Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:38 PM GMT

PDB ID	:	1L8N
Title	:	The 1.5A crystal structure of alpha-D-glucuronidase from Bacillus stearothermophilus T-1, complexed with 4-O-methyl-glucuronic acid and xylotriose
Authors	:	Golan, G.; Shallom, D.; Teplitsky, A.; Zaide, G.; Shulami, S.; Baasov, T.; Stojanoff, V.; Thompson, A.; Shoham, Y.; Shoham, G.
Deposited on	:	2002-03-21
Resolution	:	1.50 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:

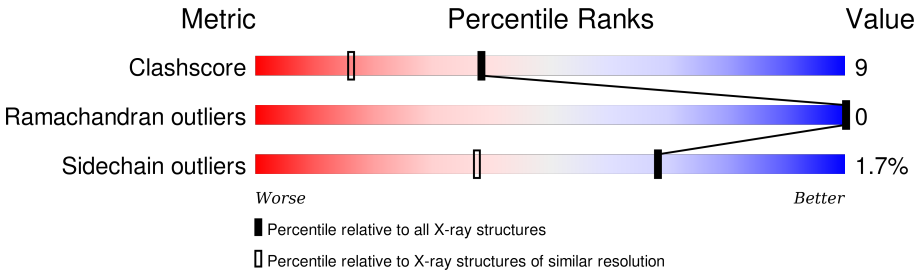
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)

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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	679	82% 16% ••

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	XYP	A	702[A]	X	-	-	-
4	GOL	A	752	-	-	X	-
4	GOL	A	754	-	-	X	-
4	GOL	A	755	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	756	-	-	X	-
4	GOL	A	760	-	-	X	-
4	GOL	A	761	-	-	X	-

2 Entry composition

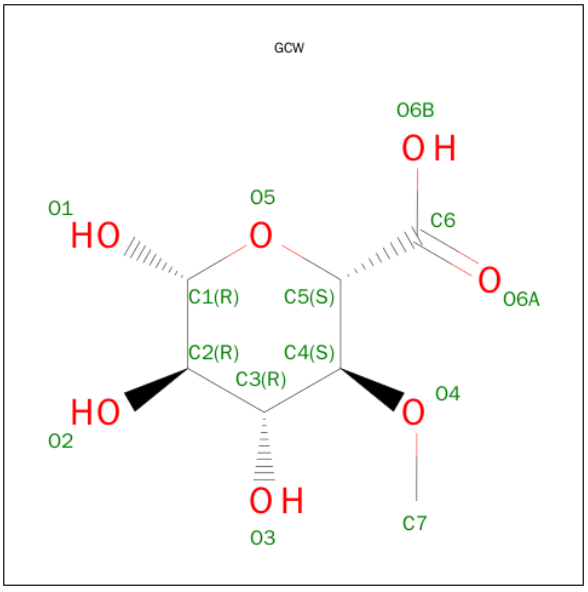
There are 5 unique types of molecules in this entry. The entry contains 6401 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	671	5617	3600	953	1042	22	0	42	0

- Molecule 2 is SUGAR (4-O-METHYL-BETA-D-GLUCURONIC ACID) (three-letter code: GCW) (formula: $C_7H_{12}O_7$).

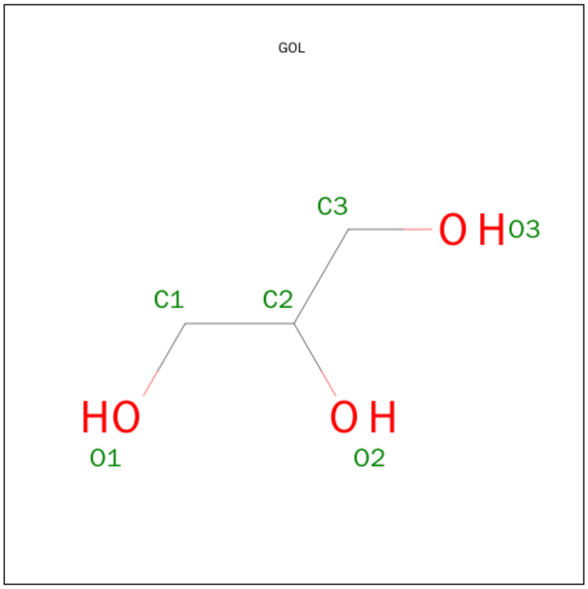


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	14	7	7	0	0

- Molecule 3 is a polymer of unknown type called SUGAR (XYP-XYP).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	2	19	10	9	0	1

