wwPDB X-ray Structure Validation Summary Report (i)

Sep 28, 2024 – 08:16 AM EDT

PDB ID	:	5U7M
Title	:	Crystal Structure of HIV-1 BG505 SOSIP.664 Prefusion Env Trimer Bound to Small Molecule HIV-1 Entry Inhibitor BMS-378806 in Complex with Human Antibodies PGT122 and 35O22 at 3.8 Angstrom
Authors	:	Pancera, M.; Lai, Y.-T.; Kwong, P.D.
Deposited on	:	2016-12-12
Resolution	:	3.02 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:

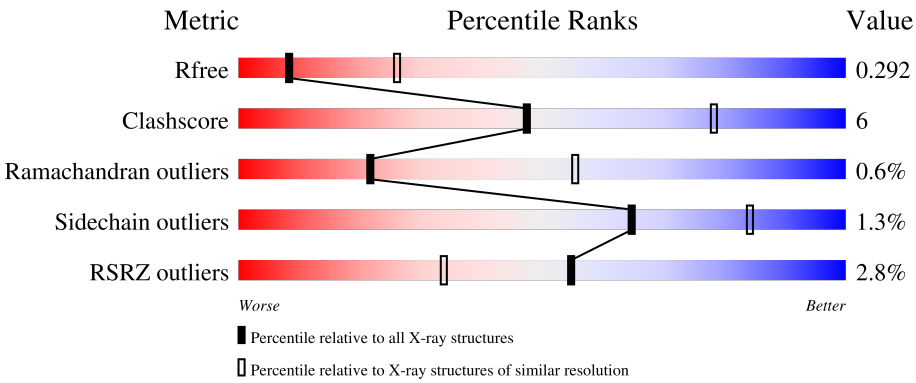
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & 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 3.02 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	2927 (3.04-3.00)
Clashscore	180529	3300 (3.04-3.00)
Ramachandran outliers	177936	3188 (3.04-3.00)
Sidechain outliers	177891	3191 (3.04-3.00)
RSRZ outliers	164620	2939 (3.04-3.00)

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	2%, 71%, 12%, 18%
2	D	243	7%, 87%, 12%
3	E	216	%, 89%, 9% •
4	G	481	%, 77%, 14% • 8%

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Mol	Chain	Length	Quality of chain
5	H	235	3% 79% 17%
6	L	213	3% 81% 16%
7	A	7	29% 57% 14%
8	C	3	33% 67%
8	S	3	100%
9	F	5	60% 40%
10	I	2	50% 50%
10	J	2	50% 50%
10	M	2	100%
10	N	2	100%
10	P	2	100%
10	Q	2	100%
10	R	2	100%
11	K	6	33% 67%
12	O	10	20% 80%

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 12026 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	126	1001	633	172	190	6	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S5
B	605	CYS	THR	engineered mutation	UNP Q2N0S5

- Molecule 2 is a protein called 35O22 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	242	1832	1165	306	353	8	0	0	0

- Molecule 3 is a protein called 35O22 FAB LIGHT CHAIN.

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

- Molecule 4 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	G	442	3472	2183	614	648	27	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	332	ASN	THR	engineered mutation	UNP Q2N0S5
G	501	CYS	ALA	engineered mutation	UNP Q2N0S5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	509	ARG	GLU	engineered mutation	UNP Q2N0S5
G	510	ARG	LYS	engineered mutation	UNP Q2N0S5
G	512	ARG	ALA	engineered mutation	UNP Q2N0S5
G	513	ARG	VAL	engineered mutation	UNP Q2N0S5

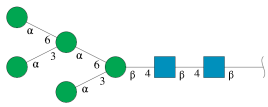
- Molecule 5 is a protein called PGT122 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	H	228	1742	1109	295	333	5	0	0	0

- Molecule 6 is a protein called PGT122 FAB LIGHT CHAIN.

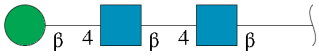
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	L	208	1577	990	265	318	4	0	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

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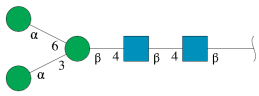
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
8	S	3	39	22	2	15	0	0	0

- Molecule 9 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.

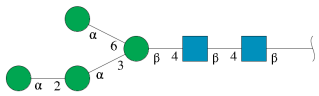


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	F	5	61	34	2	25	0	0	0

- Molecule 10 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

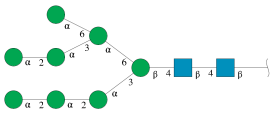
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	I	2	28	16	2	10	0	0	0
10	J	2	28	16	2	10	0	0	0
10	M	2	28	16	2	10	0	0	0
10	N	2	28	16	2	10	0	0	0
10	P	2	28	16	2	10	0	0	0
10	Q	2	28	16	2	10	0	0	0
10	R	2	28	16	2	10	0	0	0

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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.



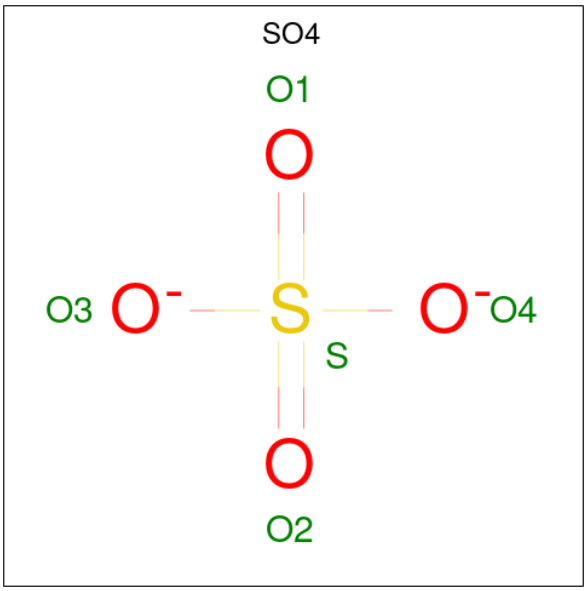
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
11	K	6	72	40	2	30	0	0	0

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-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			
12	O	10	116	64	2	50	0	0	0

- Molecule 13 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
13	B	1	5	4	1	0	0

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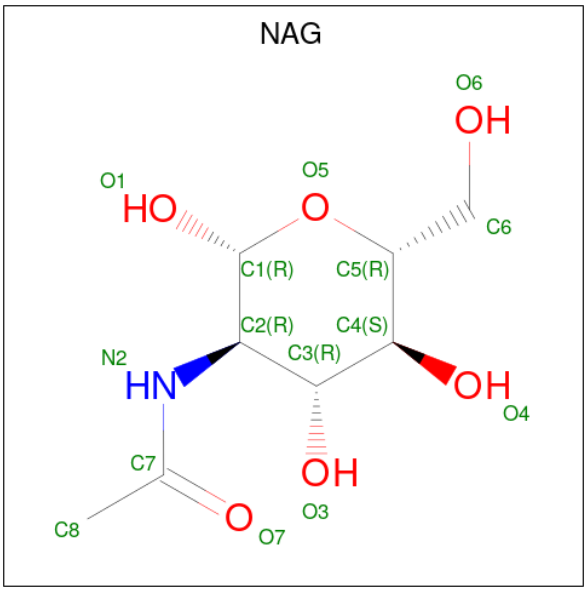
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
13	G	1	5	4	1		0	0
			Total	O	S			
13	G	1	5	4	1		0	0
			Total	O	S			
13	G	1	5	4	1		0	0
			Total	O	S			
13	L	1	5	4	1		0	0

- 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
			Total	C	N	O		
14	B	1	14	8	1	5	0	0
			Total	C	N	O		
14	B	1	14	8	1	5	0	0
			Total	C	N	O		
14	G	1	14	8	1	5	0	0
			Total	C	N	O		
14	G	1	14	8	1	5	0	0
			Total	C	N	O		
14	G	1	14	8	1	5	0	0
			Total	C	N	O		
14	G	1	14	8	1	5	0	0

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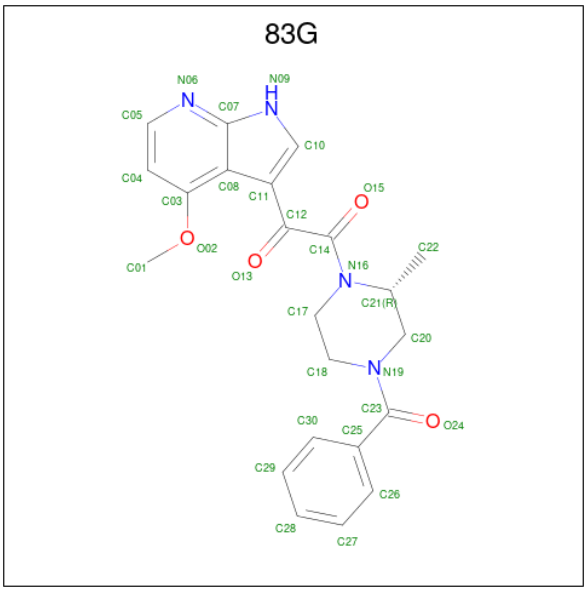
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
14	G	1	14	8	1	5	0	0
			Total	C	N	O		
14	H	1	14	8	1	5	0	0

- Molecule 15 is 1-[(2R)-4-(benzenecarbonyl)-2-methylpiperazin-1-yl]-2-(4-methoxy-1H-pyrrolo[2,3-b]pyridin-3-yl)ethane-1,2-dione (three-letter code: 83G) (formula: $C_{22}H_{22}N_4O_4$).



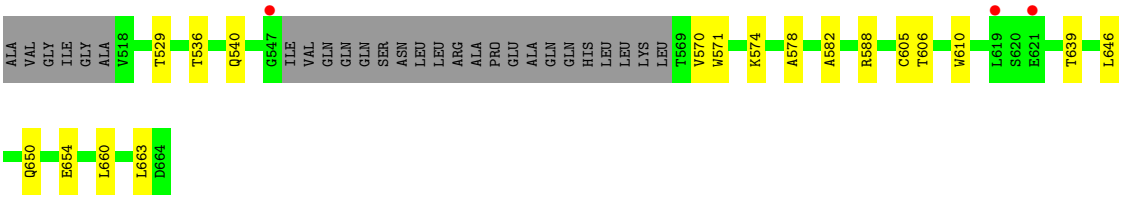
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
15	G	1	30	22	4	4	0	0

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.

