



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 08:50 AM BST

PDB ID : 1AGM
Title : Refined structure for the complex of acarbose with glucoamylase from *Aspergillus awamori* var. x100 to 2.4 angstroms resolution
Authors : Aleshin, A.E.; Firsov, L.M.; Honzatko, R.B.
Deposited on : 1994-05-13
Resolution : 2.30 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 ⓘ symbol.

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) : 2.13.1

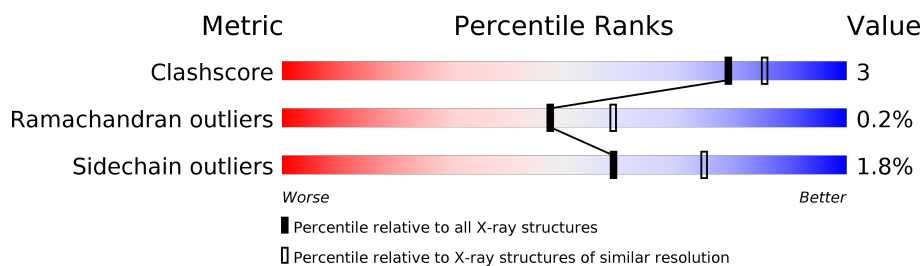
1 Overall quality at a glance

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 on 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 $\leq 5\%$.

Note EDS was not executed.

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

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	GLC	D	1[A]	X	-	-	-

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 4461 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.

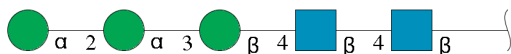
- Molecule 1 is a protein called GLUCOAMYLASE-471.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	470	3573	2239	585	741	8	0	4	0

There are 3 discrepancies between the modelled and reference sequences:

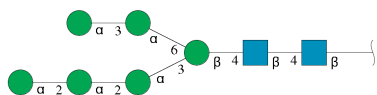
Chain	Residue	Modelled	Actual	Comment	Reference
A	58	LEU	ILE	conflict	UNP P23176
A	60	ILE	LEU	conflict	UNP P23176
A	117	THR	ALA	conflict	UNP P23176

- 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.

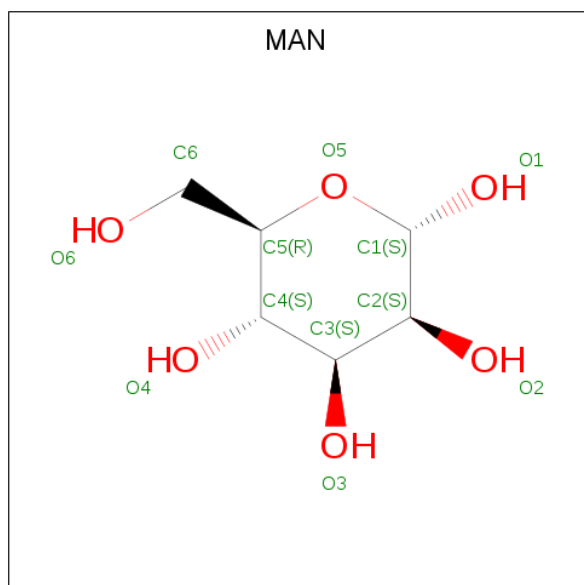


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 4 is an oligosaccharide called 4,6-dideoxy-4-[[[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino]-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	3	Total	C	N	O	0	3	0
			44	25	1	18			
4	E	3	Total	C	N	O	0	3	0
			44	25	1	18			

- Molecule 5 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



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

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

- Molecule 6 is water.

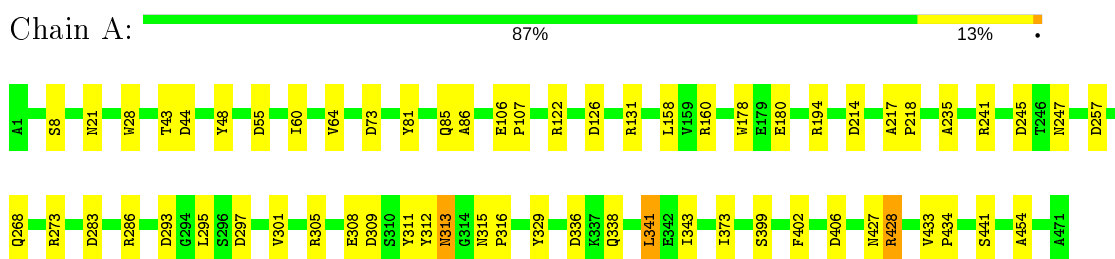
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	535	Total	O	0	0
			535	535		

