wwPDB X-ray Structure Validation Summary Report (i)

Dec 15, 2024 – 10:13 AM EST

PDB ID	:	6MDT
Title	:	Crystal structure of the B41 SOSIP.664 Env trimer with PGT124 and 35O22 Fabs, in P63 space group
Authors	:	Kumar, S.; Sarkar, A.; Wilson, I.A.
Deposited on	:	2018-09-05
Resolution	:	3.82 Å(reported)

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

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

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

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

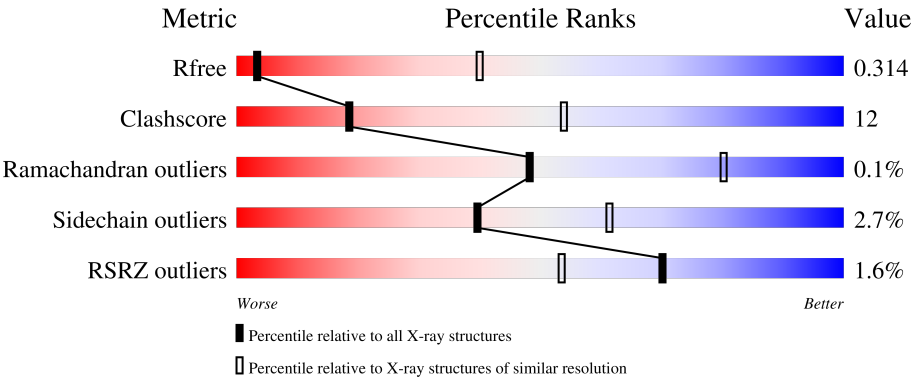
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 3.82 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	1155 (4.00-3.64)
Clashscore	180529	1222 (4.00-3.64)
Ramachandran outliers	177936	1182 (4.00-3.64)
Sidechain outliers	177891	1174 (4.00-3.64)
RSRZ outliers	164620	1156 (4.00-3.64)

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	B	153	3% 73% 14% 11%
2	G	482	% 67% 26% 6%
3	D	243	79% 20%
4	E	216	83% 15%
5	H	236	3% 67% 30%

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Mol	Chain	Length	Quality of chain
6	L	214	2% 77% 21%
7	A	5	40% 40% 20%
7	I	5	60% 20% 20%
7	K	5	40% 20% 40%
7	Q	5	40% 40% 20%
8	C	7	14% 57% 29%
9	F	2	100%
10	J	3	33% 33% 33%
10	M	3	33% 33% 33%
10	O	3	33% 67%
10	S	3	67% 33%
11	N	4	75% 25%
11	P	4	50% 50%
12	R	4	50% 50%
13	T	9	33% 33% 33%

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 12314 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 Transmembrane protein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	136	Total	C	N	O	S	0	0	0
			1077	688	181	201	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	605	CYS	THR	conflict	UNP B3UES2

- Molecule 2 is a protein called Surface protein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	455	Total	C	N	O	S	0	0	0
			3562	2237	628	671	26			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	501	CYS	ALA	conflict	UNP B3UF58

- Molecule 3 is a protein called 35O22 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	240	Total	C	N	O	S	0	0	0
			1813	1150	303	352	8			

- Molecule 4 is a protein called 35O22 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	213	Total	C	N	O	S	0	0	0
			1615	1012	267	328	8			

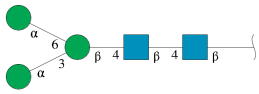
- Molecule 5 is a protein called PGT124 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	231	Total	C	N	O	S	0	0	0
			1754	1111	293	345	5			

- Molecule 6 is a protein called PGT124 Fab light chain.

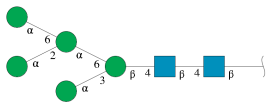
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	211	Total	C	N	O	S	0	0	0
			1601	1008	271	317	5			

- Molecule 7 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				ZeroOcc	AltConf	Trace
7	A	5	Total	C	N	O	0	0	0
			61	34	2	25			
7	I	5	Total	C	N	O	0	0	0
			61	34	2	25			
7	K	5	Total	C	N	O	0	0	0
			61	34	2	25			
7	Q	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-[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.

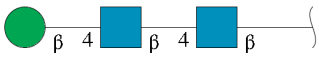


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	C	7	Total	C	N	O	0	0	0
			83	46	2	35			

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

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

- Molecule 10 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
10	J	3	Total C N O 39 22 2 15	0	0	0
10	M	3	Total C N O 39 22 2 15	0	0	0
10	O	3	Total C N O 39 22 2 15	0	0	0
10	S	3	Total C N O 39 22 2 15	0	0	0

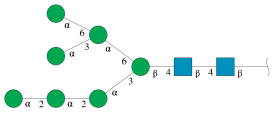
- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	N	4	Total C N O 50 28 2 20	0	0	0
11	P	4	Total C N O 50 28 2 20	0	0	0

- Molecule 12 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.

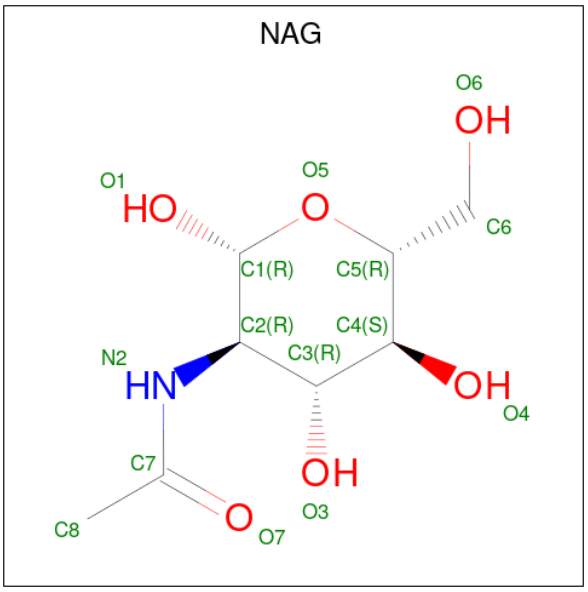
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
12	R	4	50	28	2	20	0	0	0

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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				ZeroOcc	AltConf	Trace
			Total	C	N	O			
13	T	9	105	58	2	45	0	0	0

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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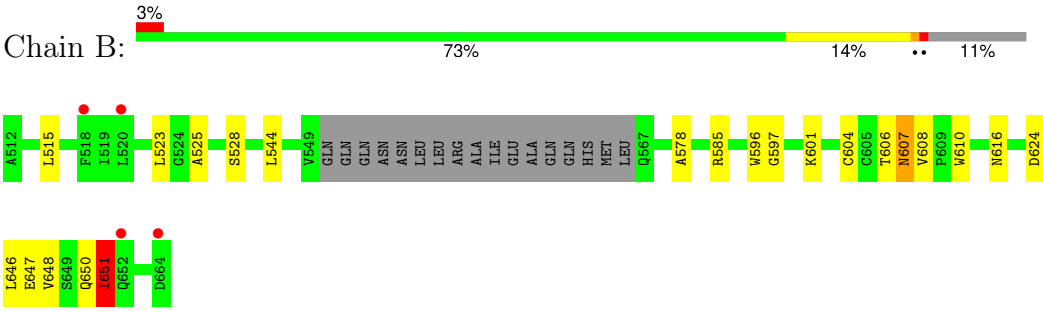
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	B	1	Total 14	C 8	N 1	O 5	0	0
14	B	1	Total 14	C 8	N 1	O 5	0	0
14	G	1	Total 14	C 8	N 1	O 5	0	0
14	G	1	Total 14	C 8	N 1	O 5	0	0
14	G	1	Total 14	C 8	N 1	O 5	0	0
14	G	1	Total 14	C 8	N 1	O 5	0	0
14	G	1	Total 14	C 8	N 1	O 5	0	0
14	G	1	Total 14	C 8	N 1	O 5	0	0

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.

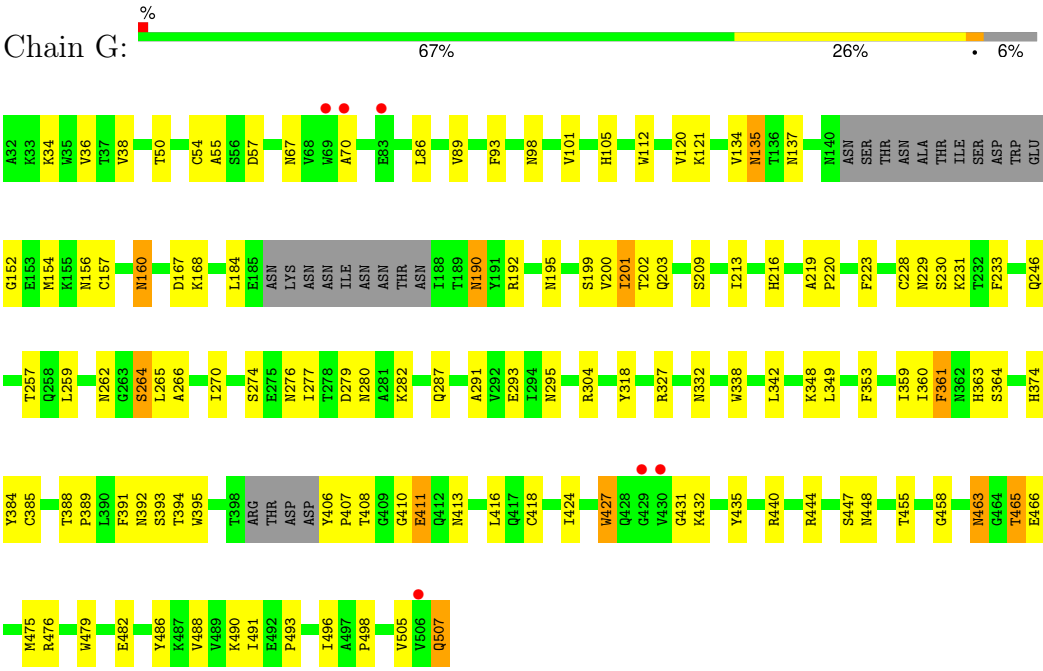
- Molecule 1: Transmembrane protein gp41

Chain B:



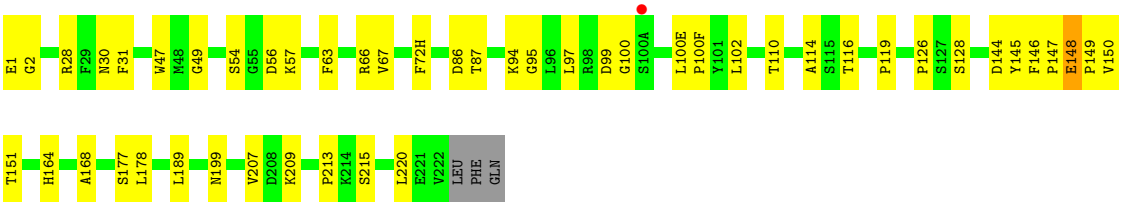
- Molecule 2: Surface protein gp120

Chain G:



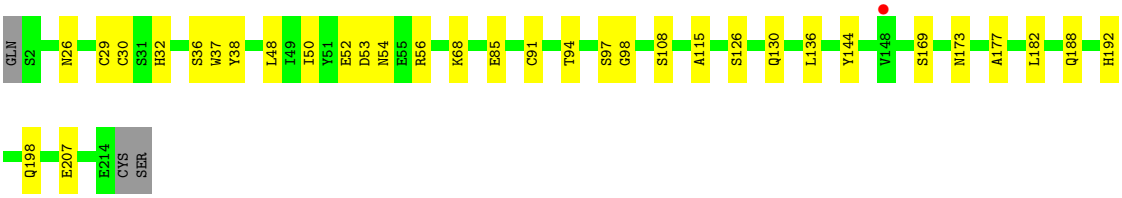
- Molecule 3: 35O22 Fab heavy chain

Chain D:



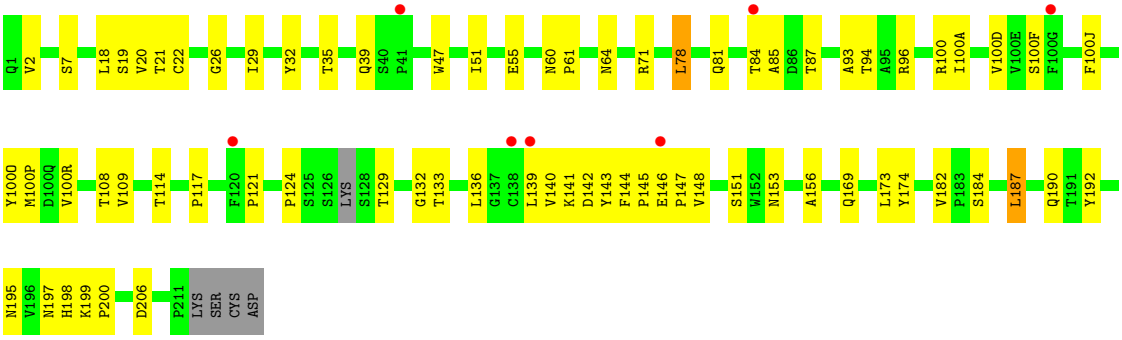
• Molecule 4: 35O22 Fab light chain

Chain E:



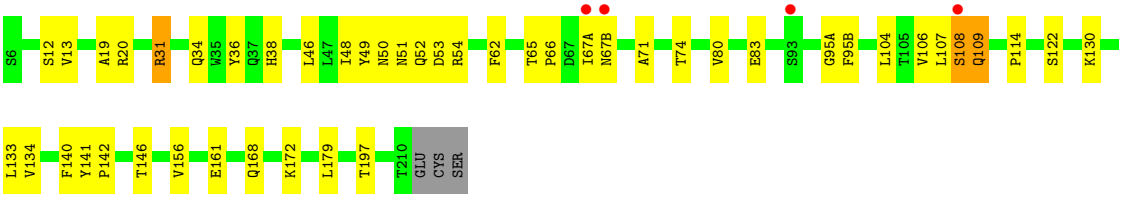
• Molecule 5: PGT124 Fab heavy chain

Chain H:



• Molecule 6: PGT124 Fab light chain

Chain L:



• Molecule 7: 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

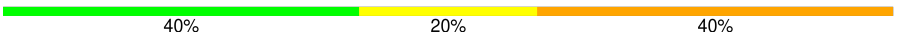
Chain A:

• Molecule 7: 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:

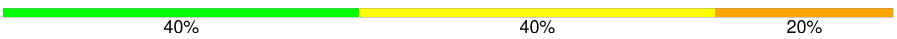
• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



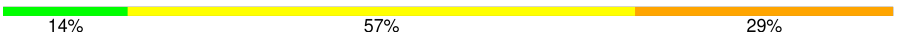
• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



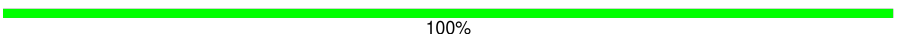
• Molecule 8: alpha-D-mannopyranose-(1-2)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



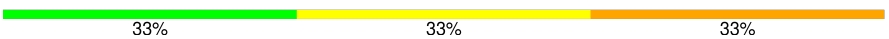
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



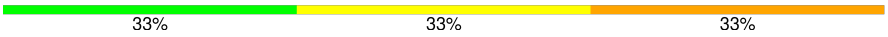
• Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



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

Chain M:



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

Chain O:

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

Chain S:

• Molecule 11: 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 N:

• Molecule 11: 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

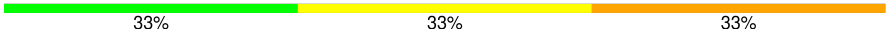
Chain P:

• Molecule 12: 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 R:

• Molecule 13: alpha-D-mannopyranose-(1-2)-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 T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	129.34Å 129.34Å 313.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.96 – 3.82 41.96 – 3.82	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.96-3.82) 99.8 (41.96-3.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 3.76Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.294 , 0.311 0.300 , 0.314	Depositor DCC
R_{free} test set	1363 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å^2)	98.9	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 38.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.35$, $< L^2 > = 0.17$	Xtriage
Estimated twinning fraction	0.177 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	12314	wwPDB-VP
Average B, all atoms (Å^2)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, BMA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	B	0.27	0/1096	0.46	0/1487
2	G	0.29	0/3637	0.49	0/4946
3	D	0.24	0/1860	0.45	0/2533
4	E	0.24	0/1659	0.45	0/2269
5	H	0.28	0/1797	0.58	1/2453 (0.0%)
6	L	0.30	0/1644	0.52	4/2246 (0.2%)
All	All	0.27	0/11693	0.49	5/15934 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	85	ALA	N-CA-CB	8.14	121.50	110.10
6	L	109	GLN	N-CA-C	-6.07	94.60	111.00
6	L	108	SER	CA-C-O	5.19	131.00	120.10
6	L	108	SER	CA-C-N	-5.04	106.11	117.20
6	L	108	SER	CB-CA-C	-5.01	100.59	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1077	0	1066	23	0
2	G	3562	0	3486	108	0
3	D	1813	0	1781	33	0
4	E	1615	0	1544	21	0
5	H	1754	0	1719	72	0
6	L	1601	0	1544	33	0
7	A	61	0	52	4	0
7	I	61	0	52	1	0
7	K	61	0	52	3	0
7	Q	61	0	52	3	0
8	C	83	0	70	7	0
9	F	28	0	25	0	0
10	J	39	0	34	2	0
10	M	39	0	34	3	0
10	O	39	0	34	2	0
10	S	39	0	34	1	0
11	N	50	0	43	0	0
11	P	50	0	43	1	0
12	R	50	0	43	5	0
13	T	105	0	86	11	0
14	B	42	0	39	1	0
14	G	84	0	78	1	0
All	All	12314	0	11911	286	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 12.

The worst 5 of 286 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:G:413:ASN:HD21	12:R:1:NAG:C1	1.51	1.24
5:H:29:ILE:HB	5:H:71:ARG:HD2	1.20	1.18
2:G:413:ASN:ND2	12:R:1:NAG:C1	2.09	1.15
5:H:29:ILE:HD13	5:H:71:ARG:HE	1.20	1.01
5:H:94:THR:HG22	5:H:100(R):VAL:HB	1.43	0.99

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 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	B	132/153 (86%)	120 (91%)	11 (8%)	1 (1%)	16 51
2	G	447/482 (93%)	411 (92%)	36 (8%)	0	100 100
3	D	238/243 (98%)	229 (96%)	9 (4%)	0	100 100
4	E	211/216 (98%)	197 (93%)	14 (7%)	0	100 100
5	H	227/236 (96%)	215 (95%)	12 (5%)	0	100 100
6	L	209/214 (98%)	191 (91%)	18 (9%)	0	100 100
All	All	1464/1544 (95%)	1363 (93%)	100 (7%)	1 (0%)	48 80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	651	ILE

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	B	115/130 (88%)	111 (96%)	4 (4%)	31 56
2	G	401/427 (94%)	381 (95%)	20 (5%)	20 46
3	D	203/206 (98%)	201 (99%)	2 (1%)	73 81
4	E	186/189 (98%)	185 (100%)	1 (0%)	86 90
5	H	199/204 (98%)	195 (98%)	4 (2%)	50 69
6	L	177/180 (98%)	174 (98%)	3 (2%)	56 72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1281/1336 (96%)	1247 (97%)	34 (3%)	40 61

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	H	78	LEU
5	H	187	LEU
6	L	95(B)	PHE
2	G	327	ARG
2	G	264	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	363	HIS
2	G	413	ASN
6	L	51	ASN
2	G	463	ASN
2	G	287	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)

