



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 05:11 PM BST

PDB ID : 6GSZ
Title : Crystal structure of native alfa-L-rhamnosidase from *Aspergillus terreus*
Authors : Pachl, P.; Rezacova, P.; Skerlova, J.
Deposited on : 2018-06-15
Resolution : 1.38 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 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)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

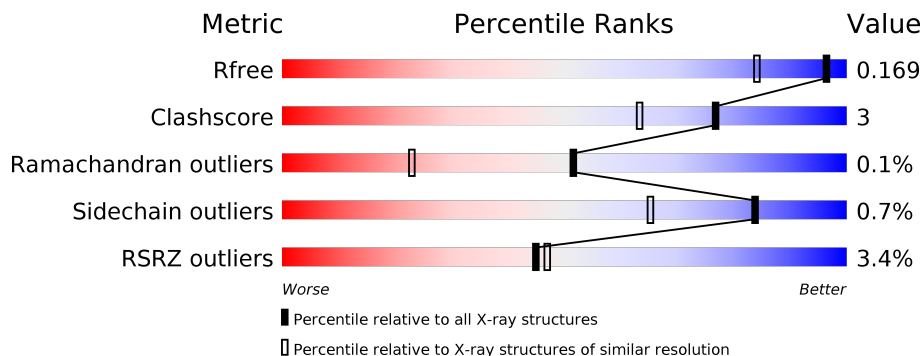
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.38 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}	130704	2907 (1.40-1.36)
Clashscore	141614	3037 (1.40-1.36)
Ramachandran outliers	138981	2970 (1.40-1.36)
Sidechain outliers	138945	2969 (1.40-1.36)
RSRZ outliers	127900	2846 (1.40-1.36)

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 $\leq 5\%$. 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	870	 3% 94% 5%
2	B	4	 100%
3	C	7	 43% 57%
4	D	5	 40% 60%
5	E	2	 50% 50%
6	F	6	 33% 50% 17%

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
15	ACT	A	962[A]	-	-	X	-
15	ACT	A	962[B]	-	-	X	-
15	ACT	A	965	-	-	X	-

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 8788 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 Alpha-L-rhamnosidase.

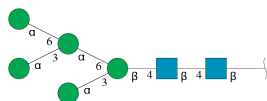
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	863	6963	4423	1189	1335	16	0	34	0

- Molecule 2 is an oligosaccharide called 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.



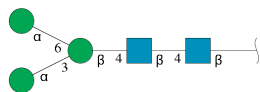
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	4	50	28	2	20	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[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
			Total	C	N	O			
3	C	7	83	46	2	35	0	0	0

- Molecule 4 is an oligosaccharide called 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.



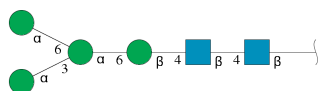
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	5	61	34	2	25	0	0	0

- Molecule 5 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
			Total	C	N	O			
5	E	2	28	16	2	10	0	0	0

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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			
6	F	6	72	40	2	30	0	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

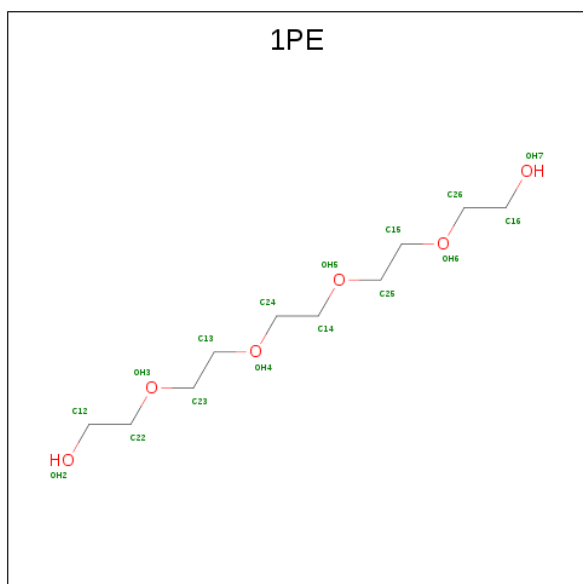


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
7	A	1	Total	C	N	O	0	1
			28	16	2	10		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

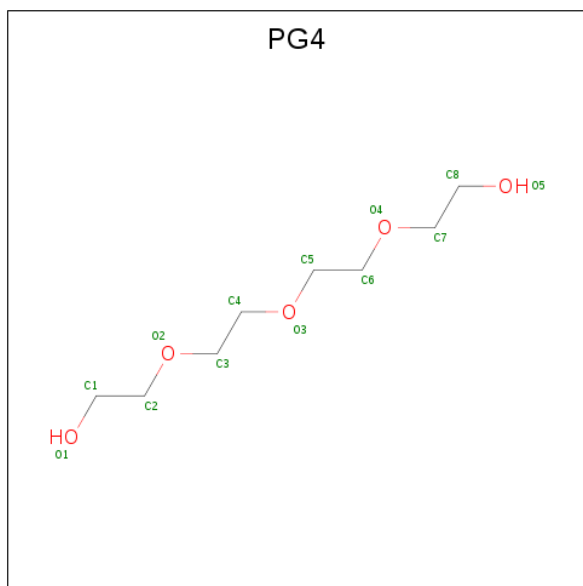
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	21	Total	Ca	0	0
			21	21		

- Molecule 9 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



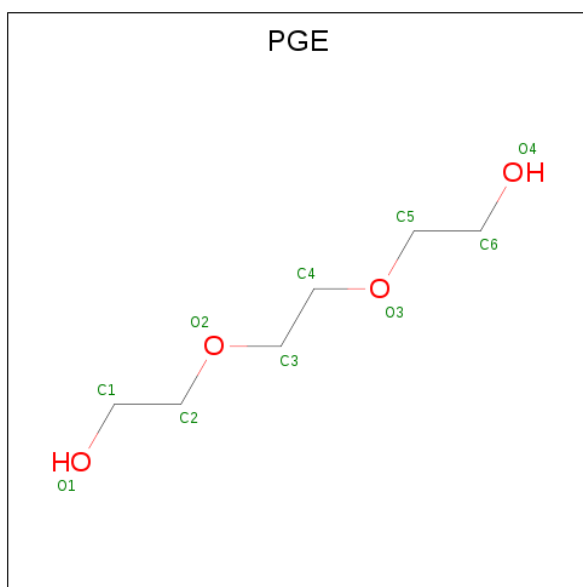
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			16	10	6		
9	A	1	Total	C	O	0	0
			15	10	5		
9	A	1	Total	C	O	0	1
			16	10	6		

- Molecule 10 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



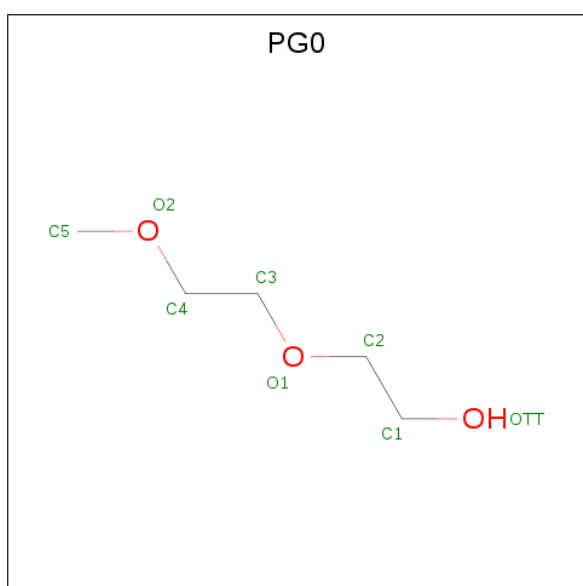
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 11 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



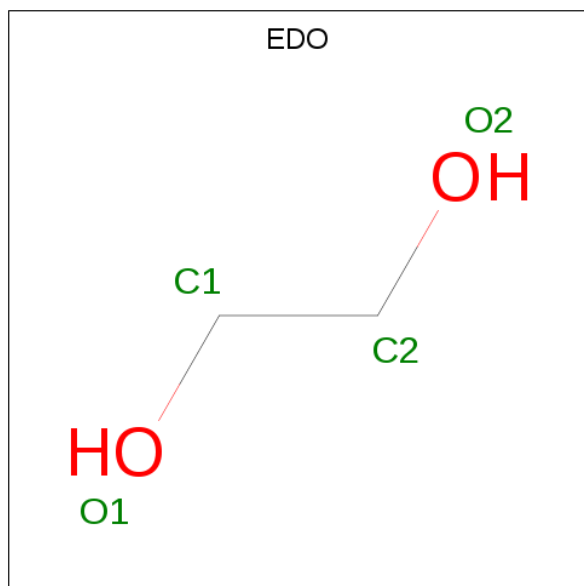
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			9	6	3		
11	A	1	Total	C	O	0	0
			9	6	3		
11	A	1	Total	C	O	0	0
			10	6	4		
11	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 12 is 2-(2-METHOXYETHOXY)ETHANOL (three-letter code: PG0) (formula: $C_5H_{12}O_3$).



