Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2023 – 05:35 AM EDT

PDB ID	:	6V7Z
Title	:	Human CD1d presenting alpha-Galactosylceramide in complex with VHH nanobody 1D22
Authors	:	Shahine, A.; Rossjohn, J.
Deposited on	:	2019-12-10
Resolution	:	2.75 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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 (1)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.75 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 7908 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 Antigen-presenting glycoprotein CD1d.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	275	2181	1396	376	401	8	0	0	0
1	C	263	2052	1319	344	382	7	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	initiating methionine	UNP P15813
C	4	MET	-	initiating methionine	UNP P15813

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	99	817	522	141	151	3	0	1	0
2	D	96	752	485	124	141	2	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
D	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Nanobody VHH ID22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	117	884	551	156	173	4	0	1	0
3	F	117	864	537	150	173	4	0	1	0

- Molecule 4 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			
4	G	2	28	16	2	10	0	0	0
4	J	2	28	16	2	10	0	0	0

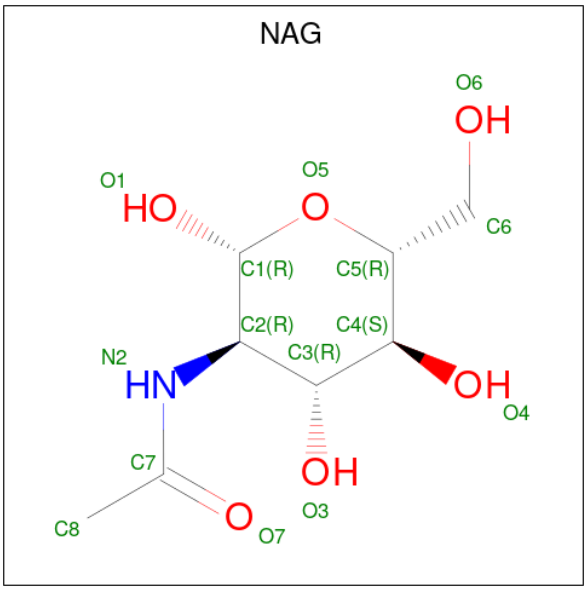
- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	H	2	25	14	1	10	0	0	0

- Molecule 6 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.

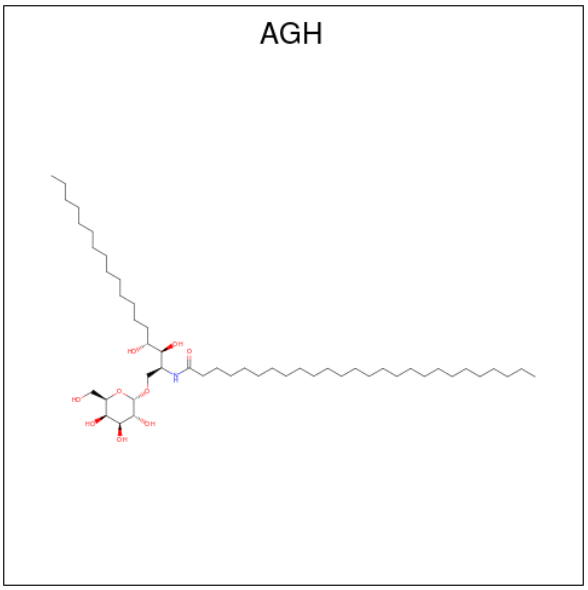
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	I	3	39	22	2	15	0	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



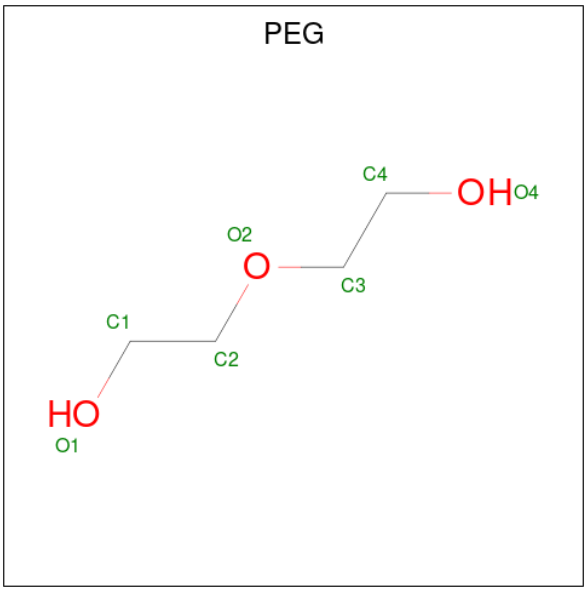
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	14	8	1	5	0	0

- Molecule 8 is N-{(1S,2R,3S)-1-[(ALPHA-D-GALACTOPYRANOSYLOXY)METHYL]-2,3-DIHYDROXYHEPTADECYL}HEXACOSANAMIDE (three-letter code: AGH) (formula: $C_{50}H_{99}NO_9$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	A	1	60	50	1	9	0	0
8	C	1	60	50	1	9	0	0

