wwPDB X-ray Structure Validation Summary Report (i)

Oct 3, 2023 – 06:47 AM EDT

PDB ID	:	6OEJ
Title	:	CRYSTAL STRUCTURE OF THE NON-NEUTRALIZING AND ADCC-POTENT ANTIBODY C11 IN COMPLEX WITH HIV-1 CLADE A/E GP120
Authors	:	Tolbert, W.D.; Pazgier, M.
Deposited on	:	2019-03-27
Resolution	:	3.45 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
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 3.45 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 5 unique types of molecules in this entry. The entry contains 12140 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 clade A/E 93TH057 HIV-1 gp120 core.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	319	Total	C	N	O	S	0	0	0
			2497	1574	423	478	22			
1	A	322	Total	C	N	O	S	0	0	0
			2524	1591	429	481	23			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	31	CYS	-	see sequence details	UNP A0A0M3KKW9
G	32	ASP	-	see sequence details	UNP A0A0M3KKW9
G	33	ASN	-	see sequence details	UNP A0A0M3KKW9
G	34	LEU	-	see sequence details	UNP A0A0M3KKW9
G	35	TRP	-	see sequence details	UNP A0A0M3KKW9
G	36	VAL	-	see sequence details	UNP A0A0M3KKW9
G	37	THR	-	see sequence details	UNP A0A0M3KKW9
G	38	VAL	-	see sequence details	UNP A0A0M3KKW9
G	39	TYR	-	see sequence details	UNP A0A0M3KKW9
G	40	TYR	-	see sequence details	UNP A0A0M3KKW9
G	41	GLY	-	see sequence details	UNP A0A0M3KKW9
G	42	VAL	-	see sequence details	UNP A0A0M3KKW9
G	43	PRO	-	see sequence details	UNP A0A0M3KKW9
G	80	CYS	ASN	engineered mutation	UNP A0A0M3KKW9
G	375	SER	HIS	engineered mutation	UNP A0A0M3KKW9
G	493	PRO	-	see sequence details	UNP A0A0M3KKW9
G	494	LEU	-	see sequence details	UNP A0A0M3KKW9
G	495	GLY	-	see sequence details	UNP A0A0M3KKW9
G	496	ILE	-	see sequence details	UNP A0A0M3KKW9
G	497	ALA	-	see sequence details	UNP A0A0M3KKW9
G	498	PRO	-	see sequence details	UNP A0A0M3KKW9
G	499	THR	-	see sequence details	UNP A0A0M3KKW9
G	500	LYS	-	see sequence details	UNP A0A0M3KKW9
G	501	ALA	-	see sequence details	UNP A0A0M3KKW9
G	502	LYS	-	see sequence details	UNP A0A0M3KKW9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	503	ARG	-	see sequence details	UNP A0A0M3KKW9
G	504	ARG	-	see sequence details	UNP A0A0M3KKW9
G	505	VAL	-	see sequence details	UNP A0A0M3KKW9
G	506	VAL	-	see sequence details	UNP A0A0M3KKW9
G	507	GLN	-	see sequence details	UNP A0A0M3KKW9
G	508	ARG	-	see sequence details	UNP A0A0M3KKW9
G	509	GLU	-	see sequence details	UNP A0A0M3KKW9
G	510	LYS	-	see sequence details	UNP A0A0M3KKW9
G	511	ARG	-	see sequence details	UNP A0A0M3KKW9
A	31	CYS	-	see sequence details	UNP A0A0M3KKW9
A	32	ASP	-	see sequence details	UNP A0A0M3KKW9
A	33	ASN	-	see sequence details	UNP A0A0M3KKW9
A	34	LEU	-	see sequence details	UNP A0A0M3KKW9
A	35	TRP	-	see sequence details	UNP A0A0M3KKW9
A	36	VAL	-	see sequence details	UNP A0A0M3KKW9
A	37	THR	-	see sequence details	UNP A0A0M3KKW9
A	38	VAL	-	see sequence details	UNP A0A0M3KKW9
A	39	TYR	-	see sequence details	UNP A0A0M3KKW9
A	40	TYR	-	see sequence details	UNP A0A0M3KKW9
A	41	GLY	-	see sequence details	UNP A0A0M3KKW9
A	42	VAL	-	see sequence details	UNP A0A0M3KKW9
A	43	PRO	-	see sequence details	UNP A0A0M3KKW9
A	80	CYS	ASN	engineered mutation	UNP A0A0M3KKW9
A	375	SER	HIS	engineered mutation	UNP A0A0M3KKW9
A	493	PRO	-	see sequence details	UNP A0A0M3KKW9
A	494	LEU	-	see sequence details	UNP A0A0M3KKW9
A	495	GLY	-	see sequence details	UNP A0A0M3KKW9
A	496	ILE	-	see sequence details	UNP A0A0M3KKW9
A	497	ALA	-	see sequence details	UNP A0A0M3KKW9
A	498	PRO	-	see sequence details	UNP A0A0M3KKW9
A	499	THR	-	see sequence details	UNP A0A0M3KKW9
A	500	LYS	-	see sequence details	UNP A0A0M3KKW9
A	501	ALA	-	see sequence details	UNP A0A0M3KKW9
A	502	LYS	-	see sequence details	UNP A0A0M3KKW9
A	503	ARG	-	see sequence details	UNP A0A0M3KKW9
A	504	ARG	-	see sequence details	UNP A0A0M3KKW9
A	505	VAL	-	see sequence details	UNP A0A0M3KKW9
A	506	VAL	-	see sequence details	UNP A0A0M3KKW9
A	507	GLN	-	see sequence details	UNP A0A0M3KKW9
A	508	ARG	-	see sequence details	UNP A0A0M3KKW9
A	509	GLU	-	see sequence details	UNP A0A0M3KKW9
A	510	LYS	-	see sequence details	UNP A0A0M3KKW9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	511	ARG	-	see sequence details	UNP A0A0M3KKW9

