



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 04:12 AM UTC

PDB ID : 5JUV / pdb_00005juv
Title : STRUCTURE OF E298Q-BETA-GALACTOSIDASE FROM AS-
PERGILLUS NIGER IN COMPLEX WITH 6-b-Galactopyranosyl galactose
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cerra, M.; Sanz-Aparicio, J.
Deposited on : 2016-05-10
Resolution : 2.27 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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

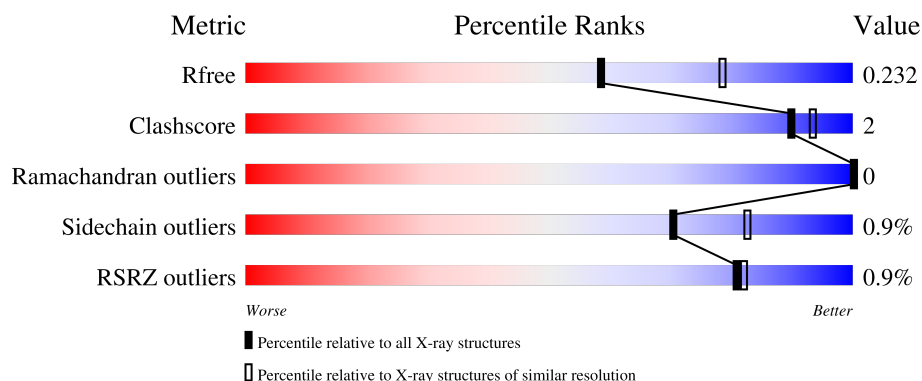
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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))
R_{free}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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 ≥ 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1013	89% 6% .
2	B	8	12% 88%
3	C	10	30% 70%
4	D	6	100%
5	E	2	50% 50%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 8098 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.

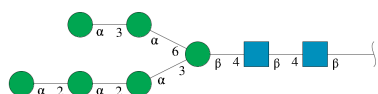
- Molecule 1 is a protein called Probable beta-galactosidase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	968	7482	4780	1220	1471	11	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

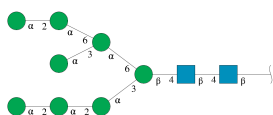
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLN	GLU	engineered mutation	UNP A2QAN3
A	1008	HIS	-	expression tag	UNP A2QAN3
A	1009	HIS	-	expression tag	UNP A2QAN3
A	1010	HIS	-	expression tag	UNP A2QAN3
A	1011	HIS	-	expression tag	UNP A2QAN3
A	1012	HIS	-	expression tag	UNP A2QAN3
A	1013	HIS	-	expression tag	UNP A2QAN3

- Molecule 2 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.



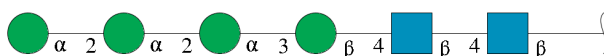
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	8	94	52	2	40	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]-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.



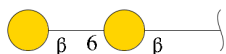
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 5 is an oligosaccharide called beta-D-galactopyranose-(1-6)-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	E	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 8 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			16	10	6		

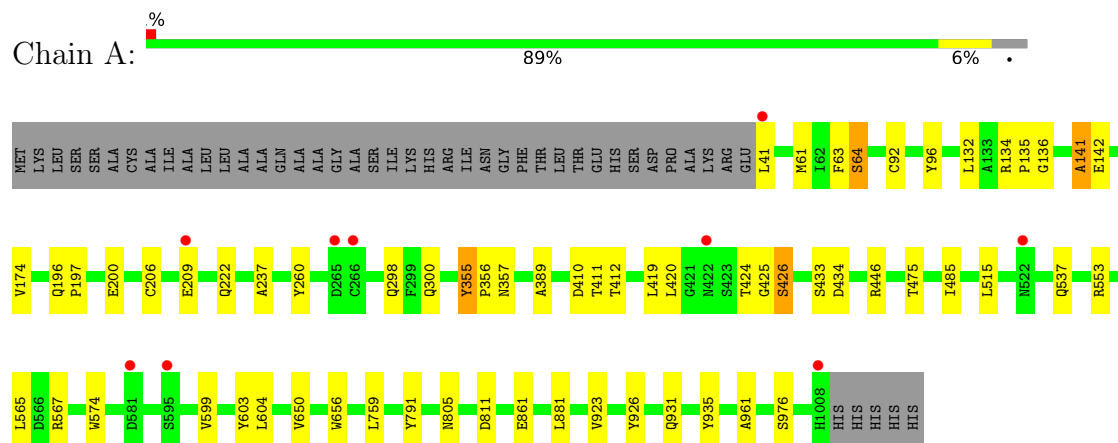
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	224	Total	O	0	0
			224	224		

3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

- Molecule 1: Probable beta-galactosidase A



- Molecule 2: 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 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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: alpha-D-mannopyranose-(1-2)-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

Chain D:  100%

MAG1
MAG2
BGA3
MAN4
MAN5
MAN6

- Molecule 5: beta-D-galactopyranose-(1-6)-beta-D-galactopyranose

Chain E:  50%  50%

GAL1
GAL2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.10Å 106.39Å 83.72Å 90.00° 99.18° 90.00°	Depositor
Resolution (Å)	82.65 – 2.27 82.65 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.9 (82.65-2.27) 99.9 (82.65-2.27)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.179 , 0.232 0.188 , 0.232	Depositor DCC
R_{free} test set	2413 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 28.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8098	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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, GAL, CL, NAG, 1PE

