



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 04:51 PM UTC

PDB ID : 6Q7I / pdb_00006q7i
Title : GH3 exo-beta-xylosidase (XlnD)
Authors : Davies, G.J.; Rowland, R.J.; Wu, L.; Moroz, O.; Blagova, E.
Deposited on : 2018-12-13
Resolution : 1.48 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 ⓘ 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

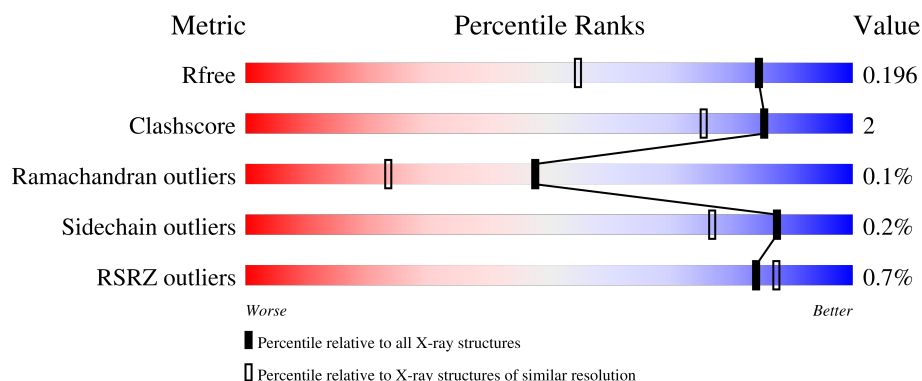
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.48 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	6779 (1.50-1.46)
Clashscore	190562	7025 (1.50-1.46)
Ramachandran outliers	187476	6917 (1.50-1.46)
Sidechain outliers	187428	6914 (1.50-1.46)
RSRZ outliers	180081	6781 (1.50-1.46)

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	785	
1	B	785	
2	C	9	
3	D	2	
3	F	2	

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Mol	Chain	Length	Quality of chain
4	E	10	

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
6	EDO	B	925	-	-	X	-

2 Entry composition [i](#)

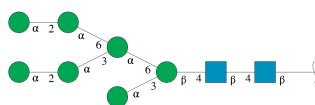
There are 10 unique types of molecules in this entry. The entry contains 14338 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Exo-1,4-beta-xylosidase xlnD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	769	Total	C	N	O	S	0	8	0
			5945	3752	982	1195	16			
1	A	770	Total	C	N	O	S	0	11	0
			5987	3775	993	1203	16			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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
2	C	9	Total	C	N	O	0	0	0
			105	58	2	45			

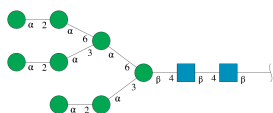
- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

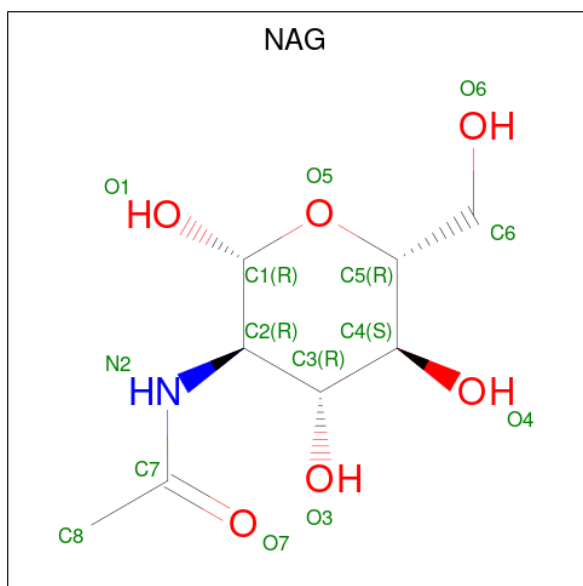
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

ose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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	E	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



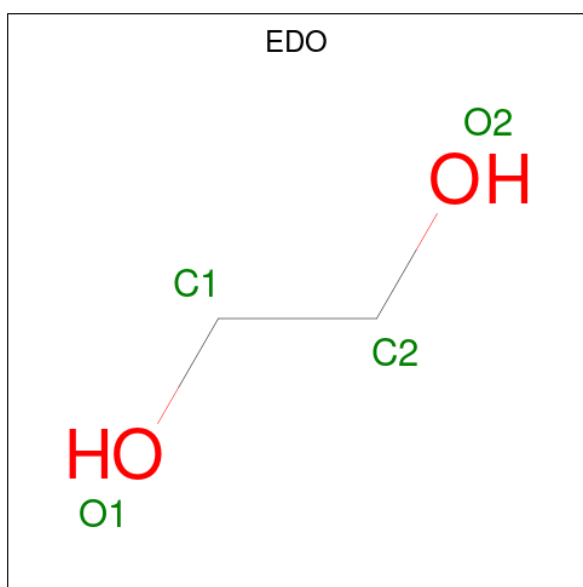
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

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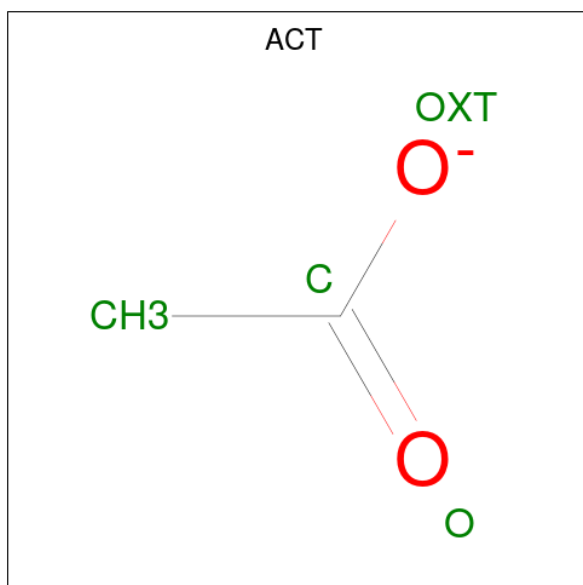
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1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

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	3	Total	K	0	0
			3	3		
9	A	1	Total	K	0	0
			1	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	873	Total	O	0	0
			873	873		
10	A	948	Total	O	0	0
			948	948		

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

Chain F:  100%

MAG1
MAG2

- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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 E:  10%  90%

