



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:56 PM UTC

PDB ID : 2BVW / pdb_00002bvw
Title : CELLOBIOHYDROLASE II (CEL6A) FROM HUMICOLA INSOLENS IN
COMPLEX WITH GLUCOSE AND CELLOTETRAOSE
Authors : Varrot, A.; Davies, G.J.; Schulein, M.
Deposited on : 1999-02-18
Resolution : 1.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

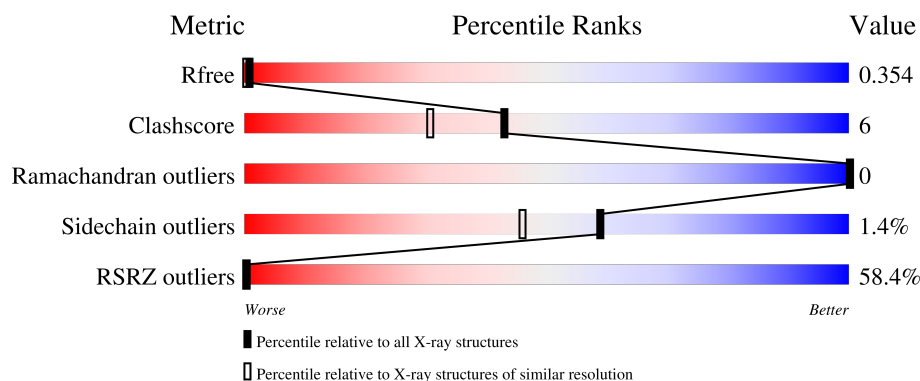
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	362	38% 85% 13% .
1	B	362	78% 86% 12% ..
2	C	4	50% 50%
3	D	3	100%

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
3	GLC	D	1	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6474 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 CELLOBIOHYDROLASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	8	0
			2850	1803	502	535	10			
1	B	360	Total	C	N	O	S	0	7	0
			2834	1795	493	536	10			

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



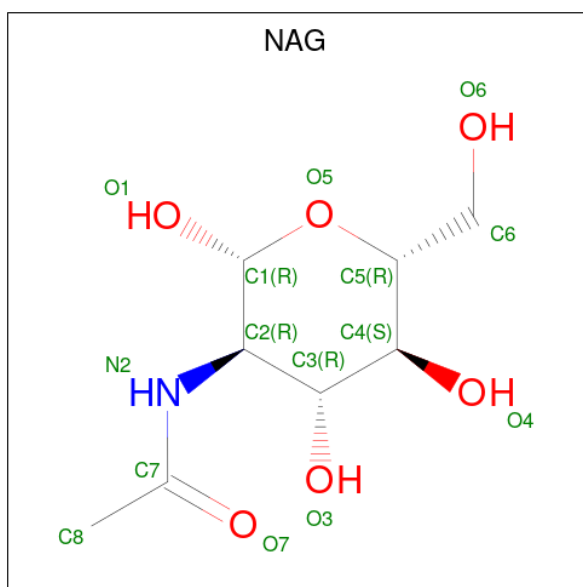
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	4	Total	C	O	0	0	0
			45	24	21			

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



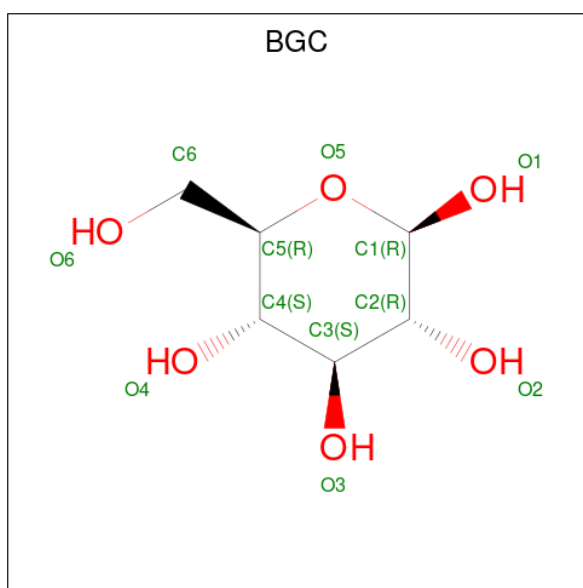
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



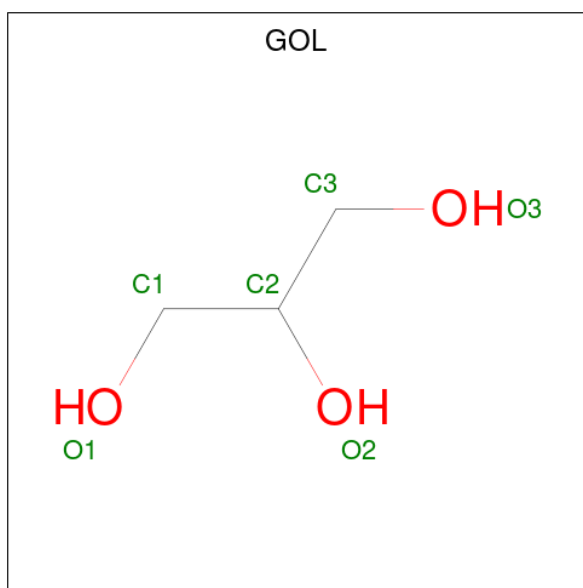
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is beta-D-glucopyranose (CCD ID: BGC) (formula: $C_6H_{12}O_6$).