3 Residue-property plots

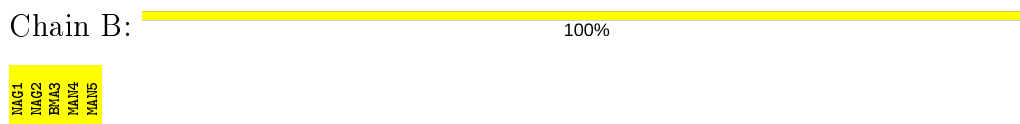
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

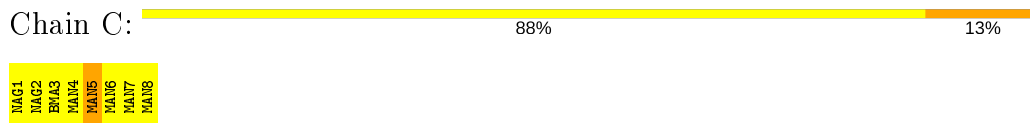
- Molecule 1: GLUCOAMYLASE-471



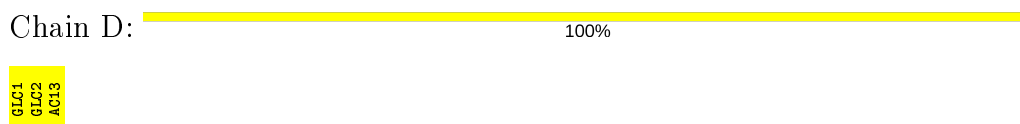
- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose




- 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



- Molecule 4: 4,6-dideoxy-4-{\{(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl\}amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 4: 4,6-dideoxy-4-{\{(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl\}amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain E:  100%

GLG1
GLG2
ACT3

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, α , β , γ	116.70Å 103.90Å 48.34Å 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}	0.124 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4461	wwPDB-VP
Average B, all atoms (Å ²)	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: GLC, AC1, BMA, NAG, MAN

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	0.89	0/3684	1.37	29/5040 (0.6%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	ARG	NE-CZ-NH1	14.02	127.31	120.30
1	A	273	ARG	NE-CZ-NH2	-11.54	114.53	120.30
1	A	194	ARG	NE-CZ-NH2	-10.31	115.15	120.30
1	A	48	TYR	CB-CG-CD1	8.59	126.15	121.00
1	A	160	ARG	NE-CZ-NH1	8.35	124.47	120.30
1	A	428	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	A	131	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	A	329	TYR	CB-CG-CD1	7.22	125.33	121.00
1	A	48	TYR	CB-CG-CD2	-7.20	116.68	121.00
1	A	309	ASP	CB-CG-OD2	7.16	124.74	118.30
1	A	126	ASP	CB-CG-OD1	7.13	124.72	118.30
1	A	454	ALA	N-CA-CB	7.03	119.95	110.10
1	A	341	LEU	CA-CB-CG	6.99	131.38	115.30
1	A	293	ASP	CB-CG-OD1	6.81	124.43	118.30
1	A	406	ASP	CB-CG-OD1	6.79	124.42	118.30
1	A	428	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	A	131	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	214	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	297	ASP	CB-CG-OD1	-5.77	113.11	118.30
1	A	122	ARG	NE-CZ-NH2	5.72	123.16	120.30
1	A	283	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	A	73	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	241	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	257	ASP	CB-CG-OD2	5.46	123.21	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	286	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	308	GLU	OE1-CD-OE2	-5.45	116.76	123.30
1	A	329	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	A	336	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	311	TYR	CB-CG-CD2	-5.07	117.96	121.00

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	3573	0	3313	21	0
2	B	61	0	52	0	0
3	C	94	0	79	2	0
4	D	44	0	16	0	0
4	E	44	0	17	0	0
5	A	110	0	100	0	0
6	A	535	0	0	2	0
All	All	4461	0	3577	21	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 3.

