



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 10:13 am BST

PDB ID : 4AYG  
Title : Lactobacillus reuteri N-terminally truncated glucansucrase GTF180 in orthorhombic apo-form  
Authors : Pijning, T.; Vujicic-Zagar, A.; Kralj, S.; Dijkhuizen, L.; Dijkstra, B.W.  
Deposited on : 2012-06-21  
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

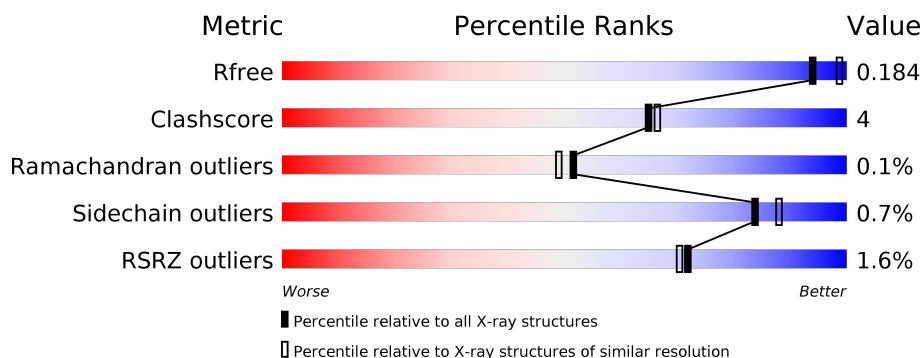
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 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	1039	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>7%</div> </div> </div>
1	B	1039	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>6%</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
3	GOL	A	2778	-	-	X	-
3	GOL	A	2790	-	-	X	-
3	GOL	A	2796	-	-	X	-
3	GOL	A	2799	-	-	X	-
3	GOL	A	2800	-	-	X	-
3	GOL	A	2802	-	-	X	-
3	GOL	B	2777	-	-	X	-
3	GOL	B	2791	-	-	X	-
5	ACY	A	2816	-	-	X	-
5	ACY	B	2806	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 19034 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 GLUCANSUCRASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1028	Total	C	N	O	S	0	8	0
			8193	5123	1385	1661	24			
1	B	1027	Total	C	N	O	S	0	4	0
			8150	5096	1379	1652	23			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	740	MET	-	expression tag	UNP Q5SBN3
A	741	GLY	-	expression tag	UNP Q5SBN3
A	1674	LEU	PHE	cloning artifact	UNP Q5SBN3
A	1773	HIS	-	expression tag	UNP Q5SBN3
A	1774	HIS	-	expression tag	UNP Q5SBN3
A	1775	HIS	-	expression tag	UNP Q5SBN3
A	1776	HIS	-	expression tag	UNP Q5SBN3
A	1777	HIS	-	expression tag	UNP Q5SBN3
A	1778	HIS	-	expression tag	UNP Q5SBN3
B	740	MET	-	expression tag	UNP Q5SBN3
B	741	GLY	-	expression tag	UNP Q5SBN3
B	1674	LEU	PHE	cloning artifact	UNP Q5SBN3
B	1773	HIS	-	expression tag	UNP Q5SBN3
B	1774	HIS	-	expression tag	UNP Q5SBN3
B	1775	HIS	-	expression tag	UNP Q5SBN3
B	1776	HIS	-	expression tag	UNP Q5SBN3
B	1777	HIS	-	expression tag	UNP Q5SBN3
B	1778	HIS	-	expression tag	UNP Q5SBN3

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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		

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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		
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		
3	A	1	Total	C	O	0	0
			6	3	3		

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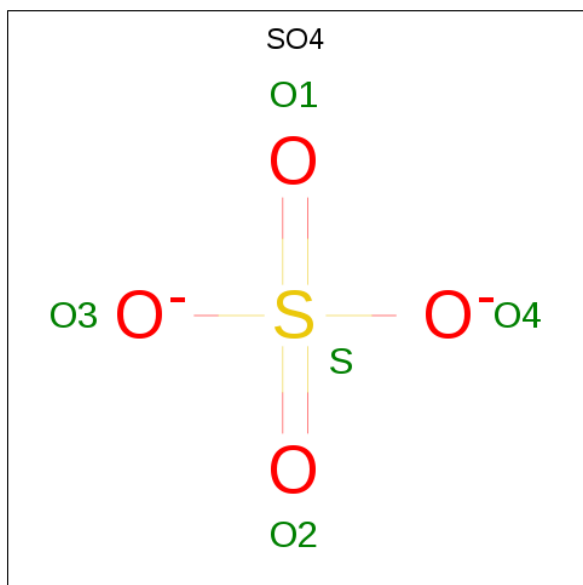
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total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