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	667	Total	O	0	0
			667	667		

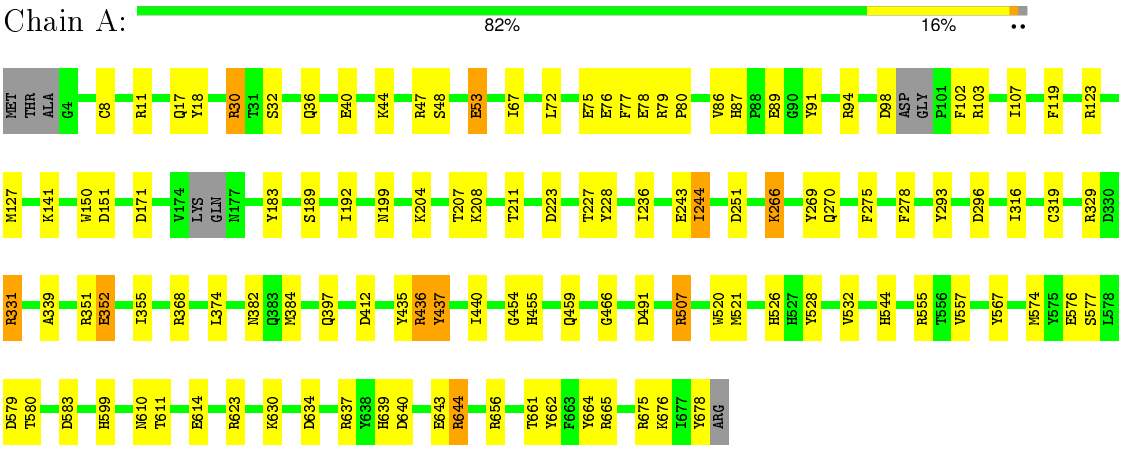
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

- Molecule 1: ALPHA-D-GLUCURONIDASE

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	73.95Å 73.95Å 331.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.50	Depositor
% Data completeness (in resolution range)	95.1 (10.00-1.50)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.140 , 0.172	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6401	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: XYP, GOL, GCW

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	0.62	0/5960	1.20	44/8084 (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
3	A	3	0

