



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 04:21 PM BST

PDB ID : 1T0O
Title : The structure of alpha-galactosidase from *Trichoderma reesei* complexed with beta-D-galactose
Authors : Golubev, A.M.; Nagem, R.A.P.; Brandao Neto, J.R.; Neustroev, K.N.; Eneyskaya, E.V.; Kulminskaya, A.A.; Shabalin, K.A.; Savel'ev, A.N.; Polikarpov, I.
Deposited on : 2004-04-12
Resolution : 1.96 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

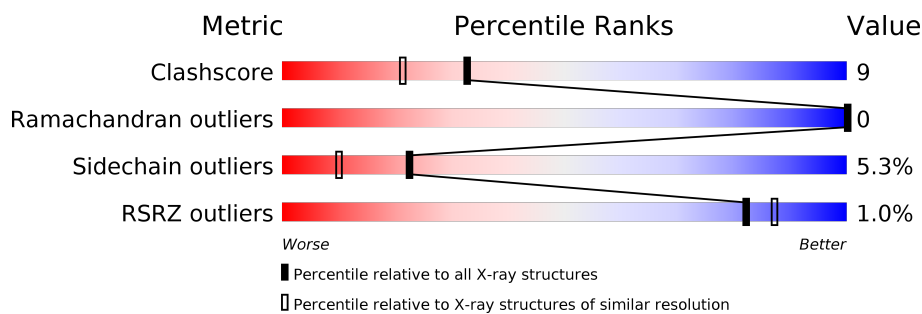
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	417	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 79%, green 19%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 79% 19% </div> </div>
2	B	2	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 50%, orange 50%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 50% 50% </div> </div>
2	E	2	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 50%, orange 50%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 50% 50% </div> </div>
3	C	7	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 100% </div> </div>
4	D	4	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 75%, orange 25%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 75% 25% </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3798 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-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3213	2039	539	618	17			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	LEU	VAL	SEE REMARK 999	GB 1580816
A	70	PRO	VAL	SEE REMARK 999	GB 1580816
A	72	ALA	THR	SEE REMARK 999	GB 1580816
A	88	ALA	ASP	SEE REMARK 999	GB 1580816
A	148	ASN	ALA	SEE REMARK 999	GB 1580816
A	151	PHE	ALA	SEE REMARK 999	GB 1580816
A	153	LYS	GLN	SEE REMARK 999	GB 1580816
A	161	THR	SER	SEE REMARK 999	GB 1580816
A	165	ASP	GLU	SEE REMARK 999	GB 1580816
A	167	THR	ASN	SEE REMARK 999	GB 1580816
A	185	GLY	ASN	SEE REMARK 999	GB 1580816
A	196	HIS	ARG	SEE REMARK 999	GB 1580816
A	202	MET	LEU	SEE REMARK 999	GB 1580816
A	207	GLN	VAL	SEE REMARK 999	GB 1580816
A	216	SER	GLU	SEE REMARK 999	GB 1580816
A	225	ASP	GLY	SEE REMARK 999	GB 1580816
A	230	ASN	GLU	SEE REMARK 999	GB 1580816
A	236	ARG	HIS	SEE REMARK 999	GB 1580816
A	238	LEU	ILE	SEE REMARK 999	GB 1580816
A	240	LEU	MET	SEE REMARK 999	GB 1580816
A	245	LEU	MET	SEE REMARK 999	GB 1580816
A	249	ASP	GLY	SEE REMARK 999	GB 1580816
A	258	MET	ILE	SEE REMARK 999	GB 1580816
A	297	ASN	GLU	SEE REMARK 999	GB 1580816
A	300	ASN	GLU	SEE REMARK 999	GB 1580816
A	327	ILE	VAL	SEE REMARK 999	GB 1580816
A	335	VAL	TYR	SEE REMARK 999	GB 1580816

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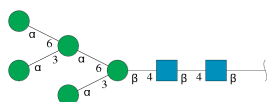
Chain	Residue	Modelled	Actual	Comment	Reference
A	337	TYR	ASN	SEE REMARK 999	GB 1580816
A	341	PHE	TYR	SEE REMARK 999	GB 1580816
A	355	VAL	MET	SEE REMARK 999	GB 1580816
A	360	ILE	HIS	SEE REMARK 999	GB 1580816
A	362	ALA	VAL	SEE REMARK 999	GB 1580816
A	363	THR	ARG	SEE REMARK 999	GB 1580816
A	369	ASN	SER	SEE REMARK 999	GB 1580816
A	378	HIS	ARG	SEE REMARK 999	GB 1580816
A	386	SER	THR	SEE REMARK 999	GB 1580816
A	389	ASP	SER	SEE REMARK 999	GB 1580816
A	398	ALA	THR	SEE REMARK 999	GB 1580816
A	415	GLN	ARG	SEE REMARK 999	GB 1580816
A	416	ARG	ASN	SEE REMARK 999	GB 1580816

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

- 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
3	C	7	Total	C	N	O	0	0	0
			83	46	2	35			

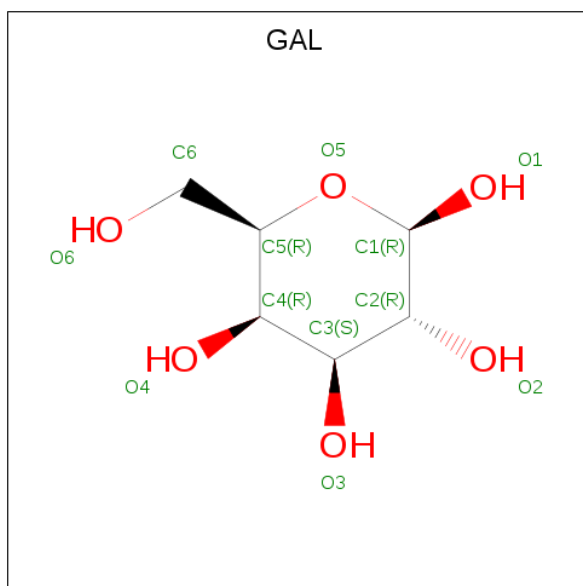
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

pyranose.



