



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 11:12 PM EDT

PDB ID : 1DOG  
Title : REFINED STRUCTURE FOR THE COMPLEX OF 1-DEOXYNOJIRIMYCIN WITH GLUCOAMYLASE FROM (ASPERGILLUS AWAMORI) VAR. X100 TO 2.4 ANGSTROMS RESOLUTION  
Authors : Harris, E.; Aleshin, A.; Firsov, L.; Honzatko, R.B.  
Deposited on : 1993-01-12  
Resolution : 2.30 Å(reported)

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We welcome your comments at [validation@mail.wwpdb.org](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (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) : 2.36.2

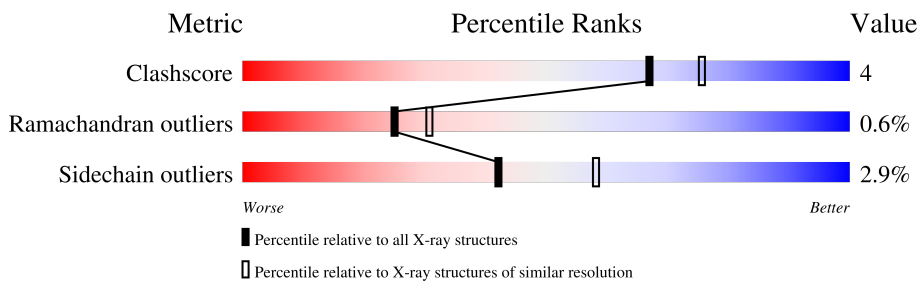
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	470	
2	B	5	
3	C	8	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4472 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.

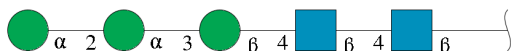
- Molecule 1 is a protein called GLUCOAMYLASE-471.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	470	3580	2242	586	744	8	0	5	0

There are 3 discrepancies between the modelled and reference sequences:

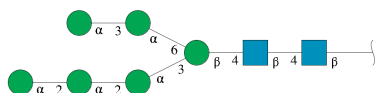
Chain	Residue	Modelled	Actual	Comment	Reference
A	58	LEU	ILE	conflict	UNP P23176
A	60	ILE	LEU	conflict	UNP P23176
A	117	THR	ALA	conflict	UNP P23176

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



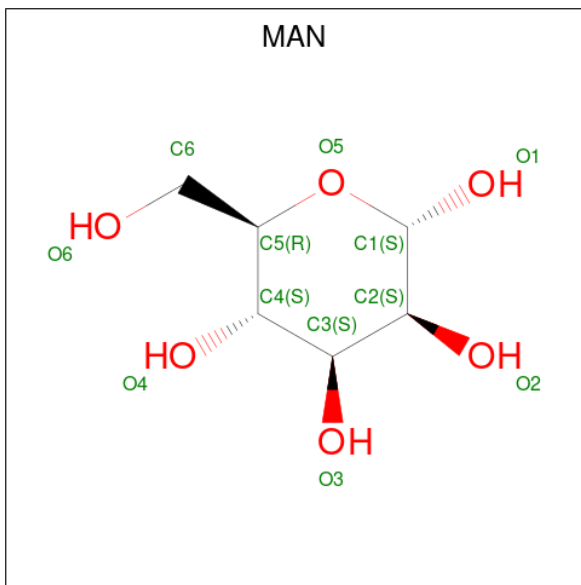
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	5	61	34	2	25	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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.



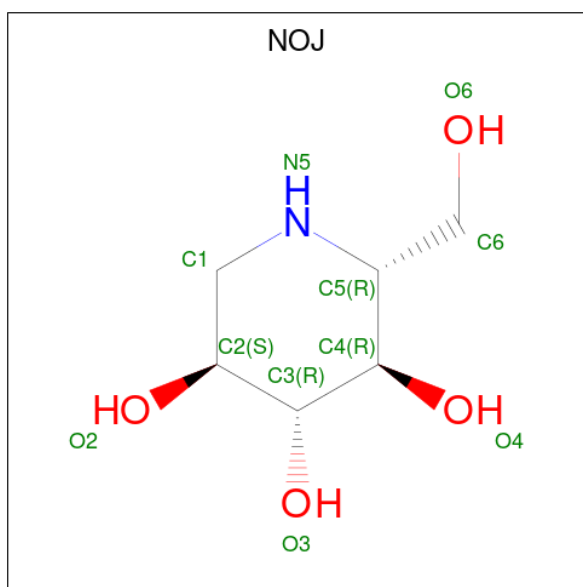
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	8	94	52	2	40	0	0	0

- Molecule 4 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	11	6	5	0	0
4	A	1	11	6	5	0	0
4	A	1	11	6	5	0	0
4	A	1	11	6	5	0	0
4	A	1	11	6	5	0	0
4	A	1	11	6	5	0	0
4	A	1	11	6	5	0	0
4	A	1	11	6	5	0	0
4	A	1	11	6	5	0	0

- Molecule 5 is 1-DEOXYNOJIRIMYCIN (three-letter code: NOJ) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	11	6	1	4	0	0
5	A	1	11	6	1	4	0	0

- Molecule 6 is water.