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



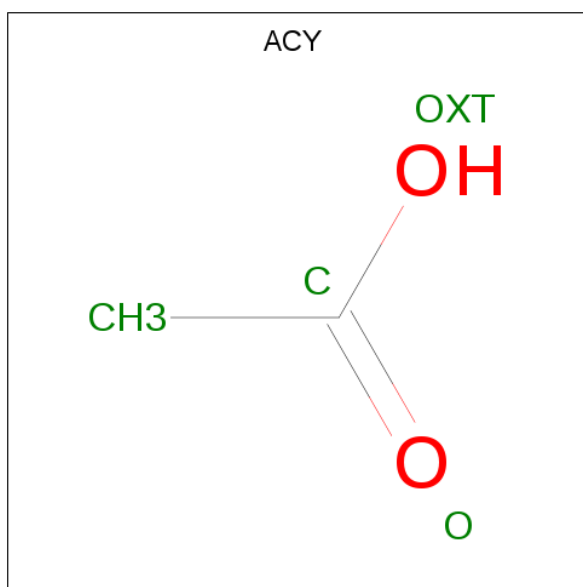
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

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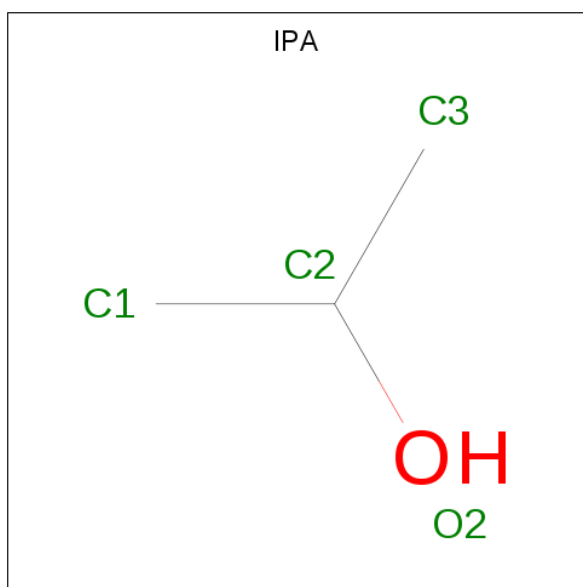
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C<sub>3</sub>H<sub>8</sub>O).



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

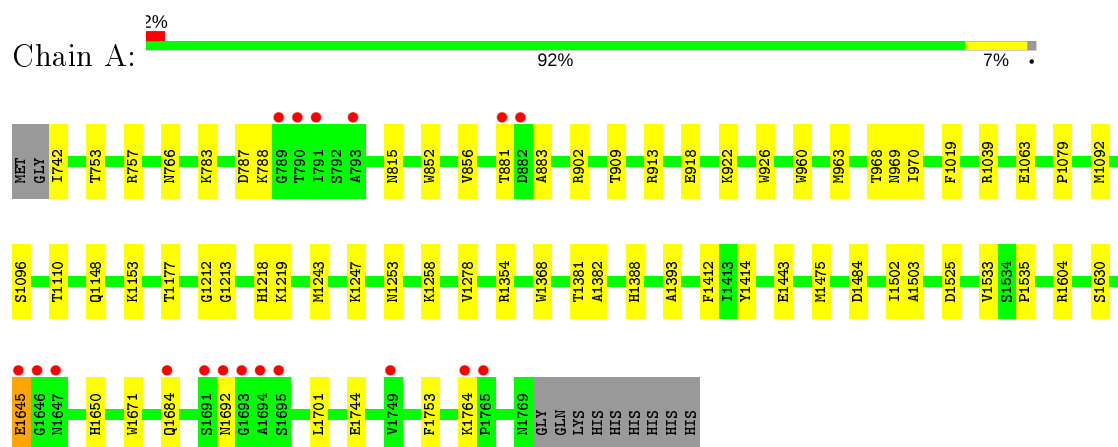
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1148	Total	O	0	0
			1148	1148		
7	B	1040	Total	O	0	0
			1040	1040		

