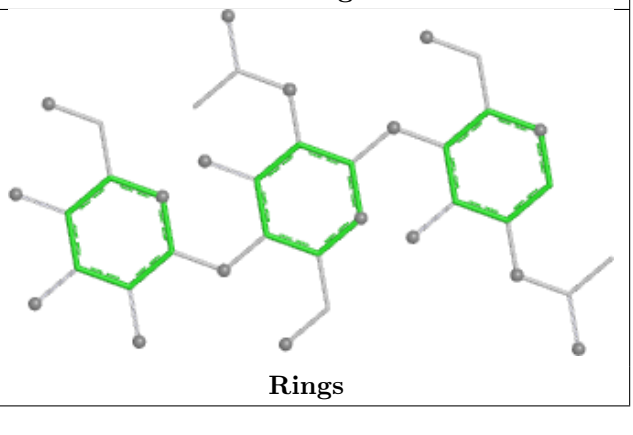
Bond lengths



Bond angles

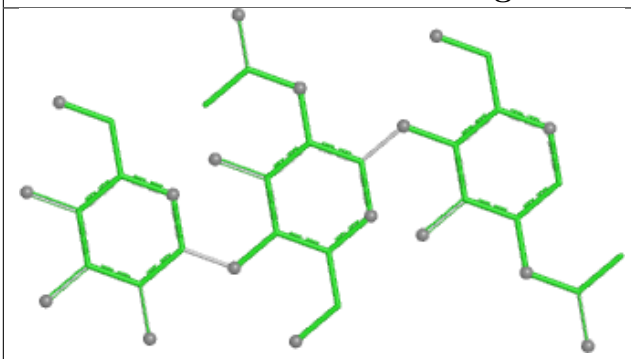


Torsions

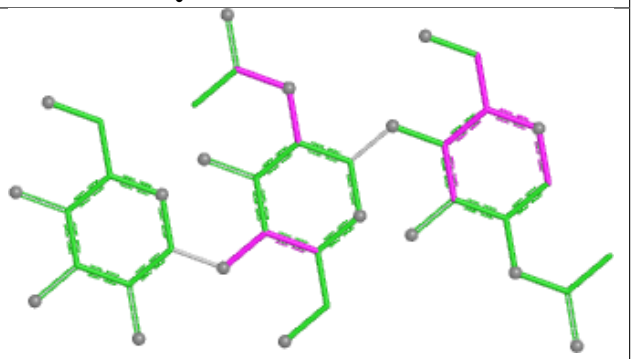


Rings

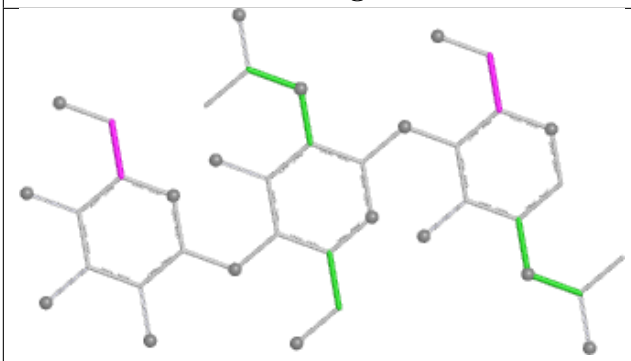
Oligosaccharide Chain Q



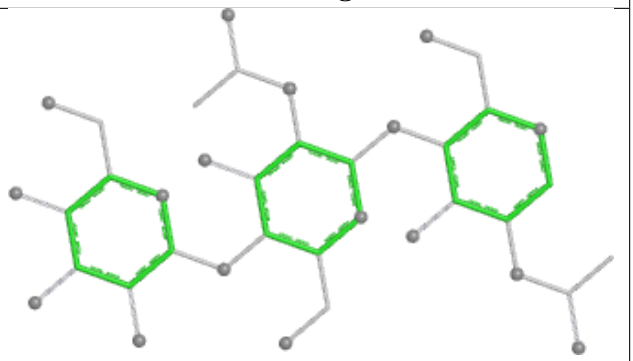
Bond lengths



Bond angles

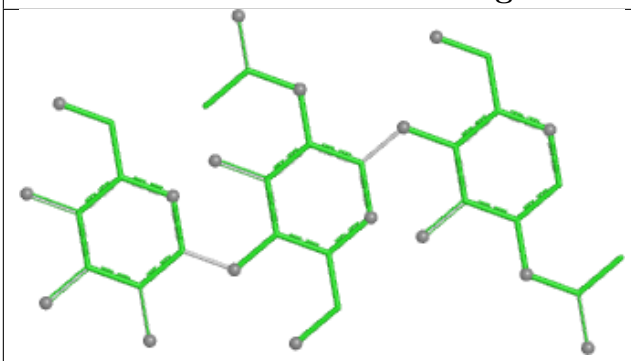


Torsions

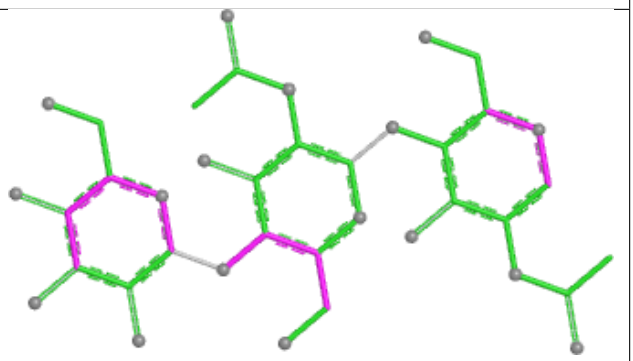


Rings

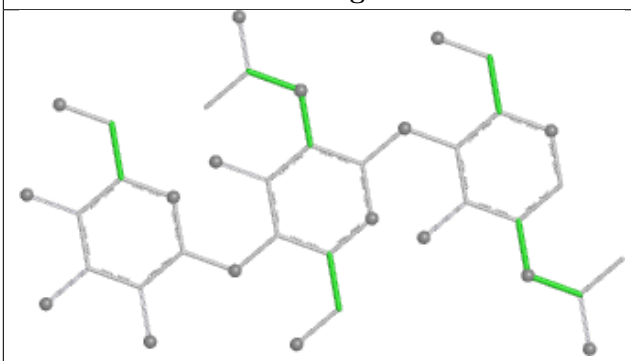