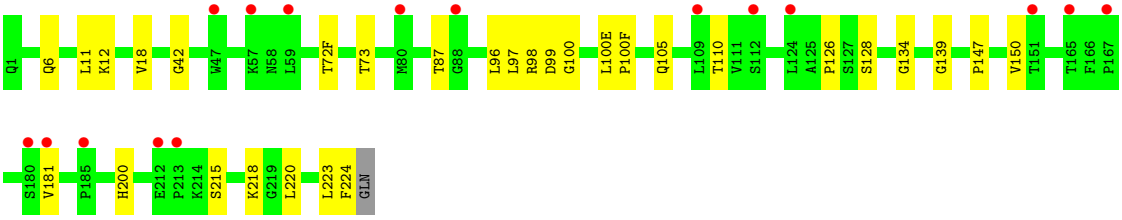
• Molecule 1: Envelope glycoprotein gp160

Chain B:



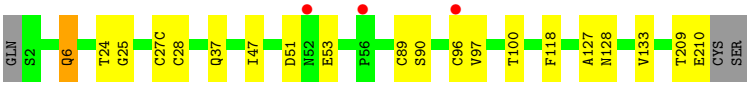
• Molecule 2: 35O22 FAB HEAVY CHAIN

Chain D:



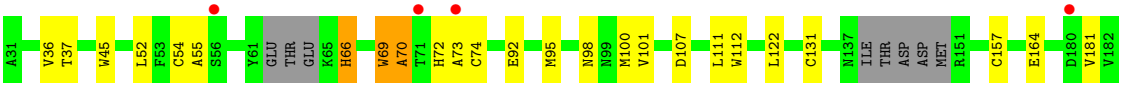
• Molecule 3: 35O22 FAB LIGHT CHAIN

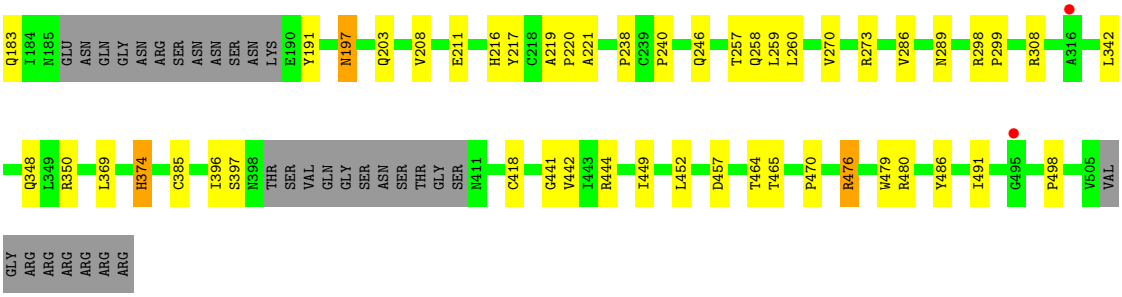
Chain E:



• Molecule 4: Envelope glycoprotein gp160

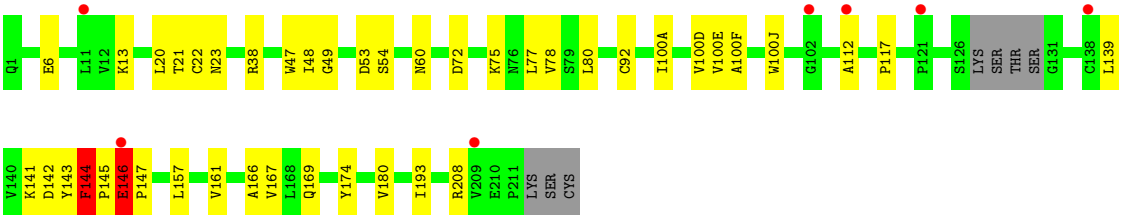
Chain G:





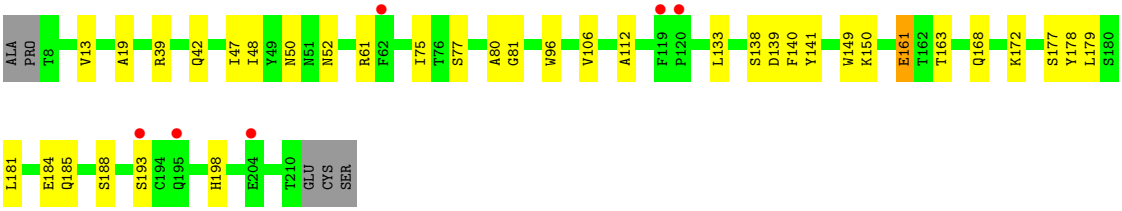
• Molecule 5: PGT122 FAB HEAVY CHAIN

Chain H:



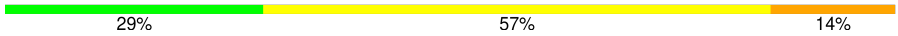
• Molecule 6: PGT122 FAB LIGHT CHAIN

Chain L:



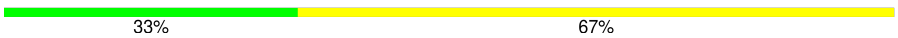
• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:



• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S: 100%

NAG1 NAG2 BMA3

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

Chain F: 60% 40%

NAG1 NAG2 BMA3 MAN4 MAN5

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

Chain I: 50% 50%

NAG1 NAG2

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

Chain J: 50% 50%

NAG1 NAG2

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

Chain M: 100%

NAG1 NAG2

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

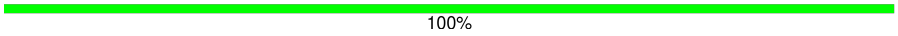
Chain N: 100%

NAG1 NAG2

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

Chain P: 100%

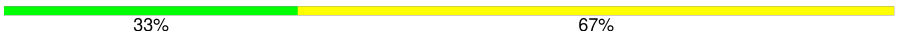
• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

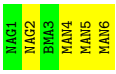
Chain Q: 

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

Chain R:

• Molecule 11: alpha-D-mannopyranose-(1-2)-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 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-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 O:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	129.19Å 129.19Å 312.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.82 – 3.02 40.82 – 3.02	Depositor EDS
% Data completeness (in resolution range)	51.7 (40.82-3.02) 51.7 (40.82-3.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.65 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.245 , 0.289 0.246 , 0.292	Depositor DCC
R_{free} test set	1526 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å^2)	71.8	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 56.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.096 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	12026	wwPDB-VP
Average B, all atoms (Å^2)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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: MAN, NAG, BMA, SO4, 83G

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	0.23	0/1019	0.38	0/1382
2	D	0.24	0/1880	0.44	0/2560
3	E	0.24	0/1659	0.44	0/2269
4	G	0.24	0/3544	0.43	0/4811
5	H	0.24	0/1789	0.47	1/2443 (0.0%)
6	L	0.23	0/1619	0.43	0/2217
All	All	0.24	0/11510	0.43	1/15682 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	H	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	146	GLU	C-N-CD	-6.24	106.87	120.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	H	144	PHE	Peptide

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	B	1001	0	975	16	0
2	D	1832	0	1806	16	0
3	E	1615	0	1542	12	0
4	G	3472	0	3404	47	0
5	H	1742	0	1715	26	0
6	L	1577	0	1518	24	0
7	A	83	0	70	1	0
8	C	39	0	34	1	0
8	S	39	0	34	0	0
9	F	61	0	52	0	0
10	I	28	0	25	1	0
10	J	28	0	25	1	0
10	M	28	0	25	0	0
10	N	28	0	25	0	0
10	P	28	0	25	0	0
10	Q	28	0	25	0	0
10	R	28	0	25	0	0
11	K	72	0	61	1	0
12	O	116	0	97	1	0
13	B	5	0	0	1	0
13	G	15	0	0	0	0
13	L	5	0	0	0	0
14	B	42	0	39	1	0
14	G	70	0	65	1	0
14	H	14	0	13	0	0
15	G	30	0	0	0	0
All	All	12026	0	11600	131	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 6.

The worst 5 of 131 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)
6:L:39:ARG:NH1	6:L:81:GLY:O	2.08	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:55:ALA:HB3	4:G:216:HIS:HB2	1.69	0.75
1:B:536:THR:O	1:B:540:GLN:NE2	2.27	0.68
6:L:61:ARG:NH1	6:L:77:SER:O	2.28	0.66
6:L:19:ALA:HB3	6:L:75:ILE:HB	1.78	0.66

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	122/153 (80%)	116 (95%)	6 (5%)	0	100	100
2	D	240/243 (99%)	227 (95%)	12 (5%)	1 (0%)	30	64
3	E	211/216 (98%)	194 (92%)	16 (8%)	1 (0%)	25	59
4	G	432/481 (90%)	392 (91%)	35 (8%)	5 (1%)	11	39
5	H	224/235 (95%)	211 (94%)	11 (5%)	2 (1%)	14	47
6	L	206/213 (97%)	189 (92%)	17 (8%)	0	100	100
All	All	1435/1541 (93%)	1329 (93%)	97 (7%)	9 (1%)	22	55

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	H	147	PRO
4	G	70	ALA
4	G	374	HIS
3	E	51	ASP
5	H	142	ASP

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	108/129 (84%)	107 (99%)	1 (1%)	75	89
2	D	205/206 (100%)	205 (100%)	0	100	100
3	E	186/189 (98%)	185 (100%)	1 (0%)	86	94
4	G	392/428 (92%)	383 (98%)	9 (2%)	45	74
5	H	198/205 (97%)	194 (98%)	4 (2%)	50	77
6	L	177/181 (98%)	176 (99%)	1 (1%)	84	92
All	All	1266/1338 (95%)	1250 (99%)	16 (1%)	65	84

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	H	146	GLU
5	H	144	PHE
4	G	444	ARG
5	H	100(J)	TRP
4	G	369	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
4	G	66	HIS
4	G	72	HIS
4	G	203	GLN
4	G	246	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)

