



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 07:28 am BST

PDB ID : 5GQU  
Title : Crystal structure of branching enzyme from *Cyanothece* sp. ATCC 51142  
Authors : Suzuki, R.; Suzuki, E.  
Deposited on : 2016-08-08  
Resolution : 1.85 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](mailto: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.

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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) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

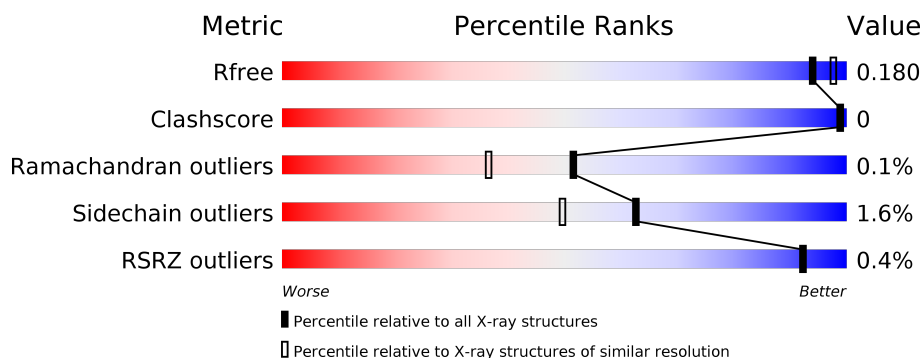
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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))
$R_{free}$	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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  $\geq 3$ , 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	793	

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	GOL	A	801	-	X	-	-
2	GOL	A	807	-	X	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7177 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 1,4-alpha-glucan branching enzyme GlgB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	755	Total	C	N	O	S	0	1	0
			6279	4061	1043	1151	24			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP B1WPM8
A	-18	GLY	-	expression tag	UNP B1WPM8
A	-17	SER	-	expression tag	UNP B1WPM8
A	-16	SER	-	expression tag	UNP B1WPM8
A	-15	HIS	-	expression tag	UNP B1WPM8
A	-14	HIS	-	expression tag	UNP B1WPM8
A	-13	HIS	-	expression tag	UNP B1WPM8
A	-12	HIS	-	expression tag	UNP B1WPM8
A	-11	HIS	-	expression tag	UNP B1WPM8
A	-10	HIS	-	expression tag	UNP B1WPM8
A	-9	SER	-	expression tag	UNP B1WPM8
A	-8	SER	-	expression tag	UNP B1WPM8
A	-7	GLY	-	expression tag	UNP B1WPM8
A	-6	LEU	-	expression tag	UNP B1WPM8
A	-5	VAL	-	expression tag	UNP B1WPM8
A	-4	PRO	-	expression tag	UNP B1WPM8
A	-3	ARG	-	expression tag	UNP B1WPM8
A	-2	GLY	-	expression tag	UNP B1WPM8
A	-1	SER	-	expression tag	UNP B1WPM8
A	0	HIS	-	expression tag	UNP B1WPM8

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Mg	0	0
			4	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	852	Total	O	0	0
			852	852		



- Molecule 1: 1,4-alpha-glucan branching enzyme GlgB

GLU	R694	D434	V182	GLY	MET
Y703	M439	P183	P183	SER	GLY
K725	K447	E194	E194	SER	SER
V758	S466	S187	S187	HIS	HIS
P759	P480	Y191	Y191	HIS	HIS
GLY	G481	S206	S206	HIS	HIS
THR	E491	D207	D207	SER	SER
ILE	D517	R216	R216	GLY	GLY
LYS	D520	D225	D225	VAL	VAL
GLU	D525	R241	R241	PRO	PRO
ILE	D525	R242	R242	ARG	ARG
ALA	F528	R243	R243	GLY	GLY
ASP	R529	S244	S244	SER	SER
GLU	G530	D245	D245	HIS	HIS
GLU	Y531	Q249	Q249	MET	MET
GLU	Y542	R270	R270	THR	THR
	D571	N274	N274	THR	THR
	E572	K285	K285	I5	I5
	R580	R290	R290	D8	D8
	E600	E296	E296	Y15	Y15
	S605	E299	E299	N16	N16
	W610	R308	R308	N35	N35
	G611	E314	E314	R42	R42
	D612	R340	R340	P46	P46
	E621	R343	R343	R47	R47
	E640	E345	E345	E58	E58
	Y644	H369	H369	V67	V67
	D647	D373	D373	H68	H68
	Y650	S374	S374	Y85	Y85
	E654	D381	D381	E91	E91
	G658	Y386	Y386	D100	D100
	T662	R412	R412	D111	D111
	R671	N413	N413	S118	S118
	D674	R432	R432	R124	R124
	D677	Y432	Y432	E135	E135
		E470	E470	D164	D164
				E170	E170

