



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 11:49 pm GMT

PDB ID : 2BVW
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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

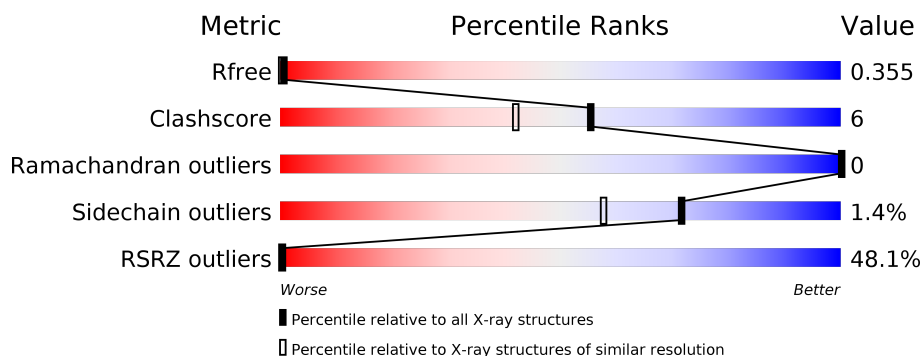
1 Overall quality at a glance

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}	100719	3453 (1.70-1.70)
Clashscore	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (1.70-1.70)
RSRZ outliers	101464	3491 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>29%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
1	B	362	<div> <div>67%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>

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
5	GOL	A	604	-	-	-	X
5	GOL	A	610	-	-	-	X
6	CTR	B	601	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.

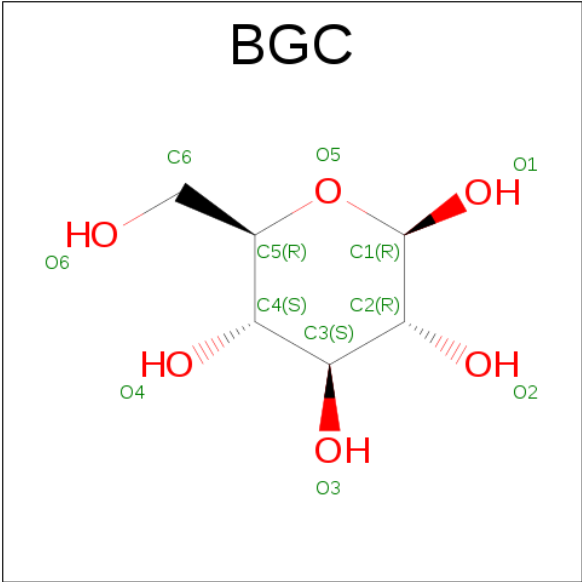
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	8	0
			2850	1803	502	535	10			
1	B	360	Total	C	N	O	S	0	7	0
			2834	1795	493	536	10			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



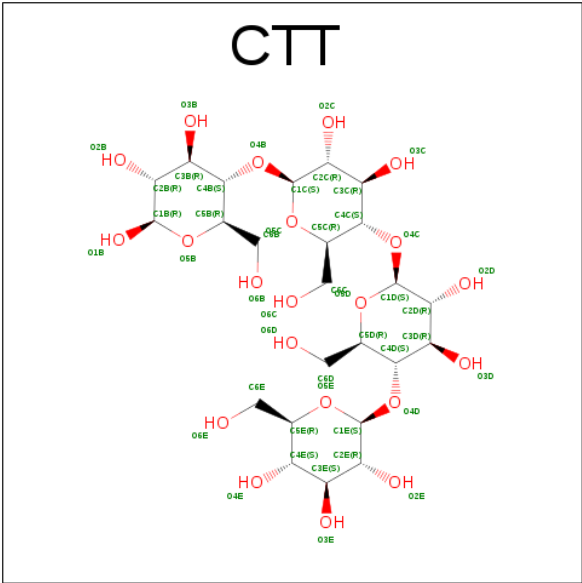
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is GLUCOSE (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



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

- Molecule 4 is CELLOTETRAOSE (three-letter code: CTT) (formula: C₂₄H₄₂O₂₁).