48 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	4,7	14,14,15	0.32	0	17,19,21	0.50	0
7	NAG	A	2	7	14,14,15	0.48	0	17,19,21	1.35	2 (11%)
7	BMA	A	3	7	11,11,12	0.63	0	15,15,17	0.71	0
7	MAN	A	4	7	11,11,12	0.82	1 (9%)	15,15,17	1.22	2 (13%)
7	MAN	A	5	7	11,11,12	0.63	0	15,15,17	1.03	2 (13%)
7	MAN	A	6	7	11,11,12	0.63	0	15,15,17	1.11	2 (13%)
7	MAN	A	7	7	11,11,12	0.63	0	15,15,17	1.07	2 (13%)
8	NAG	C	1	8,4	14,14,15	0.30	0	17,19,21	0.43	0
8	NAG	C	2	8	14,14,15	0.23	0	17,19,21	0.40	0
8	BMA	C	3	8	11,11,12	0.53	0	15,15,17	0.82	0
9	NAG	F	1	4,9	14,14,15	0.22	0	17,19,21	0.47	0
9	NAG	F	2	9	14,14,15	0.24	0	17,19,21	0.42	0
9	BMA	F	3	9	11,11,12	0.64	0	15,15,17	0.65	0
9	MAN	F	4	9	11,11,12	0.64	0	15,15,17	1.05	2 (13%)
9	MAN	F	5	9	11,11,12	0.65	0	15,15,17	1.12	2 (13%)
10	NAG	I	1	4,10	14,14,15	0.30	0	17,19,21	0.49	0
10	NAG	I	2	10	14,14,15	0.46	0	17,19,21	1.33	2 (11%)
10	NAG	J	1	4,10	14,14,15	0.38	0	17,19,21	0.60	0
10	NAG	J	2	10	14,14,15	0.25	0	17,19,21	0.49	0
11	NAG	K	1	4,11	14,14,15	0.21	0	17,19,21	0.49	0
11	NAG	K	2	11	14,14,15	0.34	0	17,19,21	0.41	0
11	BMA	K	3	11	11,11,12	0.70	0	15,15,17	0.68	0
11	MAN	K	4	11	11,11,12	0.66	0	15,15,17	1.03	2 (13%)
11	MAN	K	5	11	11,11,12	0.74	0	15,15,17	1.12	2 (13%)
11	MAN	K	6	11	11,11,12	0.65	0	15,15,17	1.03	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	NAG	M	1	4,10	14,14,15	0.22	0	17,19,21	0.52	0
10	NAG	M	2	10	14,14,15	0.22	0	17,19,21	0.43	0
10	NAG	N	1	4,10	14,14,15	0.20	0	17,19,21	0.42	0
10	NAG	N	2	10	14,14,15	0.23	0	17,19,21	0.45	0
12	NAG	O	1	12,4	14,14,15	0.21	0	17,19,21	0.44	0
12	MAN	O	10	12	11,11,12	0.70	0	15,15,17	0.98	2 (13%)
12	NAG	O	2	12	14,14,15	0.24	0	17,19,21	0.60	0
12	BMA	O	3	12	11,11,12	0.76	0	15,15,17	0.90	0
12	MAN	O	4	12	11,11,12	0.60	0	15,15,17	1.14	1 (6%)
12	MAN	O	5	12	11,11,12	0.61	0	15,15,17	1.02	2 (13%)
12	MAN	O	6	12	11,11,12	0.63	0	15,15,17	1.30	2 (13%)
12	MAN	O	7	12	11,11,12	0.71	0	15,15,17	0.96	2 (13%)
12	MAN	O	8	12	11,11,12	0.75	0	15,15,17	1.07	1 (6%)
12	MAN	O	9	12	11,11,12	0.79	0	15,15,17	1.12	2 (13%)
10	NAG	P	1	4,10	14,14,15	0.21	0	17,19,21	0.51	0
10	NAG	P	2	10	14,14,15	0.23	0	17,19,21	0.48	0
10	NAG	Q	1	4,10	14,14,15	0.27	0	17,19,21	0.67	0
10	NAG	Q	2	10	14,14,15	0.23	0	17,19,21	0.46	0
10	NAG	R	1	4,10	14,14,15	0.24	0	17,19,21	0.45	0
10	NAG	R	2	10	14,14,15	0.31	0	17,19,21	0.53	0
8	NAG	S	1	8,4	14,14,15	0.22	0	17,19,21	0.60	0
8	NAG	S	2	8	14,14,15	0.20	0	17,19,21	0.41	0
8	BMA	S	3	8	11,11,12	0.58	0	15,15,17	0.77	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	4,7	-	2/6/23/26	0/1/1/1
7	NAG	A	2	7	-	4/6/23/26	0/1/1/1
7	BMA	A	3	7	-	2/2/19/22	0/1/1/1
7	MAN	A	4	7	-	0/2/19/22	0/1/1/1
7	MAN	A	5	7	-	0/2/19/22	0/1/1/1
7	MAN	A	6	7	-	0/2/19/22	0/1/1/1
7	MAN	A	7	7	-	0/2/19/22	0/1/1/1
8	NAG	C	1	8,4	-	2/6/23/26	0/1/1/1
8	NAG	C	2	8	-	2/6/23/26	0/1/1/1
8	BMA	C	3	8	-	0/2/19/22	0/1/1/1

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	4	MAN	C1-C2	2.15	1.57	1.52

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	2	NAG	C2-N2-C7	4.62	129.09	122.90
10	I	2	NAG	C2-N2-C7	4.58	129.04	122.90
12	O	6	MAN	C1-O5-C5	4.09	117.67	112.19
12	O	9	MAN	C1-O5-C5	3.26	116.55	112.19
11	K	5	MAN	C1-O5-C5	3.26	116.55	112.19

There are no chirality outliers.

5 of 67 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	N	1	NAG	O5-C5-C6-O6
7	A	3	BMA	C4-C5-C6-O6
8	C	2	NAG	O5-C5-C6-O6
8	C	1	NAG	O5-C5-C6-O6
7	A	3	BMA	O5-C5-C6-O6

All (2) ring outliers are listed below:

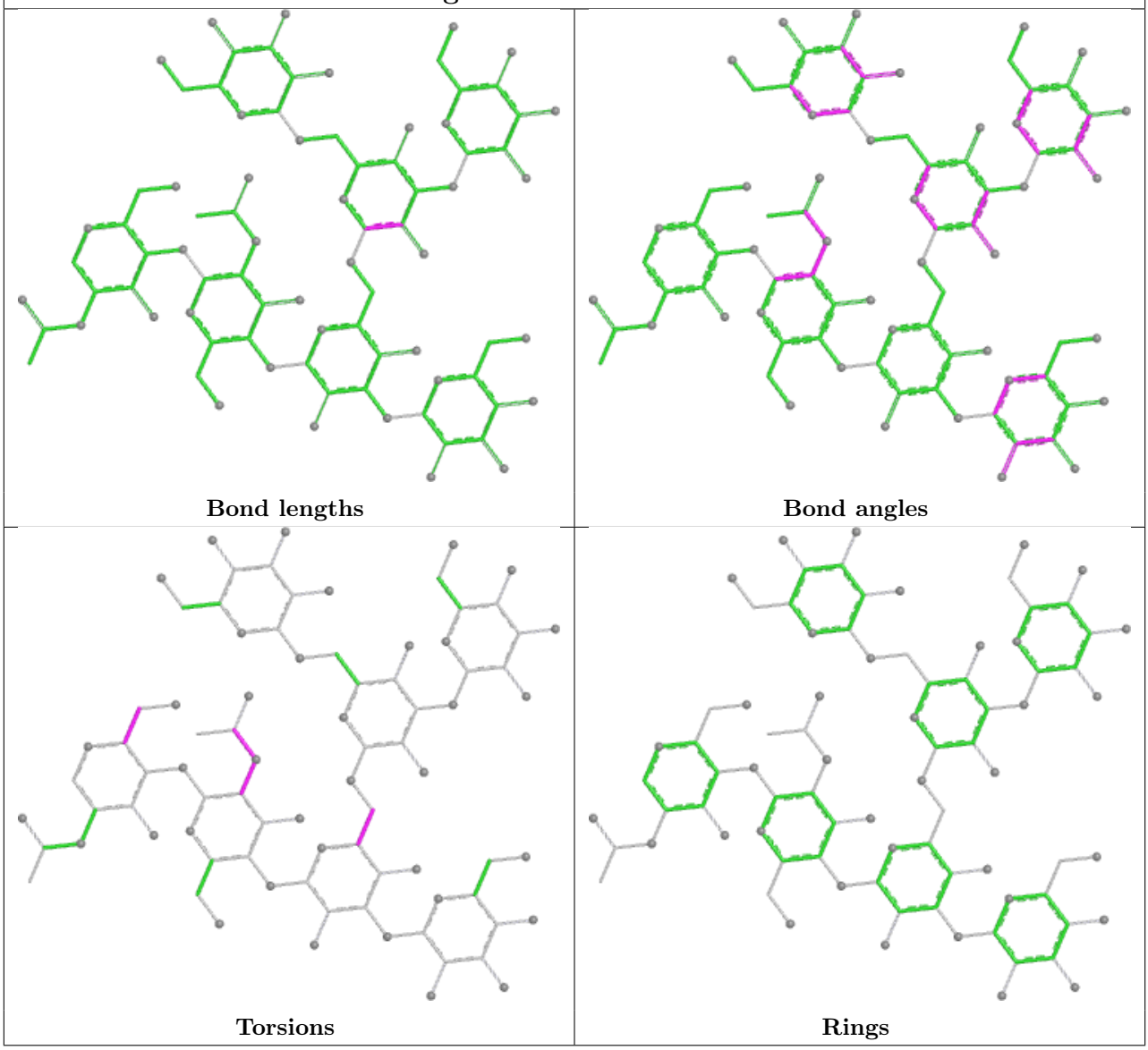
Mol	Chain	Res	Type	Atoms
12	O	9	MAN	C1-C2-C3-C4-C5-O5
11	K	5	MAN	C1-C2-C3-C4-C5-O5

7 monomers are involved in 6 short contacts:

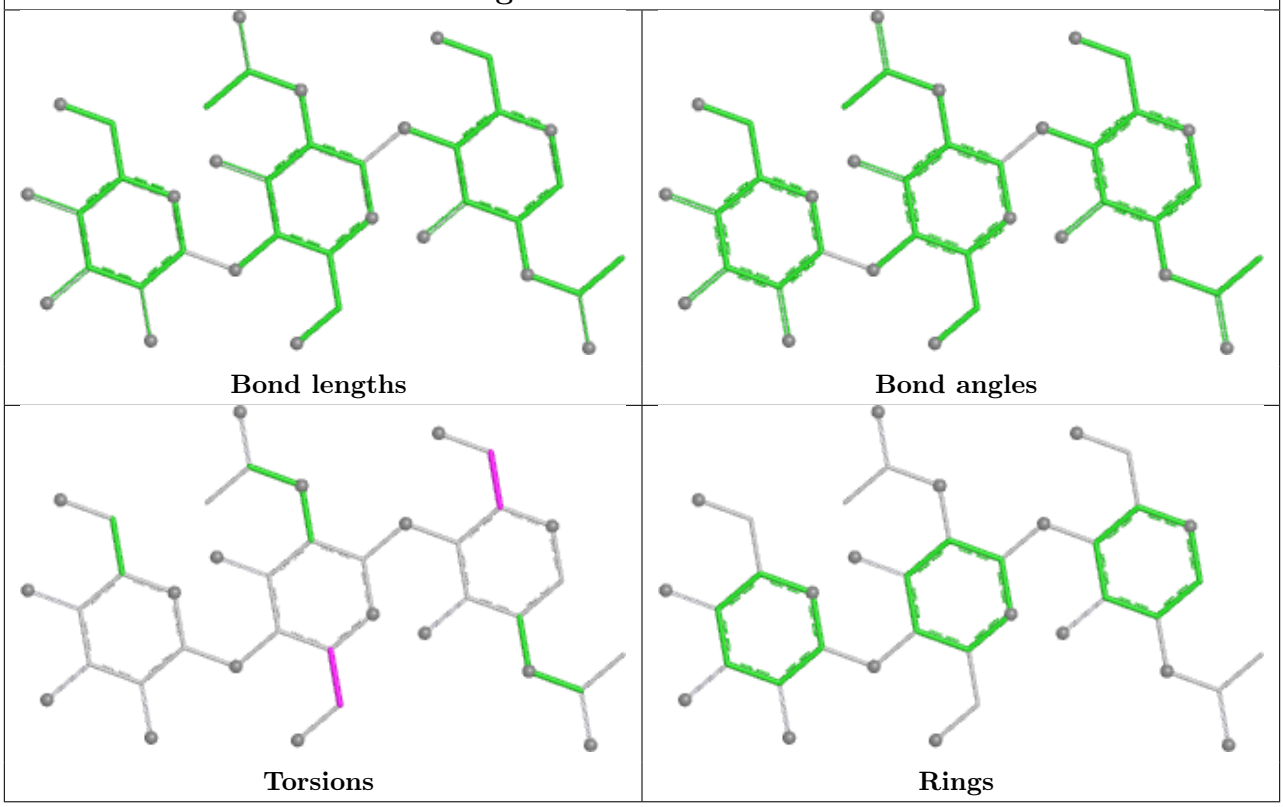
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	J	1	NAG	1	0
10	I	2	NAG	1	0
8	C	2	NAG	1	0
11	K	2	NAG	1	0
8	C	3	BMA	1	0
7	A	2	NAG	1	0
12	O	2	NAG	1	0