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.75Å 133.75Å 185.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.29 – 1.85 38.50 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.29-1.85) 100.0 (38.50-1.85)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	9.72 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.147 , 0.170 0.160 , 0.180	Depositor DCC
$R_{free}$ test set	7187 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.5	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 48.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7177	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, MG

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	1.44	43/6502 (0.7%)	1.29	47/8848 (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	2

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	242	ARG	CZ-NH1	9.75	1.45	1.33
1	A	58	GLU	CD-OE2	9.40	1.35	1.25
1	A	285	TRP	CB-CG	-8.90	1.34	1.50
1	A	299	GLU	CD-OE2	8.57	1.35	1.25
1	A	658	CYS	CB-SG	-8.21	1.68	1.82
1	A	654	GLU	CD-OE2	-8.03	1.16	1.25
1	A	343	ARG	CZ-NH2	-7.83	1.22	1.33
1	A	412	ARG	CZ-NH2	7.67	1.43	1.33
1	A	412	ARG	CD-NE	-7.56	1.33	1.46
1	A	187	SER	CB-OG	-7.50	1.32	1.42
1	A	91	GLU	CD-OE1	-7.12	1.17	1.25
1	A	135	GLU	CD-OE2	7.05	1.33	1.25
1	A	703	TYR	CG-CD1	6.90	1.48	1.39
1	A	662	THR	CB-CG2	-6.77	1.30	1.52
1	A	481	GLY	CA-C	6.58	1.62	1.51
1	A	58	GLU	CG-CD	6.51	1.61	1.51
1	A	654	GLU	CD-OE1	-6.50	1.18	1.25
1	A	621	GLU	CD-OE1	-6.50	1.18	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	TYR	CB-CG	-6.43	1.42	1.51
1	A	481	GLY	N-CA	6.27	1.55	1.46
1	A	314	GLU	CD-OE1	-6.12	1.19	1.25
1	A	605	SER	CB-OG	-6.05	1.34	1.42
1	A	610	TRP	CZ3-CH2	-6.04	1.30	1.40
1	A	206	SER	CB-OG	5.93	1.50	1.42
1	A	542	TYR	CG-CD2	5.87	1.46	1.39
1	A	434	ASP	N-CA	5.84	1.58	1.46
1	A	466	SER	CB-OG	-5.81	1.34	1.42
1	A	600	GLU	CG-CD	5.74	1.60	1.51
1	A	542	TYR	CB-CG	5.61	1.60	1.51
1	A	274	ASN	N-CA	5.56	1.57	1.46
1	A	135	GLU	CG-CD	5.45	1.60	1.51
1	A	531	TYR	CE1-CZ	-5.40	1.31	1.38
1	A	244	SER	CB-OG	-5.32	1.35	1.42
1	A	572	GLU	CD-OE2	-5.32	1.19	1.25
1	A	179	GLU	CG-CD	5.31	1.59	1.51
1	A	285	TRP	CG-CD1	5.27	1.44	1.36
1	A	296	GLU	CD-OE2	5.23	1.31	1.25
1	A	15	TYR	CG-CD1	5.20	1.46	1.39
1	A	374	SER	CB-OG	-5.18	1.35	1.42
1	A	179	GLU	CD-OE2	-5.13	1.20	1.25
1	A	644	TYR	CE1-CZ	-5.10	1.31	1.38
1	A	191	TYR	CB-CG	5.05	1.59	1.51
1	A	650	TYR	CB-CG	-5.05	1.44	1.51