- Molecule 2 is a protein called C11 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	227	Total	C	N	O	S	0	0	0
			1708	1079	288	334	7			
2	B	227	Total	C	N	O	S	0	0	0
			1709	1079	288	335	7			

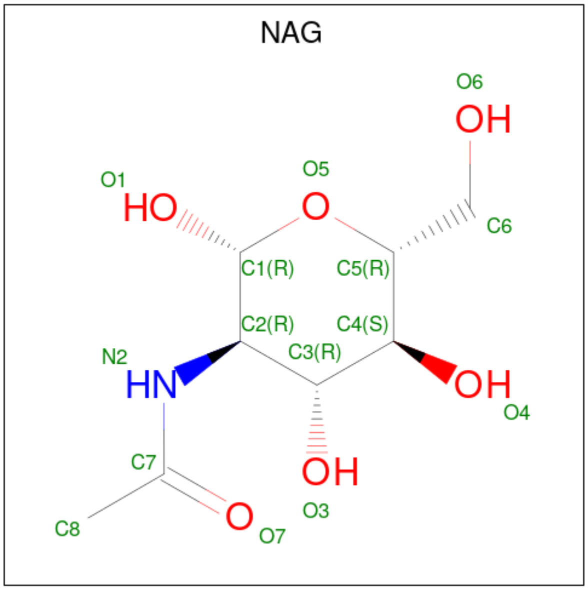
- Molecule 3 is a protein called C11 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	215	Total	C	N	O	S	0	0	0
			1646	1035	277	328	6			
3	C	216	Total	C	N	O	S	0	0	0
			1650	1037	278	329	6			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	4	Total	C	N	O	0	0	0
			49	28	2	19			
4	E	4	Total	C	N	O	0	0	0
			49	28	2	19			

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

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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	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	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	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

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	89.37Å 110.96Å 217.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.42 – 3.45	Depositor
% Data completeness (in resolution range)	91.1 (49.42-3.45)	Depositor
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.231 , 0.284	Depositor
Wilson B-factor (Å^2)	98.9	Xtriage
Anisotropy	0.773	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12140	wwPDB-VP
Average B, all atoms (Å^2)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% 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

