wwPDB X-ray Structure Validation Summary Report (i)

Dec 4, 2023 – 03:37 am GMT

PDB ID	:	1GYC
Title	:	CRYSTAL STRUCTURE DETERMINATION AT ROOM TEMPERATURE OF A LACCASE FROM TRAMETES VERSICOLOR IN ITS OXIDISED FORM CONTAINING A FULL COMPLEMENT OF COPPER IONS
Authors	:	Choinowski, T.; Antorini, M.; Piontek, K.
Deposited on	:	2002-04-23
Resolution	:	1.90 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	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
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)	:	2.36

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 1.90 Å.

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

MolProbity failed to run properly; EDS was not executed - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4600 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 LACCASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	499	3872	2479	665	720	8	0	9	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	ALA	VAL	SEE REMARK 999	UNP Q12718
A	31	PHE	VAL	SEE REMARK 999	UNP Q12718
A	49	VAL	ASP	variant	UNP Q12718
A	56	THR	SER	SEE REMARK 999	UNP Q12718
A	259	ILE	VAL	SEE REMARK 999	UNP Q12718
A	343	SER	THR	SEE REMARK 999	UNP Q12718
A	460	GLU	ASP	SEE REMARK 999	UNP Q12718

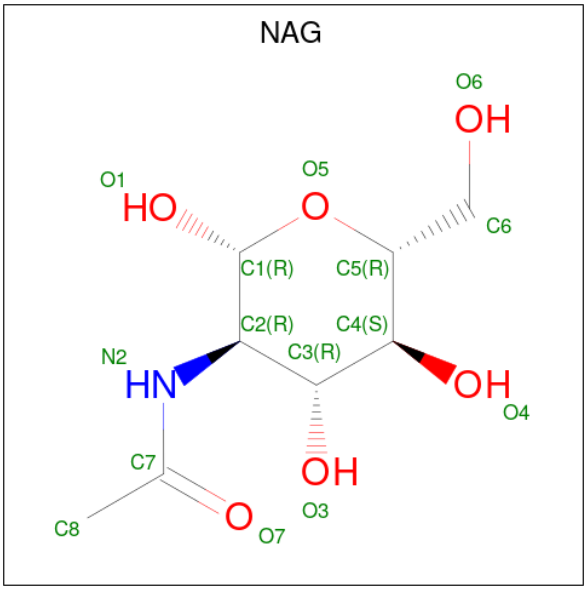
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

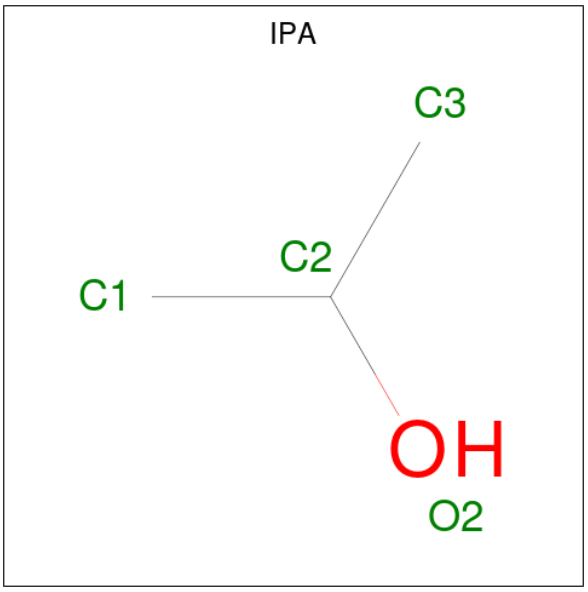
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total Cu 4 4	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 3 1	0	0
5	A	1	Total C O 4 3 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	590	Total O 590 590	0	0

MolProbity failed to run properly; EDS was not executed - this section is therefore empty.

3 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.68Å 84.98Å 91.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.90 – 1.90	Depositor
% Data completeness (in resolution range)	99.4 (17.90-1.90)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.159 , 0.212	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4600	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

4 Model quality

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

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

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

4.5 Carbohydrates

6 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	$\#\|Z\|>2$
2	NAG	B	1	1,2	14,14,15	1.22	2 (14%)	17,19,21	1.34	2 (11%)
2	NAG	B	2	2	14,14,15	1.21	1 (7%)	17,19,21	1.33	3 (17%)
2	NAG	C	1	1,2	14,14,15	1.20	1 (7%)	17,19,21	0.98	0
2	NAG	C	2	2	14,14,15	1.62	2 (14%)	17,19,21	5.88	8 (47%)
2	NAG	D	1	1,2	14,14,15	1.16	1 (7%)	17,19,21	0.86	0
2	NAG	D	2	2	14,14,15	1.45	1 (7%)	17,19,21	2.62	7 (41%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	1/6/23/26	0/1/1/1
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	5/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	3/6/23/26	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAG	O7-C7	-3.85	1.14	1.23
2	C	1	NAG	O7-C7	-3.82	1.14	1.23
2	C	2	NAG	C2-N2	-3.71	1.40	1.46
2	C	2	NAG	O7-C7	-3.63	1.15	1.23
2	D	1	NAG	O7-C7	-3.42	1.15	1.23