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	0.76	18/7685 (0.2%)	0.80	7/10488 (0.1%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	135	PRO	C-O	-7.69	1.16	1.23
1	A	433	SER	C-O	-7.42	1.15	1.24
1	A	142	GLU	C-O	-6.68	1.15	1.23
1	A	197	PRO	C-O	-6.39	1.15	1.24
1	A	567	ARG	C-O	-6.25	1.16	1.24
1	A	485	ILE	C-O	-5.78	1.17	1.24
1	A	424	THR	C-O	-5.77	1.16	1.24
1	A	426	SER	C-O	-5.72	1.16	1.23
1	A	412	THR	C-O	-5.70	1.16	1.24
1	A	599	VAL	C-O	-5.58	1.18	1.24
1	A	200	GLU	C-O	-5.47	1.17	1.23
1	A	446	ARG	C-O	-5.46	1.17	1.24
1	A	420	LEU	C-O	-5.45	1.17	1.24
1	A	196	GLN	C-O	-5.45	1.18	1.24
1	A	425	GLY	C-O	-5.44	1.18	1.24
1	A	209	GLU	C-O	-5.42	1.17	1.23
1	A	419	LEU	C-O	-5.15	1.18	1.23
1	A	136	GLY	C-O	-5.11	1.17	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	410	ASP	N-CA-C	7.29	121.60	113.21
1	A	206	CYS	N-CA-C	6.98	121.11	111.90
1	A	603	TYR	N-CA-C	6.35	118.73	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	565	LEU	N-CA-C	6.01	119.01	109.81
1	A	434	ASP	N-CA-C	-5.92	97.56	107.99
1	A	141	ALA	N-CA-C	5.78	119.63	112.24
1	A	64	SER	N-CA-C	5.19	117.56	109.52

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	7482	0	7183	26	0
2	B	94	0	79	0	0
3	C	116	0	97	0	0
4	D	72	0	61	0	0
5	E	23	0	21	2	0
6	A	70	0	65	2	0
7	A	1	0	0	0	0
8	A	16	0	22	0	0
9	A	224	0	0	0	0
All	All	8098	0	7528	26	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 2.

All (26) 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:61:MET:HE1	1:A:63:PHE:HB2	1.48	0.95
1:A:791:TYR:CE2	6:A:1760:NAG:H82	2.32	0.65
1:A:134:ARG:HH12	1:A:298:GLN:HE21	1.46	0.64
1:A:64:SER:HB2	1:A:92:CYS:HB3	1.80	0.64
1:A:96:TYR:CE2	1:A:141:ALA:HB2	2.32	0.64
1:A:805:ASN:HD21	1:A:811:ASP:HA	1.66	0.59
1:A:861:GLU:OE2	1:A:926:TYR:OH	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:MET:CE	1:A:63:PHE:HB2	2.30	0.56
1:A:61:MET:HE2	1:A:389:ALA:HB1	1.87	0.55
1:A:237:ALA:O	5:E:1:GAL:O3	2.23	0.52
1:A:174:VAL:HG11	1:A:222:GLN:HB3	1.94	0.50
1:A:260:TYR:HD1	5:E:1:GAL:H3	1.78	0.49
1:A:355:TYR:CZ	1:A:357:ASN:HB2	2.47	0.49
1:A:260:TYR:HA	1:A:300:GLN:HB2	1.94	0.49
1:A:355:TYR:HB2	1:A:356:PRO:HD2	1.96	0.47
1:A:759:LEU:HD11	1:A:791:TYR:CD2	2.50	0.47
1:A:650:VAL:HG22	1:A:656:TRP:CD1	2.49	0.46
1:A:61:MET:HE2	1:A:389:ALA:CB	2.45	0.46
1:A:881:LEU:HD11	1:A:976:SER:HA	1.98	0.46
1:A:426:SER:HB2	1:A:475:THR:OG1	2.15	0.46
1:A:515:LEU:C	1:A:515:LEU:HD12	2.43	0.43
1:A:926:TYR:HB2	1:A:961:ALA:HB3	2.00	0.43
1:A:791:TYR:CZ	6:A:1760:NAG:H82	2.54	0.42
1:A:923:VAL:HB	1:A:935:TYR:HB3	2.01	0.42
1:A:574:TRP:CZ2	1:A:604:LEU:HA	2.56	0.40
1:A:96:TYR:CD2	1:A:141:ALA:HB2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	966/1013 (95%)	928 (96%)	38 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	808/842 (96%)	801 (99%)	7 (1%)	70 82

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LEU
1	A	132	LEU
1	A	355	TYR
1	A	411	THR
1	A	537	GLN
1	A	553	ARG
1	A	931	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	298	GLN
1	A	349	ASN
1	A	458	GLN
1	A	466	ASN
1	A	577	GLN
1	A	648	HIS
1	A	687	GLN
1	A	805	ASN
1	A	924	GLN
1	A	931	GLN
1	A	1008	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

26 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	0.72	0	17,19,21	1.42	2 (11%)
2	NAG	B	2	2	14,14,15	0.68	0	17,19,21	0.85	0
2	BMA	B	3	2	11,11,12	0.95	0	15,15,17	2.20	6 (40%)
2	MAN	B	4	2	11,11,12	1.84	3 (27%)	15,15,17	1.92	3 (20%)
2	MAN	B	5	2	11,11,12	1.37	1 (9%)	15,15,17	2.30	4 (26%)
2	MAN	B	6	2	11,11,12	0.63	0	15,15,17	1.71	4 (26%)
2	MAN	B	7	2	11,11,12	0.61	0	15,15,17	1.28	2 (13%)
2	MAN	B	8	2	11,11,12	0.49	0	15,15,17	1.52	3 (20%)
3	NAG	C	1	3,1	14,14,15	0.57	0	17,19,21	1.36	3 (17%)
3	MAN	C	10	3	11,11,12	0.52	0	15,15,17	1.07	1 (6%)
3	NAG	C	2	3	14,14,15	0.77	0	17,19,21	1.02	2 (11%)
3	BMA	C	3	3	11,11,12	0.47	0	15,15,17	0.80	0
3	MAN	C	4	3	11,11,12	0.66	0	15,15,17	1.58	2 (13%)
3	MAN	C	5	3	11,11,12	0.58	0	15,15,17	1.07	2 (13%)
3	MAN	C	6	3	11,11,12	0.62	0	15,15,17	0.79	1 (6%)
3	MAN	C	7	3	11,11,12	0.85	0	15,15,17	0.67	0
3	MAN	C	8	3	11,11,12	0.68	0	15,15,17	1.31	2 (13%)
3	MAN	C	9	3	11,11,12	0.68	0	15,15,17	0.84	0
4	NAG	D	1	4,1	14,14,15	0.72	0	17,19,21	1.14	2 (11%)
4	NAG	D	2	4	14,14,15	0.65	0	17,19,21	1.06	1 (5%)
4	BMA	D	3	4	11,11,12	0.56	0	15,15,17	1.66	3 (20%)
4	MAN	D	4	4	11,11,12	0.62	0	15,15,17	1.66	3 (20%)
4	MAN	D	5	4	11,11,12	0.74	0	15,15,17	2.17	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	D	6	4	11,11,12	0.56	0	15,15,17	3.57	9 (60%)
5	GAL	E	1	5	12,12,12	0.76	0	17,17,17	3.05	5 (29%)
5	GAL	E	2	5	11,11,12	0.72	0	15,15,17	1.67	4 (26%)