Oligosaccharide Chain T



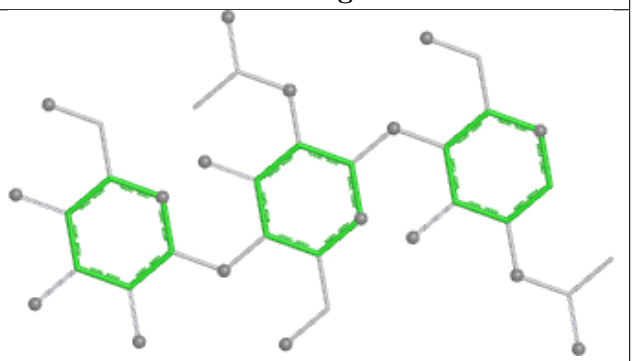
Bond lengths



Bond angles

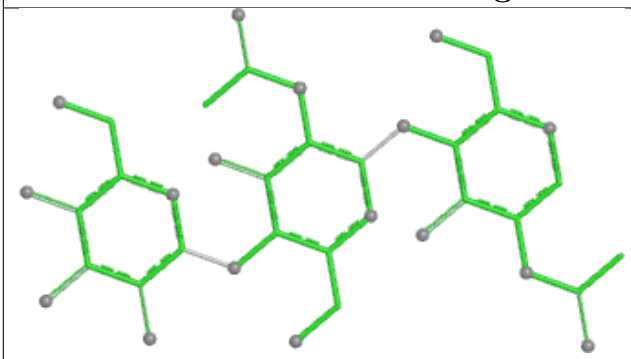


Torsions

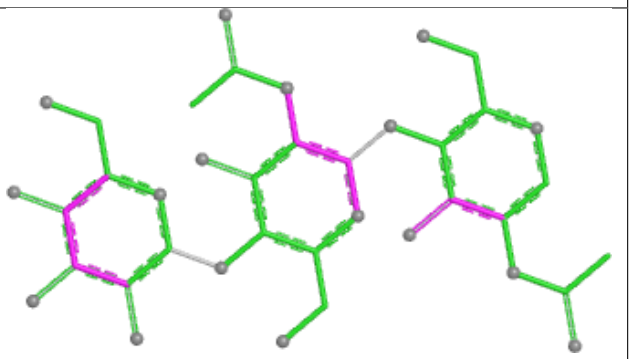


Rings

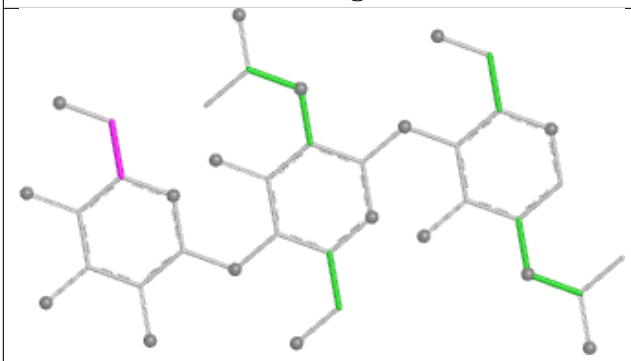
Oligosaccharide Chain V



Bond lengths



Bond angles



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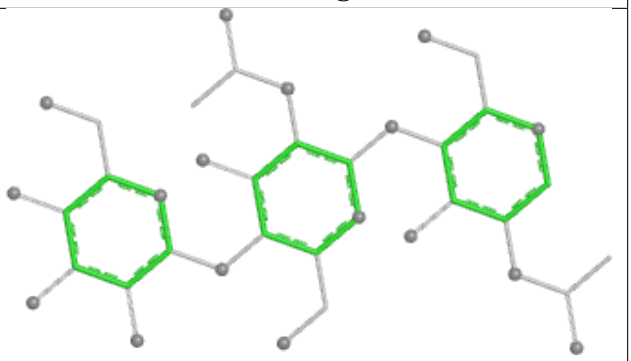
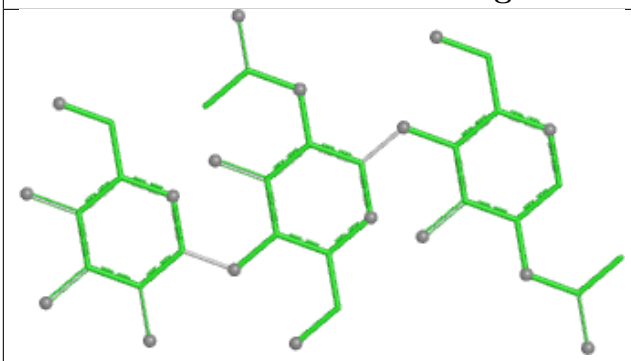
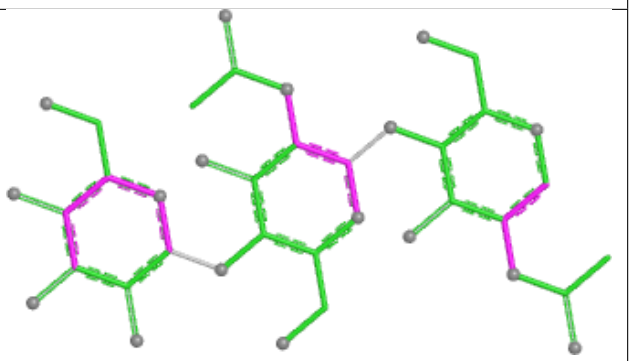