MAG1
MAG2
ENAG
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.47Å 90.58Å 244.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.24 – 1.48 33.24 – 1.48	Depositor EDS
% Data completeness (in resolution range)	99.9 (33.24-1.48) 99.9 (33.24-1.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 1.48Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.159 , 0.193 0.162 , 0.196	Depositor DCC
R_{free} test set	13022 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14338	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 11.20% 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: BMA, MAN, ACT, EDO, NAG, K, GOL, PCA

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	1.10	5/6127 (0.1%)	1.18	5/8373 (0.1%)
1	B	1.09	4/6086 (0.1%)	1.21	6/8320 (0.1%)
All	All	1.10	9/12213 (0.1%)	1.19	11/16693 (0.1%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	478	HIS	CE1-NE2	6.54	1.39	1.32
1	A	668	HIS	CE1-NE2	6.16	1.38	1.32
1	A	417	ASP	N-CA	5.67	1.49	1.46
1	B	108	ALA	CA-CB	-5.44	1.49	1.53
1	B	111	GLY	C-O	5.42	1.30	1.23

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	724	ASP	CA-CB-CG	7.31	119.91	112.60
1	A	788	VAL	CA-C-O	-6.36	109.99	120.80
1	B	392	ASP	CA-CB-CG	6.30	118.90	112.60
1	B	514	GLU	CB-CG-CD	6.15	123.05	112.60
1	B	387	ARG	CG-CD-NE	-6.08	98.63	112.00

There are no chirality outliers.

There are no planarity outliers.

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	5987	0	5631	21	0
1	B	5945	0	5589	19	0
2	C	105	0	88	0	0
3	D	28	0	25	0	0
3	F	28	0	25	0	0
4	E	116	0	97	0	0
5	A	112	0	104	0	0
5	B	126	0	117	0	0
6	A	28	0	41	8	0
6	B	16	0	24	9	0
7	B	4	0	3	1	0
8	A	6	0	8	0	0
8	B	12	0	16	3	0
9	A	1	0	0	0	0
9	B	3	0	0	0	0
10	A	948	0	0	13	0
10	B	873	0	0	7	0
All	All	14338	0	11768	53	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.

The worst 5 of 53 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)
6:A:921:EDO:H11	10:A:1522:HOH:O	1.79	0.83
1:B:208:GLY:HA2	6:B:925:EDO:H21	1.62	0.79
6:A:923:EDO:H22	10:A:1782:HOH:O	1.80	0.79
6:B:924:EDO:O1	6:B:925:EDO:O1	1.92	0.76
6:A:923:EDO:C2	10:A:1782:HOH:O	2.38	0.70

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	780/785 (99%)	753 (96%)	26 (3%)	1 (0%)	48	23
1	B	775/785 (99%)	750 (97%)	24 (3%)	1 (0%)	48	23
All	All	1555/1570 (99%)	1503 (97%)	50 (3%)	2 (0%)	48	23

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	SER
1	B	231	SER

5.3.2 Protein sidechains ⓘ

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	641/647 (99%)	640 (100%)	1 (0%)	87	77
1	B	636/647 (98%)	635 (100%)	1 (0%)	87	77
All	All	1277/1294 (99%)	1275 (100%)	2 (0%)	87	77

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	233	ASN
1	A	647	THR

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	478	HIS
1	A	492	GLN
1	A	515	ASN

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Mol	Chain	Res	Type
1	A	313	ASN
1	B	743	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	PCA	B	19	1	7,8,9	0.53	0	9,10,12	0.78	0
1	PCA	A	19	1	7,8,9	0.61	0	9,10,12	1.01	1 (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
1	PCA	B	19	1	-	0/0/11/13	0/1/1/1
1	PCA	A	19	1	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	19	PCA	O-C-CA	-2.13	119.29	124.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

23 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	C	1	2,1	14,14,15	0.94	1 (7%)	17,19,21	1.71	3 (17%)
2	NAG	C	2	2	14,14,15	0.59	0	17,19,21	1.27	1 (5%)
2	BMA	C	3	2	11,11,12	1.50	1 (9%)	15,15,17	1.13	1 (6%)
2	MAN	C	4	2	11,11,12	0.67	0	15,15,17	1.14	2 (13%)
2	MAN	C	5	2	11,11,12	0.88	0	15,15,17	1.43	3 (20%)
2	MAN	C	6	2	11,11,12	0.65	0	15,15,17	1.10	2 (13%)
2	MAN	C	7	2	11,11,12	0.69	0	15,15,17	1.29	1 (6%)
2	MAN	C	8	2	11,11,12	1.05	0	15,15,17	0.92	0
2	MAN	C	9	2	11,11,12	0.90	1 (9%)	15,15,17	1.72	4 (26%)
3	NAG	D	1	1,3	14,14,15	0.68	0	17,19,21	1.27	1 (5%)
3	NAG	D	2	3	14,14,15	0.76	0	17,19,21	1.30	3 (17%)
4	NAG	E	1	1,4	14,14,15	1.54	3 (21%)	17,19,21	2.30	4 (23%)
4	MAN	E	10	4	11,11,12	0.99	0	15,15,17	1.40	3 (20%)
4	NAG	E	2	4	14,14,15	0.96	1 (7%)	17,19,21	1.50	4 (23%)
4	BMA	E	3	4	11,11,12	0.65	0	15,15,17	1.66	2 (13%)
4	MAN	E	4	4	11,11,12	0.79	0	15,15,17	1.46	4 (26%)
4	MAN	E	5	4	11,11,12	0.84	0	15,15,17	2.92	5 (33%)
4	MAN	E	6	4	11,11,12	1.28	1 (9%)	15,15,17	2.56	4 (26%)
4	MAN	E	7	4	11,11,12	0.48	0	15,15,17	0.97	1 (6%)
4	MAN	E	8	4	11,11,12	0.48	0	15,15,17	1.02	0
4	MAN	E	9	4	11,11,12	0.62	0	15,15,17	1.47	4 (26%)
3	NAG	F	1	1,3	14,14,15	0.75	0	17,19,21	1.40	3 (17%)
3	NAG	F	2	3	14,14,15	0.93	0	17,19,21	1.78	6 (35%)

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1	NAG	C1-C2	4.07	1.57	1.52
2	C	3	BMA	O5-C1	-3.89	1.37	1.43
4	E	6	MAN	O5-C1	-2.78	1.39	1.43
4	E	1	NAG	C8-C7	2.73	1.56	1.50
4	E	2	NAG	C1-C2	2.52	1.55	1.52

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	5	MAN	O2-C2-C3	-8.21	93.16	110.15

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1	NAG	O5-C1-C2	-7.66	99.45	111.29
4	E	6	MAN	C1-O5-C5	6.40	120.77	112.19
4	E	6	MAN	O5-C5-C6	-5.13	97.68	107.66
2	C	1	NAG	O5-C1-C2	-5.05	103.48	111.29

There are no chirality outliers.