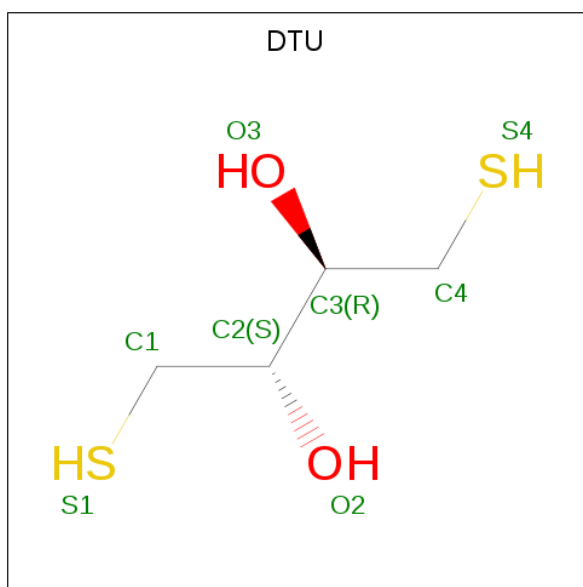
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			7	4	3		
12	A	1	Total	C	O	0	0
			8	5	3		
12	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 13 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



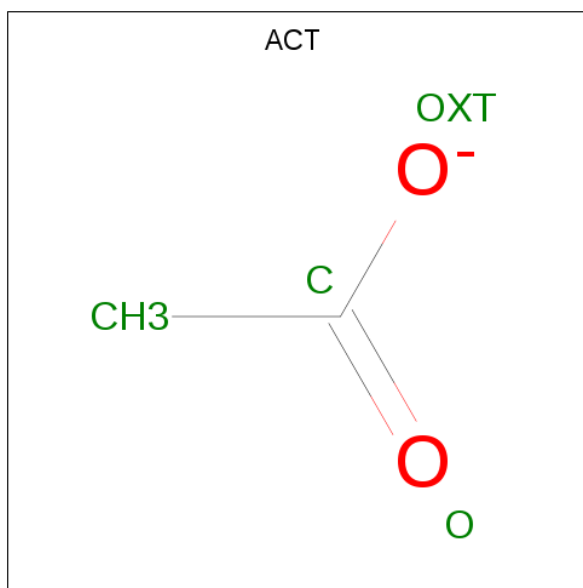
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 14 is (2R,3S)-1,4-DIMERCAPTOBUTANE-2,3-DIOL (three-letter code: DTU) (formula: C₄H₁₀O₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	O			S
14	A	1	16	8	4	4	0	1

- Molecule 15 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



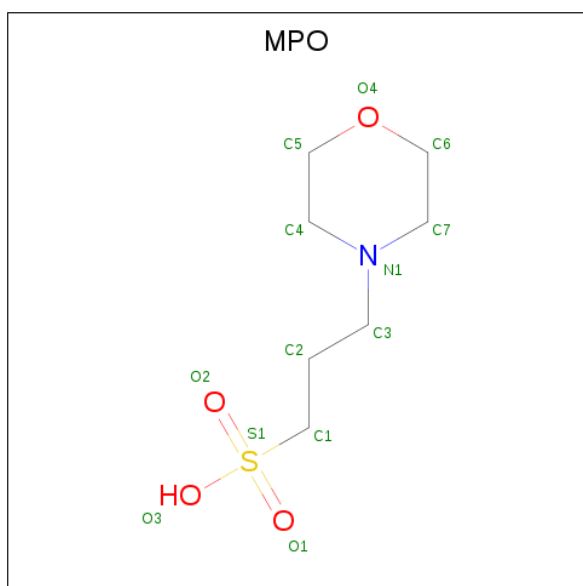
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
15	A	1	4	2	2	0	0
15	A	1	8	4	4	0	1
15	A	1	4	2	2	0	0

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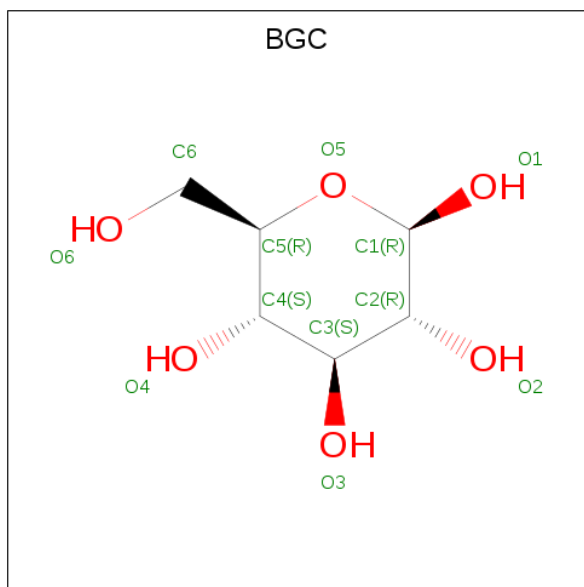
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	A	1	Total	C	O	0	0
			4	2	2		
15	A	1	Total	C	O	0	0
			4	2	2		
15	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 16 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO) (formula: $C_7H_{15}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	A	1	Total	C	N	O	S	0	1
			13	7	1	4	1		

- Molecule 17 is beta-D-glucopyranose (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total C O 12 6 6	0	1

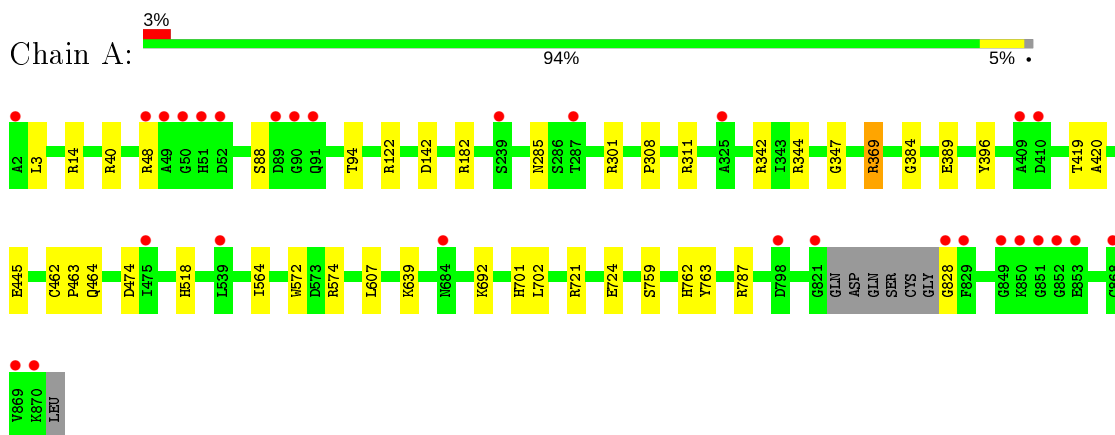
- Molecule 18 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1254	Total O 1275 1275	0	41

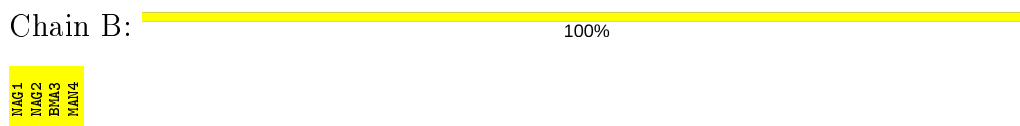
3 Residue-property plots [i](#)

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.