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

- Molecule 5 is beta-D-galactopyranose (three-letter code: GAL) (formula: C₆H₁₂O₆).



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

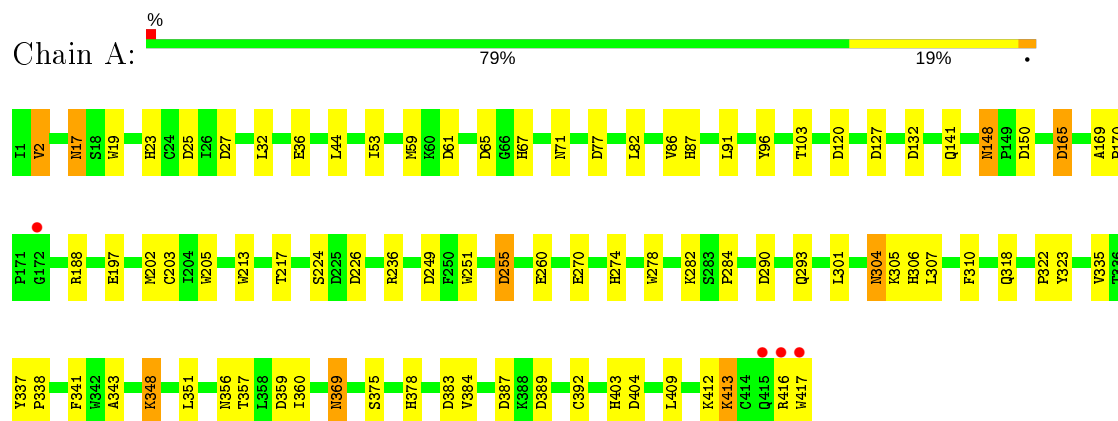
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	384	Total	O	0	0
			384	384		

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-galactosidase



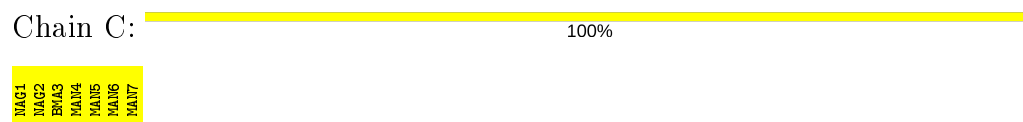
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

Chain D:



MAN1
MAN2
MAN3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.83Å 58.31Å 153.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	9.00 – 1.96 9.86 – 1.96	Depositor EDS
% Data completeness (in resolution range)	72.3 (9.00-1.96) 70.4 (9.86-1.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.65 (at 1.96Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.151 , 0.205 0.158 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtriage
Anisotropy	0.554	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.078 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3798	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.30% 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, GAL, BMA, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/3304	0.85	10/4512 (0.2%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	ASP	CB-CG-OD2	7.51	125.06	118.30
1	A	61	ASP	CB-CG-OD2	6.24	123.92	118.30
1	A	77	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	255	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	404	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	65	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	25	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	359	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	389	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	383	ASP	CB-CG-OD2	5.07	122.86	118.30

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	3213	0	3045	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	28	0	25	0	0
2	E	28	0	25	1	0
3	C	83	0	70	2	0
4	D	50	0	43	1	0
5	A	12	0	12	1	0
6	A	384	0	0	11	0
All	All	3798	0	3220	58	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 9.

All (58) 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:306:HIS:HD2	6:A:1060:HOH:O	1.56	0.87
1:A:260:GLU:H	1:A:274:HIS:HE1	1.24	0.85
1:A:270:GLU:OE2	1:A:403:HIS:HD2	1.62	0.81
1:A:87:HIS:HE1	1:A:127:ASP:OD2	1.65	0.79
1:A:165:ASP:HB2	6:A:945:HOH:O	1.84	0.77
1:A:17:ASN:ND2	1:A:19:TRP:H	1.85	0.74
1:A:67:HIS:HD2	1:A:120:ASP:OD2	1.72	0.73
1:A:260:GLU:H	1:A:274:HIS:CE1	2.09	0.69
1:A:226:ASP:OD1	5:A:901:GAL:O2	2.09	0.68
1:A:23:HIS:HD2	6:A:1032:HOH:O	1.77	0.68
1:A:2:VAL:HG23	6:A:1156:HOH:O	1.95	0.67
1:A:403:HIS:HE1	6:A:994:HOH:O	1.81	0.62
1:A:132:ASP:HA	1:A:203:CYS:HB3	1.80	0.61
1:A:348:LYS:HG2	6:A:1060:HOH:O	2.02	0.60
1:A:304:ASN:HD22	1:A:307:LEU:H	1.51	0.58
1:A:306:HIS:HE1	1:A:387:ASP:OD2	1.87	0.58
1:A:23:HIS:HE1	6:A:1014:HOH:O	1.85	0.58
1:A:2:VAL:HG22	4:D:1:NAG:H62	1.86	0.57
1:A:2:VAL:HG13	1:A:251:TRP:CE2	2.40	0.56
1:A:290:ASP:OD2	1:A:293:GLN:NE2	2.38	0.56
1:A:378:HIS:HB3	1:A:392:CYS:SG	2.46	0.56
1:A:17:ASN:HD22	1:A:19:TRP:H	1.53	0.55
1:A:67:HIS:CD2	1:A:120:ASP:OD2	2.57	0.55
1:A:369:ASN:HD22	1:A:369:ASN:N	2.08	0.52
6:A:1282:HOH:O	3:C:6:MAN:H62	2.10	0.52
1:A:2:VAL:HG13	1:A:251:TRP:NE1	2.24	0.51
1:A:338:PRO:HD2	1:A:357:THR:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LEU:HD13	1:A:91:LEU:HD23	1.94	0.49
1:A:87:HIS:CE1	1:A:127:ASP:OD2	2.56	0.49
1:A:53:ILE:HD11	1:A:82:LEU:HD23	1.94	0.49
1:A:87:HIS:HD2	6:A:1133:HOH:O	1.94	0.48
1:A:255:ASP:HA	1:A:284:PRO:HD2	1.96	0.48
1:A:86:VAL:HG13	1:A:91:LEU:HB2	1.95	0.47
1:A:249:ASP:OD2	1:A:318:GLN:NE2	2.47	0.46
1:A:59:MET:SD	1:A:71:ASN:HA	2.56	0.46
1:A:2:VAL:HA	1:A:251:TRP:CD2	2.50	0.46
1:A:304:ASN:ND2	1:A:307:LEU:H	2.13	0.46
1:A:343:ALA:HA	1:A:351:LEU:O	2.17	0.45
1:A:148:ASN:HD22	1:A:148:ASN:C	2.20	0.45
6:A:1282:HOH:O	3:C:6:MAN:C6	2.64	0.45
1:A:2:VAL:CG1	1:A:251:TRP:CE2	3.00	0.44
1:A:337:TYR:CD1	2:E:1:NAG:H5	2.53	0.43
1:A:348:LYS:HB3	1:A:409:LEU:HD21	1.99	0.43
1:A:205:TRP:HA	1:A:224:SER:O	2.18	0.43
1:A:335:VAL:HG12	6:A:937:HOH:O	2.17	0.43
1:A:202:MET:HE3	1:A:213:TRP:CZ3	2.54	0.42
1:A:306:HIS:HB2	1:A:384:VAL:HG13	2.01	0.42
1:A:202:MET:HE3	1:A:213:TRP:HZ3	1.85	0.42
1:A:150:ASP:OD2	1:A:236:ARG:HD2	2.20	0.42
1:A:282:LYS:HE2	1:A:310:PHE:O	2.19	0.41
1:A:356:ASN:O	1:A:403:HIS:HA	2.20	0.41
1:A:32:LEU:O	1:A:36:GLU:HG2	2.20	0.41
1:A:188:ARG:HD3	1:A:217:THR:HA	2.02	0.41
1:A:323:TYR:CZ	1:A:341:PHE:HB3	2.56	0.41
1:A:169:ALA:HA	1:A:170:PRO:HD2	1.90	0.41
1:A:96:TYR:HE1	1:A:103:THR:HB	1.86	0.40
1:A:378:HIS:O	1:A:413:LYS:HG3	2.21	0.40
1:A:322:PRO:HA	1:A:341:PHE:O	2.22	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	415/417 (100%)	407 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	340/340 (100%)	322 (95%)	18 (5%)	22	10