Rings

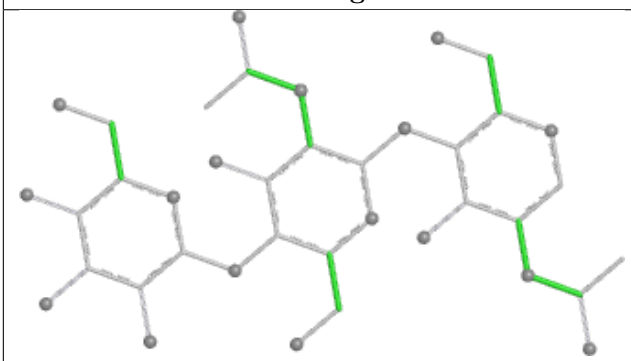
Oligosaccharide Chain X



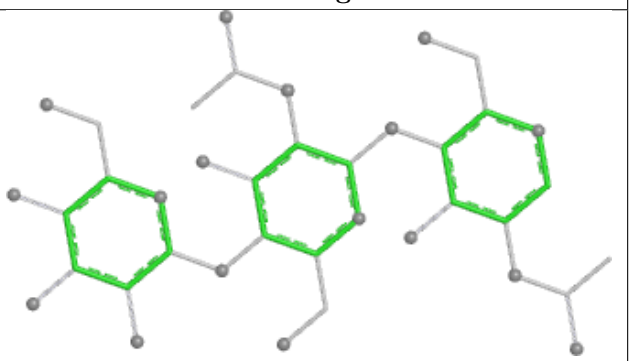
Bond lengths



Bond angles

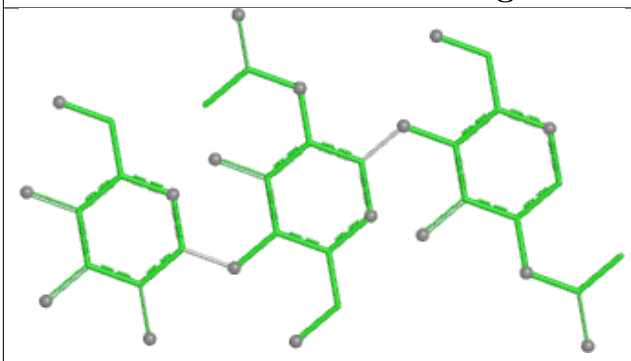


Torsions

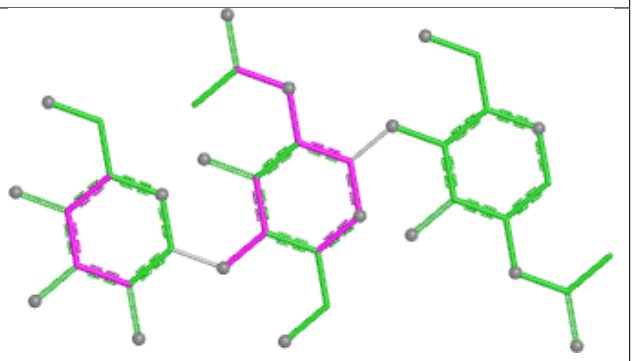


Rings

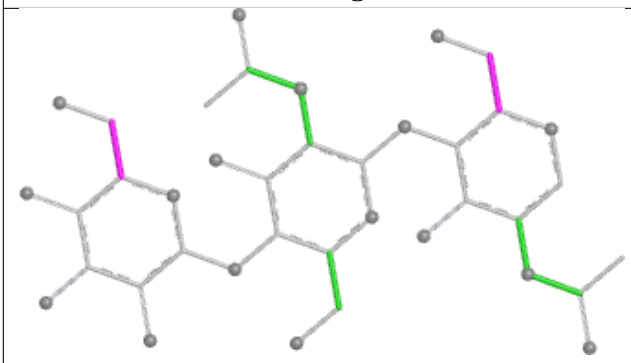
Oligosaccharide Chain Z



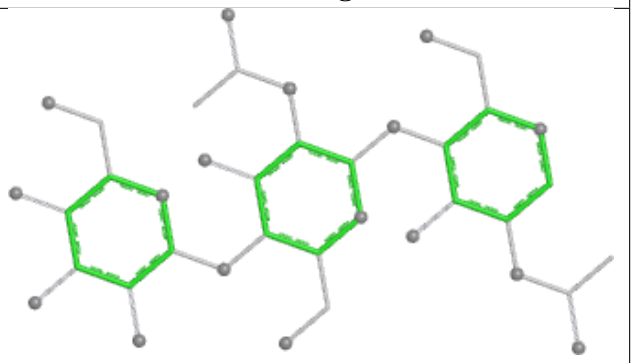
Bond lengths



Bond angles

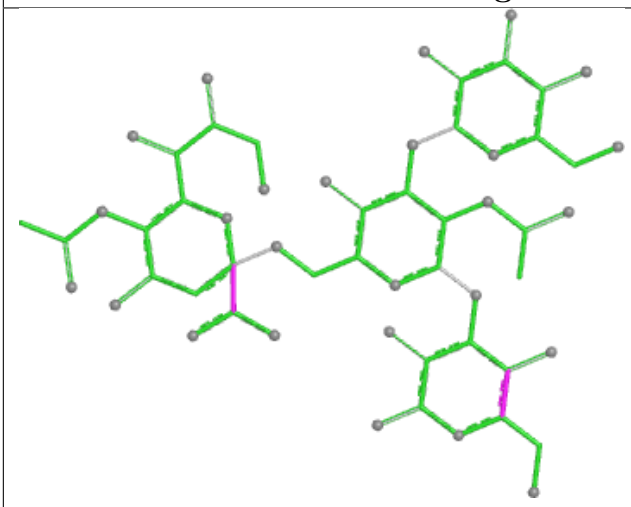


Torsions