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

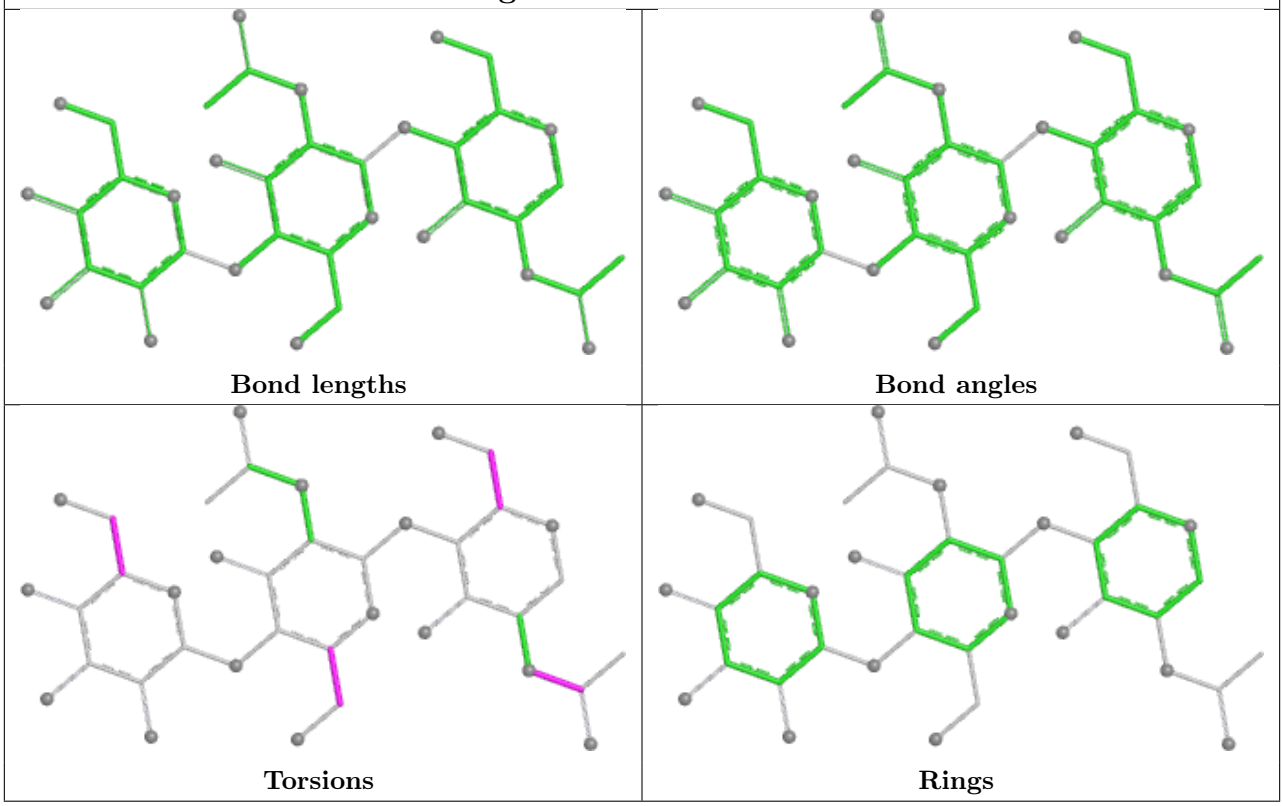
Oligosaccharide Chain A



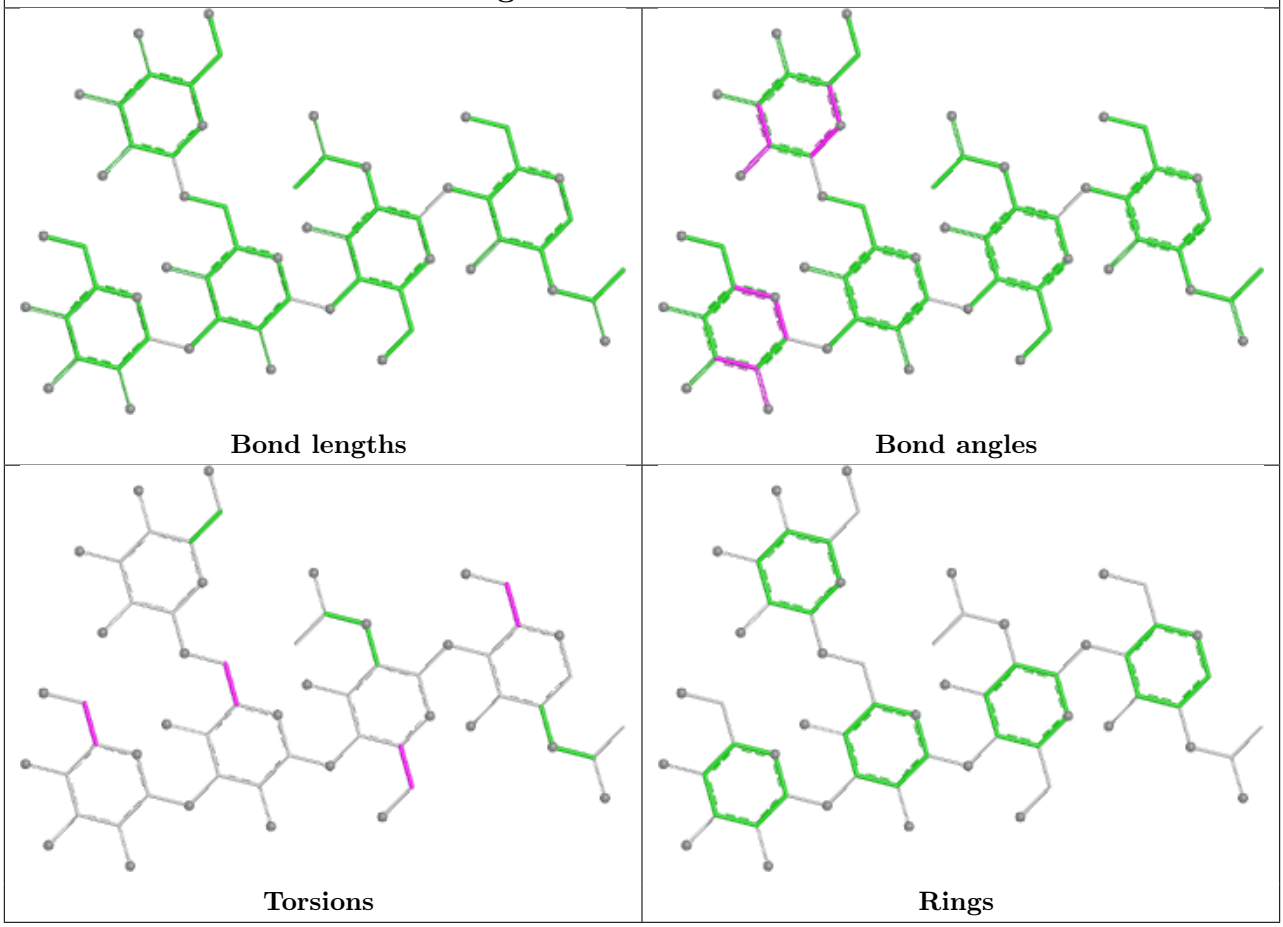
Oligosaccharide Chain C



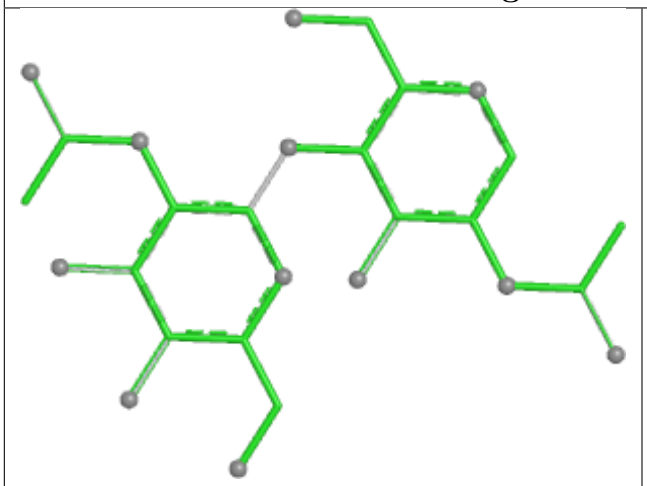
Oligosaccharide Chain S



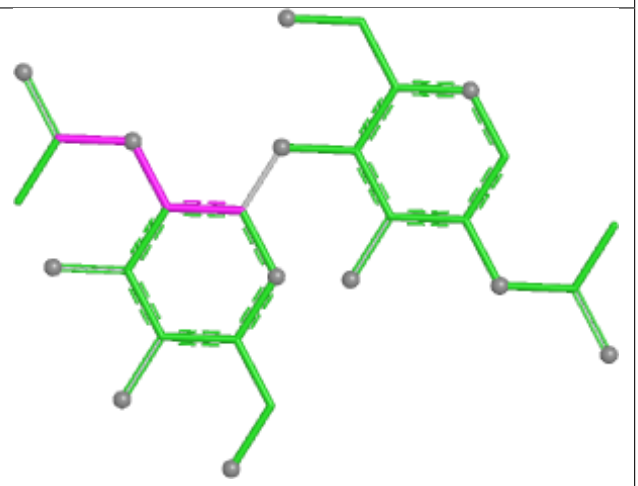
Oligosaccharide Chain F



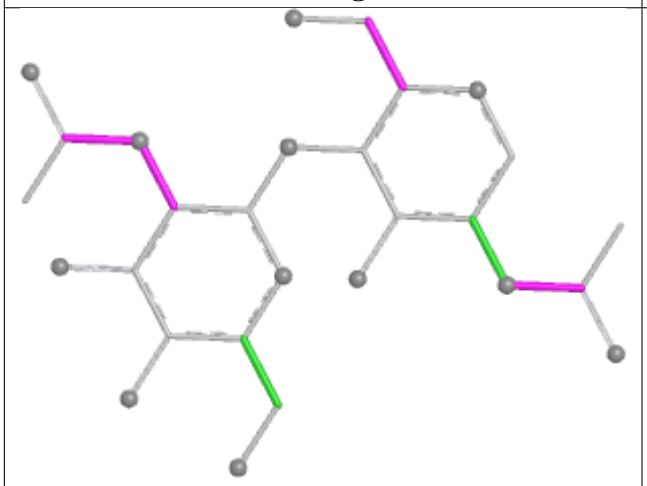
Oligosaccharide Chain I



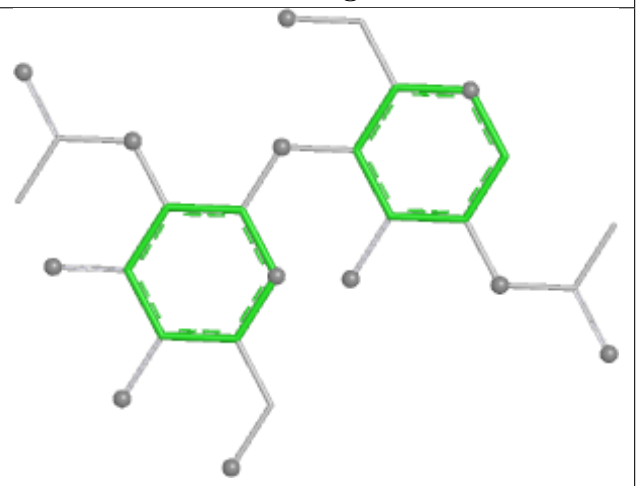
Bond lengths



Bond angles