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	NAG	C2-N2-C7	20.70	152.37	122.90
2	C	2	NAG	C1-C2-N2	7.31	122.97	110.49
2	C	2	NAG	O7-C7-N2	-6.04	110.85	121.95
2	D	2	NAG	O5-C1-C2	-5.96	101.88	111.29
2	D	2	NAG	C2-N2-C7	4.86	129.83	122.90

There are no chirality outliers.

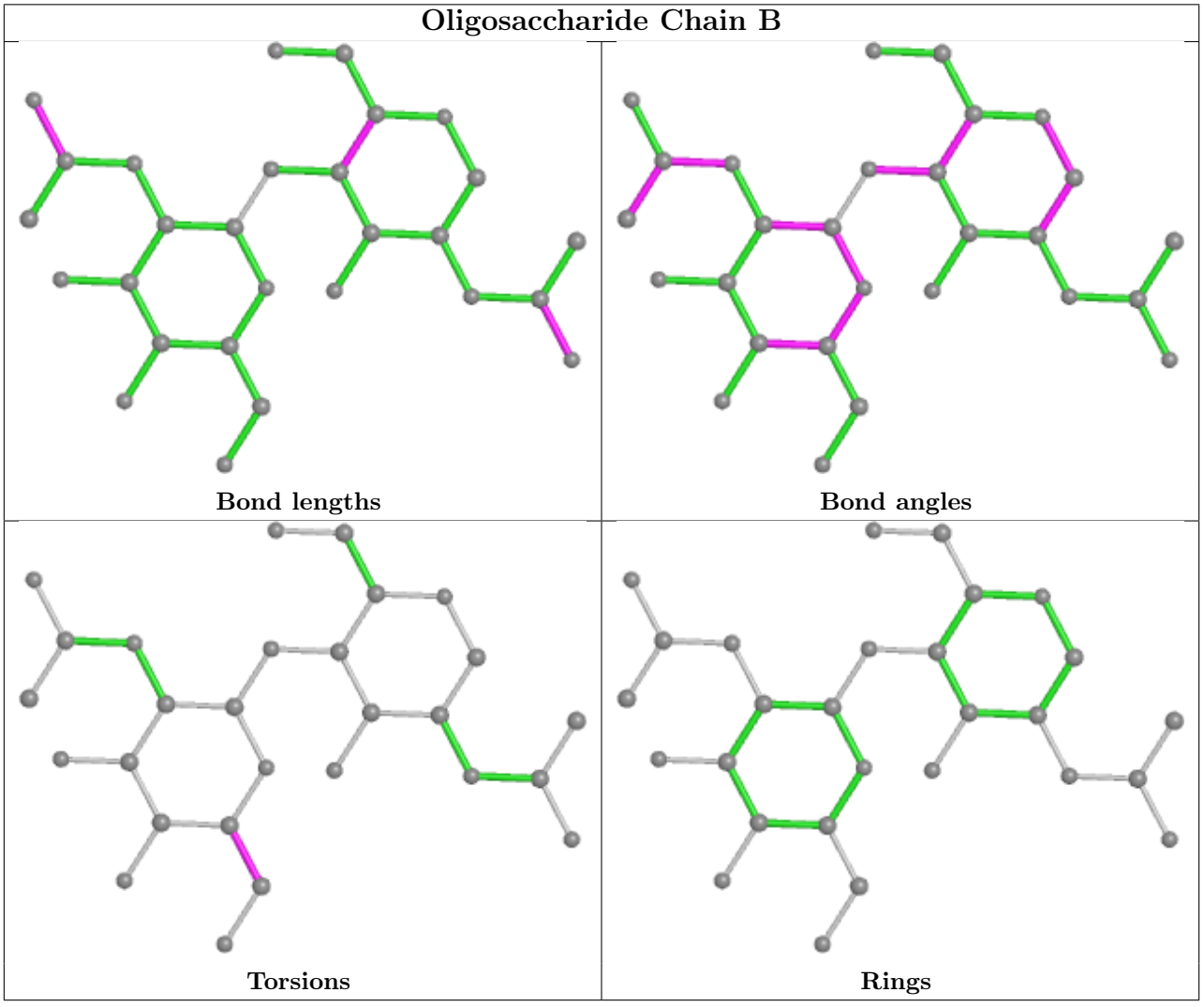
5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C1-C2-N2-C7
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	C	1	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6