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	17	ASN
1	A	141	GLN
1	A	148	ASN
1	A	165	ASP
1	A	197	GLU
1	A	278	TRP
1	A	301	LEU
1	A	304	ASN
1	A	305	LYS
1	A	348	LYS
1	A	360	ILE
1	A	369	ASN
1	A	375	SER
1	A	412	LYS
1	A	413	LYS
1	A	416	ARG
1	A	417	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	23	HIS
1	A	67	HIS
1	A	87	HIS
1	A	135	ASN
1	A	141	GLN
1	A	148	ASN
1	A	246	ASN
1	A	274	HIS
1	A	293	GLN
1	A	304	ASN
1	A	306	HIS
1	A	369	ASN
1	A	378	HIS
1	A	403	HIS

5.3.3 RNA ⓘ

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 ⓘ

15 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	0.62	0	17,19,21	0.99	1 (5%)
2	NAG	B	2	2	14,14,15	0.60	0	17,19,21	0.78	0
3	NAG	C	1	1,3	14,14,15	0.76	0	17,19,21	1.32	2 (11%)
3	NAG	C	2	3	14,14,15	0.78	0	17,19,21	1.28	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	C	3	3	11,11,12	0.76	0	15,15,17	1.65	4 (26%)
3	MAN	C	4	3	11,11,12	0.96	1 (9%)	15,15,17	1.34	2 (13%)
3	MAN	C	5	3	11,11,12	0.71	0	15,15,17	1.48	2 (13%)
3	MAN	C	6	3	11,11,12	0.54	0	15,15,17	0.87	0
3	MAN	C	7	3	11,11,12	0.66	0	15,15,17	1.43	3 (20%)
4	NAG	D	1	1,4	14,14,15	0.77	0	17,19,21	1.50	2 (11%)
4	NAG	D	2	4	14,14,15	0.86	1 (7%)	17,19,21	0.81	0
4	BMA	D	3	4	11,11,12	0.54	0	15,15,17	1.14	2 (13%)
4	MAN	D	4	4	11,11,12	0.63	0	15,15,17	1.35	2 (13%)
2	NAG	E	1	1,2	14,14,15	0.82	0	17,19,21	1.47	3 (17%)
2	NAG	E	2	2	14,14,15	0.69	0	17,19,21	1.10	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
2	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	MAN	C	5	3	-	0/2/19/22	0/1/1/1
3	MAN	C	6	3	-	2/2/19/22	0/1/1/1
3	MAN	C	7	3	-	2/2/19/22	0/1/1/1
4	NAG	D	1	1,4	-	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	-	2/2/19/22	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2	NAG	O5-C1	-2.30	1.40	1.43
3	C	4	MAN	O5-C1	-2.17	1.40	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	NAG	O5-C1-C2	-4.55	104.11	111.29
3	C	1	NAG	O5-C1-C2	-4.24	104.59	111.29
3	C	7	MAN	C1-O5-C5	-3.72	107.15	112.19
3	C	2	NAG	C1-O5-C5	3.46	116.88	112.19
3	C	3	BMA	O5-C5-C6	3.32	112.40	107.20
3	C	3	BMA	C3-C4-C5	-3.12	104.68	110.24
4	D	4	MAN	C3-C4-C5	3.03	115.65	110.24
4	D	3	BMA	C1-C2-C3	2.98	113.33	109.67
2	E	1	NAG	O5-C1-C2	-2.82	106.83	111.29
3	C	5	MAN	O2-C2-C1	-2.64	103.74	109.15
2	E	1	NAG	C1-C2-N2	2.64	115.00	110.49
4	D	1	NAG	O4-C4-C5	-2.52	103.05	109.30
3	C	4	MAN	O2-C2-C1	-2.50	104.04	109.15
3	C	3	BMA	C1-O5-C5	-2.38	108.97	112.19
3	C	7	MAN	O5-C5-C6	2.38	110.93	107.20
4	D	3	BMA	O5-C5-C6	2.37	110.93	107.20
2	E	1	NAG	C6-C5-C4	-2.36	107.47	113.00
2	E	2	NAG	C1-O5-C5	2.25	115.25	112.19
3	C	5	MAN	O5-C1-C2	2.14	114.07	110.77
3	C	1	NAG	O4-C4-C5	-2.11	104.07	109.30
2	E	2	NAG	C6-C5-C4	-2.09	108.11	113.00
3	C	7	MAN	O5-C1-C2	-2.09	107.55	110.77
4	D	4	MAN	O5-C5-C6	2.08	110.46	107.20
2	B	1	NAG	C4-C3-C2	2.07	114.06	111.02
3	C	4	MAN	O5-C1-C2	-2.06	107.59	110.77
3	C	3	BMA	O6-C6-C5	-2.06	104.24	111.29