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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

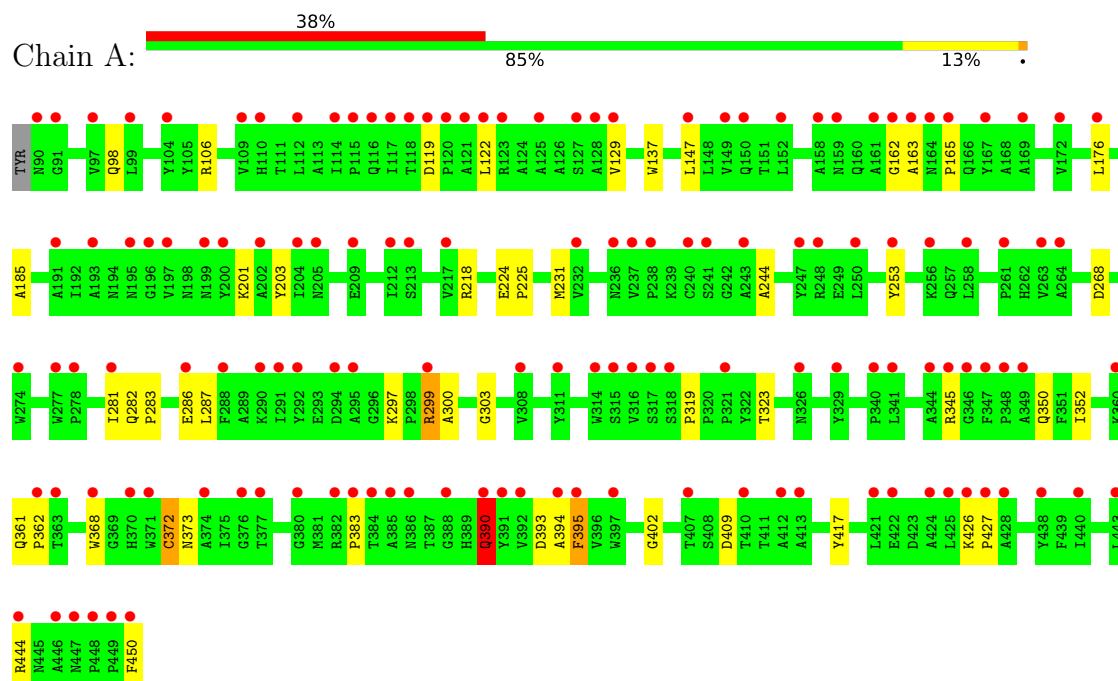
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	355	Total	O	0	0
			355	355		
7	B	262	Total	O	0	0
			262	262		

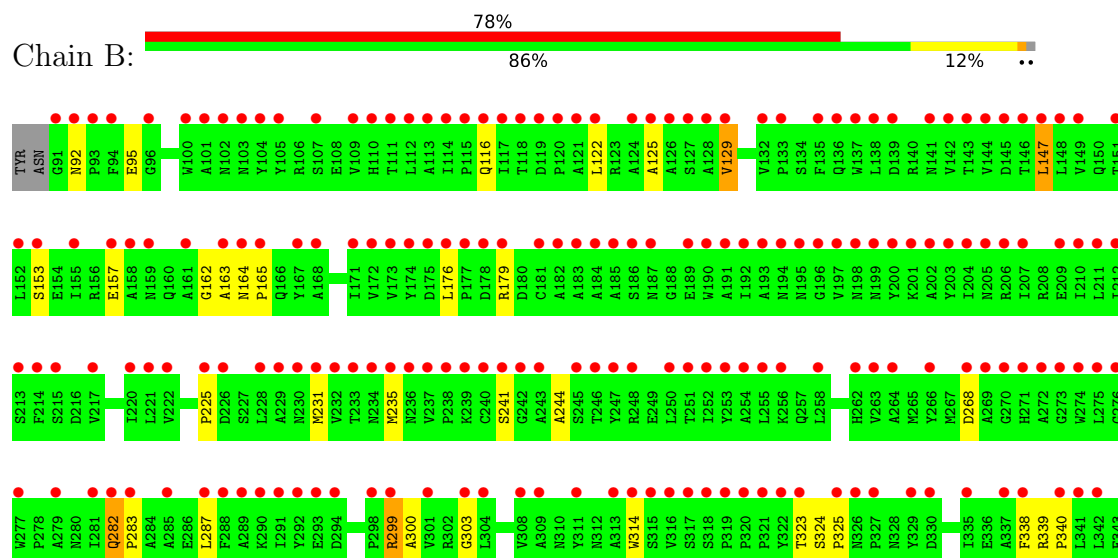
3 Residue-property plots

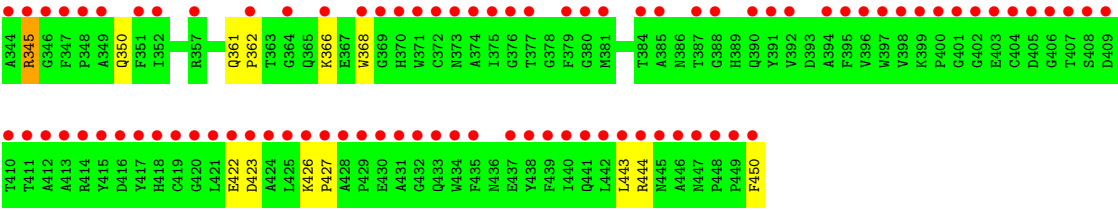
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: CELLOBIOHYDROLASE II



• Molecule 1: CELLOBIOHYDROLASE II





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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.56Å 154.43Å 51.04Å 90.00° 119.31° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 20.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	89.6 (20.00-1.70) 89.6 (20.00-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 1.67Å)	Xtriage
Refinement program	CCP4	Depositor
R, R_{free}	0.175 , 0.226 0.336 , 0.354	Depositor DCC
R_{free} test set	3313 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	13.7	Xtriage
Anisotropy	0.570	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	6474	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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, GOL, GLC, 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	0.56	0/2972	1.30	10/4063 (0.2%)
1	B	0.54	0/2951	1.27	4/4035 (0.1%)
All	All	0.55	0/5923	1.29	14/8098 (0.2%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	338	PHE	CA-CB-CG	8.61	122.41	113.80
1	B	314	TRP	N-CA-C	-8.31	102.17	111.14
1	A	390	GLN	CG-CD-NE2	7.60	127.80	116.40
1	A	390	GLN	OE1-CD-NE2	-6.60	116.00	122.60
1	A	372	CYS	N-CA-C	6.43	119.19	108.96
1	A	402	GLY	N-CA-C	-6.07	107.09	113.58
1	A	203	TYR	CA-CB-CG	5.70	124.16	113.90
1	A	281	ILE	N-CA-C	5.52	116.29	110.72
1	A	185	ALA	N-CA-C	5.47	117.25	111.28
1	A	319	PRO	N-CA-C	5.43	117.32	110.70
1	A	352	ILE	N-CA-CB	5.42	120.34	111.44
1	B	345	ARG	CD-NE-CZ	5.23	131.72	124.40
1	B	147	LEU	N-CA-C	5.22	116.97	111.28
1	A	395	PHE	N-CA-C	-5.09	101.42	109.76