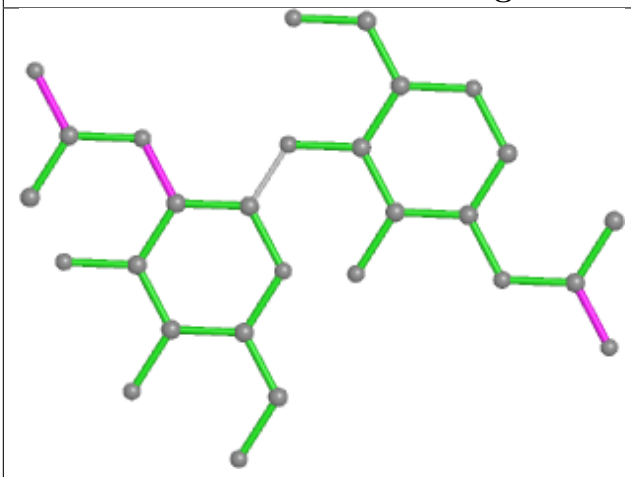
There are no ring outliers.

No monomer is involved in short contacts.

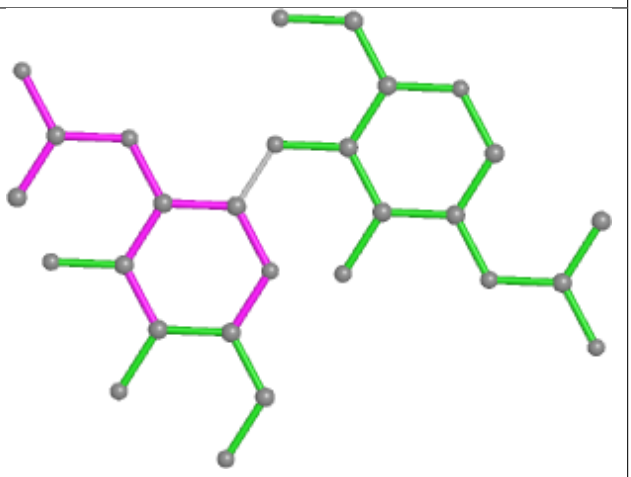
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