All (21) 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)
1:A:312:TYR:O	1:A:313:ASN:HB2	2.02	0.59
1:A:295:LEU:HD12	1:A:301:VAL:HG12	1.93	0.51
1:A:43:THR:HG23	3:C:5:MAN:H61	1.91	0.51
1:A:217:ALA:HB3	1:A:218:PRO:HD3	1.93	0.51
1:A:338:GLN:HG3	6:A:1315:HOH:O	2.11	0.51
1:A:81:TYR:O	1:A:85:GLN:HG2	2.10	0.50
1:A:60:ILE:O	1:A:64:VAL:HG23	2.12	0.50
1:A:43:THR:CG2	3:C:5:MAN:H61	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:ARG:CZ	1:A:434:PRO:HD3	2.43	0.49
1:A:178:TRP:O	1:A:180:GLU:HG3	2.16	0.46
1:A:316:PRO:HD2	1:A:402:PHE:O	2.15	0.46
1:A:433:VAL:HB	1:A:434:PRO:HD2	1.99	0.44
1:A:235:ALA:HB2	1:A:245:ASP:HB3	2.00	0.43
1:A:315:ASN:HB3	1:A:316:PRO:HD2	2.01	0.42
1:A:427:ASN:HA	1:A:427:ASN:HD22	1.70	0.42
1:A:86:ALA:HA	1:A:158:LEU:HD21	2.02	0.42
1:A:268:GLN:HA	6:A:781:HOH:O	2.19	0.42
1:A:178:TRP:CD2	1:A:305:ARG:HD2	2.55	0.41
1:A:21:ASN:ND2	1:A:28:TRP:HE3	2.19	0.41
1:A:343:ILE:HD11	1:A:373:ILE:CD1	2.51	0.40
1:A:106:GLU:HA	1:A:107:PRO:HD3	1.89	0.40

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	472/470 (100%)	453 (96%)	18 (4%)	1 (0%)	47 58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	313	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	389/385 (101%)	381 (98%)	8 (2%)	53 70

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	44[A]	ASP
1	A	44[B]	ASP
1	A	55	ASP
1	A	247	ASN
1	A	341	LEU
1	A	399	SER
1	A	441	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

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

19 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	0.90	1 (7%)	17,19,21	1.32	2 (11%)
2	NAG	B	2	2	14,14,15	1.02	1 (7%)	17,19,21	1.42	3 (17%)
2	BMA	B	3	2	11,11,12	0.58	0	15,15,17	1.50	2 (13%)
2	MAN	B	4	2	11,11,12	0.75	0	15,15,17	1.58	1 (6%)
2	MAN	B	5	2	11,11,12	0.83	0	15,15,17	1.65	4 (26%)
3	NAG	C	1	1,3	14,14,15	1.11	1 (7%)	17,19,21	1.66	5 (29%)
3	NAG	C	2	3	14,14,15	0.97	1 (7%)	17,19,21	1.53	2 (11%)
3	BMA	C	3	3	11,11,12	0.50	0	15,15,17	1.08	1 (6%)
3	MAN	C	4	3	11,11,12	0.40	0	15,15,17	1.68	1 (6%)
3	MAN	C	5	3	11,11,12	0.62	0	15,15,17	1.36	2 (13%)
3	MAN	C	6	3	11,11,12	0.52	0	15,15,17	1.32	1 (6%)
3	MAN	C	7	3	11,11,12	0.57	0	15,15,17	1.06	1 (6%)
3	MAN	C	8	3	11,11,12	0.72	0	15,15,17	1.46	1 (6%)
4	GLC	D	1[A]	4	12,12,12	0.86	0	17,17,17	1.28	4 (23%)
4	GLC	D	2[A]	4	11,11,12	1.37	1 (9%)	15,15,17	1.70	3 (20%)
4	AC1	D	3[A]	4	21,22,23	1.35	3 (14%)	22,32,34	1.23	4 (18%)
4	GLC	E	1[B]	4	12,12,12	1.09	0	17,17,17	1.71	4 (23%)
4	GLC	E	2[B]	4	11,11,12	1.39	1 (9%)	15,15,17	1.78	4 (26%)
4	AC1	E	3[B]	4	21,22,23	1.35	3 (14%)	22,32,34	1.21	4 (18%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	C	4	3	-	1/2/19/22	0/1/1/1
3	MAN	C	5	3	-	0/2/19/22	0/1/1/1
3	MAN	C	6	3	-	1/2/19/22	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
4	GLC	D	1[A]	4	1/1/5/5	2/2/22/22	0/1/1/1
4	GLC	D	2[A]	4	-	0/2/19/22	0/1/1/1
4	AC1	D	3[A]	4	-	1/6/43/46	0/2/2/2
4	GLC	E	1[B]	4	-	2/2/22/22	0/1/1/1
4	GLC	E	2[B]	4	-	0/2/19/22	0/1/1/1
4	AC1	E	3[B]	4	-	1/6/43/46	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2[A]	GLC	C2-C3	3.33	1.57	1.52
4	E	2[B]	GLC	C2-C3	3.30	1.57	1.52
4	E	3[B]	AC1	C7B-C5B	3.27	1.37	1.32
4	D	3[A]	AC1	C7B-C5B	3.19	1.37	1.32
3	C	1	NAG	C8-C7	3.11	1.57	1.50
2	B	1	NAG	C8-C7	2.82	1.56	1.50
3	C	2	NAG	C8-C7	2.80	1.56	1.50
2	B	2	NAG	C8-C7	2.66	1.56	1.50
4	D	3[A]	AC1	C2B-C1B	2.24	1.55	1.52
4	E	3[B]	AC1	C2B-C1B	2.19	1.55	1.52
4	E	3[B]	AC1	C4A-C5B	2.13	1.53	1.51
4	D	3[A]	AC1	C4A-C5B	2.10	1.53	1.51