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	47	ARG	NE-CZ-NH1	11.71	126.15	120.30
1	A	30	ARG	NE-CZ-NH1	-11.50	114.55	120.30
1	A	30	ARG	NE-CZ-NH2	9.40	125.00	120.30
1	A	555	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	A	637	ARG	NE-CZ-NH1	-8.99	115.80	120.30
1	A	296	ASP	CB-CG-OD1	8.50	125.95	118.30
1	A	103	ARG	NE-CZ-NH2	-8.13	116.24	120.30
1	A	368	ARG	NE-CZ-NH2	-7.65	116.48	120.30
1	A	98	ASP	CB-CG-OD1	7.51	125.06	118.30
1	A	293	TYR	CB-CG-CD1	-7.44	116.54	121.00
1	A	644	ARG	NE-CZ-NH1	-7.35	116.62	120.30
1	A	47	ARG	CD-NE-CZ	7.28	133.79	123.60
1	A	675	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	A	351	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	A	507	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	A	507	ARG	NE-CZ-NH2	-7.00	116.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	555	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	A	183	TYR	CB-CG-CD1	6.59	124.95	121.00
1	A	623	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	296	ASP	CB-CG-OD2	-6.34	112.60	118.30
1	A	183	TYR	CB-CG-CD2	-6.29	117.22	121.00
1	A	435	TYR	CB-CG-CD1	6.04	124.62	121.00
1	A	18	TYR	CB-CG-CD1	-5.96	117.42	121.00
1	A	91	TYR	CB-CG-CD2	5.82	124.49	121.00
1	A	435	TYR	CB-CG-CD2	-5.82	117.51	121.00
1	A	251	ASP	CB-CG-OD1	5.81	123.53	118.30
1	A	412	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	53	GLU	OE1-CD-OE2	5.53	129.93	123.30
1	A	329	ARG	NE-CZ-NH1	-5.53	117.54	120.30
1	A	102	PHE	CB-CG-CD2	-5.50	116.95	120.80
1	A	331	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	A	662	TYR	CB-CG-CD1	5.33	124.20	121.00
1	A	491	ASP	CB-CG-OD2	5.33	123.09	118.30
1	A	293	TYR	CG-CD1-CE1	-5.32	117.04	121.30
1	A	171	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	352	GLU	OE1-CD-OE2	-5.29	116.95	123.30
1	A	437	TYR	CB-CG-CD2	-5.19	117.88	121.00
1	A	47	ARG	NH1-CZ-NH2	-5.19	113.69	119.40
1	A	436	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	634	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	A	11	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	A	228	TYR	CB-CG-CD1	-5.07	117.96	121.00
1	A	567	TYR	CD1-CE1-CZ	-5.04	115.26	119.80
1	A	53	GLU	CG-CD-OE1	-5.03	108.24	118.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	702[A]	XYP	C4B,C2B,C3B

There are no planarity outliers.

5.2 Too-close contacts (i)

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	5617	0	5430	98	0
2	A	14	0	11	0	0
3	A	19	0	16	1	0
4	A	84	0	110	48	0
5	A	667	0	0	20	0
All	All	6401	0	5567	103	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 9.

