



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2024 – 08:58 pm GMT

PDB ID : 2BWC
Title : Structure of Endoglucanase 12A (Cel12A) from *Rhodothermus marinus* in complex with cellopentaose (5 minute soak)
Authors : Crennell, S.J.; Nordberg-Karlsson, E.
Deposited on : 2005-07-13
Resolution : 2.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

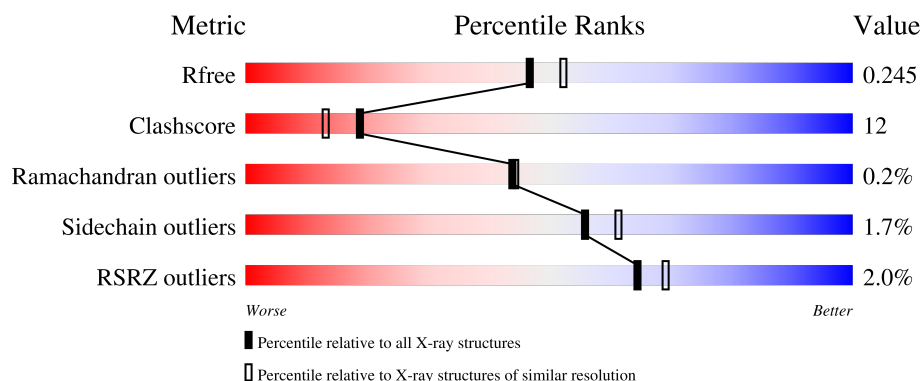
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




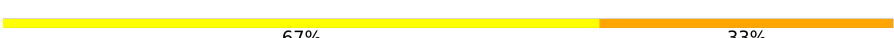
The reported resolution of this entry is 2.15 Å.

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}	164625	1881 (2.16-2.16)
Clashscore	180529	2047 (2.16-2.16)
Ramachandran outliers	177936	2027 (2.16-2.16)
Sidechain outliers	177891	2026 (2.16-2.16)
RSRZ outliers	164620	1882 (2.16-2.16)

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	227	
1	B	227	
2	C	3	
3	D	3	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	C	1	X	-	X	-
3	BGC	D	1[B]	-	-	X	-
4	GOL	A	1001	-	X	-	-
4	GOL	A	1002	-	X	-	-
4	GOL	A	1003[A]	-	X	-	-
4	GOL	A	1003[B]	-	X	X	-
4	GOL	A	1234	-	X	-	-
4	GOL	A	1235	-	X	-	-
4	GOL	B	1001	-	X	-	-
4	GOL	B	1002[A]	-	X	-	-
4	GOL	B	1237	-	X	-	-
6	GLC	B	1003[B]	X	-	X	-

2 Entry composition [i](#)

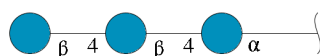
There are 7 unique types of molecules in this entry. The entry contains 4225 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ENDOGLUCANASE.

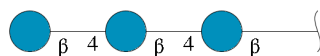
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	8	0
			1842	1160	320	356	6			
1	B	226	Total	C	N	O	S	0	7	0
			1839	1160	324	349	6			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	3	Total	C	O	0	0	0
			34	18	16			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	3	Total	C	O	0	3	0
			67	36	31			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



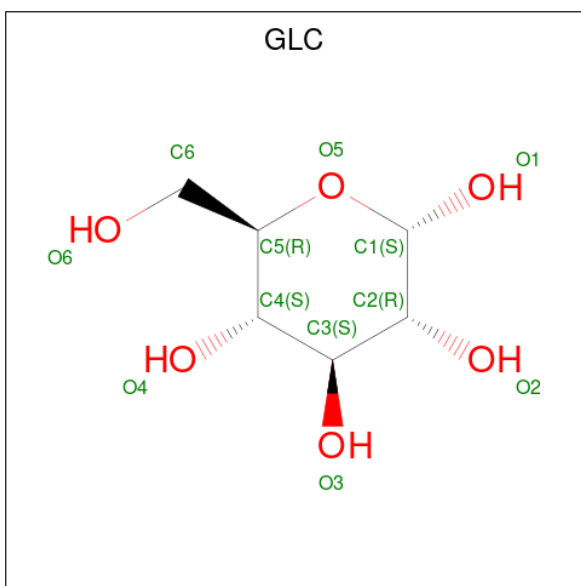
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	1
			12	6	6		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	1
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is alpha-D-glucopyranose (three-letter code: GLC) (formula: C₆H₁₂O₆).



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


- Molecule 7 is water.

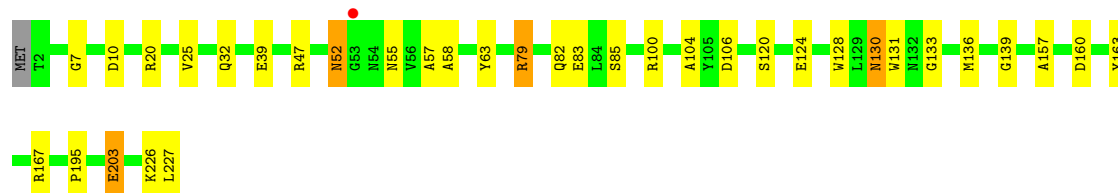
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	214	Total 214	O 214	0	0
7	B	158	Total 158	O 158	0	0

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.