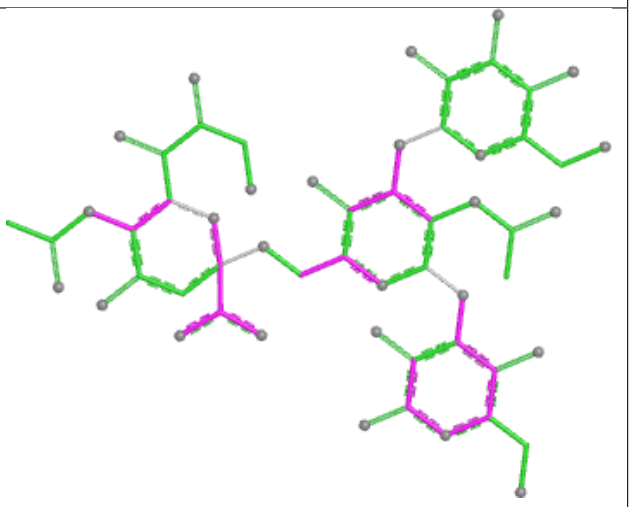


Rings

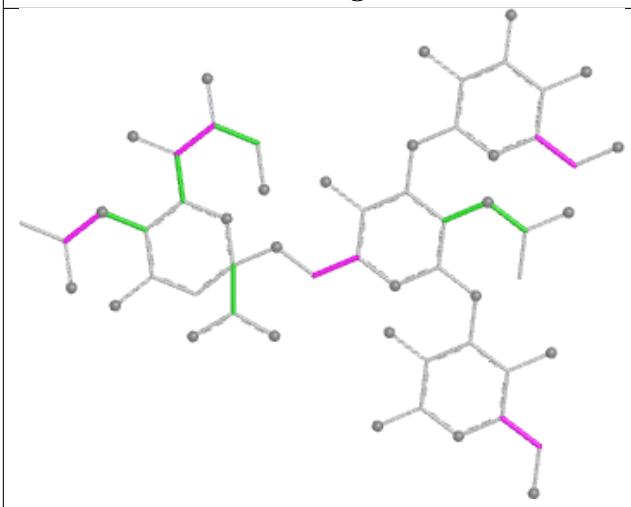
Oligosaccharide Chain O



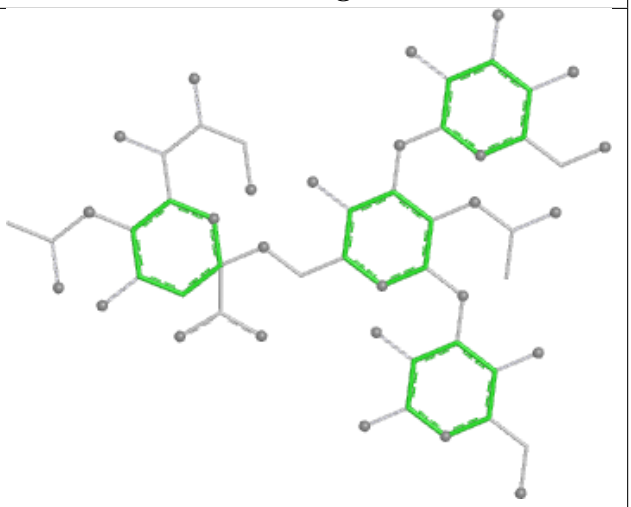
Bond lengths



Bond angles

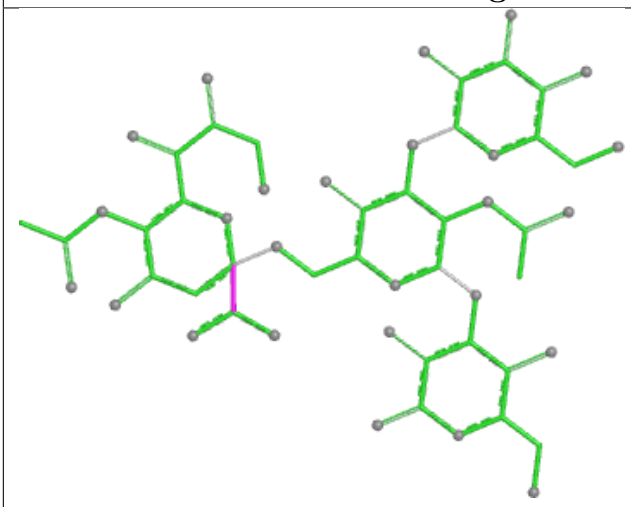


Torsions

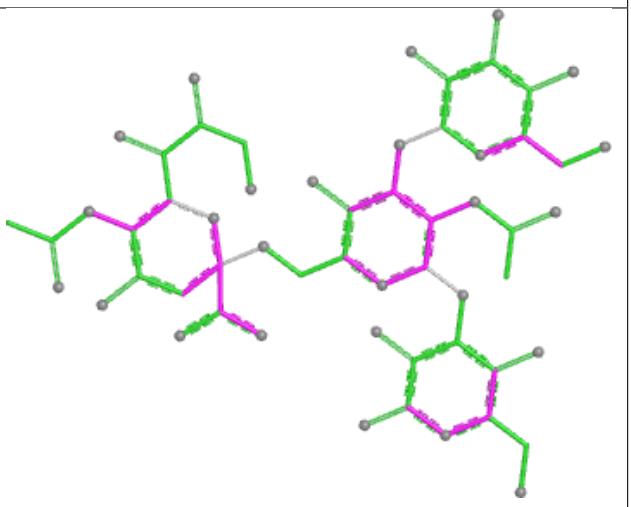


Rings

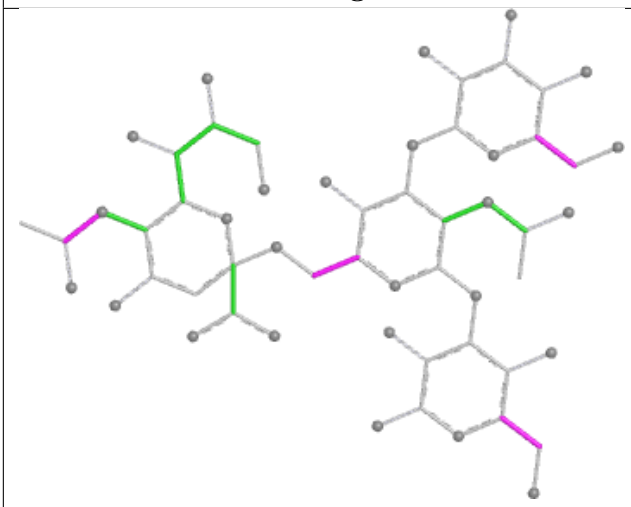
Oligosaccharide Chain W



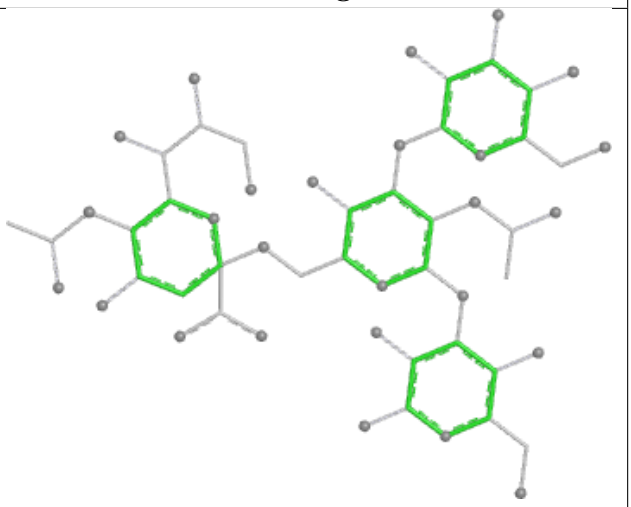
Bond lengths



Bond angles

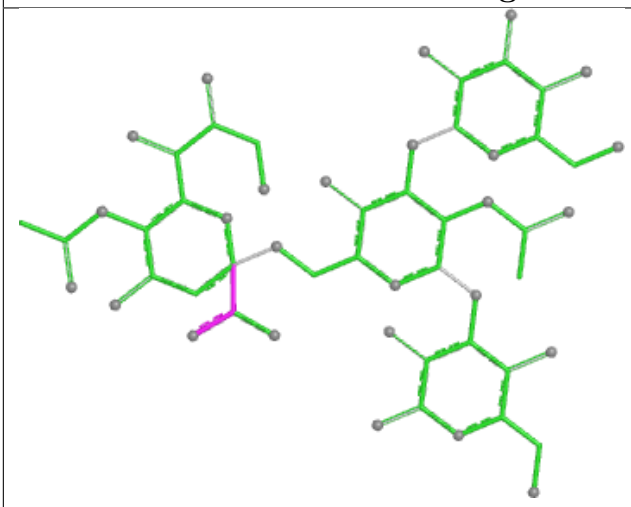


Torsions

