



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 04:29 PM BST

PDB ID : 1MQQ
Title : THE CRYSTAL STRUCTURE OF ALPHA-D-GLUCURONIDASE FROM BACILLUS STEAROTHERMOPHILUS T-1 COMPLEXED WITH GLUCURONIC ACID
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Deposited on : 2002-09-17
Resolution : 1.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

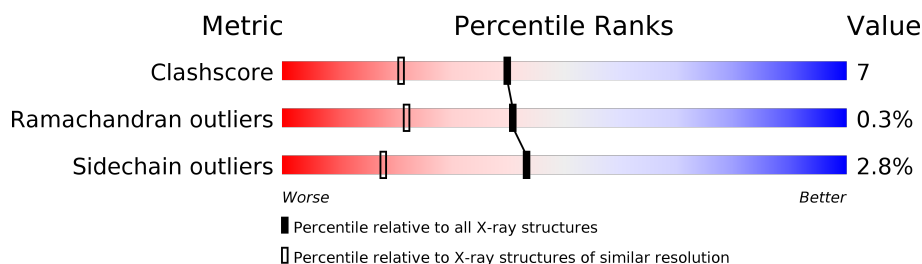
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	679	<div>84% 13% ..</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
2	GCU	A	701[A]	X	-	-	-
3	GOL	A	757	-	-	X	-
3	GOL	A	759	-	-	X	-
3	GOL	A	761	-	-	X	-
3	GOL	A	762	-	-	X	-

2 Entry composition [i](#)

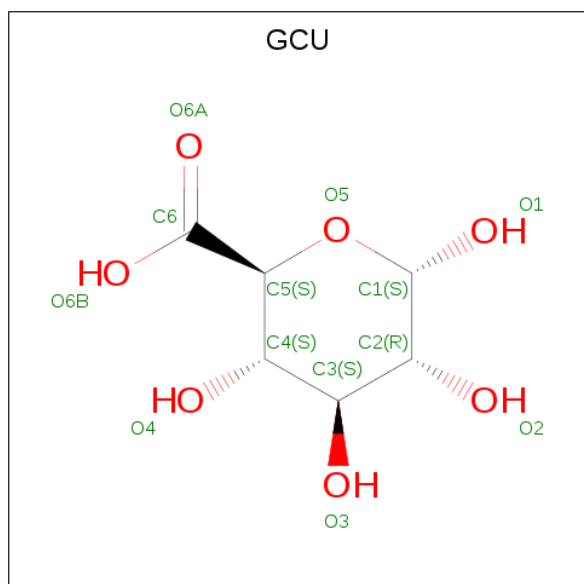
There are 4 unique types of molecules in this entry. The entry contains 6429 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ALPHA-D-GLUCURONIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	675	5681	3651	959	1051	20	0	43	0

- Molecule 2 is alpha-D-glucopyranuronic acid (three-letter code: GCU) (formula: C₆H₁₀O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	26	12	14	0	1

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	656	Total	O	0	0
			656	656		

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	74.09 Å 74.09 Å 331.86 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.65	Depositor
% Data completeness (in resolution range)	98.9 (40.00-1.65)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97, CNS	Depositor
R, R_{free}	0.185 , 0.229	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6429	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, GCU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/6009	1.19	24/8153 (0.3%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	436	ARG	CD-NE-CZ	13.31	142.24	123.60
1	A	176	GLN	C-N-CA	10.09	146.93	121.70
1	A	436	ARG	NE-CZ-NH1	9.78	125.19	120.30
1	A	597	ARG	NE-CZ-NH2	-9.48	115.56	120.30
1	A	204	LYS	CA-CB-CG	-8.15	95.47	113.40
1	A	226	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	A	91	TYR	CB-CG-CD1	-7.16	116.70	121.00
1	A	340	TYR	CB-CG-CD1	6.95	125.17	121.00
1	A	91	TYR	CB-CG-CD2	6.71	125.02	121.00
1	A	597	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	340	TYR	CB-CG-CD2	-6.24	117.26	121.00
1	A	435	TYR	CB-CG-CD1	6.00	124.60	121.00
1	A	57	VAL	C-N-CA	-5.92	106.90	121.70
1	A	429	ASP	CB-CG-OD1	5.89	123.60	118.30
1	A	662	TYR	CB-CG-CD1	5.84	124.50	121.00
1	A	103	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	463	TYR	CB-CG-CD1	-5.82	117.51	121.00
1	A	548	ARG	CD-NE-CZ	5.75	131.64	123.60
1	A	228	TYR	CB-CG-CD1	-5.65	117.61	121.00
1	A	467	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	A	583	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	A	465	PHE	CB-CG-CD1	-5.13	117.21	120.80
1	A	583	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	121	PHE	CB-CG-CD1	-5.05	117.27	120.80