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	2850	0	2721	37	4
1	B	2834	0	2697	33	3
2	C	45	0	39	0	0
3	D	34	0	30	1	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
5	A	12	0	12	1	0
5	B	12	0	12	0	0
6	A	36	0	48	3	0
6	B	6	0	8	0	0
7	A	355	0	0	2	7
7	B	262	0	0	6	1
All	All	6474	0	5593	71	8

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 6.

All (71) 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:129[A]:VAL:HG22	1:A:450:PHE:CZ	1.95	0.99
1:A:129[A]:VAL:HG22	1:A:450:PHE:CE2	2.10	0.87
1:B:299[B]:ARG:NH2	7:B:798:HOH:O	2.10	0.83
1:B:299[B]:ARG:NH1	7:B:858:HOH:O	2.15	0.79
1:A:286:GLU:HG2	1:A:345[B]:ARG:HE	1.50	0.77
1:A:390:GLN:H	1:A:390:GLN:HE21	1.34	0.76
1:B:444[A]:ARG:HG3	1:B:444[A]:ARG:HH11	1.51	0.75
1:B:129[A]:VAL:HG13	1:B:450:PHE:CZ	2.24	0.73
1:A:444[B]:ARG:HH11	1:A:444[B]:ARG:HG2	1.55	0.71
1:A:299[A]:ARG:HH11	1:A:299[A]:ARG:HG2	1.56	0.71
1:A:390:GLN:H	1:A:390:GLN:NE2	1.90	0.68
1:A:129[A]:VAL:HG22	1:A:450:PHE:CE1	2.30	0.66
1:B:92:ASN:O	1:B:95[B]:GLU:HG2	1.98	0.63
1:A:287:LEU:HD12	7:A:835:HOH:O	1.98	0.63
1:B:235:MET:O	1:B:241:SER:HB3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129[A]:VAL:HG21	1:B:443:LEU:HD21	1.83	0.60
1:A:426:LYS:HB3	1:A:427:PRO:HA	1.84	0.59
1:B:129[A]:VAL:CG2	1:B:443:LEU:HD21	2.34	0.58
1:B:444[A]:ARG:HG3	1:B:444[A]:ARG:NH1	2.15	0.58
1:B:225:PRO:HA	1:B:268:ASP:CB	2.35	0.57
1:A:106:ARG:HH22	6:A:605:GOL:H12	1.70	0.56
1:B:426:LYS:HB3	1:B:427:PRO:HA	1.86	0.56
7:B:610:HOH:O	3:D:1:GLC:H61	2.05	0.55
1:A:361:GLN:HA	1:A:362:PRO:C	2.32	0.53
1:B:129[A]:VAL:HG21	1:B:443:LEU:CD2	2.38	0.53
1:A:129[A]:VAL:CG2	1:A:450:PHE:CE2	2.88	0.52
1:A:282:GLN:O	1:A:286:GLU:HG3	2.10	0.52
1:B:125:ALA:O	1:B:129[A]:VAL:HG23	2.11	0.51
1:A:282:GLN:HB2	1:A:283:PRO:HD3	1.94	0.49
1:B:231:MET:SD	1:B:244:ALA:HA	2.53	0.49
1:A:299[A]:ARG:HG2	1:A:299[A]:ARG:NH1	2.27	0.48
1:A:303:GLY:HA3	1:A:350:GLN:O	2.13	0.48
1:A:225:PRO:HA	1:A:268:ASP:CG	2.39	0.48
1:A:225:PRO:HA	1:A:268:ASP:CB	2.44	0.47
1:B:366:LYS:HE3	1:B:423:ASP:HB3	1.96	0.47
1:B:225:PRO:HA	1:B:268:ASP:CG	2.40	0.47
1:B:366:LYS:HB3	7:B:609:HOH:O	2.14	0.47
1:B:176:LEU:O	1:B:179:ARG:HB2	2.15	0.46
1:A:299[A]:ARG:HG3	7:A:698:HOH:O	2.15	0.46
1:B:361:GLN:HA	1:B:362:PRO:C	2.40	0.46
1:A:444[B]:ARG:HG2	1:A:444[B]:ARG:NH1	2.24	0.46
1:B:122:LEU:HD22	1:B:444[B]:ARG:NH2	2.30	0.46
1:B:282:GLN:N	1:B:283:PRO:HD2	2.30	0.46
1:A:129[A]:VAL:HG22	1:A:450:PHE:CD2	2.51	0.45
1:A:286:GLU:HG2	1:A:345[A]:ARG:CZ	2.46	0.45
1:B:303:GLY:HA3	1:B:350:GLN:O	2.17	0.45
1:B:339:ARG:HB3	1:B:340:PRO:HD3	1.98	0.45
1:A:137:TRP:CE3	5:A:602:BGC:H5	2.52	0.45
1:B:299[A]:ARG:HG2	7:B:773:HOH:O	2.17	0.44
1:A:323:THR:HA	1:A:368:TRP:CE3	2.52	0.44
1:B:345:ARG:HH11	1:B:345:ARG:HG3	1.83	0.43
1:A:98:GLN:HG3	1:A:165:PRO:HG2	1.99	0.43
1:B:323:THR:HA	1:B:368:TRP:CE3	2.53	0.43
1:A:299[A]:ARG:HD2	1:A:300:ALA:N	2.33	0.43
1:A:372:CYS:O	1:A:373:ASN:C	2.61	0.43
1:A:383:PRO:HA	1:A:395:PHE:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:MET:SD	1:A:244:ALA:HA	2.59	0.43
1:B:162:GLY:O	1:B:163:ALA:C	2.59	0.43
1:A:417:TYR:HD1	6:A:610:GOL:HO3	1.66	0.42
1:B:324:SER:HA	1:B:325:PRO:HA	1.79	0.42
1:B:366:LYS:NZ	1:B:422:GLU:HB2	2.33	0.42
1:A:162:GLY:O	1:A:163:ALA:C	2.61	0.42
1:A:393:ASP:O	1:A:394:ALA:HB2	2.20	0.42
1:B:299[A]:ARG:HG3	1:B:300:ALA:N	2.34	0.42
1:A:176:LEU:HG	1:A:224:GLU:CD	2.46	0.41
1:A:218:ARG:CZ	6:A:609:GOL:H12	2.50	0.41
1:B:164:ASN:HA	1:B:165:PRO:C	2.46	0.41
1:B:147:LEU:HD23	7:B:676:HOH:O	2.21	0.41
1:B:116:GLN:HE21	1:B:116:GLN:HB3	1.68	0.41
1:A:129[A]:VAL:CG2	1:A:450:PHE:CD2	3.05	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:TYR:OH	7:A:824:HOH:O[1_454]	1.62	0.58
1:B:116:GLN:OE1	7:A:920:HOH:O[1_454]	1.97	0.23
7:A:860:HOH:O	7:B:711:HOH:O[1_656]	2.02	0.18
1:B:157[B]:GLU:CG	7:A:753:HOH:O[1_454]	2.04	0.16
1:A:119:ASP:OD1	7:A:694:HOH:O[1_656]	2.07	0.13
1:A:201:LYS:NZ	7:A:850:HOH:O[1_454]	2.14	0.06
1:B:153:SER:O	7:A:753:HOH:O[1_454]	2.18	0.02
1:A:297:LYS:NZ	1:A:409:ASP:OD1[1_554]	2.19	0.01