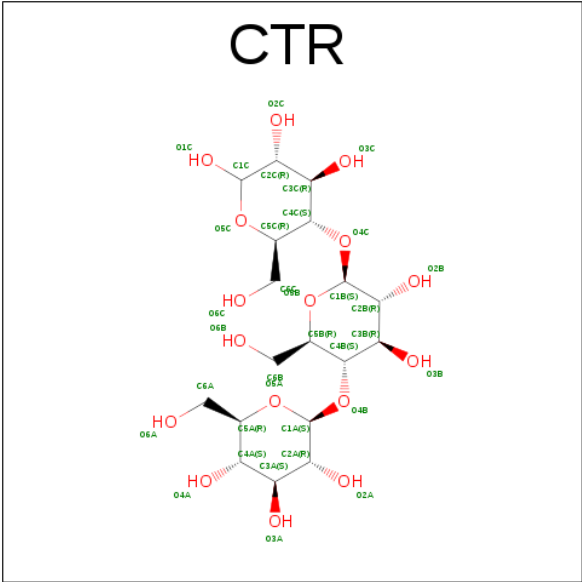
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			45	24	21		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is SUGAR (CELLOTRIOSE) (three-letter code: CTR) (formula: C₁₈H₃₂O₁₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			34	18	16		

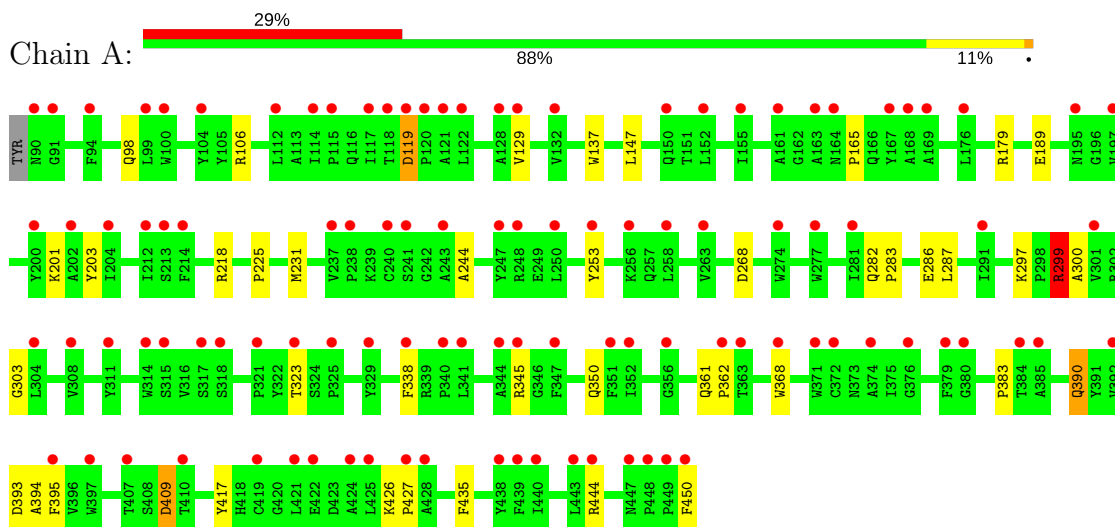
- Molecule 7 is water.