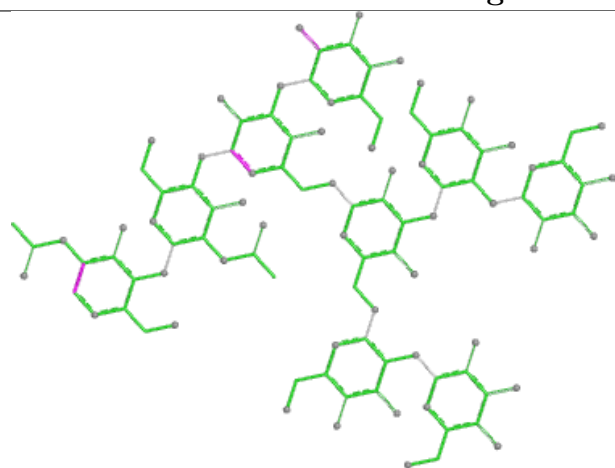
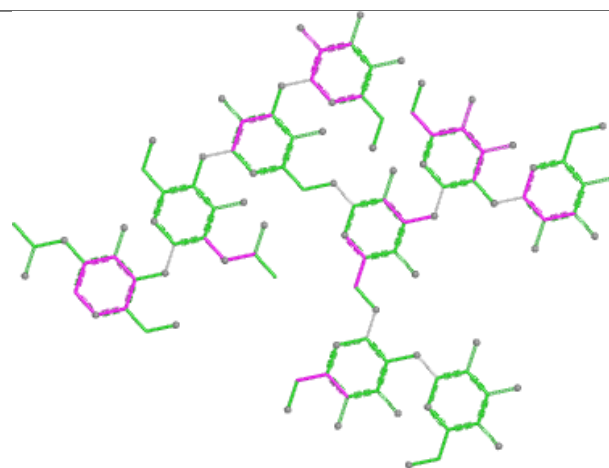
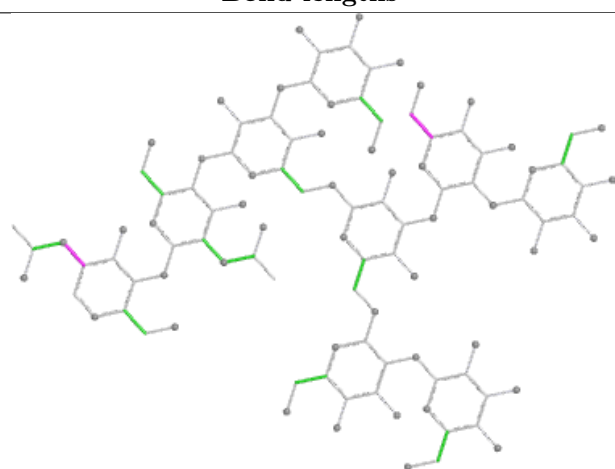
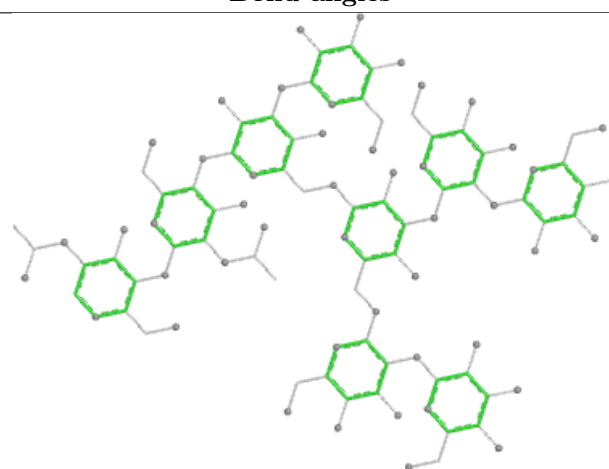
5 of 13 torsion outliers are listed below:

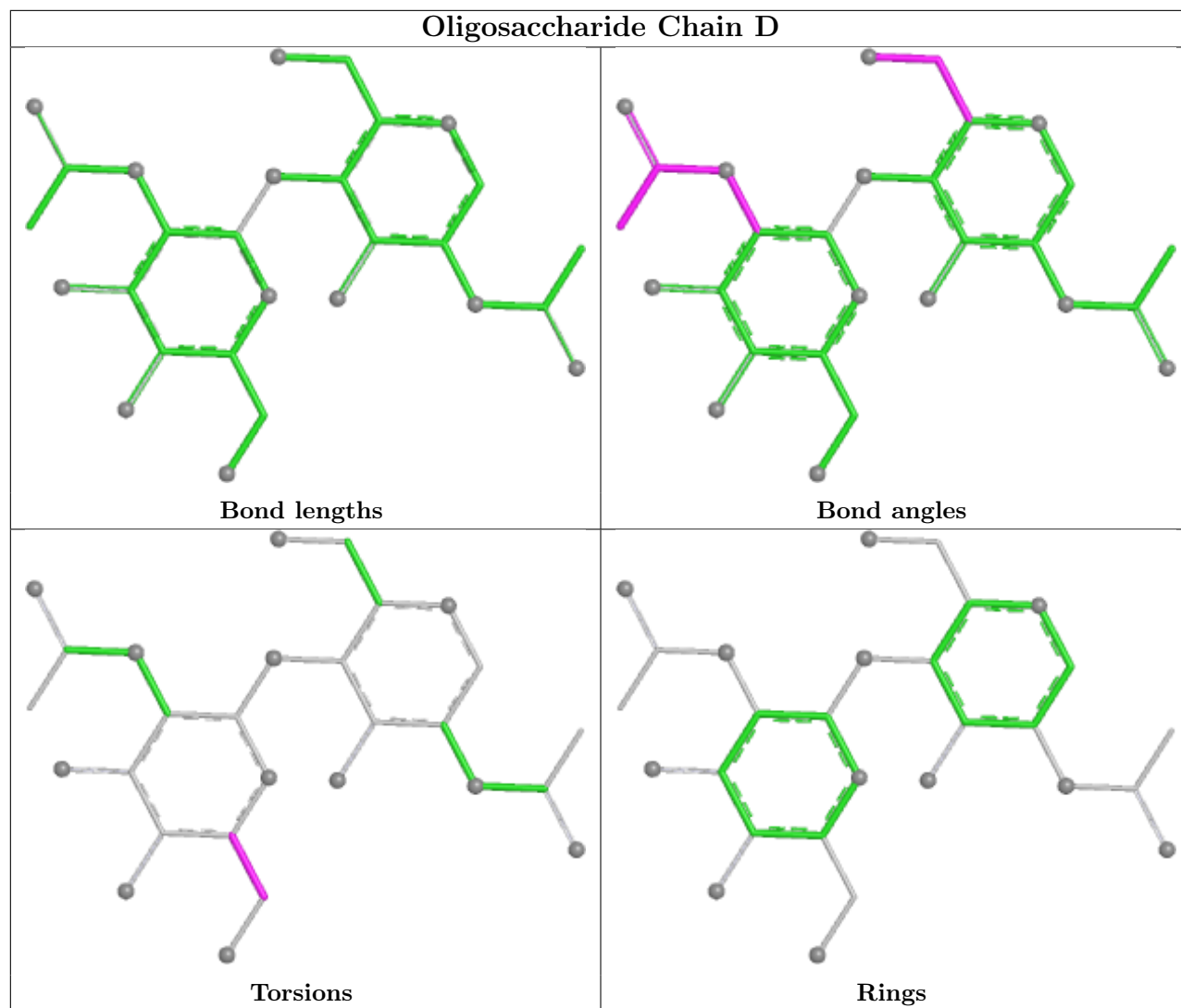
Mol	Chain	Res	Type	Atoms
3	D	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
4	E	9	MAN	O5-C5-C6-O6
4	E	6	MAN	O5-C5-C6-O6
2	C	5	MAN	O5-C5-C6-O6