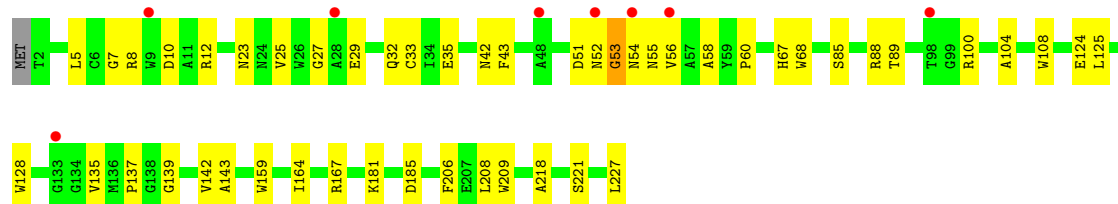
- Molecule 1: ENDOGLUCANASE

Chain A: 



- Molecule 1: ENDOGLUCANASE

Chain B: 



- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain C: 



- Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.89Å 67.33Å 131.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.65 – 2.15 36.65 – 2.15	Depositor EDS
% Data completeness (in resolution range)	94.5 (36.65-2.15) 94.5 (36.65-2.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 2.16Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.184 , 0.233 0.198 , 0.245	Depositor DCC
R_{free} test set	1309 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 66.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4225	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% 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, GLC, SO4, GOL

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	0.34	0/1895	0.63	0/2593
1	B	0.32	0/1892	0.61	0/2586
All	All	0.33	0/3787	0.62	0/5179

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1842	0	1690	26	0
1	B	1839	0	1706	44	0
2	C	34	0	30	7	0
3	D	67	0	58	13	0
4	A	36	0	24	7	0
4	B	18	0	13	6	0
5	A	5	0	0	0	0
6	B	12	0	11	8	0
7	A	214	0	0	4	0
7	B	158	0	0	0	0
All	All	4225	0	3532	86	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 12.