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

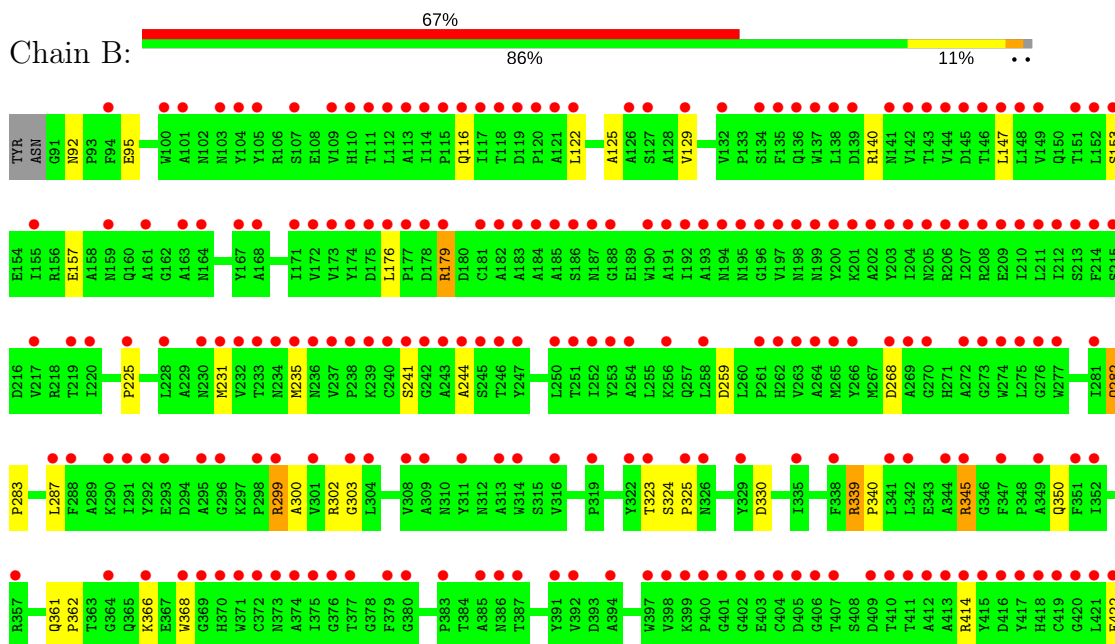
3 Residue-property plots

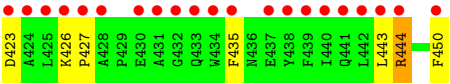
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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





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 19.80 – 1.67	Depositor EDS
% Data completeness (in resolution range)	89.6 (20.00-1.70) 86.3 (19.80-1.67)	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 , 0.355	Depositor DCC
R_{free} test set	3278 reflections (5.10%)	DCC
Wilson B-factor (Å ²)	13.7	Xtriage
Anisotropy	0.570	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.4	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: CTT, GOL, BGC, NAG, CTR

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	0.44	0/2972	1.03	8/4063 (0.2%)
1	B	0.44	0/2951	1.02	11/4035 (0.3%)
All	All	0.44	0/5923	1.03	19/8098 (0.2%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	ASP	CB-CG-OD1	8.05	125.55	118.30
1	A	299[A]	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	A	299[B]	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	B	330	ASP	CB-CG-OD1	7.14	124.72	118.30
1	B	345	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	B	414	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	B	345	ARG	CD-NE-CZ	5.80	131.72	123.60
1	B	259	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	189	GLU	OE1-CD-OE2	-5.71	116.45	123.30
1	A	203	TYR	CA-CB-CG	5.66	124.16	113.40
1	A	409	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	B	444[A]	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	B	444[B]	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	179	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	140	ARG	NE-CZ-NH2	5.37	122.98	120.30
1	B	302	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	B	339	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	338	PHE	CB-CG-CD2	-5.30	117.09	120.80
1	B	179	ARG	NE-CZ-NH1	5.30	122.95	120.30

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	35	4
1	B	2834	0	2697	32	3
2	A	14	0	13	0	0
2	B	14	0	13	0	0
3	A	12	0	12	1	0
3	B	12	0	12	0	0
4	A	45	0	42	0	0
5	A	36	0	48	3	0
5	B	6	0	8	0	0
6	B	34	0	32	1	0
7	A	355	0	0	3	7
7	B	262	0	0	7	1
All	All	6474	0	5598	68	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 (68) 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:444[B]:ARG:NH1	7:A:722:HOH:O	1.81	1.14
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[A]:ARG:NH2	7:B:858:HOH:O	2.12	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:HE21	1:A:390:GLN:H	1.34	0.76
1:B:444[A]:ARG:HH11	1:B:444[A]:ARG:HG3	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:HG2	1:A:299[A]:ARG:HH11	1.56	0.71
1:A:390:GLN:NE2	1:A:390:GLN:H	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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	5:A:605:GOL:H12	1.70	0.56
1:B:426:LYS:HB3	1:B:427:PRO:HA	1.86	0.56
6:B:601:CTR:H6C1	7:B:610:HOH:O	2.05	0.55
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:A:361:GLN:HA	1:A:362:PRO:C	2.32	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:CB	2.44	0.47
1:B:366:LYS:HE3	1:B:423:ASP:HB3	1.96	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:A:444[B]:ARG:NH1	1:A:444[B]:ARG:HG2	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	3: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:225:PRO:HA	1:A:268:ASP:CG	2.39	0.43
1:A:299[A]:ARG:HD2	1:A:300:ALA:N	2.33	0.43
1:A:383:PRO:HA	1:A:395:PHE:O	2.19	0.43
1:A:231:MET:SD	1:A:244:ALA:HA	2.59	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:TYR:HD1	5: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:B:361:GLN:HA	1:B:362:PRO:C	2.40	0.42
1:B:225:PRO:HA	1:B:268:ASP:CG	2.40	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:218:ARG:CZ	5:A:609:GOL:H12	2.50	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	66	50
1	B	294/289 (102%)	289 (98%)	5 (2%)	66	50
All	All	590/578 (102%)	580 (98%)	10 (2%)	71	50