62 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	A	1	7	14,14,15	0.58	0	17,19,21	0.67	0
7	NAG	A	2	7	14,14,15	0.27	0	17,19,21	1.12	1 (5%)
7	BMA	A	3	7	11,11,12	0.59	0	15,15,17	1.50	2 (13%)
7	MAN	A	4	7	11,11,12	0.55	0	15,15,17	0.71	0
7	MAN	A	5	7	11,11,12	0.45	0	15,15,17	0.55	0
8	NAG	C	1	2,8	14,14,15	0.53	0	17,19,21	0.44	0
8	NAG	C	2	8	14,14,15	0.39	0	17,19,21	0.52	0
8	BMA	C	3	8	11,11,12	0.26	0	15,15,17	1.18	2 (13%)
8	MAN	C	4	8	11,11,12	0.91	1 (9%)	15,15,17	2.38	5 (33%)
8	MAN	C	5	8	11,11,12	0.52	0	15,15,17	1.09	0
8	MAN	C	6	8	11,11,12	0.28	0	15,15,17	0.69	0
8	MAN	C	7	8	11,11,12	0.26	0	15,15,17	0.72	0
9	NAG	F	1	9,2	14,14,15	0.20	0	17,19,21	0.50	0
9	NAG	F	2	9	14,14,15	0.35	0	17,19,21	0.48	0
7	NAG	I	1	2,7	14,14,15	0.31	0	17,19,21	0.48	0
7	NAG	I	2	7	14,14,15	1.23	1 (7%)	17,19,21	1.37	1 (5%)
7	BMA	I	3	7	11,11,12	0.36	0	15,15,17	1.07	1 (6%)
7	MAN	I	4	7	11,11,12	0.44	0	15,15,17	0.77	0
7	MAN	I	5	7	11,11,12	0.36	0	15,15,17	0.71	0
10	NAG	J	1	2,10	14,14,15	0.93	1 (7%)	17,19,21	1.84	5 (29%)
10	NAG	J	2	10	14,14,15	0.98	1 (7%)	17,19,21	0.84	1 (5%)
10	BMA	J	3	10	11,11,12	0.40	0	15,15,17	0.69	0
7	NAG	K	1	7	14,14,15	1.07	1 (7%)	17,19,21	0.52	0
7	NAG	K	2	7	14,14,15	0.14	0	17,19,21	0.49	0
7	BMA	K	3	7	11,11,12	0.43	0	15,15,17	1.06	1 (6%)
7	MAN	K	4	7	11,11,12	0.56	0	15,15,17	0.78	0
7	MAN	K	5	7	11,11,12	0.42	0	15,15,17	0.62	0
10	NAG	M	1	2,10	14,14,15	0.71	0	17,19,21	0.57	0
10	NAG	M	2	10	14,14,15	0.40	0	17,19,21	1.39	3 (17%)
10	BMA	M	3	10	11,11,12	0.38	0	15,15,17	0.69	0
11	NAG	N	1	2,11	14,14,15	0.28	0	17,19,21	0.56	0
11	NAG	N	2	11	14,14,15	0.41	0	17,19,21	0.56	0
11	BMA	N	3	11	11,11,12	0.70	0	15,15,17	1.11	0
11	MAN	N	4	11	11,11,12	0.79	0	15,15,17	1.20	2 (13%)
10	NAG	O	1	2,10	14,14,15	0.44	0	17,19,21	0.57	0
10	NAG	O	2	10	14,14,15	0.57	0	17,19,21	0.48	0
10	BMA	O	3	10	11,11,12	0.62	0	15,15,17	0.72	0
11	NAG	P	1	2,11	14,14,15	0.35	0	17,19,21	0.65	0
11	NAG	P	2	11	14,14,15	0.54	0	17,19,21	0.65	0
11	BMA	P	3	11	11,11,12	0.24	0	15,15,17	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	MAN	P	4	11	11,11,12	0.24	0	15,15,17	0.47	0
7	NAG	Q	1	2,7	14,14,15	0.32	0	17,19,21	0.49	0
7	NAG	Q	2	7	14,14,15	0.52	0	17,19,21	0.98	1 (5%)
7	BMA	Q	3	7	11,11,12	0.54	0	15,15,17	1.03	1 (6%)
7	MAN	Q	4	7	11,11,12	0.30	0	15,15,17	0.70	0
7	MAN	Q	5	7	11,11,12	0.32	0	15,15,17	0.67	0
12	NAG	R	1	12	14,14,15	0.68	1 (7%)	17,19,21	0.56	0
12	NAG	R	2	12	14,14,15	0.56	0	17,19,21	1.50	2 (11%)
12	BMA	R	3	12	11,11,12	0.32	0	15,15,17	0.66	0
12	MAN	R	4	12	11,11,12	0.59	0	15,15,17	0.57	0
10	NAG	S	1	2,10	14,14,15	0.32	0	17,19,21	0.52	0
10	NAG	S	2	10	14,14,15	0.39	0	17,19,21	0.61	0
10	BMA	S	3	10	11,11,12	0.41	0	15,15,17	0.71	0
13	NAG	T	1	13	14,14,15	0.49	0	17,19,21	0.62	0
13	NAG	T	2	13	14,14,15	0.91	1 (7%)	17,19,21	0.95	2 (11%)
13	BMA	T	3	13	11,11,12	0.81	0	15,15,17	2.38	5 (33%)
13	MAN	T	4	13	11,11,12	0.36	0	15,15,17	1.44	2 (13%)
13	MAN	T	5	13	11,11,12	0.48	0	15,15,17	1.56	2 (13%)
13	MAN	T	6	13	11,11,12	0.24	0	15,15,17	0.63	0
13	MAN	T	7	13	11,11,12	0.32	0	15,15,17	0.80	0
13	MAN	T	8	13	11,11,12	0.36	0	15,15,17	0.52	0
13	MAN	T	9	13	11,11,12	0.41	0	15,15,17	0.73	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	A	1	7	-	0/6/23/26	0/1/1/1
7	NAG	A	2	7	-	2/6/23/26	0/1/1/1
7	BMA	A	3	7	-	1/2/19/22	0/1/1/1
7	MAN	A	4	7	-	0/2/19/22	0/1/1/1
7	MAN	A	5	7	-	2/2/19/22	0/1/1/1
8	NAG	C	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	C	2	8	-	1/6/23/26	0/1/1/1
8	BMA	C	3	8	-	2/2/19/22	0/1/1/1
8	MAN	C	4	8	-	2/2/19/22	0/1/1/1
8	MAN	C	5	8	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MAN	C	6	8	-	2/2/19/22	0/1/1/1
8	MAN	C	7	8	-	2/2/19/22	0/1/1/1
9	NAG	F	1	9,2	-	0/6/23/26	0/1/1/1
9	NAG	F	2	9	-	2/6/23/26	0/1/1/1
7	NAG	I	1	2,7	-	1/6/23/26	0/1/1/1
7	NAG	I	2	7	-	5/6/23/26	0/1/1/1
7	BMA	I	3	7	-	2/2/19/22	0/1/1/1
7	MAN	I	4	7	-	0/2/19/22	0/1/1/1
7	MAN	I	5	7	-	2/2/19/22	0/1/1/1
10	NAG	J	1	2,10	-	3/6/23/26	0/1/1/1
10	NAG	J	2	10	-	2/6/23/26	0/1/1/1
10	BMA	J	3	10	-	0/2/19/22	0/1/1/1
7	NAG	K	1	7	-	0/6/23/26	0/1/1/1
7	NAG	K	2	7	-	0/6/23/26	0/1/1/1
7	BMA	K	3	7	-	2/2/19/22	0/1/1/1
7	MAN	K	4	7	-	0/2/19/22	0/1/1/1
7	MAN	K	5	7	-	0/2/19/22	0/1/1/1
10	NAG	M	1	2,10	-	5/6/23/26	0/1/1/1
10	NAG	M	2	10	-	2/6/23/26	0/1/1/1
10	BMA	M	3	10	-	0/2/19/22	0/1/1/1
11	NAG	N	1	2,11	-	2/6/23/26	0/1/1/1
11	NAG	N	2	11	-	4/6/23/26	0/1/1/1
11	BMA	N	3	11	-	1/2/19/22	0/1/1/1
11	MAN	N	4	11	-	1/2/19/22	0/1/1/1
10	NAG	O	1	2,10	-	1/6/23/26	0/1/1/1
10	NAG	O	2	10	-	2/6/23/26	0/1/1/1
10	BMA	O	3	10	-	1/2/19/22	0/1/1/1
11	NAG	P	1	2,11	-	3/6/23/26	0/1/1/1
11	NAG	P	2	11	-	2/6/23/26	0/1/1/1
11	BMA	P	3	11	-	1/2/19/22	0/1/1/1
11	MAN	P	4	11	-	0/2/19/22	0/1/1/1
7	NAG	Q	1	2,7	-	4/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	0/6/23/26	0/1/1/1
7	BMA	Q	3	7	-	2/2/19/22	0/1/1/1
7	MAN	Q	4	7	-	0/2/19/22	0/1/1/1
7	MAN	Q	5	7	-	0/2/19/22	0/1/1/1
12	NAG	R	1	12	-	2/6/23/26	0/1/1/1
12	NAG	R	2	12	-	6/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	BMA	R	3	12	-	0/2/19/22	0/1/1/1
12	MAN	R	4	12	-	1/2/19/22	0/1/1/1
10	NAG	S	1	2,10	-	2/6/23/26	0/1/1/1
10	NAG	S	2	10	-	0/6/23/26	0/1/1/1
10	BMA	S	3	10	-	0/2/19/22	0/1/1/1
13	NAG	T	1	13	-	2/6/23/26	0/1/1/1
13	NAG	T	2	13	-	1/6/23/26	0/1/1/1
13	BMA	T	3	13	-	1/2/19/22	0/1/1/1
13	MAN	T	4	13	-	2/2/19/22	0/1/1/1
13	MAN	T	5	13	-	0/2/19/22	0/1/1/1
13	MAN	T	6	13	-	0/2/19/22	0/1/1/1
13	MAN	T	7	13	-	2/2/19/22	0/1/1/1
13	MAN	T	8	13	-	2/2/19/22	0/1/1/1
13	MAN	T	9	13	-	0/2/19/22	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	2	NAG	C1-C2	4.26	1.58	1.52
7	K	1	NAG	O5-C1	-3.87	1.37	1.43
10	J	2	NAG	O5-C1	-3.41	1.38	1.43
10	J	1	NAG	O5-C1	-2.56	1.39	1.43
13	T	2	NAG	O5-C1	-2.42	1.39	1.43

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	4	MAN	C1-C2-C3	-5.22	102.04	109.64
13	T	3	BMA	O5-C1-C2	4.94	122.57	110.79
13	T	3	BMA	O3-C3-C2	-4.82	100.21	110.05
8	C	4	MAN	O2-C2-C3	4.80	120.10	110.15
12	R	2	NAG	C2-N2-C7	4.74	129.26	122.90

There are no chirality outliers.

5 of 89 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	2	NAG	C1-C2-N2-C7
10	J	1	NAG	C1-C2-N2-C7
10	J	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
11	P	1	NAG	O5-C5-C6-O6
7	K	3	BMA	C4-C5-C6-O6

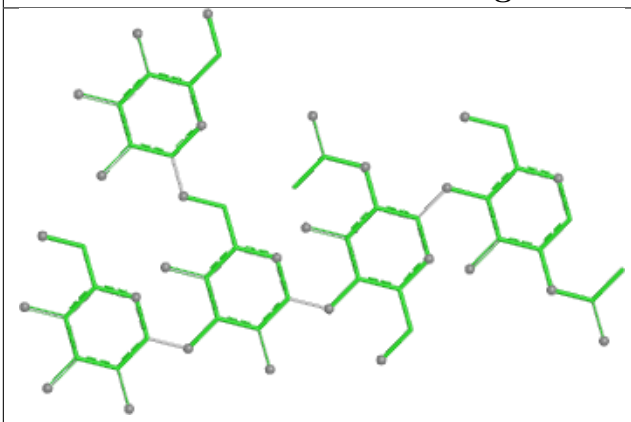
There are no ring outliers.