All (103) 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:521:MET:H	4:A:752:GOL:H31	1.34	0.93
1:A:520:TRP:HB2	4:A:752:GOL:H2	1.50	0.92
1:A:676:LYS:HB2	4:A:755:GOL:H2	1.53	0.90
1:A:243[B]:GLU:CD	1:A:243[B]:GLU:CG	2.41	0.88
1:A:630:LYS:HD2	4:A:750:GOL:H11	1.56	0.87
1:A:577:SER:HB3	1:A:580[A]:THR:HG22	1.59	0.84
1:A:644:ARG:HG3	4:A:754:GOL:H11	1.61	0.80
1:A:80:PRO:HG3	5:A:1321:HOH:O	1.84	0.77
1:A:574:MET:O	1:A:580[A]:THR:HG23	1.86	0.75
1:A:532:VAL:O	4:A:752:GOL:H32	1.86	0.75
4:A:762:GOL:H11	5:A:1401:HOH:O	1.85	0.75
1:A:352:GLU:HB2	1:A:436:ARG:HH21	1.51	0.74
1:A:223:ASP:O	1:A:227[B]:THR:HG23	1.88	0.74
1:A:521:MET:N	4:A:752:GOL:H31	2.04	0.72
1:A:611:THR:HG22	4:A:756:GOL:H2	1.72	0.71
1:A:676:LYS:N	4:A:755:GOL:H32	2.05	0.71
1:A:454:GLY:O	4:A:754:GOL:H12	1.90	0.71
1:A:526:HIS:HD2	1:A:528:TYR:H	1.38	0.70
4:A:755:GOL:H12	5:A:917:HOH:O	1.90	0.70
1:A:72:LEU:HA	5:A:1316:HOH:O	1.94	0.68
1:A:44:LYS:NZ	4:A:760:GOL:H12	2.09	0.67
1:A:580[A]:THR:HG21	5:A:1026:HOH:O	1.94	0.67
1:A:319[B]:CYS:SG	1:A:339:ALA:HB1	2.35	0.66
1:A:520:TRP:CB	4:A:752:GOL:H2	2.25	0.66
1:A:526:HIS:CD2	1:A:528:TYR:H	2.15	0.64
1:A:507:ARG:HH11	1:A:507:ARG:HG3	1.62	0.63
1:A:78:GLU:HB3	5:A:1398:HOH:O	1.98	0.63
1:A:79:ARG:HG2	5:A:1348:HOH:O	1.98	0.62
1:A:639:HIS:O	1:A:643:GLU:HG3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:GLU:HG3	5:A:1316:HOH:O	1.98	0.61
1:A:48[A]:SER:OG	4:A:760:GOL:H2	2.01	0.61
1:A:207:THR:HG21	1:A:243[B]:GLU:OE1	2.01	0.60
1:A:656:ARG:HH22	4:A:757:GOL:C3	2.15	0.59
1:A:192[A]:ILE:HD11	1:A:466:GLY:HA2	1.86	0.57
1:A:640:ASP:HB3	4:A:754:GOL:O2	2.04	0.57
1:A:544:HIS:HD2	4:A:752:GOL:O2	1.89	0.56
1:A:644:ARG:HE	4:A:754:GOL:C3	2.18	0.56
4:A:756:GOL:H32	5:A:1084:HOH:O	2.05	0.56
1:A:77:PHE:HB2	5:A:1348:HOH:O	2.07	0.55
1:A:107:ILE:HG23	5:A:1316:HOH:O	2.06	0.54
1:A:644:ARG:CG	4:A:754:GOL:H11	2.35	0.54
1:A:665:ARG:CG	4:A:761:GOL:H2	2.38	0.53
1:A:610:ASN:HB3	4:A:756:GOL:O2	2.09	0.53
1:A:665:ARG:HE	4:A:761:GOL:C2	2.23	0.52
1:A:557[B]:VAL:HG22	1:A:576:GLU:OE2	2.11	0.51
1:A:208[A]:LYS:HZ2	1:A:244[A]:ILE:HD13	1.75	0.51
1:A:208[A]:LYS:NZ	1:A:244[A]:ILE:HD13	2.25	0.51
1:A:266:LYS:O	1:A:270[B]:GLN:HG3	2.11	0.51
1:A:644:ARG:HE	4:A:754:GOL:H32	1.76	0.51
1:A:150:TRP:HA	1:A:199:ASN:HA	1.93	0.51
1:A:665:ARG:HG2	4:A:761:GOL:H2	1.93	0.50