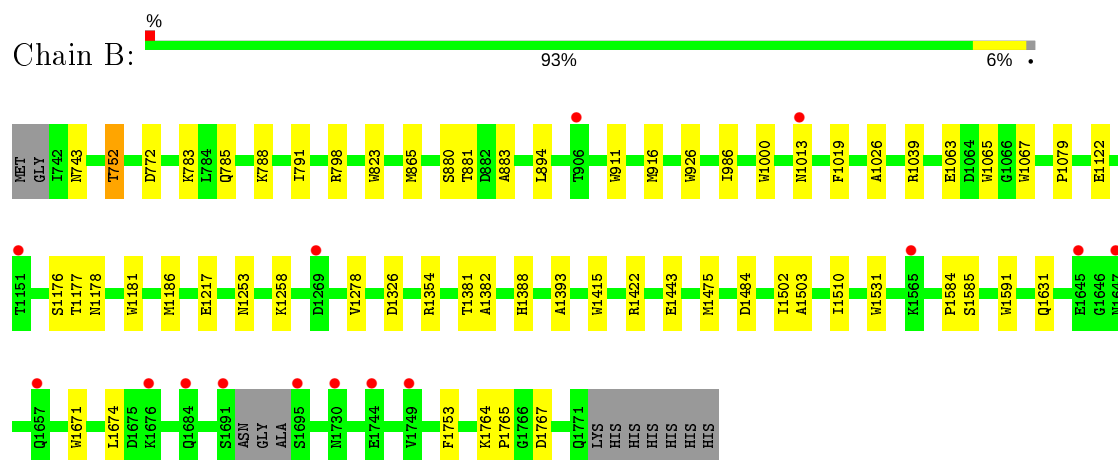
### 3 Residue-property plots [i](#)

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



#### • Molecule 1: GLUCANSUCRASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.79Å 147.36Å 244.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 47.09 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.8 (50.00-2.00) 93.9 (47.09-2.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.75 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.155 , 0.183 0.156 , 0.184	Depositor DCC
$R_{free}$ test set	10644 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.1	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 53.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	19034	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACY, GOL, CA, IPA, SO4

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	0.63	5/8390 (0.1%)	0.65	1/11411 (0.0%)
1	B	0.59	11/8342 (0.1%)	0.62	1/11344 (0.0%)
All	All	0.61	16/16732 (0.1%)	0.63	2/22755 (0.0%)

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1181	TRP	CD2-CE2	5.60	1.48	1.41
1	B	1000	TRP	CD2-CE2	5.55	1.48	1.41
1	B	911	TRP	CD2-CE2	5.55	1.48	1.41
1	A	1671	TRP	CD2-CE2	5.44	1.47	1.41
1	A	960	TRP	CD2-CE2	5.29	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1186	MET	CG-SD-CE	-5.92	90.73	100.20
1	A	1525	ASP	CB-CG-OD1	5.10	122.89	118.30

There are no chirality outliers.

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	8193	0	7729	68	0
1	B	8150	0	7696	50	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	198	0	264	47	0
3	B	138	0	184	27	0
4	A	55	0	0	1	0
4	B	50	0	0	0	0
5	A	32	0	24	2	0
5	B	20	0	15	2	0
6	A	4	0	8	0	0
6	B	4	0	8	2	0
7	A	1148	0	0	17	0
7	B	1040	0	0	5	0
All	All	19034	0	15928	133	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 4.

The worst 5 of 133 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)
3:A:2790:GOL:H2	7:A:3140:HOH:O	1.51	1.11
3:B:2773:GOL:H11	7:B:3142:HOH:O	1.58	1.04
3:B:2776:GOL:H12	7:B:3999:HOH:O	1.64	0.97
1:A:856:VAL:HG22	1:A:881:THR:CG2	1.94	0.97
1:B:1382:ALA:H	3:B:2791:GOL:H11	1.28	0.96

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	1034/1039 (100%)	1009 (98%)	24 (2%)	1 (0%)	51	49
1	B	1027/1039 (99%)	1002 (98%)	24 (2%)	1 (0%)	51	49
All	All	2061/2078 (99%)	2011 (98%)	48 (2%)	2 (0%)	51	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	743	ASN
1	A	1692	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	882/883 (100%)	876 (99%)	6 (1%)	84	88
1	B	878/883 (99%)	870 (99%)	8 (1%)	78	83
All	All	1760/1766 (100%)	1746 (99%)	14 (1%)	84	86