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	6	MAN	O5-C5-C6-O6
3	C	3	BMA	O5-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
3	C	3	BMA	C4-C5-C6-O6
3	C	7	MAN	O5-C5-C6-O6
3	C	6	MAN	C4-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
3	C	7	MAN	C4-C5-C6-O6
4	D	4	MAN	O5-C5-C6-O6
4	D	3	BMA	C4-C5-C6-O6

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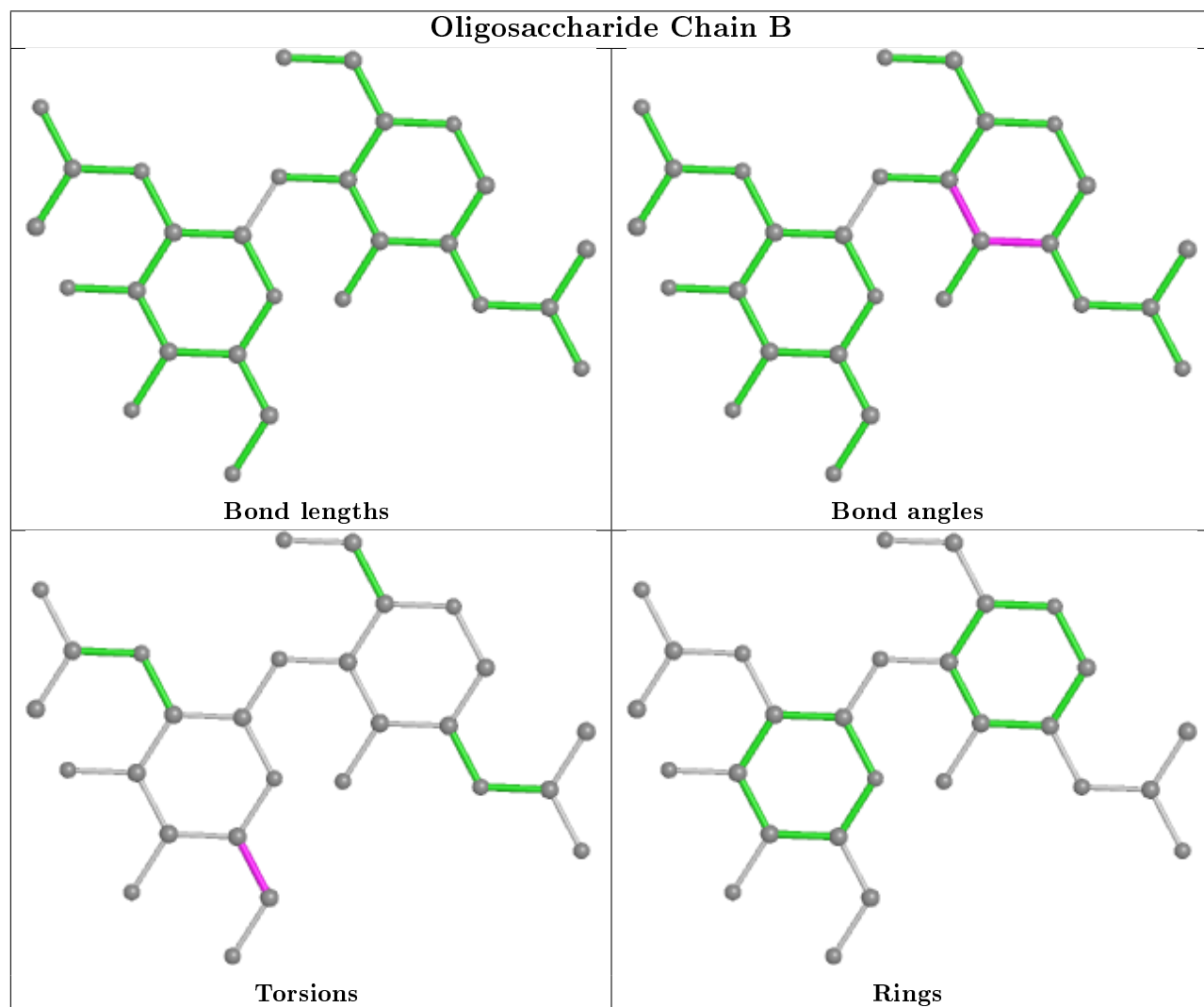
Mol	Chain	Res	Type	Atoms
4	D	4	MAN	C4-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6