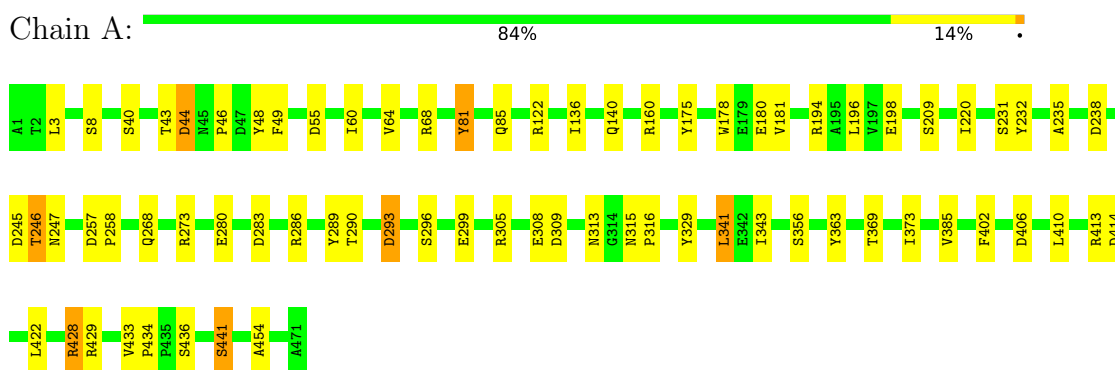
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	605	605	605	0	0

### 3 Residue-property plots

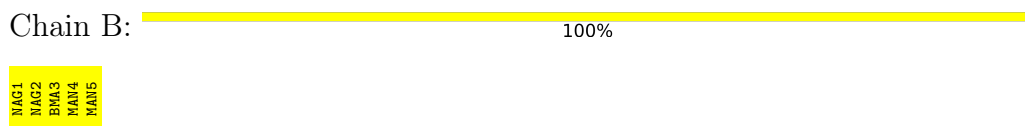
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

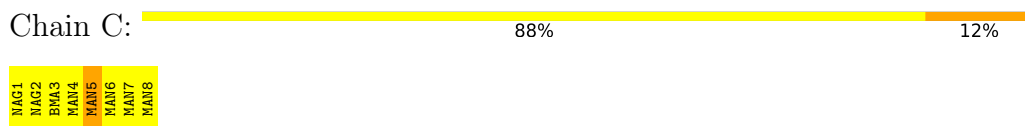
- Molecule 1: GLUCOAMYLASE-471



- Molecule 2: alpha-D-mannopyranose-(1-2)-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



- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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



## 4 Data and refinement statistics

Xtrriage (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, $\alpha$ , $\beta$ , $\gamma$	116.60Å 103.60Å 48.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.30)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.119 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4472	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

## 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, BMA, NOJ, NAG

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	0.87	0/3692	1.40	33/5051 (0.7%)

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
1	A	0	4

There are no bond length outliers.

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	273	ARG	NE-CZ-NH1	17.87	129.24	120.30
1	A	273	ARG	NE-CZ-NH2	-16.32	112.14	120.30
1	A	122	ARG	NE-CZ-NH2	10.05	125.33	120.30
1	A	428	ARG	NE-CZ-NH1	9.85	125.22	120.30
1	A	429	ARG	NE-CZ-NH1	8.77	124.69	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	246[B]	THR	Mainchain
1	A	428	ARG	Sidechain
1	A	44[A]	ASP	Sidechain
1	A	44[B]	ASP	Sidechain



## 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	A	3580	0	3308	25	0
2	B	61	0	52	0	0
3	C	94	0	79	2	0
4	A	110	0	100	0	0
5	A	22	0	26	4	0
6	A	605	0	0	6	0
All	All	4472	0	3565	29	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 4.