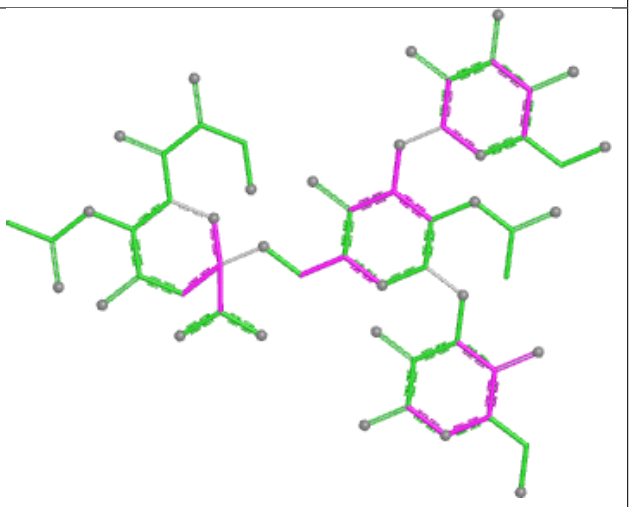


Rings

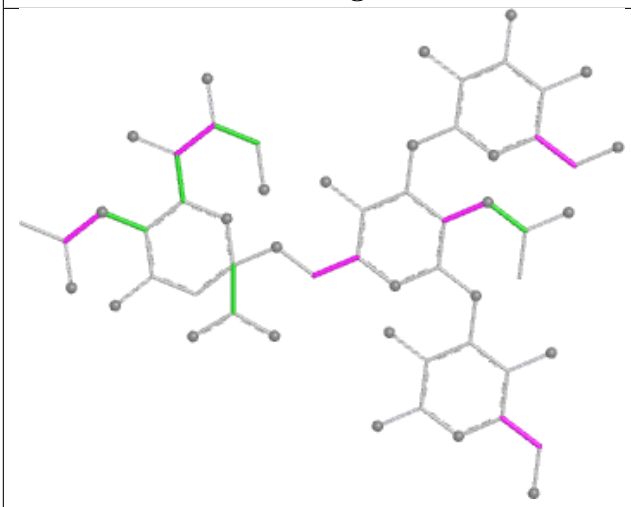
Oligosaccharide Chain a



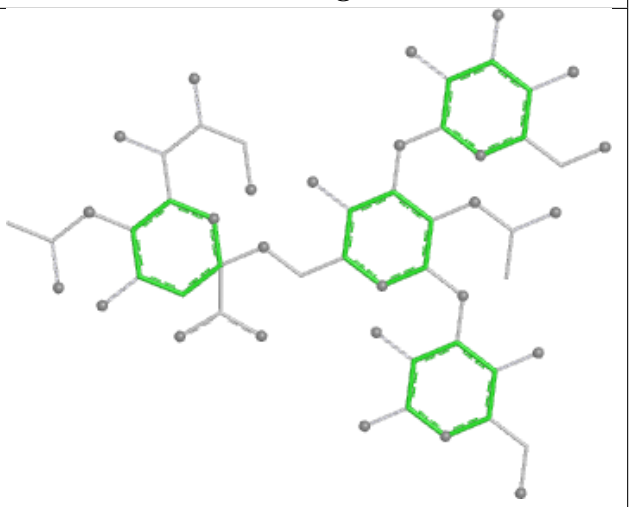
Bond lengths



Bond angles

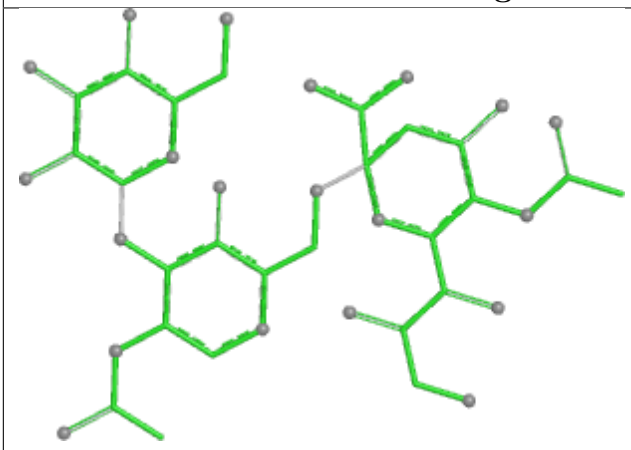


Torsions

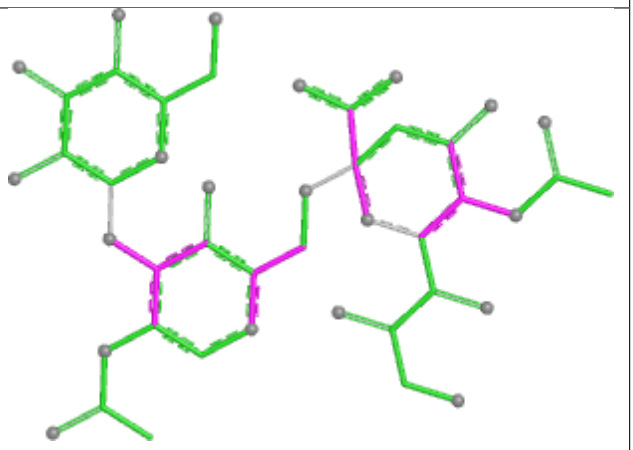


Rings

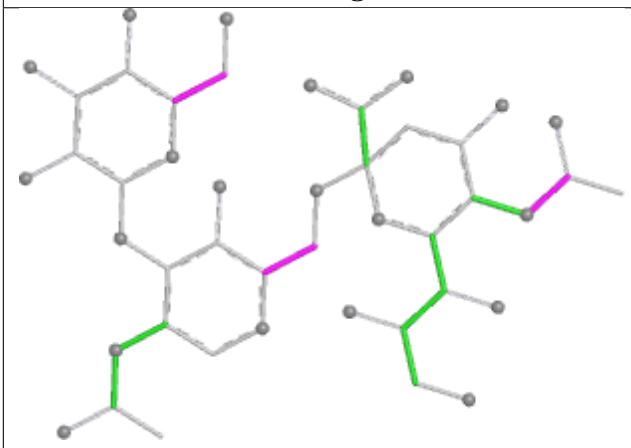
Oligosaccharide Chain R



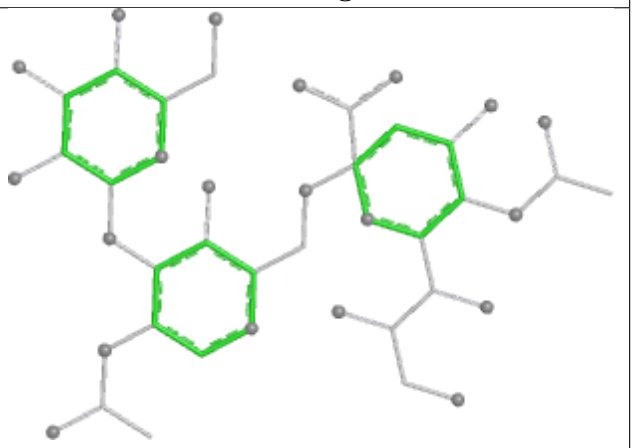
Bond lengths



Bond angles

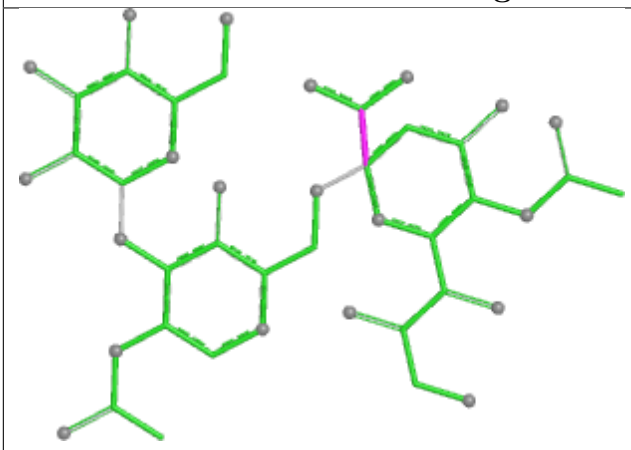


