



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:55 PM UTC

PDB ID : 1MQR / pdb_00001mqr
Title : THE CRYSTAL STRUCTURE OF ALPHA-D-GLUCURONIDASE (E386Q)
FROM BACILLUS STEAROTHERMOPHILUS T-6
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Stojanoff, V.; Thompson, A.; Shoham, Y.; Shoham, G.
Deposited on : 2002-09-17
Resolution : 2.00 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

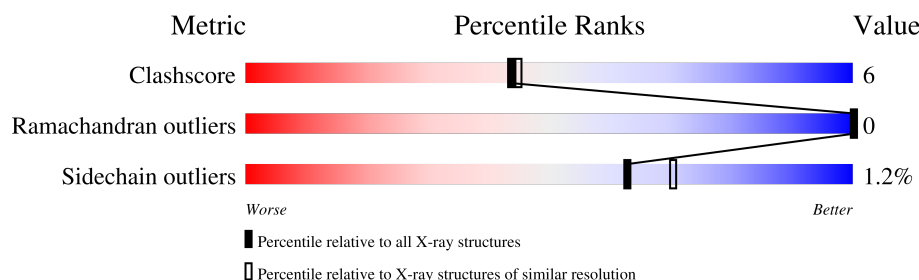
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	679	 83% 14% ...

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6118 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.

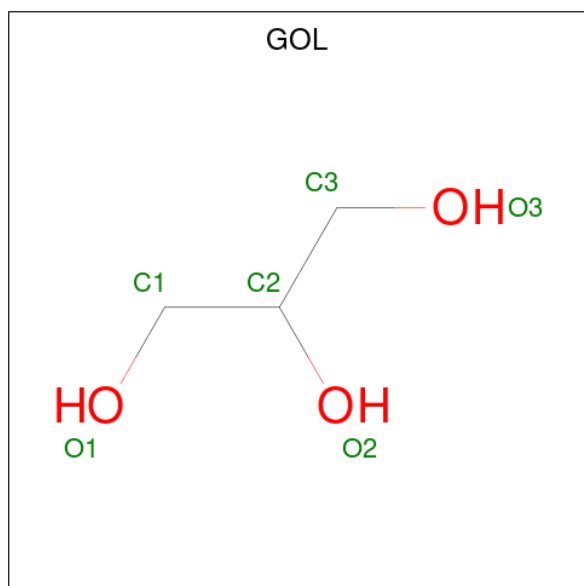
- Molecule 1 is a protein called ALPHA-D-GLUCURONIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	674	5616	3588	969	1040	19	0	13	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	386	GLN	GLU	engineered mutation	UNP Q9ZFM3

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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

- Molecule 3 is water.

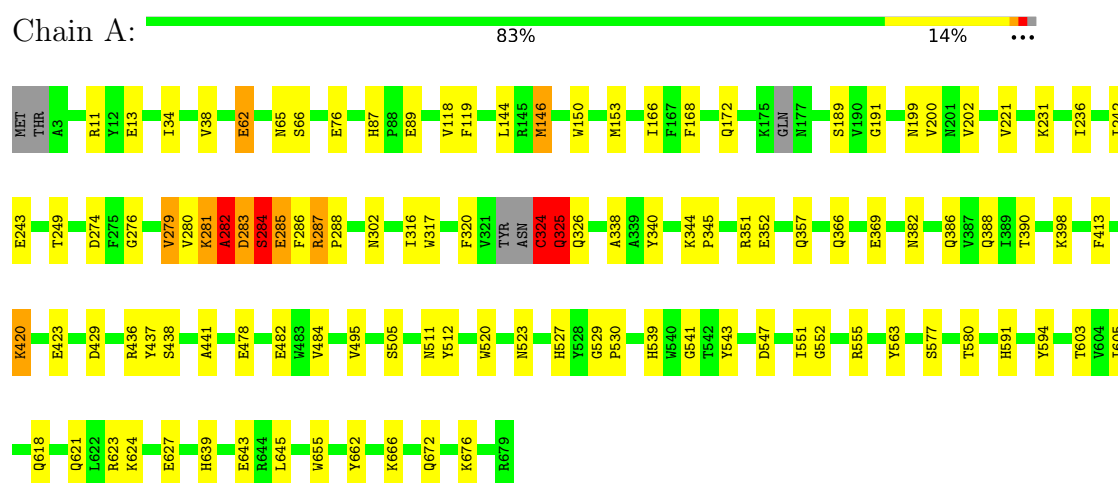
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	466	Total	O	0	0
			466	466		

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. 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. 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.

