wwPDB X-ray Structure Validation Summary Report (i)

Sep 29, 2024 – 02:16 AM EDT

PDB ID	:	1JV2
Title	:	CRYSTAL STRUCTURE OF THE EXTRACELLULAR SEGMENT OF INTEGRIN ALPHAVBETA3
Authors	:	Xiong, J.P.; Stehle, T.; Diefenbach, B.; Zhang, R.; Dunker, R.; Scott, D.; Joachimiak, A.; Goodman, S.L.; Arnaout, M.A.
Deposited on	:	2001-08-28
Resolution	:	3.10 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:

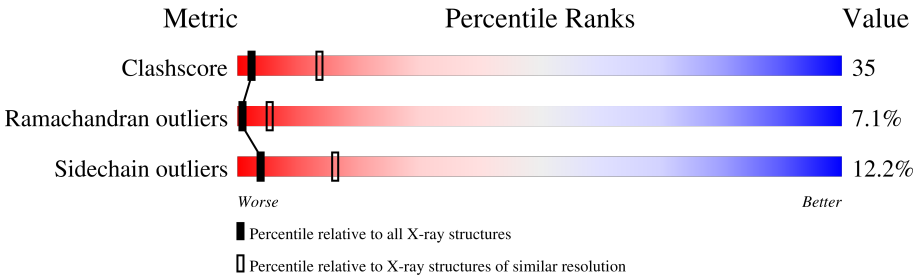
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.10 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))
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	957	44% 44% 8%
2	B	692	32% 36% 10% 22%
3	C	2	100%
3	D	2	100%
3	E	2	50% 50%
3	G	2	100%
4	F	2	50% 50%
4	H	2	50% 50%

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Mol	Chain	Length	Quality of chain
4	I	2	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NDG	I	2	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11656 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 INTEGRIN, ALPHA V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	927	Total	C	N	O	S	0	0	0
			7216	4568	1224	1389	35			

- Molecule 2 is a protein called PLATELET MEMBRANE GLYCOPROTEIN IIIA BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	539	Total	C	N	O	S	0	0	0
			4182	2594	700	842	46			

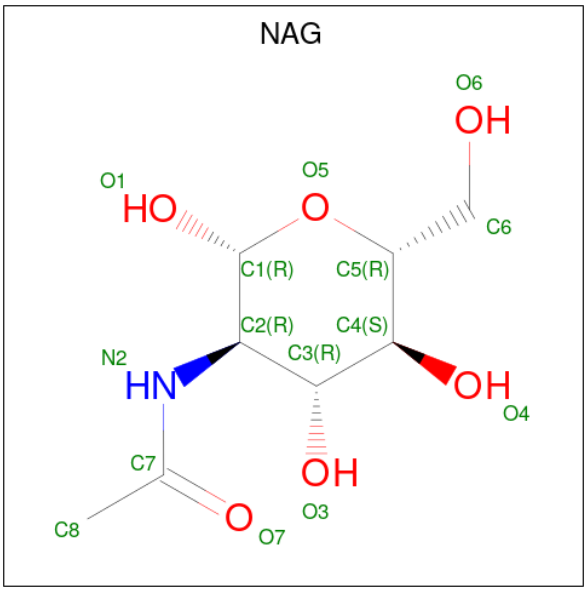
- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	5	Total Ca 5 5	0	0
6	B	1	Total Ca 1 1	0	0

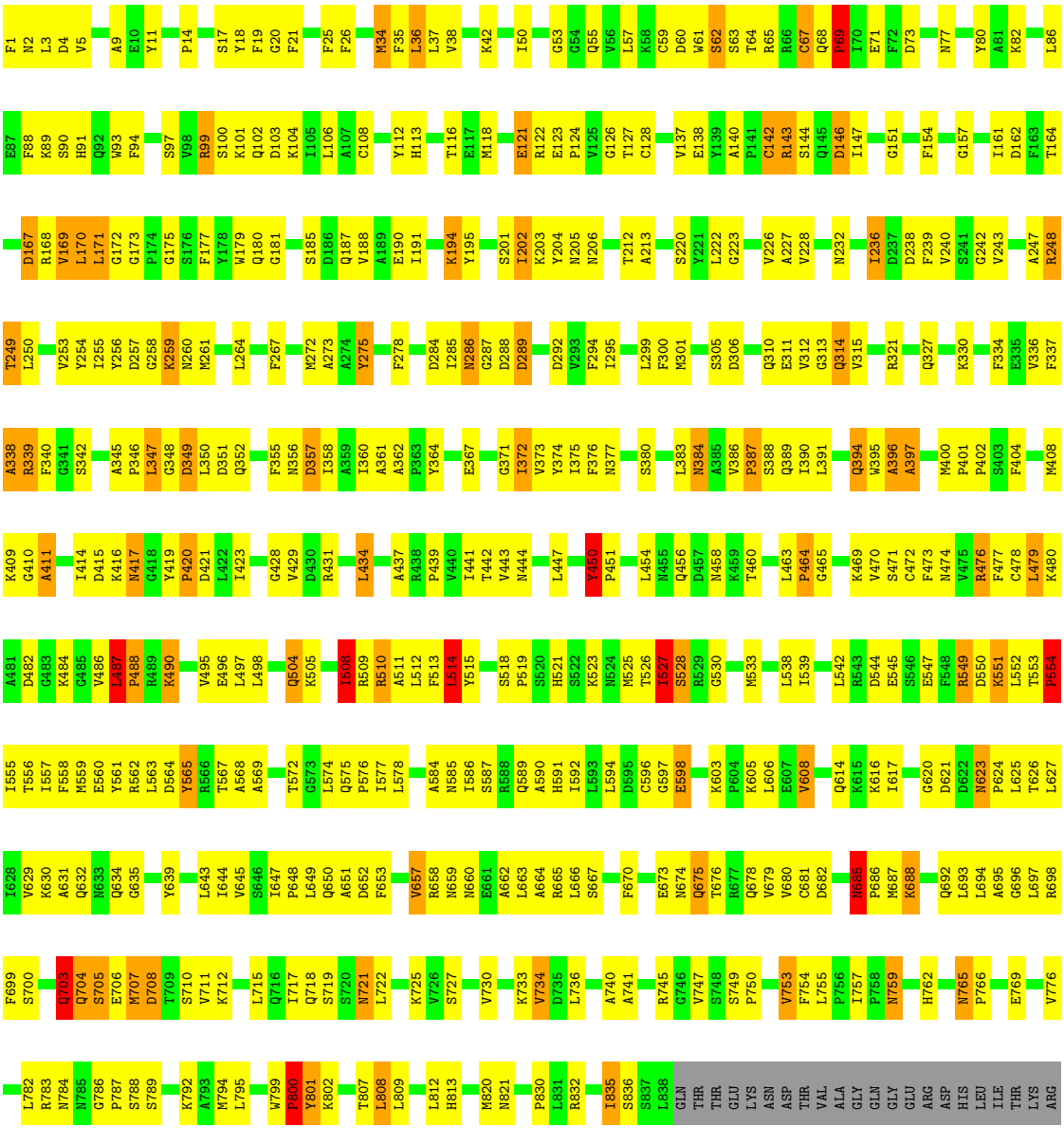
3 Residue-property plots (i)