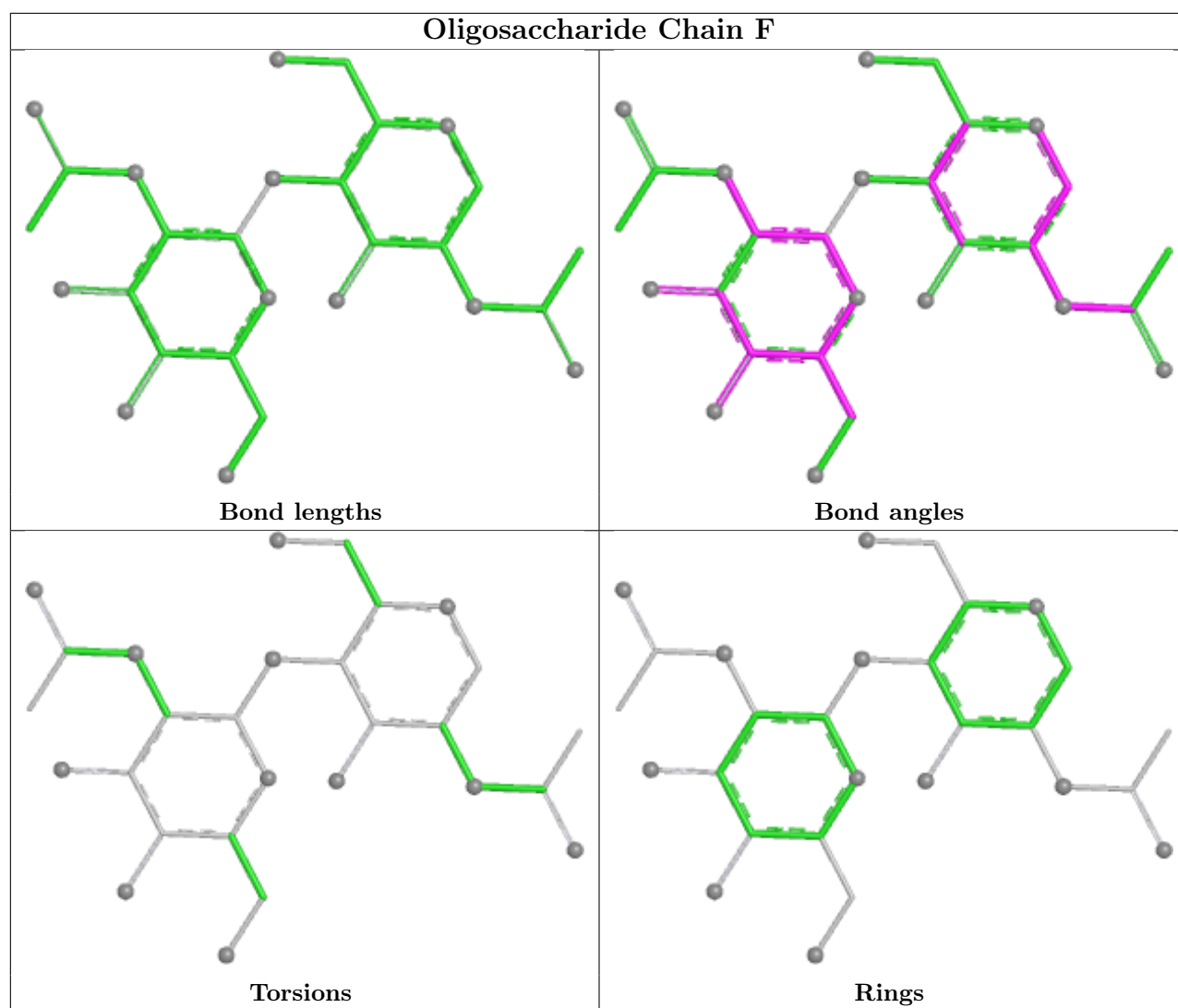
There are no ring outliers.