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	-	0/2/19/22	0/1/1/1
2	MAN	B	4	2	-	0/2/19/22	0/1/1/1
2	MAN	B	5	2	-	0/2/19/22	0/1/1/1
2	MAN	B	6	2	-	2/2/19/22	0/1/1/1
2	MAN	B	7	2	-	1/2/19/22	0/1/1/1
2	MAN	B	8	2	-	2/2/19/22	0/1/1/1
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	MAN	C	10	3	-	2/2/19/22	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	1/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	MAN	C	5	3	-	2/2/19/22	0/1/1/1
3	MAN	C	6	3	-	2/2/19/22	0/1/1/1
3	MAN	C	7	3	-	1/2/19/22	0/1/1/1
3	MAN	C	8	3	-	0/2/19/22	0/1/1/1
3	MAN	C	9	3	-	2/2/19/22	0/1/1/1
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	2/2/19/22	0/1/1/1
4	MAN	D	4	4	-	0/2/19/22	0/1/1/1
4	MAN	D	5	4	-	2/2/19/22	0/1/1/1
4	MAN	D	6	4	-	2/2/19/22	0/1/1/1
5	GAL	E	1	5	-	1/2/22/22	0/1/1/1
5	GAL	E	2	5	-	2/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	MAN	O5-C1	-4.08	1.36	1.43
2	B	5	MAN	O5-C1	-2.99	1.38	1.43
2	B	4	MAN	C2-C3	-2.73	1.48	1.52
2	B	4	MAN	O3-C3	-2.21	1.37	1.43

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1	GAL	O6-C6-C5	10.07	145.64	111.33
4	D	6	MAN	C1-O5-C5	8.78	123.96	112.19
2	B	5	MAN	C1-O5-C5	7.47	122.20	112.19
4	D	5	MAN	C1-O5-C5	6.34	120.69	112.19
2	B	4	MAN	C1-C2-C3	-5.62	101.47	109.64
3	C	4	MAN	C1-O5-C5	4.59	118.33	112.19
2	B	3	BMA	C6-C5-C4	-4.45	102.08	113.02
4	D	6	MAN	C3-C4-C5	-4.40	102.25	110.23
4	D	6	MAN	O3-C3-C4	4.36	120.66	110.38
4	D	6	MAN	O4-C4-C3	4.09	120.03	110.38
5	E	1	GAL	O5-C1-C2	3.89	117.14	110.30
2	B	3	BMA	C1-O5-C5	3.87	117.38	112.19
5	E	1	GAL	C1-O5-C5	3.86	121.11	113.65
4	D	3	BMA	C1-O5-C5	3.72	117.17	112.19
2	B	8	MAN	O4-C4-C3	-3.72	101.61	110.38
4	D	4	MAN	O2-C2-C3	-3.71	102.46	110.15
4	D	6	MAN	O5-C5-C6	-3.67	100.52	107.66
2	B	3	BMA	O3-C3-C4	-3.64	101.81	110.38
2	B	6	MAN	C1-O5-C5	3.47	116.84	112.19
4	D	6	MAN	C2-C3-C4	-3.40	104.89	110.86
3	C	8	MAN	C1-O5-C5	3.33	116.65	112.19
5	E	2	GAL	O5-C5-C6	3.29	114.07	107.66
4	D	6	MAN	C1-C2-C3	-3.25	104.92	109.64
2	B	1	NAG	O5-C1-C2	-3.22	106.30	111.29
5	E	2	GAL	C3-C4-C5	-3.12	104.57	110.23
2	B	6	MAN	O3-C3-C4	3.03	117.53	110.38
4	D	1	NAG	C1-O5-C5	-3.03	108.12	112.19
4	D	3	BMA	C3-C4-C5	3.00	115.67	110.23
5	E	1	GAL	O5-C5-C6	2.94	113.73	106.44
4	D	6	MAN	O2-C2-C3	2.93	116.22	110.15
5	E	2	GAL	C1-C2-C3	2.91	113.87	109.64
2	B	6	MAN	C2-C3-C4	-2.76	106.00	110.86
2	B	1	NAG	C1-C2-N2	2.75	114.76	110.43
5	E	1	GAL	C1-C2-C3	2.71	115.88	110.36
4	D	5	MAN	O2-C2-C3	-2.68	104.59	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3	BMA	C1-C2-C3	2.65	113.50	109.64
4	D	4	MAN	C1-O5-C5	2.61	115.69	112.19
2	B	4	MAN	O3-C3-C2	-2.57	104.82	110.05
2	B	5	MAN	C1-C2-C3	2.54	113.35	109.64
2	B	5	MAN	C2-C3-C4	-2.53	106.41	110.86
4	D	4	MAN	O2-C2-C1	2.49	114.93	109.22
2	B	7	MAN	O3-C3-C2	-2.49	104.97	110.05
2	B	7	MAN	C1-O5-C5	2.48	115.51	112.19
2	B	4	MAN	O5-C1-C2	2.48	116.69	110.79
3	C	8	MAN	C2-C3-C4	-2.47	106.51	110.86
2	B	6	MAN	C3-C4-C5	-2.45	105.79	110.23
4	D	5	MAN	C3-C4-C5	-2.44	105.81	110.23
3	C	2	NAG	C1-O5-C5	2.40	115.41	112.19
2	B	8	MAN	C1-C2-C3	2.36	113.08	109.64
2	B	3	BMA	O5-C5-C6	2.34	112.21	107.66
4	D	2	NAG	O7-C7-C8	-2.30	117.96	122.05
4	D	5	MAN	O5-C5-C4	-2.26	105.33	110.83
3	C	10	MAN	O5-C5-C6	2.24	112.02	107.66
2	B	8	MAN	C1-O5-C5	2.21	115.15	112.19
3	C	5	MAN	C1-O5-C5	2.20	115.14	112.19
3	C	2	NAG	O7-C7-C8	-2.19	118.16	122.05
3	C	5	MAN	C3-C4-C5	2.19	114.20	110.23
4	D	6	MAN	O5-C1-C2	-2.19	105.57	110.79
4	D	5	MAN	O5-C5-C6	-2.17	103.43	107.66
2	B	3	BMA	C3-C4-C5	2.13	114.10	110.23
5	E	2	GAL	O5-C5-C4	-2.12	105.68	110.83
3	C	1	NAG	C1-C2-N2	2.11	113.75	110.43
2	B	3	BMA	O3-C3-C2	2.10	114.33	110.05
3	C	1	NAG	O7-C7-N2	2.10	125.69	121.98
3	C	4	MAN	O2-C2-C3	-2.04	105.93	110.15
3	C	1	NAG	O5-C1-C2	-2.03	108.15	111.29
2	B	5	MAN	O2-C2-C3	-2.02	105.97	110.15
3	C	6	MAN	C1-O5-C5	2.01	114.88	112.19
4	D	1	NAG	O5-C1-C2	-2.01	108.18	111.29