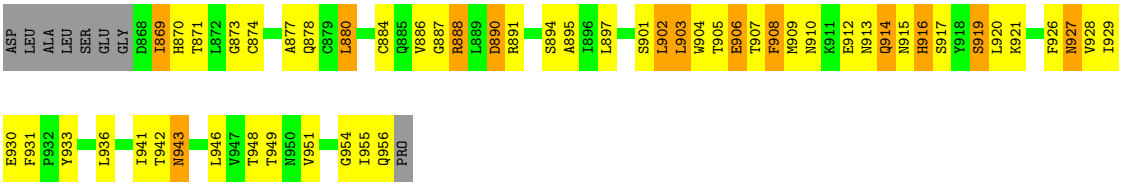
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: INTEGRIN, ALPHA V

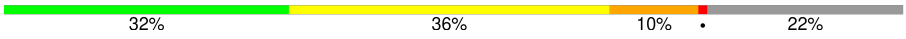
Chain A:

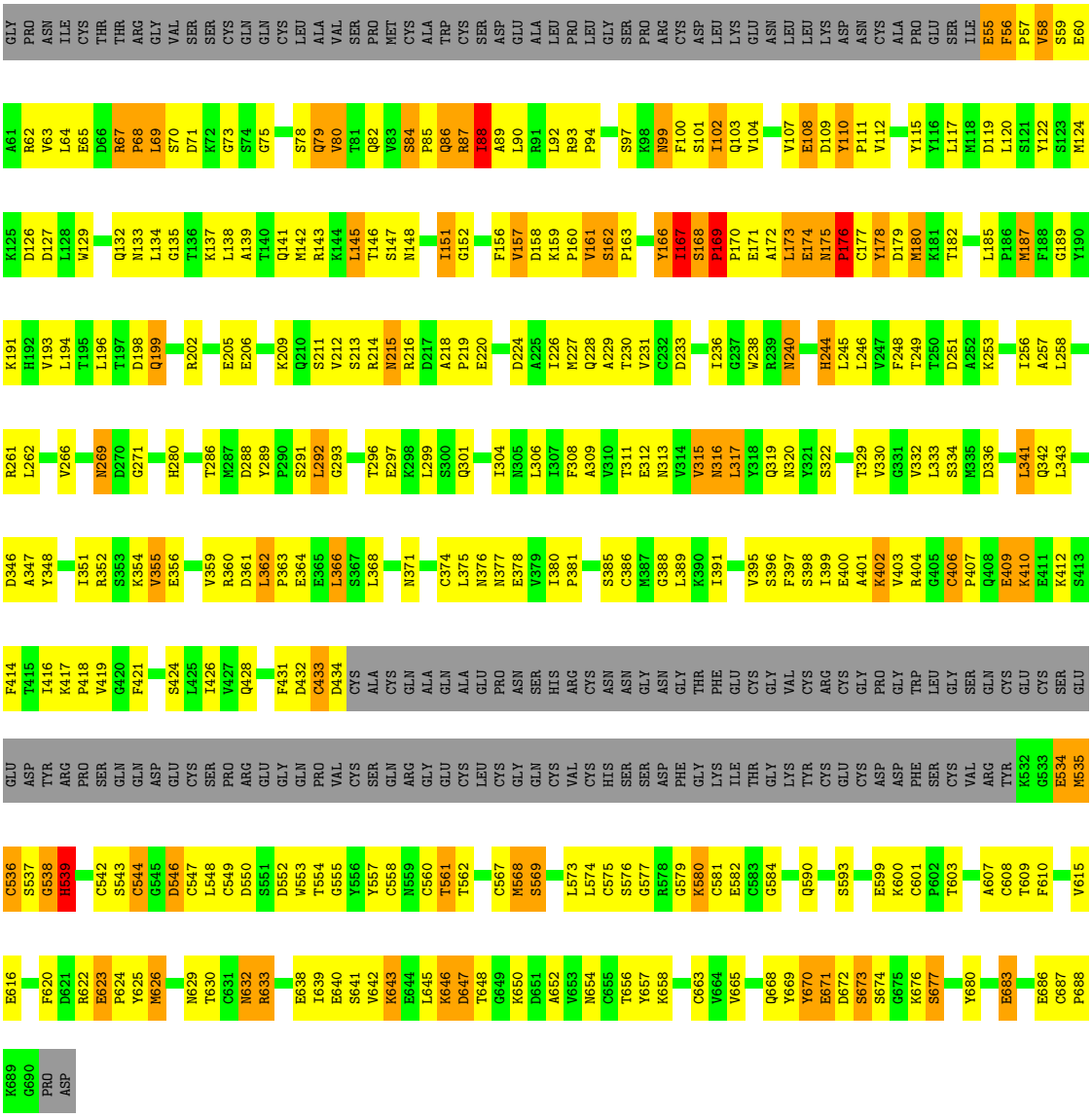




• Molecule 2: PLATELET MEMBRANE GLYCOPROTEIN IIIA BETA SUBUNIT

Chain B:





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

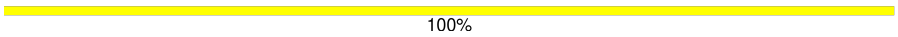
Chain D:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

Chain F:

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

Chain H:

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

Chain I:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	130.00Å 130.00Å 307.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.255 , 0.335	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11656	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.48	0/7372	0.80	12/9994 (0.1%)
2	B	0.48	0/4256	0.79	6/5754 (0.1%)
All	All	0.48	0/11628	0.79	18/15748 (0.1%)

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	912	GLU	N-CA-C	8.62	134.26	111.00
1	A	703	GLN	N-CA-C	7.21	130.47	111.00
2	B	378	GLU	N-CA-C	-6.11	94.52	111.00
2	B	169	PRO	C-N-CD	5.90	140.79	128.40
1	A	687	MET	N-CA-C	-5.89	95.10	111.00

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	A	7216	0	7036	492	0
2	B	4182	0	4030	308	0
3	C	28	0	25	3	0
3	D	28	0	25	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	28	0	25	3	0
3	G	28	0	25	1	0
4	F	28	0	24	7	0
4	H	28	0	24	3	0
4	I	28	0	24	10	0
5	A	28	0	26	8	0
5	B	28	0	26	5	0
6	A	5	0	0	0	0
6	B	1	0	0	0	0
All	All	11656	0	11290	800	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 35.

The worst 5 of 800 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)
4:F:2:NDG:H2	4:F:2:NDG:H6C2	1.19	1.12
1:A:585:ASN:HD22	3:E:1:NAG:H62	1.13	1.10
2:B:69:LEU:HD22	2:B:80:VAL:HA	1.34	1.08
1:A:127:THR:HG22	1:A:140:ALA:HB2	1.39	1.03
2:B:648:THR:HA	4:I:2:NDG:C1	1.89	1.02

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	A	923/957 (96%)	708 (77%)	157 (17%)	58 (6%)	1	7
2	B	535/692 (77%)	388 (72%)	102 (19%)	45 (8%)	0	4
All	All	1458/1649 (88%)	1096 (75%)	259 (18%)	103 (7%)	1	5

5 of 103 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	SER
1	A	69	PRO
1	A	118	MET
1	A	169	VAL
1	A	205	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	787/812 (97%)	702 (89%)	85 (11%)	5	21
2	B	484/616 (79%)	414 (86%)	70 (14%)	2	11
All	All	1271/1428 (89%)	1116 (88%)	155 (12%)	4	16

5 of 155 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	224	ASP
2	B	561	THR
2	B	269	ASN
2	B	355	VAL
2	B	646	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	913	ASN
2	B	240	ASN
1	A	915	ASN
2	B	133	ASN
2	B	279	ASN

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)

14 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	C	1	1,3	14,14,15	0.53	0	17,19,21	0.83	1 (5%)
3	NAG	C	2	3	14,14,15	0.87	1 (7%)	17,19,21	0.72	0
3	NAG	D	1	1,3	14,14,15	0.49	0	17,19,21	1.35	2 (11%)
3	NAG	D	2	3	14,14,15	0.79	1 (7%)	17,19,21	0.71	0
3	NAG	E	1	1,3	14,14,15	0.73	0	17,19,21	0.92	1 (5%)
3	NAG	E	2	3	14,14,15	0.53	0	17,19,21	0.64	0
4	NAG	F	1	1,4	14,14,15	0.80	1 (7%)	17,19,21	0.92	1 (5%)
4	NDG	F	2	4	14,14,15	0.59	0	17,19,21	0.71	0
3	NAG	G	1	1,3	14,14,15	0.49	0	17,19,21	0.84	0
3	NAG	G	2	3	14,14,15	0.47	0	17,19,21	0.64	0
4	NAG	H	1	4,2	14,14,15	0.44	0	17,19,21	1.15	1 (5%)
4	NDG	H	2	4	14,14,15	0.47	0	17,19,21	0.70	0
4	NAG	I	1	4,2	14,14,15	0.55	0	17,19,21	1.31	2 (11%)
4	NDG	I	2	4	14,14,15	0.79	0	17,19,21	0.82	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
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	4/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	3/6/23/26	0/1/1/1
4	NDG	F	2	4	-	1/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
4	NAG	H	1	4,2	-	1/6/23/26	0/1/1/1
4	NDG	H	2	4	-	1/6/23/26	0/1/1/1
4	NAG	I	1	4,2	-	0/6/23/26	0/1/1/1
4	NDG	I	2	4	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	NAG	C1-C2	2.38	1.55	1.52
4	F	1	NAG	C1-C2	2.31	1.55	1.52
3	D	2	NAG	C1-C2	2.11	1.55	1.52

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1	NAG	C4-C3-C2	-3.92	105.28	111.02
4	H	1	NAG	C2-N2-C7	-3.53	118.17	122.90
3	D	1	NAG	O5-C1-C2	-2.83	106.91	111.29
4	F	1	NAG	C2-N2-C7	-2.81	119.14	122.90
4	I	1	NAG	C1-O5-C5	2.41	115.42	112.19

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
4	I	2	NDG	O5-C5-C6-O6
4	I	2	NDG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6

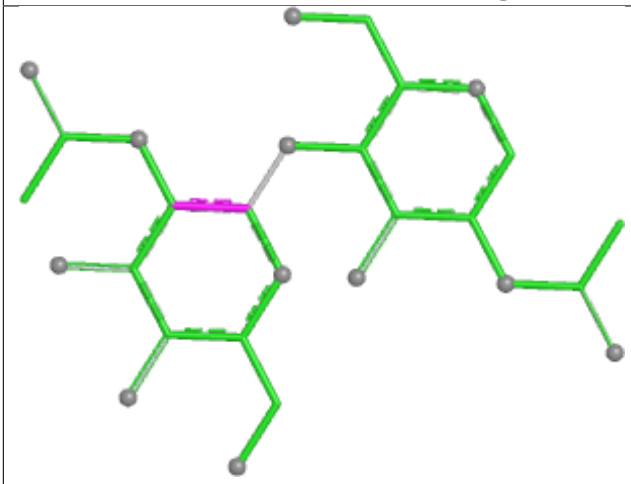
There are no ring outliers.