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	367/362 (101%)	356 (97%)	11 (3%)	0	100	100
1	B	365/362 (101%)	353 (97%)	12 (3%)	0	100	100
All	All	732/724 (101%)	709 (97%)	23 (3%)	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	296/289 (102%)	291 (98%)	5 (2%)	53	38
1	B	294/289 (102%)	288 (98%)	6 (2%)	48	32
All	All	590/578 (102%)	579 (98%)	11 (2%)	59	34

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	LEU
1	A	147	LEU
1	A	299[A]	ARG
1	A	299[B]	ARG
1	A	390	GLN
1	B	129[A]	VAL
1	B	129[B]	VAL
1	B	282	GLN
1	B	287	LEU
1	B	299[A]	ARG
1	B	299[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	164	ASN

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Mol	Chain	Res	Type
1	A	166	GLN
1	A	282	GLN
1	A	390	GLN
1	A	445	ASN
1	B	116	GLN
1	B	136	GLN
1	B	150	GLN
1	B	230	ASN
1	B	234	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 ⓘ

7 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	BGC	C	1	2	12,12,12	0.75	0	17,17,17	0.96	0
2	BGC	C	2	2	11,11,12	0.68	0	15,15,17	1.22	1 (6%)
2	BGC	C	3	2	11,11,12	0.43	0	15,15,17	1.11	1 (6%)
2	BGC	C	4	2	11,11,12	0.90	0	15,15,17	0.96	0
3	GLC	D	1	3	12,12,12	0.50	0	17,17,17	0.89	0
3	BGC	D	2	3	11,11,12	0.76	0	15,15,17	1.11	1 (6%)
3	BGC	D	3	3	11,11,12	0.51	0	15,15,17	0.83	1 (6%)

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	BGC	C	1	2	-	0/2/22/22	0/1/1/1
2	BGC	C	2	2	-	0/2/19/22	0/1/1/1
2	BGC	C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	C	4	2	-	0/2/19/22	0/1/1/1
3	GLC	D	1	3	1/1/5/5	0/2/22/22	0/1/1/1
3	BGC	D	2	3	-	0/2/19/22	0/1/1/1
3	BGC	D	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	BGC	O3-C3-C2	-3.07	103.79	110.05
3	D	2	BGC	C1-O5-C5	2.30	115.27	112.19
2	C	3	BGC	O3-C3-C2	-2.24	105.48	110.05
3	D	3	BGC	O5-C5-C4	-2.07	105.79	110.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	1	GLC	C1