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

8 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	D	1	4,2	14,14,15	0.28	0	17,19,21	0.51	0
4	NAG	D	2	4	14,14,15	0.54	0	17,19,21	0.49	0
4	BMA	D	3	4	11,11,12	0.67	0	15,15,17	0.78	0
4	FUC	D	4	4	10,10,11	0.82	0	14,14,16	1.01	1 (7%)
4	NAG	E	1	4,2	14,14,15	0.26	0	17,19,21	0.54	0
4	NAG	E	2	4	14,14,15	0.20	0	17,19,21	0.53	0
4	BMA	E	3	4	11,11,12	0.59	0	15,15,17	0.79	0
4	FUC	E	4	4	10,10,11	0.83	0	14,14,16	1.33	2 (14%)

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	D	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	4/6/23/26	0/1/1/1
4	BMA	D	3	4	-	2/2/19/22	0/1/1/1
4	FUC	D	4	4	-	-	0/1/1/1
4	NAG	E	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	1/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	FUC	E	4	4	-	-	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})
4	E	4	FUC	O5-C5-C4	3.04	114.97	109.52
4	E	4	FUC	C1-O5-C5	2.22	117.81	112.78
4	D	4	FUC	O5-C5-C4	2.22	113.50	109.52

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	D	3	BMA	C4-C5-C6-O6
4	D	2	NAG	C1-C2-N2-C7

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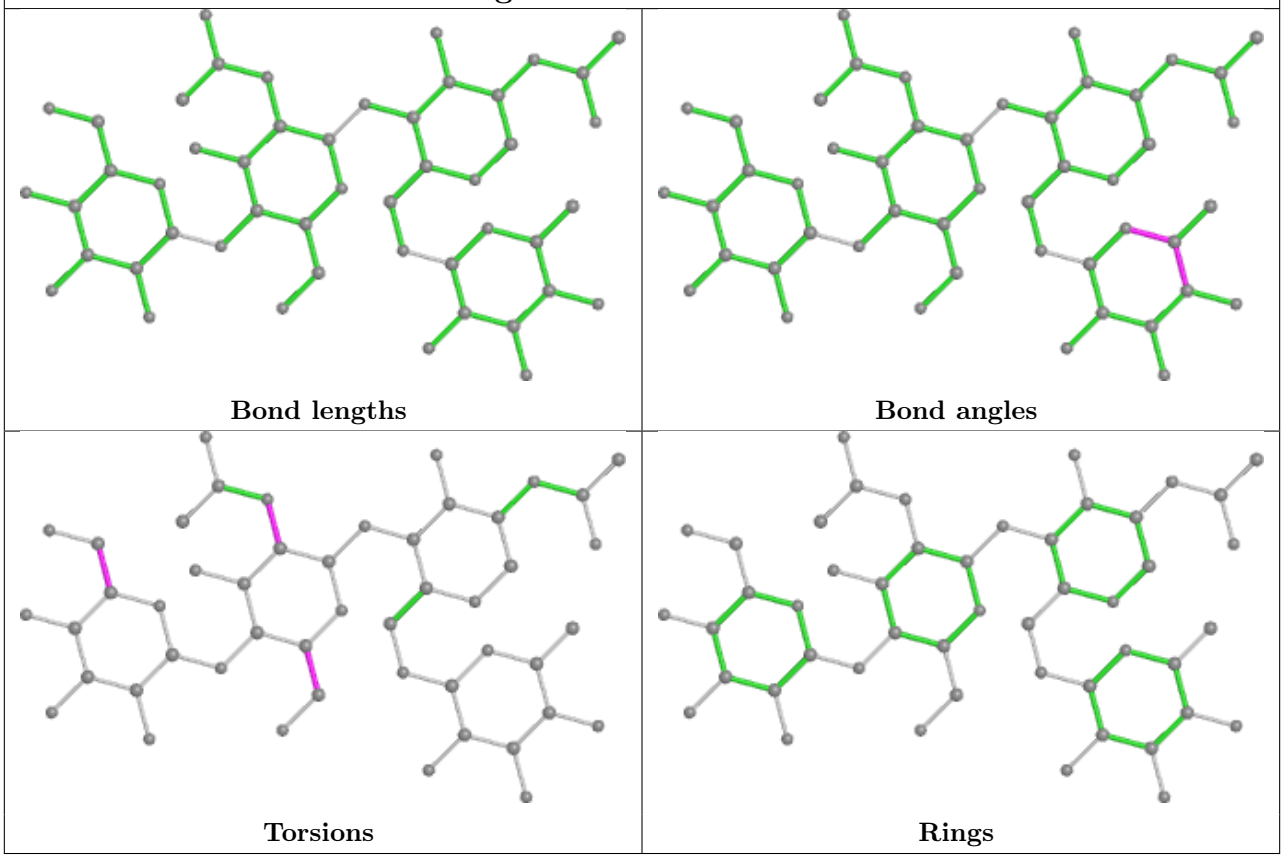
Mol	Chain	Res	Type	Atoms
4	D	3	BMA	O5-C5-C6-O6