All (86) 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)
4:B:1002[A]:GOL:C1	4:B:1002[A]:GOL:O1	1.64	1.43
4:A:1003[B]:GOL:H12	2:C:1:GLC:O1	1.20	1.26
6:B:1003[B]:GLC:C4	3:D:1[B]:BGC:O1	2.11	0.99
6:B:1003[B]:GLC:C4	3:D:1[B]:BGC:HA	1.78	0.97
6:B:1003[B]:GLC:O4	3:D:1[B]:BGC:O1	1.82	0.96
4:A:1003[A]:GOL:C2	2:C:1:GLC:O1	2.22	0.88
1:B:8[A]:ARG:HG3	1:B:25:VAL:HB	1.54	0.88
1:B:124:GLU:OE2	3:D:1[B]:BGC:H1	1.74	0.87
1:A:39[A]:GLU:HG3	7:A:2048:HOH:O	1.81	0.79
4:A:1003[A]:GOL:C3	2:C:1:GLC:O1	2.34	0.74
1:A:79:ARG:HH11	1:A:79:ARG:HB2	1.53	0.73
6:B:1003[B]:GLC:H4	3:D:1[B]:BGC:O1	1.86	0.73
1:B:5:LEU:HD21	1:B:12[A]:ARG:HE	1.53	0.72
1:A:130:ASN:HD22	1:A:131:TRP:H	1.38	0.71
1:B:8[B]:ARG:HG3	1:B:25:VAL:HB	1.73	0.70
1:B:54:ASN:H	1:B:100:ARG:NH2	1.90	0.69
1:A:82:GLN:HG2	1:A:195:PRO:O	1.93	0.69
1:A:106:ASP:O	1:A:203:GLU:HG3	1.94	0.68
1:B:139:GLY:H	4:B:1001:GOL:H11	1.60	0.67
4:A:1003[B]:GOL:H12	2:C:1:GLC:C1	2.23	0.66
1:B:32:GLN:NE2	1:B:208:LEU:HD12	2.08	0.66
1:A:7:GLY:HA3	1:A:10[A]:ASP:OD1	1.94	0.66
1:A:63:TYR:HB3	1:A:203:GLU:HB3	1.77	0.66
1:B:54:ASN:H	1:B:100:ARG:HH21	1.46	0.62
4:B:1002[A]:GOL:O2	3:D:1[A]:BGC:C1	2.48	0.62
4:B:1002[A]:GOL:C1	4:B:1002[A]:GOL:HO1	2.08	0.61
1:A:124:GLU:OE2	2:C:1:GLC:H1	1.99	0.61
1:B:164:ILE:HD12	1:B:164:ILE:N	2.17	0.60
6:B:1003[B]:GLC:O4	3:D:1[B]:BGC:C1	2.48	0.60
1:B:181[A]:LYS:HE2	1:B:185:ASP:OD1	2.02	0.60
1:B:67:HIS:CD2	3:D:3[A]:BGC:H6C2	2.37	0.59
1:B:25:VAL:HA	1:B:58:ALA:CB	2.34	0.58
1:B:29[B]:GLU:H	1:B:29[B]:GLU:CD	2.08	0.57
1:B:51:ASP:OD1	1:B:51:ASP:O	2.24	0.55
1:B:67:HIS:NE2	3:D:3[A]:BGC:H6C2	2.22	0.55
1:B:25:VAL:HA	1:B:58:ALA:HB2	1.88	0.55
1:A:20:ARG:HD3	1:A:63:TYR:OH	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:HIS:CD2	3:D:3[B]:BGC:H6C2	2.44	0.53
6:B:1003[B]:GLC:C3	3:D:1[B]:BGC:HA	2.23	0.52
1:A:52:ASN:HB2	1:A:57:ALA:HB2	1.90	0.52
1:A:226:LYS:HG2	7:A:2207:HOH:O	2.10	0.52
1:A:85:SER:HB3	1:A:227:LEU:HD23	1.91	0.51
1:B:60:PRO:HD2	1:B:206:PHE:O	2.09	0.51
1:A:104:ALA:HB2	1:A:128:TRP:HA	1.92	0.51
1:B:85:SER:HB3	1:B:227:LEU:HD23	1.94	0.50
1:B:5:LEU:O	1:B:33:CYS:HA	2.12	0.50
1:A:130:ASN:HD22	1:A:131:TRP:N	2.08	0.50
1:B:88:ARG:HH22	4:B:1237:GOL:H12	1.77	0.49
1:A:100:ARG:HG2	1:A:133:GLY:HA3	1.94	0.49
1:B:27:GLY:HA3	1:B:56:VAL:O	2.13	0.48
1:A:100:ARG:HD2	7:A:2114:HOH:O	2.13	0.48
1:B:53:GLY:HA2	1:B:100:ARG:HH21	1.78	0.48
1:B:108:TRP:CZ3	1:B:124:GLU:HB2	2.48	0.48
1:A:120:SER:HA	1:A:160[B]:ASP:OD1	2.13	0.48
1:B:8[A]:ARG:NH1	1:B:25:VAL:HG11	2.29	0.48
1:A:25:VAL:HA	1:A:58:ALA:CB	2.45	0.47
1:A:83[B]:GLU:O	1:A:83[B]:GLU:HG3	2.15	0.47
1:B:159:TRP:CH2	6:B:1003[B]:GLC:H61	2.49	0.47
1:B:100:ARG:HH11	1:B:100:ARG:HG2	1.79	0.46
1:B:135:VAL:HG11	1:B:209:TRP:CE3	2.50	0.46
1:A:32:GLN:HA	1:A:47:ARG:O	2.16	0.46
1:A:136:MET:SD	1:A:167:ARG:NH1	2.87	0.46
1:B:53:GLY:C	1:B:55:ASN:H	2.19	0.46
4:A:1003[B]:GOL:C2	2:C:1:GLC:O1	2.49	0.46
1:B:104:ALA:HB2	1:B:128:TRP:HA	1.97	0.45
1:B:8[A]:ARG:HG3	1:B:8[A]:ARG:HH11	1.80	0.45
1:B:128:TRP:HB2	1:B:167:ARG:HA	1.99	0.44
1:B:125:LEU:C	1:B:125:LEU:HD23	2.39	0.43
4:A:1003[B]:GOL:C3	2:C:1:GLC:O1	2.62	0.43
1:B:137:PRO:HD3	1:B:167:ARG:NH1	2.34	0.43
1:B:35:GLU:O	1:B:43:PHE:HA	2.18	0.42
1:A:52:ASN:HB3	1:A:55:ASN:O	2.19	0.42
1:A:157:ALA:HB3	1:A:163:TYR:HB3	2.01	0.42
1:B:139:GLY:N	4:B:1001:GOL:H11	2.32	0.42
1:B:5:LEU:HD11	1:B:12[A]:ARG:HG2	2.01	0.42
1:B:142:VAL:O	1:B:143:ALA:HB2	2.20	0.42
1:B:7:GLY:N	1:B:10:ASP:OD1	2.50	0.41
1:B:42:ASN:OD1	1:B:218:ALA:HA	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:LEU:CD2	1:B:12[A]:ARG:HE	2.27	0.41
1:A:139:GLY:H	4:A:1001:GOL:C2	2.34	0.41
1:A:167:ARG:NH1	7:A:2153:HOH:O	2.54	0.41
6:B:1003[B]:GLC:O4	3:D:1[B]:BGC:H2	2.20	0.41
1:B:68:TRP:CH2	3:D:2[A]:BGC:H4	2.56	0.41
1:A:25:VAL:HA	1:A:58:ALA:HB2	2.04	0.40
1:B:137:PRO:HD3	1:B:167:ARG:HH11	1.86	0.40
1:B:89:THR:HA	1:B:221:SER:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	232/227 (102%)	227 (98%)	5 (2%)	0	100	100
1	B	231/227 (102%)	222 (96%)	8 (4%)	1 (0%)	30	27
All	All	463/454 (102%)	449 (97%)	13 (3%)	1 (0%)	44	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	53	GLY