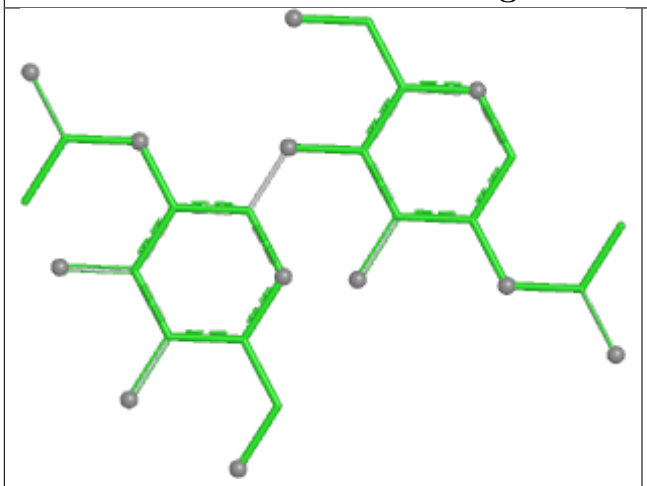


Torsions

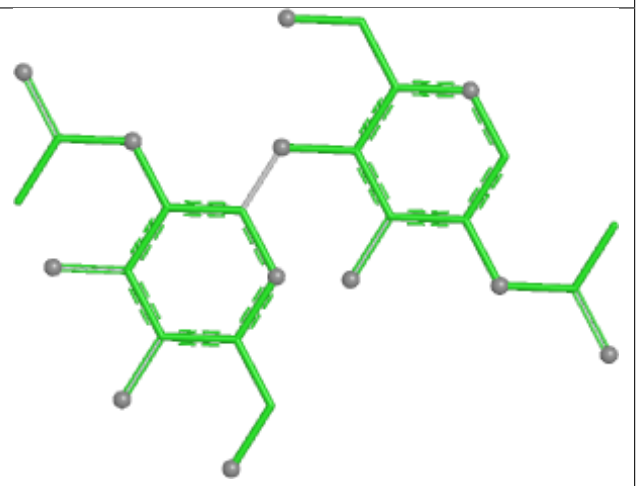


Rings

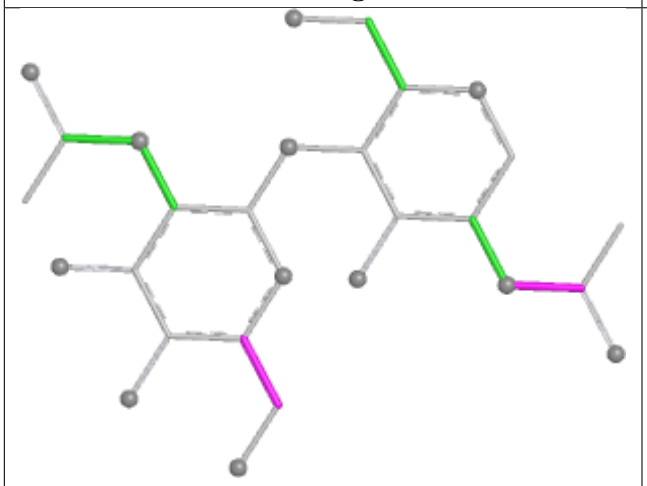
Oligosaccharide Chain J



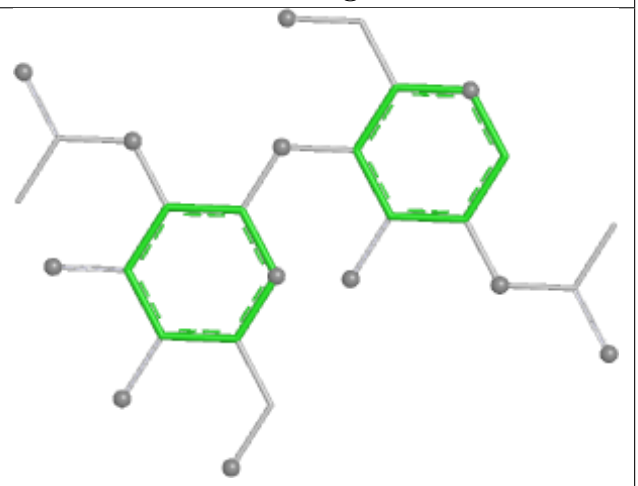
Bond lengths



Bond angles

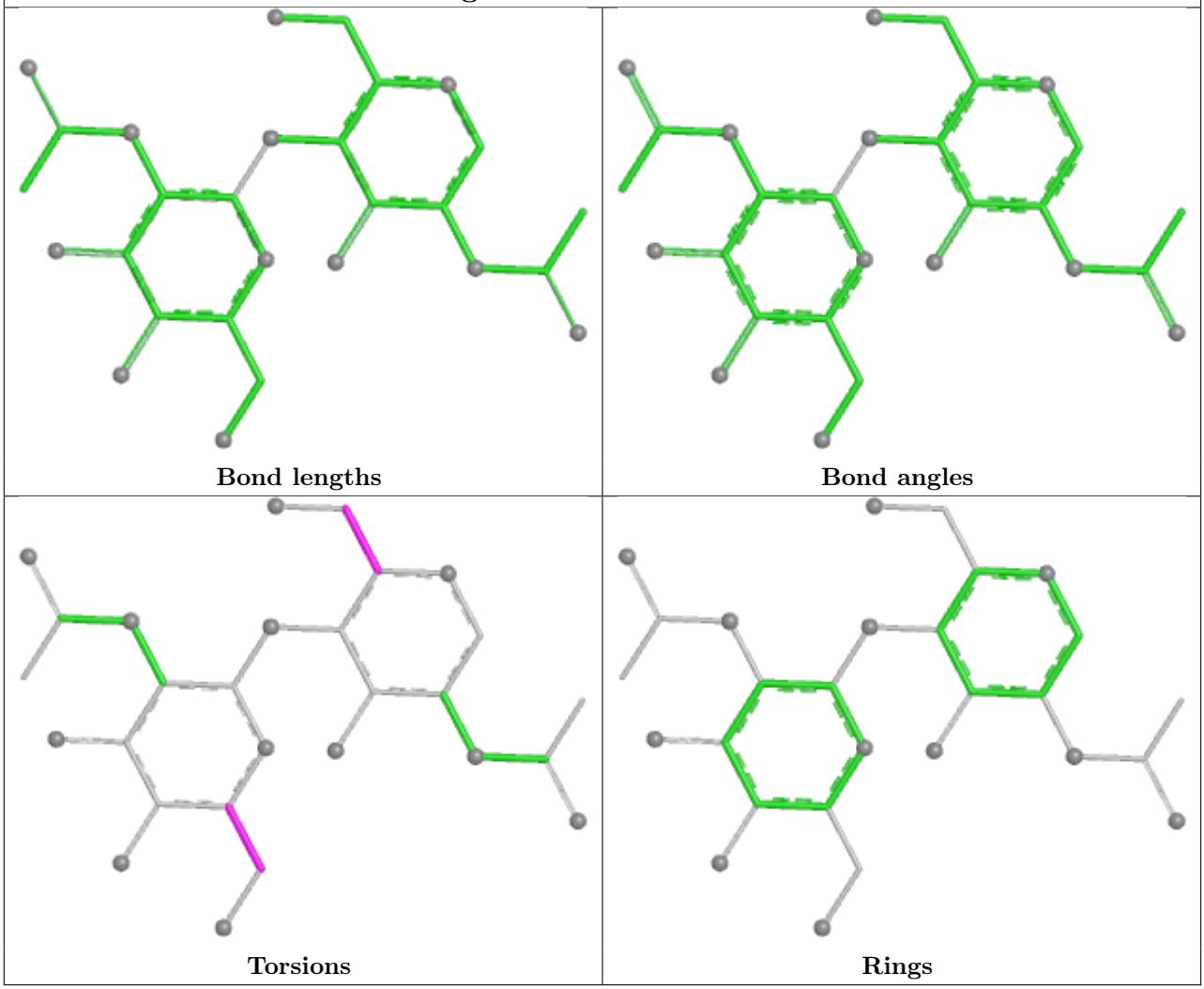


Torsions

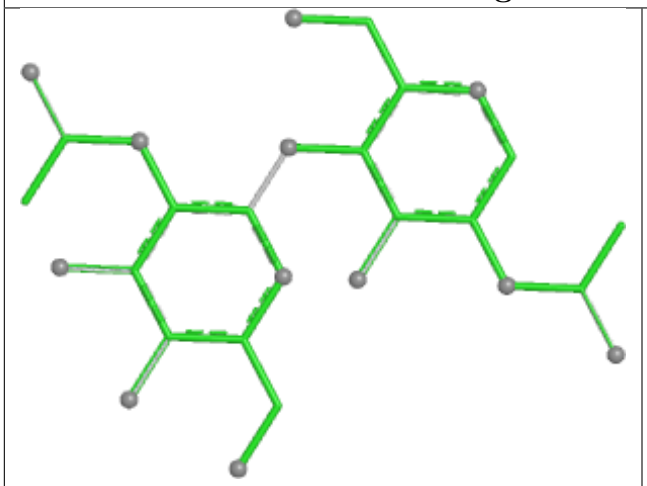


Rings

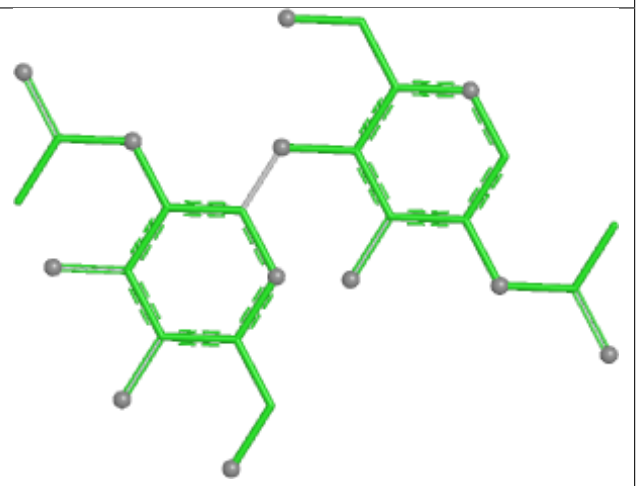
Oligosaccharide Chain M



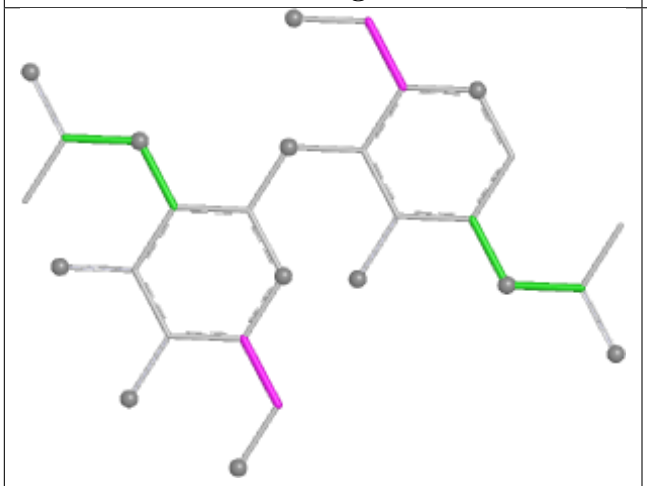
Oligosaccharide Chain N