29 monomers are involved in 43 short contacts:

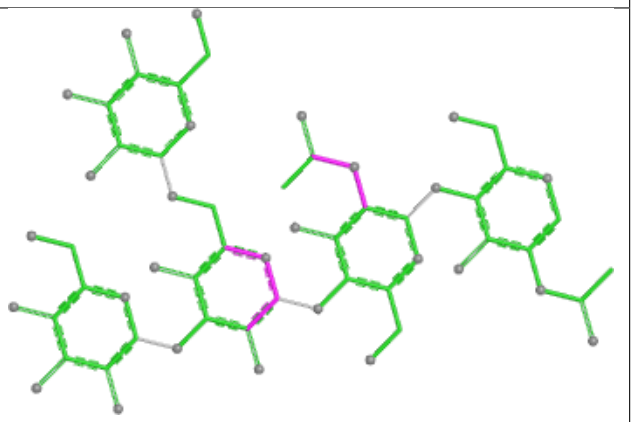
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	5	MAN	1	0
10	O	3	BMA	1	0
7	I	2	NAG	1	0
8	C	6	MAN	1	0
10	O	2	NAG	2	0
13	T	4	MAN	1	0
7	A	2	NAG	2	0
7	Q	1	NAG	2	0
7	K	1	NAG	2	0
8	C	1	NAG	3	0
7	K	3	BMA	1	0
8	C	3	BMA	1	0
12	R	1	NAG	3	0
12	R	2	NAG	2	0
13	T	1	NAG	5	0
10	J	1	NAG	2	0
11	P	3	BMA	1	0
13	T	6	MAN	1	0
13	T	5	MAN	4	0
8	C	4	MAN	2	0
11	P	4	MAN	1	0
7	A	1	NAG	2	0
7	K	4	MAN	1	0
10	M	1	NAG	3	0
10	S	1	NAG	1	0
13	T	2	NAG	1	0
8	C	7	MAN	1	0
10	M	2	NAG	1	0
7	Q	2	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.