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	186/179 (104%)	182 (98%)	4 (2%)	47	51
1	B	185/179 (103%)	183 (99%)	2 (1%)	70	75
All	All	371/358 (104%)	365 (98%)	6 (2%)	56	64

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	79	ARG
1	A	130	ASN
1	A	203	GLU
1	B	23	ASN
1	B	52	ASN

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

Mol	Chain	Res	Type
1	A	24	ASN
1	A	52	ASN
1	A	130	ASN
1	A	162	ASN
1	B	23	ASN
1	B	24	ASN
1	B	32	GLN
1	B	52	ASN
1	B	54	ASN
1	B	117	ASN
1	B	132	ASN
1	B	162	ASN

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 ⓘ

9 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	GLC	C	1	4,2	12,12,12	0.35	0	17,17,17	0.35	0
2	BGC	C	2	2	11,11,12	0.47	0	15,15,17	0.47	0
2	BGC	C	3	2	11,11,12	0.52	0	15,15,17	0.56	0
3	BGC	D	1[A]	3	11,11,12	0.67	0	15,15,17	1.17	1 (6%)
3	BGC	D	1[B]	3	12,12,12	0.38	0	17,17,17	0.41	0
3	BGC	D	2[A]	3	11,11,12	0.53	0	15,15,17	0.35	0
3	BGC	D	2[B]	3	11,11,12	0.49	0	15,15,17	0.40	0
3	BGC	D	3[A]	3	11,11,12	0.46	0	15,15,17	0.29	0
3	BGC	D	3[B]	3	11,11,12	0.44	0	15,15,17	0.29	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	GLC	C	1	4,2	1/1/5/5	0/2/22/22	0/1/1/1
2	BGC	C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	C	3	2	-	2/2/19/22	0/1/1/1
3	BGC	D	1[A]	3	-	2/2/19/22	0/1/1/1
3	BGC	D	1[B]	3	-	0/2/22/22	0/1/1/1
3	BGC	D	2[A]	3	-	2/2/19/22	0/1/1/1
3	BGC	D	2[B]	3	-	2/2/19/22	0/1/1/1
3	BGC	D	3[A]	3	-	2/2/19/22	0/1/1/1
3	BGC	D	3[B]	3	-	2/2/19/22	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(°)	Ideal(°)
3	D	1[A]	BGC	C1-C2-C3	3.18	113.57	109.67

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1	GLC	C1

All (14) torsion outliers are listed below:

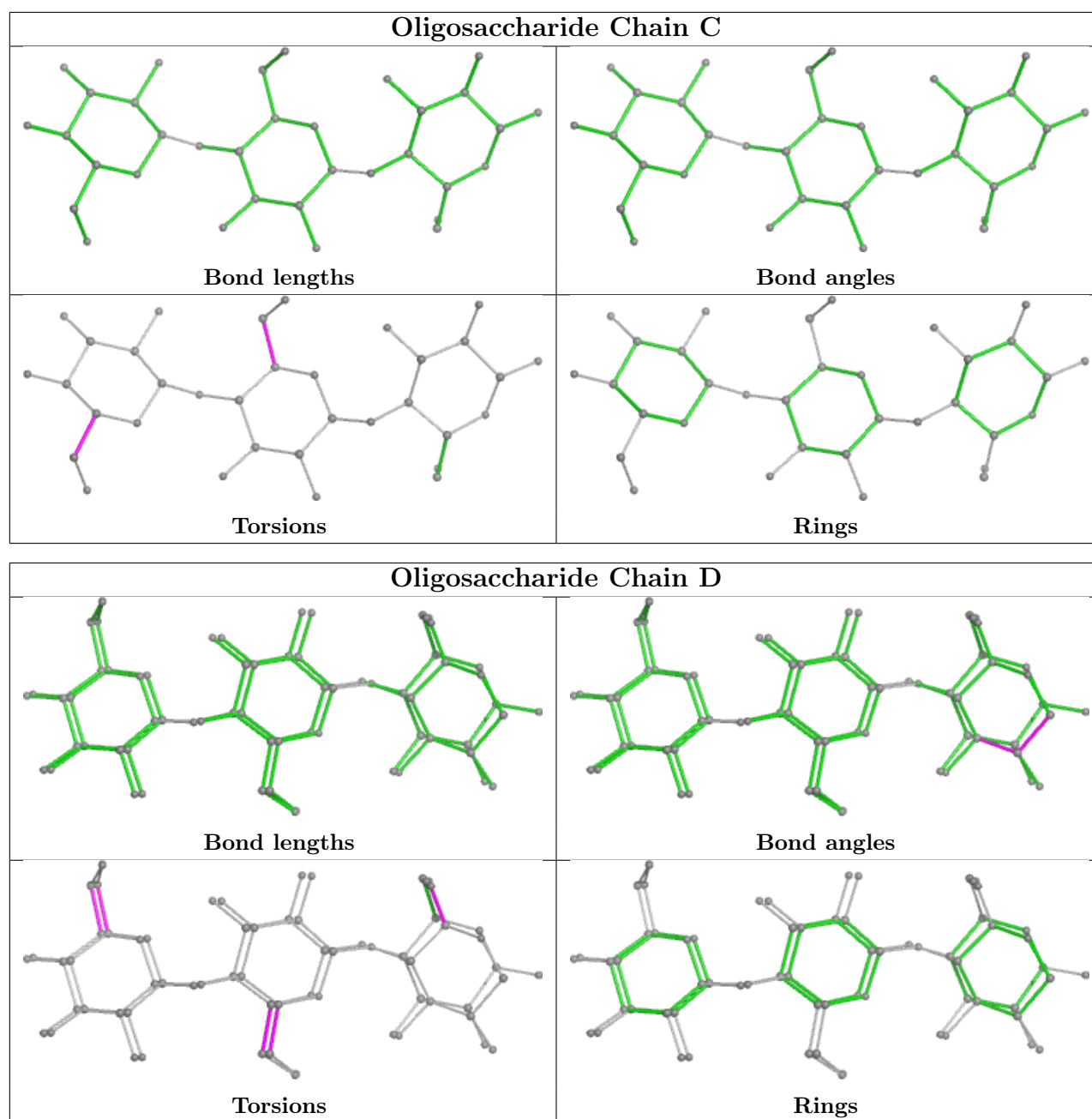
Mol	Chain	Res	Type	Atoms
3	D	2[B]	BGC	O5-C5-C6-O6
2	C	2	BGC	O5-C5-C6-O6
3	D	2[A]	BGC	O5-C5-C6-O6
3	D	2[B]	BGC	C4-C5-C6-O6
2	C	3	BGC	O5-C5-C6-O6
2	C	2	BGC	C4-C5-C6-O6
2	C	3	BGC	C4-C5-C6-O6
3	D	2[A]	BGC	C4-C5-C6-O6
3	D	3[B]	BGC	O5-C5-C6-O6
3	D	3[B]	BGC	C4-C5-C6-O6
3	D	3[A]	BGC	C4-C5-C6-O6
3	D	1[A]	BGC	O5-C5-C6-O6
3	D	3[A]	BGC	O5-C5-C6-O6
3	D	1[A]	BGC	C4-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1[A]	BGC	1	0
3	D	2[A]	BGC	1	0
3	D	3[B]	BGC	1	0
3	D	3[A]	BGC	2	0
2	C	1	GLC	7	0
3	D	1[B]	BGC	8	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](#)