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	5	MAN	C4-C5-C6-O6
4	D	5	MAN	O5-C5-C6-O6
3	C	6	MAN	O5-C5-C6-O6

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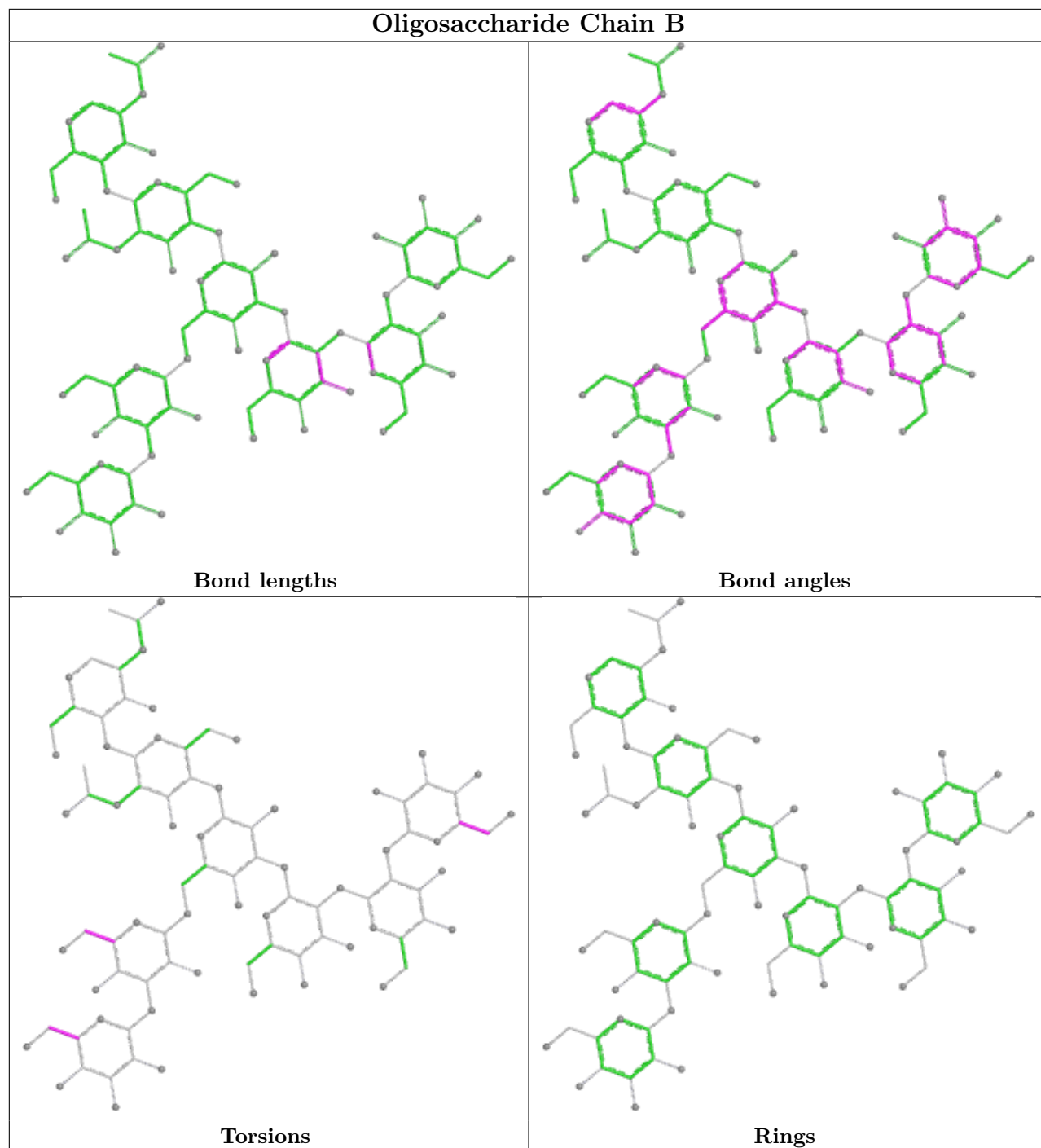
Mol	Chain	Res	Type	Atoms
2	B	6	MAN	O5-C5-C6-O6
3	C	10	MAN	O5-C5-C6-O6
2	B	8	MAN	O5-C5-C6-O6
3	C	9	MAN	C4-C5-C6-O6
5	E	2	GAL	O5-C5-C6-O6
3	C	10	MAN	C4-C5-C6-O6
3	C	6	MAN	C4-C5-C6-O6
5	E	2	GAL	C4-C5-C6-O6
3	C	9	MAN	O5-C5-C6-O6
2	B	8	MAN	C4-C5-C6-O6
2	B	6	MAN	C4-C5-C6-O6
3	C	5	MAN	C4-C5-C6-O6
4	D	3	BMA	C4-C5-C6-O6
3	C	5	MAN	O5-C5-C6-O6
4	D	6	MAN	C4-C5-C6-O6
2	B	7	MAN	O5-C5-C6-O6
5	E	1	GAL	O5-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
4	D	6	MAN	O5-C5-C6-O6
3	C	3	BMA	C4-C5-C6-O6
3	C	7	MAN	C4-C5-C6-O6