13 monomers are involved in 30 short contacts:

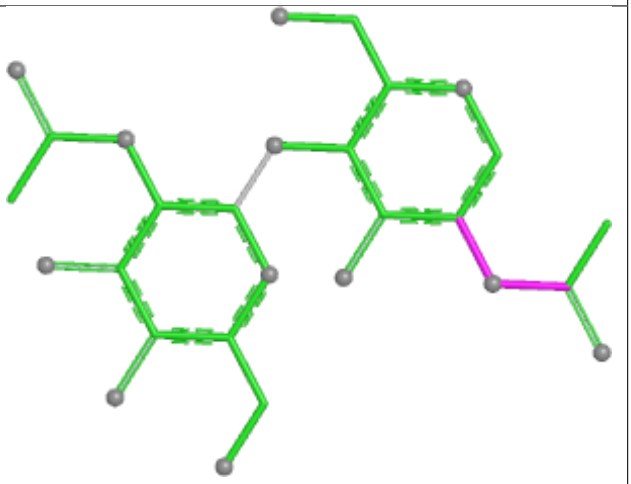
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	2	NDG	3	0
4	I	2	NDG	7	0
4	H	2	NDG	3	0
3	E	1	NAG	3	0
3	G	1	NAG	1	0
4	F	1	NAG	4	0
3	C	1	NAG	2	0
4	I	1	NAG	3	0
3	C	2	NAG	3	0
4	H	1	NAG	1	0
3	D	2	NAG	1	0
3	D	1	NAG	2	0
3	G	2	NAG	1	0