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	1003[B]	2	5,5,5	4.52	5 (100%)	5,5,5	5.78	3 (60%)
6	GLC	B	1003[B]	-	12,12,12	0.49	0	17,17,17	0.61	0
5	SO4	A	1236	-	4,4,4	0.21	0	6,6,6	0.14	0
4	GOL	A	1235	-	5,5,5	4.53	5 (100%)	5,5,5	5.75	3 (60%)
4	GOL	A	1002	-	5,5,5	4.55	5 (100%)	5,5,5	5.76	3 (60%)
4	GOL	B	1001	-	5,5,5	4.53	5 (100%)	5,5,5	5.77	3 (60%)
4	GOL	B	1237	-	5,5,5	4.55	5 (100%)	5,5,5	5.75	3 (60%)
4	GOL	A	1234	-	5,5,5	4.57	5 (100%)	5,5,5	5.77	3 (60%)
4	GOL	A	1003[A]	-	5,5,5	4.54	5 (100%)	5,5,5	5.75	3 (60%)
4	GOL	B	1002[A]	-	5,5,5	4.90	4 (80%)	5,5,5	5.82	3 (60%)
4	GOL	A	1001	-	5,5,5	4.54	5 (100%)	5,5,5	5.79	3 (60%)

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
4	GOL	A	1003[B]	2	-	2/4/4/4	-
6	GLC	B	1003[B]	-	1/1/5/5	1/2/22/22	0/1/1/1
4	GOL	A	1235	-	-	2/4/4/4	-
4	GOL	A	1002	-	-	2/4/4/4	-
4	GOL	B	1001	-	-	2/4/4/4	-
4	GOL	B	1237	-	-	2/4/4/4	-
4	GOL	A	1003[A]	-	-	2/4/4/4	-
4	GOL	A	1234	-	-	3/4/4/4	-
4	GOL	B	1002[A]	-	-	2/4/4/4	-
4	GOL	A	1001	-	-	2/4/4/4	-