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	MAN	C1-O5-C5	5.72	119.94	112.19
3	C	8	MAN	O5-C1-C2	4.35	117.49	110.77
2	B	4	MAN	O5-C1-C2	-4.25	104.21	110.77
3	C	6	MAN	C1-O5-C5	4.14	117.80	112.19
3	C	5	MAN	C1-O5-C5	4.04	117.67	112.19
4	E	1[B]	GLC	C1-O5-C5	3.95	121.11	113.66
2	B	3	BMA	C1-O5-C5	3.91	117.49	112.19
2	B	1	NAG	C1-O5-C5	3.86	117.43	112.19
3	C	2	NAG	O4-C4-C5	-3.82	99.82	109.30
4	E	2[B]	GLC	C1-O5-C5	3.67	117.17	112.19
4	D	2[A]	GLC	C1-O5-C5	3.53	116.98	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	O5-C1-C2	-3.43	105.87	111.29
4	E	2[B]	GLC	O2-C2-C1	3.27	115.84	109.15
3	C	2	NAG	C1-O5-C5	3.25	116.60	112.19
2	B	5	MAN	C1-C2-C3	3.22	113.63	109.67
3	C	1	NAG	C6-C5-C4	3.09	120.25	113.00
4	E	2[B]	GLC	O5-C1-C2	-3.06	106.04	110.77
4	D	2[A]	GLC	O2-C2-C1	3.06	115.41	109.15
2	B	5	MAN	O5-C5-C4	-3.05	103.42	110.83
3	C	1	NAG	O5-C5-C4	-2.91	103.76	110.83
4	D	2[A]	GLC	O5-C1-C2	-2.85	106.37	110.77
2	B	3	BMA	O5-C1-C2	-2.80	106.45	110.77
4	E	1[B]	GLC	O2-C2-C1	2.78	115.61	109.16
2	B	2	NAG	C1-O5-C5	2.54	115.63	112.19
4	E	1[B]	GLC	O5-C1-C2	2.49	114.73	110.28
3	C	7	MAN	C1-O5-C5	2.44	115.50	112.19
4	D	1[A]	GLC	O4-C4-C3	-2.36	104.89	110.35
2	B	5	MAN	C6-C5-C4	2.34	118.48	113.00
3	C	5	MAN	O5-C1-C2	-2.30	107.22	110.77
3	C	1	NAG	O4-C4-C5	-2.30	103.59	109.30
2	B	2	NAG	C8-C7-N2	-2.29	112.23	116.10
4	D	3[A]	AC1	C7B-C1B-N4A	2.27	114.08	110.68
3	C	3	BMA	O2-C2-C3	-2.26	105.61	110.14
2	B	2	NAG	O5-C5-C4	-2.23	105.39	110.83
4	E	3[B]	AC1	C7B-C1B-N4A	2.22	114.02	110.68
4	D	3[A]	AC1	O6B-C6B-C5B	-2.20	107.25	112.50
3	C	1	NAG	C3-C4-C5	-2.19	106.33	110.24
4	D	1[A]	GLC	O5-C5-C4	2.19	113.67	109.69
2	B	5	MAN	C3-C4-C5	-2.19	106.33	110.24
4	D	1[A]	GLC	O2-C2-C1	2.17	114.18	109.16
4	E	3[B]	AC1	C1-O5-C5	2.15	117.65	112.78
4	D	3[A]	AC1	C1-O5-C5	2.13	117.60	112.78
2	B	1	NAG	C1-C2-N2	2.11	114.09	110.49
4	D	1[A]	GLC	C1-O5-C5	2.11	117.64	113.66
4	E	3[B]	AC1	O6B-C6B-C5B	-2.08	107.51	112.50
4	E	1[B]	GLC	O2-C2-C3	-2.04	105.63	110.35
4	D	3[A]	AC1	O2-C2-C1	2.04	113.32	109.15
4	E	2[B]	GLC	O4-C4-C3	2.01	115.00	110.35
4	E	3[B]	AC1	O2-C2-C1	2.00	113.25	109.15

All (1) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
4	D	1[A]	GLC	C1

All (13) torsion outliers are listed below:

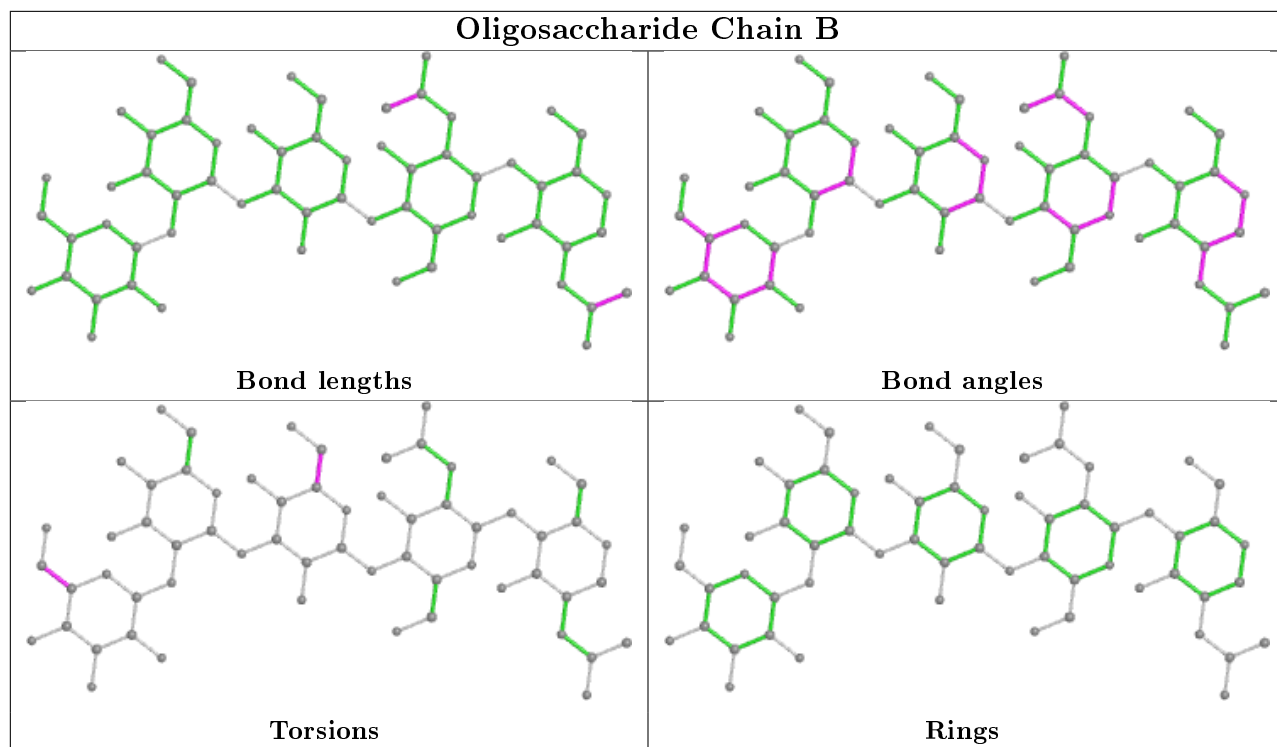
Mol	Chain	Res	Type	Atoms
2	B	3	BMA	O5-C5-C6-O6
2	B	5	MAN	O5-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
4	E	1[B]	GLC	C4-C5-C6-O6
4	D	1[A]	GLC	C4-C5-C6-O6
2	B	5	MAN	C4-C5-C6-O6
4	E	1[B]	GLC	O5-C5-C6-O6
3	C	6	MAN	O5-C5-C6-O6
4	D	1[A]	GLC	O5-C5-C6-O6
4	D	3[A]	AC1	C5-C4-N4A-C1B
4	E	3[B]	AC1	C5-C4-N4A-C1B
3	C	4	MAN	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6