Torsions

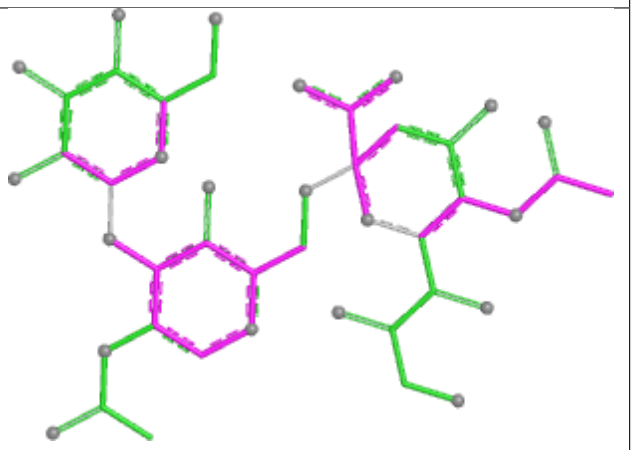


Rings

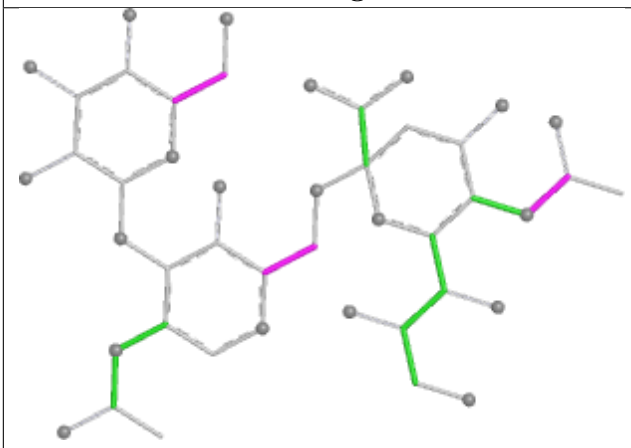
Oligosaccharide Chain Y



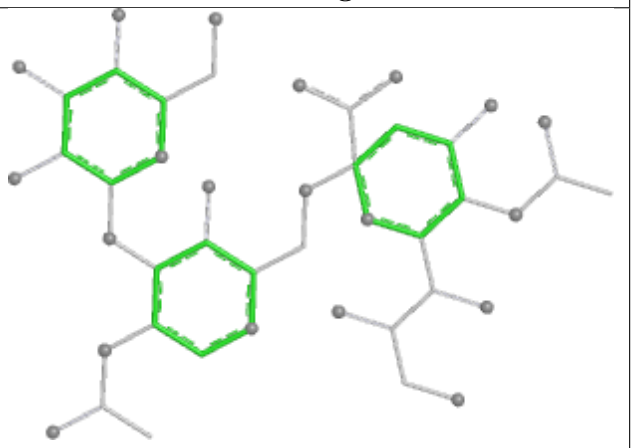
Bond lengths



Bond angles

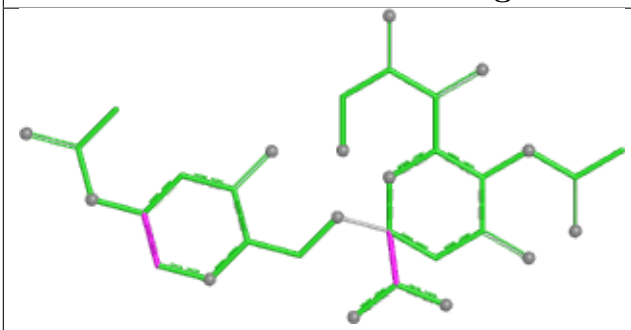


Torsions

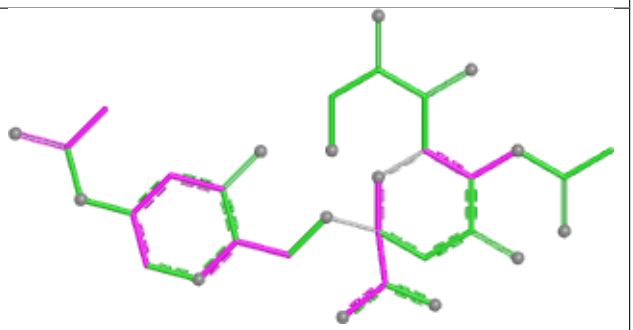


Rings

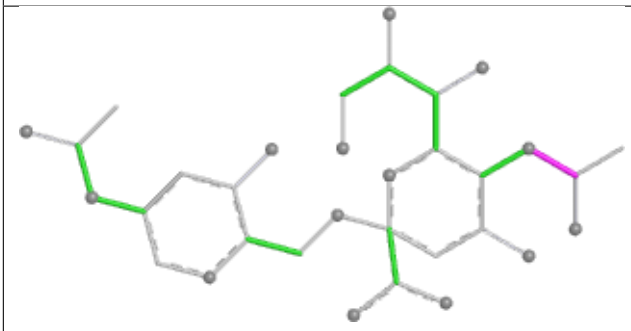
Oligosaccharide Chain U



Bond lengths



Bond angles