1:A:630:LYS:NZ	4:A:750:GOL:H31	2.26	0.50
1:A:316[A]:ILE:CD1	1:A:355:ILE:HD12	2.42	0.50
1:A:521:MET:HA	4:A:752:GOL:H31	1.94	0.50
1:A:644:ARG:CG	4:A:754:GOL:H31	2.41	0.49
1:A:521:MET:CA	4:A:752:GOL:H31	2.43	0.49
1:A:664:TYR:CD2	4:A:761:GOL:H32	2.48	0.49
1:A:676:LYS:CA	4:A:755:GOL:H32	2.43	0.48
1:A:507:ARG:NH1	1:A:507:ARG:HG3	2.28	0.48
1:A:76:GLU:HG3	5:A:1359:HOH:O	2.14	0.48
1:A:44:LYS:HG3	4:A:760:GOL:H11	1.94	0.48
3:A:703:XYP:H5B2	5:A:1370:HOH:O	2.13	0.48
1:A:557[B]:VAL:HG22	1:A:576:GLU:CD	2.34	0.47
1:A:455:HIS:HA	4:A:754:GOL:H12	1.95	0.47
1:A:79:ARG:HG2	5:A:1317:HOH:O	2.15	0.47
1:A:577:SER:HB3	1:A:580[A]:THR:CG2	2.40	0.47
1:A:678:TYR:O	4:A:761:GOL:H11	2.15	0.46
1:A:30:ARG:HD2	1:A:30:ARG:HH11	1.51	0.46
1:A:236[A]:ILE:HD13	1:A:278:PHE:CD2	2.50	0.46
1:A:656:ARG:HH22	4:A:757:GOL:H31	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:ARG:CD	4:A:754:GOL:H11	2.46	0.46
1:A:331:ARG:NH1	5:A:1416:HOH:O	2.49	0.46
1:A:44:LYS:HZ1	4:A:760:GOL:H12	1.81	0.45
1:A:656:ARG:NH2	4:A:757:GOL:O3	2.50	0.45
1:A:79:ARG:NE	5:A:1348:HOH:O	2.50	0.45
1:A:507:ARG:NH2	5:A:1047:HOH:O	2.50	0.45
1:A:94:ARG:NH2	5:A:1317:HOH:O	2.49	0.44
1:A:630:LYS:HZ3	4:A:750:GOL:H31	1.82	0.44
1:A:664:TYR:HD2	4:A:761:GOL:H32	1.80	0.44
1:A:86:VAL:HG23	1:A:87[A]:HIS:CD2	2.53	0.44
1:A:32:SER:O	1:A:36[A]:GLN:HG2	2.17	0.44
1:A:208[A]:LYS:HE3	5:A:1038:HOH:O	2.17	0.44
1:A:123:ARG:O	1:A:127[B]:MET:HG3	2.18	0.43
1:A:211:THR:HG21	1:A:244[A]:ILE:HD13	2.00	0.43
1:A:644:ARG:HG2	4:A:754:GOL:H31	2.01	0.43
1:A:382:ASN:HB3	1:A:437:TYR:O	2.19	0.43
1:A:611:THR:HA	4:A:756:GOL:H2	2.02	0.42
1:A:79:ARG:N	5:A:1317:HOH:O	2.49	0.42
1:A:384[B]:MET:HG3	1:A:440:ILE:HA	2.01	0.42
1:A:614:GLU:OE1	4:A:756:GOL:O2	2.28	0.42
1:A:319[B]:CYS:SG	1:A:374:LEU:CD1	3.08	0.41
1:A:455:HIS:HA	4:A:754:GOL:C1	2.50	0.41
1:A:269:TYR:CE2	1:A:275:PHE:HB3	2.55	0.41
1:A:119:PHE:CG	1:A:189:SER:HA	2.55	0.41
1:A:577:SER:CB	1:A:580[A]:THR:HG22	2.40	0.41
1:A:661:THR:HG23	4:A:761:GOL:H12	2.03	0.41
1:A:665:ARG:HE	4:A:761:GOL:C1	2.34	0.41
1:A:583:ASP:OD1	1:A:599:HIS:HD2	2.04	0.41
1:A:8[B]:CYS:SG	1:A:459:GLN:HB3	2.60	0.41
1:A:87[B]:HIS:HE1	1:A:89:GLU:OE1	2.03	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	705/679 (104%)	691 (98%)	14 (2%)	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	619/586 (106%)	606 (98%)	13 (2%)	61 27