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	752	THR
1	B	798	ARG
1	B	1013	ASN
1	A	1744	GLU
1	B	894	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 94 ligands modelled in this entry, 2 are monoatomic - leaving 92 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	$\# Z  > 2$
3	GOL	B	2792	-	5,5,5	0.43	0	5,5,5	0.13	0
4	SO4	B	2798	-	4,4,4	0.38	0	6,6,6	0.40	0
4	SO4	B	2796	-	4,4,4	0.38	0	6,6,6	0.29	0
3	GOL	A	2789	-	5,5,5	0.50	0	5,5,5	0.49	0
3	GOL	A	2782	-	5,5,5	0.46	0	5,5,5	1.02	0
3	GOL	A	2798	-	5,5,5	0.27	0	5,5,5	0.26	0
3	GOL	A	2796	-	5,5,5	0.33	0	5,5,5	0.62	0
4	SO4	A	2812	-	4,4,4	0.48	0	6,6,6	0.20	0
3	GOL	B	2793	-	5,5,5	0.31	0	5,5,5	0.62	0
5	ACY	A	2818	-	1,3,3	1.83	0	0,3,3	0.00	-
3	GOL	B	2782	-	5,5,5	0.15	0	5,5,5	0.33	0
3	GOL	A	2801	-	5,5,5	0.42	0	5,5,5	0.42	0
5	ACY	A	2819	-	1,3,3	1.42	0	0,3,3	0.00	-
3	GOL	A	2792	-	5,5,5	0.41	0	5,5,5	0.33	0
5	ACY	B	2807	-	1,3,3	1.51	0	0,3,3	0.00	-
3	GOL	A	2783	-	5,5,5	0.24	0	5,5,5	0.46	0
3	GOL	B	2785[A]	-	5,5,5	0.29	0	5,5,5	0.50	0
4	SO4	B	2802	-	4,4,4	0.40	0	6,6,6	0.17	0
4	SO4	B	2804	-	4,4,4	0.38	0	6,6,6	0.15	0
3	GOL	B	2775	-	5,5,5	0.27	0	5,5,5	0.31	0
5	ACY	B	2808	-	1,3,3	1.86	0	0,3,3	0.00	-
3	GOL	B	2787	-	5,5,5	0.34	0	5,5,5	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	A	2805	-	4,4,4	0.37	0	6,6,6	0.11	0
4	SO4	A	2811	-	4,4,4	0.36	0	6,6,6	0.50	0
4	SO4	A	2810	-	4,4,4	0.46	0	6,6,6	0.25	0
4	SO4	B	2797	-	4,4,4	0.36	0	6,6,6	0.35	0
3	GOL	A	2776	-	5,5,5	0.32	0	5,5,5	0.54	0
3	GOL	B	2789	-	5,5,5	0.38	0	5,5,5	0.60	0
3	GOL	A	2797	-	5,5,5	0.42	0	5,5,5	0.26	0
5	ACY	A	2817	-	1,3,3	1.32	0	0,3,3	0.00	-
3	GOL	B	2774	-	5,5,5	0.29	0	5,5,5	0.46	0
4	SO4	A	2808	-	4,4,4	0.43	0	6,6,6	0.28	0
3	GOL	B	2783	-	5,5,5	0.43	0	5,5,5	0.41	0
3	GOL	A	2781	-	5,5,5	0.48	0	5,5,5	0.66	0
5	ACY	A	2815	-	1,3,3	1.53	0	0,3,3	0.00	-
4	SO4	A	2807	-	4,4,4	0.41	0	6,6,6	0.23	0
3	GOL	B	2777	-	5,5,5	0.30	0	5,5,5	0.96	0
3	GOL	B	2784	-	5,5,5	0.25	0	5,5,5	0.41	0
4	SO4	A	2809	-	4,4,4	0.27	0	6,6,6	0.19	0
3	GOL	A	2771	-	5,5,5	0.39	0	5,5,5	0.17	0
3	GOL	B	2778	-	5,5,5	0.46	0	5,5,5	0.33	0
3	GOL	B	2786	-	5,5,5	0.47	0	5,5,5	0.42	0
4	SO4	A	2823	-	4,4,4	0.41	0	6,6,6	0.25	0
3	GOL	A	2785	-	5,5,5	0.25	0	5,5,5	0.26	0
4	SO4	A	2813	-	4,4,4	0.34	0	6,6,6	0.17	0
6	IPA	B	2810	-	3,3,3	0.58	0	3,3,3	0.27	0