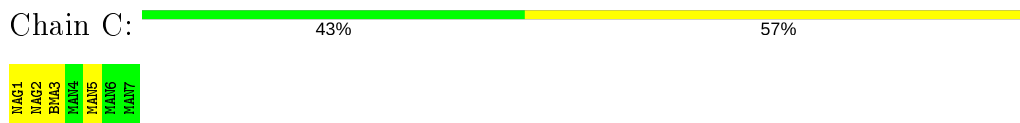
- Molecule 1: Alpha-L-rhamnosidase



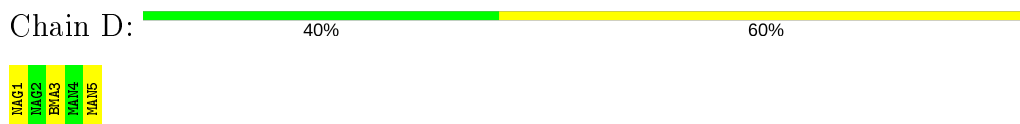
- Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- Molecule 4: 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 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  50% 50%

MAG1
MAG2

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

Chain F:  33% 50% 17%

MAG1
MAG2
MAN3
MAN4
MAN5
MAN6

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.26Å 106.25Å 119.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.82 – 1.38 45.78 – 1.38	Depositor EDS
% Data completeness (in resolution range)	90.9 (45.82-1.38) 90.9 (45.78-1.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 1.38Å)	Xtrriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.134 , 0.168 0.138 , 0.169	Depositor DCC
R_{free} test set	10709 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	13.3	Xtrriage
Anisotropy	0.474	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	8788	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, NAG, MPO, CA, EDO, 1PE, PG4, PGE, BMA, PG0, ACT, DTU, 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	0.62	0/7261	0.81	4/9886 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	396	TYR	CB-CG-CD1	7.51	125.50	121.00
1	A	787	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	369	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	A	182	ARG	NE-CZ-NH2	-5.09	117.75	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	48	ARG	Sidechain
1	A	721	ARG	Sidechain

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	6963	0	6683	33	0
2	B	50	0	43	0	0
3	C	83	0	68	0	0
4	D	61	0	51	0	0
5	E	28	0	25	0	0
6	F	72	0	61	2	0
7	A	42	0	39	1	0
8	A	21	0	0	0	0
9	A	47	0	63	2	0
10	A	13	0	18	0	0
11	A	38	0	50	1	0
12	A	22	0	29	2	0
13	A	4	0	6	1	0
14	A	16	0	18	5	0
15	A	28	0	21	11	0
16	A	13	0	14	1	0
17	A	12	0	11	1	0
18	A	1275	0	0	12	0
All	All	8788	0	7200	44	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.

The worst 5 of 44 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:344[B]:ARG:HG2	1:A:389[B]:GLU:HG2	1.57	0.86
17:A:968[A]:BGC:H1	18:A:1168:HOH:O	1.79	0.81
1:A:14:ARG:HB2	15:A:962[A]:ACT:H3	1.64	0.77
18:A:1002:HOH:O	6:F:6:MAN:O6	2.04	0.75
1:A:308:PRO:HD2	13:A:958:EDO:O2	1.93	0.69

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	893/870 (103%)	875 (98%)	17 (2%)	1 (0%)	51 23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	463	PRO

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	756/734 (103%)	751 (99%)	5 (1%)	84 65

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	301	ARG
1	A	464	GLN
1	A	474	ASP
1	A	759	SER
1	A	763	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS

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](#)

24 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	0.67	0	17,19,21	1.13	1 (5%)
2	NAG	B	2	2	14,14,15	0.59	0	17,19,21	1.59	4 (23%)
2	BMA	B	3	2	11,11,12	0.48	0	15,15,17	1.07	1 (6%)
2	MAN	B	4	2	11,11,12	0.50	0	15,15,17	1.57	3 (20%)
3	NAG	C	1	1,3	14,14,15	0.91	1 (7%)	17,19,21	0.68	0
3	NAG	C	2	8,3	14,14,15	0.74	0	17,19,21	1.51	5 (29%)
3	BMA	C	3	3	11,11,12	0.44	0	15,15,17	0.91	1 (6%)
3	MAN	C	4	3	11,11,12	0.53	0	15,15,17	0.64	0
3	MAN	C	5	8,3	11,11,12	1.37	2 (18%)	15,15,17	1.68	4 (26%)
3	MAN	C	6	3	11,11,12	0.47	0	15,15,17	0.79	0
3	MAN	C	7	3	11,11,12	0.32	0	15,15,17	0.78	0
4	NAG	D	1	1,4	14,14,15	1.39	2 (14%)	17,19,21	0.96	1 (5%)
4	NAG	D	2	4	14,14,15	0.62	0	17,19,21	0.75	0
4	BMA	D	3	4	11,11,12	0.90	1 (9%)	15,15,17	1.34	1 (6%)
4	MAN	D	4	8,4	11,11,12	0.52	0	15,15,17	1.19	0
4	MAN	D	5	4	11,11,12	1.41	2 (18%)	15,15,17	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	E	1	1,5	14,14,15	0.69	0	17,19,21	1.80	5 (29%)
5	NAG	E	2	5	14,14,15	0.41	0	17,19,21	0.99	0
6	NAG	F	1	1,6	14,14,15	0.63	1 (7%)	17,19,21	1.38	4 (23%)
6	NAG	F	2	8,6	14,14,15	0.60	0	17,19,21	1.01	1 (5%)
6	BMA	F	3	6	11,11,12	1.03	2 (18%)	15,15,17	1.53	3 (20%)
6	MAN	F	4	6	11,11,12	0.60	0	15,15,17	1.11	0
6	MAN	F	5	6	11,11,12	0.84	0	15,15,17	0.72	0
6	MAN	F	6	6	11,11,12	1.01	1 (9%)	15,15,17	1.03	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
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
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	8,3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	MAN	C	5	8,3	-	0/2/19/22	0/1/1/1
3	MAN	C	6	3	-	0/2/19/22	0/1/1/1
3	MAN	C	7	3	-	2/2/19/22	0/1/1/1
4	NAG	D	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	8,4	-	2/2/19/22	0/1/1/1
4	MAN	D	5	4	-	1/2/19/22	0/1/1/1
5	NAG	E	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
6	NAG	F	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	F	2	8,6	-	0/6/23/26	0/1/1/1
6	BMA	F	3	6	-	0/2/19/22	0/1/1/1
6	MAN	F	4	6	-	0/2/19/22	0/1/1/1
6	MAN	F	5	6	-	0/2/19/22	0/1/1/1
6	MAN	F	6	6	-	0/2/19/22	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	NAG	O5-C1	-3.44	1.38	1.43
4	D	1	NAG	C1-C2	2.99	1.56	1.52
3	C	5	MAN	O2-C2	2.97	1.49	1.43
4	D	5	MAN	O4-C4	2.94	1.49	1.43
6	F	6	MAN	O4-C4	2.71	1.49	1.43

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	MAN	O5-C5-C6	4.14	113.69	107.20
4	D	3	BMA	C1-O5-C5	3.93	117.52	112.19
2	B	2	NAG	C1-O5-C5	3.34	116.71	112.19
2	B	2	NAG	C4-C3-C2	3.25	115.78	111.02
2	B	1	NAG	O5-C1-C2	-3.22	106.20	111.29

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

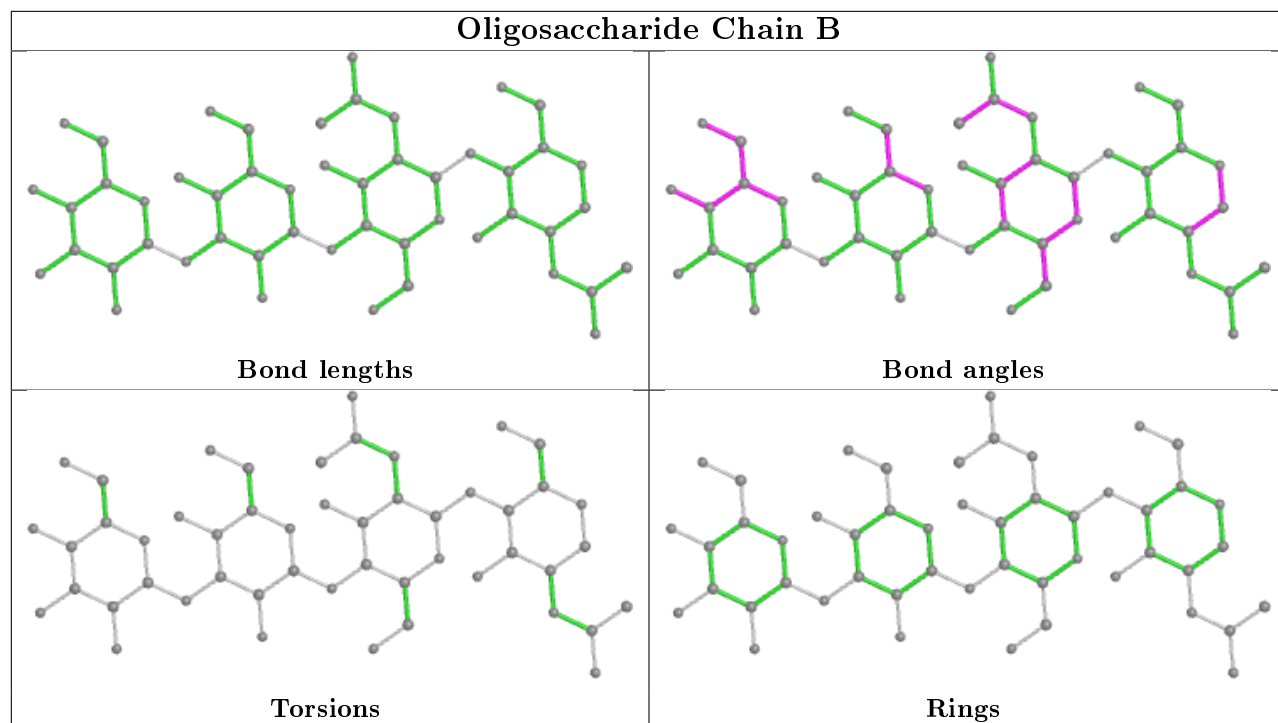
Mol	Chain	Res	Type	Atoms
3	C	7	MAN	O5-C5-C6-O6
4	D	4	MAN	C4-C5-C6-O6
3	C	7	MAN	C4-C5-C6-O6
4	D	4	MAN	O5-C5-C6-O6
5	E	1	NAG	C3-C2-N2-C7