Note EDS was not executed.

• Molecule 1: ALPHA-D-GLUCURONIDASE



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	73.54Å 73.54Å 328.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.03 – 2.00	Depositor
% Data completeness (in resolution range)	99.8 (49.03-2.00)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.179 , 0.203	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6118	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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

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	0.67	12/5768 (0.2%)	1.11	42/7819 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	325	GLN	C-N	-21.66	1.03	1.33
1	A	284	SER	C-N	-19.66	1.03	1.33
1	A	324	CYS	C-N	-18.22	1.03	1.33
1	A	282	ALA	C-N	-16.86	1.10	1.33
1	A	386	GLN	C-N	-10.64	1.20	1.33
1	A	281	LYS	C-N	-6.18	1.25	1.33
1	A	618	GLN	CD-OE1	5.17	1.33	1.23
1	A	357	GLN	CD-OE1	5.14	1.33	1.23
1	A	511	ASN	CG-OD1	5.13	1.33	1.23
1	A	172	GLN	CD-OE1	5.07	1.33	1.23
1	A	326	GLN	CD-OE1	5.07	1.33	1.23
1	A	672	GLN	CD-OE1	5.02	1.33	1.23

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	282	ALA	O-C-N	-19.52	99.90	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	CYS	N-CA-C	18.45	162.65	111.00
1	A	324	CYS	O-C-N	-17.86	94.42	123.00
1	A	325	GLN	N-CA-C	16.89	137.88	107.99
1	A	324	CYS	CB-CA-C	-15.97	79.75	110.10
1	A	320	PHE	O-C-N	15.61	141.66	122.93
1	A	283	ASP	CA-C-N	-14.37	99.40	122.53
1	A	283	ASP	C-N-CA	-14.37	99.40	122.53
1	A	320	PHE	CA-C-N	-13.13	98.07	121.70
1	A	320	PHE	C-N-CA	-13.13	98.07	121.70
1	A	386	GLN	OE1-CD-NE2	-9.87	112.73	122.60
1	A	325	GLN	OE1-CD-NE2	-9.75	112.85	122.60
1	A	325	GLN	CA-C-N	-8.68	107.52	123.05
1	A	325	GLN	C-N-CA	-8.68	107.52	123.05
1	A	398	LYS	N-CA-C	-8.16	101.82	112.68
1	A	282	ALA	N-CA-C	7.86	119.93	111.36
1	A	324	CYS	CA-C-N	7.48	133.74	123.11
1	A	324	CYS	C-N-CA	7.48	133.74	123.11
1	A	505	SER	N-CA-C	7.47	120.07	111.11
1	A	279	VAL	N-CA-C	-7.31	97.94	108.17
1	A	283	ASP	O-C-N	6.79	131.83	123.21
1	A	325	GLN	N-CA-CB	-6.74	99.28	110.47
1	A	386	GLN	CG-CD-NE2	6.67	126.41	116.40
1	A	280	VAL	N-CA-C	6.65	118.37	108.46
1	A	325	GLN	CG-CD-NE2	6.63	126.35	116.40
1	A	603	THR	N-CA-C	-6.62	101.61	110.55
1	A	146	MET	N-CA-C	6.42	120.15	109.95
1	A	676	LYS	N-CA-C	6.34	118.29	109.15
1	A	166	ILE	N-CA-C	-6.17	106.72	112.83
1	A	338	ALA	N-CA-C	6.13	118.50	111.02
1	A	284	SER	CA-C-N	-5.85	111.37	121.66
1	A	284	SER	C-N-CA	-5.85	111.37	121.66
1	A	243	GLU	N-CA-C	5.72	117.55	111.31
1	A	529	GLY	CA-C-N	5.28	125.04	119.76
1	A	529	GLY	C-N-CA	5.28	125.04	119.76
1	A	191	GLY	N-CA-C	5.22	122.30	115.36
1	A	520	TRP	N-CA-C	5.22	116.90	108.08
1	A	76	GLU	N-CA-C	-5.10	105.90	112.68
1	A	66	SER	N-CA-C	5.05	116.87	109.24
1	A	65	ASN	N-CA-C	-5.04	102.17	109.59
1	A	591	HIS	N-CA-C	-5.03	100.53	108.73
1	A	221	VAL	N-CA-C	-5.02	105.65	110.72