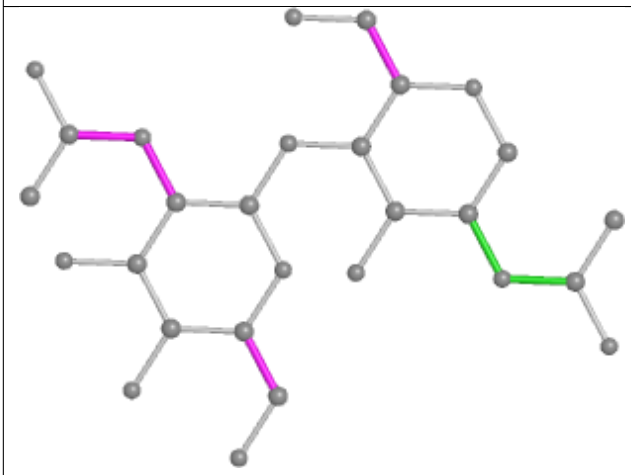
Oligosaccharide Chain C



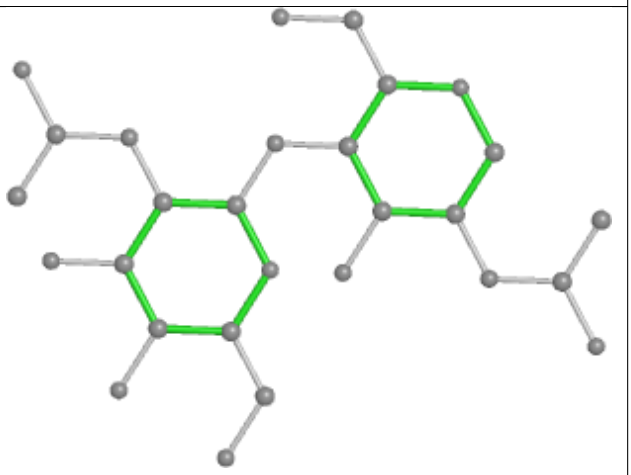
Bond lengths



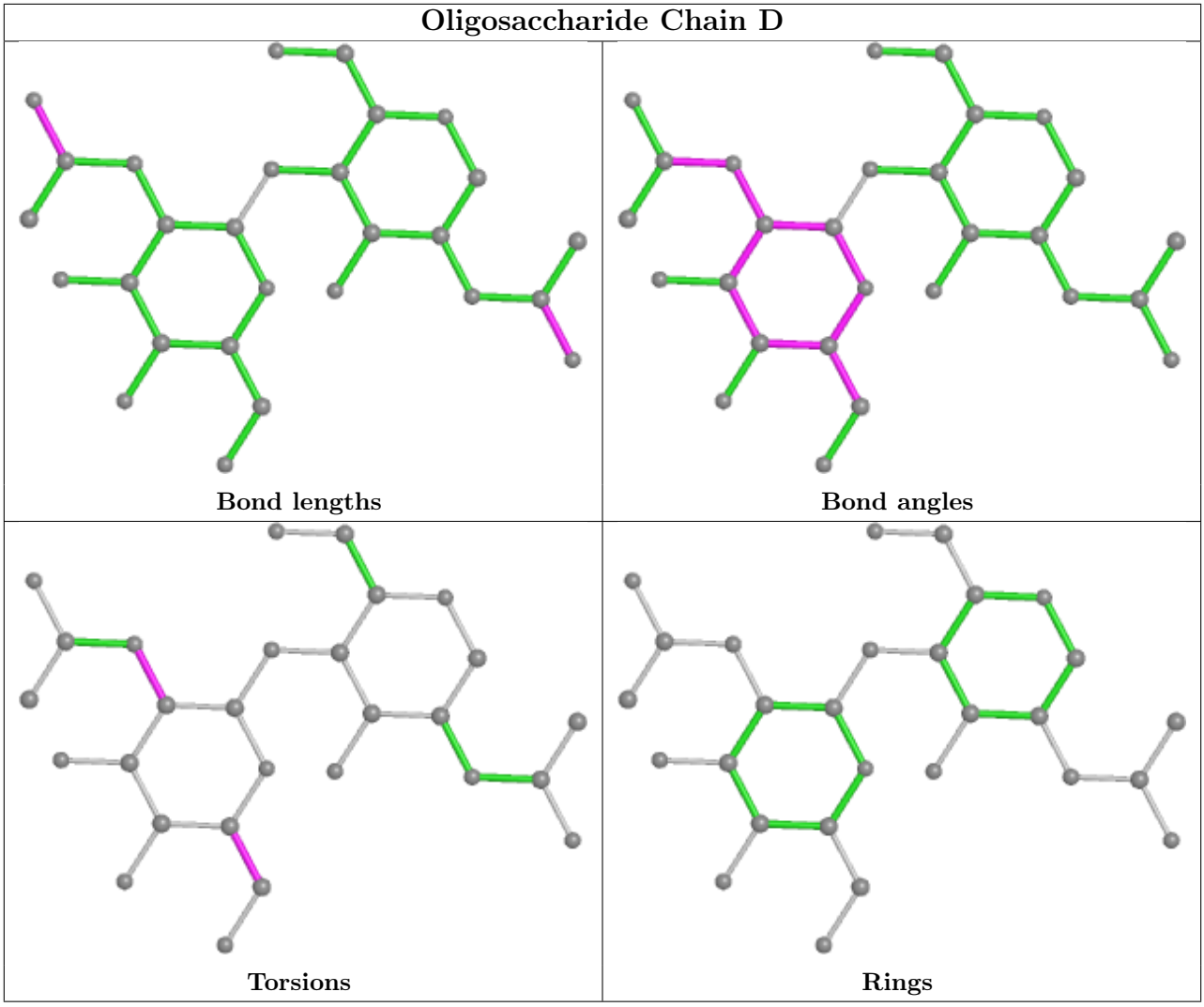
Bond angles



Torsions



Rings



4.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	IPA	A	1513	-	3,3,3	1.09	0	3,3,3	0.95	0
4	NAG	A	1512	1	14,14,15	1.25	2 (14%)	17,19,21	1.03	0
5	IPA	A	1514	-	3,3,3	1.04	0	3,3,3	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	A	1508	1	14,14,15	1.35	1 (7%)	17,19,21	1.83	4 (23%)
4	NAG	A	1509	1	14,14,15	1.11	1 (7%)	17,19,21	1.13	3 (17%)

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	A	1508	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1512	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1509	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1508	NAG	O7-C7	-3.57	1.15	1.23
4	A	1512	NAG	O7-C7	-3.51	1.15	1.23
4	A	1509	NAG	O7-C7	-3.35	1.15	1.23
4	A	1512	NAG	C2-N2	2.18	1.50	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1508	NAG	C4-C3-C2	4.27	117.27	111.02
4	A	1508	NAG	O5-C1-C2	-3.66	105.50	111.29
4	A	1508	NAG	C3-C4-C5	3.18	115.91	110.24
4	A	1509	NAG	C1-O5-C5	-2.29	109.09	112.19
4	A	1509	NAG	O5-C5-C4	-2.28	105.29	110.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1508	NAG	C8-C7-N2-C2
4	A	1508	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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

5.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

5.3 Carbohydrates

EDS was not executed - this section is therefore empty.

5.4 Ligands

EDS was not executed - this section is therefore empty.

5.5 Other polymers

EDS was not executed - this section is therefore empty.