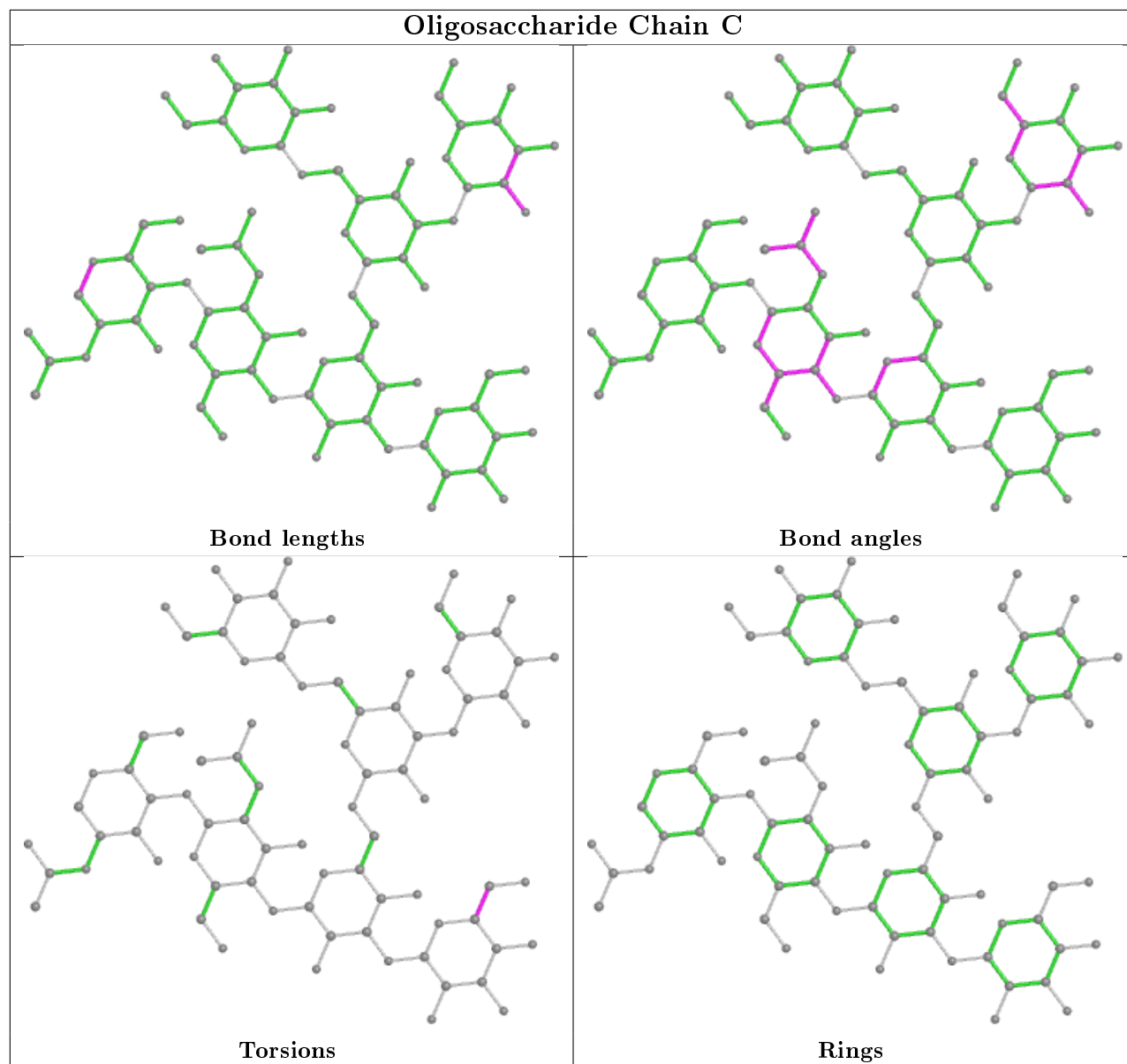
There are no ring outliers.

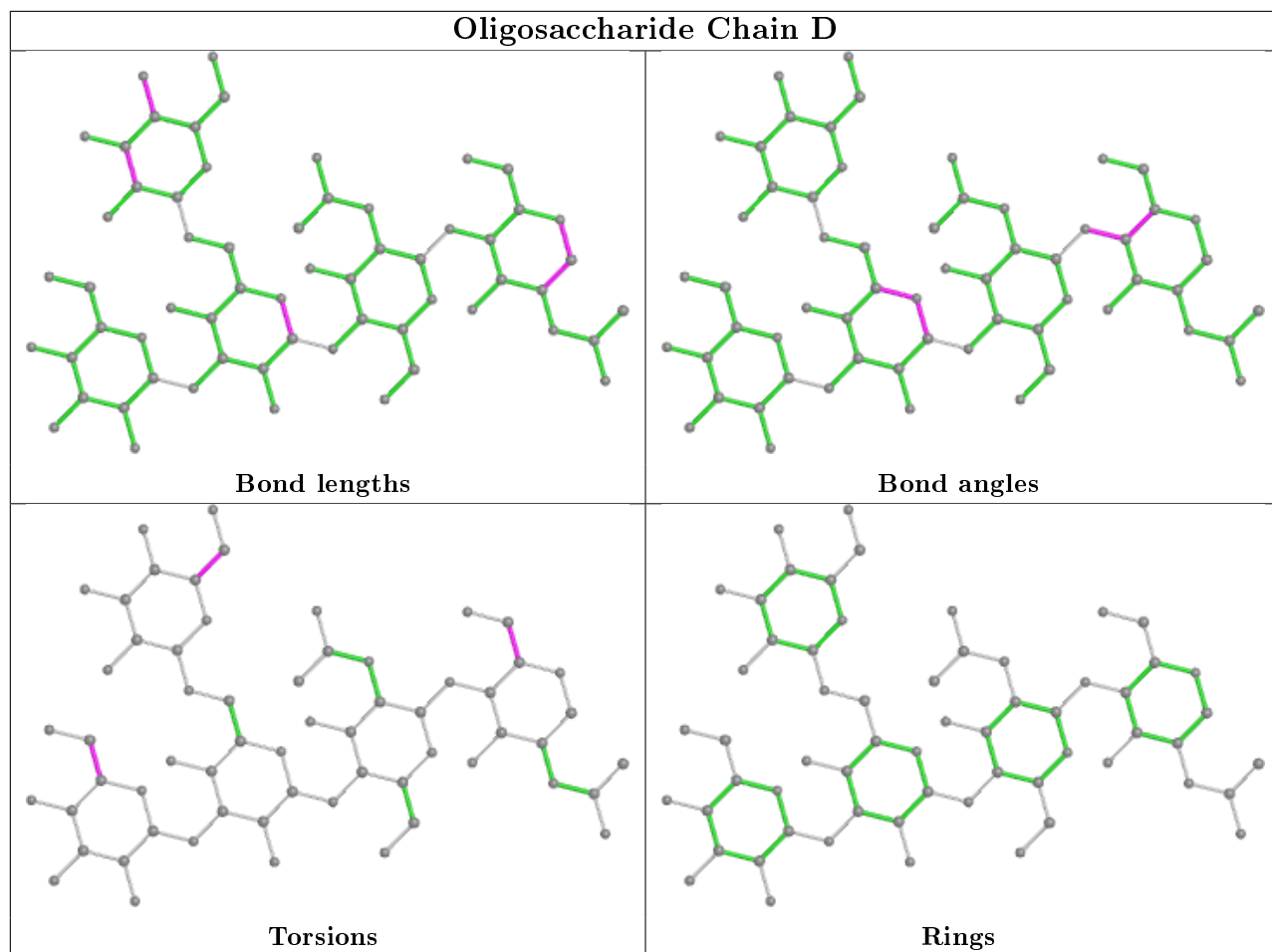
1 monomer is involved in 2 short contacts:

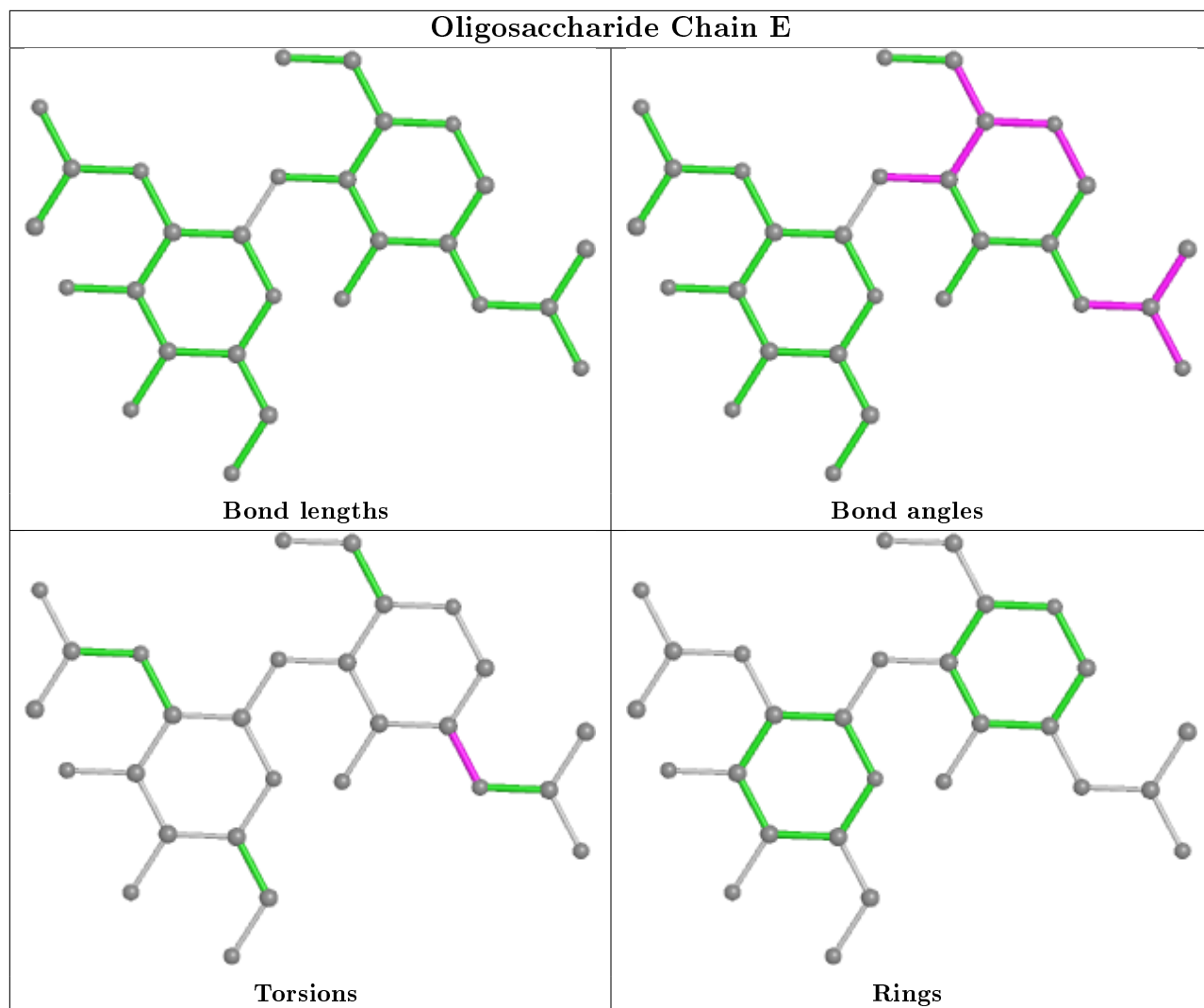
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	6	MAN	2	0

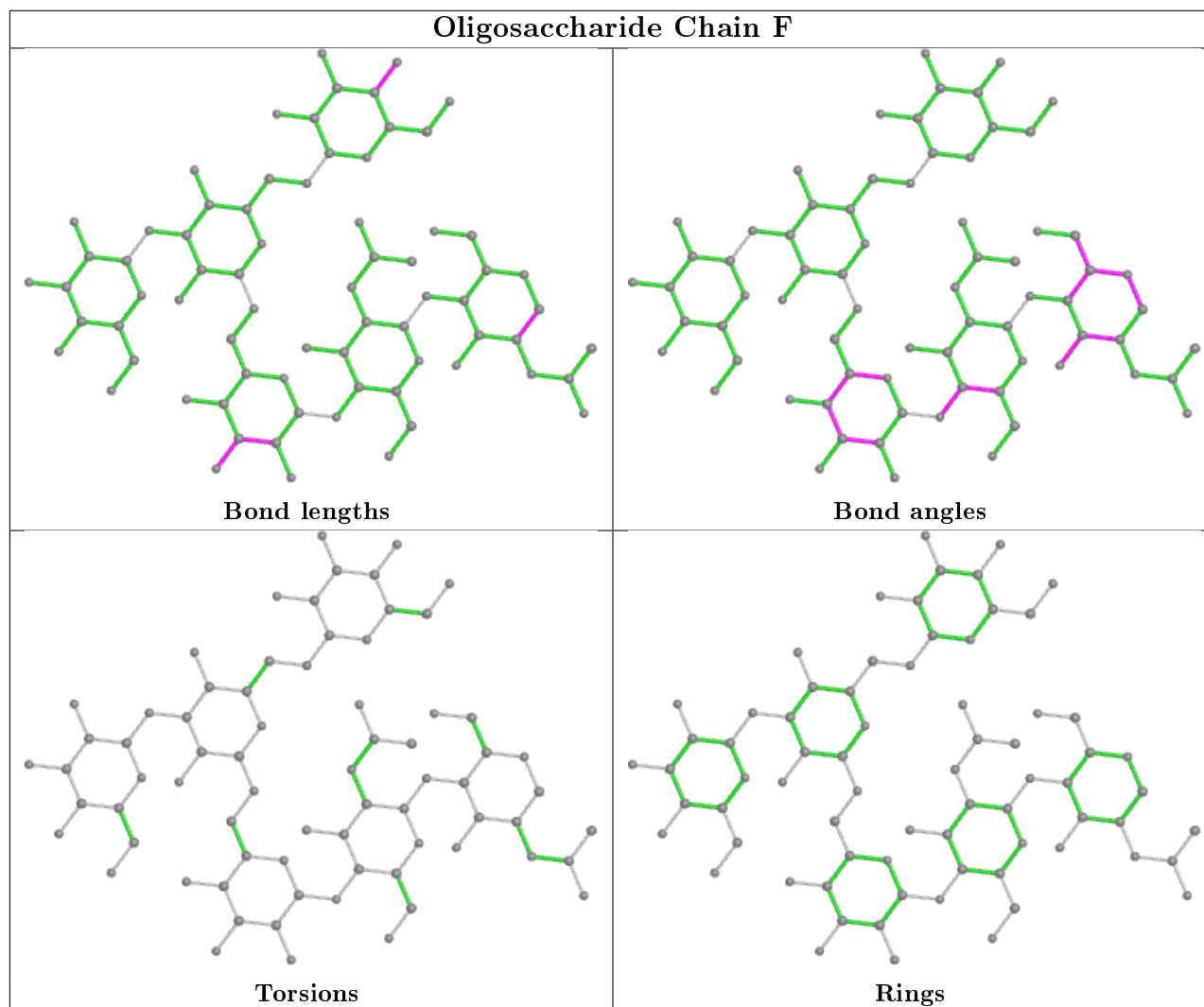
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 47 ligands modelled in this entry, 21 are monoatomic - leaving 26 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	$\# Z > 2$
14	DTU	A	960[B]	1	7,7,7	0.99	0	4,8,8	2.03	1 (25%)
12	PG0	A	952	-	7,7,7	0.36	0	6,6,6	0.57	0
9	1PE	A	948	-	15,15,15	0.64	0	14,14,14	0.92	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	1PE	A	955[A]	-	15,15,15	0.54	0	14,14,14	0.77	0
11	PGE	A	950	-	8,8,9	0.61	0	7,7,8	0.78	0
15	ACT	A	964	-	1,3,3	2.62	1 (100%)	0,3,3	0.00	-
15	ACT	A	966	-	1,3,3	2.06	1 (100%)	0,3,3	0.00	-
11	PGE	A	956	-	9,9,9	0.81	0	8,8,8	1.11	0
15	ACT	A	961	-	1,3,3	1.18	0	0,3,3	0.00	-
17	BGC	A	968[A]	-	12,12,12	1.68	2 (16%)	17,17,17	2.65	10 (58%)
13	EDO	A	958	-	3,3,3	1.13	0	2,2,2	0.30	0
15	ACT	A	962[A]	-	1,3,3	0.39	0	0,3,3	0.00	-
10	PG4	A	949	-	12,12,12	0.64	0	11,11,11	1.11	1 (9%)
15	ACT	A	962[B]	-	1,3,3	0.63	0	0,3,3	0.00	-
15	ACT	A	963	-	1,3,3	2.07	1 (100%)	0,3,3	0.00	-
15	ACT	A	965	-	1,3,3	2.29	1 (100%)	0,3,3	0.00	-
12	PG0	A	957	8	6,6,7	0.84	0	5,5,6	0.70	0
9	1PE	A	954	-	14,14,15	0.62	0	13,13,14	0.94	1 (7%)
7	NAG	A	920	1	14,14,15	0.62	0	17,19,21	1.03	2 (11%)
7	NAG	A	917[B]	1	14,14,15	1.14	2 (14%)	17,19,21	2.39	5 (29%)
16	MPO	A	967[A]	-	13,13,13	2.24	2 (15%)	17,17,17	1.73	2 (11%)
7	NAG	A	917[A]	1	14,14,15	1.52	4 (28%)	17,19,21	1.85	6 (35%)
12	PG0	A	951	-	6,6,7	0.44	0	5,5,6	0.70	0
11	PGE	A	959	-	9,9,9	0.45	0	8,8,8	1.00	0
11	PGE	A	953	-	8,8,9	0.40	0	7,7,8	0.60	0
14	DTU	A	960[A]	1	7,7,7	0.96	0	4,8,8	1.12	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
14	DTU	A	960[B]	1	-	4/8/8/8	-
9	1PE	A	948	-	-	2/13/13/13	-
9	1PE	A	954	-	-	4/12/12/13	-
7	NAG	A	920	1	-	0/6/23/26	0/1/1/1
7	NAG	A	917[B]	1	-	2/6/23/26	0/1/1/1
16	MPO	A	967[A]	-	-	0/7/15/15	0/1/1/1
7	NAG	A	917[A]	1	-	0/6/23/26	0/1/1/1
12	PG0	A	952	-	-	2/5/5/5	-
12	PG0	A	951	-	-	2/4/4/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	PGE	A	950	-	-	2/6/6/7	-
11	PGE	A	956	-	-	3/7/7/7	-
10	PG4	A	949	-	-	3/10/10/10	-
11	PGE	A	953	-	-	2/6/6/7	-
17	BGC	A	968[A]	-	-	0/2/22/22	0/1/1/1
13	EDO	A	958	-	-	1/1/1/1	-
9	1PE	A	955[A]	-	-	3/13/13/13	-
14	DTU	A	960[A]	1	-	5/8/8/8	-
12	PG0	A	957	8	-	1/4/4/5	-
11	PGE	A	959	-	-	3/7/7/7	-