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

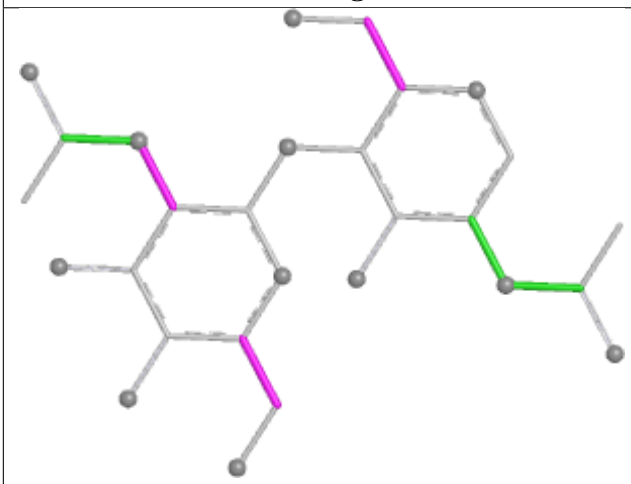
Oligosaccharide Chain C



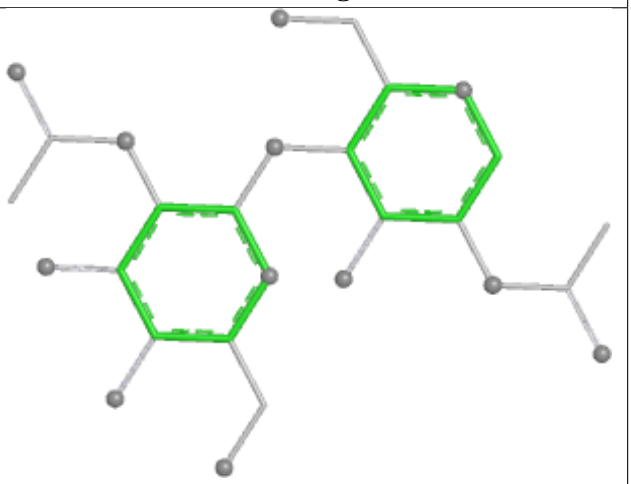
Bond lengths



Bond angles

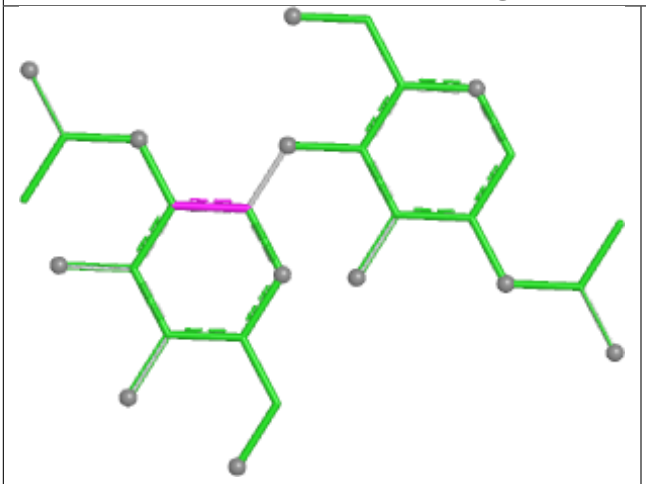


Torsions

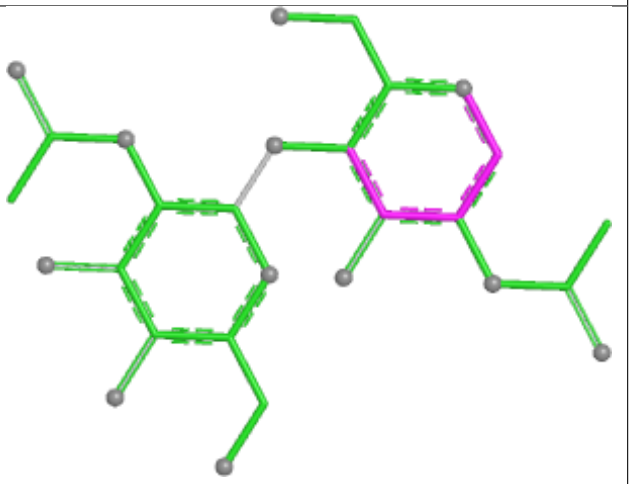


Rings

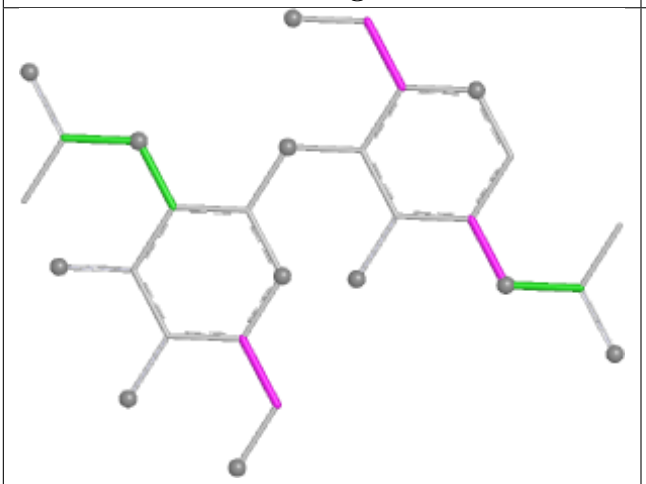
Oligosaccharide Chain D



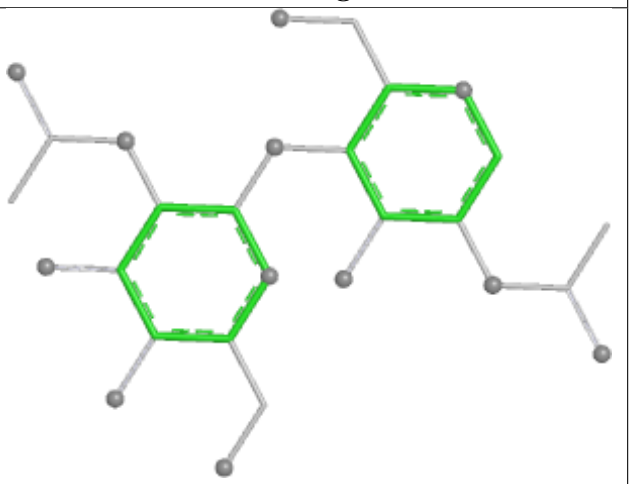
Bond lengths



Bond angles

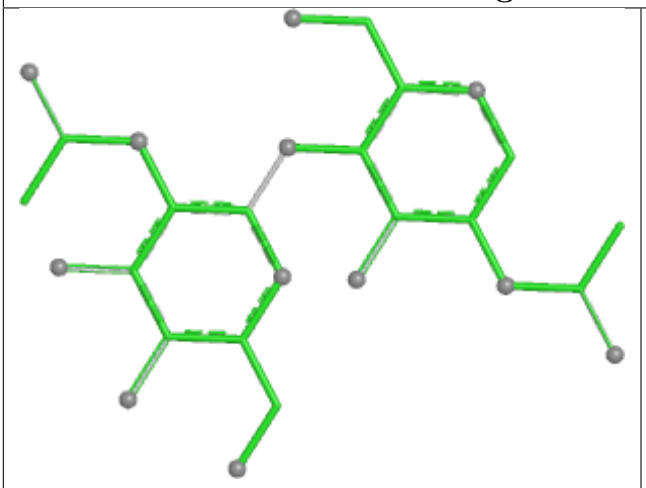


Torsions

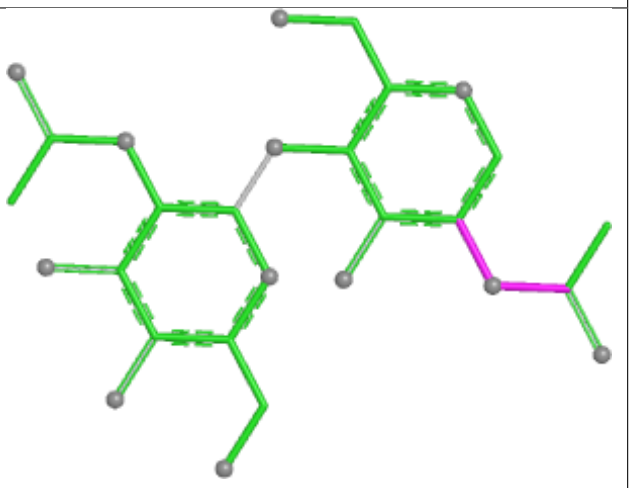


Rings

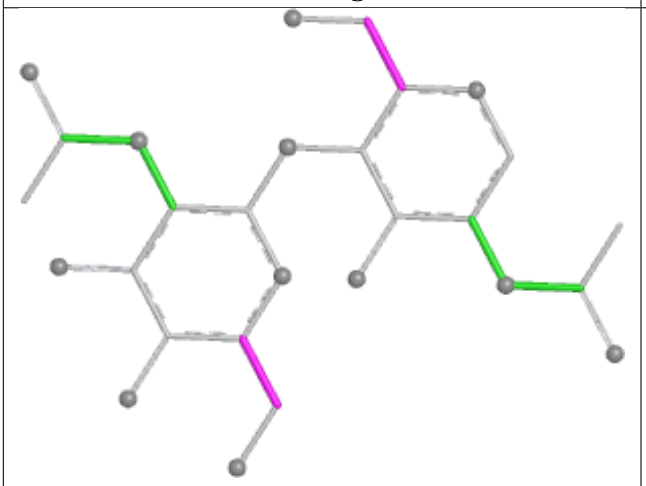
Oligosaccharide Chain E