The worst 5 of 29 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)
5:A:496:NOJ:H12	6:A:1200:HOH:O	1.12	1.26
5:A:496:NOJ:C1	6:A:1200:HOH:O	1.91	0.68
5:A:495:NOJ:H11	5:A:496:NOJ:O2	1.98	0.63
1:A:43:THR:HG23	3:C:5:MAN:H61	1.81	0.63
1:A:235:ALA:HB2	1:A:245:ASP:HB3	1.81	0.62

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	473/470 (101%)	454 (96%)	15 (3%)	4 (1%)	<b>19</b> <b>23</b>

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	238	ASP
1	A	313	ASN
1	A	246[A]	THR
1	A	246[B]	THR

### 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	390/385 (101%)	378 (97%)	12 (3%)	40 55

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	247	ASN
1	A	341	LEU
1	A	441	SER
1	A	356	SER
1	A	44[B]	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	313	ASN
1	A	426	ASN
1	A	427	ASN
1	A	168	GLN
1	A	21	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](#)

13 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	2,1	14,14,15	1.01	1 (7%)	17,19,21	1.48	2 (11%)
2	NAG	B	2	2	14,14,15	0.94	1 (7%)	17,19,21	1.24	3 (17%)
2	BMA	B	3	2	11,11,12	0.62	0	15,15,17	1.34	3 (20%)
2	MAN	B	4	2	11,11,12	0.88	0	15,15,17	1.81	3 (20%)
2	MAN	B	5	2	11,11,12	0.73	0	15,15,17	1.22	3 (20%)
3	NAG	C	1	1,3	14,14,15	1.01	1 (7%)	17,19,21	1.28	2 (11%)
3	NAG	C	2	3	14,14,15	0.88	1 (7%)	17,19,21	1.33	2 (11%)
3	BMA	C	3	3	11,11,12	0.72	0	15,15,17	1.40	1 (6%)
3	MAN	C	4	3	11,11,12	0.37	0	15,15,17	1.63	3 (20%)
3	MAN	C	5	3	11,11,12	0.54	0	15,15,17	1.20	1 (6%)
3	MAN	C	6	3	11,11,12	0.62	0	15,15,17	1.34	1 (6%)
3	MAN	C	7	3	11,11,12	0.56	0	15,15,17	1.10	2 (13%)
3	MAN	C	8	3	11,11,12	0.57	0	15,15,17	1.31	2 (13%)

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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	B	4	2	-	0/2/19/22	0/1/1/1
2	MAN	B	5	2	-	2/2/19/22	0/1/1/1
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	1/2/19/22	0/1/1/1
3	MAN	C	5	3	-	1/2/19/22	0/1/1/1
3	MAN	C	6	3	-	2/2/19/22	0/1/1/1
3	MAN	C	7	3	-	0/2/19/22	0/1/1/1
3	MAN	C	8	3	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	NAG	C8-C7	3.08	1.56	1.50
2	B	1	NAG	C8-C7	2.93	1.56	1.50
3	C	2	NAG	C8-C7	2.86	1.56	1.50
2	B	2	NAG	C8-C7	2.69	1.56	1.50

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	MAN	C1-O5-C5	4.71	118.58	112.19
3	C	6	MAN	C1-O5-C5	4.32	118.05	112.19
2	B	1	NAG	C1-O5-C5	4.02	117.64	112.19
3	C	2	NAG	C1-O5-C5	3.64	117.12	112.19
2	B	2	NAG	C1-O5-C5	3.44	116.85	112.19