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	40[A]	GLU
1	A	40[B]	GLU
1	A	53	GLU
1	A	141	LYS
1	A	151	ASP
1	A	204	LYS
1	A	244[A]	ILE
1	A	244[B]	ILE
1	A	266	LYS
1	A	397	GLN
1	A	579[A]	ASP
1	A	579[B]	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	526	HIS
1	A	599	HIS

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Mol	Chain	Res	Type
1	A	639	HIS
1	A	672	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)

2 carbohydrates 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	XYP	A	702[A]	3	9,9,10	1.39	1 (11%)	12,12,14	0.98	0
3	XYP	A	703	3	10,10,10	1.35	2 (20%)	12,14,14	1.84	1 (8%)

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	XYP	A	702[A]	3	3/3/3/4	0/0/14/17	0/1/1/1
3	XYP	A	703	3	-	0/0/17/17	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702[A]	XYP	O5B-C1B	2.02	1.46	1.42
3	A	703	XYP	O5B-C1B	2.10	1.46	1.43
3	A	703	XYP	O5B-C5B	2.10	1.47	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	703	XYP	O4A-C1B-O5B	5.90	126.71	109.90

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	702[A]	XYP	C4B
3	A	702[A]	XYP	C2B
3	A	702[A]	XYP	C3B

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	A	703	XYP	1	0

5.6 Ligand geometry (i)

15 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	GCW	A	701	-	11,14,14	1.64	3 (27%)	14,20,20	1.32	1 (7%)
4	GOL	A	750	-	5,5,5	0.57	0	5,5,5	0.65	0
4	GOL	A	751	-	5,5,5	0.69	0	5,5,5	0.40	0
4	GOL	A	752	-	5,5,5	1.04	0	5,5,5	2.49	1 (20%)
4	GOL	A	753	-	5,5,5	0.74	0	5,5,5	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	A	754	-	5,5,5	0.61	0	5,5,5	1.91	3 (60%)
4	GOL	A	755	-	5,5,5	0.94	0	5,5,5	2.26	2 (40%)
4	GOL	A	756	-	5,5,5	0.88	0	5,5,5	0.99	0
4	GOL	A	757	-	5,5,5	0.75	0	5,5,5	0.71	0
4	GOL	A	758	-	5,5,5	0.67	0	5,5,5	1.82	2 (40%)
4	GOL	A	759	-	5,5,5	0.42	0	5,5,5	1.70	2 (40%)
4	GOL	A	760	-	5,5,5	0.56	0	5,5,5	0.74	0
4	GOL	A	761	-	5,5,5	0.50	0	5,5,5	1.68	1 (20%)
4	GOL	A	762	-	5,5,5	0.51	0	5,5,5	0.67	0
4	GOL	A	763[B]	-	5,5,5	0.57	0	5,5,5	0.34	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	GCW	A	701	-	-	0/2/26/26	0/1/1/1
4	GOL	A	750	-	-	0/4/4/4	0/0/0/0
4	GOL	A	751	-	-	0/4/4/4	0/0/0/0
4	GOL	A	752	-	-	0/4/4/4	0/0/0/0
4	GOL	A	753	-	-	0/4/4/4	0/0/0/0
4	GOL	A	754	-	-	0/4/4/4	0/0/0/0
4	GOL	A	755	-	-	0/4/4/4	0/0/0/0
4	GOL	A	756	-	-	0/4/4/4	0/0/0/0
4	GOL	A	757	-	-	0/4/4/4	0/0/0/0
4	GOL	A	758	-	-	0/4/4/4	0/0/0/0
4	GOL	A	759	-	-	0/4/4/4	0/0/0/0
4	GOL	A	760	-	-	0/4/4/4	0/0/0/0
4	GOL	A	761	-	-	0/4/4/4	0/0/0/0
4	GOL	A	762	-	-	0/4/4/4	0/0/0/0
4	GOL	A	763[B]	-	-	0/4/4/4	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	GCW	C1-C2	2.15	1.57	1.52
2	A	701	GCW	O5-C5	2.79	1.47	1.43
2	A	701	GCW	C4-C5	3.22	1.58	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	GCW	O1-C1-O5	-3.12	101.72	110.25
4	A	759	GOL	C3-C2-C1	2.01	119.01	111.12
4	A	754	GOL	O3-C3-C2	2.16	120.68	110.18
4	A	754	GOL	O1-C1-C2	2.21	120.89	110.18
4	A	754	GOL	O2-C2-C3	2.24	118.93	108.65
4	A	758	GOL	O2-C2-C3	2.27	119.06	108.65
4	A	755	GOL	C3-C2-C1	2.35	120.33	111.12
4	A	761	GOL	O1-C1-C2	2.48	122.21	110.18
4	A	758	GOL	O2-C2-C1	2.72	121.11	108.65
4	A	759	GOL	O2-C2-C3	2.83	121.63	108.65
4	A	755	GOL	O3-C3-C2	4.30	131.04	110.18
4	A	752	GOL	O3-C3-C2	4.96	134.24	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	750	GOL	3	0
4	A	752	GOL	8	0
4	A	754	GOL	11	0
4	A	755	GOL	4	0
4	A	756	GOL	5	0
4	A	757	GOL	3	0
4	A	760	GOL	4	0
4	A	761	GOL	8	0
4	A	762	GOL	2	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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.