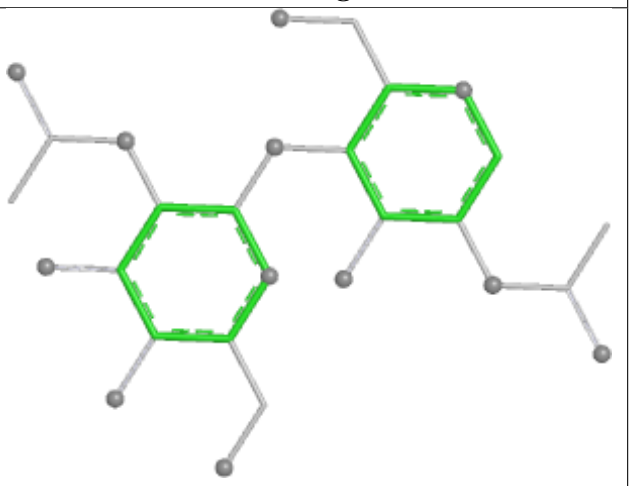
Bond lengths



Bond angles

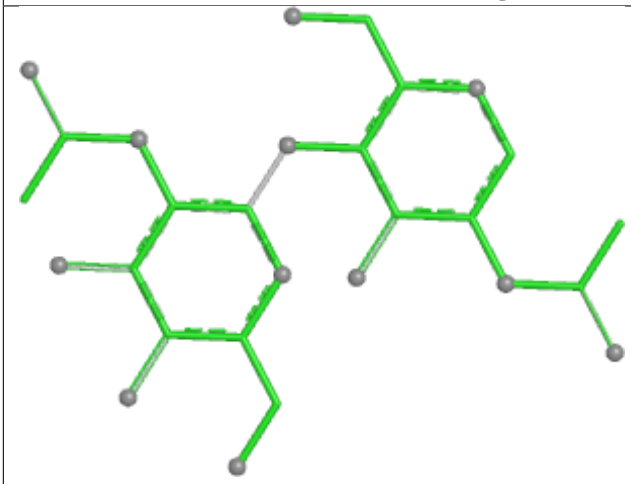


Torsions

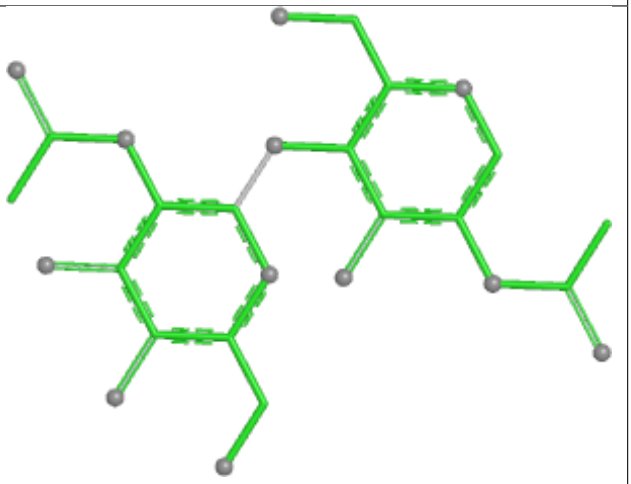


Rings

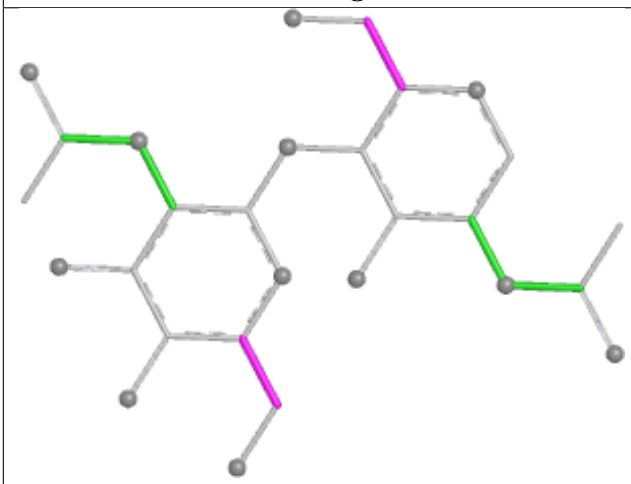
Oligosaccharide Chain G



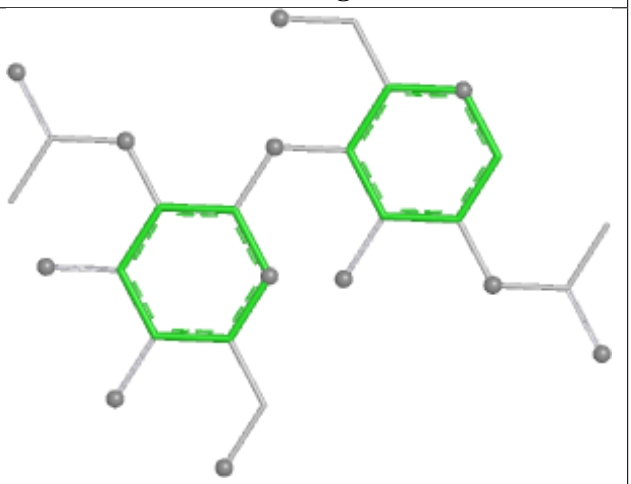
Bond lengths



Bond angles

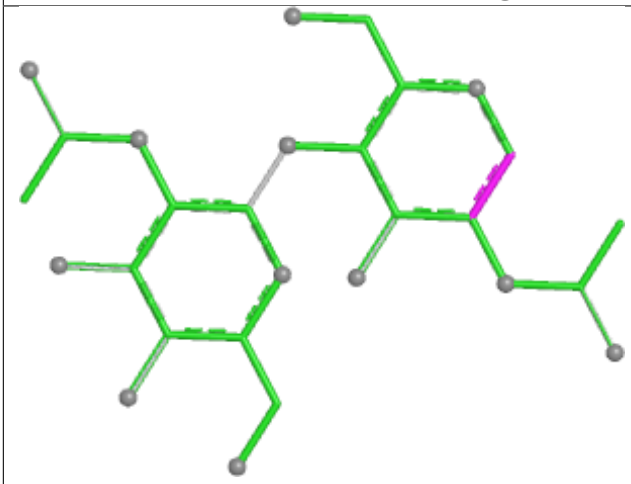


Torsions

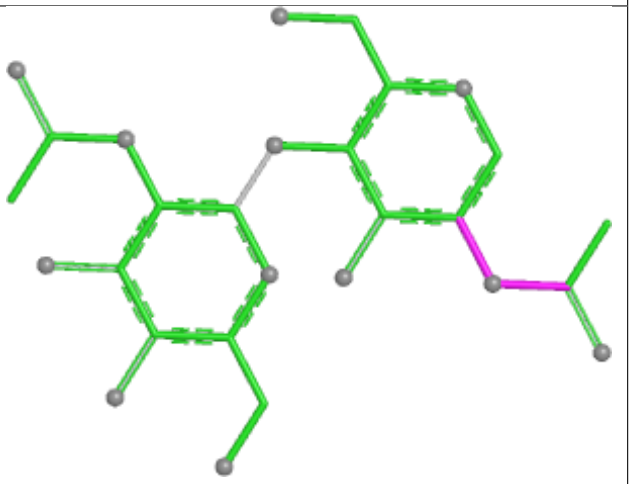


Rings

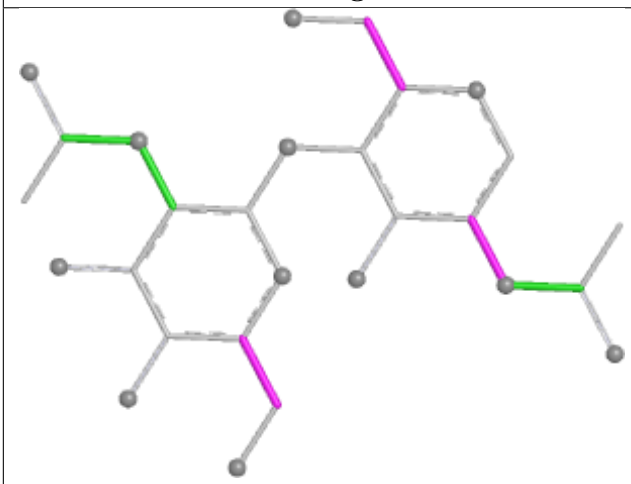
Oligosaccharide Chain F



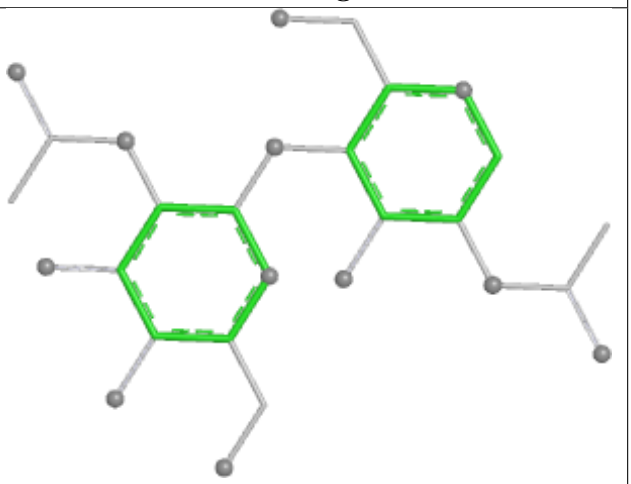
Bond lengths



Bond angles

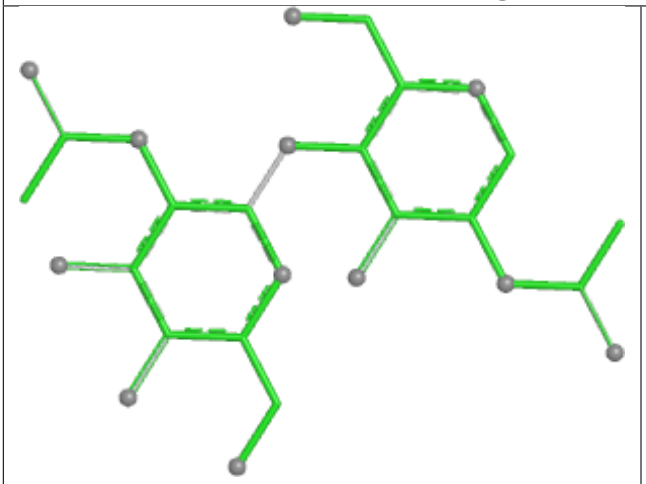


Torsions