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	967[A]	MPO	O2-S1	5.93	1.62	1.45
16	A	967[A]	MPO	C1-S1	-4.71	1.70	1.77
17	A	968[A]	BGC	O3-C3	-4.18	1.33	1.43
7	A	917[A]	NAG	C1-C2	3.69	1.57	1.52
17	A	968[A]	BGC	C4-C5	-3.56	1.45	1.53

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	917[B]	NAG	C1-O5-C5	-7.59	101.91	112.19
16	A	967[A]	MPO	O3-S1-C1	6.09	115.61	105.77
17	A	968[A]	BGC	O2-C2-C1	-4.72	98.21	109.16
7	A	917[A]	NAG	O3-C3-C4	-4.05	100.98	110.35
17	A	968[A]	BGC	O3-C3-C4	-3.70	101.80	110.35

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	960[B]	DTU	S1-C1-C2-O2
14	A	960[B]	DTU	S1-C1-C2-C3
14	A	960[B]	DTU	C2-C3-C4-S4
14	A	960[B]	DTU	O3-C3-C4-S4
14	A	960[A]	DTU	S1-C1-C2-C3

There are no ring outliers.

12 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	960[B]	DTU	3	0
9	A	955[A]	1PE	2	0
11	A	956	PGE	1	0
17	A	968[A]	BGC	1	0
13	A	958	EDO	1	0
15	A	962[A]	ACT	6	0
15	A	962[B]	ACT	3	0
15	A	965	ACT	2	0
12	A	957	PG0	2	0
7	A	917[B]	NAG	1	0
16	A	967[A]	MPO	1	0
14	A	960[A]	DTU	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	863/870 (99%)	-0.06	29 (3%) 45 47	10, 15, 31, 70	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	50	GLY	7.3
1	A	829	PHE	7.2
1	A	868	CYS	6.7
1	A	49	ALA	5.8
1	A	828	GLY	5.5

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.

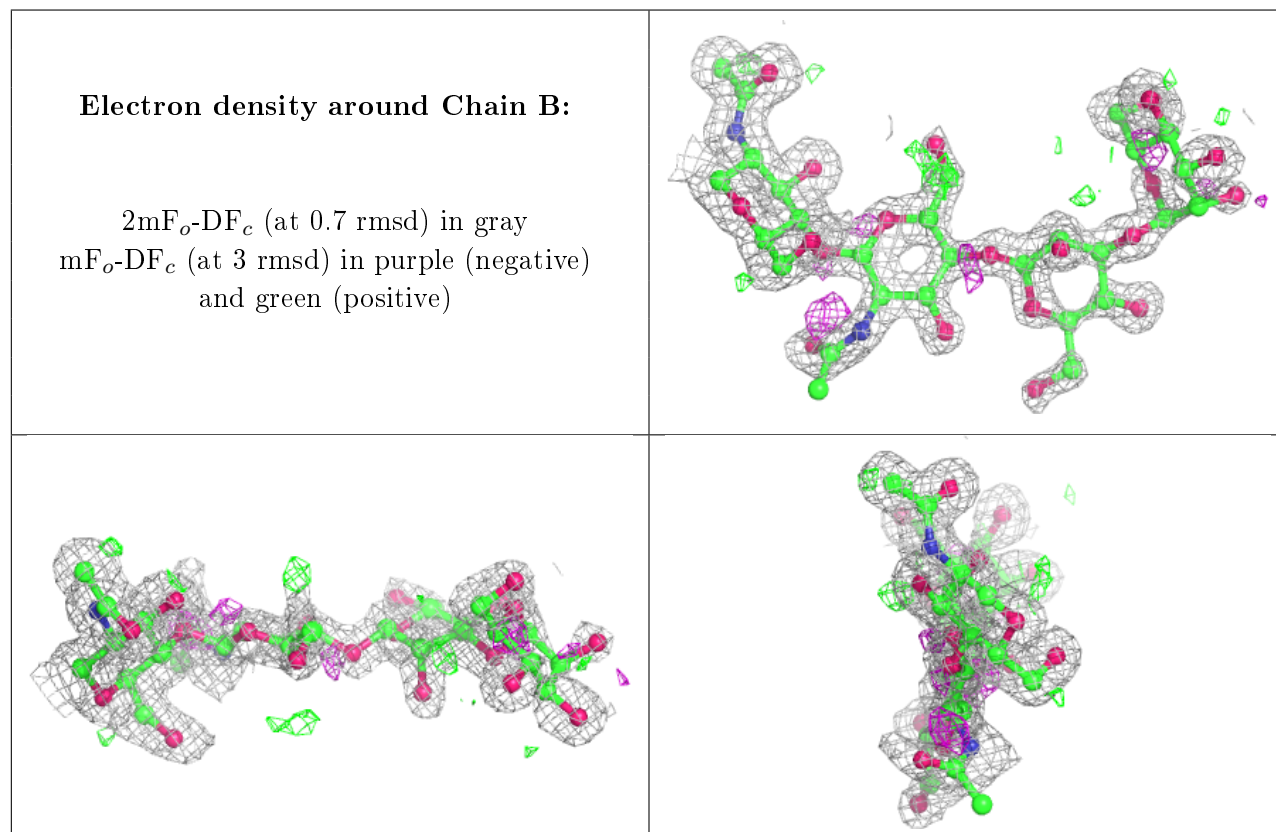
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAN	D	5	11/12	0.45	0.36	43,46,54,55	0
3	MAN	C	7	11/12	0.58	0.28	43,46,48,59	11
6	MAN	F	6	11/12	0.66	0.24	23,26,29,30	11
2	MAN	B	4	11/12	0.69	0.25	21,31,33,33	11
3	MAN	C	5	11/12	0.72	0.17	35,40,47,53	11
6	BMA	F	3	11/12	0.73	0.28	27,30,35,37	11
3	MAN	C	6	11/12	0.78	0.15	28,30,33,39	11