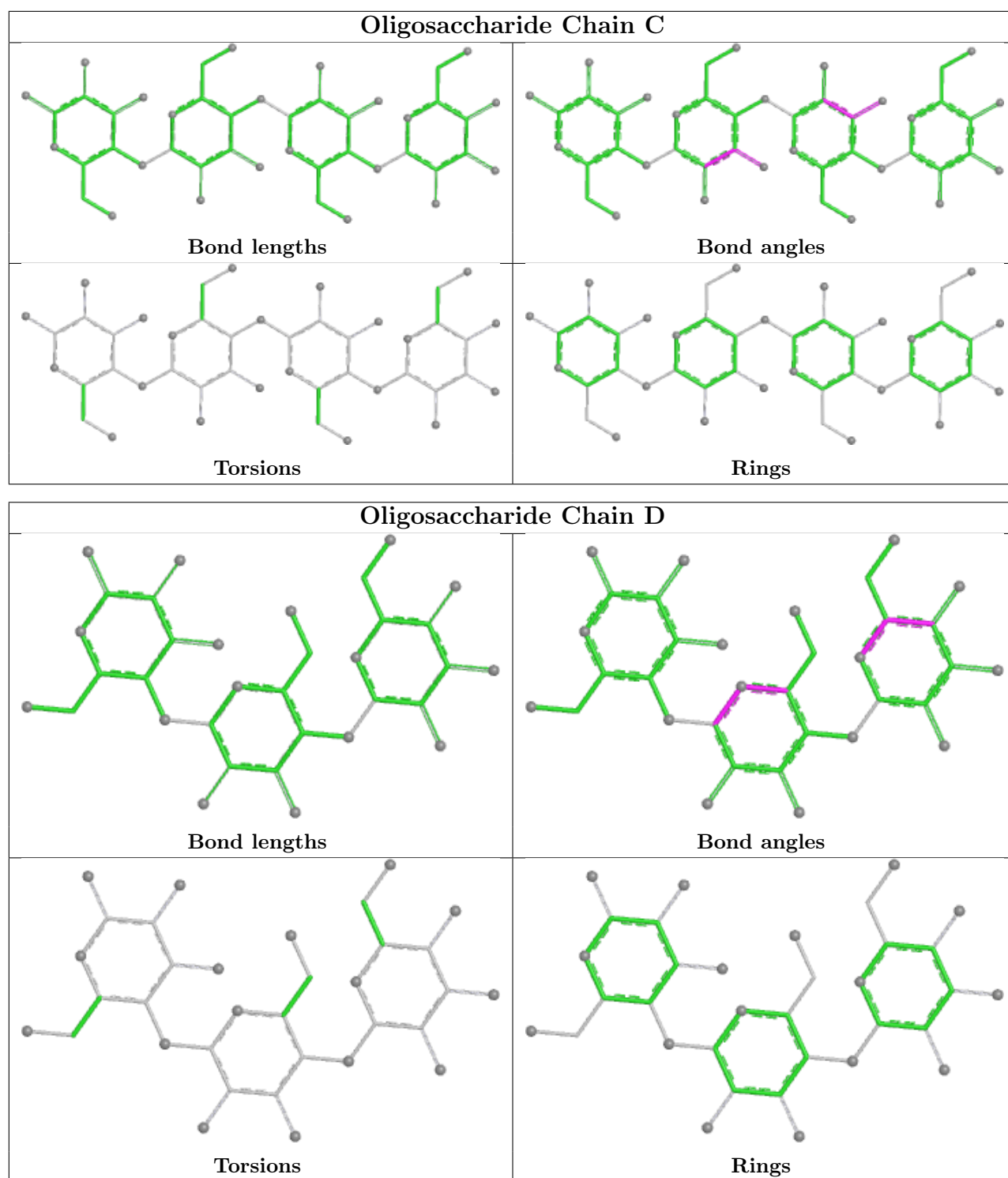
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	GLC	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](#)

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
6	GOL	A	605	-	5,5,5	0.43	0	5,5,5	0.84	0
4	NAG	A	500	1	14,14,15	1.12	1 (7%)	17,19,21	0.93	0
6	GOL	A	607	-	5,5,5	0.60	0	5,5,5	0.47	0
6	GOL	A	610	-	5,5,5	0.59	0	5,5,5	0.64	0
5	BGC	B	603	-	12,12,12	0.76	0	17,17,17	0.85	0
6	GOL	A	604	-	5,5,5	0.70	0	5,5,5	0.58	0
6	GOL	B	608	-	5,5,5	0.52	0	5,5,5	0.50	0
4	NAG	B	500	1	14,14,15	1.41	2 (14%)	17,19,21	1.19	1 (5%)
6	GOL	A	606	-	5,5,5	0.66	0	5,5,5	0.55	0
6	GOL	A	609	-	5,5,5	0.75	0	5,5,5	0.63	0
5	BGC	A	602	-	12,12,12	0.67	0	17,17,17	1.02	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	605	-	-	2/4/4/4	-
4	NAG	A	500	1	-	0/6/23/26	0/1/1/1
6	GOL	A	607	-	-	4/4/4/4	-
6	GOL	A	610	-	-	2/4/4/4	-
5	BGC	B	603	-	-	0/2/22/22	0/1/1/1
6	GOL	A	604	-	-	2/4/4/4	-
6	GOL	B	608	-	-	4/4/4/4	-
4	NAG	B	500	1	-	0/6/23/26	0/1/1/1
6	GOL	A	606	-	-	0/4/4/4	-
6	GOL	A	609	-	-	1/4/4/4	-
5	BGC	A	602	-	-	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)
4	B	500	NAG	O7-C7	-3.65	1.15	1.23
4	A	500	NAG	O7-C7	-3.51	1.15	1.23
4	B	500	NAG	C2-N2	2.05	1.49	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	500	NAG	O5-C1-C2	-2.17	107.94	111.29

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	607	GOL	O1-C1-C2-C3
6	A	610	GOL	C1-C2-C3-O3
6	B	608	GOL	C1-C2-C3-O3
6	A	607	GOL	O1-C1-C2-O2
6	A	605	GOL	C1-C2-C3-O3
6	A	607	GOL	C1-C2-C3-O3
6	B	608	GOL	O1-C1-C2-C3
6	B	608	GOL	O2-C2-C3-O3
6	A	610	GOL	O2-C2-C3-O3
6	A	604	GOL	O1-C1-C2-O2
6	A	605	GOL	O2-C2-C3-O3
6	A	607	GOL	O2-C2-C3-O3
6	A	609	GOL	O1-C1-C2-O2
6	B	608	GOL	O1-C1-C2-O2
6	A	604	GOL	O1-C1-C2-C3

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	605	GOL	1	0
6	A	610	GOL	1	0
6	A	609	GOL	1	0
5	A	602	BGC	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

6.1 Protein, DNA and RNA chains

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	361/362 (99%)	1.78	139 (38%) 1 0	8, 16, 27, 36	8 (2%)
1	B	360/362 (99%)	3.00	282 (78%) 0 0	9, 17, 28, 35	7 (1%)
All	All	721/724 (99%)	2.39	421 (58%) 0 0	8, 16, 27, 36	15 (2%)