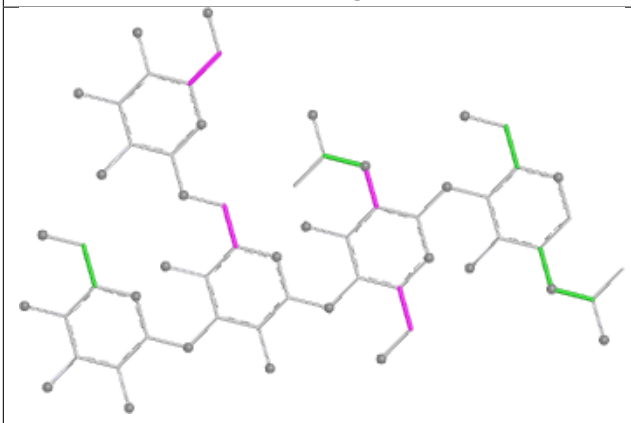
Oligosaccharide Chain A



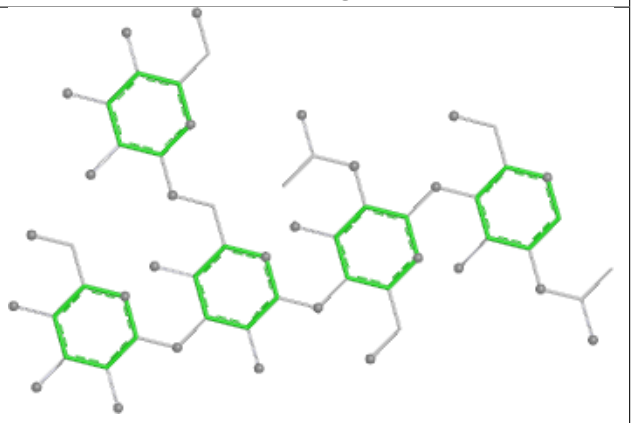
Bond lengths



Bond angles

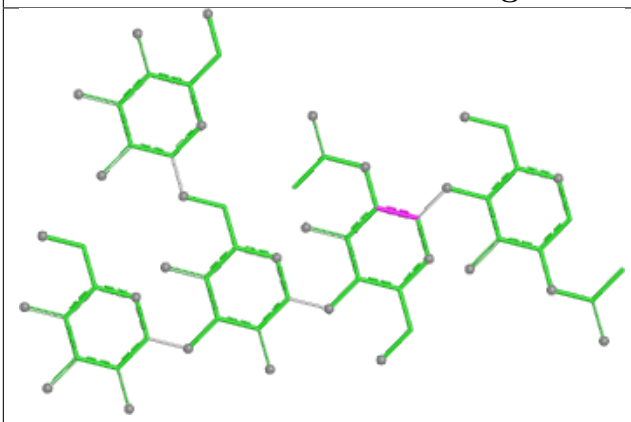


Torsions

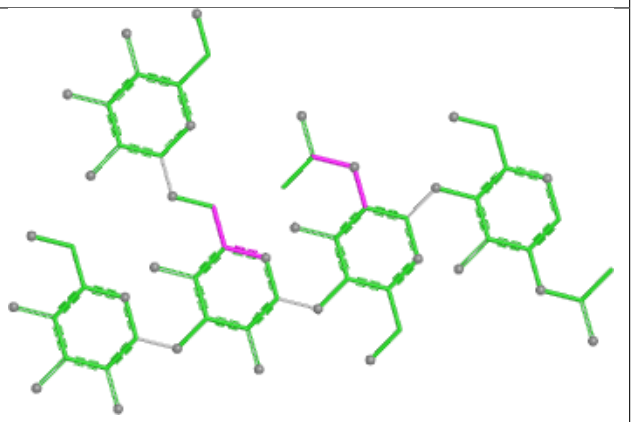


Rings

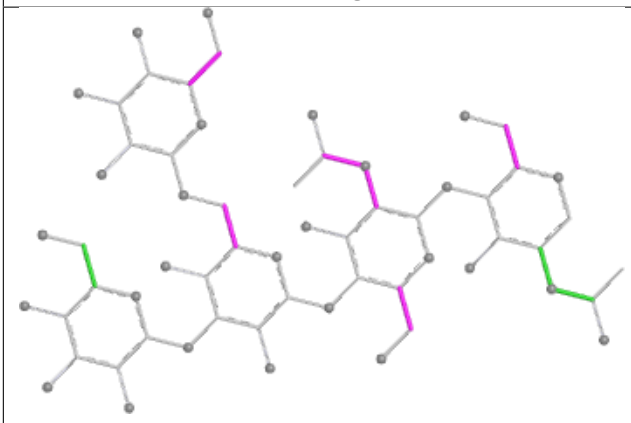
Oligosaccharide Chain I



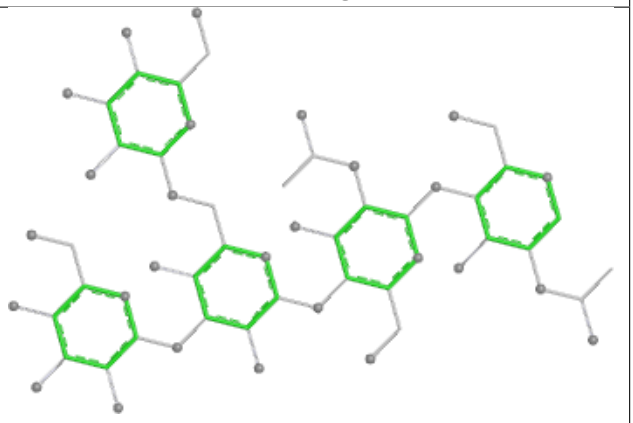
Bond lengths



Bond angles

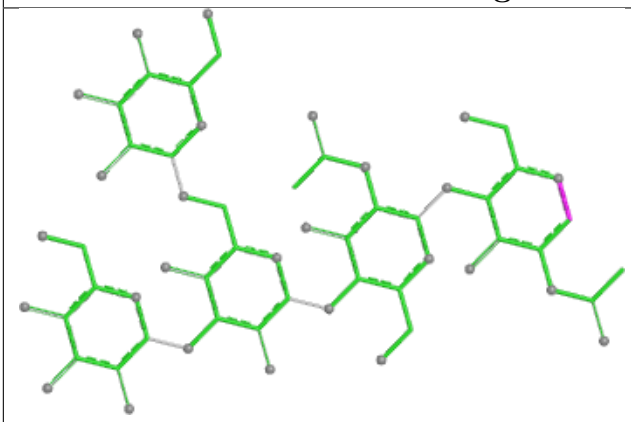


Torsions

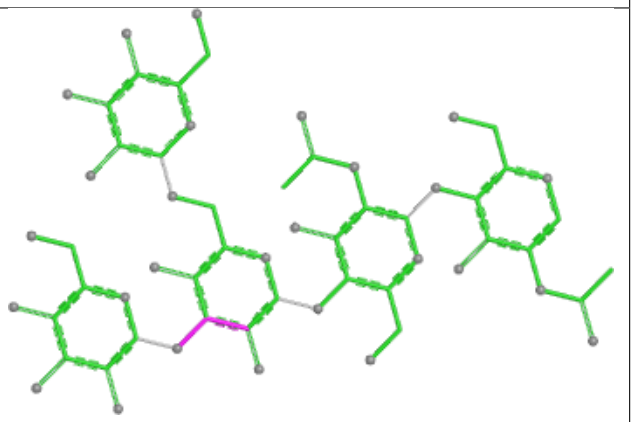


Rings

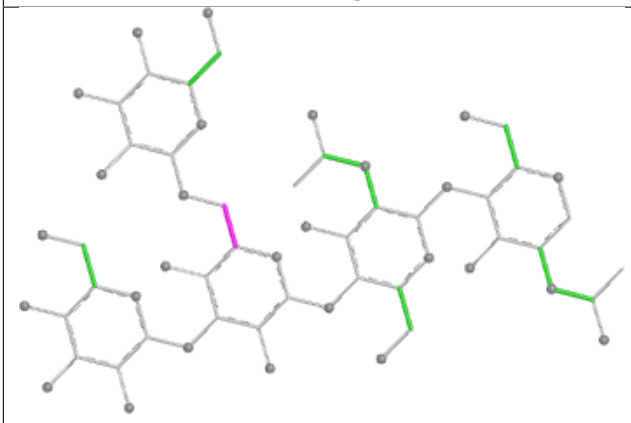
Oligosaccharide Chain K



Bond lengths



Bond angles



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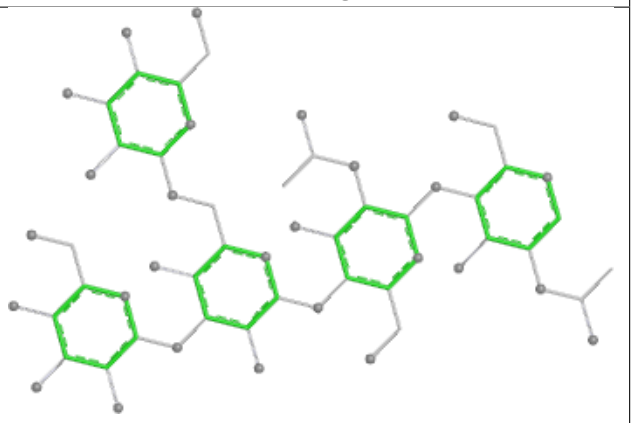
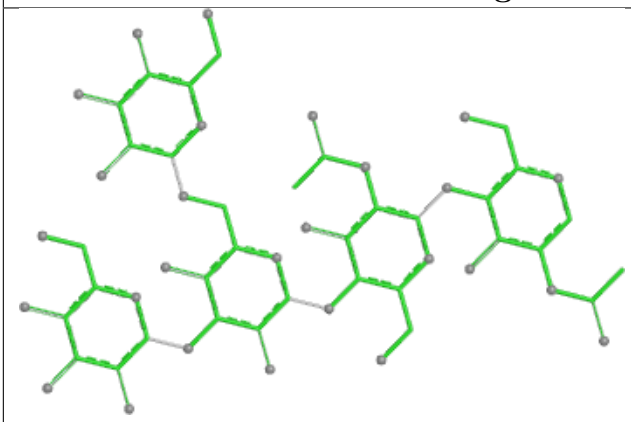
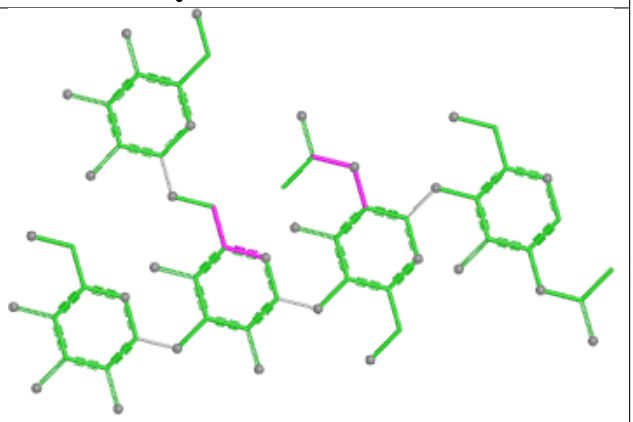