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	LEU
1	A	299[A]	ARG
1	A	299[B]	ARG
1	A	390	GLN
1	A	435	PHE
1	B	282	GLN
1	B	287	LEU
1	B	299[A]	ARG
1	B	299[B]	ARG
1	B	435	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	166	GLN
1	A	390	GLN
1	A	445	ASN
1	B	116	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	136	GLN
1	B	166	GLN
1	B	230	ASN
1	B	234	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

13 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	$\# Z > 2$
2	NAG	A	500	1	14,14,15	1.07	1 (7%)	15,19,21	0.90	0
4	CTT	A	600	-	48,48,48	0.64	0	71,71,71	1.19	4 (5%)
3	BGC	A	602	-	12,12,12	0.67	0	17,17,17	1.07	0
5	GOL	A	604	-	5,5,5	0.65	0	5,5,5	0.51	0
5	GOL	A	605	-	5,5,5	0.40	0	5,5,5	0.77	0
5	GOL	A	606	-	5,5,5	0.62	0	5,5,5	0.49	0
5	GOL	A	607	-	5,5,5	0.55	0	5,5,5	0.41	0
5	GOL	A	609	-	5,5,5	0.73	0	5,5,5	0.59	0
5	GOL	A	610	-	5,5,5	0.55	0	5,5,5	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	500	1	14,14,15	1.36	1 (7%)	15,19,21	1.21	1 (6%)
6	CTR	B	601	-	36,36,36	0.51	0	53,53,53	1.00	2 (3%)
3	BGC	B	603	-	12,12,12	0.77	0	17,17,17	0.88	0
5	GOL	B	608	-	5,5,5	0.47	0	5,5,5	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	500	1	-	0/6/23/26	0/1/1/1
4	CTT	A	600	-	-	0/20/100/100	0/4/4/4
3	BGC	A	602	-	-	0/2/22/22	0/1/1/1
5	GOL	A	604	-	-	0/4/4/4	0/0/0/0
5	GOL	A	605	-	-	0/4/4/4	0/0/0/0
5	GOL	A	606	-	-	0/4/4/4	0/0/0/0
5	GOL	A	607	-	-	0/4/4/4	0/0/0/0
5	GOL	A	609	-	-	0/4/4/4	0/0/0/0
5	GOL	A	610	-	-	0/4/4/4	0/0/0/0
2	NAG	B	500	1	-	0/6/23/26	0/1/1/1
6	CTR	B	601	-	1/1/15/15	0/14/74/74	0/3/3/3
3	BGC	B	603	-	-	0/2/22/22	0/1/1/1
5	GOL	B	608	-	-	0/4/4/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	NAG	O7-C7	-3.49	1.15	1.23
2	A	500	NAG	O7-C7	-3.35	1.15	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	CTT	O3C-C3C-C2C	-3.02	103.79	110.36
2	B	500	NAG	O5-C1-C2	-2.54	107.94	111.47
6	B	601	CTR	O4B-C1A-O5A	-2.45	104.76	110.70
4	A	600	CTT	O3D-C3D-C2D	-2.24	105.48	110.36
6	B	601	CTR	O5A-C5A-C4A	-2.10	105.79	109.66
4	A	600	CTT	O4C-C4C-C3C	2.13	112.31	107.19
4	A	600	CTT	O4D-C4D-C3D	2.22	112.53	107.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	601	CTR	C1C

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	BGC	1	0
5	A	605	GOL	1	0
5	A	609	GOL	1	0
5	A	610	GOL	1	0
6	B	601	CTR	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%)	1.51	105 (29%) 1 0	8, 16, 27, 36	0
1	B	360/362 (99%)	2.98	242 (67%) 0 0	9, 17, 28, 35	0
All	All	721/724 (99%)	2.24	347 (48%) 0 0	8, 17, 27, 36	0