All (421) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	412	ALA	10.0
1	B	191	ALA	7.5
1	B	190	TRP	7.4
1	B	120	PRO	6.3
1	B	175	ASP	6.3
1	B	194	ASN	6.1
1	B	420	GLY	6.1
1	A	120	PRO	5.8
1	B	115	PRO	5.7
1	B	193	ALA	5.7
1	B	148	LEU	5.7
1	B	184	ALA	5.7
1	A	161	ALA	5.7
1	B	147	LEU	5.7
1	B	192	ILE	5.6
1	B	404	CYS	5.6
1	A	121	ALA	5.5
1	B	434	TRP	5.4
1	A	449	PRO	5.4
1	B	413	ALA	5.3
1	B	432	GLY	5.3
1	B	309	ALA	5.3
1	A	344	ALA	5.3
1	B	202	ALA	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	371	TRP	5.2
1	B	407	THR	5.2
1	B	291	ILE	5.0
1	B	138	LEU	5.0
1	A	450	PHE	4.9
1	B	402	GLY	4.9
1	B	181	CYS	4.9
1	B	410	THR	4.9
1	B	421	LEU	4.8
1	B	182	ALA	4.8
1	A	119	ASP	4.7
1	B	112	LEU	4.7
1	B	425	LEU	4.7
1	A	195	ASN	4.6
1	B	199	ASN	4.6
1	B	207	ILE	4.6
1	B	118	THR	4.6
1	B	287	LEU	4.6
1	A	115	PRO	4.6
1	B	253	TYR	4.6
1	B	411	THR	4.6
1	A	443	LEU	4.6
1	B	177	PRO	4.6
1	B	195	ASN	4.5
1	B	440	ILE	4.5
1	B	419	CYS	4.5
1	B	142	VAL	4.5
1	B	183	ALA	4.5
1	B	212	ILE	4.4
1	B	236	ASN	4.4
1	B	247	TYR	4.4
1	B	245	SER	4.4
1	B	417	TYR	4.3
1	B	444[A]	ARG	4.3
1	B	272	ALA	4.3
1	B	275	LEU	4.3
1	B	237	VAL	4.3
1	B	377	THR	4.3
1	B	174	TYR	4.2
1	B	172	VAL	4.2
1	A	163	ALA	4.2
1	B	196	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	235	MET	4.1
1	B	435	PHE	4.1
1	B	441	GLN	4.1
1	A	321	PRO	4.1
1	B	232	VAL	4.1
1	B	316	VAL	4.1
1	B	198	ASN	4.1
1	B	228	LEU	4.0
1	B	311	TYR	4.0
1	B	438	TYR	4.0
1	A	256	LYS	4.0
1	B	114	ILE	4.0
1	B	121	ALA	4.0
1	B	137	TRP	4.0
1	A	90	ASN	4.0
1	B	214	PHE	4.0
1	B	301	VAL	4.0
1	B	428	ALA	4.0
1	B	335	ILE	3.9
1	A	314	TRP	3.9
1	B	415	TYR	3.9
1	B	424	ALA	3.9
1	B	197	VAL	3.9
1	B	104	TYR	3.9
1	B	385	ALA	3.9
1	B	231	MET	3.9
1	B	325	PRO	3.9
1	B	366	LYS	3.9
1	B	414	ARG	3.9
1	B	100	TRP	3.9
1	B	338	PHE	3.9
1	B	204	ILE	3.8
1	A	444[A]	ARG	3.8
1	A	374	ALA	3.8
1	B	126	ALA	3.8
1	A	291	ILE	3.8
1	B	109	VAL	3.8
1	A	424	ALA	3.8
1	B	185	ALA	3.8
1	B	144	VAL	3.8
1	B	173	VAL	3.8
1	A	422	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	425	LEU	3.8
1	B	238	PRO	3.8
1	B	94	PHE	3.7
1	B	277	TRP	3.7
1	B	250	LEU	3.7
1	A	237	VAL	3.7
1	B	233	THR	3.7
1	B	329	TYR	3.7
1	B	127	SER	3.7
1	B	397	TRP	3.6
1	B	210	ILE	3.6
1	B	321	PRO	3.6
1	B	242	GLY	3.6
1	B	230	ASN	3.5
1	A	91	GLY	3.5
1	B	187	ASN	3.5
1	B	292	TYR	3.5
1	B	293	GLU	3.5
1	B	110	HIS	3.5
1	B	122	LEU	3.5
1	B	153	SER	3.5
1	B	225	PRO	3.5
1	B	400	PRO	3.5
1	B	178	ASP	3.5
1	B	241	SER	3.5
1	B	246	THR	3.5
1	A	428	ALA	3.4
1	B	347	PHE	3.4
1	B	149	VAL	3.4
1	B	119	ASP	3.4
1	B	427	PRO	3.4
1	B	391	TYR	3.4
1	B	101	ALA	3.4
1	A	421	LEU	3.4
1	A	368	TRP	3.4
1	A	315	SER	3.4
1	B	201	LYS	3.4
1	A	122	LEU	3.4
1	B	369	GLY	3.4
1	A	118	THR	3.4
1	A	164	ASN	3.4
1	B	213[A]	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	128	ALA	3.3
1	B	254	ALA	3.3
1	B	431	ALA	3.3
1	B	379	PHE	3.3
1	B	368	TRP	3.3
1	A	114	ILE	3.3
1	A	340	PRO	3.3
1	B	348	PRO	3.3
1	B	113	ALA	3.3
1	B	128	ALA	3.3
1	B	344	ALA	3.3
1	A	281	ILE	3.3
1	B	437	GLU	3.3
1	A	197	VAL	3.3
1	B	430	GLU	3.2
1	B	105	TYR	3.2
1	A	410	THR	3.2
1	B	152	LEU	3.2
1	A	447	ASN	3.2
1	B	270	GLY	3.2
1	B	273	GLY	3.2
1	B	426	LYS	3.2
1	A	392	VAL	3.2
1	A	345[A]	ARG	3.2
1	B	251	THR	3.2
1	A	117	ILE	3.2
1	B	239	LYS	3.2
1	B	299[A]	ARG	3.2
1	B	303	GLY	3.2
1	B	269	ALA	3.2
1	B	439	PHE	3.2
1	B	418	HIS	3.2
1	B	111	THR	3.2
1	B	167	TYR	3.1
1	B	450	PHE	3.1
1	A	363	THR	3.1
1	B	317	SER	3.1
1	A	204	ILE	3.1
1	B	252	ILE	3.1
1	B	352	ILE	3.1
1	B	314	TRP	3.1
1	B	217	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	448	PRO	3.1
1	B	209	GLU	3.1
1	B	409	ASP	3.1
1	B	203	TYR	3.1
1	B	388	GLY	3.1
1	B	116	GLN	3.1
1	B	117	ILE	3.1
1	B	211	LEU	3.1
1	B	234	ASN	3.1
1	B	387	THR	3.1
1	B	351	PHE	3.1
1	A	232	VAL	3.0
1	B	448	PRO	3.0
1	B	380	GLY	3.0
1	B	200	TYR	3.0
1	B	171	ILE	3.0
1	A	427	PRO	3.0
1	B	165	PRO	3.0