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	5681	0	5468	82	0
2	A	26	0	18	0	0
3	A	66	0	88	30	0
4	A	656	0	0	10	0
All	All	6429	0	5574	83	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 7.

All (83) 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:11:ARG:HH12	3:A:761:GOL:H12	1.24	1.03
1:A:13[B]:GLU:OE2	3:A:761:GOL:H32	1.64	0.97
1:A:13[B]:GLU:OE2	3:A:761:GOL:C3	2.13	0.97
1:A:436:ARG:HH11	1:A:436:ARG:HB2	1.36	0.90
1:A:13[B]:GLU:CD	3:A:761:GOL:H32	2.06	0.77
1:A:125:LEU:HD22	3:A:755:GOL:H31	1.68	0.73
1:A:656:ARG:HH22	3:A:757:GOL:H32	1.53	0.73
1:A:653:LYS:HE2	3:A:757:GOL:H2	1.71	0.72
1:A:31:THR:HG22	4:A:1305:HOH:O	1.89	0.70
1:A:47:ARG:HD3	1:A:53:GLU:OE2	1.90	0.70
1:A:553:VAL:HG13	3:A:759:GOL:H11	1.75	0.68
1:A:11:ARG:NH1	3:A:761:GOL:H12	2.05	0.68
1:A:77:PHE:HB3	1:A:79:ARG:NH1	2.09	0.68
3:A:756:GOL:O1	3:A:762:GOL:H2	1.93	0.67
1:A:94:ARG:HH12	3:A:762:GOL:H31	1.58	0.66
1:A:77:PHE:HB2	3:A:762:GOL:O1	1.99	0.63
1:A:590:HIS:HB3	3:A:758:GOL:O2	1.98	0.63
1:A:223:ASP:O	1:A:227[B]:THR:HG23	2.00	0.61
1:A:243:GLU:HG3	4:A:1330:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:ARG:NH2	3:A:757:GOL:H32	2.17	0.58
1:A:436:ARG:NH1	1:A:436:ARG:HB2	2.12	0.58
1:A:94:ARG:HH12	3:A:762:GOL:C3	2.18	0.57
1:A:58[A]:GLN:HG3	4:A:1149:HOH:O	2.04	0.57
1:A:590:HIS:CE1	3:A:758:GOL:HO3	2.23	0.57
1:A:266:LYS:O	1:A:270[A]:GLN:HG2	2.07	0.55
1:A:624[A]:LYS:HG3	4:A:1398:HOH:O	2.07	0.54
1:A:13[B]:GLU:OE2	3:A:761:GOL:H31	2.05	0.53
1:A:436:ARG:HD2	1:A:437:TYR:CE2	2.42	0.53
1:A:547:ASP:O	1:A:666:LYS:HG2	2.10	0.52
1:A:30[A]:ARG:HB3	1:A:30[A]:ARG:HH11	1.75	0.52
1:A:58[B]:GLN:HG2	4:A:1149:HOH:O	2.10	0.52
1:A:13[B]:GLU:OE1	3:A:761:GOL:H32	2.10	0.51
1:A:32:SER:O	1:A:36[B]:GLN:HG3	2.11	0.51
1:A:590:HIS:HB3	3:A:758:GOL:HO2	1.76	0.51
1:A:67[A]:ILE:HD11	1:A:121:PHE:CZ	2.46	0.50
1:A:13[B]:GLU:CD	3:A:761:GOL:C3	2.74	0.49
1:A:150:TRP:HA	1:A:199:ASN:HA	1.94	0.49
1:A:656:ARG:HH22	3:A:757:GOL:C3	2.23	0.48
1:A:545:TYR:CE2	3:A:759:GOL:H32	2.48	0.48
1:A:123:ARG:O	1:A:127[A]:MET:HG3	2.14	0.48
1:A:14:ARG:CZ	1:A:51:GLU:HG3	2.44	0.48