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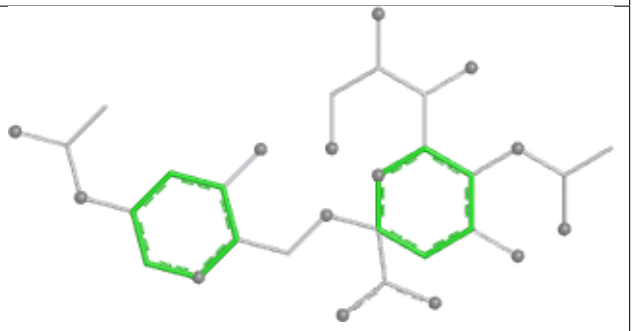

Rings

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	NAG	D	500	2	14,14,15	0.89	1 (7%)	17,19,21	2.08	4 (23%)
9	NAG	B	500	2	14,14,15	1.00	1 (7%)	17,19,21	1.73	4 (23%)
9	NAG	H	500	2	14,14,15	1.13	2 (14%)	17,19,21	2.43	7 (41%)
9	NAG	J	500	2	14,14,15	1.27	2 (14%)	17,19,21	2.61	9 (52%)
9	NAG	L	500	2	14,14,15	1.25	2 (14%)	17,19,21	3.02	5 (29%)
9	NAG	F	500	2	14,14,15	1.00	1 (7%)	17,19,21	2.58	7 (41%)