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	412	ARG	NE-CZ-NH2	-24.49	108.05	120.30
1	A	412	ARG	NE-CZ-NH1	17.23	128.92	120.30
1	A	242	ARG	NE-CZ-NH2	-16.65	111.98	120.30
1	A	412	ARG	CD-NE-CZ	12.67	141.33	123.60
1	A	612	ASP	CB-CG-OD1	-9.27	109.96	118.30
1	A	580	ARG	NE-CZ-NH1	8.23	124.41	120.30
1	A	658	CYS	CB-CA-C	7.86	126.12	110.40
1	A	480	PRO	C-N-CA	-7.51	106.53	122.30
1	A	671	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	A	340	ARG	NE-CZ-NH2	7.01	123.80	120.30
1	A	674	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	A	207	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	A	8	ASP	CB-CG-OD1	6.77	124.40	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	571	ASP	CB-CG-OD1	6.49	124.14	118.30
1	A	381	ASP	CB-CG-OD1	6.46	124.11	118.30
1	A	225	ASP	CB-CG-OD2	-6.33	112.61	118.30
1	A	674	ASP	CB-CG-OD1	6.32	123.99	118.30
1	A	662	THR	N-CA-CB	-6.28	98.37	110.30
1	A	647	ASP	CB-CG-OD1	6.27	123.94	118.30
1	A	520	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	A	434	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	58	GLU	CA-CB-CG	5.70	125.93	113.40
1	A	100	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	A	517	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	A	216	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	290	ARG	NE-CZ-NH2	5.61	123.11	120.30
1	A	677	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	A	345	GLU	OE1-CD-OE2	-5.53	116.66	123.30
1	A	529	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	68	HIS	N-CA-C	5.50	125.85	111.00
1	A	118	SER	CA-CB-OG	-5.46	96.45	111.20
1	A	111	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	640	GLU	OE1-CD-OE2	5.44	129.83	123.30
1	A	386	TYR	CB-CG-CD2	5.42	124.25	121.00
1	A	241	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	432	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	164	ASP	CB-CG-OD1	5.35	123.12	118.30
1	A	242	ARG	NH1-CZ-NH2	5.31	125.24	119.40
1	A	439	MET	CG-SD-CE	-5.29	91.73	100.20
1	A	525	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	124	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	A	245	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	A	270	MET	CG-SD-CE	5.15	108.44	100.20
1	A	67	VAL	CG1-CB-CG2	-5.13	102.69	110.90
1	A	694	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	A	308	MET	CA-CB-CG	5.12	122.00	113.30
1	A	42	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	184	GLU	Mainchain
1	A	412	ARG	Sidechain

## 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	6279	0	5865	4	0
2	A	42	0	56	2	0
3	A	4	0	0	0	0
4	A	852	0	0	1	0
All	All	7177	0	5921	5	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 0.

All (5) 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:46:PRO:O	1:A:47:LYS:HB2	2.05	0.56
2:A:801:GOL:H2	4:A:967:HOH:O	2.16	0.45
1:A:182:VAL:HA	1:A:183:PRO:HD2	1.94	0.42
1:A:244:SER:HB3	1:A:249:GLN:NE2	2.36	0.40
1:A:528:PHE:CD2	2:A:802:GOL:H2	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	754/793 (95%)	734 (97%)	19 (2%)	1 (0%)	51 36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	HIS

### 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	669/700 (96%)	658 (98%)	11 (2%)	62 49

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

Mol	Chain	Res	Type
1	A	16	ASN
1	A	184	GLU
1	A	216	ARG
1	A	369	HIS
1	A	373	ASP
1	A	413	ASN
1	A	434	ASP
1	A	447	LYS
1	A	491	GLU
1	A	662	THR
1	A	725	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	9	GLN
1	A	16	ASN
1	A	634	ASN

### 5.3.3 RNA ⓘ

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](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 for Mogul analysis.