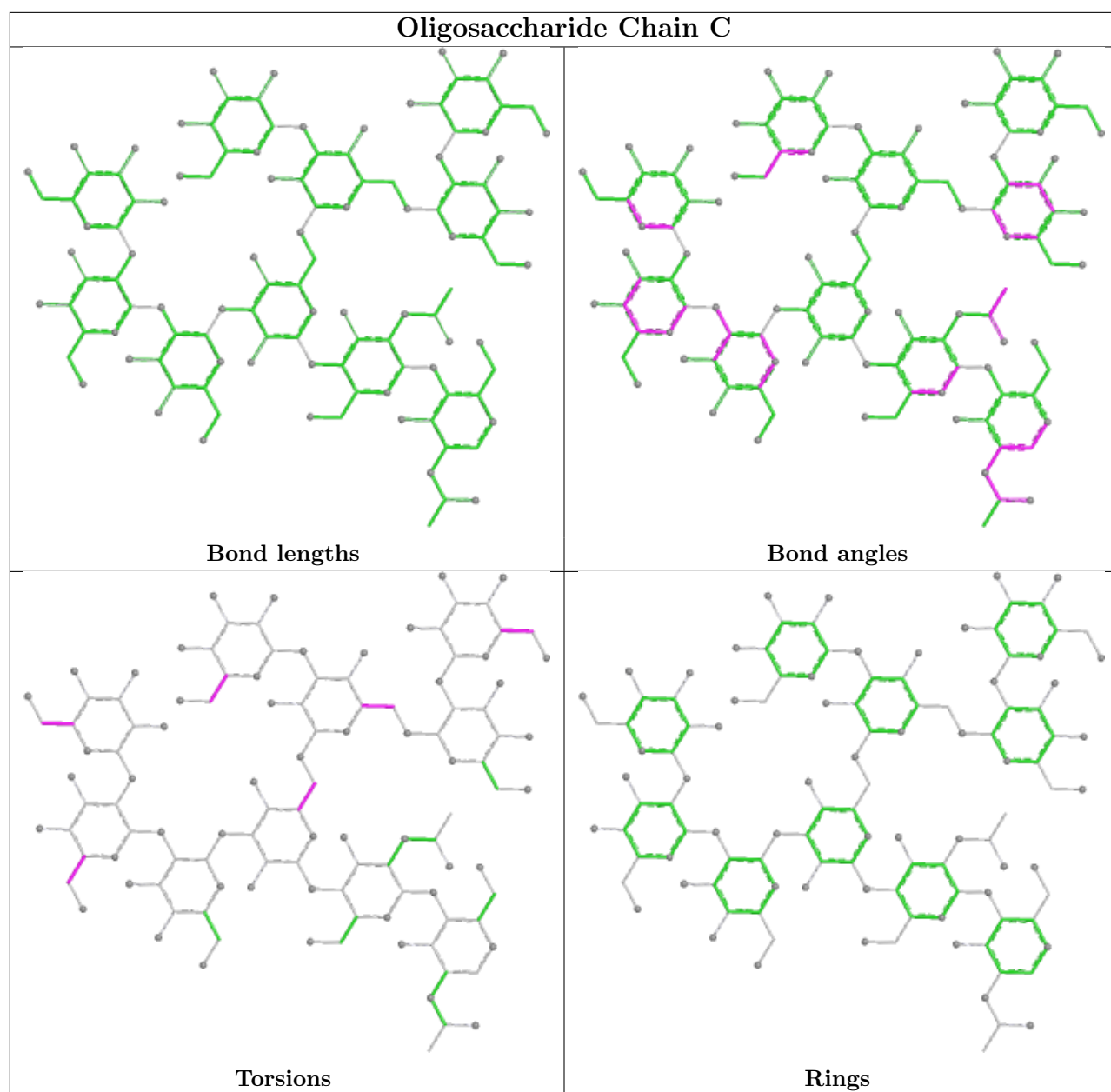
There are no ring outliers.

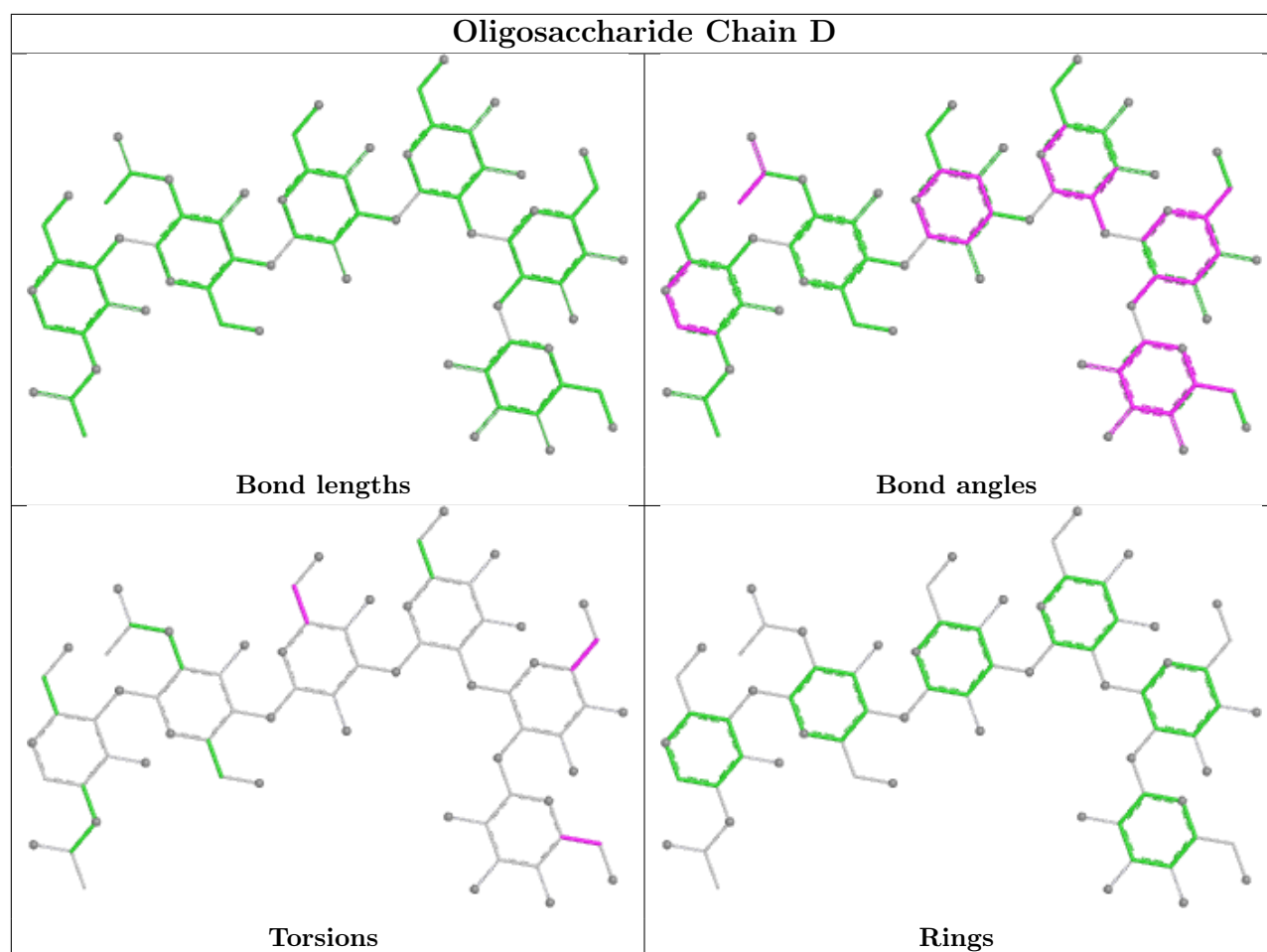
1 monomer is involved in 2 short contacts:

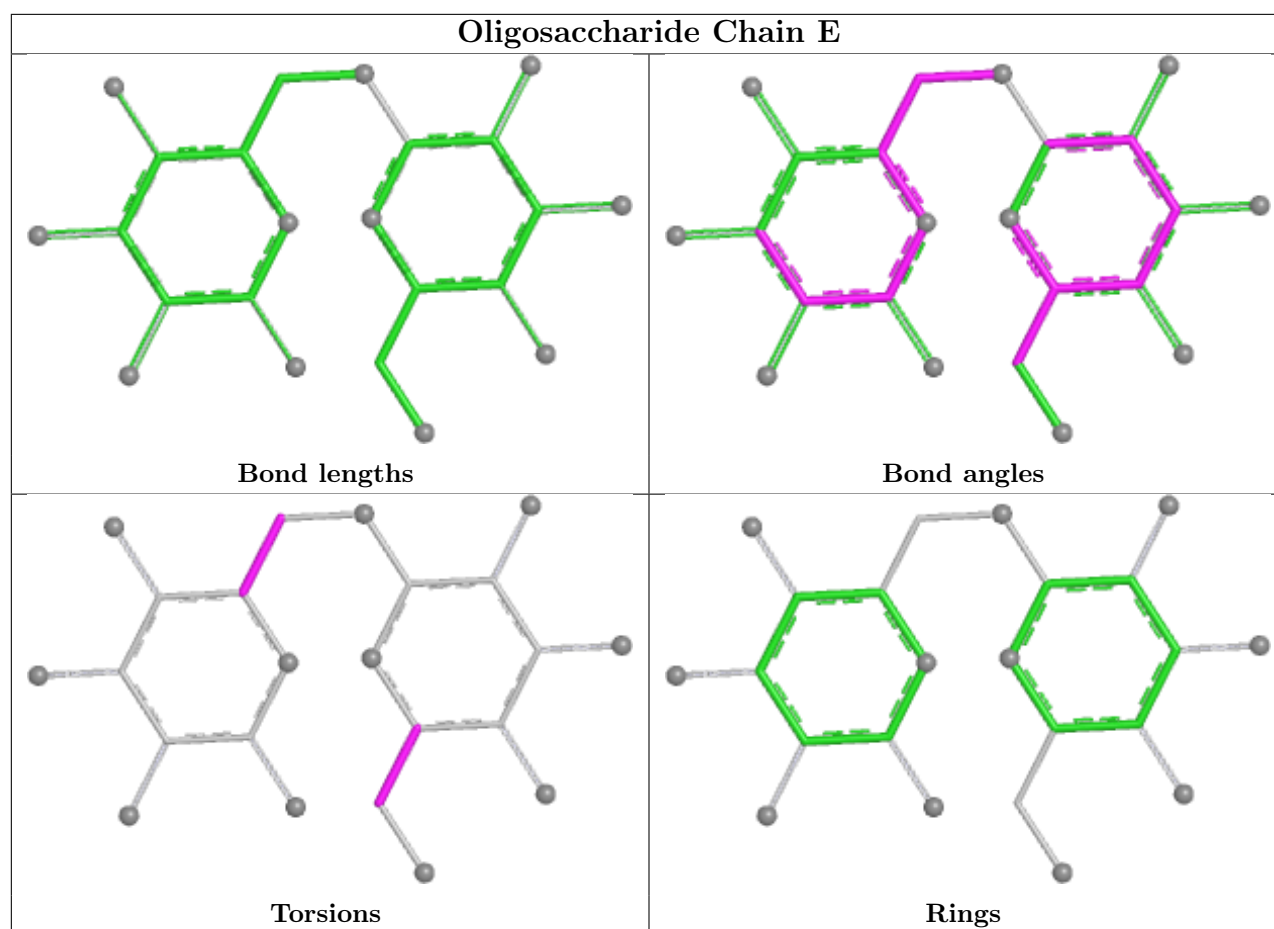
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1	GAL	2	0

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](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	$\# Z > 2$
6	NAG	A	1760	1	14,14,15	0.42	0	17,19,21	1.56	3 (17%)
8	1PE	A	3001	-	15,15,15	0.36	0	14,14,14	0.43	0
6	NAG	A	1478	1	14,14,15	0.44	0	17,19,21	1.04	1 (5%)
6	NAG	A	1156	1	14,14,15	0.58	0	17,19,21	0.95	1 (5%)
6	NAG	A	1777	1	14,14,15	0.62	0	17,19,21	0.97	2 (11%)
6	NAG	A	1739	1	14,14,15	0.62	0	17,19,21	1.03	2 (11%)