All (347) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	194	ASN	11.6
1	B	412	ALA	11.3
1	B	190	TRP	9.8
1	B	413	ALA	8.5
1	B	191	ALA	8.4
1	B	404	CYS	7.3
1	B	238	PRO	7.1
1	B	411	THR	6.8
1	B	163	ALA	6.8
1	B	434	TRP	6.7
1	B	420	GLY	6.5
1	B	193	ALA	6.3
1	B	118	THR	6.2
1	B	192	ILE	6.2
1	B	235	MET	6.2
1	B	253	TYR	6.1
1	B	371	TRP	6.1
1	B	115	PRO	5.8
1	B	291	ILE	5.8
1	B	231	MET	5.8
1	B	184	ALA	5.8
1	B	410	THR	5.7
1	B	142	VAL	5.6
1	A	120	PRO	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	207	ILE	5.6
1	B	245	SER	5.5
1	B	177	PRO	5.5
1	B	147	LEU	5.5
1	A	450	PHE	5.4
1	B	236	ASN	5.3
1	B	112	LEU	5.3
1	B	414	ARG	5.2
1	B	181	CYS	5.2
1	B	104	TYR	5.1
1	B	287	LEU	5.1
1	B	204	ILE	5.1
1	B	187	ASN	5.1
1	B	149	VAL	5.0
1	B	275	LEU	5.0
1	B	148	LEU	4.9
1	B	175	ASP	4.9
1	B	254	ALA	4.9
1	B	199	ASN	4.8
1	B	213[A]	SER	4.8
1	B	424	ALA	4.8
1	B	385	ALA	4.8
1	B	435	PHE	4.8
1	B	440	ILE	4.7
1	B	247	TYR	4.7
1	B	174	TYR	4.7
1	B	195	ASN	4.7
1	B	242	GLY	4.7
1	B	421	LEU	4.7
1	B	309	ALA	4.7
1	B	198	ASN	4.6
1	B	428	ALA	4.5
1	B	419	CYS	4.5
1	B	417	TYR	4.5
1	B	127	SER	4.5
1	B	214	PHE	4.4
1	B	212	ILE	4.4
1	B	228	LEU	4.4
1	B	144	VAL	4.4
1	B	182	ALA	4.4
1	B	432	GLY	4.4
1	A	443	LEU	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	311	TYR	4.3
1	B	203	TYR	4.3
1	B	415	TYR	4.3
1	B	202	ALA	4.3
1	B	197	VAL	4.3
1	A	204	ILE	4.2
1	B	402	GLY	4.2
1	B	246	THR	4.2
1	B	335	ILE	4.2
1	B	137	TRP	4.2
1	B	126	ALA	4.2
1	B	120	PRO	4.2
1	B	138	LEU	4.2
1	B	400	PRO	4.1
1	B	196	GLY	4.1
1	B	425	LEU	4.1
1	B	338	PHE	4.1
1	A	161	ALA	4.1
1	B	299[A]	ARG	4.0
1	A	121	ALA	4.0
1	B	230	ASN	4.0
1	B	450	PHE	4.0
1	B	352	ILE	4.0
1	B	368	TRP	4.0
1	B	200	TYR	4.0
1	B	438	TYR	4.0
1	B	292	TYR	3.9
1	B	252	ILE	3.9
1	B	100	TRP	3.9
1	B	377	THR	3.9
1	B	272	ALA	3.8
1	B	316	VAL	3.8
1	B	430	GLU	3.8
1	B	407	THR	3.8
1	B	173	VAL	3.8
1	A	374	ALA	3.8
1	A	176	LEU	3.8
1	B	351	PHE	3.7
1	B	277	TRP	3.7
1	B	209	GLU	3.7
1	B	234	ASN	3.7
1	B	418	HIS	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	439	PHE	3.7
1	B	269	ALA	3.7
1	B	397	TRP	3.7
1	B	172	VAL	3.7
1	B	210	ILE	3.6
1	A	444[A]	ARG	3.6
1	B	122	LEU	3.6
1	B	109	VAL	3.6
1	B	111	THR	3.5
1	B	152	LEU	3.5
1	B	431	ALA	3.5
1	B	132	VAL	3.5
1	A	344	ALA	3.5
1	B	341	LEU	3.5
1	B	369	GLY	3.5
1	A	195	ASN	3.5
1	B	250	LEU	3.5
1	B	117	ILE	3.5