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

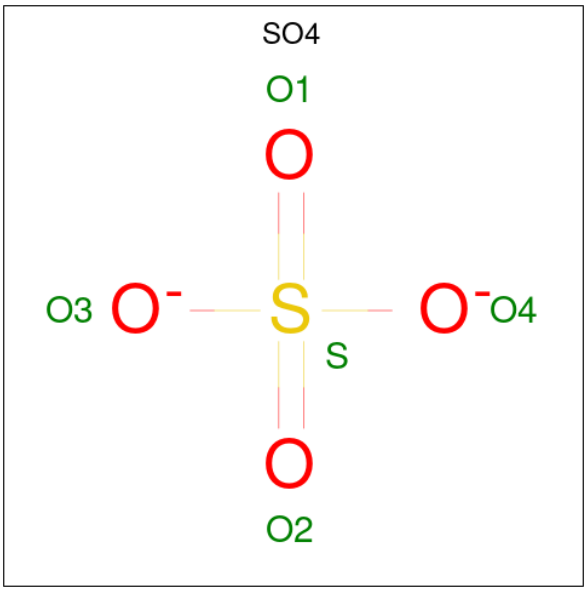


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	A	1	7	4	3	0	0
			Total	C	O		
9	A	1	7	4	3	0	0
			Total	C	O		
9	E	1	7	4	3	0	0

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

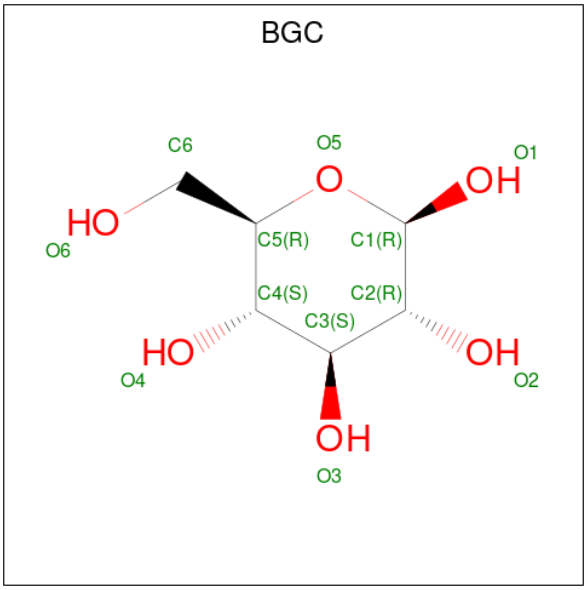
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
10	A	1	1	1	0	0

- Molecule 11 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 12 is beta-D-glucopyranose (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total C O 12 6 6	0	0

- Molecule 13 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
13	D	1	1	1	0	0

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
14	A	13	13	13	0	0
			Total	O		
14	B	17	17	17	0	0
			Total	O		
14	C	19	19	19	0	0
			Total	O		
14	D	5	5	5	0	0
			Total	O		
14	E	4	4	4	0	0
			Total	O		
14	F	6	6	6	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.72Å 121.93Å 172.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.31 – 2.75	Depositor
% Data completeness (in resolution range)	99.9 (45.31-2.75)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.186 , 0.252	Depositor
Wilson B-factor (Å^2)	71.1	Xtriage
Anisotropy	0.361	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7908	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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.

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates (i)

9 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	$\#\|Z\| > 2$
4	NAG	G	1	1,4	14,14,15	0.37	0	17,19,21	0.52	0
4	NAG	G	2	4	14,14,15	0.23	0	17,19,21	0.46	0
5	NAG	H	1	1,5	14,14,15	0.35	0	17,19,21	0.59	0
5	BMA	H	2	5	11,11,12	1.52	2 (18%)	15,15,17	1.25	1 (6%)
6	NAG	I	1	1,6	14,14,15	0.64	1 (7%)	17,19,21	0.54	0
6	NAG	I	2	6	14,14,15	0.34	0	17,19,21	0.55	0
6	BMA	I	3	6	11,11,12	1.01	0	15,15,17	0.76	0
4	NAG	J	1	1,4	14,14,15	0.60	0	17,19,21	0.89	1 (5%)
4	NAG	J	2	4	14,14,15	1.61	1 (7%)	17,19,21	1.13	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
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
5	NAG	H	1	1,5	-	1/6/23/26	0/1/1/1
5	BMA	H	2	5	-	0/2/19/22	0/1/1/1
6	NAG	I	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	I	2	6	-	2/6/23/26	0/1/1/1
6	BMA	I	3	6	-	1/2/19/22	0/1/1/1
4	NAG	J	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	2	NAG	O5-C1	5.70	1.52	1.43
5	H	2	BMA	C1-C2	3.21	1.59	1.52
5	H	2	BMA	C2-C3	2.89	1.56	1.52
6	I	1	NAG	O5-C1	2.18	1.47	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	2	NAG	C1-O5-C5	4.47	118.25	112.19
4	J	1	NAG	C1-O5-C5	2.82	116.02	112.19
5	H	2	BMA	C1-C2-C3	2.19	112.36	109.67

There are no chirality outliers.