Rings

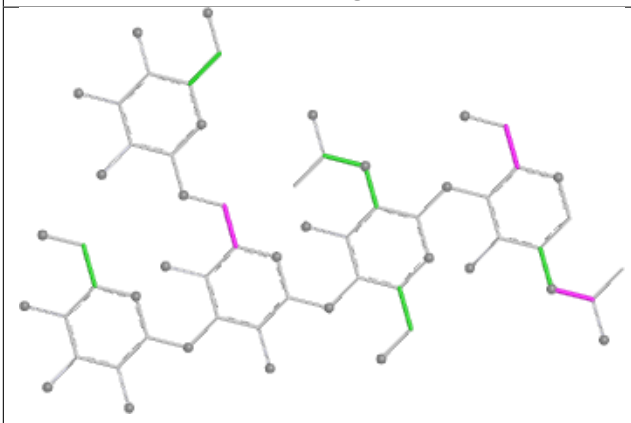
Oligosaccharide Chain Q



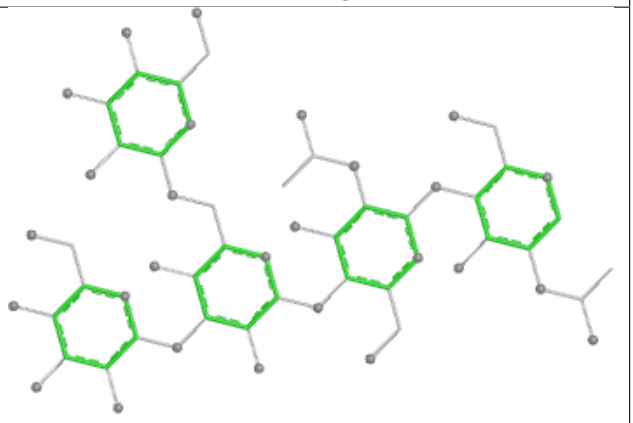
Bond lengths



Bond angles

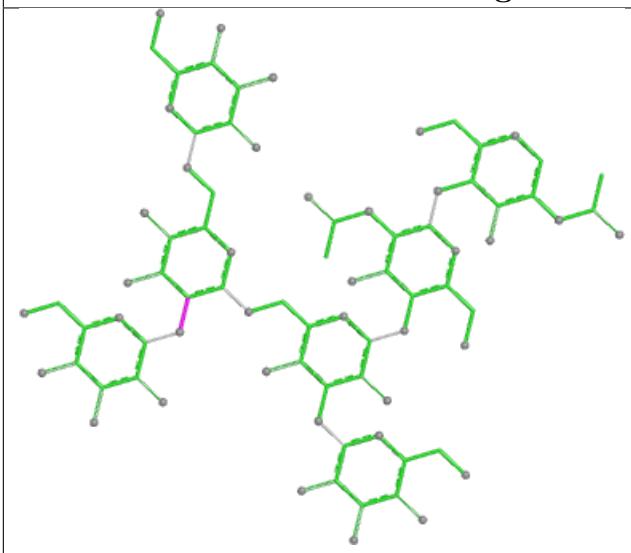


Torsions

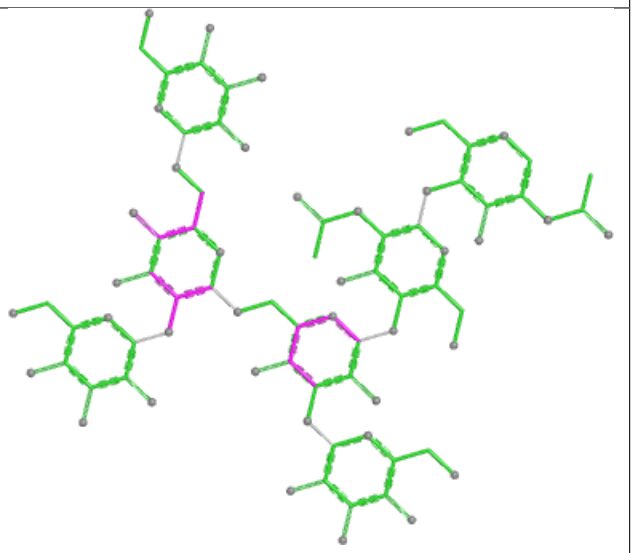


Rings

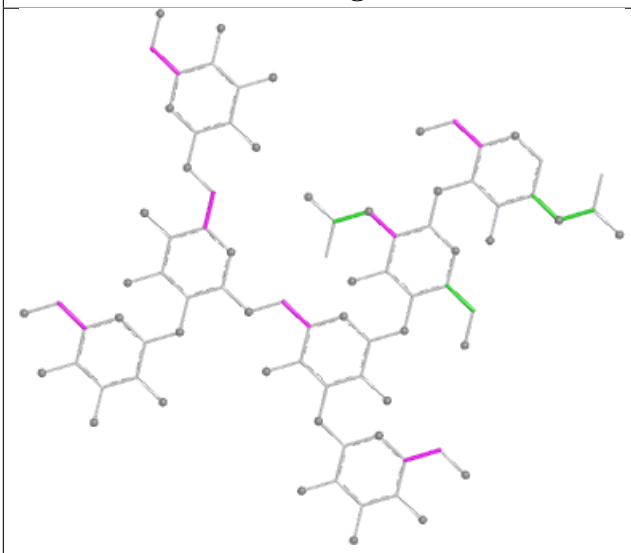
Oligosaccharide Chain C



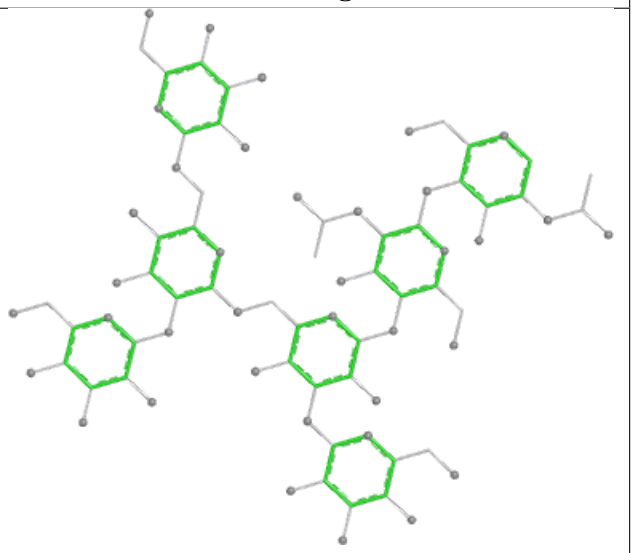
Bond lengths



Bond angles

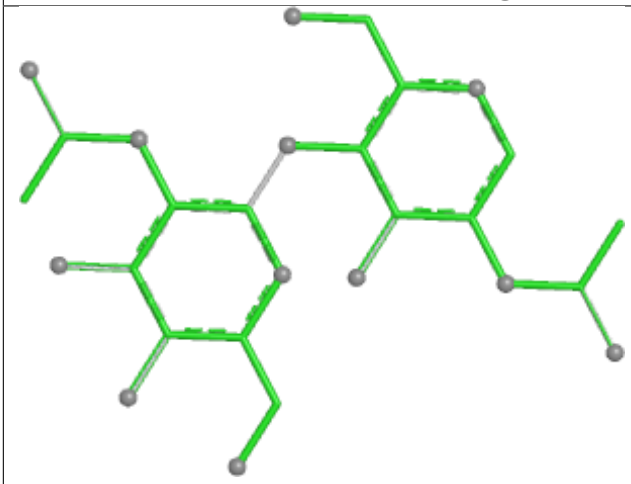


Torsions

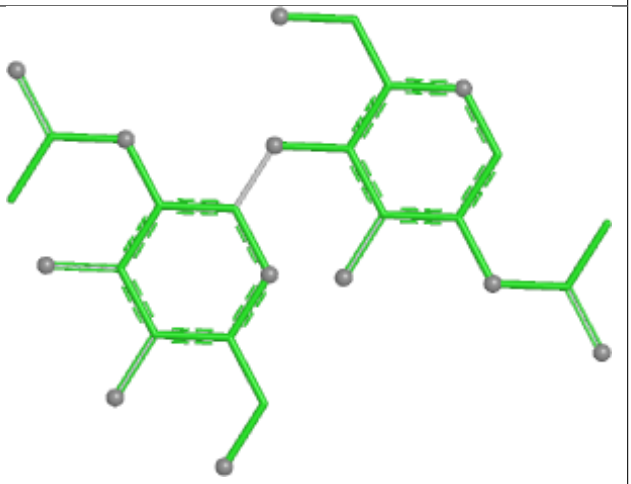


Rings

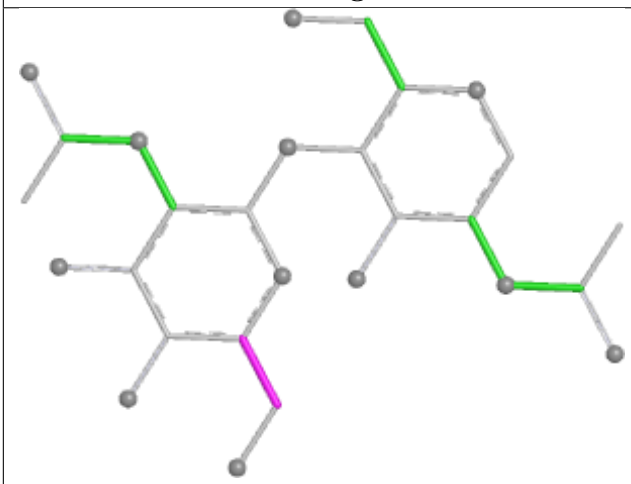
Oligosaccharide Chain F



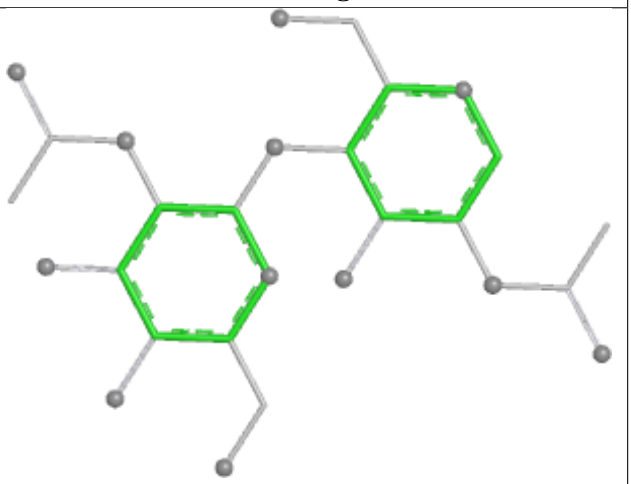
Bond lengths



Bond angles

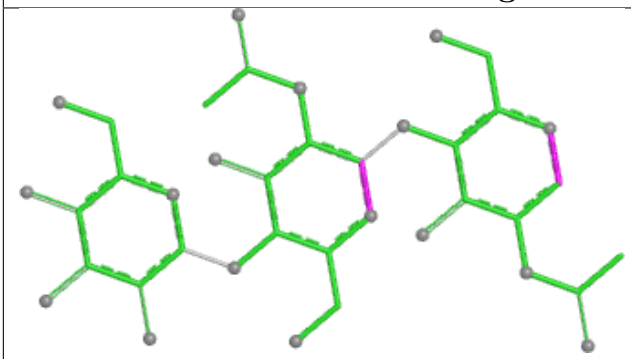


Torsions

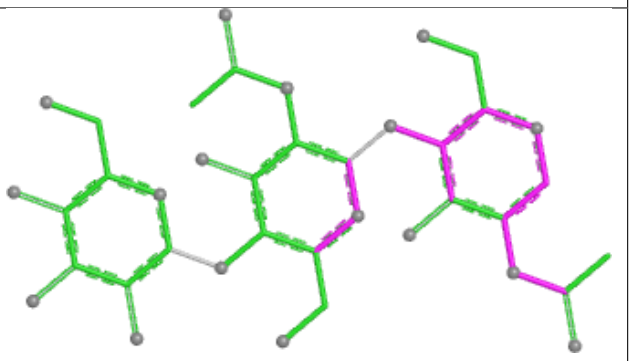


Rings

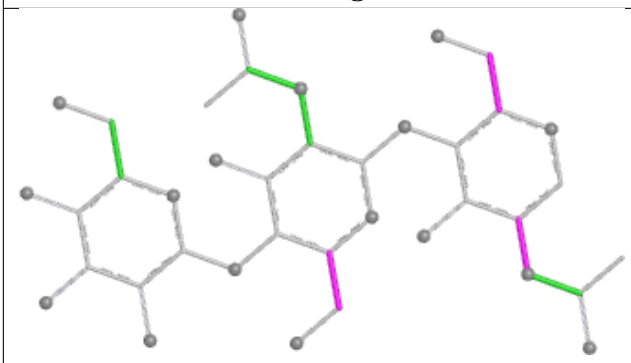
Oligosaccharide Chain J



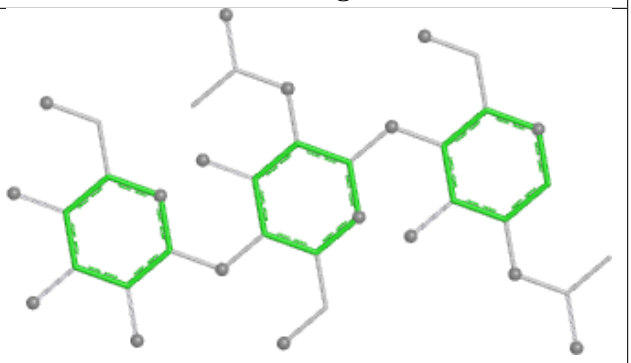
Bond lengths



Bond angles

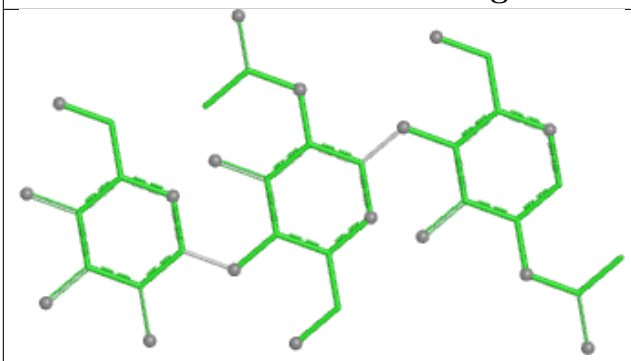


Torsions

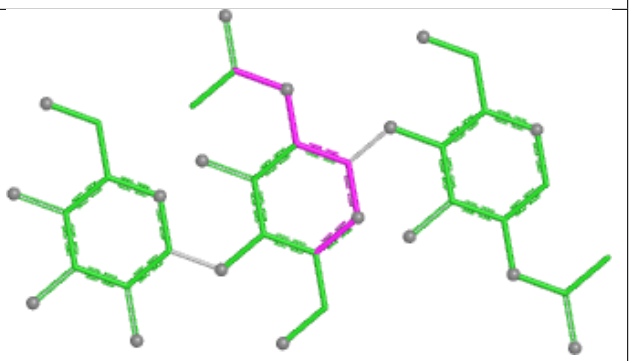


Rings

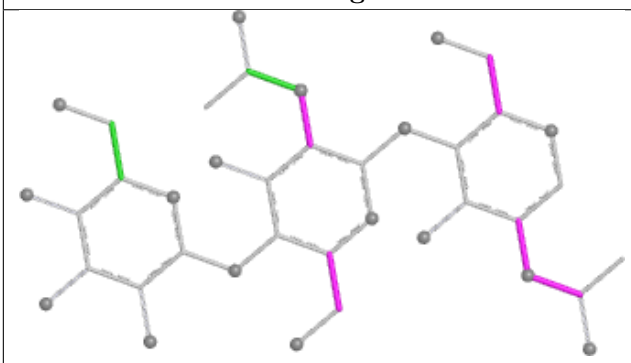
Oligosaccharide Chain M



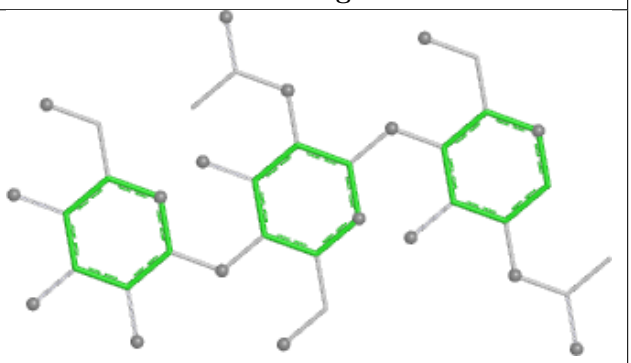
Bond lengths



Bond angles

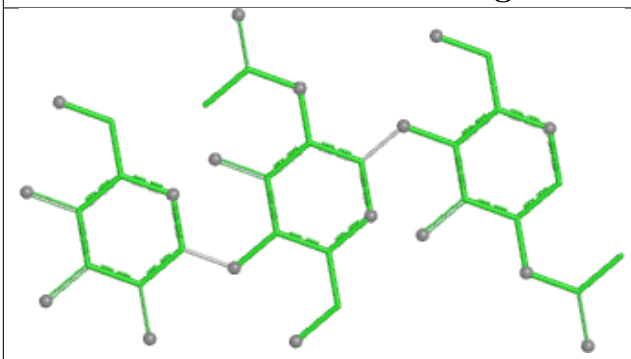


Torsions

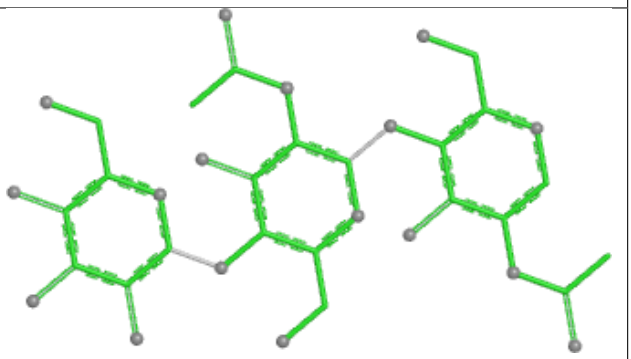


Rings

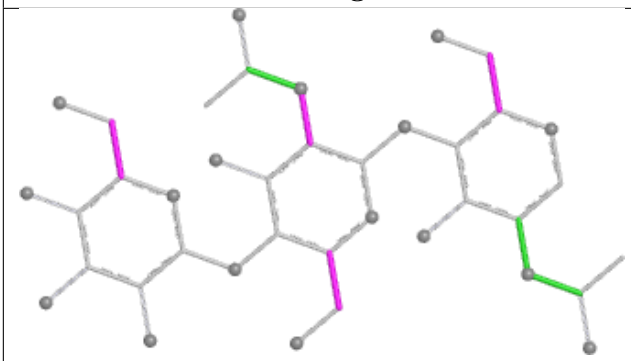
Oligosaccharide Chain O



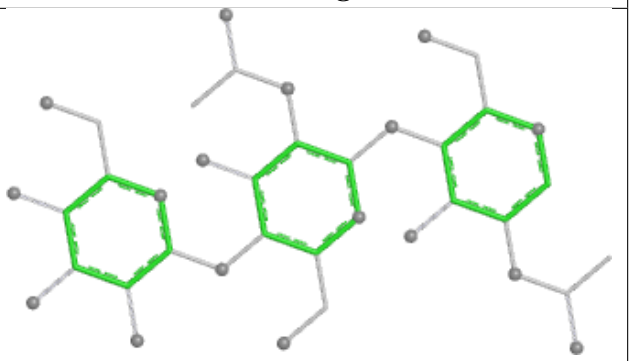
Bond lengths



Bond angles

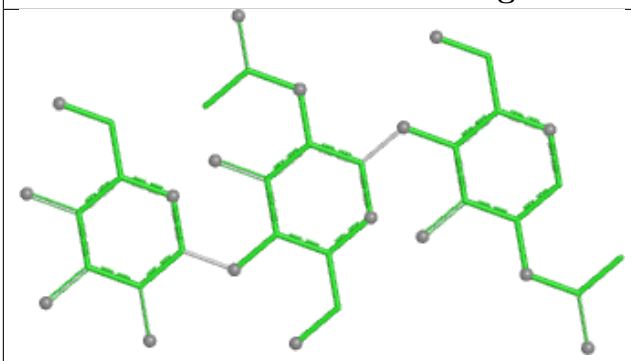


Torsions

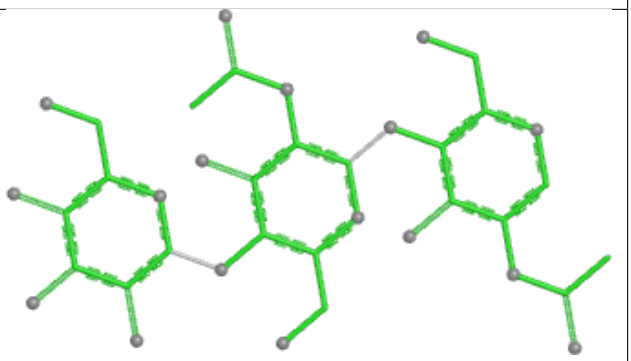


Rings

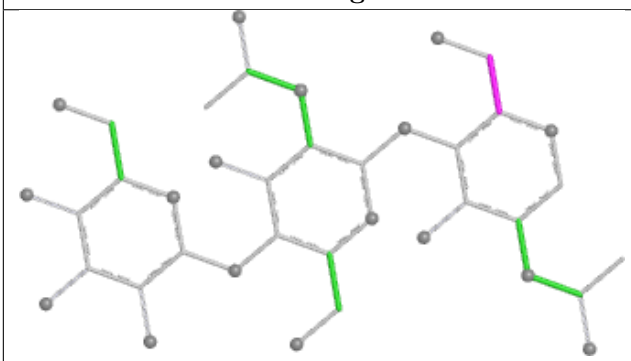
Oligosaccharide Chain S



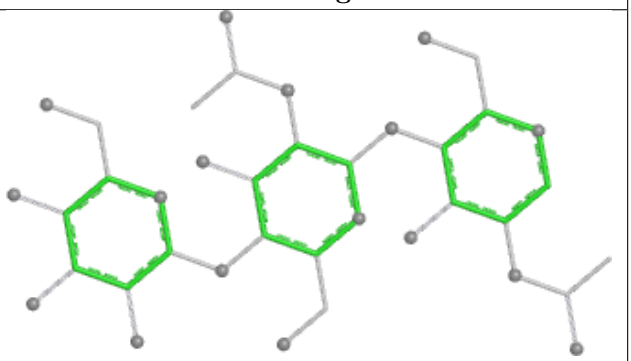
Bond lengths



Bond angles