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	282	ALA	Mainchain
1	A	283	ASP	Mainchain
1	A	324	CYS	Peptide,Mainchain
1	A	325	GLN	Mainchain

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	5616	0	5388	68	0
2	A	36	0	48	0	0
3	A	466	0	0	1	0
All	All	6118	0	5436	68	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 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:324:CYS:O	1:A:325:GLN:HG2	1.43	1.19
1:A:324:CYS:O	1:A:325:GLN:CG	2.15	0.95
1:A:202:VAL:O	1:A:287[A]:ARG:NH1	2.01	0.92
1:A:324:CYS:SG	1:A:325:GLN:N	2.49	0.83
1:A:324:CYS:HG	1:A:325:GLN:N	1.82	0.78
1:A:87:HIS:HD2	1:A:89:GLU:H	1.30	0.76
1:A:62:GLU:H	1:A:62:GLU:CD	1.99	0.70
1:A:242[A]:ILE:HD11	1:A:249:THR:C	2.16	0.70
1:A:242[A]:ILE:HD11	1:A:249:THR:CA	2.21	0.70
1:A:231[B]:LYS:HD2	1:A:274:ASP:O	1.98	0.63
1:A:436:ARG:HD2	1:A:437:TYR:CE2	2.33	0.63
1:A:242[B]:ILE:HD12	1:A:288[B]:PRO:HG3	1.78	0.63
1:A:231[A]:LYS:HD3	1:A:276:GLY:HA2	1.81	0.62
1:A:38:VAL:CG1	1:A:118:VAL:HG21	2.33	0.59
1:A:150:TRP:HA	1:A:199:ASN:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:SER:HG	1:A:285:GLU:N	2.00	0.58
1:A:623:ARG:O	1:A:627:GLU:HG3	2.04	0.58
1:A:325:GLN:NE2	1:A:539:HIS:CE1	2.72	0.57
1:A:38:VAL:HG13	1:A:118:VAL:HG21	1.87	0.57
1:A:87:HIS:CD2	1:A:89:GLU:H	2.18	0.57
1:A:236:ILE:HD12	1:A:236:ILE:C	2.31	0.56
1:A:541:GLY:HA2	1:A:543:TYR:CE2	2.41	0.55
1:A:639:HIS:O	1:A:643:GLU:HG3	2.07	0.55
1:A:285:GLU:HG2	1:A:286:PHE:CD2	2.41	0.55
1:A:344:LYS:HB3	1:A:345:PRO:HD3	1.90	0.54
1:A:382:ASN:HB3	1:A:437:TYR:O	2.08	0.54
1:A:478:GLU:O	1:A:482:GLU:HG3	2.09	0.53
1:A:555:ARG:HB3	1:A:563:TYR:HB3	1.92	0.52
1:A:621:GLN:OE1	1:A:624:LYS:HD3	2.10	0.52
1:A:200:VAL:HG22	1:A:281:LYS:HB2	1.92	0.51
1:A:325:GLN:CD	1:A:539:HIS:ND1	2.69	0.51
1:A:236:ILE:HD12	1:A:236:ILE:O	2.11	0.51
1:A:484:VAL:HG11	1:A:495:VAL:HA	1.93	0.50
1:A:282:ALA:HB2	1:A:317:TRP:CH2	2.46	0.49
1:A:279:VAL:HA	1:A:316:ILE:HB	1.95	0.49
1:A:242[A]:ILE:HD11	1:A:249:THR:N	2.27	0.49
1:A:366:GLN:HB2	1:A:369:GLU:HG3	1.94	0.49
1:A:388:GLN:HG2	1:A:390:THR:O	2.13	0.48
1:A:325:GLN:CD	1:A:539:HIS:CE1	2.92	0.48
1:A:551:ILE:HG12	1:A:552:GLY:N	2.29	0.48
1:A:285:GLU:HG2	1:A:286:PHE:CE2	2.49	0.47
1:A:325:GLN:HB3	1:A:539:HIS:HB2	1.97	0.47
1:A:119:PHE:CG	1:A:189:SER:HA	2.50	0.47
1:A:340:TYR:CZ	1:A:344:LYS:HG3	2.50	0.46
1:A:352:GLU:HB2	1:A:436:ARG:HE	1.79	0.46
1:A:34:ILE:O	1:A:38:VAL:HG23	2.17	0.45
1:A:144[B]:LEU:HD23	1:A:438:SER:O	2.17	0.45
1:A:302:ASN:CG	1:A:351:ARG:HG2	2.43	0.44
1:A:285:GLU:CG	1:A:286:PHE:CE2	3.01	0.44
1:A:623:ARG:HA	1:A:645:LEU:HD13	2.00	0.44
1:A:153:MET:HA	1:A:168:PHE:CB	2.48	0.43
1:A:512:TYR:O	1:A:655:TRP:HB3	2.19	0.43
1:A:523:ASN:O	1:A:527:HIS:HA	2.19	0.43
1:A:285:GLU:O	1:A:285:GLU:HG3	2.19	0.42
1:A:146:MET:O	1:A:441:ALA:HA	2.19	0.42
1:A:547:ASP:O	1:A:666:LYS:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:PHE:O	1:A:423:GLU:HA	2.20	0.41
1:A:594:TYR:HB3	1:A:605:ILE:HB	2.02	0.41
1:A:231[A]:LYS:HG2	1:A:276:GLY:CA	2.51	0.41
1:A:420:LYS:HE3	3:A:987:HOH:O	2.20	0.41
1:A:429:ASP:OD1	1:A:429:ASP:C	2.64	0.41
1:A:344:LYS:HD3	1:A:344:LYS:O	2.20	0.41
1:A:285:GLU:CG	1:A:286:PHE:CD2	3.03	0.41
1:A:530:PRO:HB3	1:A:655:TRP:CE3	2.55	0.41
1:A:287[B]:ARG:HE	1:A:287[B]:ARG:HB2	1.57	0.40
1:A:577:SER:HB3	1:A:580:THR:OG1	2.21	0.40
1:A:662:TYR:CD1	1:A:662:TYR:C	2.99	0.40
1:A:11:ARG:CZ	1:A:13[B]:GLU:HG3	2.51	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	681/679 (100%)	660 (97%)	21 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	594/587 (101%)	586 (99%)	8 (1%)	61	68