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1002[A]	GOL	C3-C2	-8.31	1.17	1.51
4	A	1234	GOL	C3-C2	-7.50	1.20	1.51
4	A	1002	GOL	C3-C2	-7.46	1.21	1.51
4	A	1235	GOL	C3-C2	-7.45	1.21	1.51
4	A	1003[B]	GOL	C3-C2	-7.41	1.21	1.51
4	A	1003[A]	GOL	C3-C2	-7.37	1.21	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	GOL	C3-C2	-7.35	1.21	1.51
4	B	1001	GOL	C3-C2	-7.35	1.21	1.51
4	B	1237	GOL	C3-C2	-7.32	1.21	1.51
4	B	1002[A]	GOL	O1-C1	5.20	1.64	1.42
4	B	1237	GOL	O1-C1	4.62	1.61	1.42
4	A	1003[A]	GOL	O1-C1	4.61	1.61	1.42
4	A	1234	GOL	O1-C1	4.60	1.61	1.42
4	A	1003[B]	GOL	O1-C1	4.57	1.61	1.42
4	A	1001	GOL	O1-C1	4.56	1.61	1.42
4	B	1001	GOL	O1-C1	4.55	1.61	1.42
4	A	1235	GOL	O1-C1	4.51	1.61	1.42
4	A	1002	GOL	O1-C1	4.36	1.60	1.42
4	B	1002[A]	GOL	O3-C3	3.87	1.58	1.42
4	B	1237	GOL	O3-C3	3.43	1.56	1.42
4	B	1001	GOL	O3-C3	3.38	1.56	1.42
4	A	1001	GOL	O3-C3	3.37	1.56	1.42
4	A	1003[B]	GOL	O3-C3	3.35	1.56	1.42
4	A	1002	GOL	O3-C3	3.33	1.56	1.42
4	A	1235	GOL	O3-C3	3.31	1.56	1.42
4	A	1003[A]	GOL	O3-C3	3.29	1.56	1.42
4	A	1234	GOL	O3-C3	3.28	1.56	1.42
4	A	1002	GOL	C1-C2	-3.01	1.39	1.51
4	A	1001	GOL	O2-C2	-3.00	1.34	1.43
4	A	1003[A]	GOL	O2-C2	-2.97	1.34	1.43
4	A	1002	GOL	O2-C2	-2.96	1.34	1.43
4	A	1234	GOL	O2-C2	-2.93	1.34	1.43
4	B	1237	GOL	O2-C2	-2.91	1.34	1.43
4	B	1001	GOL	O2-C2	-2.89	1.34	1.43
4	B	1237	GOL	C1-C2	-2.87	1.39	1.51
4	B	1001	GOL	C1-C2	-2.87	1.39	1.51
4	A	1235	GOL	C1-C2	-2.84	1.40	1.51
4	A	1001	GOL	C1-C2	-2.83	1.40	1.51
4	A	1003[A]	GOL	C1-C2	-2.82	1.40	1.51
4	A	1235	GOL	O2-C2	-2.81	1.35	1.43
4	A	1003[B]	GOL	C1-C2	-2.76	1.40	1.51
4	A	1234	GOL	C1-C2	-2.76	1.40	1.51
4	A	1003[B]	GOL	O2-C2	-2.73	1.35	1.43
4	B	1002[A]	GOL	C1-C2	-2.48	1.41	1.51

All (27) bond angle outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
-----	-------	-----	------	-------	---	-------------	----------

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	GOL	O3-C3-C2	10.60	161.02	110.20
4	A	1003[A]	GOL	O3-C3-C2	10.50	160.57	110.20
4	A	1003[B]	GOL	O3-C3-C2	10.49	160.52	110.20
4	B	1001	GOL	O3-C3-C2	10.49	160.50	110.20
4	B	1237	GOL	O3-C3-C2	10.45	160.33	110.20
4	A	1234	GOL	O3-C3-C2	10.45	160.30	110.20
4	A	1002	GOL	O3-C3-C2	10.44	160.25	110.20
4	A	1235	GOL	O3-C3-C2	10.37	159.92	110.20
4	B	1002[A]	GOL	O3-C3-C2	10.31	159.64	110.20
4	B	1002[A]	GOL	O2-C2-C3	6.85	139.30	109.12
4	A	1002	GOL	O2-C2-C3	6.83	139.21	109.12
4	A	1234	GOL	O2-C2-C3	6.76	138.90	109.12
4	B	1001	GOL	O2-C2-C3	6.76	138.89	109.12
4	A	1235	GOL	O2-C2-C3	6.76	138.89	109.12
4	A	1003[B]	GOL	O2-C2-C3	6.75	138.86	109.12
4	A	1001	GOL	O2-C2-C3	6.75	138.84	109.12
4	B	1237	GOL	O2-C2-C3	6.73	138.75	109.12
4	A	1003[A]	GOL	O2-C2-C3	6.66	138.47	109.12
4	B	1002[A]	GOL	O1-C1-C2	3.84	128.59	110.20
4	A	1235	GOL	O1-C1-C2	3.36	126.32	110.20
4	A	1234	GOL	O1-C1-C2	3.31	126.07	110.20
4	A	1003[B]	GOL	O1-C1-C2	3.27	125.88	110.20
4	A	1003[A]	GOL	O1-C1-C2	3.22	125.63	110.20
4	B	1237	GOL	O1-C1-C2	3.21	125.58	110.20
4	B	1001	GOL	O1-C1-C2	3.21	125.57	110.20
4	A	1002	GOL	O1-C1-C2	3.14	125.28	110.20
4	A	1001	GOL	O1-C1-C2	3.10	125.08	110.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	1003[B]	GLC	C1