1	B	444[A]	ARG	3.4
1	B	129[A]	VAL	3.4
1	B	232	VAL	3.4
1	B	329	TYR	3.4
1	B	178	ASP	3.4
1	B	256	LYS	3.4
1	B	301	VAL	3.4
1	A	281	ILE	3.4
1	A	164	ASN	3.4
1	A	314	TRP	3.4
1	B	243	ALA	3.3
1	A	424	ALA	3.3
1	B	183	ALA	3.3
1	B	441	GLN	3.3
1	B	322	TYR	3.3
1	B	105	TYR	3.3
1	A	115	PRO	3.3
1	B	208	ARG	3.3
1	B	442	LEU	3.3
1	B	185	ALA	3.3
1	B	263	VAL	3.2
1	B	239	LYS	3.2
1	B	394	ALA	3.2
1	B	241	SER	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	113	ALA	3.2
1	B	201	LYS	3.2
1	B	94	PHE	3.2
1	B	288	PHE	3.2
1	B	206	ARG	3.2
1	A	114	ILE	3.2
1	B	409	ASP	3.2
1	B	146	THR	3.1
1	A	152	LEU	3.1
1	A	425	LEU	3.1
1	B	374	ALA	3.1
1	B	274	TRP	3.1
1	B	392	VAL	3.1
1	B	296	GLY	3.1
1	B	136	GLN	3.1
1	B	211	LEU	3.1
1	B	426	LYS	3.1
1	A	247	TYR	3.1
1	B	391	TYR	3.1
1	B	114	ILE	3.0
1	B	171	ILE	3.0
1	A	163	ALA	3.0
1	B	240	CYS	3.0
1	B	347	PHE	3.0
1	B	375	ILE	3.0
1	A	345[A]	ARG	3.0
1	A	91	GLY	3.0
1	B	153	SER	3.0
1	B	176	LEU	3.0
1	B	437	GLU	3.0
1	B	372	CYS	3.0
1	A	129[A]	VAL	3.0
1	A	392	VAL	3.0
1	B	103	ASN	2.9
1	A	122	LEU	2.9
1	B	237	VAL	2.9
1	B	119	ASP	2.9
1	A	214	PHE	2.9
1	A	351	PHE	2.9
1	B	303	GLY	2.9
1	A	99	LEU	2.9
1	A	169	ALA	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	101	ALA	2.9
1	B	370	HIS	2.9
1	A	438	TYR	2.9
1	B	379	PHE	2.9
1	B	308	VAL	2.9
1	B	268	ASP	2.9
1	B	205	ASN	2.9
1	A	197	VAL	2.8
1	A	321	PRO	2.8
1	B	323	THR	2.8
1	B	349	ALA	2.8
1	B	366	LYS	2.8
1	B	143	THR	2.8
1	B	270	GLY	2.8
1	B	273	GLY	2.8
1	B	110	HIS	2.8
1	B	398	VAL	2.8
1	A	363	THR	2.8
1	A	379	PHE	2.8
1	B	233	THR	2.8
1	B	159	ASN	2.8
1	A	304	LEU	2.7
1	B	293	GLU	2.7
1	A	440	ILE	2.7
1	B	251	THR	2.7
1	B	167	TYR	2.7
1	B	217	VAL	2.7
1	A	119	ASP	2.7
1	B	141	ASN	2.7
1	A	428	ALA	2.7
1	A	371	TRP	2.7
1	A	447	ASN	2.7
1	A	238	PRO	2.6
1	B	225	PRO	2.6
1	B	399	LYS	2.6
1	B	427	PRO	2.6
1	A	243	ALA	2.6
1	B	357	ARG	2.6
1	A	449	PRO	2.6
1	A	258	LEU	2.6
1	B	161	ALA	2.6
1	B	107	SER	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	179	ARG	2.6
1	A	291	ILE	2.6
1	A	202	ALA	2.6
1	A	421	LEU	2.6
1	B	262	HIS	2.6
1	B	151	THR	2.5
1	A	352	ILE	2.5
1	B	220	ILE	2.5
1	B	325	PRO	2.5
1	B	342	LEU	2.5
1	A	167	TYR	2.5
1	A	200	TYR	2.5
1	A	253	TYR	2.5
1	B	406	GLY	2.5
1	B	290	LYS	2.5
1	A	380	GLY	2.5
1	B	116	GLN	2.5
1	B	266	TYR	2.5
1	A	315	SER	2.5
1	B	145	ASP	2.5
1	B	168	ALA	2.5
1	B	188	GLY	2.5