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	GLU
1	A	284	SER
1	A	285	GLU
1	A	287[A]	ARG
1	A	287[B]	ARG
1	A	324	CYS
1	A	325	GLN
1	A	420	LYS

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

Mol	Chain	Res	Type
1	A	87	HIS
1	A	142	ASN
1	A	325	GLN
1	A	349	GLN
1	A	360	ASN
1	A	382	ASN
1	A	386	GLN
1	A	618	GLN
1	A	628	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

6 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	GOL	A	701	-	5,5,5	0.79	0	5,5,5	0.46	0
2	GOL	A	703	-	5,5,5	0.79	0	5,5,5	0.42	0
2	GOL	A	705	-	5,5,5	0.81	0	5,5,5	0.28	0
2	GOL	A	706[B]	-	5,5,5	0.81	0	5,5,5	0.70	0
2	GOL	A	706[A]	-	5,5,5	0.81	0	5,5,5	0.69	0
2	GOL	A	704	-	5,5,5	0.73	0	5,5,5	0.43	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	GOL	A	701	-	-	0/4/4/4	-
2	GOL	A	703	-	-	0/4/4/4	-
2	GOL	A	705	-	-	0/4/4/4	-
2	GOL	A	706[B]	-	-	3/4/4/4	-
2	GOL	A	706[A]	-	-	4/4/4/4	-
2	GOL	A	704	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	706[A]	GOL	C1-C2-C3-O3
2	A	706[A]	GOL	O1-C1-C2-C3
2	A	706[B]	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	A	706[A]	GOL	O2-C2-C3-O3
2	A	706[B]	GOL	O2-C2-C3-O3
2	A	704	GOL	O1-C1-C2-C3
2	A	706[A]	GOL	O1-C1-C2-O2
2	A	706[B]	GOL	O1-C1-C2-O2
2	A	704	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	282:ALA	C	283:ASP	N	1.10
1	A	284:SER	C	285:GLU	N	1.03
1	A	324:CYS	C	325:GLN	N	1.03
1	A	325:GLN	C	326:GLN	N	1.03

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.