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	GOL	C1-C2-C3-O3
4	A	1002	GOL	C1-C2-C3-O3
4	A	1003[A]	GOL	C1-C2-C3-O3
4	A	1003[B]	GOL	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	1234	GOL	C1-C2-C3-O3
4	A	1235	GOL	C1-C2-C3-O3
4	B	1001	GOL	O1-C1-C2-O2
4	B	1001	GOL	C1-C2-C3-O3
4	B	1002[A]	GOL	C1-C2-C3-O3
4	B	1237	GOL	C1-C2-C3-O3
4	A	1235	GOL	O1-C1-C2-O2
4	A	1002	GOL	O1-C1-C2-C3
4	A	1003[A]	GOL	O1-C1-C2-C3
4	A	1234	GOL	O1-C1-C2-C3
4	A	1001	GOL	O1-C1-C2-O2
4	A	1003[B]	GOL	O1-C1-C2-O2
4	A	1234	GOL	O1-C1-C2-O2
4	B	1237	GOL	O1-C1-C2-O2
4	B	1002[A]	GOL	O1-C1-C2-O2
6	B	1003[B]	GLC	O5-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1003[B]	GOL	4	0
6	B	1003[B]	GLC	8	0
4	B	1001	GOL	2	0
4	B	1237	GOL	1	0
4	A	1003[A]	GOL	2	0
4	B	1002[A]	GOL	3	0
4	A	1001	GOL	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	226/227 (99%)	0.07	1 (0%) 89 90	10, 20, 35, 58	8 (3%)
1	B	226/227 (99%)	0.22	8 (3%) 47 53	11, 27, 48, 70	7 (3%)
All	All	452/454 (99%)	0.14	9 (1%) 64 69	10, 23, 44, 70	15 (3%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	52	ASN	4.9
1	B	133	GLY	2.6
1	B	28	ALA	2.6
1	B	48	ALA	2.5
1	B	56	VAL	2.4
1	B	98	THR	2.3
1	A	53	GLY	2.3
1	B	54	ASN	2.2
1	B	9	TRP	2.2

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.

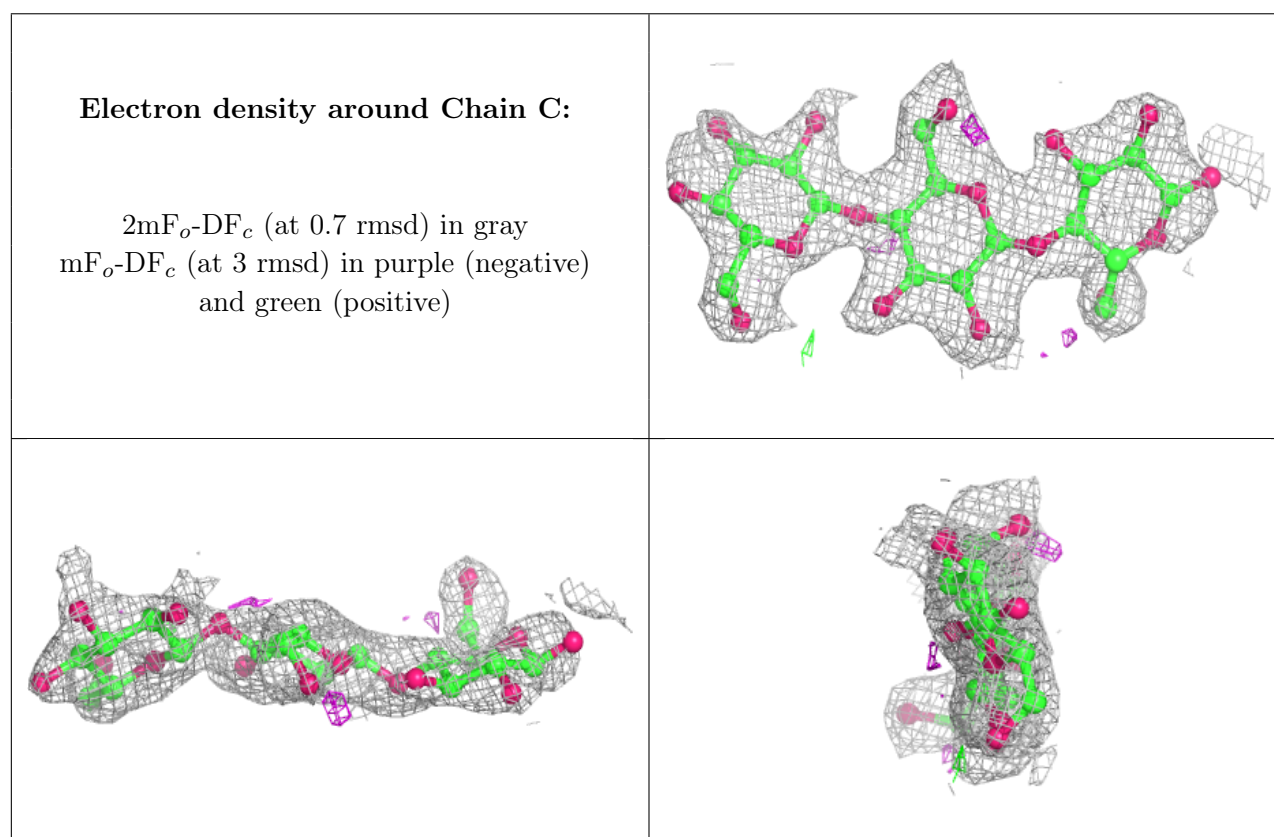
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BGC	D	3[A]	11/12	0.78	0.18	58,61,62,62	11