All (10) torsion outliers are listed below:

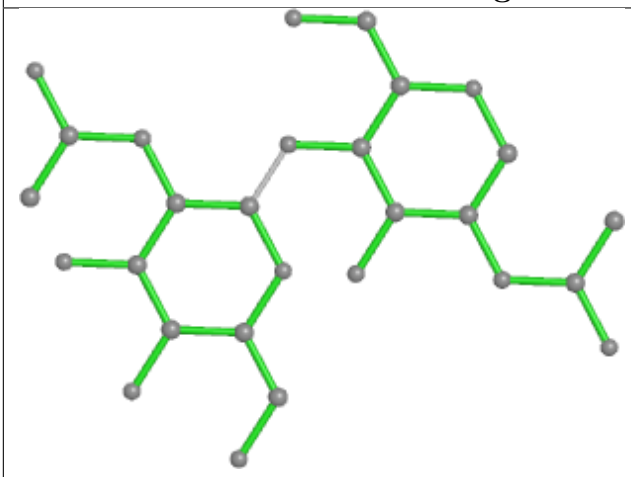
Mol	Chain	Res	Type	Atoms
4	G	1	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
6	I	3	BMA	O5-C5-C6-O6
6	I	1	NAG	C4-C5-C6-O6
6	I	1	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
6	I	2	NAG	C4-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6

There are no ring outliers.

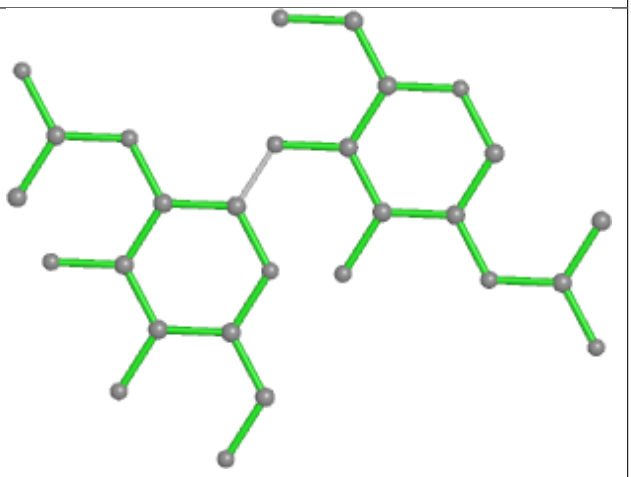
No monomer is involved in short contacts.