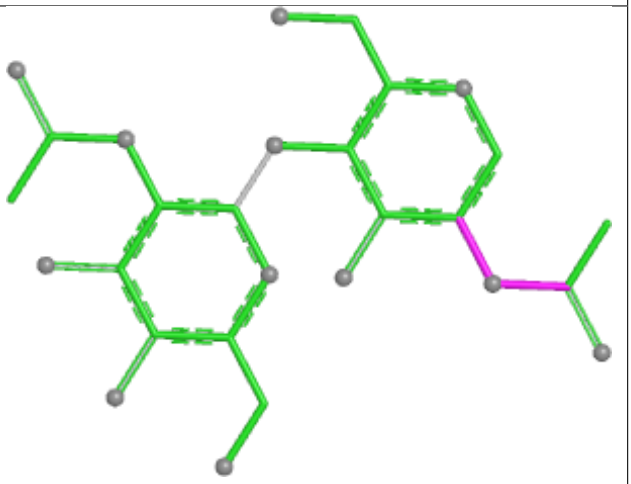


Rings

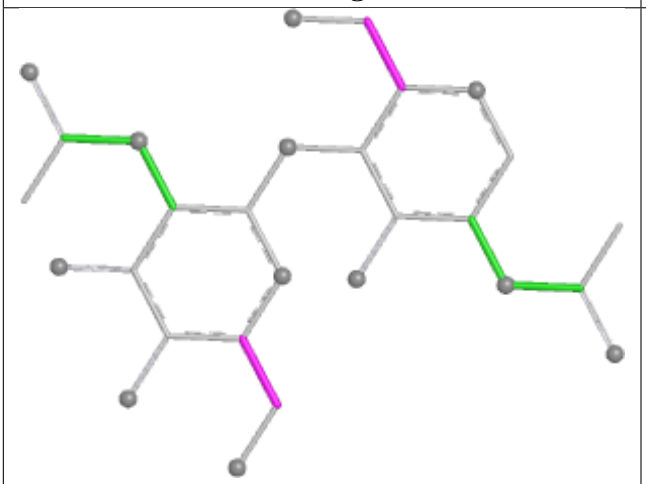
Oligosaccharide Chain H



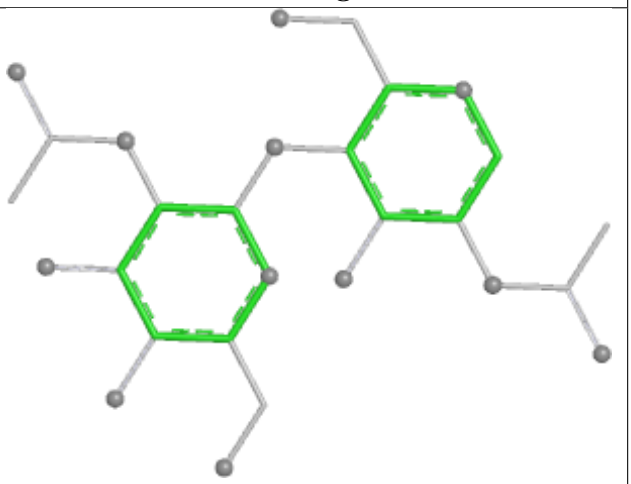
Bond lengths



Bond angles

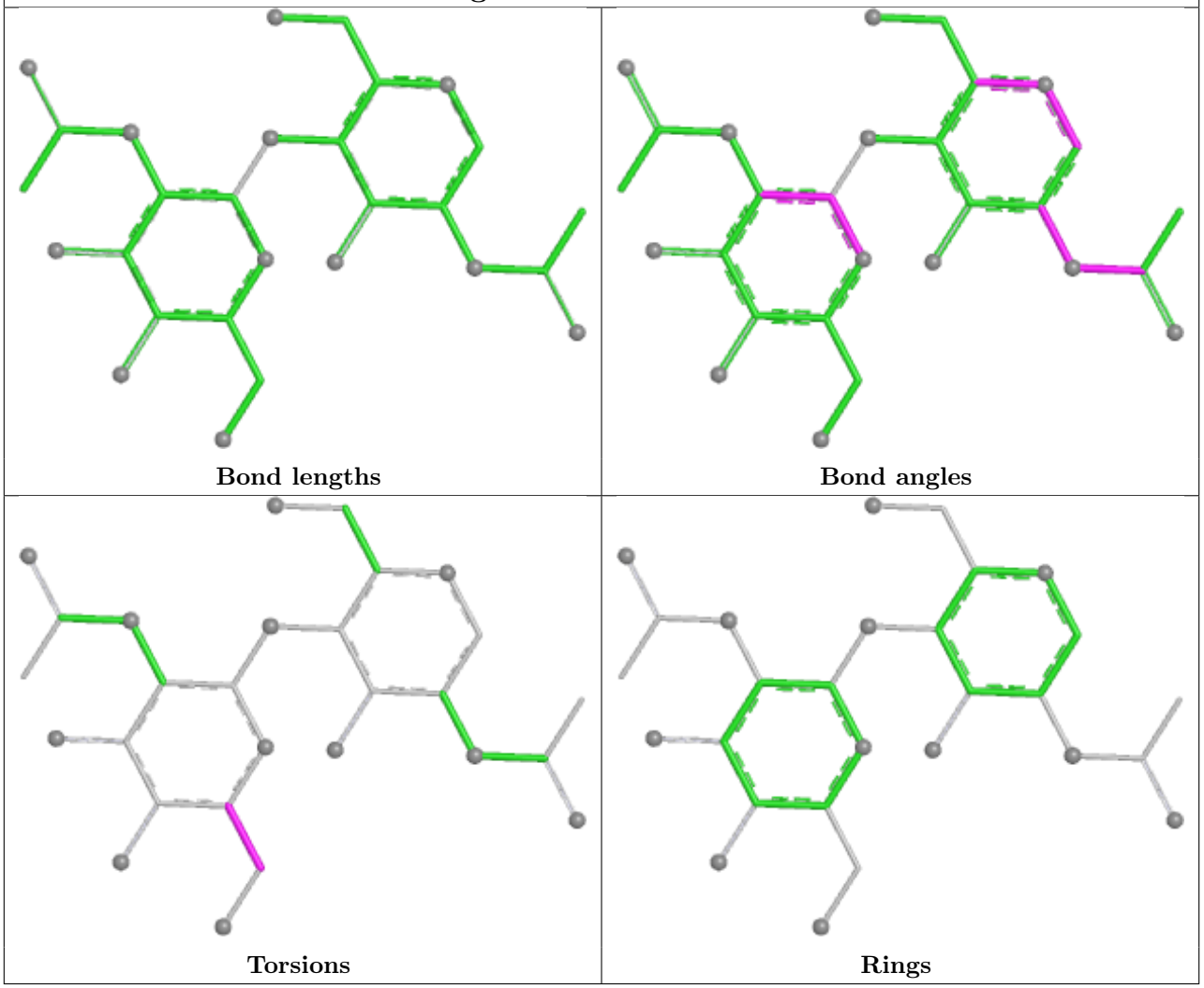


Torsions



Rings

Oligosaccharide Chain I



5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	B	3320	2	14,14,15	0.45	0	17,19,21	0.86	1 (5%)
5	NAG	A	2458	1	14,14,15	0.74	0	17,19,21	0.85	1 (5%)
5	NAG	A	2260	1	14,14,15	0.50	0	17,19,21	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	B	3371	2	14,14,15	0.59	0	17,19,21	1.12	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
5	NAG	B	3320	2	-	1/6/23/26	0/1/1/1
5	NAG	A	2458	1	-	1/6/23/26	0/1/1/1
5	NAG	A	2260	1	-	3/6/23/26	0/1/1/1
5	NAG	B	3371	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	3371	NAG	C2-N2-C7	-3.10	118.75	122.90
5	A	2458	NAG	C2-N2-C7	-2.27	119.86	122.90
5	B	3320	NAG	C2-N2-C7	-2.15	120.02	122.90

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	3371	NAG	O5-C5-C6-O6
5	B	3371	NAG	C4-C5-C6-O6
5	B	3320	NAG	O5-C5-C6-O6
5	A	2260	NAG	O5-C5-C6-O6
5	A	2260	NAG	C1-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	3320	NAG	1	0
5	A	2458	NAG	5	0
5	A	2260	NAG	3	0
5	B	3371	NAG	4	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.