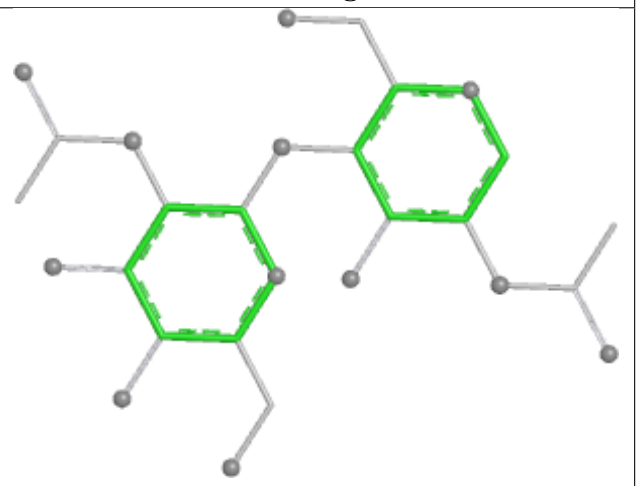
Bond lengths



Bond angles

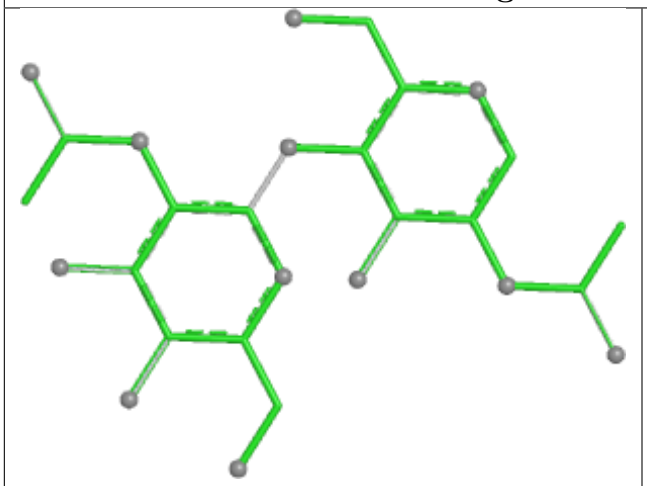


Torsions

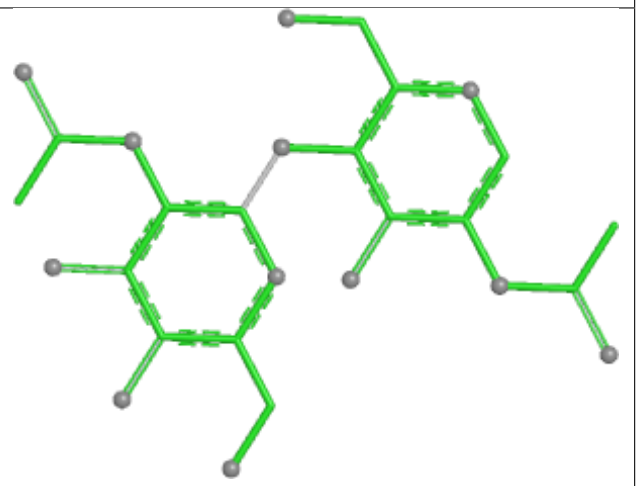


Rings

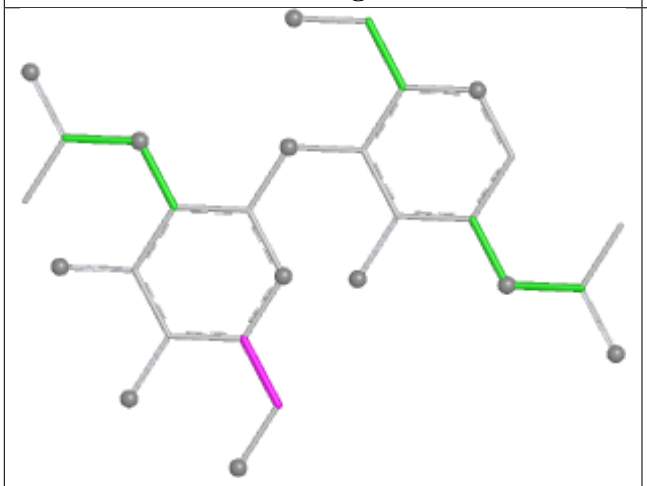
Oligosaccharide Chain P



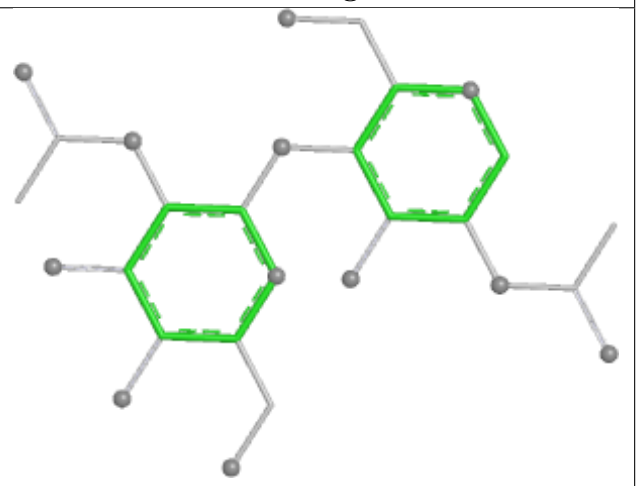
Bond lengths



Bond angles

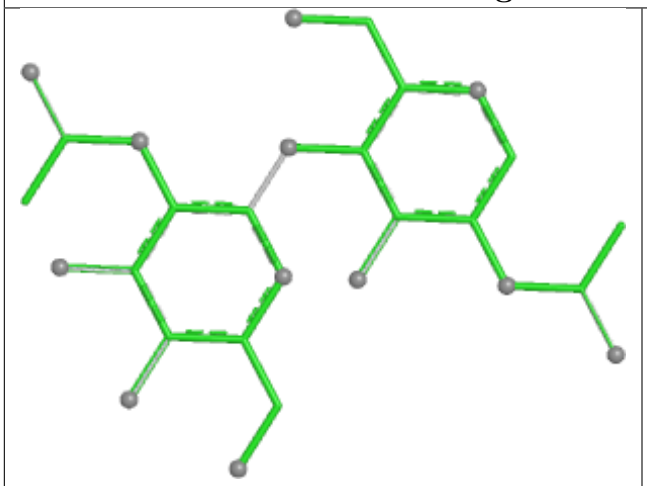


Torsions

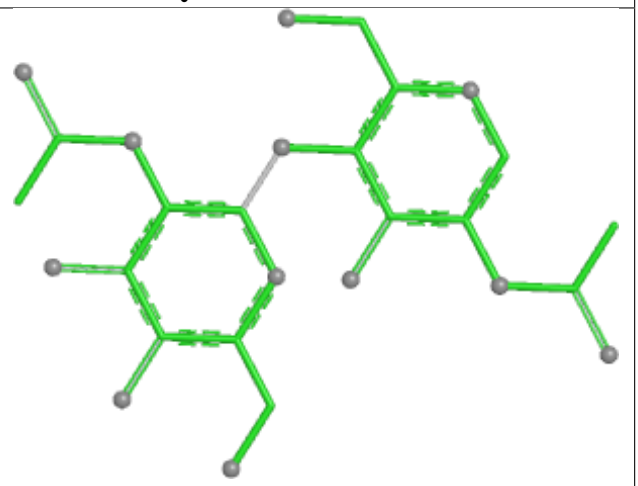


Rings

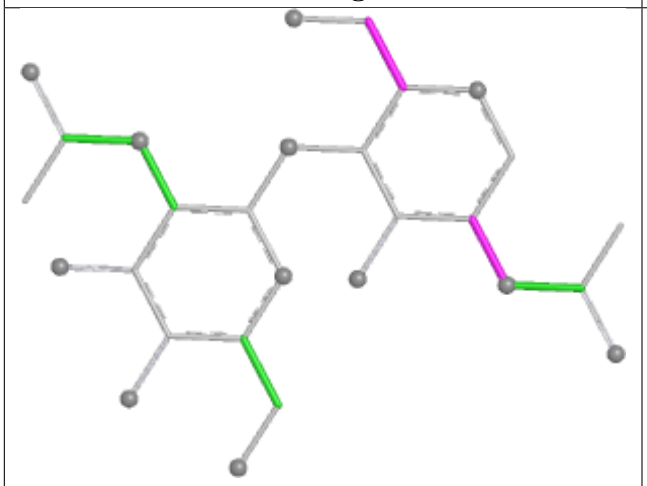