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

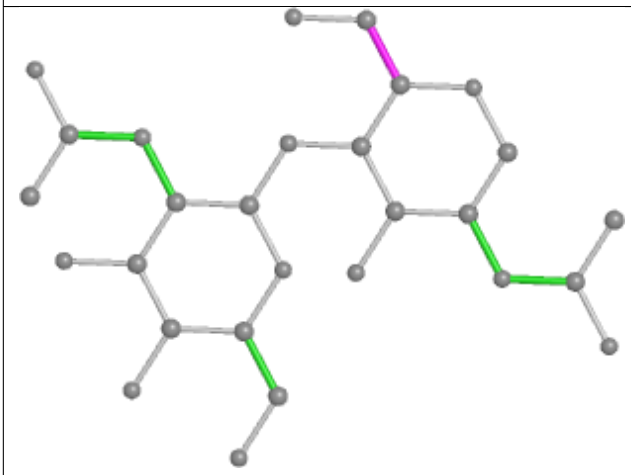
Oligosaccharide Chain G



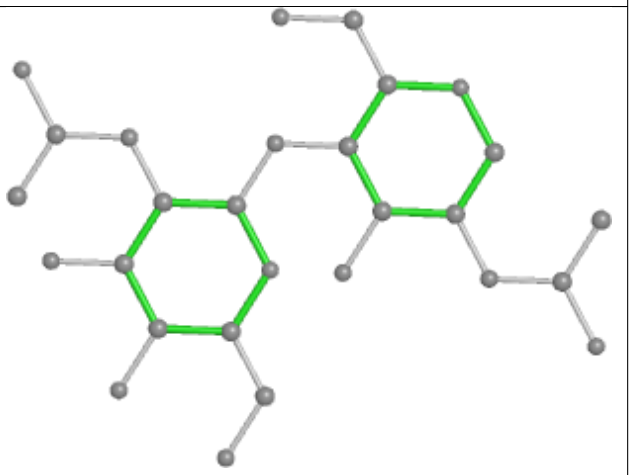
Bond lengths



Bond angles

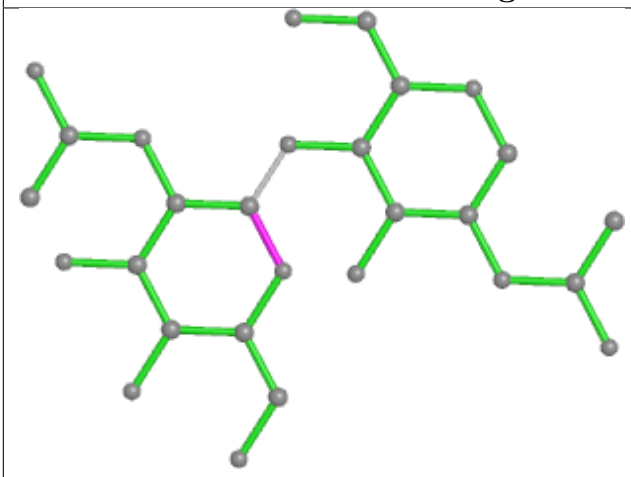


Torsions

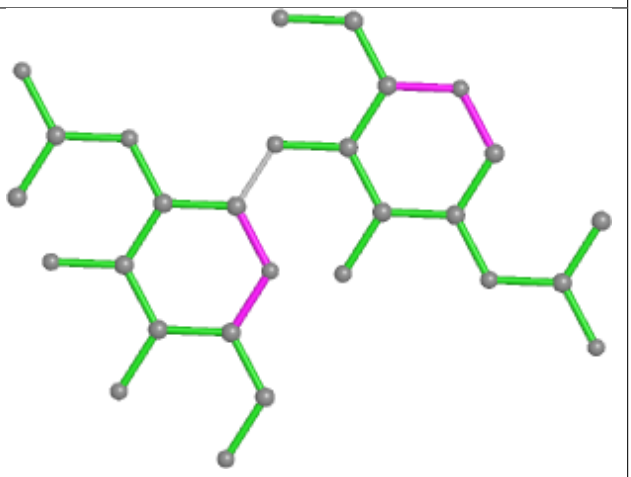


Rings

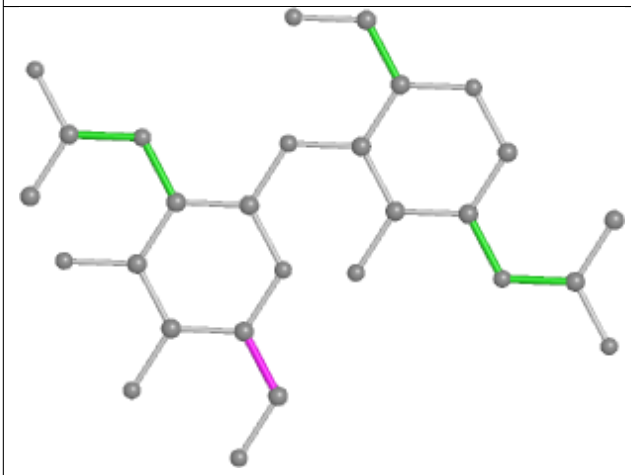
Oligosaccharide Chain J



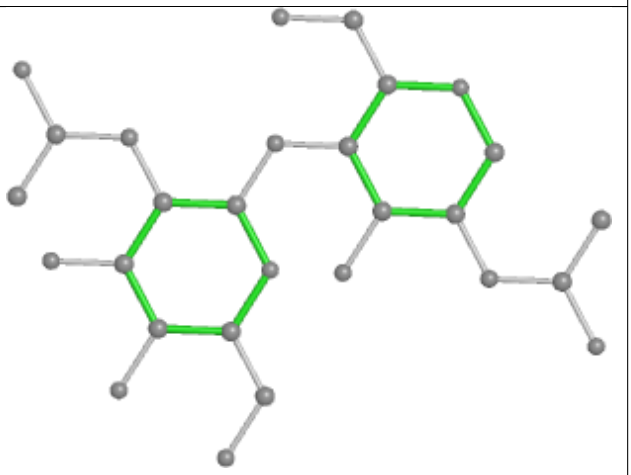
Bond lengths



Bond angles

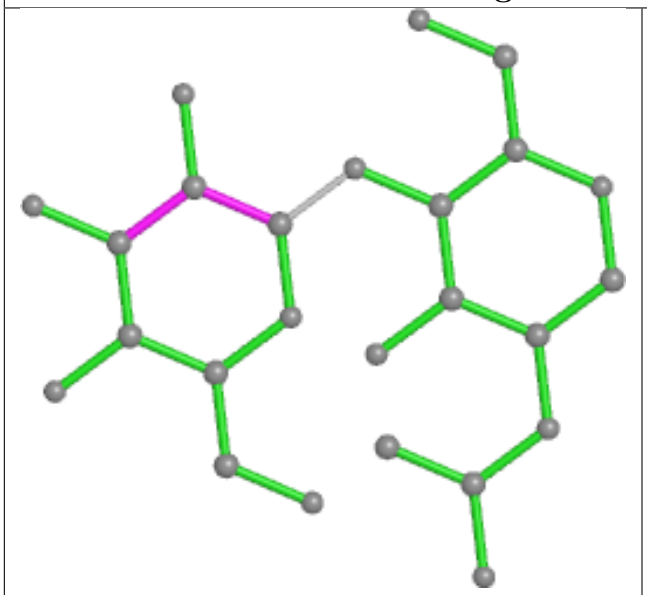


Torsions

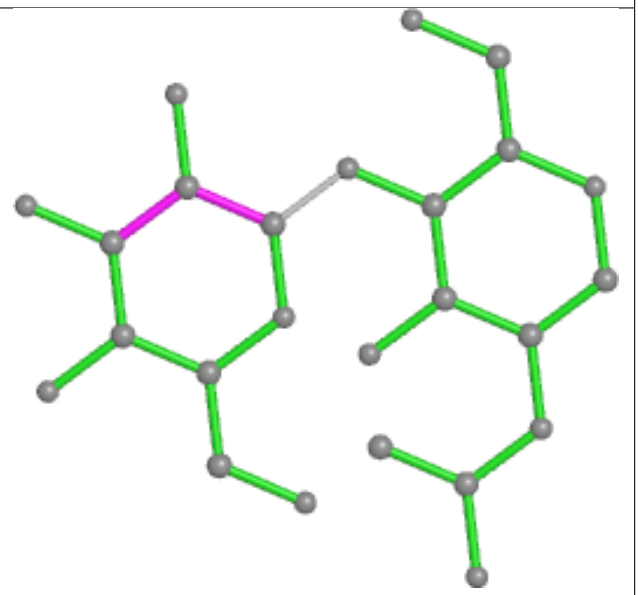


Rings

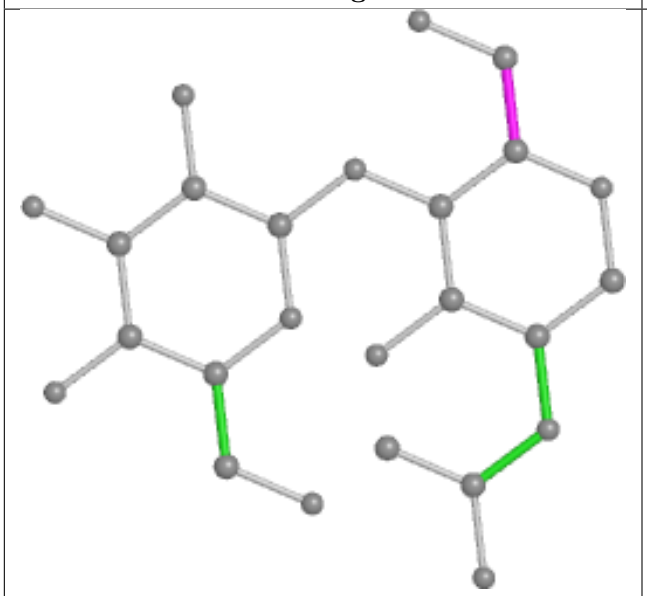
Oligosaccharide Chain H



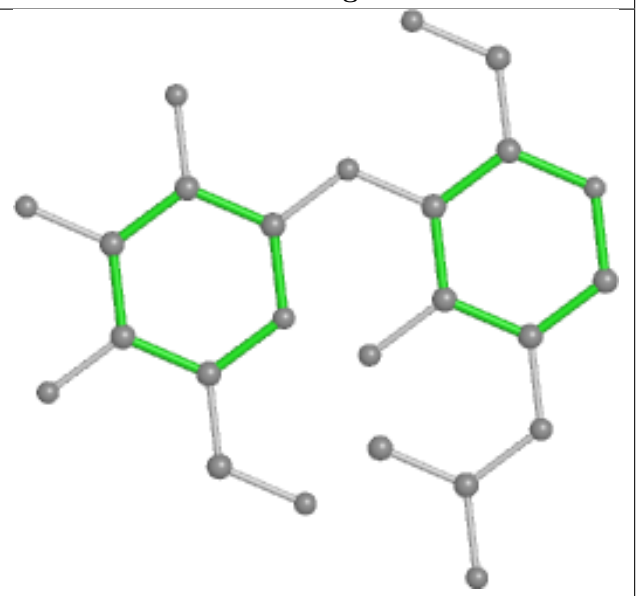
Bond lengths



Bond angles

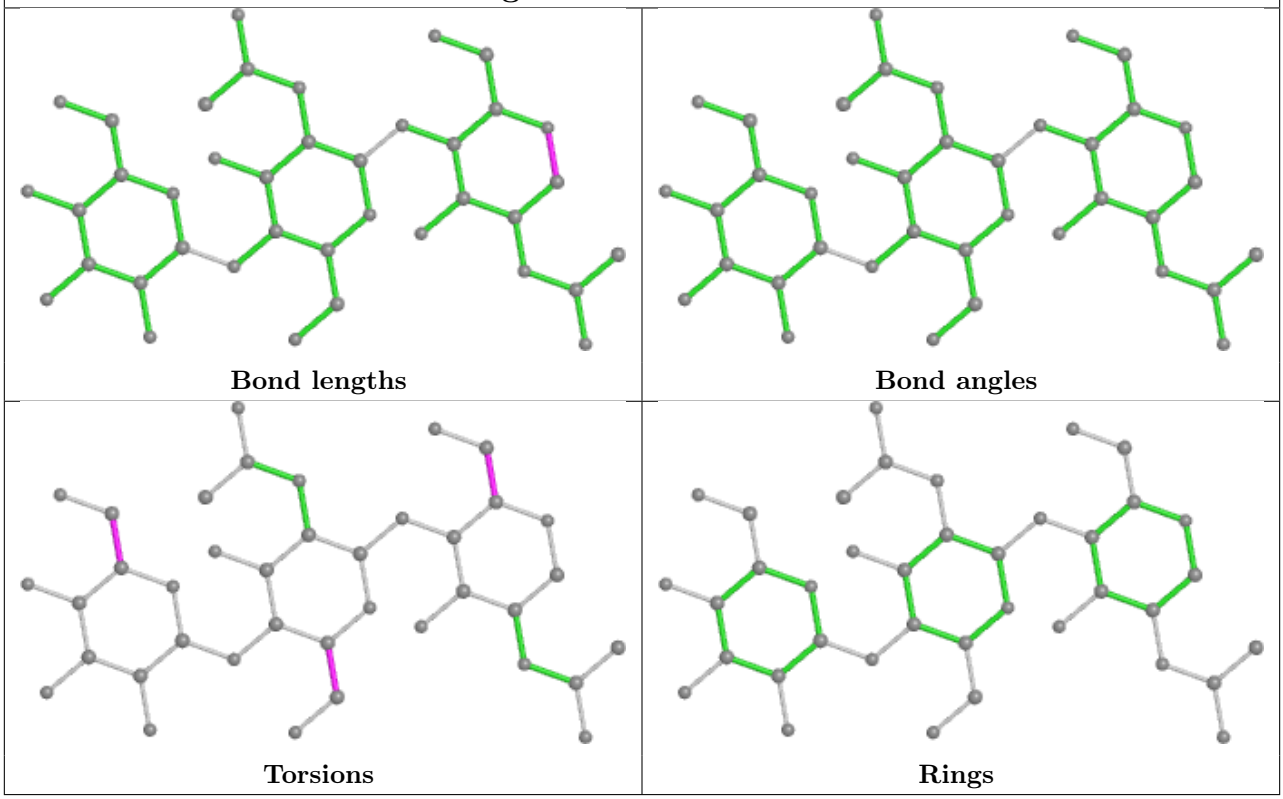


Torsions



Rings

Oligosaccharide Chain I



4.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	PEG	E	201	-	6,6,6	0.52	0	5,5,5	0.35	0
9	PEG	A	404	-	6,6,6	0.53	0	5,5,5	0.39	0