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	804	-	5,5,5	1.09	0	5,5,5	1.34	1 (20%)
2	GOL	A	801	-	5,5,5	1.71	2 (40%)	5,5,5	2.75	3 (60%)
2	GOL	A	805	-	5,5,5	0.34	0	5,5,5	1.24	1 (20%)
2	GOL	A	802	-	5,5,5	2.68	3 (60%)	5,5,5	2.11	1 (20%)
2	GOL	A	806	-	5,5,5	0.82	0	5,5,5	1.88	1 (20%)
2	GOL	A	803	-	5,5,5	0.95	0	5,5,5	0.50	0
2	GOL	A	807	-	5,5,5	2.04	2 (40%)	5,5,5	2.14	2 (40%)

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	804	-	-	2/4/4/4	-
2	GOL	A	801	-	-	2/4/4/4	-
2	GOL	A	805	-	-	4/4/4/4	-
2	GOL	A	802	-	-	0/4/4/4	-
2	GOL	A	806	-	-	0/4/4/4	-
2	GOL	A	803	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	807	-	-	3/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	802	GOL	O3-C3	4.18	1.60	1.42
2	A	807	GOL	O3-C3	3.78	1.58	1.42
2	A	802	GOL	C3-C2	2.78	1.63	1.51
2	A	801	GOL	O2-C2	2.75	1.51	1.43
2	A	802	GOL	O2-C2	2.64	1.51	1.43
2	A	807	GOL	O2-C2	-2.19	1.36	1.43
2	A	801	GOL	C3-C2	2.15	1.60	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	GOL	O2-C2-C3	4.49	128.91	109.12
2	A	802	GOL	O3-C3-C2	3.84	128.63	110.20
2	A	806	GOL	C3-C2-C1	3.35	124.71	111.70
2	A	801	GOL	O1-C1-C2	3.28	125.93	110.20
2	A	807	GOL	O1-C1-C2	3.15	125.31	110.20
2	A	807	GOL	O3-C3-C2	2.76	123.42	110.20
2	A	804	GOL	O3-C3-C2	2.53	122.34	110.20
2	A	801	GOL	C3-C2-C1	-2.30	102.75	111.70
2	A	805	GOL	O1-C1-C2	2.09	120.23	110.20

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	804	GOL	C1-C2-C3-O3
2	A	804	GOL	O2-C2-C3-O3
2	A	801	GOL	C1-C2-C3-O3
2	A	805	GOL	O1-C1-C2-C3
2	A	805	GOL	C1-C2-C3-O3
2	A	807	GOL	O1-C1-C2-C3
2	A	805	GOL	O2-C2-C3-O3
2	A	801	GOL	O2-C2-C3-O3
2	A	805	GOL	O1-C1-C2-O2
2	A	807	GOL	O1-C1-C2-O2
2	A	807	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	GOL	1	0
2	A	802	GOL	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	755/793 (95%)	-0.44	3 (0%) 92 92	14, 21, 42, 77	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	758	VAL	3.7
1	A	35	ASN	3.5
1	A	759	PRO	2.5

### 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](#)

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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	GOL	A	801	6/6	0.75	0.28	33,41,43,51	0
2	GOL	A	804	6/6	0.83	0.32	37,54,58,58	0
2	GOL	A	802	6/6	0.85	0.16	27,43,55,55	0
2	GOL	A	805	6/6	0.87	0.30	45,53,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	A	811	1/1	0.89	0.26	44,44,44,44	0
2	GOL	A	806	6/6	0.91	0.21	33,53,59,60	0
2	GOL	A	807	6/6	0.92	0.14	27,41,44,45	0
2	GOL	A	803	6/6	0.94	0.12	33,34,35,35	0
3	MG	A	809	1/1	0.98	0.04	22,22,22,22	0
3	MG	A	810	1/1	0.98	0.07	23,23,23,23	0
3	MG	A	808	1/1	0.98	0.13	40,40,40,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.