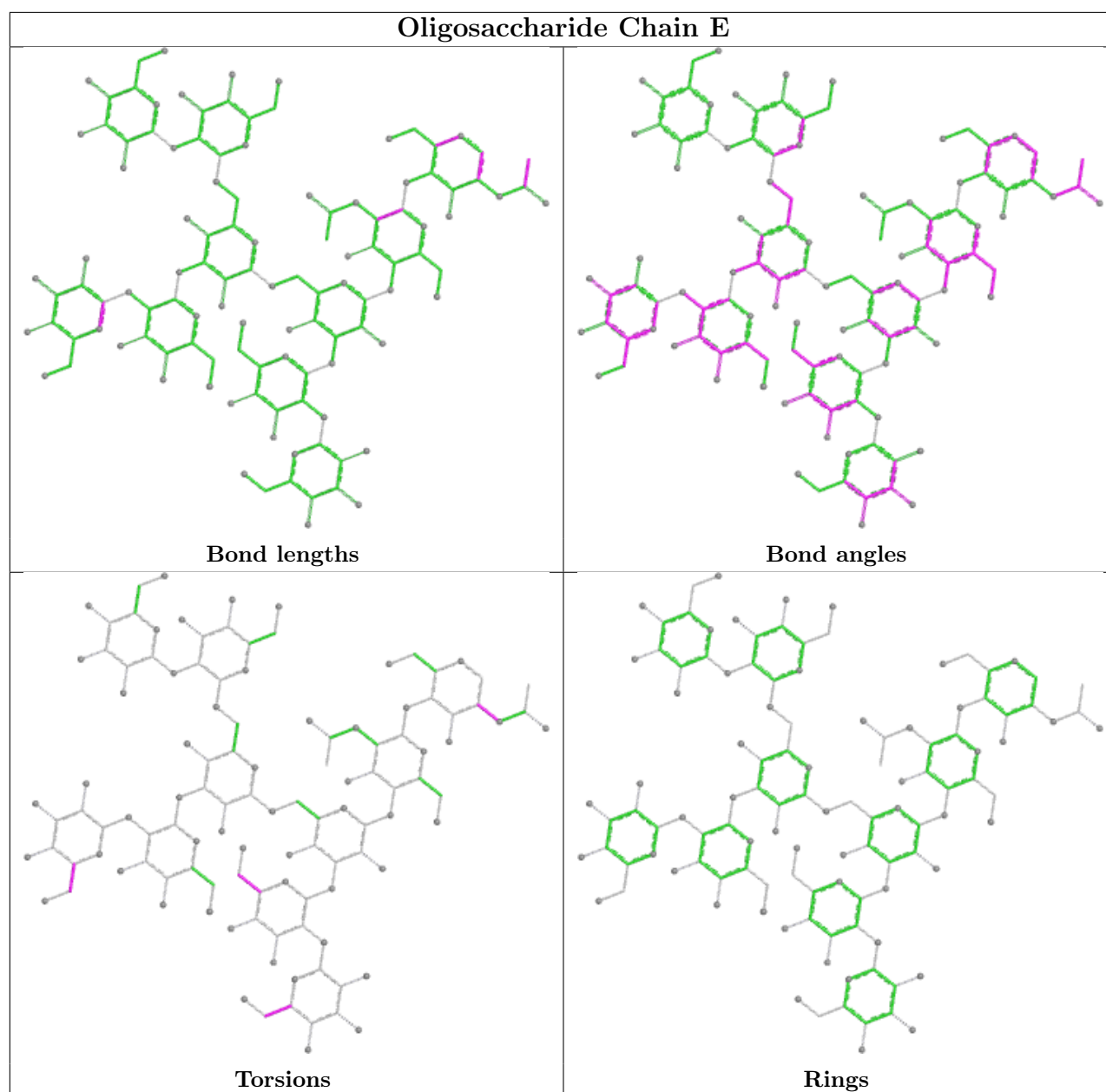
No monomer is involved in short contacts.

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

Oligosaccharide Chain C**Bond lengths****Bond angles****Torsions****Rings**







5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 4 are monoatomic - leaving 32 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	EDO	A	925	-	3,3,3	0.32	0	2,2,2	0.35	0
5	NAG	A	915	1	14,14,15	0.51	0	17,19,21	1.22	1 (5%)
7	ACT	B	922	-	3,3,3	0.82	0	3,3,3	1.32	0
5	NAG	A	917	1	14,14,15	0.72	0	17,19,21	1.52	4 (23%)
6	EDO	A	923	-	3,3,3	0.50	0	2,2,2	0.08	0
5	NAG	B	920	1	14,14,15	1.39	2 (14%)	17,19,21	1.88	2 (11%)
5	NAG	A	920	1	14,14,15	0.96	1 (7%)	17,19,21	1.82	5 (29%)
5	NAG	B	913	1	14,14,15	0.68	0	17,19,21	0.88	0
5	NAG	B	914	1	14,14,15	0.97	1 (7%)	17,19,21	1.66	4 (23%)
6	EDO	A	924	-	3,3,3	0.55	0	2,2,2	0.53	0
5	NAG	B	918	1	14,14,15	0.54	0	17,19,21	1.24	3 (17%)
5	NAG	B	919	1	14,14,15	0.81	1 (7%)	17,19,21	1.03	1 (5%)
5	NAG	A	901	1	14,14,15	0.89	0	17,19,21	1.46	5 (29%)
6	EDO	A	927	6	3,3,3	0.26	0	2,2,2	0.49	0
5	NAG	A	914	1	14,14,15	1.14	1 (7%)	17,19,21	2.18	5 (29%)
6	EDO	B	921	-	3,3,3	0.32	0	2,2,2	0.28	0
6	EDO	B	925	-	3,3,3	0.45	0	2,2,2	1.13	0
6	EDO	A	922	-	3,3,3	0.11	0	2,2,2	0.63	0
5	NAG	A	916	1	14,14,15	0.87	1 (7%)	17,19,21	1.08	1 (5%)
8	GOL	B	926	-	5,5,5	0.19	0	5,5,5	1.15	0
6	EDO	A	926	6	3,3,3	0.26	0	2,2,2	0.38	0
6	EDO	B	924	-	3,3,3	0.33	0	2,2,2	0.13	0
6	EDO	B	923	-	3,3,3	0.66	0	2,2,2	0.53	0
5	NAG	A	918	1	14,14,15	1.01	0	17,19,21	1.58	2 (11%)
8	GOL	A	928	-	5,5,5	0.08	0	5,5,5	0.51	0
5	NAG	B	917	1	14,14,15	0.60	0	17,19,21	2.35	8 (47%)
8	GOL	B	927	-	5,5,5	0.11	0	5,5,5	0.36	0
5	NAG	B	911	1	14,14,15	0.60	0	17,19,21	0.98	0
5	NAG	B	912	1	14,14,15	0.75	0	17,19,21	0.98	1 (5%)
5	NAG	A	919	1	14,14,15	0.52	0	17,19,21	0.79	0
5	NAG	B	901	1	14,14,15	1.20	2 (14%)	17,19,21	2.28	3 (17%)
6	EDO	A	921	-	3,3,3	0.15	0	2,2,2	0.18	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
6	EDO	A	925	-	-	1/1/1/1	-
5	NAG	A	915	1	-	0/6/23/26	0/1/1/1
5	NAG	A	917	1	-	0/6/23/26	0/1/1/1
6	EDO	A	923	-	-	1/1/1/1	-
5	NAG	B	920	1	-	0/6/23/26	0/1/1/1
5	NAG	A	920	1	-	0/6/23/26	0/1/1/1
5	NAG	B	913	1	-	0/6/23/26	0/1/1/1
5	NAG	B	914	1	-	0/6/23/26	0/1/1/1
6	EDO	A	924	-	-	1/1/1/1	-
5	NAG	B	918	1	-	0/6/23/26	0/1/1/1
5	NAG	B	919	1	-	0/6/23/26	0/1/1/1
5	NAG	A	901	1	-	0/6/23/26	0/1/1/1
6	EDO	A	927	6	-	0/1/1/1	-
5	NAG	A	914	1	-	0/6/23/26	0/1/1/1
6	EDO	B	921	-	-	1/1/1/1	-
6	EDO	B	925	-	-	0/1/1/1	-
6	EDO	A	922	-	-	1/1/1/1	-
5	NAG	A	916	1	-	0/6/23/26	0/1/1/1
8	GOL	B	926	-	-	3/4/4/4	-
6	EDO	A	926	6	-	1/1/1/1	-
6	EDO	B	924	-	-	0/1/1/1	-
6	EDO	B	923	-	-	1/1/1/1	-
5	NAG	A	918	1	-	0/6/23/26	0/1/1/1
8	GOL	A	928	-	-	0/4/4/4	-
5	NAG	B	917	1	-	2/6/23/26	0/1/1/1
8	GOL	B	927	-	-	0/4/4/4	-
5	NAG	B	911	1	-	0/6/23/26	0/1/1/1
5	NAG	B	912	1	-	0/6/23/26	0/1/1/1
5	NAG	A	919	1	-	0/6/23/26	0/1/1/1
5	NAG	B	901	1	-	1/6/23/26	0/1/1/1
6	EDO	A	921	-	-	0/1/1/1	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	920	NAG	C1-C2	3.88	1.57	1.52
5	B	901	NAG	C8-C7	2.86	1.56	1.50
5	A	914	NAG	O7-C7	2.52	1.28	1.23
5	B	914	NAG	O5-C5	2.51	1.48	1.43
5	B	919	NAG	C1-C2	2.49	1.55	1.52