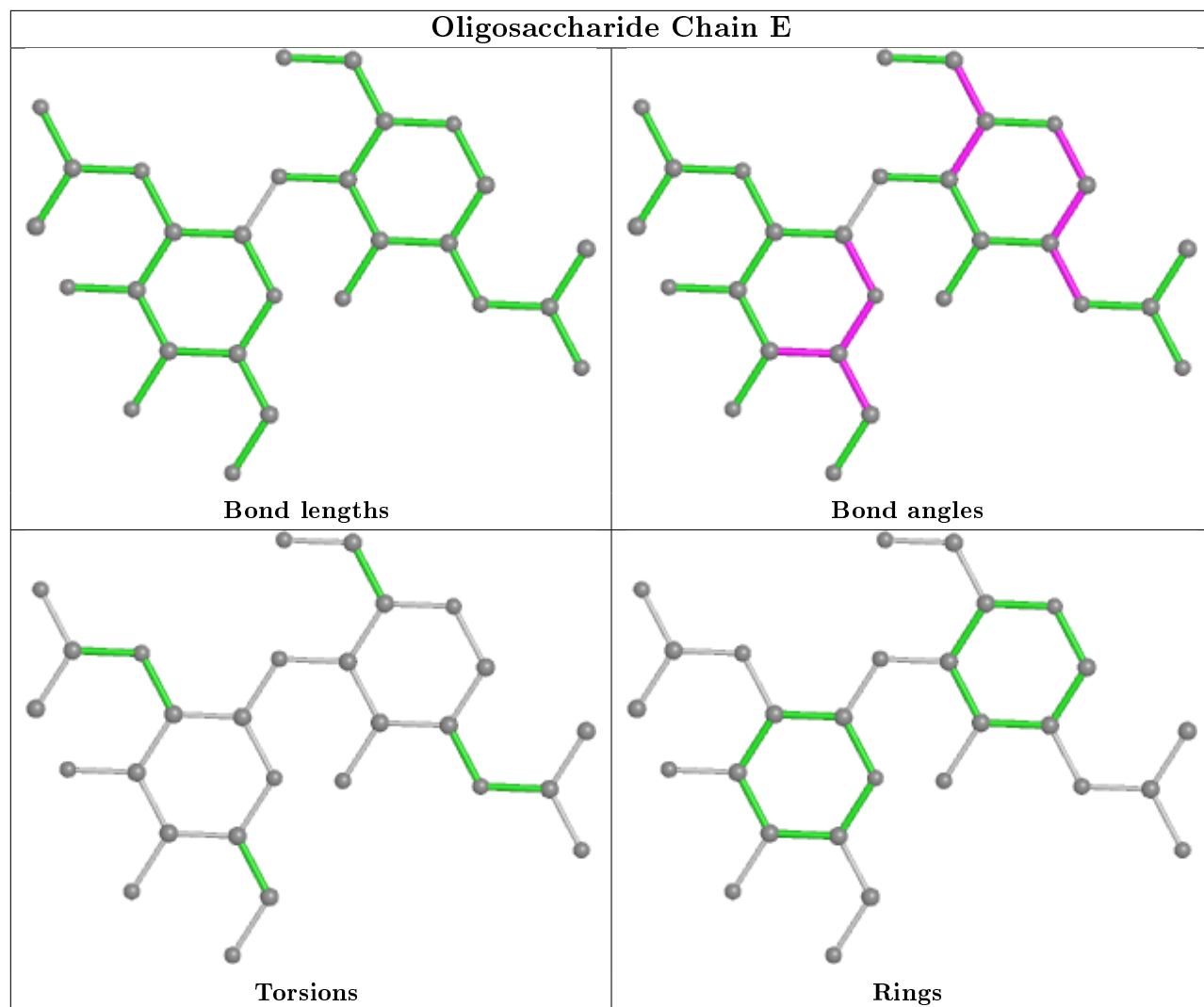
There are no ring outliers.

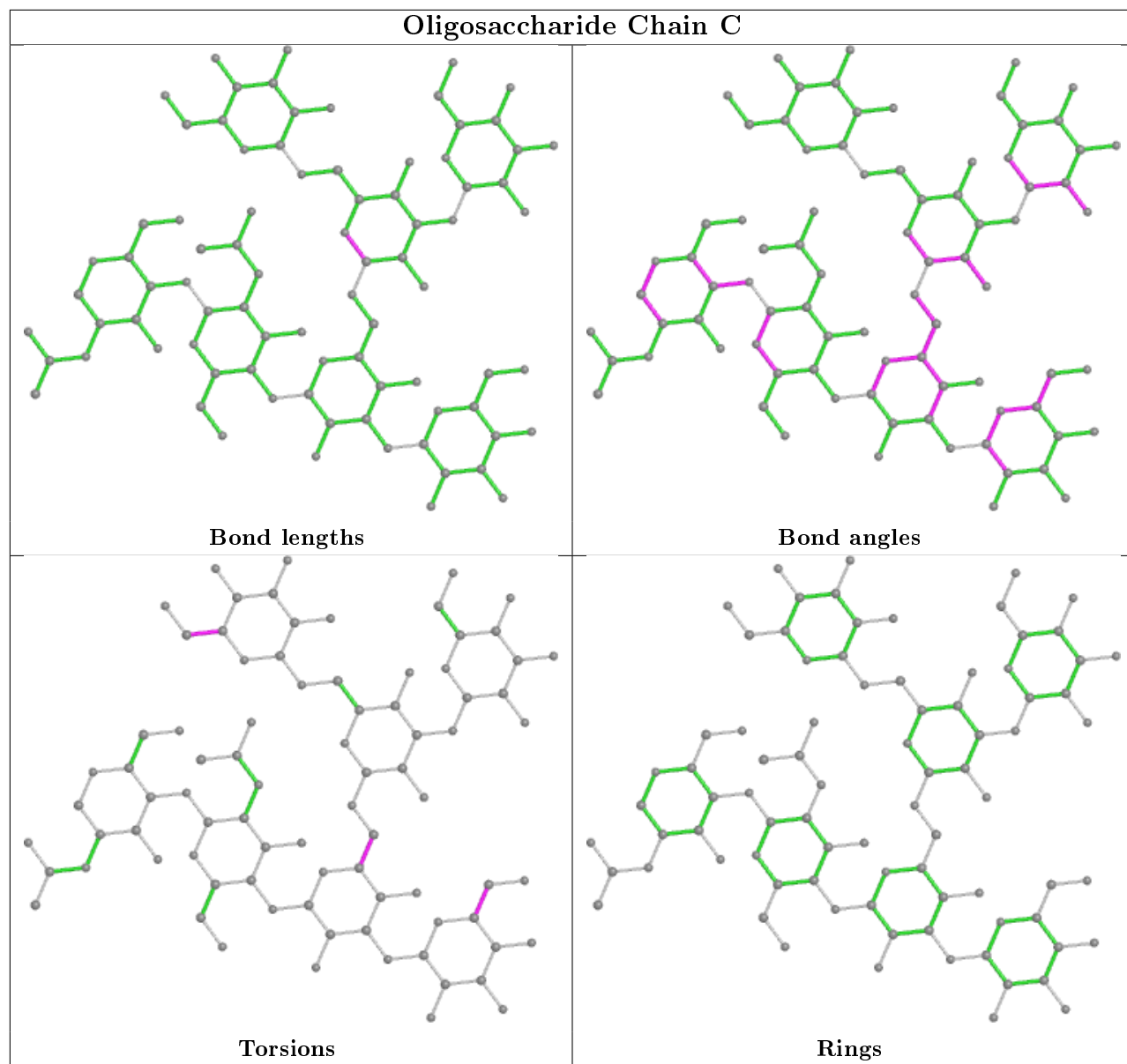
3 monomers are involved in 4 short contacts:

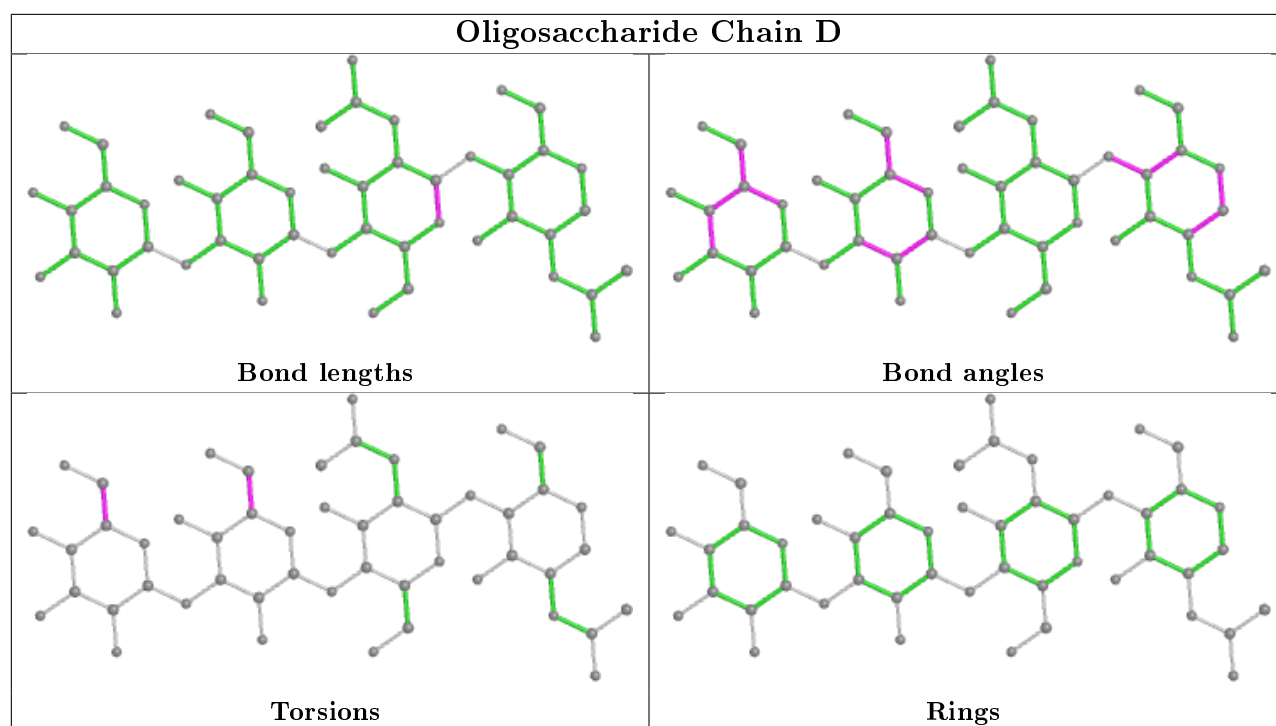
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	1	0
3	C	6	MAN	2	0
2	E	1	NAG	1	0

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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GAL	A	901	-	12,12,12	2.31	3 (25%)	17,17,17	2.05	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
5	GAL	A	901	-	-	0/2/22/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	901	GAL	C3-C2	-4.53	1.40	1.52
5	A	901	GAL	C1-C2	4.41	1.62	1.52
5	A	901	GAL	O3-C3	3.80	1.51	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	901	GAL	O4-C4-C5	-4.48	98.17	109.30
5	A	901	GAL	O5-C5-C4	4.22	117.36	109.69
5	A	901	GAL	O4-C4-C3	-2.93	103.57	110.35
5	A	901	GAL	O3-C3-C4	-2.07	105.56	110.35
5	A	901	GAL	C4-C3-C2	2.05	114.39	110.82
5	A	901	GAL	C6-C5-C4	2.04	117.78	113.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	901	GAL	1	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	417/417 (100%)	-0.49	4 (0%) 82 87	12, 21, 35, 71	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	417	TRP	11.4
1	A	416	ARG	4.1
1	A	415	GLN	2.8
1	A	172	GLY	2.3

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.