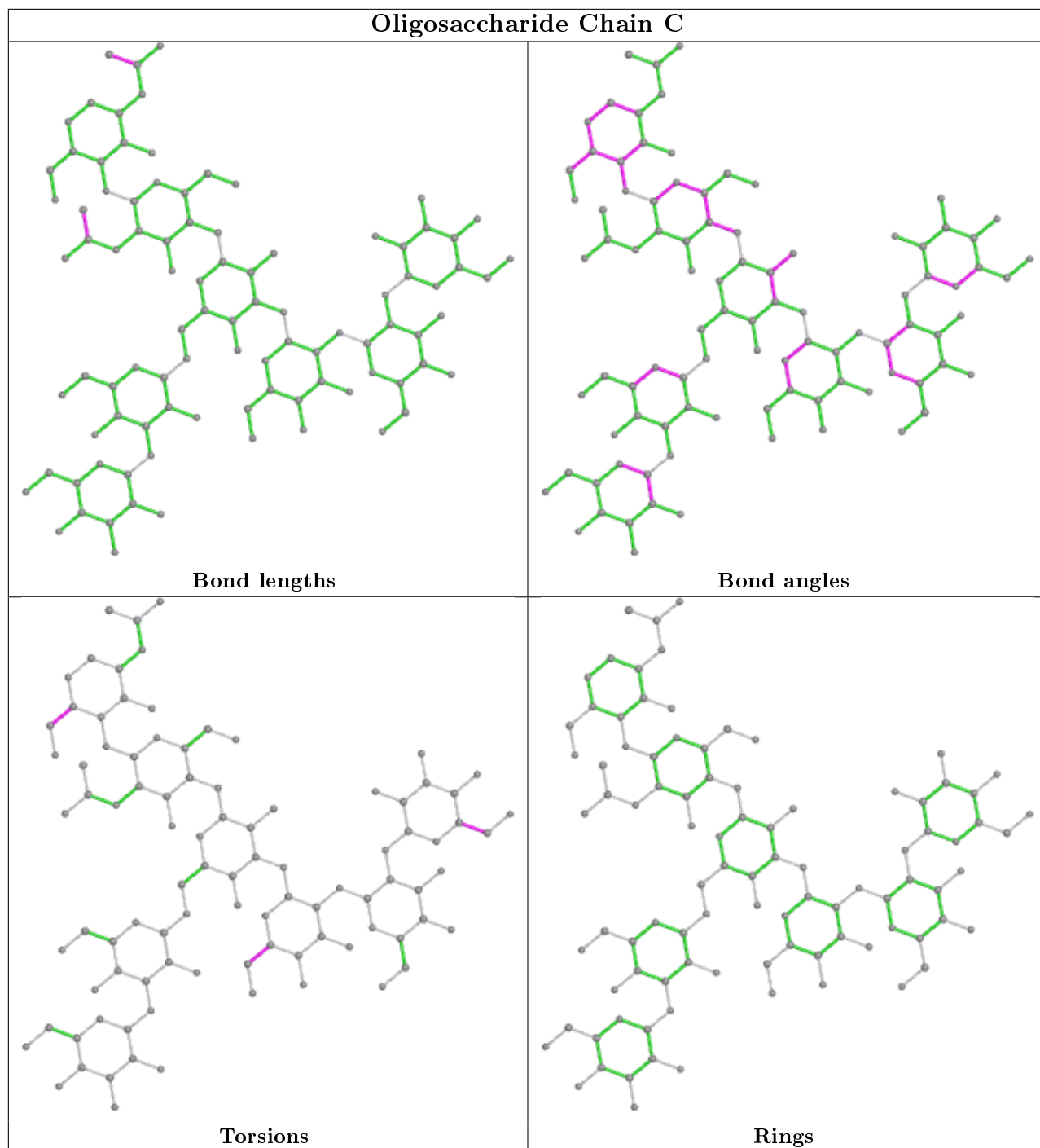
There are no ring outliers.