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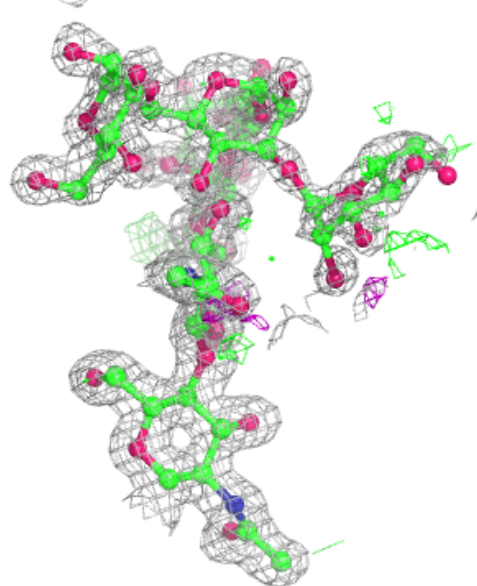
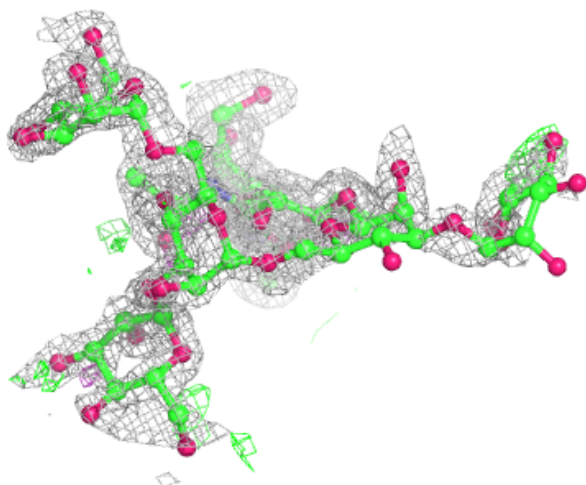
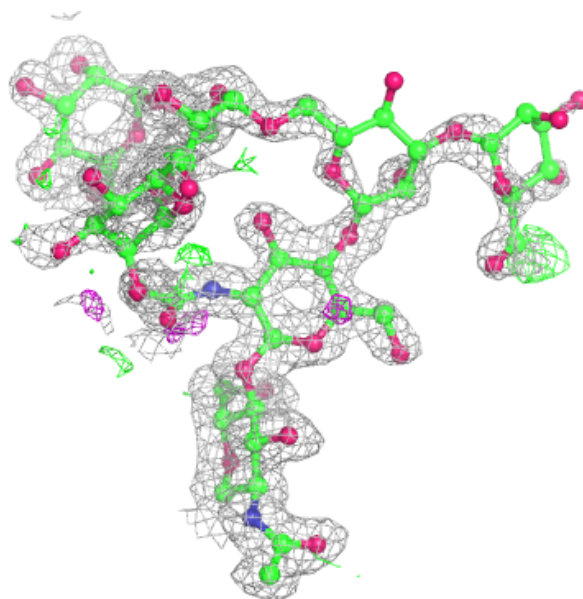
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MAN	F	5	11/12	0.78	0.28	19,33,38,38	11
2	BMA	B	3	11/12	0.79	0.20	31,33,40,43	11
6	NAG	F	2	14/15	0.79	0.21	31,36,44,50	14
6	MAN	F	4	11/12	0.83	0.20	25,27,30,30	11
3	MAN	C	4	11/12	0.84	0.13	29,31,33,35	11
4	MAN	D	4	11/12	0.84	0.32	42,47,53,60	0
3	BMA	C	3	11/12	0.86	0.24	35,35,42,47	11
6	NAG	F	1	14/15	0.89	0.28	34,42,61,69	0
3	NAG	C	2	14/15	0.89	0.14	32,39,44,53	0
5	NAG	E	2	14/15	0.90	0.21	36,46,57,67	14
2	NAG	B	2	14/15	0.93	0.29	31,40,57,60	0
4	BMA	D	3	11/12	0.94	0.17	26,33,41,49	0
2	NAG	B	1	14/15	0.94	0.10	17,21,27,31	0
3	NAG	C	1	14/15	0.94	0.06	18,25,30,32	0
5	NAG	E	1	14/15	0.95	0.14	24,32,38,39	0
4	NAG	D	2	14/15	0.96	0.05	15,18,25,30	0
4	NAG	D	1	14/15	0.98	0.05	14,16,20,23	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.



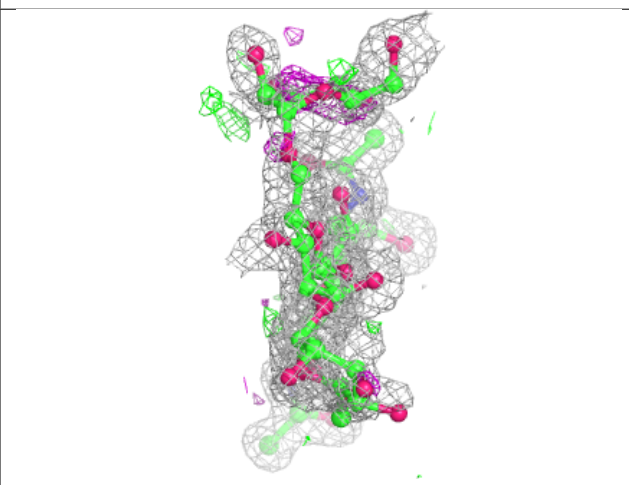
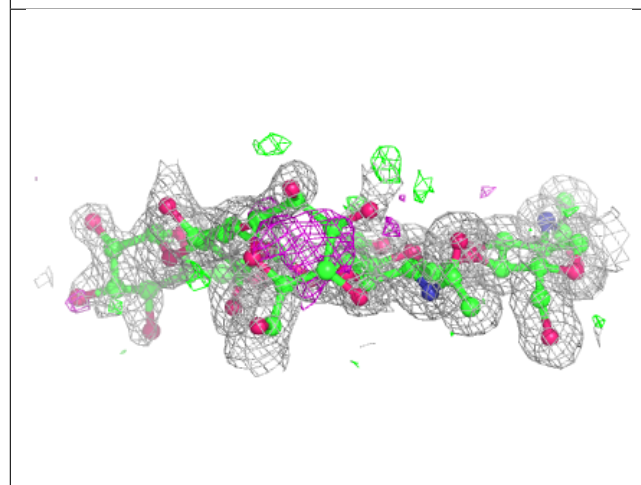
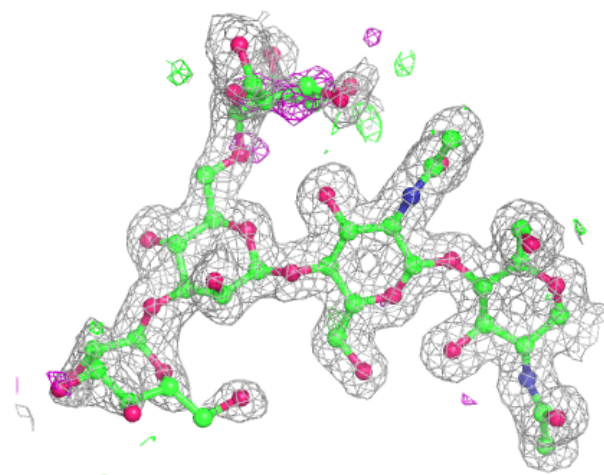
Electron density around Chain C:

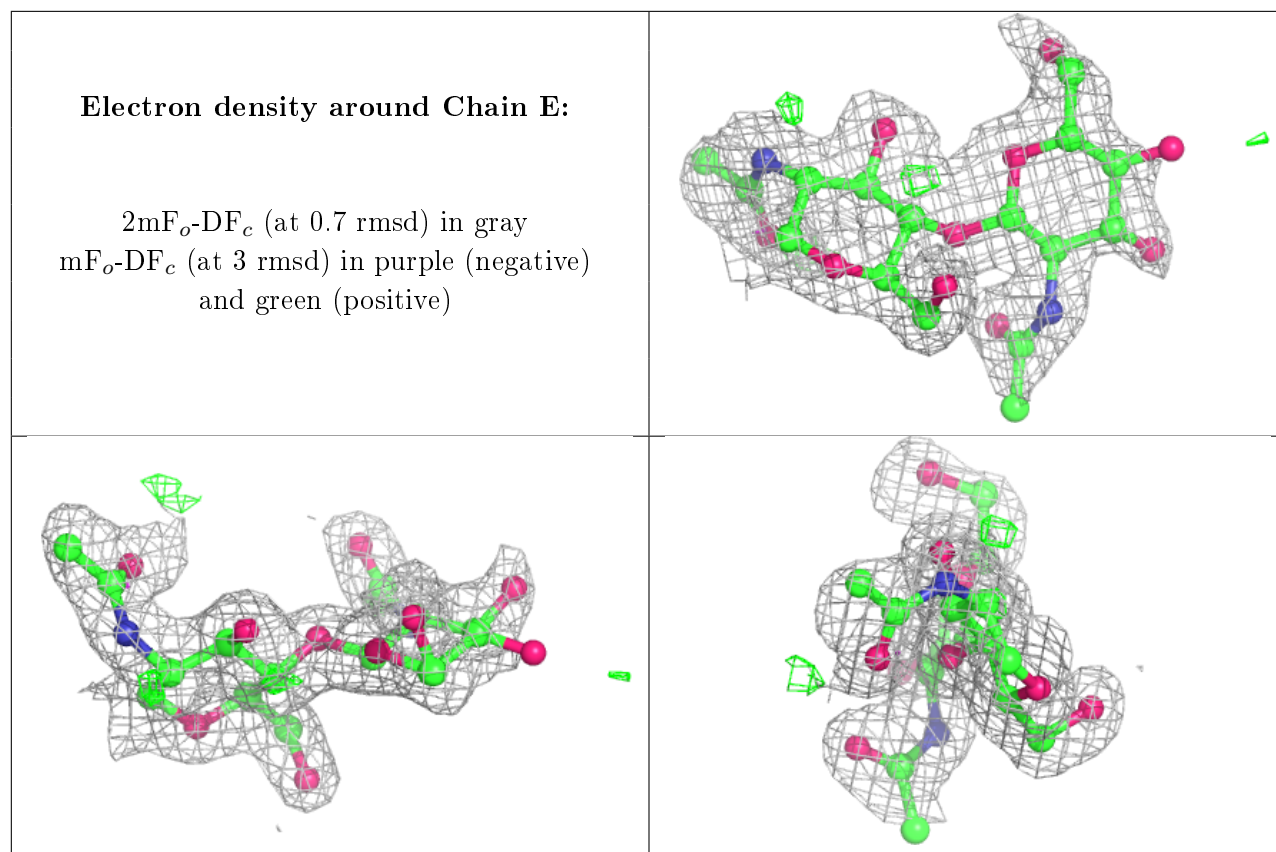
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