12	BGC	B	102	-	12,12,12	1.24	1 (8%)	17,17,17	1.79	5 (29%)
8	AGH	A	402	-	60,60,60	1.43	5 (8%)	65,69,69	1.01	3 (4%)
9	PEG	A	403	-	6,6,6	0.48	0	5,5,5	0.44	0
11	SO4	B	101	-	4,4,4	0.11	0	6,6,6	0.16	0
8	AGH	C	401	-	60,60,60	1.36	5 (8%)	65,69,69	1.75	8 (12%)
7	NAG	A	401	1	14,14,15	0.63	1 (7%)	17,19,21	0.66	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
9	PEG	E	201	-	-	3/4/4/4	-
9	PEG	A	404	-	-	2/4/4/4	-
12	BGC	B	102	-	-	2/2/22/22	0/1/1/1
8	AGH	A	402	-	-	18/58/78/78	0/1/1/1
9	PEG	A	403	-	-	1/4/4/4	-
8	AGH	C	401	-	-	22/58/78/78	0/1/1/1
7	NAG	A	401	1	-	0/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	402	AGH	CAA-N2	6.85	1.48	1.34
8	C	401	AGH	CAA-N2	6.06	1.47	1.34
8	A	402	AGH	OAA-CAA	-3.13	1.16	1.23
8	C	401	AGH	OAA-CAA	-3.06	1.17	1.23
12	B	102	BGC	O5-C1	2.98	1.50	1.42
8	C	401	AGH	O6A-C1A	2.53	1.48	1.41
8	A	402	AGH	O6A-C1A	2.40	1.47	1.41
8	A	402	AGH	CAB-CAA	2.15	1.55	1.51