Oligosaccharide Chain Q



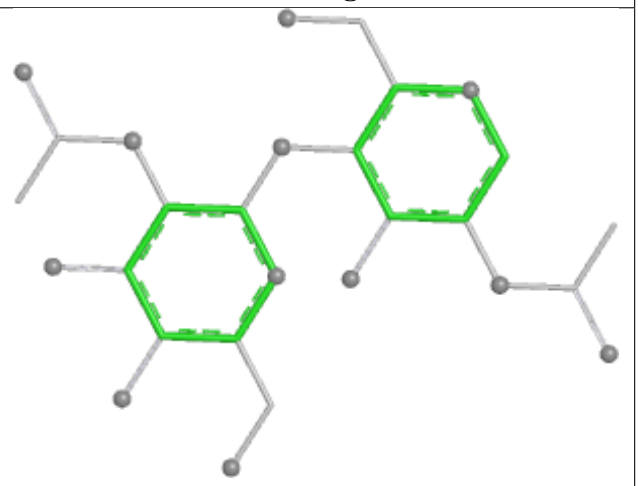
Bond lengths



Bond angles

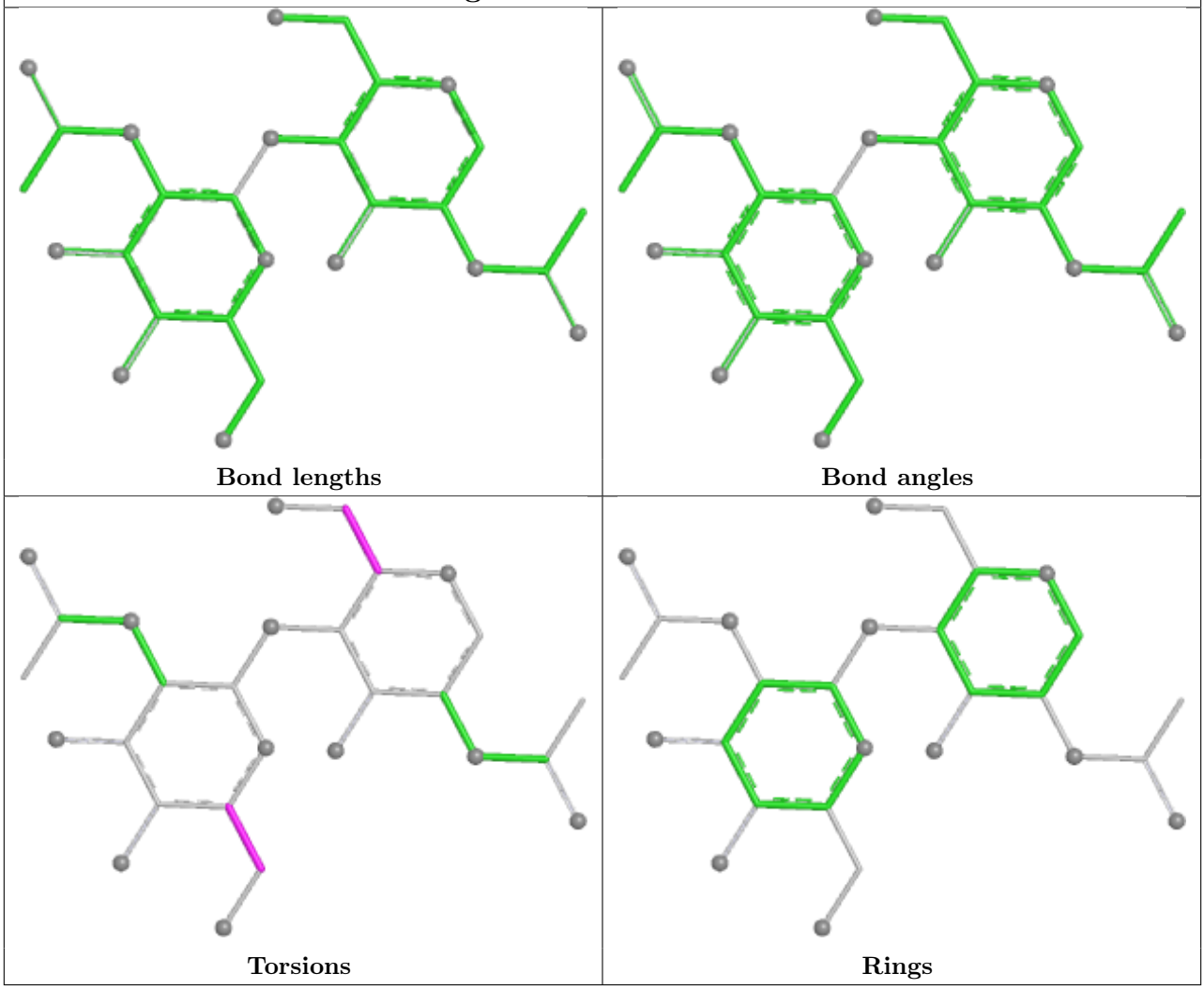


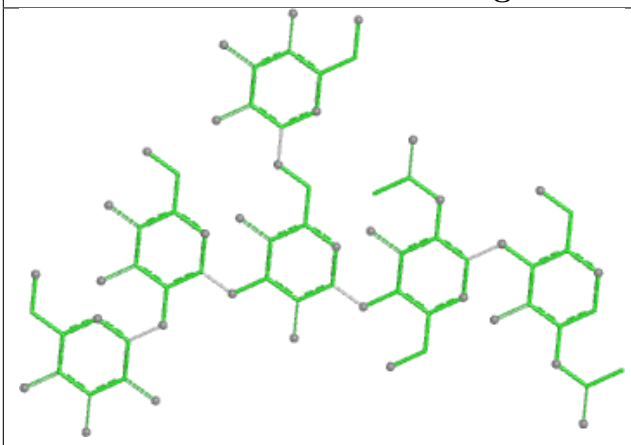
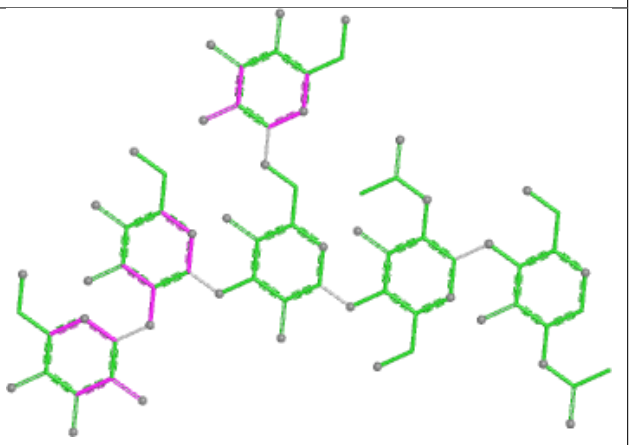
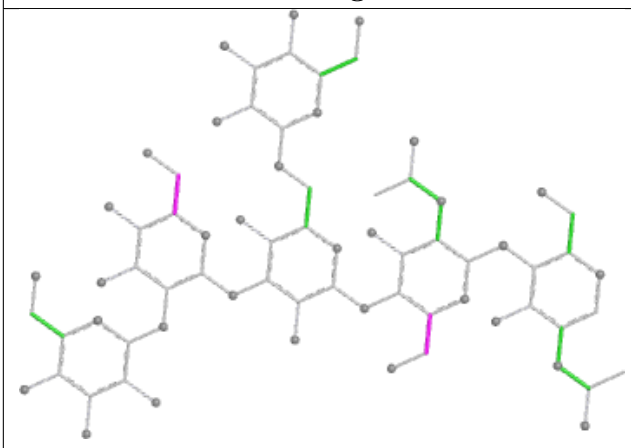
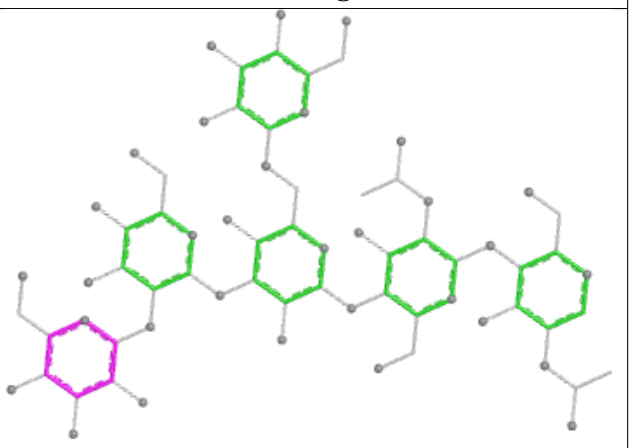
Torsions



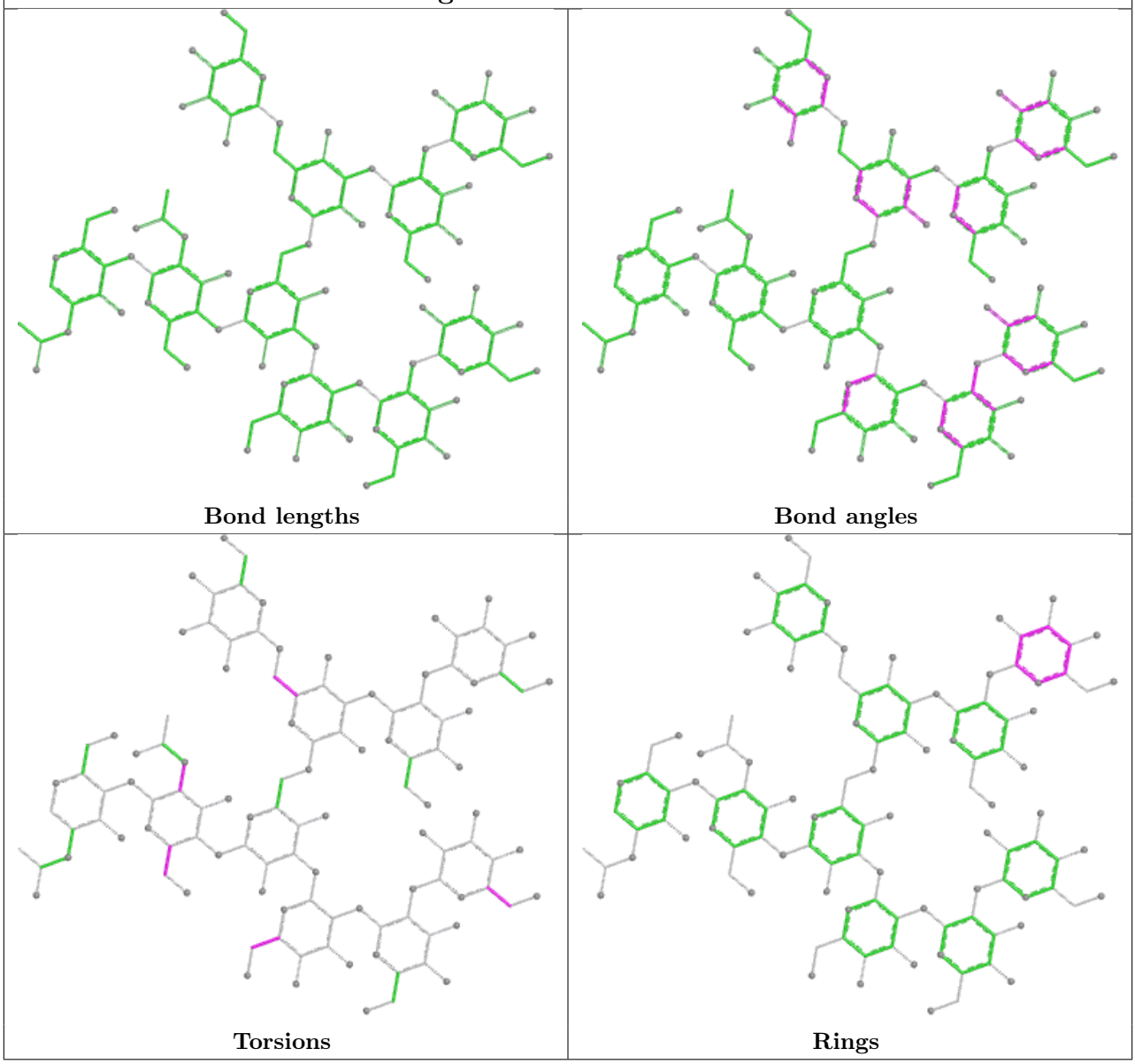
Rings

Oligosaccharide Chain R



Oligosaccharide Chain K	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain O