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
6	NAG	A	1760	1	-	0/6/23/26	0/1/1/1
8	1PE	A	3001	-	-	6/13/13/13	-
6	NAG	A	1478	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1156	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1777	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1739	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1760	NAG	C1-O5-C5	4.93	118.79	112.19
6	A	1739	NAG	C1-O5-C5	2.69	115.79	112.19
6	A	1760	NAG	C3-C4-C5	-2.43	105.83	110.23
6	A	1156	NAG	O7-C7-C8	-2.27	118.00	122.05
6	A	1478	NAG	O5-C1-C2	-2.25	107.81	111.29
6	A	1739	NAG	O7-C7-C8	-2.19	118.15	122.05
6	A	1777	NAG	C4-C3-C2	-2.14	107.88	111.02
6	A	1777	NAG	O5-C5-C4	-2.08	105.78	110.83
6	A	1760	NAG	O7-C7-C8	-2.03	118.44	122.05

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	3001	1PE	C15-C25-OH5-C14
8	A	3001	1PE	OH4-C13-C23-OH3
8	A	3001	1PE	OH2-C12-C22-OH3
8	A	3001	1PE	OH6-C15-C25-OH5
8	A	3001	1PE	C25-C15-OH6-C26
8	A	3001	1PE	C16-C26-OH6-C15
6	A	1478	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
6	A	1760	NAG	2	0

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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	968/1013 (95%)	-0.15	9 (0%) 81 82	13, 22, 37, 56	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1008	HIS	3.9
1	A	422	ASN	3.7
1	A	41	LEU	2.3
1	A	265	ASP	2.2
1	A	595	SER	2.2
1	A	522	ASN	2.1
1	A	209	GLU	2.1
1	A	581	ASP	2.1
1	A	266	CYS	2.0

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	B	6	11/12	0.51	0.18	63,66,70,70	0
3	MAN	C	6	11/12	0.57	0.20	60,64,65,66	0
2	MAN	B	7	11/12	0.58	0.20	61,69,74,74	0

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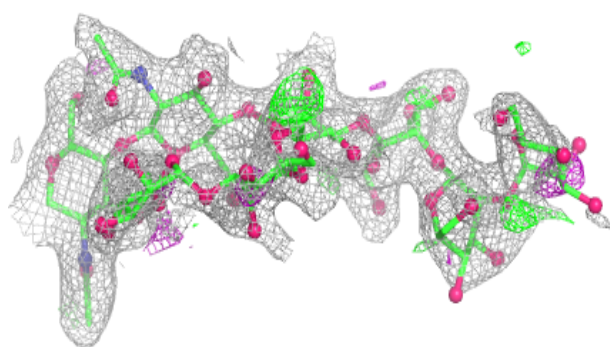
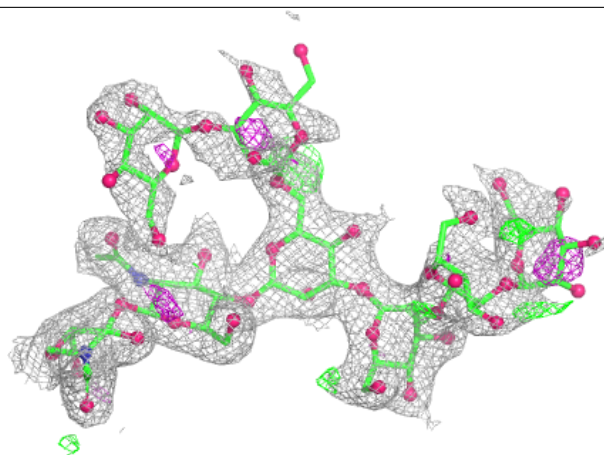
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MAN	B	5	11/12	0.69	0.18	48,53,58,61	0
4	MAN	D	6	11/12	0.69	0.20	74,79,86,88	0
5	GAL	E	1	12/12	0.74	0.20	39,57,60,61	0
2	MAN	B	8	11/12	0.75	0.20	69,74,75,77	0
4	MAN	D	5	11/12	0.76	0.15	64,65,67,74	0
4	BMA	D	3	11/12	0.79	0.13	39,44,46,46	0
3	MAN	C	5	11/12	0.79	0.15	49,50,52,58	0
3	NAG	C	1	14/15	0.86	0.11	21,22,25,25	0
4	MAN	D	4	11/12	0.87	0.11	43,48,52,57	0
2	BMA	B	3	11/12	0.87	0.10	25,30,38,47	0
4	NAG	D	2	14/15	0.89	0.09	25,27,30,33	0
3	MAN	C	10	11/12	0.89	0.09	27,29,31,32	0
5	GAL	E	2	11/12	0.89	0.11	29,32,34,35	0
3	MAN	C	8	11/12	0.90	0.09	27,27,28,29	0
2	MAN	B	4	11/12	0.90	0.09	32,34,36,41	0
3	NAG	C	2	14/15	0.90	0.10	17,20,22,25	0
3	MAN	C	4	11/12	0.91	0.09	32,35,37,42	0
3	MAN	C	9	11/12	0.92	0.09	29,31,34,37	0
4	NAG	D	1	14/15	0.94	0.07	17,19,20,22	0
3	BMA	C	3	11/12	0.94	0.07	22,22,24,28	0
3	MAN	C	7	11/12	0.95	0.06	22,23,25,26	0
2	NAG	B	1	14/15	0.95	0.06	18,18,19,19	0
2	NAG	B	2	14/15	0.96	0.06	19,19,21,23	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