8	C	401	AGH	O3A-C3A	2.11	1.48	1.43
7	A	401	NAG	C1-C2	2.11	1.55	1.52
8	C	401	AGH	CAB-CAA	2.06	1.55	1.51
8	A	402	AGH	O6A-C5M	2.06	1.49	1.44

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	401	AGH	C6-C5-C4	-9.88	97.93	114.18
12	B	102	BGC	C4-C3-C2	3.66	117.21	110.82
8	C	401	AGH	C2-N2-CAA	-3.21	118.06	123.48
12	B	102	BGC	O3-C3-C4	-3.12	103.14	110.35
8	C	401	AGH	O6A-C5M-C4A	2.67	114.55	109.69
8	A	402	AGH	C1-O1A-C1A	2.64	118.91	113.74
12	B	102	BGC	O1-C1-C2	2.64	116.47	109.03
8	C	401	AGH	OAA-CAA-N2	-2.55	118.64	122.95
12	B	102	BGC	O3-C3-C2	2.38	115.85	110.35
8	C	401	AGH	C8-C7-C6	-2.35	102.52	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	401	AGH	CAE-CAD-CAC	-2.32	102.64	114.42
8	C	401	AGH	CAC-CAB-CAA	-2.29	106.84	113.26
12	B	102	BGC	C1-O5-C5	-2.23	109.46	113.66
8	A	402	AGH	O3-C3-C4	2.20	114.12	108.81
8	C	401	AGH	CAB-CAA-N2	2.05	119.38	115.83
8	A	402	AGH	O6A-C5M-C6A	2.04	111.51	106.44