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
9	NAG	D	500	2	-	0/6/23/26	0/1/1/1
9	NAG	B	500	2	-	1/6/23/26	0/1/1/1
9	NAG	H	500	2	-	0/6/23/26	0/1/1/1
9	NAG	J	500	2	-	0/6/23/26	0/1/1/1
9	NAG	L	500	2	-	0/6/23/26	0/1/1/1
9	NAG	F	500	2	-	0/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	500	NAG	C1-C2	3.14	1.56	1.52
9	F	500	NAG	C1-C2	2.90	1.56	1.52
9	B	500	NAG	C1-C2	2.76	1.56	1.52
9	H	500	NAG	O7-C7	2.63	1.29	1.23
9	D	500	NAG	C1-C2	2.57	1.55	1.52
9	L	500	NAG	O7-C7	2.55	1.28	1.23
9	L	500	NAG	C1-C2	2.50	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	H	500	NAG	C1-C2	2.22	1.55	1.52
9	J	500	NAG	O7-C7	2.20	1.28	1.23

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	L	500	NAG	C2-N2-C7	6.72	131.90	122.90
9	F	500	NAG	C1-C2-N2	6.32	120.39	110.43
9	L	500	NAG	O7-C7-N2	6.25	133.03	121.98
9	H	500	NAG	C1-O5-C5	5.51	119.57	112.19
9	J	500	NAG	C1-O5-C5	5.20	119.16	112.19
9	F	500	NAG	O7-C7-N2	4.99	130.80	121.98
9	L	500	NAG	C1-O5-C5	4.76	118.56	112.19
9	J	500	NAG	O7-C7-N2	4.71	130.31	121.98
9	L	500	NAG	C8-C7-N2	-4.62	108.46	116.12
9	D	500	NAG	O7-C7-N2	4.44	129.82	121.98
9	F	500	NAG	C1-O5-C5	4.13	117.72	112.19
9	D	500	NAG	C1-C2-N2	4.01	116.75	110.43
9	D	500	NAG	C1-O5-C5	4.01	117.55	112.19
9	H	500	NAG	O7-C7-N2	4.00	129.05	121.98
9	J	500	NAG	C8-C7-N2	-3.98	109.52	116.12
9	H	500	NAG	C8-C7-N2	-3.97	109.54	116.12
9	H	500	NAG	C2-N2-C7	3.80	127.99	122.90
9	J	500	NAG	C2-N2-C7	3.68	127.83	122.90
9	B	500	NAG	O7-C7-N2	3.65	128.43	121.98
9	B	500	NAG	C1-O5-C5	3.56	116.95	112.19
9	F	500	NAG	O7-C7-C8	-3.14	116.46	122.05
9	B	500	NAG	C8-C7-N2	-2.91	111.30	116.12
9	H	500	NAG	C4-C3-C2	-2.81	106.90	111.02
9	F	500	NAG	O5-C1-C2	-2.77	107.00	111.29
9	D	500	NAG	C8-C7-N2	-2.77	111.53	116.12
9	J	500	NAG	O3-C3-C2	2.64	114.88	109.40
9	J	500	NAG	C3-C4-C5	-2.58	105.56	110.23
9	L	500	NAG	C1-C2-N2	2.54	114.44	110.43
9	J	500	NAG	O4-C4-C5	2.53	115.55	109.32
9	H	500	NAG	O3-C3-C2	2.48	114.56	109.40
9	J	500	NAG	C1-C2-N2	2.48	114.34	110.43
9	J	500	NAG	O5-C1-C2	-2.29	107.75	111.29
9	F	500	NAG	C2-N2-C7	2.25	125.92	122.90
9	H	500	NAG	O4-C4-C5	2.22	114.80	109.32
9	B	500	NAG	C2-N2-C7	2.16	125.79	122.90
9	F	500	NAG	C8-C7-N2	-2.04	112.74	116.12

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	500	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
9	F	500	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 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	316/325 (97%)	-1.18	1 (0%) 90 88	39, 58, 82, 97	1 (0%)
1	C	316/325 (97%)	-1.19	0 100 100	38, 58, 83, 97	1 (0%)
1	E	316/325 (97%)	-1.23	0 100 100	39, 58, 81, 98	1 (0%)
1	G	316/325 (97%)	-1.16	0 100 100	42, 60, 83, 104	1 (0%)
1	I	316/325 (97%)	-1.18	0 100 100	43, 60, 85, 101	1 (0%)
1	K	316/325 (97%)	-1.18	0 100 100	41, 60, 83, 105	1 (0%)
2	B	167/181 (92%)	-1.18	0 100 100	35, 60, 89, 129	0
2	D	167/181 (92%)	-1.21	0 100 100	34, 59, 87, 124	0
2	F	167/181 (92%)	-1.18	0 100 100	34, 60, 88, 120	0
2	H	167/181 (92%)	-1.16	0 100 100	37, 58, 80, 135	0
2	J	167/181 (92%)	-1.23	0 100 100	35, 58, 84, 138	0
2	L	167/181 (92%)	-1.16	0 100 100	36, 59, 81, 133	0
All	All	2898/3036 (95%)	-1.19	1 (0%) 100 100	34, 59, 85, 138	6 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	84	SER	2.1

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

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

6.3 Carbohydrates

SUGAR-RSR INFOmissingINFO

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	NAG	J	500	14/15	0.96	0.09	76,87,94,99	0
9	NAG	L	500	14/15	0.96	0.07	72,78,82,82	0
9	NAG	D	500	14/15	0.97	0.06	65,86,97,105	0
9	NAG	H	500	14/15	0.97	0.06	65,73,76,76	0
9	NAG	B	500	14/15	0.98	0.06	70,81,92,94	0
8	CA	A	412	1/1	0.98	0.03	75,75,75,75	0
9	NAG	F	500	14/15	0.98	0.06	78,87,98,100	0
8	CA	E	410	1/1	0.99	0.06	75,75,75,75	0
8	CA	G	408	1/1	0.99	0.04	77,77,77,77	0
8	CA	I	407	1/1	0.99	0.05	77,77,77,77	0
8	CA	K	408	1/1	0.99	0.06	77,77,77,77	0
8	CA	C	411	1/1	0.99	0.04	76,76,76,76	0

6.5 Other polymers (i)

There are no such residues in this entry.