1	B	295	ALA	2.5
1	B	314	TRP	2.5
1	A	341	LEU	2.5
1	B	258	LEU	2.5
1	B	364	GLY	2.5
1	A	237	VAL	2.5
1	A	368	TRP	2.5
1	A	256	LYS	2.4
1	A	407	THR	2.4
1	B	276	GLY	2.4
1	B	319	PRO	2.4
1	A	419	CYS	2.4
1	A	395	PHE	2.4
1	B	304	LEU	2.4
1	A	240	CYS	2.4
1	A	117	ILE	2.4
1	A	347	PHE	2.4
1	B	135	PHE	2.4
1	A	427	PRO	2.4
1	A	448	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	104	TYR	2.4
1	A	150[A]	GLN	2.4
1	A	329	TYR	2.4
1	B	345	ARG	2.4
1	B	264	ALA	2.4
1	B	401	GLY	2.4
1	B	387	THR	2.4
1	A	132	VAL	2.3
1	B	433	GLN	2.4
1	A	112	LEU	2.3
1	A	155	ILE	2.3
1	B	261	PRO	2.3
1	B	281	ILE	2.3
1	A	318	SER	2.3
1	A	274	TRP	2.3
1	B	326	ASN	2.3
1	B	155	ILE	2.3
1	B	422	GLU	2.3
1	A	263	VAL	2.3
1	B	186	SER	2.3
1	B	313	ALA	2.3
1	B	403	GLU	2.3
1	A	439	PHE	2.3
1	A	308	VAL	2.2
1	A	325	PRO	2.2
1	B	215	SER	2.2
1	A	128	ALA	2.2
1	B	344	ALA	2.2
1	A	340	PRO	2.2
1	B	443	LEU	2.2
1	A	212	ILE	2.2
1	A	397	TRP	2.2
1	B	416	ASP	2.2
1	A	376	GLY	2.2
1	B	139	ASP	2.2
1	A	362	PRO	2.2
1	A	338	PHE	2.2
1	A	422	GLU	2.2
1	A	248	ARG	2.2
1	A	168	ALA	2.2
1	B	121	ALA	2.2
1	B	134	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	94	PHE	2.1
1	A	90	ASN	2.1
1	B	164	ASN	2.1
1	B	298	PRO	2.1
1	B	423	ASP	2.1
1	A	384	THR	2.1
1	A	301	VAL	2.1
1	A	118	THR	2.1
1	A	372	CYS	2.1
1	B	219	THR	2.1
1	A	213	SER	2.1
1	A	241	SER	2.1
1	A	317	SER	2.1
1	B	244	ALA	2.1
1	A	323	THR	2.1
1	A	356	GLY	2.1
1	B	376	GLY	2.1
1	A	410	THR	2.1
1	A	311	TYR	2.1
1	A	277	TRP	2.1
1	B	383	PRO	2.1
1	B	380	GLY	2.1
1	B	265	MET	2.0
1	B	373	ASN	2.0
1	B	386	ASN	2.0
1	A	250	LEU	2.0
1	B	405	ASP	2.0
1	A	385	ALA	2.0
1	A	100	TRP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
5	GOL	A	610	6/6	0.63	0.29	4.56	33,36,38,40	0
5	GOL	A	604	6/6	0.70	0.28	3.12	24,27,28,31	0
5	GOL	A	606	6/6	0.77	0.21	0.45	19,21,22,24	0
3	BGC	A	602	12/12	0.82	0.14	0.30	8,11,13,13	0
5	GOL	A	605	6/6	0.67	0.22	0.27	20,26,26,26	0
3	BGC	B	603	12/12	0.60	0.29	0.24	11,13,14,15	0
5	GOL	B	608	6/6	0.28	0.32	0.18	44,44,45,45	0
2	NAG	A	500	14/15	0.78	0.15	0.18	15,20,22,24	0
6	CTR	B	601	34/34	0.65	0.23	-0.21	11,18,30,32	0
5	GOL	A	609	6/6	0.65	0.20	-0.32	30,31,33,35	0
4	CTT	A	600	45/45	0.83	0.15	-0.34	10,19,33,35	1
2	NAG	B	500	14/15	0.49	0.28	-0.51	24,26,28,29	0
5	GOL	A	607	6/6	0.56	0.27	-	27,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.