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	401	AGH	CAA-CAB-CAC-CAD
12	B	102	BGC	O5-C5-C6-O6
8	A	402	AGH	CAJ-CAK-CAL-CAM
8	C	401	AGH	CAU-CAV-CAW-CAX
12	B	102	BGC	C4-C5-C6-O6
8	C	401	AGH	C4A-C5M-C6A-O5A
9	A	404	PEG	O1-C1-C2-O2
8	C	401	AGH	C14-C15-C16-C17
8	A	402	AGH	CAS-CAT-CAU-CAV
8	C	401	AGH	CAK-CAL-CAM-CAN
8	A	402	AGH	CAQ-CAR-CAS-CAT
8	C	401	AGH	CAC-CAD-CAE-CAF
8	C	401	AGH	CAJ-CAK-CAL-CAM
8	C	401	AGH	C7-C8-C9-C10
8	A	402	AGH	CAU-CAV-CAW-CAX
8	C	401	AGH	CAH-CAI-CAJ-CAK
8	A	402	AGH	CAG-CAH-CAI-CAJ
8	A	402	AGH	CAF-CAG-CAH-CAI
8	A	402	AGH	C4-C5-C6-C7
8	A	402	AGH	CAT-CAU-CAV-CAW
8	C	401	AGH	CAF-CAG-CAH-CAI
8	A	402	AGH	C14-C15-C16-C17
8	C	401	AGH	CAT-CAU-CAV-CAW
8	C	401	AGH	CAB-CAC-CAD-CAE
9	A	404	PEG	O2-C3-C4-O4
8	C	401	AGH	CAP-CAQ-CAR-CAS
8	C	401	AGH	CAM-CAN-CAO-CAP
8	C	401	AGH	CAR-CAS-CAT-CAU
8	C	401	AGH	C9-C10-C11-C12
8	C	401	AGH	CAV-CAW-CAX-CAY
9	E	201	PEG	C1-C2-O2-C3

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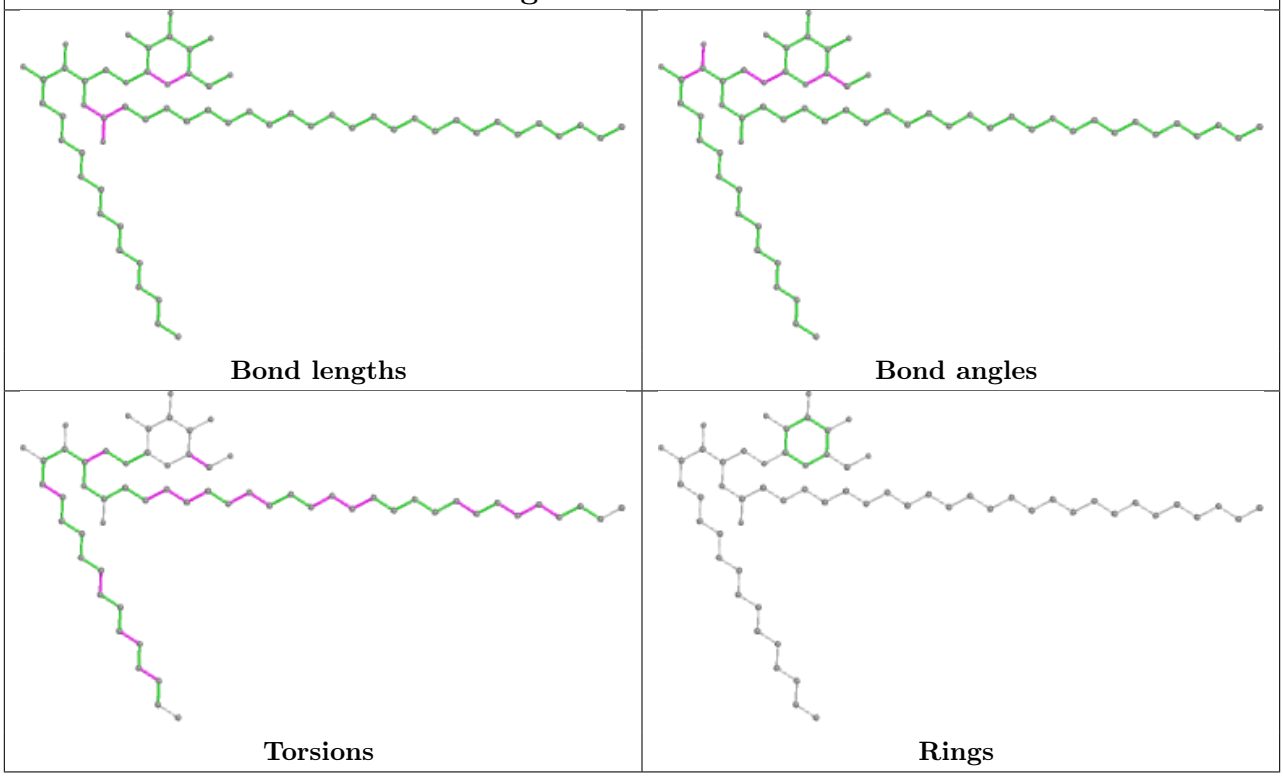
Mol	Chain	Res	Type	Atoms
8	C	401	AGH	C13-C14-C15-C16
8	A	402	AGH	C12-C13-C14-C15
8	A	402	AGH	O1A-C1-C2-C3
8	A	402	AGH	CAL-CAM-CAN-CAO
8	A	402	AGH	CAC-CAD-CAE-CAF
8	A	402	AGH	CAB-CAC-CAD-CAE
9	A	403	PEG	C1-C2-O2-C3
8	C	401	AGH	CAO-CAP-CAQ-CAR
8	A	402	AGH	CAD-CAE-CAF-CAG
8	A	402	AGH	C9-C10-C11-C12
8	C	401	AGH	CAI-CAJ-CAK-CAL
9	E	201	PEG	O1-C1-C2-O2
9	E	201	PEG	O2-C3-C4-O4
8	A	402	AGH	CAK-CAL-CAM-CAN
8	C	401	AGH	CAE-CAF-CAG-CAH
8	A	402	AGH	O6A-C5M-C6A-O5A
8	C	401	AGH	O6A-C5M-C6A-O5A