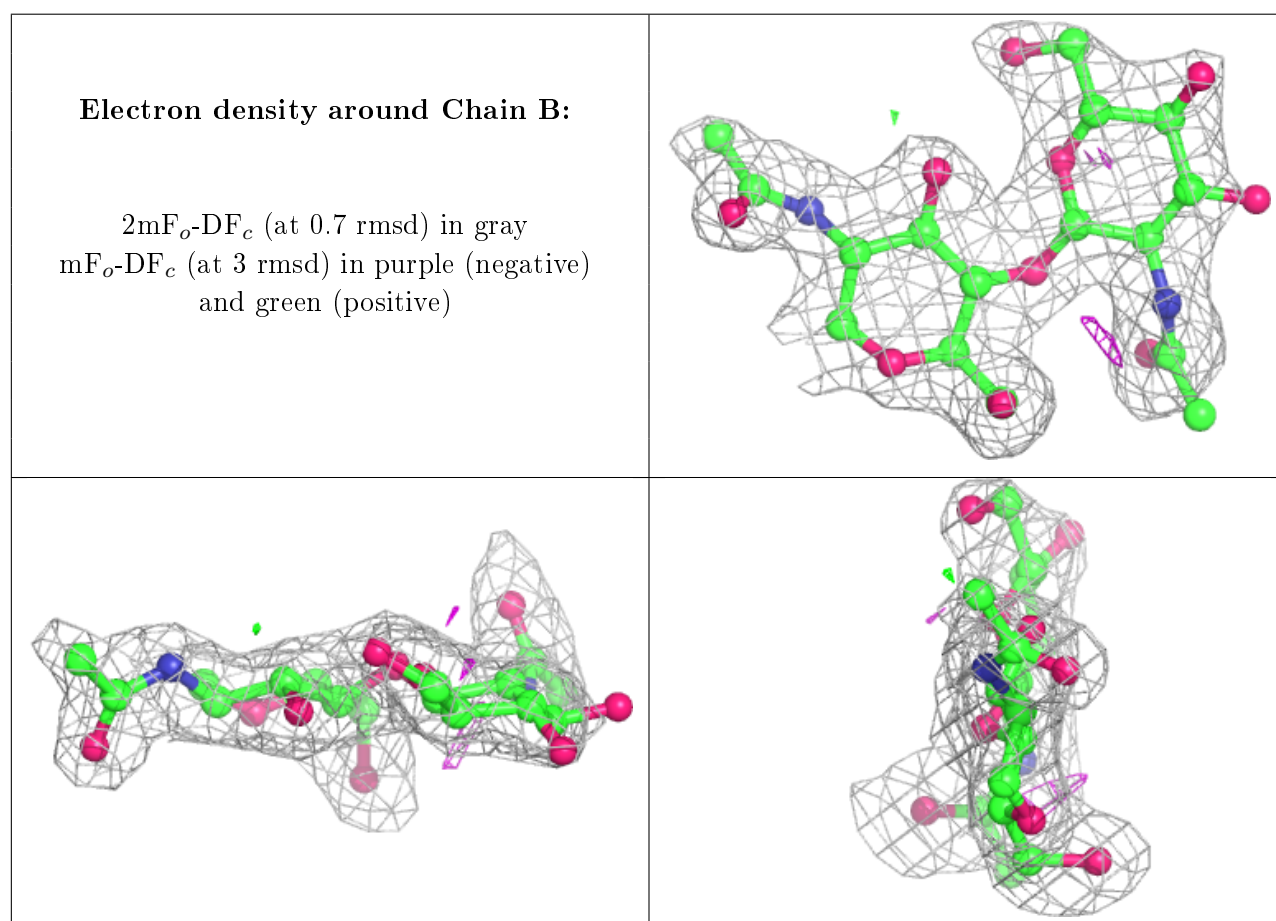
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	C	7	11/12	0.76	0.27	49,53,55,57	0
4	MAN	D	4	11/12	0.80	0.36	60,64,65,66	0
2	NAG	B	2	14/15	0.86	0.28	48,51,53,54	0
3	MAN	C	6	11/12	0.89	0.24	47,50,52,53	0
2	NAG	E	2	14/15	0.91	0.16	36,37,43,44	0
4	BMA	D	3	11/12	0.91	0.14	42,48,50,55	0
2	NAG	B	1	14/15	0.94	0.09	37,39,41,45	0
3	NAG	C	1	14/15	0.95	0.09	24,27,34,37	0

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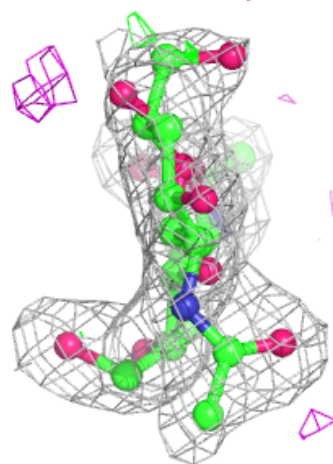
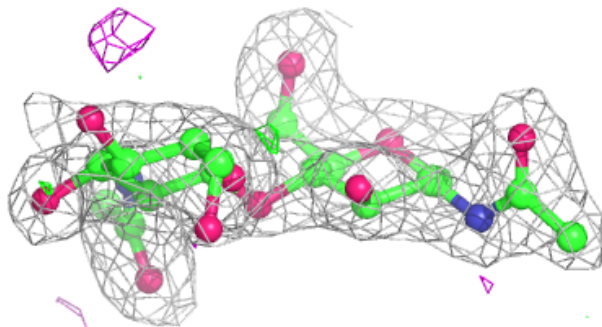
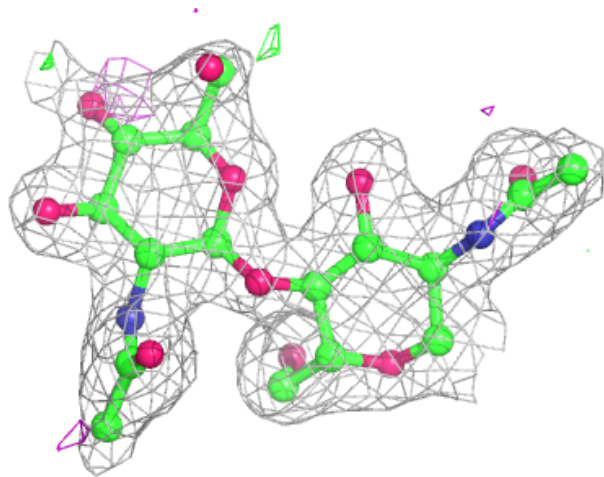
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	BMA	C	3	11/12	0.95	0.10	27,31,37,43	0
4	NAG	D	2	14/15	0.96	0.08	23,26,31,35	0
2	NAG	E	1	14/15	0.96	0.08	21,27,32,33	0
4	NAG	D	1	14/15	0.96	0.08	22,23,26,26	0
3	MAN	C	4	11/12	0.96	0.08	20,25,34,40	0
3	NAG	C	2	14/15	0.97	0.08	21,24,27,28	0
3	MAN	C	5	11/12	0.97	0.08	13,16,19,24	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.