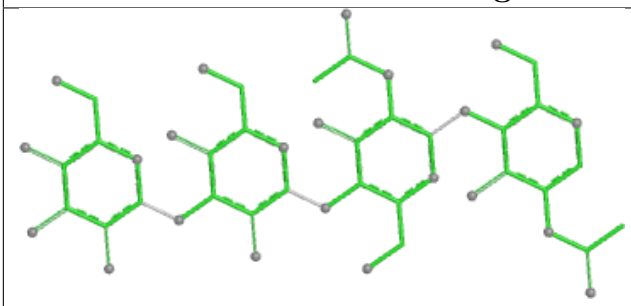


Torsions

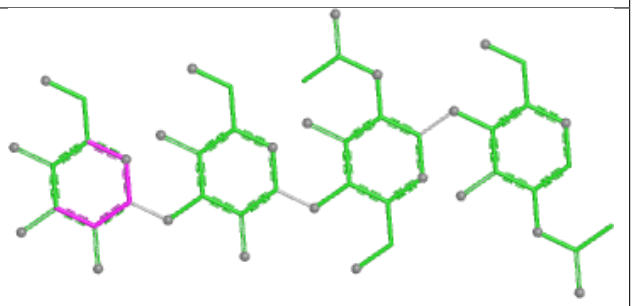


Rings

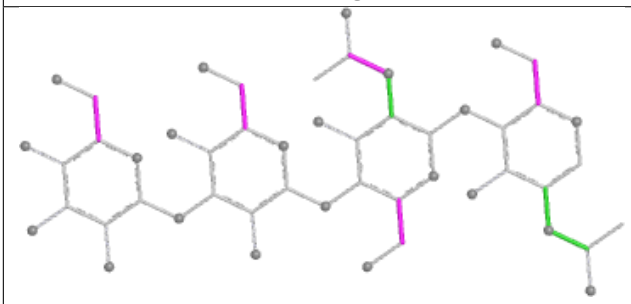
Oligosaccharide Chain N



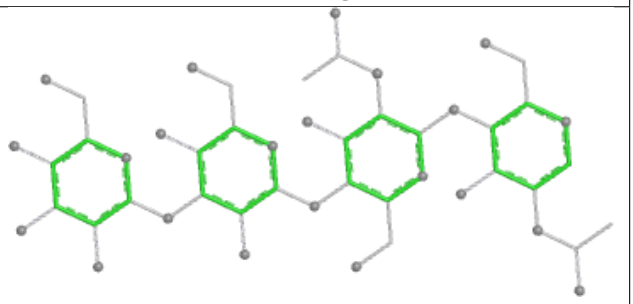
Bond lengths



Bond angles

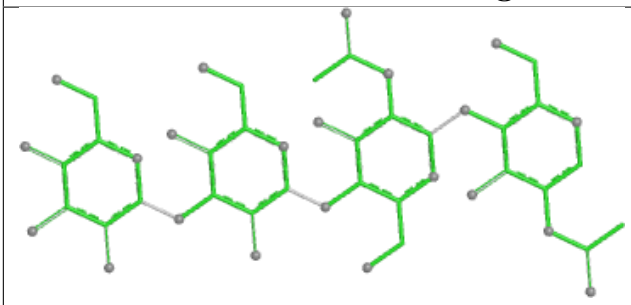


Torsions

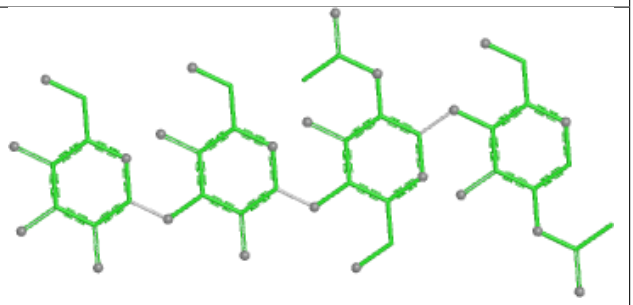


Rings

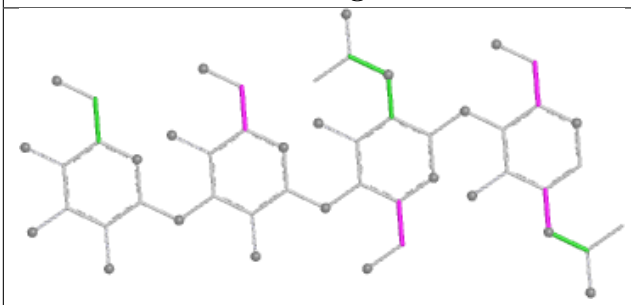
Oligosaccharide Chain P



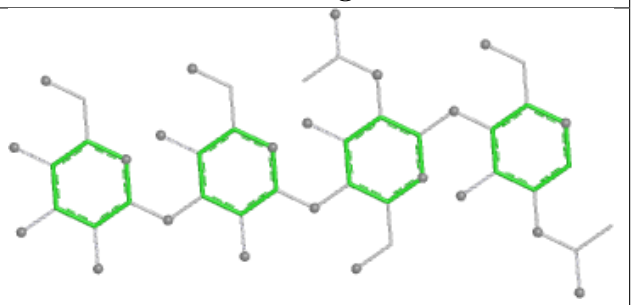
Bond lengths



Bond angles

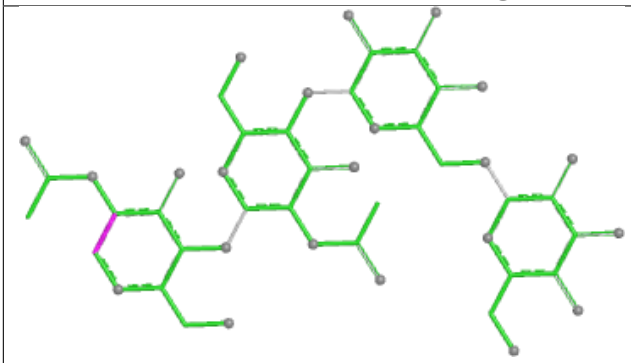


Torsions

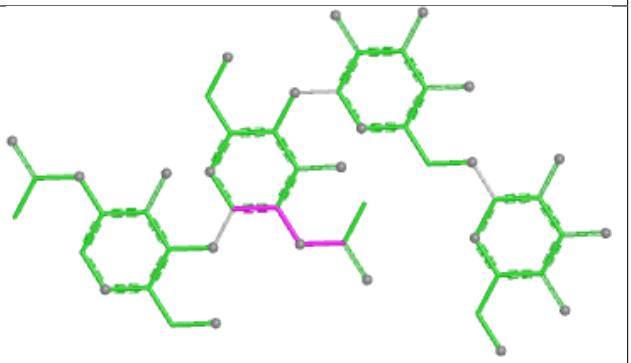


Rings

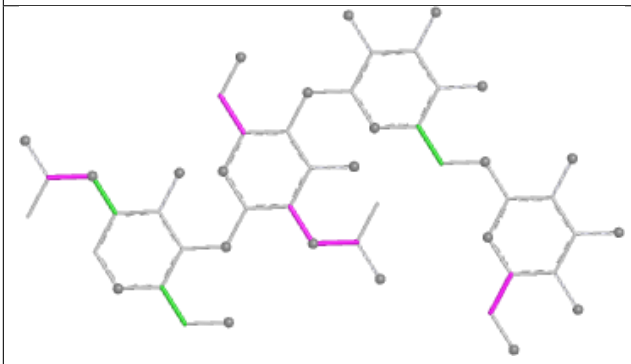
Oligosaccharide Chain R



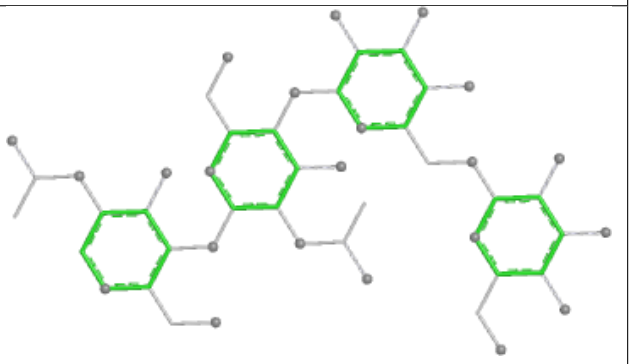
Bond lengths



Bond angles

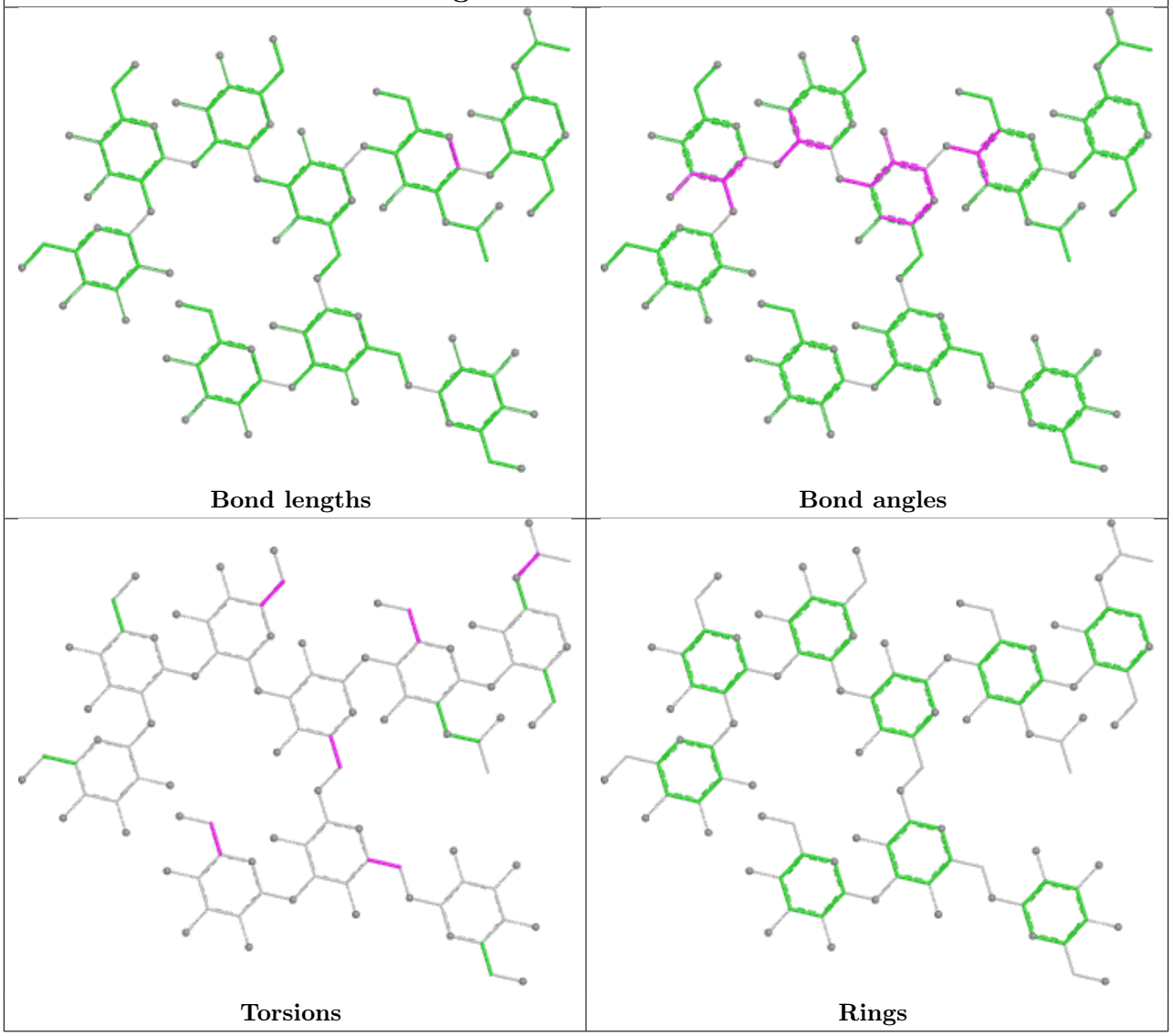


Torsions



Rings

Oligosaccharide Chain T



5.6 Ligand geometry (i)

9 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	$\#\|Z\| > 2$
14	NAG	G	601	2	14,14,15	0.38	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	NAG	B	701	1	14,14,15	0.22	0	17,19,21	0.41	0
14	NAG	B	703	1	14,14,15	0.34	0	17,19,21	0.52	0
14	NAG	G	606	2	14,14,15	0.27	0	17,19,21	0.66	0
14	NAG	G	604	2	14,14,15	0.28	0	17,19,21	0.56	0
14	NAG	B	702	1	14,14,15	0.54	0	17,19,21	0.42	0
14	NAG	G	602	2	14,14,15	0.54	0	17,19,21	0.93	1 (5%)
14	NAG	G	603	2	14,14,15	0.27	0	17,19,21	0.36	0
14	NAG	G	605	2	14,14,15	0.57	0	17,19,21	0.63	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
14	NAG	G	601	2	-	4/6/23/26	0/1/1/1
14	NAG	B	701	1	-	0/6/23/26	0/1/1/1
14	NAG	B	703	1	-	0/6/23/26	0/1/1/1
14	NAG	G	606	2	-	2/6/23/26	0/1/1/1
14	NAG	G	604	2	-	3/6/23/26	0/1/1/1