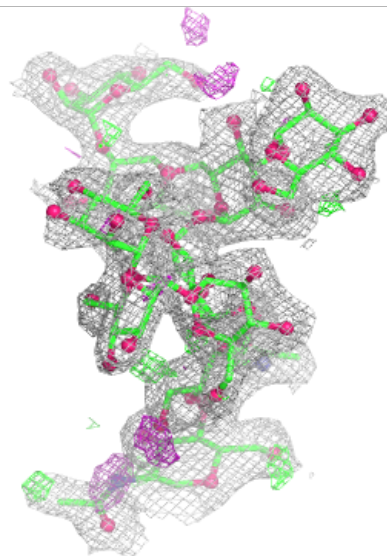
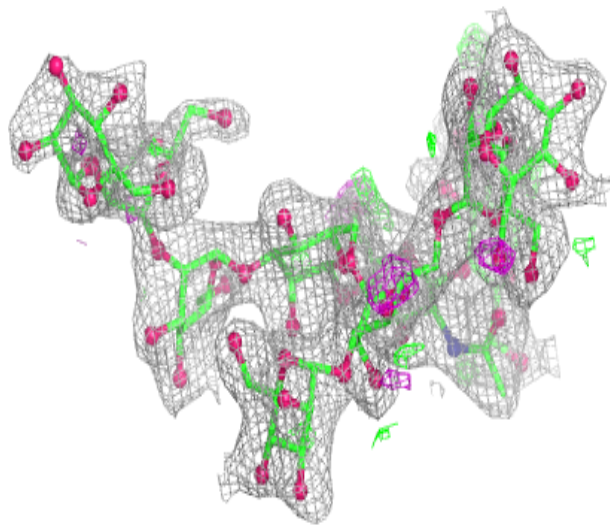
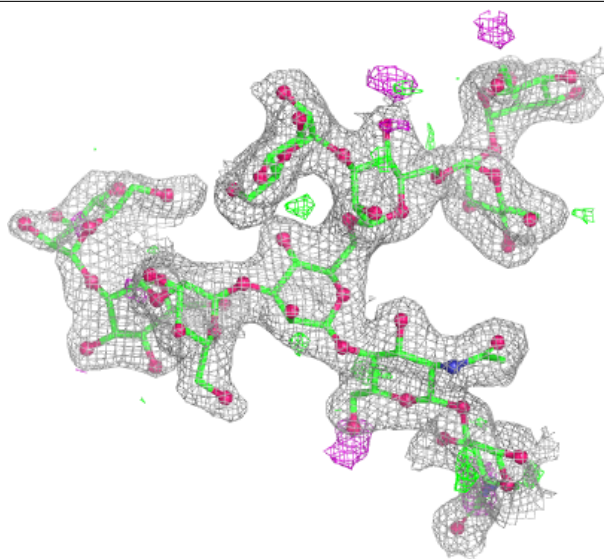
Electron density around Chain B:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



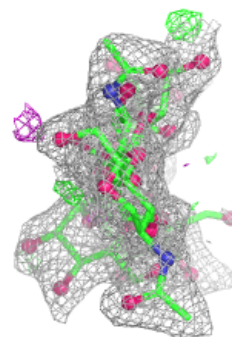
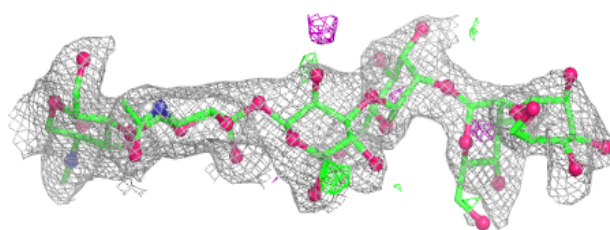
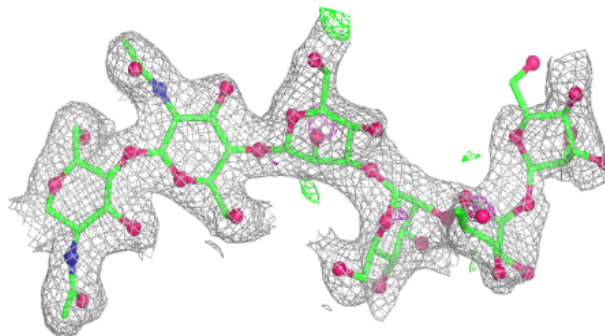
Electron density around Chain C:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

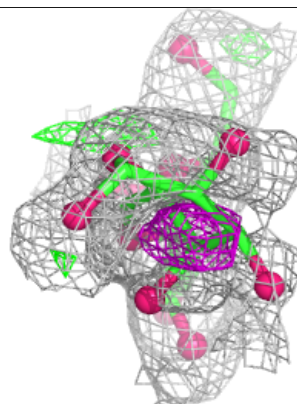
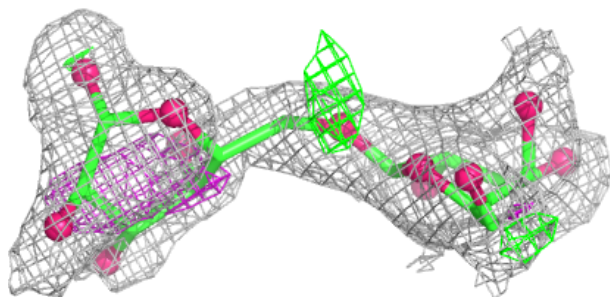
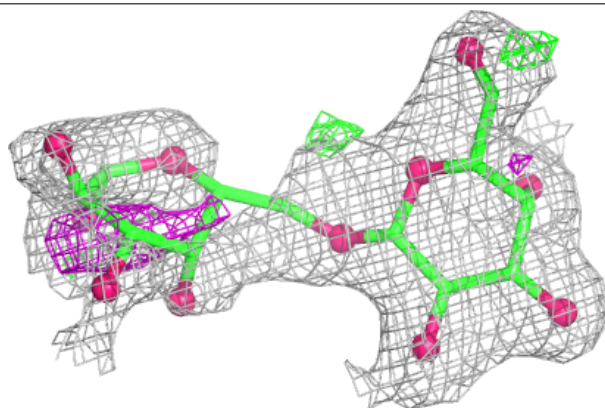


Electron density around Chain D:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain E:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	A	1156	14/15	0.48	0.24	67,74,79,82	0
6	NAG	A	1478	14/15	0.73	0.14	49,53,56,58	0
8	1PE	A	3001	16/16	0.76	0.23	44,59,69,71	0
6	NAG	A	1739	14/15	0.78	0.14	41,45,51,52	0
6	NAG	A	1760	14/15	0.88	0.09	28,30,33,34	0
6	NAG	A	1777	14/15	0.94	0.07	23,25,26,26	0
7	CL	A	2001	1/1	0.99	0.02	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.