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	901	NAG	C2-N2-C7	7.32	132.71	122.90
5	A	914	NAG	C8-C7-N2	-6.44	105.44	116.12
5	B	917	NAG	C1-O5-C5	4.94	118.81	112.19
5	B	920	NAG	C1-O5-C5	4.91	118.77	112.19
5	B	920	NAG	O5-C1-C2	-4.64	104.11	111.29

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	901	NAG	C1-C2-N2-C7
8	B	926	GOL	C1-C2-C3-O3
5	B	917	NAG	C4-C5-C6-O6
8	B	926	GOL	O1-C1-C2-O2
8	B	926	GOL	O2-C2-C3-O3

There are no ring outliers.

10 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	922	ACT	1	0
6	A	923	EDO	3	0
6	A	924	EDO	3	0
6	B	921	EDO	2	0
6	B	925	EDO	4	0
8	B	926	GOL	2	0
6	B	924	EDO	2	0
6	B	923	EDO	2	0
8	B	927	GOL	1	0
6	A	921	EDO	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	769/785 (97%)	-0.27	4 (0%) 87 90	7, 19, 30, 44	30 (3%)
1	B	768/785 (97%)	-0.11	6 (0%) 82 86	8, 21, 36, 48	22 (2%)
All	All	1537/1570 (97%)	-0.19	10 (0%) 84 87	7, 20, 33, 48	52 (3%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	57	LEU	3.4
1	A	788	VAL	3.0
1	B	478[A]	HIS	2.8
1	A	647	THR	2.6
1	A	787	PHE	2.6

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	PCA	A	19	8/9	0.96	0.06	17,19,20,20	0
1	PCA	B	19	8/9	0.98	0.04	17,18,20,20	0

6.3 Carbohydrates [i](#)

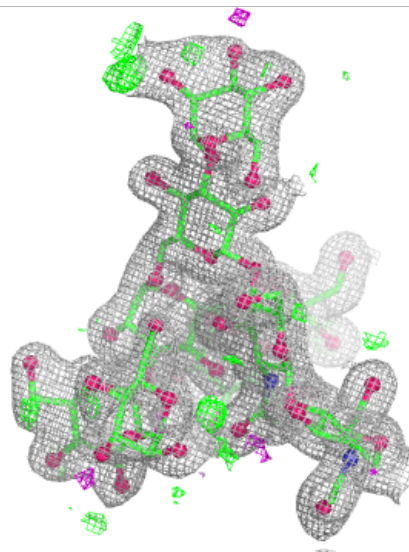
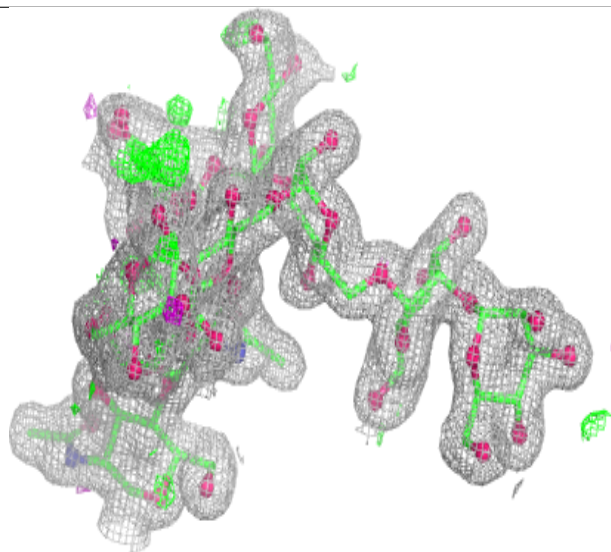
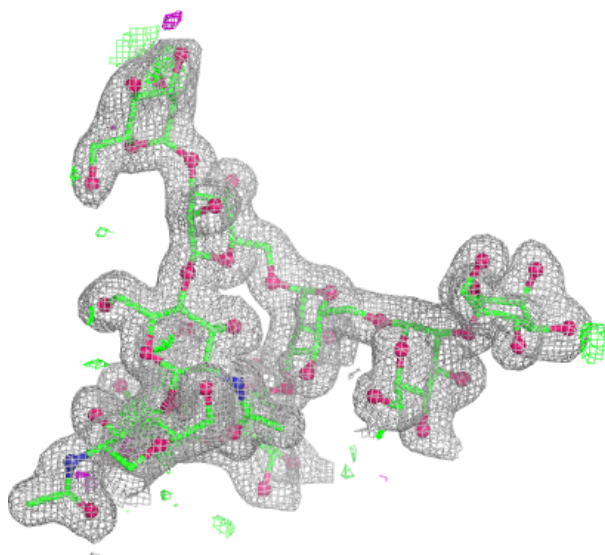
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	F	2	14/15	0.61	0.13	47,63,73,74	0
4	MAN	E	10	11/12	0.72	0.12	58,63,68,70	0
3	NAG	D	2	14/15	0.76	0.12	40,45,55,66	0
4	MAN	E	6	11/12	0.79	0.13	42,47,51,64	0
2	MAN	C	6	11/12	0.80	0.12	39,47,51,55	0
4	MAN	E	9	11/12	0.85	0.11	37,45,56,57	0
2	MAN	C	9	11/12	0.85	0.10	29,39,45,49	0
4	MAN	E	5	11/12	0.86	0.10	34,41,46,50	0
2	MAN	C	5	11/12	0.87	0.09	34,40,42,46	0
3	NAG	F	1	14/15	0.92	0.08	25,29,41,45	0
3	NAG	D	1	14/15	0.92	0.08	25,27,37,41	0
2	MAN	C	7	11/12	0.94	0.07	27,31,40,42	0
4	NAG	E	1	14/15	0.94	0.08	17,22,29,29	0
4	MAN	E	7	11/12	0.95	0.06	26,29,33,35	0
4	NAG	E	2	14/15	0.95	0.06	22,23,29,31	0
4	BMA	E	3	11/12	0.95	0.07	22,25,30,30	0
4	MAN	E	4	11/12	0.96	0.06	24,26,28,32	0
2	BMA	C	3	11/12	0.96	0.06	23,26,30,31	0
2	MAN	C	8	11/12	0.96	0.06	21,25,30,33	0
2	MAN	C	4	11/12	0.96	0.06	26,28,29,31	0
2	NAG	C	1	14/15	0.96	0.06	18,21,26,29	0
2	NAG	C	2	14/15	0.96	0.05	22,23,26,32	0
4	MAN	E	8	11/12	0.97	0.05	19,23,28,31	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.