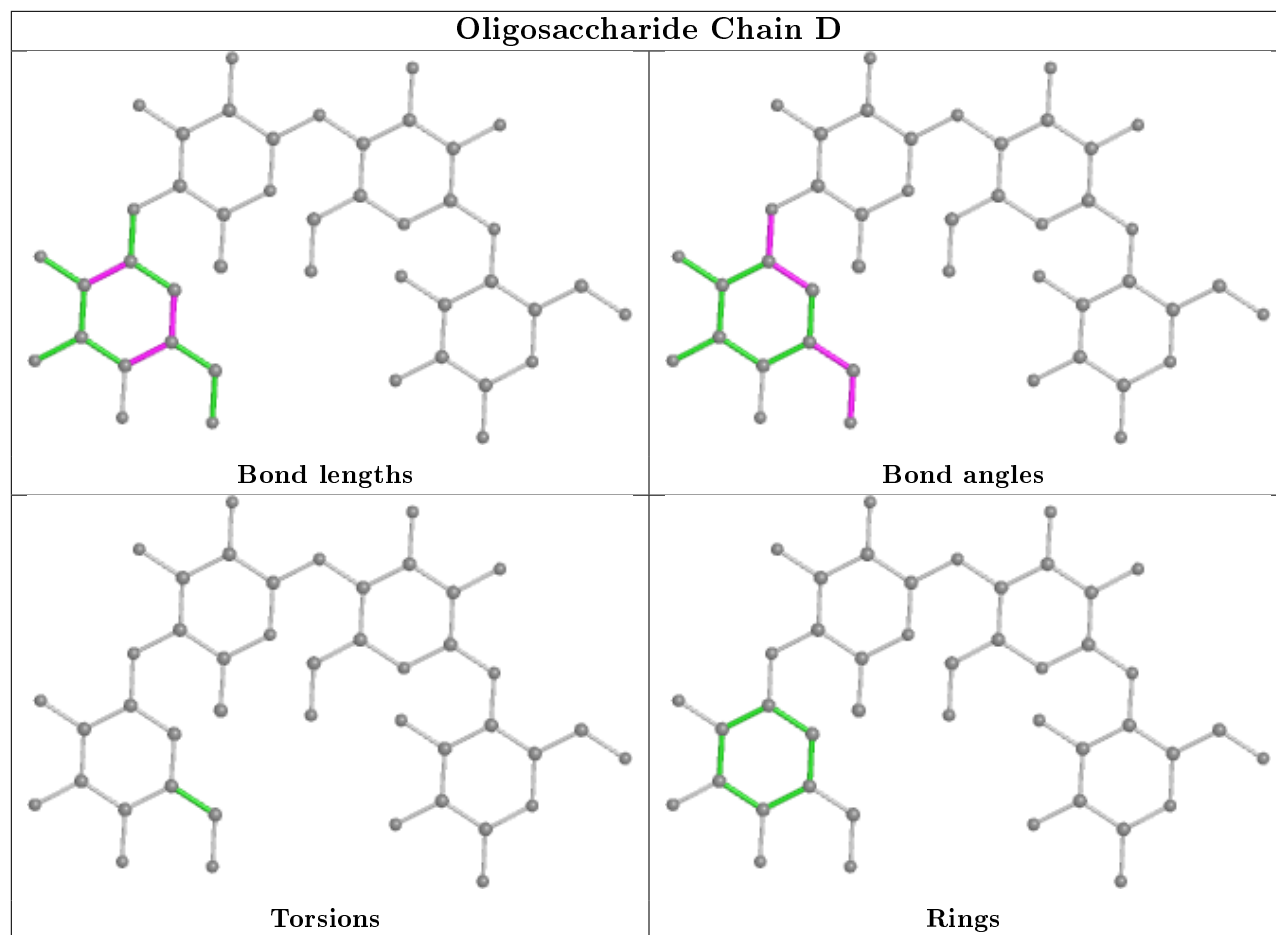
1 monomer is involved in 2 short contacts:

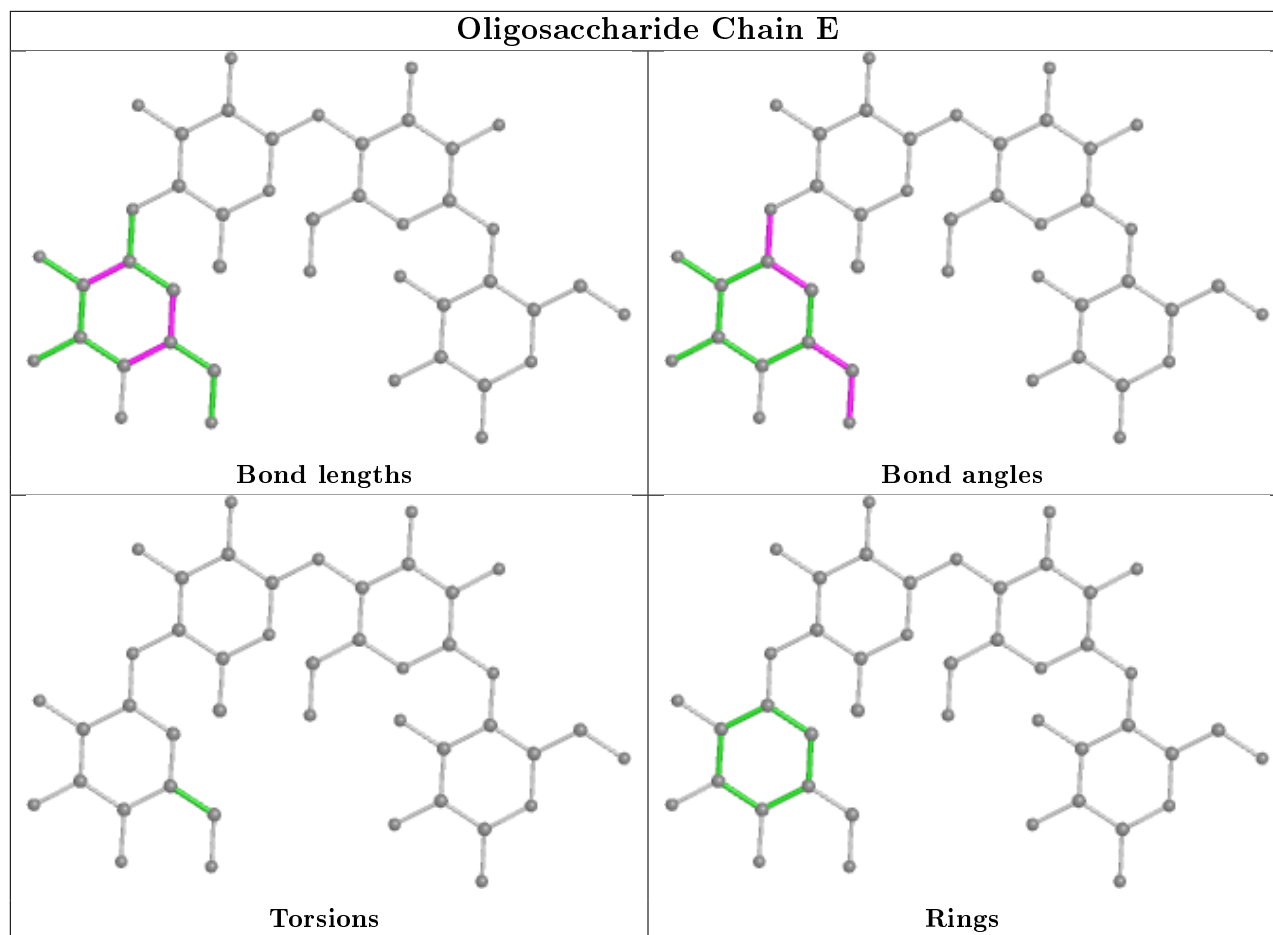
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	5	MAN	2	0