1:A:555:ARG:HB3	1:A:563:TYR:HB3	1.97	0.47
1:A:446:ILE:HA	1:A:452:TRP:O	2.15	0.47
1:A:561:THR:CG2	3:A:759:GOL:H12	2.45	0.47
1:A:79:ARG:HG2	1:A:94:ARG:NH2	2.30	0.47
1:A:75:GLU:OE2	1:A:82:GLU:OE2	2.32	0.46
1:A:532:VAL:HG11	1:A:662:TYR:CE1	2.51	0.46
1:A:270[A]:GLN:NE2	4:A:1044:HOH:O	2.50	0.45
1:A:30[A]:ARG:NH1	1:A:111:ASP:OD2	2.50	0.45
1:A:11:ARG:HH22	3:A:761:GOL:C3	2.29	0.45
1:A:577:SER:OG	1:A:579[A]:ASP:OD1	2.34	0.45
1:A:50[A]:MET:HB2	1:A:52:ILE:HG12	1.98	0.45
1:A:436:ARG:NH2	4:A:1334:HOH:O	2.49	0.45
1:A:507:ARG:NH1	1:A:510:GLU:OE1	2.50	0.45
1:A:30[A]:ARG:CB	1:A:30[A]:ARG:HH11	2.30	0.44
1:A:507:ARG:NH1	4:A:1286:HOH:O	2.50	0.44
1:A:98:ASP:OD2	1:A:100:GLY:N	2.50	0.44
1:A:331:ARG:NH1	4:A:1437:HOH:O	2.50	0.44
1:A:21:LEU:HD12	1:A:50[A]:MET:SD	2.58	0.44
1:A:557[A]:VAL:HG22	1:A:576:GLU:CD	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ALA:HB3	1:A:310:PRO:HD3	2.00	0.44
1:A:175:LYS:O	1:A:176:GLN:O	2.35	0.43
1:A:47:ARG:HH11	1:A:53:GLU:HG2	1.83	0.43
1:A:418:LYS:HE3	1:A:433:PHE:CE1	2.54	0.43
1:A:489:GLY:HA3	3:A:761:GOL:O3	2.18	0.43
1:A:554:ASP:N	3:A:759:GOL:H2	2.34	0.42
1:A:362:PRO:HG3	1:A:563:TYR:OH	2.20	0.42
1:A:30[A]:ARG:NH1	1:A:30[A]:ARG:HB3	2.33	0.42
1:A:367[B]:VAL:HG23	4:A:814:HOH:O	2.18	0.42
1:A:554:ASP:H	3:A:759:GOL:H2	1.84	0.42
1:A:331:ARG:HD3	3:A:759:GOL:H31	2.00	0.42
1:A:96:ASP:HB2	1:A:103:ARG:HB2	2.02	0.41
1:A:198:ASN:ND2	1:A:235[A]:SER:OG	2.54	0.41
1:A:624[A]:LYS:HB2	1:A:624[A]:LYS:HE2	1.24	0.41
1:A:72:LEU:HD13	1:A:78:GLU:HG3	2.02	0.41
1:A:11:ARG:HH22	3:A:761:GOL:H32	1.86	0.41
1:A:524[A]:PRO:HB3	1:A:535:TYR:CE1	2.55	0.41
1:A:408:LYS:HE3	1:A:408:LYS:HB3	1.82	0.41
1:A:79:ARG:HB2	1:A:82:GLU:CD	2.41	0.41
1:A:340:TYR:HA	1:A:374:LEU:HD21	2.03	0.40
1:A:331:ARG:HD3	3:A:759:GOL:C3	2.51	0.40
1:A:119:PHE:CG	1:A:189:SER:HA	2.57	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	716/679 (105%)	700 (98%)	14 (2%)	2 (0%)	41 22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	GLN
1	A	177	ASN

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	623/586 (106%)	596 (96%)	27 (4%)	29 7