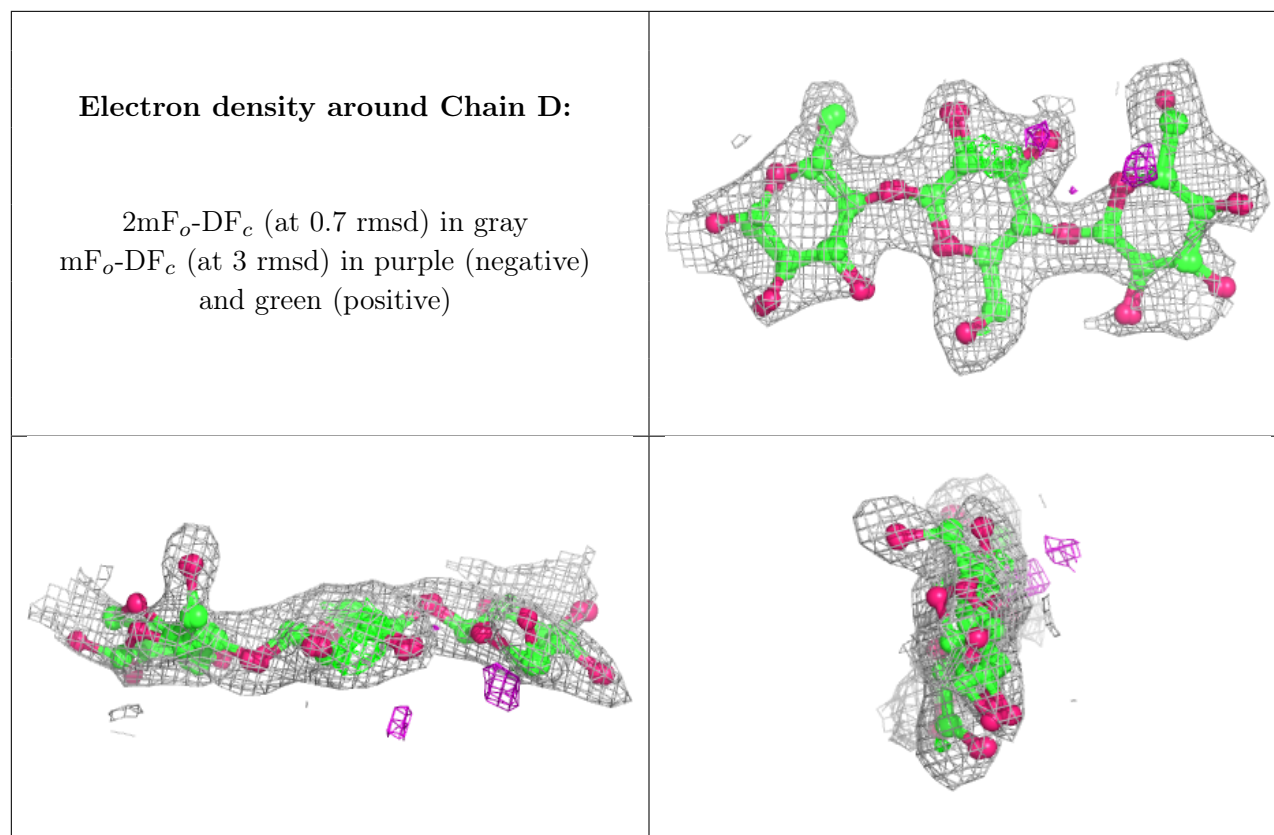
Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	BGC	D	3[B]	11/12	0.78	0.18	55,58,59,60	11
2	GLC	C	1	12/12	0.86	0.15	34,39,40,44	12
2	BGC	C	3	11/12	0.86	0.13	56,59,62,62	0
2	BGC	C	2	11/12	0.87	0.12	29,40,48,51	0
3	BGC	D	2[A]	11/12	0.89	0.15	43,48,54,55	11
3	BGC	D	2[B]	11/12	0.89	0.15	36,42,50,50	11
3	BGC	D	1[A]	11/12	0.89	0.17	49,54,57,57	11
3	BGC	D	1[B]	12/12	0.89	0.17	40,44,45,45	12

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.





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
4	GOL	B	1237	6/6	0.69	0.19	59,60,61,62	0
6	GLC	B	1003[B]	12/12	0.74	0.29	60,65,66,67	12
4	GOL	B	1002[A]	6/6	0.75	0.22	54,55,57,58	6
4	GOL	B	1001	6/6	0.77	0.16	68,69,69,70	0
4	GOL	A	1002	6/6	0.77	0.24	64,65,66,68	0
4	GOL	A	1001	6/6	0.78	0.18	61,62,63,64	0
4	GOL	A	1235	6/6	0.79	0.15	58,59,59,60	0
4	GOL	A	1003[B]	6/6	0.81	0.17	50,52,53,55	6
4	GOL	A	1003[A]	6/6	0.81	0.17	43,47,48,50	6
4	GOL	A	1234	6/6	0.84	0.17	53,59,61,63	0
5	SO4	A	1236	5/5	0.95	0.10	25,26,27,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.