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](#)

10 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	MAN	A	488	1	11,11,12	0.58	0	15,15,17	1.42	1 (6%)
5	MAN	A	487	1	11,11,12	0.75	0	15,15,17	1.17	1 (6%)
5	MAN	A	494	1	11,11,12	0.78	1 (9%)	15,15,17	1.44	2 (13%)
5	MAN	A	489	1	11,11,12	0.69	0	15,15,17	0.98	1 (6%)
5	MAN	A	493	1	11,11,12	0.70	0	15,15,17	1.33	1 (6%)
5	MAN	A	492	1	11,11,12	0.81	0	15,15,17	1.01	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	A	485	1	11,11,12	0.69	0	15,15,17	1.08	1 (6%)
5	MAN	A	491	1	11,11,12	0.52	0	15,15,17	1.06	1 (6%)
5	MAN	A	486	1	11,11,12	0.61	0	15,15,17	0.93	1 (6%)
5	MAN	A	490	1	11,11,12	1.02	1 (9%)	15,15,17	1.19	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
5	MAN	A	488	1	-	2/2/19/22	0/1/1/1
5	MAN	A	487	1	-	2/2/19/22	0/1/1/1
5	MAN	A	494	1	-	0/2/19/22	0/1/1/1
5	MAN	A	489	1	-	0/2/19/22	0/1/1/1
5	MAN	A	493	1	-	0/2/19/22	0/1/1/1
5	MAN	A	492	1	-	0/2/19/22	0/1/1/1
5	MAN	A	485	1	-	0/2/19/22	0/1/1/1
5	MAN	A	491	1	-	0/2/19/22	0/1/1/1
5	MAN	A	486	1	-	0/2/19/22	0/1/1/1
5	MAN	A	490	1	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	490	MAN	O5-C1	2.62	1.47	1.43
5	A	494	MAN	O5-C1	2.02	1.46	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	493	MAN	C1-O5-C5	4.80	118.69	112.19
5	A	494	MAN	C1-O5-C5	4.41	118.17	112.19
5	A	488	MAN	O5-C1-C2	-3.34	105.62	110.77
5	A	487	MAN	C1-O5-C5	3.05	116.32	112.19
5	A	494	MAN	O5-C1-C2	2.90	115.25	110.77
5	A	492	MAN	O3-C3-C4	-2.78	103.92	110.35
5	A	490	MAN	C1-O5-C5	2.53	115.61	112.19
5	A	486	MAN	C1-O5-C5	2.36	115.39	112.19
5	A	491	MAN	O3-C3-C4	-2.13	105.42	110.35
5	A	485	MAN	O5-C1-C2	-2.12	107.49	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	489	MAN	C6-C5-C4	2.12	117.97	113.00
5	A	490	MAN	O5-C1-C2	2.02	113.89	110.77

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	487	MAN	O5-C5-C6-O6
5	A	488	MAN	O5-C5-C6-O6
5	A	488	MAN	C4-C5-C6-O6
5	A	487	MAN	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.