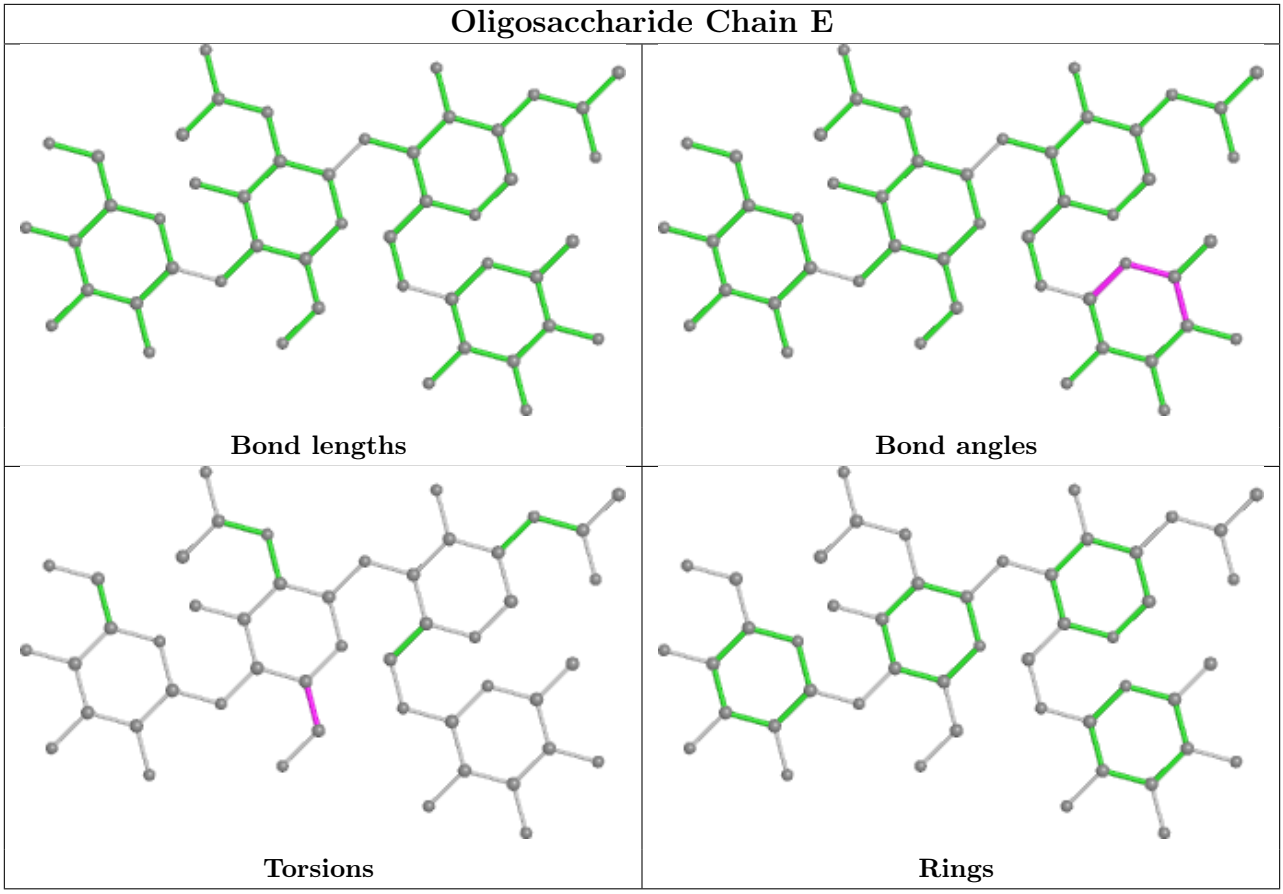
There are no ring outliers.