1	B	376	GLY	3.0
1	A	329	TYR	3.0
1	A	169	ALA	3.0
1	A	440	ILE	3.0
1	A	318	SER	3.0
1	B	340	PRO	3.0
1	A	380	GLY	3.0
1	A	384	THR	3.0
1	A	348	PRO	3.0
1	B	319	PRO	3.0
1	B	362	PRO	3.0
1	B	429	PRO	3.0
1	A	116	GLN	2.9
1	B	323	THR	2.9
1	B	161	ALA	2.9
1	B	129[A]	VAL	2.9
1	B	143	THR	2.9
1	B	243	ALA	2.9
1	B	394	ALA	2.9
1	A	341	LEU	2.9
1	B	176	LEU	2.9
1	B	342	LEU	2.9
1	B	370	HIS	2.9
1	B	146	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	392	VAL	2.9
1	B	349	ALA	2.9
1	B	322	TYR	2.9
1	A	376	GLY	2.9
1	B	416	ASP	2.9
1	B	103	ASN	2.9
1	A	104	TYR	2.8
1	B	408	SER	2.8
1	B	390	GLN	2.8
1	A	346	GLY	2.8
1	B	91	GLY	2.8
1	B	318	SER	2.8
1	B	449	PRO	2.8
1	B	151	THR	2.8
1	A	274	TRP	2.8
1	B	274	TRP	2.8
1	B	364	GLY	2.8
1	B	107	SER	2.8
1	A	316	VAL	2.8
1	A	362	PRO	2.8
1	B	240	CYS	2.8
1	B	375	ILE	2.8
1	A	162	GLY	2.8
1	A	191	ALA	2.7
1	A	129[A]	VAL	2.7
1	B	226	ASP	2.7
1	A	241	SER	2.7
1	A	217	VAL	2.7
1	B	258	LEU	2.7
1	B	155	ILE	2.7
1	B	220	ILE	2.7
1	B	163	ALA	2.7
1	B	179	ARG	2.7
1	B	288	PHE	2.7
1	B	308	VAL	2.7
1	A	264	ALA	2.7
1	B	283	PRO	2.6
1	B	186	SER	2.6
1	B	135	PHE	2.6
1	B	205	ASN	2.6
1	B	132	VAL	2.6
1	A	212	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	202	ALA	2.6
1	B	158	ALA	2.6
1	A	278	PRO	2.6
1	A	347	PHE	2.6
1	A	176	LEU	2.6
1	B	422	GLU	2.6
1	A	290	LYS	2.6
1	A	360	LYS	2.6
1	A	383	PRO	2.6
1	B	399	LYS	2.6
1	B	276	GLY	2.6
1	B	345	ARG	2.6
1	B	423	ASP	2.6
1	B	136	GLN	2.6
1	A	110	HIS	2.6
1	A	370	HIS	2.6
1	B	381	MET	2.6
1	A	158	ALA	2.6
1	A	193	ALA	2.6
1	B	374	ALA	2.6
1	B	320	PRO	2.6
1	B	406	GLY	2.5
1	A	407	THR	2.5
1	B	442	LEU	2.5
1	B	403	GLU	2.5
1	B	304	LEU	2.5
1	B	266	TYR	2.5
1	B	168	ALA	2.5
1	B	313	ALA	2.5
1	B	357	ARG	2.5
1	A	386	ASN	2.5
1	B	268	ASP	2.5
1	B	446	ALA	2.5
1	B	96	GLY	2.5
1	B	281	ILE	2.5
1	B	157[A]	GLU	2.4
1	A	438	TYR	2.4
1	B	447	ASN	2.4
1	A	294	ASP	2.4
1	A	277	TRP	2.4
1	B	298	PRO	2.4
1	B	289	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	373	ASN	2.4
1	A	253	TYR	2.4
1	A	388	GLY	2.4
1	B	327	PRO	2.4
1	A	385	ALA	2.4
1	A	299[A]	ARG	2.4
1	A	308	VAL	2.4
1	B	396	VAL	2.4
1	B	262	HIS	2.4
1	A	258	LEU	2.3
1	A	394	ALA	2.3
1	B	206	ARG	2.3
1	B	294	ASP	2.3
1	A	247	TYR	2.3
1	A	150[A]	GLN	2.3
1	B	92	ASN	2.3
1	B	102	ASN	2.3
1	A	248	ARG	2.3
1	A	240	CYS	2.3
1	B	372	CYS	2.3
1	A	152	LEU	2.3
1	A	288	PHE	2.3
1	A	395	PHE	2.3
1	A	205	ASN	2.3
1	B	159	ASN	2.3
1	A	286	GLU	2.3
1	A	97	VAL	2.3
1	A	263	VAL	2.3
1	A	426	LYS	2.3
1	A	390	GLN	2.3
1	A	99	LEU	2.3
1	B	395	PHE	2.3
1	A	196	GLY	2.3
1	A	238	PRO	2.2
1	B	271	HIS	2.2
1	B	282	GLN	2.2
1	B	445	ASN	2.2
1	B	255	LEU	2.2
1	A	317	SER	2.2
1	B	145	ASP	2.2
1	A	292	TYR	2.2
1	A	311	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	433	GLN	2.2
1	A	165	PRO	2.2
1	A	397	TRP	2.2
1	B	125	ALA	2.2
1	B	337	ALA	2.2
1	B	215	SER	2.2
1	A	112	LEU	2.2
1	B	221	LEU	2.2
1	A	209	GLU	2.2
1	B	93	PRO	2.2
1	B	384	THR	2.2
1	A	109	VAL	2.2
1	A	172	VAL	2.2
1	B	222	VAL	2.2
1	A	125	ALA	2.2
1	A	446	ALA	2.2
1	B	279	ALA	2.2
1	B	330	ASP	2.2
1	A	371	TRP	2.2
1	B	189	GLU	2.2
1	B	341	LEU	2.2
1	A	123	ARG	2.2
1	B	164	ASN	2.2
1	A	167	TYR	2.2
1	A	391	TYR	2.2
1	B	290	LYS	2.2
1	A	261	PRO	2.2
1	A	127[A]	SER	2.2
1	B	229	ALA	2.1
1	A	382[A]	ARG	2.1
1	B	346	GLY	2.1
1	B	443	LEU	2.1
1	A	326	ASN	2.1
1	B	405	ASP	2.1
1	A	413	ALA	2.1
1	B	124	ALA	2.1
1	B	285	ALA	2.1
1	A	159	ASN	2.1
1	A	199	ASN	2.1
1	B	141	ASN	2.1
1	A	213	SER	2.1
1	A	200	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	243	ALA	2.1
1	B	263	VAL	2.1
1	B	326	ASN	2.1
1	A	377	THR	2.1
1	B	401	GLY	2.0
1	A	236	ASN	2.0
1	A	295	ALA	2.0
1	A	349	ALA	2.0
1	B	139	ASP	2.0
1	B	248	ARG	2.0
1	B	315	SER	2.0
1	A	147	LEU	2.0
1	A	250	LEU	2.0
1	B	133	PRO	2.0
1	B	256	LYS	2.0
1	A	412	ALA	2.0
1	B	264	ALA	2.0
1	A	149	VAL	2.0
1	B	398	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