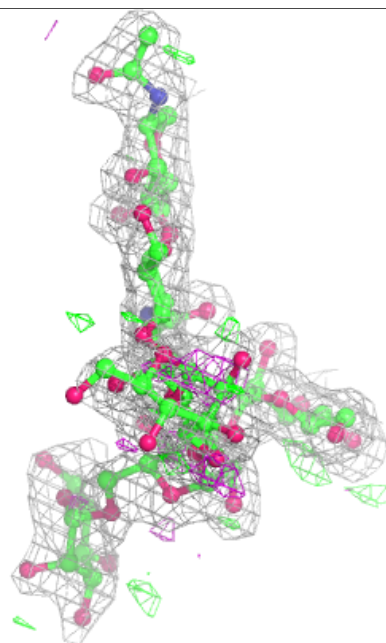
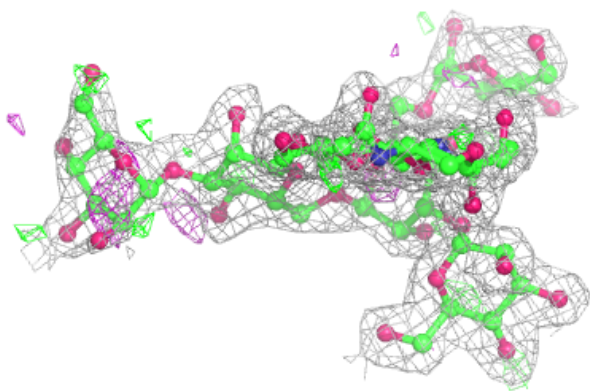
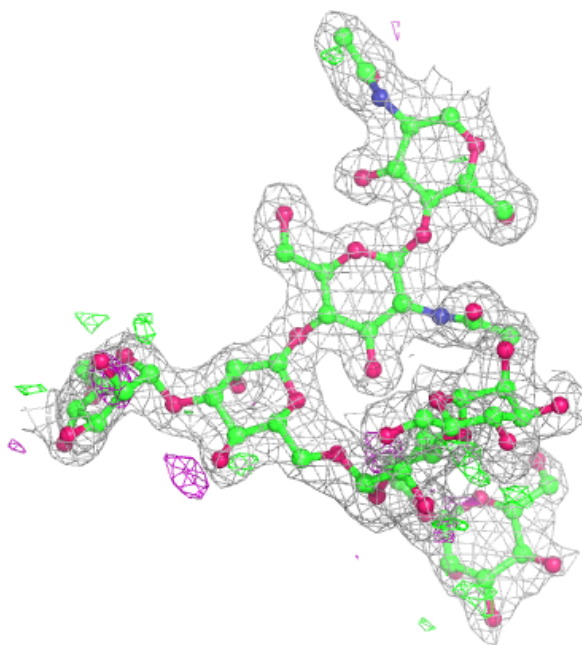
Electron density around Chain E:

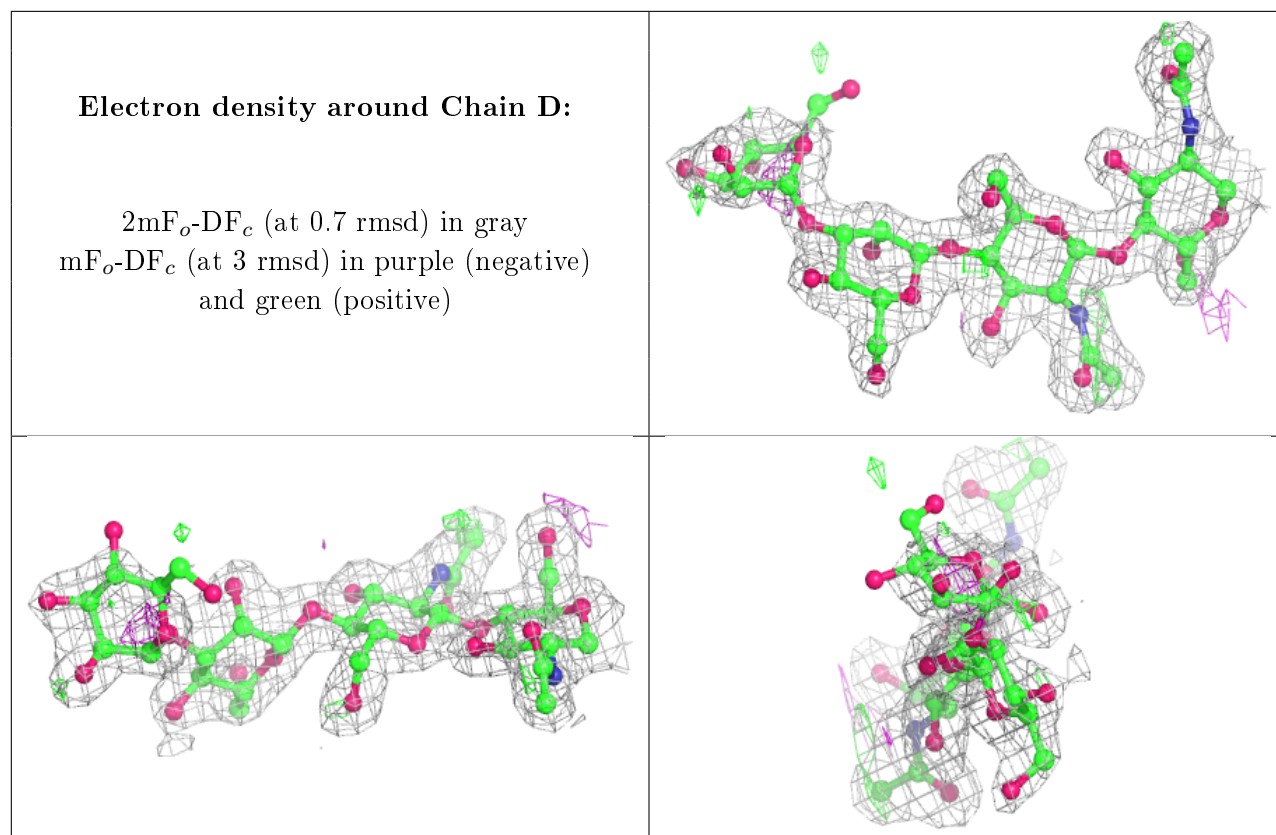
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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(\AA^2)	Q<0.9
5	GAL	A	901	12/12	0.90	0.14	20,22,24,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.