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30[A]	ARG
1	A	30[B]	ARG
1	A	50[A]	MET
1	A	50[B]	MET
1	A	58[A]	GLN
1	A	58[B]	GLN
1	A	62[A]	GLU
1	A	62[B]	GLU
1	A	66[A]	SER
1	A	66[B]	SER
1	A	67[A]	ILE
1	A	67[B]	ILE
1	A	72	LEU
1	A	73	GLU
1	A	244[A]	ILE
1	A	244[B]	ILE
1	A	344[A]	LYS
1	A	344[B]	LYS
1	A	397	GLN
1	A	436	ARG
1	A	505[A]	SER
1	A	505[B]	SER
1	A	507	ARG
1	A	579[A]	ASP
1	A	579[B]	ASP

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Mol	Chain	Res	Type
1	A	624[A]	LYS
1	A	624[B]	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	HIS
1	A	511	ASN
1	A	618	GLN

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 monosaccharides 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	$\# Z > 2$
3	GOL	A	757	-	5,5,5	0.58	0	5,5,5	0.81	0
3	GOL	A	758	-	5,5,5	0.58	0	5,5,5	0.65	0
3	GOL	A	753	-	5,5,5	0.59	0	5,5,5	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GCU	A	701[B]	-	10,13,13	1.83	2 (20%)	15,19,19	1.39	2 (13%)
3	GOL	A	754	-	5,5,5	0.63	0	5,5,5	0.34	0
3	GOL	A	759	-	5,5,5	0.43	0	5,5,5	0.93	0
3	GOL	A	755	-	5,5,5	0.64	0	5,5,5	0.40	0
3	GOL	A	756	-	5,5,5	0.50	0	5,5,5	0.60	0
3	GOL	A	751	-	5,5,5	0.58	0	5,5,5	0.45	0
3	GOL	A	761	-	5,5,5	0.59	0	5,5,5	0.52	0
3	GOL	A	752	-	5,5,5	0.72	0	5,5,5	0.30	0
3	GOL	A	762	-	5,5,5	0.45	0	5,5,5	0.74	0
2	GCU	A	701[A]	-	10,13,13	1.79	1 (10%)	15,19,19	1.36	2 (13%)

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
3	GOL	A	757	-	-	3/4/4/4	-
3	GOL	A	758	-	-	2/4/4/4	-
3	GOL	A	753	-	-	0/4/4/4	-
2	GCU	A	701[B]	-	-	0/0/24/24	0/1/1/1
3	GOL	A	754	-	-	0/4/4/4	-
3	GOL	A	759	-	-	2/4/4/4	-
3	GOL	A	755	-	-	2/4/4/4	-
3	GOL	A	756	-	-	0/4/4/4	-
3	GOL	A	751	-	-	0/4/4/4	-
3	GOL	A	761	-	-	0/4/4/4	-
3	GOL	A	752	-	-	2/4/4/4	-
3	GOL	A	762	-	-	2/4/4/4	-
2	GCU	A	701[A]	-	1/1/6/6	0/0/24/24	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701[B]	GCU	O5-C5	4.02	1.48	1.44
2	A	701[A]	GCU	O5-C5	3.95	1.48	1.44
2	A	701[B]	GCU	C1-C2	2.07	1.57	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701[B]	GCU	O5-C5-C4	2.86	113.62	108.91
2	A	701[B]	GCU	C1-O5-C5	2.72	116.37	112.31
2	A	701[A]	GCU	C1-O5-C5	2.32	115.78	112.31
2	A	701[A]	GCU	O1-C1-O5	-2.16	103.91	110.38

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	701[A]	GCU	C1

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	757	GOL	O1-C1-C2-C3
3	A	759	GOL	C1-C2-C3-O3
3	A	752	GOL	O1-C1-C2-C3
3	A	762	GOL	O1-C1-C2-O2
3	A	762	GOL	O1-C1-C2-C3
3	A	757	GOL	C1-C2-C3-O3
3	A	758	GOL	C1-C2-C3-O3
3	A	755	GOL	C1-C2-C3-O3
3	A	757	GOL	O2-C2-C3-O3
3	A	758	GOL	O2-C2-C3-O3
3	A	759	GOL	O2-C2-C3-O3
3	A	755	GOL	O2-C2-C3-O3
3	A	752	GOL	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	757	GOL	4	0
3	A	758	GOL	3	0
3	A	759	GOL	7	0
3	A	755	GOL	1	0
3	A	756	GOL	1	0
3	A	761	GOL	11	0
3	A	762	GOL	4	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.