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

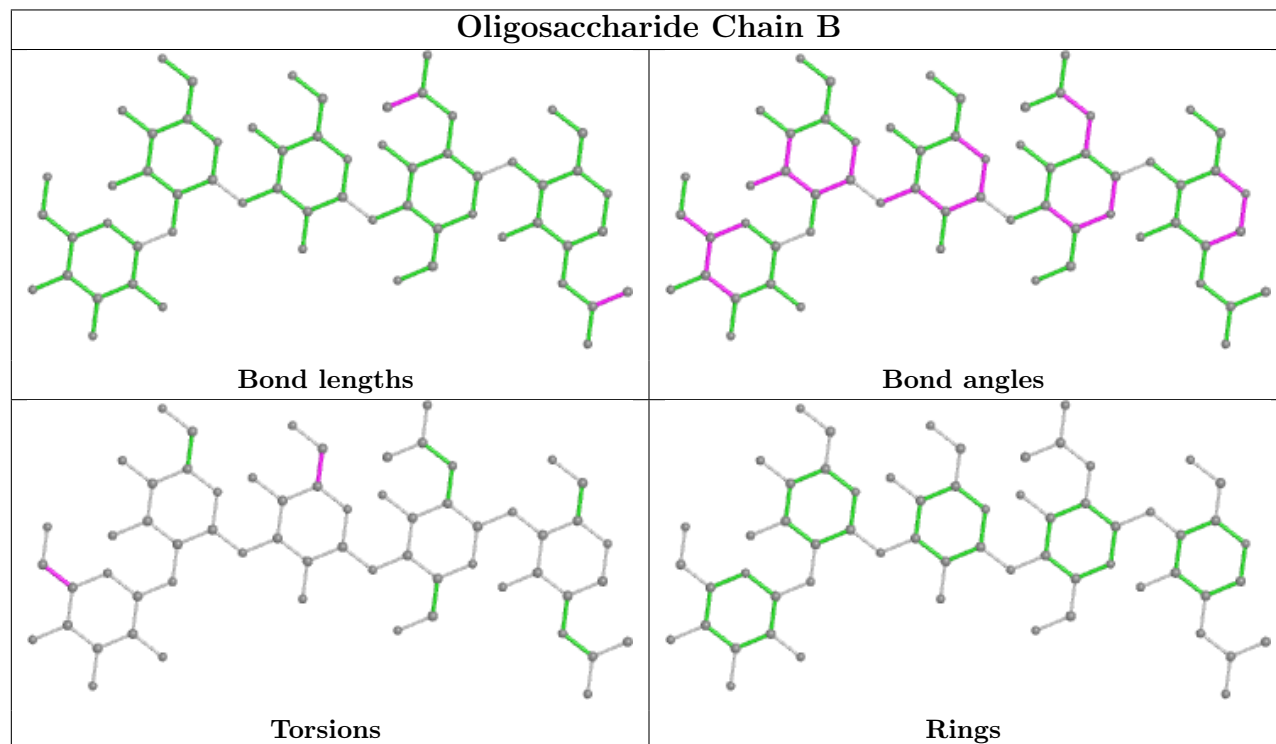
Mol	Chain	Res	Type	Atoms
2	B	3	BMA	O5-C5-C6-O6
3	C	6	MAN	O5-C5-C6-O6
2	B	5	MAN	O5-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
2	B	5	MAN	C4-C5-C6-O6

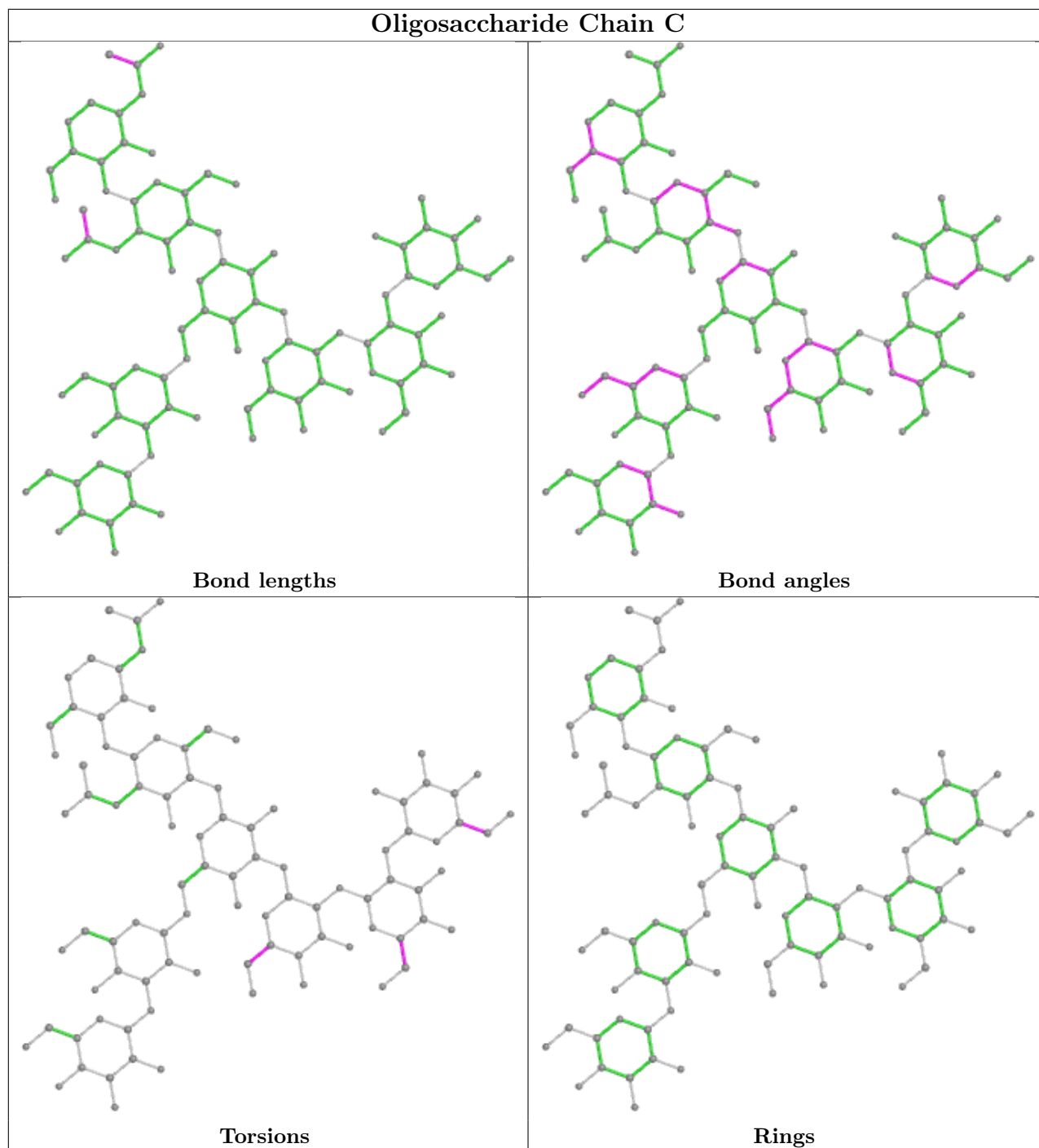
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	5	MAN	2	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.