3	GOL	A	2780	-	5,5,5	0.44	0	5,5,5	1.62	1 (20%)
3	GOL	A	2772	-	5,5,5	0.39	0	5,5,5	0.32	0
3	GOL	A	2793	-	5,5,5	0.34	0	5,5,5	0.29	0
3	GOL	B	2776	-	5,5,5	0.17	0	5,5,5	0.77	0
3	GOL	A	2800	-	5,5,5	0.28	0	5,5,5	0.90	0
3	GOL	A	2775	-	5,5,5	0.49	0	5,5,5	0.55	0
3	GOL	B	2794	-	5,5,5	0.51	0	5,5,5	0.45	0
5	ACY	A	2820	-	1,3,3	1.30	0	0,3,3	0.00	-
3	GOL	A	2788	-	5,5,5	0.36	0	5,5,5	0.55	0
3	GOL	B	2781	-	5,5,5	0.43	0	5,5,5	0.39	0
5	ACY	B	2809	-	1,3,3	1.30	0	0,3,3	0.00	-
4	SO4	B	2801	-	4,4,4	0.34	0	6,6,6	0.19	0
3	GOL	B	2773	-	5,5,5	0.47	0	5,5,5	1.58	2 (40%)
3	GOL	B	2785[B]	-	5,5,5	0.32	0	5,5,5	0.30	0
5	ACY	A	2816	-	1,3,3	1.17	0	0,3,3	0.00	-
5	ACY	B	2806	-	1,3,3	1.43	0	0,3,3	0.00	-
3	GOL	A	2774	-	5,5,5	0.23	0	5,5,5	0.62	0
3	GOL	A	2790	-	5,5,5	0.35	0	5,5,5	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	B	2799	-	4,4,4	0.32	0	6,6,6	0.27	0
4	SO4	A	2804	-	4,4,4	0.24	0	6,6,6	0.15	0
3	GOL	A	2779	-	5,5,5	0.28	0	5,5,5	0.32	0
3	GOL	A	2787	-	5,5,5	0.17	0	5,5,5	0.43	0
4	SO4	A	2806	-	4,4,4	0.33	0	6,6,6	0.44	0
3	GOL	B	2791	-	5,5,5	0.27	0	5,5,5	0.53	0
3	GOL	A	2795	-	5,5,5	0.28	0	5,5,5	0.68	0
3	GOL	A	2802	-	5,5,5	0.29	0	5,5,5	0.69	0
3	GOL	A	2791	-	5,5,5	0.76	0	5,5,5	0.72	0
3	GOL	A	2784	-	5,5,5	0.33	0	5,5,5	0.74	0
3	GOL	B	2790	-	5,5,5	0.33	0	5,5,5	0.15	0
3	GOL	A	2777	-	5,5,5	0.28	0	5,5,5	0.67	0
3	GOL	A	2803	-	5,5,5	0.63	0	5,5,5	0.25	0
3	GOL	A	2794	-	5,5,5	0.49	0	5,5,5	0.86	0
4	SO4	B	2800	-	4,4,4	0.38	0	6,6,6	0.12	0
5	ACY	A	2814	-	1,3,3	1.24	0	0,3,3	0.00	-
3	GOL	B	2779	-	5,5,5	0.35	0	5,5,5	0.36	0
3	GOL	B	2788	-	5,5,5	0.33	0	5,5,5	0.13	0
3	GOL	A	2799	-	5,5,5	0.37	0	5,5,5	0.33	0
3	GOL	B	2780	-	5,5,5	0.20	0	5,5,5	0.73	0
3	GOL	A	2786	-	5,5,5	0.23	0	5,5,5	0.91	0
4	SO4	B	2803	-	4,4,4	0.36	0	6,6,6	0.10	0
5	ACY	B	2805	-	1,3,3	1.77	0	0,3,3	0.00	-
3	GOL	A	2778	-	5,5,5	0.61	0	5,5,5	1.40	1 (20%)
6	IPA	A	2822	-	3,3,3	0.51	0	3,3,3	0.22	0
5	ACY	A	2821	-	1,3,3	1.50	0	0,3,3	0.00	-
4	SO4	B	2795	-	4,4,4	0.16	0	6,6,6	0.39	0
3	GOL	A	2773	-	5,5,5	0.21	0	5,5,5	0.71	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
3	GOL	A	2790	-	-	2/4/4/4	-
3	GOL	B	2792	-	-	2/4/4/4	-
3	GOL	A	2785	-	-	2/4/4/4	-
3	GOL	A	2776	-	-	4/4/4/4	-
3	GOL	A	2780	-	-	2/4/4/4	-
3	GOL	B	2789	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	2772	-	-	0/4/4/4	-
3	GOL	A	2779	-	-	2/4/4/4	-