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 D





4.6 Ligand geometry (i)

22 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	$\#\|Z\| > 2$
5	NAG	A	606	1	14,14,15	0.34	0	17,19,21	0.34	0
5	NAG	A	610	1	14,14,15	0.35	0	17,19,21	0.45	0
5	NAG	A	602	1	14,14,15	0.47	0	17,19,21	0.42	0
5	NAG	A	607	1	14,14,15	0.20	0	17,19,21	0.47	0
5	NAG	G	605	1	14,14,15	0.35	0	17,19,21	0.33	0
5	NAG	G	604	1	14,14,15	0.27	0	17,19,21	0.40	0
5	NAG	G	602	1	14,14,15	0.40	0	17,19,21	0.39	0
5	NAG	A	609	1	14,14,15	0.29	0	17,19,21	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	A	604	1	14,14,15	0.44	0	17,19,21	0.51	0
5	NAG	G	603	1	14,14,15	0.27	0	17,19,21	0.36	0
5	NAG	G	606	1	14,14,15	0.30	0	17,19,21	0.46	0
5	NAG	G	610	1	14,14,15	0.32	0	17,19,21	0.49	0
5	NAG	G	601	1	14,14,15	0.41	0	17,19,21	0.52	0
5	NAG	G	608	1	14,14,15	0.23	0	17,19,21	0.47	0
5	NAG	G	611	1	14,14,15	0.29	0	17,19,21	0.47	0
5	NAG	G	609	1	14,14,15	0.37	0	17,19,21	0.49	0
5	NAG	A	611	1	14,14,15	0.22	0	17,19,21	0.37	0
5	NAG	G	607	1	14,14,15	0.37	0	17,19,21	0.51	0
5	NAG	A	608	1	14,14,15	0.30	0	17,19,21	0.40	0
5	NAG	A	605	1	14,14,15	0.39	0	17,19,21	0.48	0
5	NAG	A	603	1	14,14,15	0.39	0	17,19,21	0.54	0
5	NAG	A	601	1	14,14,15	0.72	1 (7%)	17,19,21	0.67	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
5	NAG	A	606	1	-	2/6/23/26	0/1/1/1
5	NAG	A	610	1	-	0/6/23/26	0/1/1/1
5	NAG	A	602	1	-	1/6/23/26	0/1/1/1
5	NAG	A	607	1	-	2/6/23/26	0/1/1/1
5	NAG	G	605	1	-	3/6/23/26	0/1/1/1
5	NAG	G	604	1	-	2/6/23/26	0/1/1/1
5	NAG	G	602	1	-	0/6/23/26	0/1/1/1
5	NAG	A	609	1	-	2/6/23/26	0/1/1/1
5	NAG	A	604	1	-	2/6/23/26	0/1/1/1
5	NAG	G	603	1	-	2/6/23/26	0/1/1/1
5	NAG	G	606	1	-	2/6/23/26	0/1/1/1
5	NAG	G	610	1	-	0/6/23/26	0/1/1/1
5	NAG	G	601	1	-	1/6/23/26	0/1/1/1
5	NAG	G	608	1	-	2/6/23/26	0/1/1/1
5	NAG	G	611	1	-	2/6/23/26	0/1/1/1
5	NAG	G	609	1	-	1/6/23/26	0/1/1/1
5	NAG	A	611	1	-	2/6/23/26	0/1/1/1
5	NAG	G	607	1	-	0/6/23/26	0/1/1/1
5	NAG	A	608	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	605	1	-	1/6/23/26	0/1/1/1
5	NAG	A	603	1	-	0/6/23/26	0/1/1/1
5	NAG	A	601	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	NAG	C1-C2	2.56	1.56	1.52

There are no bond angle outliers.

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	608	NAG	C4-C5-C6-O6
5	G	603	NAG	O5-C5-C6-O6
5	A	611	NAG	O5-C5-C6-O6
5	A	607	NAG	O5-C5-C6-O6
5	G	608	NAG	O5-C5-C6-O6

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 failed to run properly - this section is therefore empty.

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

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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