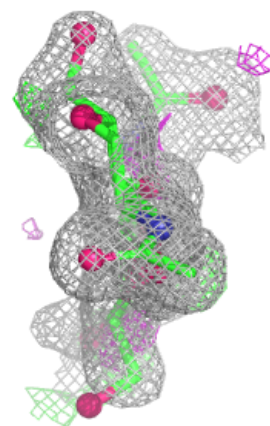
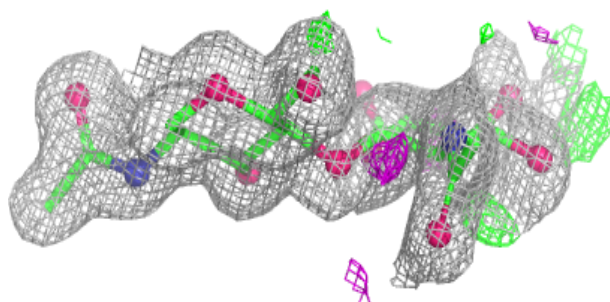
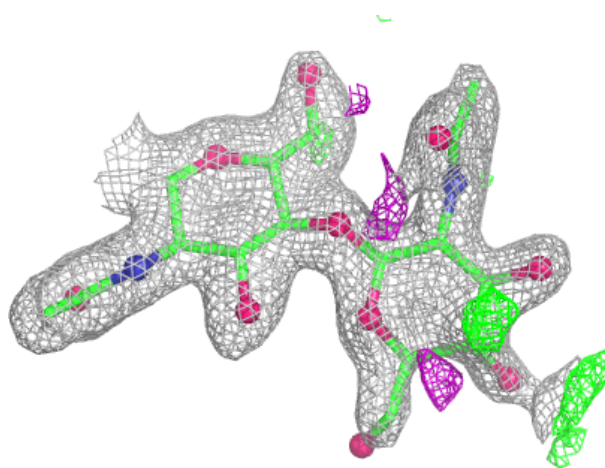
Electron density around Chain C:

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



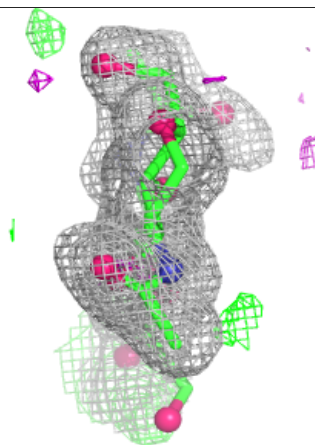
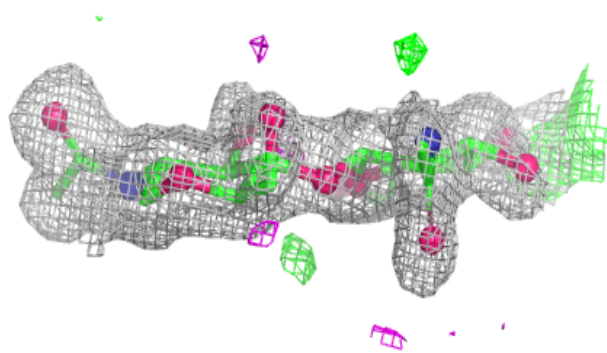
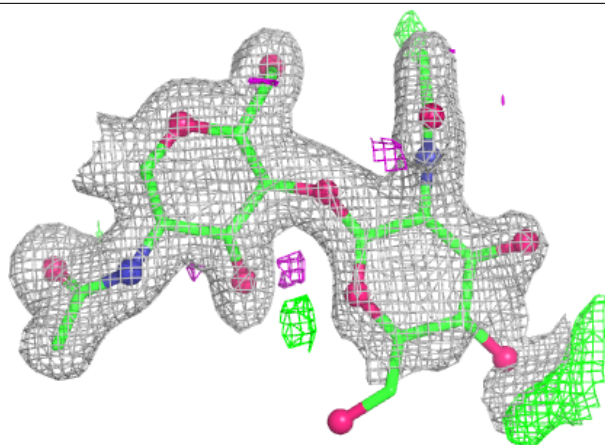
Electron density around Chain D:

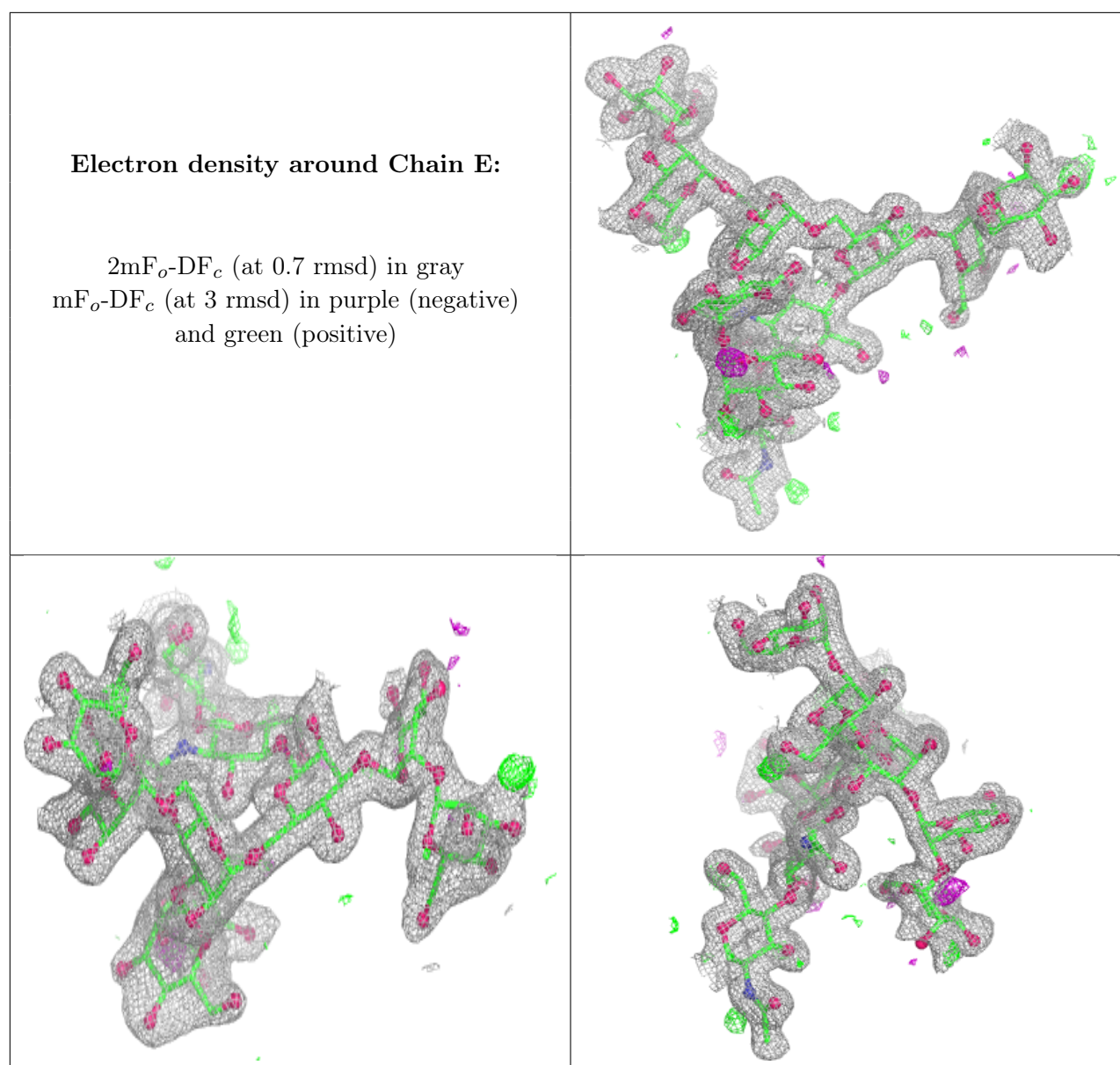
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain F:

$2mF_o - DF_c$ (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(Å ²)	Q<0.9
6	EDO	A	926	4/4	0.72	0.19	37,39,39,42	4
6	EDO	A	925	4/4	0.74	0.18	34,47,49,56	0
6	EDO	B	921	4/4	0.75	0.18	45,57,58,59	0
6	EDO	A	924	4/4	0.79	0.14	36,37,41,45	0
6	EDO	A	922	4/4	0.81	0.14	32,36,37,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	B	917	14/15	0.81	0.12	32,39,48,53	0
6	EDO	A	927	4/4	0.81	0.12	21,23,26,26	4
5	NAG	B	918	14/15	0.82	0.11	34,41,52,53	0
5	NAG	B	919	14/15	0.82	0.11	36,39,48,50	0
5	NAG	B	920	14/15	0.82	0.11	26,41,44,49	0
5	NAG	A	919	14/15	0.85	0.10	40,48,52,52	0
8	GOL	B	927	6/6	0.86	0.11	32,42,50,53	0
6	EDO	B	923	4/4	0.87	0.12	33,37,39,41	0
6	EDO	B	925	4/4	0.88	0.10	30,31,34,38	0
5	NAG	A	918	14/15	0.90	0.09	21,28,31,37	0
5	NAG	A	915	14/15	0.90	0.08	29,36,45,47	0
5	NAG	A	920	14/15	0.90	0.09	27,31,38,39	0
5	NAG	A	916	14/15	0.90	0.08	30,34,42,43	0
6	EDO	B	924	4/4	0.91	0.09	30,38,39,41	0
5	NAG	B	913	14/15	0.91	0.09	29,39,48,52	0
6	EDO	A	923	4/4	0.92	0.08	26,28,31,32	0
5	NAG	B	911	14/15	0.92	0.08	25,30,34,36	0
8	GOL	B	926	6/6	0.92	0.09	20,22,23,29	0
5	NAG	B	914	14/15	0.92	0.08	22,28,30,40	0
6	EDO	A	921	4/4	0.93	0.07	27,30,30,31	0
7	ACT	B	922	4/4	0.93	0.08	16,20,22,29	0
5	NAG	A	914	14/15	0.93	0.08	20,26,34,37	0
5	NAG	B	901	14/15	0.93	0.08	21,24,38,40	0
8	GOL	A	928	6/6	0.95	0.07	19,22,24,24	0
5	NAG	A	917	14/15	0.96	0.06	22,26,28,30	0
9	K	B	929	1/1	0.96	0.09	39,39,39,39	0
5	NAG	A	901	14/15	0.97	0.05	20,22,25,28	0
5	NAG	B	912	14/15	0.97	0.05	20,22,27,27	0
9	K	B	930	1/1	0.97	0.13	37,37,37,37	0
9	K	A	929	1/1	0.98	0.07	28,28,28,28	0
9	K	B	928	1/1	0.99	0.06	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.