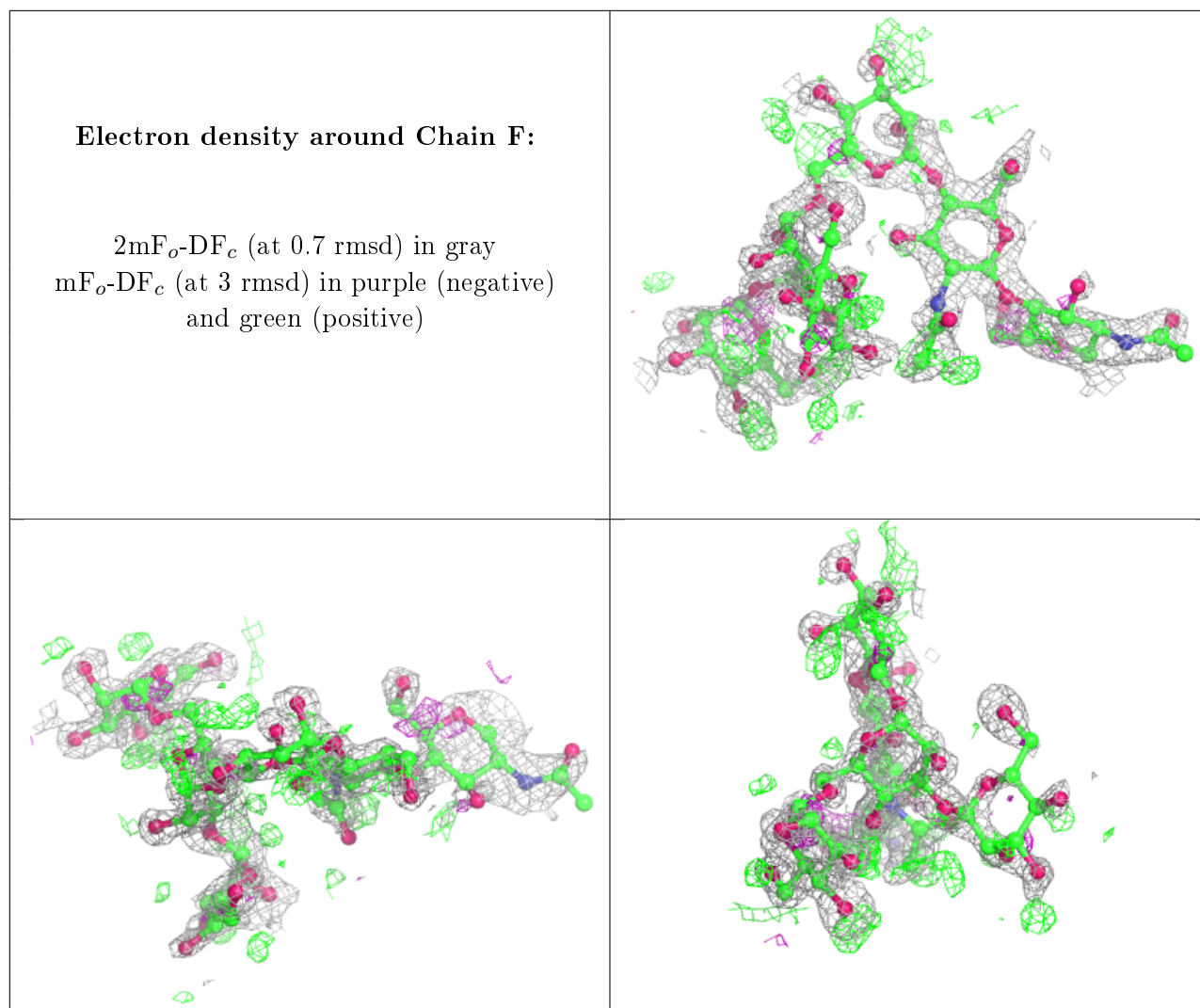


Electron density around Chain D:

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







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
14	DTU	A	960[B]	8/8	0.65	0.36	49,54,68,88	8
14	DTU	A	960[A]	8/8	0.65	0.36	45,47,51,57	8
8	CA	A	936	1/1	0.70	0.27	46,46,46,46	1
7	NAG	A	917[A]	14/15	0.74	0.26	15,25,44,45	14
11	PGE	A	959	10/10	0.74	0.25	33,39,43,44	0
7	NAG	A	917[B]	14/15	0.74	0.26	23,33,44,47	14
15	ACT	A	966	4/4	0.81	0.32	34,35,38,39	4
9	1PE	A	954	15/16	0.83	0.19	21,27,41,41	15

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	A	920	14/15	0.83	0.29	36,42,55,55	0
15	ACT	A	963	4/4	0.83	0.26	41,45,53,58	0
15	ACT	A	961	4/4	0.84	0.12	43,49,52,62	0
8	CA	A	941	1/1	0.85	0.42	41,41,41,41	1
12	PG0	A	957	7/8	0.85	0.10	27,32,33,36	0
8	CA	A	937	1/1	0.86	0.20	28,28,28,28	1
9	1PE	A	955[A]	16/16	0.86	0.15	23,32,41,41	16
12	PG0	A	952	8/8	0.87	0.10	41,45,49,50	0
12	PG0	A	951	7/8	0.87	0.17	35,39,45,46	0
13	EDO	A	958	4/4	0.87	0.29	12,13,14,16	4
11	PGE	A	953	9/10	0.88	0.14	39,42,52,53	0
11	PGE	A	956	10/10	0.88	0.12	22,39,51,62	0
15	ACT	A	965	4/4	0.89	0.13	25,27,29,42	0
16	MPO	A	967[A]	13/13	0.89	0.14	19,26,34,44	13
8	CA	A	946	1/1	0.89	0.57	42,42,42,42	1
10	PG4	A	949	13/13	0.90	0.12	21,27,35,37	0
8	CA	A	943	1/1	0.91	0.39	43,43,43,43	1
17	BGC	A	968[A]	12/12	0.91	0.19	14,25,29,37	12
8	CA	A	942	1/1	0.91	0.25	42,42,42,42	1
8	CA	A	931	1/1	0.92	0.25	40,40,40,40	0
9	1PE	A	948	16/16	0.93	0.09	18,24,39,44	0
8	CA	A	933	1/1	0.93	0.27	37,37,37,37	1
15	ACT	A	964	4/4	0.93	0.15	28,37,39,42	0
11	PGE	A	950	9/10	0.94	0.10	24,31,40,47	0
8	CA	A	947	1/1	0.94	0.33	45,45,45,45	1
8	CA	A	935	1/1	0.95	0.18	32,32,32,32	1
15	ACT	A	962[B]	4/4	0.95	0.09	14,17,17,26	4
15	ACT	A	962[A]	4/4	0.95	0.09	15,16,17,24	4
8	CA	A	944	1/1	0.95	0.21	46,46,46,46	1
8	CA	A	938	1/1	0.95	0.17	45,45,45,45	1
8	CA	A	940	1/1	0.96	0.13	37,37,37,37	1
8	CA	A	939	1/1	0.96	0.30	49,49,49,49	1
8	CA	A	932	1/1	0.96	0.10	36,36,36,36	1
8	CA	A	945	1/1	0.97	0.30	45,45,45,45	1
8	CA	A	930	1/1	0.98	0.23	31,31,31,31	1
8	CA	A	934	1/1	0.99	0.21	35,35,35,35	1
8	CA	A	927	1/1	1.00	0.05	13,13,13,13	0
8	CA	A	929	1/1	1.00	0.02	20,20,20,20	1
8	CA	A	928	1/1	1.00	0.07	22,22,22,22	1

6.5 Other polymers

There are no such residues in this entry.