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

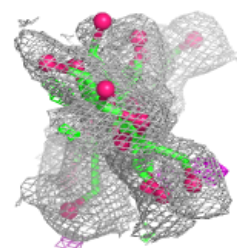
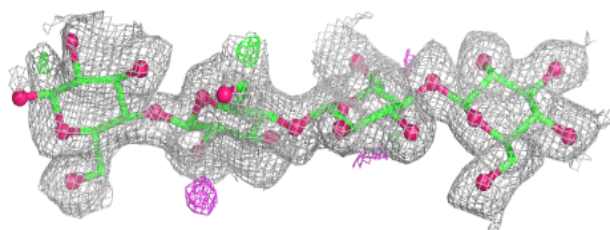
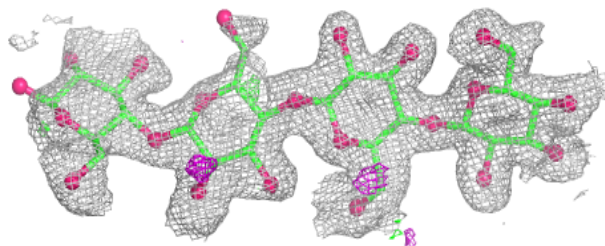
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BGC	D	3	11/12	0.55	0.18	11,15,16,18	0
3	BGC	D	2	11/12	0.66	0.15	16,18,20,22	0
3	GLC	D	1	12/12	0.66	0.17	23,30,32,32	0
2	BGC	C	2	11/12	0.73	0.15	21,25,27,29	0
2	BGC	C	1	12/12	0.79	0.14	29,31,33,35	1
2	BGC	C	3	11/12	0.86	0.09	12,15,18,19	0
2	BGC	C	4	11/12	0.90	0.09	10,13,14,15	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.

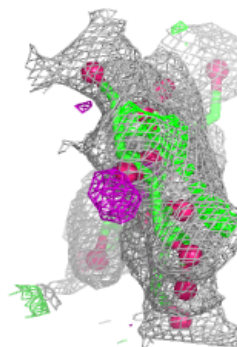
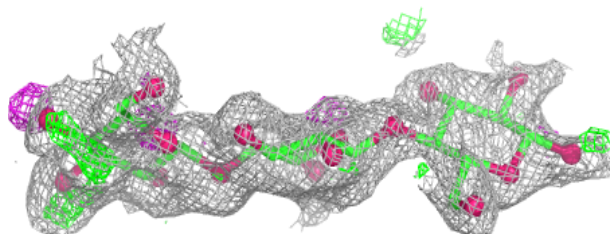
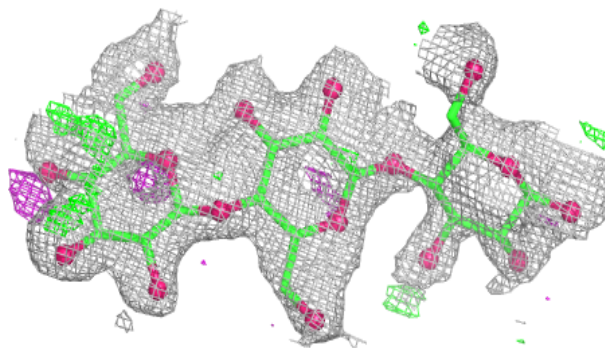
Electron density around Chain C:

$2mF_o-DF_c$ (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
6	GOL	B	608	6/6	0.20	0.25	44,44,45,45	0
4	NAG	B	500	14/15	0.53	0.20	24,26,28,29	0
6	GOL	A	607	6/6	0.54	0.23	27,33,33,33	0
5	BGC	B	603	12/12	0.56	0.18	11,13,14,15	0
6	GOL	A	604	6/6	0.63	0.18	24,27,28,31	0
6	GOL	A	609	6/6	0.65	0.18	30,31,33,35	0
6	GOL	A	610	6/6	0.68	0.20	33,36,38,40	0
6	GOL	A	605	6/6	0.74	0.18	20,26,26,26	0
6	GOL	A	606	6/6	0.74	0.17	19,21,22,24	0
4	NAG	A	500	14/15	0.78	0.13	15,20,22,24	0
5	BGC	A	602	12/12	0.81	0.10	8,11,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.