14	NAG	B	702	1	-	0/6/23/26	0/1/1/1
14	NAG	G	602	2	-	0/6/23/26	0/1/1/1
14	NAG	G	603	2	-	0/6/23/26	0/1/1/1
14	NAG	G	605	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	602	NAG	C1-O5-C5	3.47	116.84	112.19
14	G	605	NAG	C1-O5-C5	2.05	114.93	112.19

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	G	606	NAG	O5-C5-C6-O6
14	G	601	NAG	C8-C7-N2-C2
14	G	601	NAG	O7-C7-N2-C2
14	G	601	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
14	G	606	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	701	NAG	1	0
14	G	602	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	B	136/153 (88%)	-0.03	4 (2%)	54	41	46, 87, 150, 168	0
2	G	455/482 (94%)	-0.04	7 (1%)	71	55	47, 107, 175, 214	0
3	D	240/243 (98%)	-0.27	1 (0%)	89	78	62, 150, 289, 309	0
4	E	213/216 (98%)	-0.16	1 (0%)	87	74	80, 144, 226, 242	0
5	H	231/236 (97%)	-0.02	7 (3%)	52	40	56, 129, 176, 198	0
6	L	211/214 (98%)	-0.15	4 (1%)	66	50	53, 115, 142, 156	0
All	All	1486/1544 (96%)	-0.11	24 (1%)	70	53	46, 117, 219, 309	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	H	146	GLU	3.9
2	G	70	ALA	3.4
6	L	93	SER	3.1
1	B	664	ASP	3.1
5	H	120	PHE	2.9

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
14	NAG	B	701	14/15	0.38	0.14	118,118,118,118	0
14	NAG	G	604	14/15	0.51	0.10	118,118,118,118	0
14	NAG	G	605	14/15	0.55	0.10	118,118,118,118	0
14	NAG	G	601	14/15	0.68	0.09	118,118,118,118	0
14	NAG	G	602	14/15	0.73	0.09	118,118,118,118	0
14	NAG	B	702	14/15	0.75	0.17	37,37,37,37	0
14	NAG	G	603	14/15	0.76	0.09	118,118,118,118	0
14	NAG	B	703	14/15	0.81	0.16	37,37,37,37	0
14	NAG	G	606	14/15	0.86	0.12	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.