There are no ring outliers.

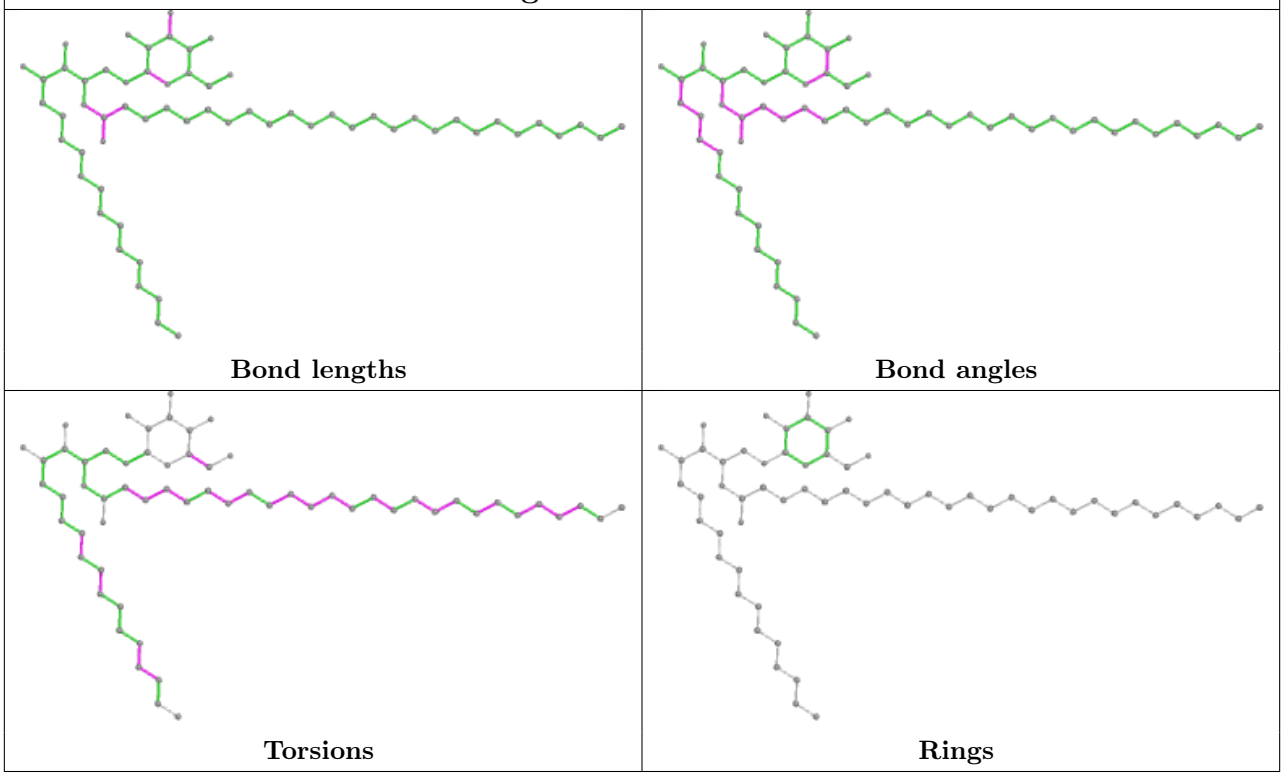
No monomer is involved in short contacts.

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 AGH A 402



Ligand AGH C 401



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.