5.6 Ligand geometry (i)

15 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	B	704	1	14,14,15	0.25	0	17,19,21	0.45	0
13	SO4	G	601	-	4,4,4	0.24	0	6,6,6	0.08	0
14	NAG	G	656	4	14,14,15	0.21	0	17,19,21	0.42	0
13	SO4	G	603	-	4,4,4	0.24	0	6,6,6	0.08	0
13	SO4	B	701	-	4,4,4	0.23	0	6,6,6	0.07	0
13	SO4	G	602	-	4,4,4	0.23	0	6,6,6	0.07	0
14	NAG	H	301	5	14,14,15	0.25	0	17,19,21	0.43	0
15	83G	G	657	-	32,33,33	2.30	12 (37%)	39,47,47	2.15	8 (20%)
14	NAG	G	631	4	14,14,15	0.47	0	17,19,21	1.35	2 (11%)
14	NAG	B	702	1	14,14,15	0.25	0	17,19,21	0.46	0
14	NAG	B	703	1	14,14,15	0.21	0	17,19,21	0.39	0
14	NAG	G	624	4	14,14,15	0.20	0	17,19,21	0.43	0
13	SO4	L	301	-	4,4,4	0.23	0	6,6,6	0.07	0
14	NAG	G	611	4	14,14,15	0.23	0	17,19,21	0.46	0
14	NAG	G	646	4	14,14,15	0.20	0	17,19,21	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	NAG	B	704	1	-	0/6/23/26	0/1/1/1
14	NAG	G	656	4	-	0/6/23/26	0/1/1/1
14	NAG	H	301	5	-	2/6/23/26	0/1/1/1
15	83G	G	657	-	-	0/18/35/35	0/4/4/4
14	NAG	G	631	4	-	6/6/23/26	0/1/1/1
14	NAG	B	702	1	-	2/6/23/26	0/1/1/1
14	NAG	G	624	4	-	2/6/23/26	0/1/1/1
14	NAG	B	703	1	-	2/6/23/26	0/1/1/1
14	NAG	G	611	4	-	3/6/23/26	0/1/1/1
14	NAG	G	646	4	-	4/6/23/26	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	G	657	83G	C14-N16	7.56	1.45	1.34
15	G	657	83G	C23-N19	5.78	1.47	1.34
15	G	657	83G	C10-N09	-3.86	1.28	1.36
15	G	657	83G	C07-N06	-3.01	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	G	657	83G	C11-C08	-2.88	1.38	1.42

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	G	657	83G	C11-C08-C07	-7.22	101.78	107.54
15	G	657	83G	C21-C20-N19	-5.47	104.74	110.99
14	G	631	NAG	C2-N2-C7	4.56	129.00	122.90
15	G	657	83G	C17-N16-C21	3.68	120.83	114.75
15	G	657	83G	C10-C11-C12	-3.67	119.97	127.72

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

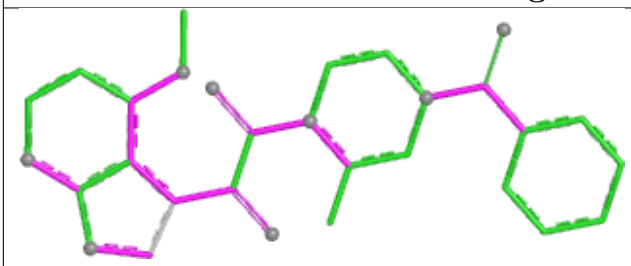
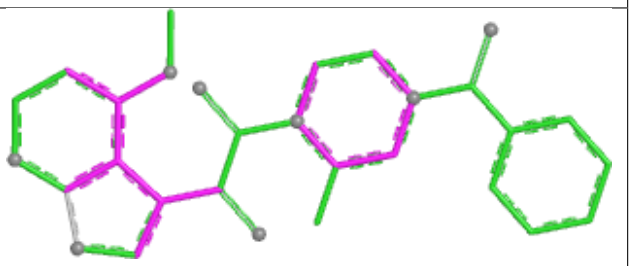
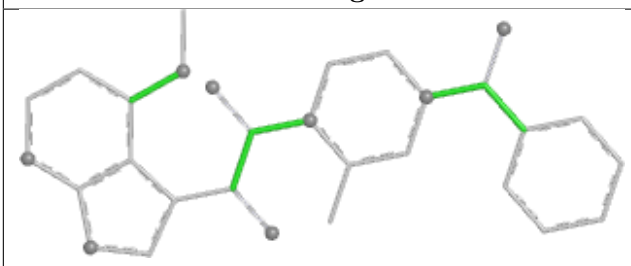
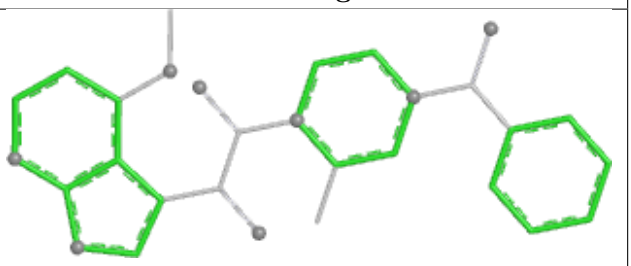
Mol	Chain	Res	Type	Atoms
14	H	301	NAG	O5-C5-C6-O6
14	B	702	NAG	O5-C5-C6-O6
14	G	631	NAG	O5-C5-C6-O6
14	B	702	NAG	C4-C5-C6-O6
14	G	646	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	701	SO4	1	0
14	G	631	NAG	1	0
14	B	703	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 83G G 657	
 Bond lengths	 Bond angles
 Torsions	 Rings

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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	126/153 (82%)	0.27	3 (2%)	59	38	40, 91, 160, 190	0
2	D	242/243 (99%)	0.53	16 (6%)	26	14	93, 197, 320, 379	0
3	E	213/216 (98%)	0.34	3 (1%)	73	52	124, 198, 291, 352	0
4	G	442/481 (91%)	0.12	6 (1%)	73	52	31, 93, 168, 215	0
5	H	228/235 (97%)	0.20	7 (3%)	51	31	83, 136, 198, 261	0
6	L	208/213 (97%)	0.21	6 (2%)	54	33	79, 116, 178, 257	0
All	All	1459/1541 (94%)	0.26	41 (2%)	55	34	31, 129, 265, 379	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	H	138	CYS	6.1
6	L	119	PHE	4.1
2	D	180	SER	3.1
4	G	73	ALA	3.1
4	G	316	ALA	3.1

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

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

6.3 Carbohydrates (i)

SUGAR-RSR INFOmissingINFO

6.4 Ligands (i)

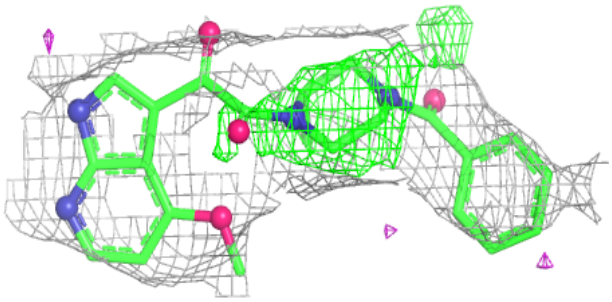
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

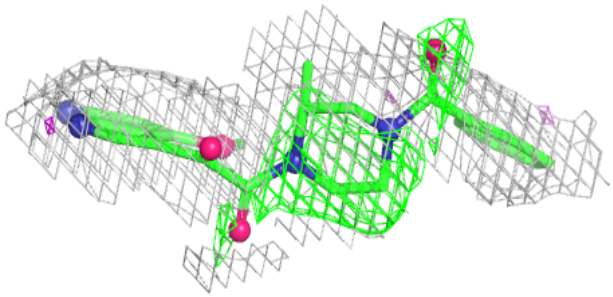
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	NAG	G	646	14/15	0.43	0.14	127,168,179,187	0
14	NAG	H	301	14/15	0.47	0.11	113,133,168,188	0
14	NAG	G	656	14/15	0.53	0.10	80,146,160,173	0
14	NAG	B	703	14/15	0.66	0.13	156,162,180,181	0
13	SO4	G	602	5/5	0.66	0.12	154,157,158,166	0
14	NAG	B	702	14/15	0.69	0.10	116,165,178,179	0
14	NAG	G	611	14/15	0.70	0.12	131,146,156,156	0
14	NAG	G	631	14/15	0.71	0.09	140,159,168,176	0
13	SO4	G	601	5/5	0.72	0.08	161,174,180,183	0
14	NAG	B	704	14/15	0.78	0.10	110,130,155,159	0
13	SO4	B	701	5/5	0.81	0.08	108,131,132,152	0
13	SO4	G	603	5/5	0.87	0.12	201,202,204,207	5
14	NAG	G	624	14/15	0.87	0.12	90,123,134,147	0
13	SO4	L	301	5/5	0.89	0.10	192,200,209,229	5
15	83G	G	657	30/30	0.92	0.18	26,74,138,232	0

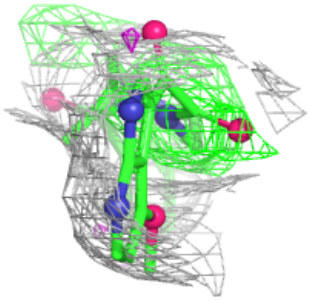
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 83G G 657:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.