## 5.6 Ligand geometry [i](#)

12 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
4	MAN	A	492	1	11,11,12	0.79	0	15,15,17	0.97	0
4	MAN	A	485	1	11,11,12	0.63	0	15,15,17	1.17	2 (13%)
4	MAN	A	487	1	11,11,12	0.92	1 (9%)	15,15,17	1.29	1 (6%)
4	MAN	A	486	1	11,11,12	0.71	0	15,15,17	0.87	0
4	MAN	A	489	1	11,11,12	0.66	0	15,15,17	0.92	0
4	MAN	A	491	1	11,11,12	0.67	0	15,15,17	1.05	1 (6%)
4	MAN	A	494	1	11,11,12	1.26	1 (9%)	15,15,17	1.62	4 (26%)
4	MAN	A	490	1	11,11,12	1.23	2 (18%)	15,15,17	1.41	4 (26%)
4	MAN	A	493	1	11,11,12	0.67	0	15,15,17	1.67	3 (20%)
5	NOJ	A	495	-	11,11,11	2.37	3 (27%)	13,15,15	1.60	1 (7%)
4	MAN	A	488	1	11,11,12	0.67	0	15,15,17	1.29	1 (6%)
5	NOJ	A	496	-	11,11,11	2.52	3 (27%)	13,15,15	2.32	2 (15%)

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	MAN	A	492	1	-	0/2/19/22	0/1/1/1
4	MAN	A	485	1	-	0/2/19/22	0/1/1/1
4	MAN	A	487	1	-	2/2/19/22	0/1/1/1
4	MAN	A	486	1	-	0/2/19/22	0/1/1/1
4	MAN	A	489	1	-	0/2/19/22	0/1/1/1
4	MAN	A	491	1	-	0/2/19/22	0/1/1/1
4	MAN	A	494	1	-	2/2/19/22	0/1/1/1
4	MAN	A	490	1	-	0/2/19/22	0/1/1/1
4	MAN	A	493	1	-	0/2/19/22	0/1/1/1
5	NOJ	A	495	-	-	0/2/19/19	0/1/1/1
4	MAN	A	488	1	-	2/2/19/22	0/1/1/1
5	NOJ	A	496	-	-	2/2/19/19	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	496	NOJ	C1-N5	-5.93	1.38	1.47
5	A	495	NOJ	C1-N5	-5.11	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	496	NOJ	C5-N5	-4.73	1.41	1.47
5	A	495	NOJ	C1-C2	4.08	1.56	1.52
5	A	495	NOJ	C5-N5	-3.53	1.42	1.47

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	496	NOJ	C1-N5-C5	6.63	123.96	109.61
5	A	495	NOJ	C1-N5-C5	4.63	119.62	109.61
4	A	493	MAN	C1-O5-C5	4.58	118.40	112.19
5	A	496	NOJ	C1-C2-C3	4.04	115.07	110.33
4	A	494	MAN	O5-C1-C2	3.58	116.30	110.77

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	496	NOJ	C4-C5-C6-O6
5	A	496	NOJ	N5-C5-C6-O6
4	A	494	MAN	O5-C5-C6-O6
4	A	488	MAN	O5-C5-C6-O6
4	A	487	MAN	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	495	NOJ	1	0
5	A	496	NOJ	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1



All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	246[B]:THR	C	247:ASN	N	1.16

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.