3	GOL	A	2797	-	-	3/4/4/4	-
3	GOL	B	2778	-	-	2/4/4/4	-
3	GOL	A	2787	-	-	2/4/4/4	-
3	GOL	A	2793	-	-	4/4/4/4	-
3	GOL	A	2789	-	-	3/4/4/4	-
3	GOL	B	2776	-	-	4/4/4/4	-
3	GOL	A	2782	-	-	0/4/4/4	-
3	GOL	B	2784	-	-	4/4/4/4	-
3	GOL	A	2775	-	-	4/4/4/4	-
3	GOL	B	2791	-	-	4/4/4/4	-
3	GOL	A	2795	-	-	4/4/4/4	-
3	GOL	A	2798	-	-	2/4/4/4	-
3	GOL	B	2786	-	-	4/4/4/4	-
3	GOL	A	2796	-	-	1/4/4/4	-
3	GOL	A	2791	-	-	4/4/4/4	-
3	GOL	B	2794	-	-	0/4/4/4	-
3	GOL	B	2774	-	-	0/4/4/4	-
3	GOL	A	2784	-	-	1/4/4/4	-
3	GOL	B	2783	-	-	4/4/4/4	-
3	GOL	A	2777	-	-	0/4/4/4	-
3	GOL	B	2793	-	-	4/4/4/4	-
3	GOL	A	2803	-	-	1/4/4/4	-
3	GOL	A	2794	-	-	0/4/4/4	-
3	GOL	B	2779	-	-	4/4/4/4	-
3	GOL	A	2781	-	-	0/4/4/4	-
3	GOL	B	2788	-	-	0/4/4/4	-
3	GOL	A	2788	-	-	1/4/4/4	-
3	GOL	B	2781	-	-	4/4/4/4	-
3	GOL	B	2782	-	-	3/4/4/4	-
3	GOL	A	2801	-	-	0/4/4/4	-
3	GOL	A	2792	-	-	0/4/4/4	-
3	GOL	B	2790	-	-	2/4/4/4	-
3	GOL	B	2777	-	-	2/4/4/4	-
3	GOL	A	2783	-	-	4/4/4/4	-
3	GOL	A	2800	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	2773	-	-	0/4/4/4	-
3	GOL	B	2780	-	-	2/4/4/4	-
3	GOL	B	2785[B]	-	-	4/4/4/4	-
3	GOL	A	2786	-	-	2/4/4/4	-
3	GOL	B	2785[A]	-	-	2/4/4/4	-
3	GOL	A	2778	-	-	2/4/4/4	-
3	GOL	A	2771	-	-	0/4/4/4	-
3	GOL	B	2787	-	-	2/4/4/4	-
3	GOL	B	2775	-	-	0/4/4/4	-
3	GOL	A	2802	-	-	4/4/4/4	-
3	GOL	A	2799	-	-	0/4/4/4	-
3	GOL	A	2774	-	-	0/4/4/4	-
3	GOL	A	2773	-	-	2/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2773	GOL	O2-C2-C3	-2.69	97.26	109.12
3	A	2780	GOL	O3-C3-C2	-2.22	99.58	110.20
3	A	2778	GOL	C3-C2-C1	-2.20	103.13	111.70
3	B	2773	GOL	O3-C3-C2	-2.00	100.59	110.20

There are no chirality outliers.

5 of 116 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2793	GOL	O1-C1-C2-C3
3	B	2793	GOL	C1-C2-C3-O3
3	B	2793	GOL	O2-C2-C3-O3
3	A	2783	GOL	O1-C1-C2-O2
3	A	2783	GOL	O1-C1-C2-C3

There are no ring outliers.

29 monomers are involved in 81 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2782	GOL	3	0
3	A	2798	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2796	GOL	4	0
3	A	2801	GOL	2	0
3	B	2785[A]	GOL	3	0
3	B	2789	GOL	2	0
3	B	2774	GOL	1	0
3	B	2783	GOL	1	0
3	B	2777	GOL	9	0
3	B	2784	GOL	1	0
4	A	2813	SO4	1	0
6	B	2810	IPA	2	0
3	A	2780	GOL	1	0
3	B	2776	GOL	1	0
3	A	2800	GOL	8	0
3	B	2773	GOL	3	0
5	A	2816	ACY	2	0
5	B	2806	ACY	2	0
3	A	2790	GOL	4	0
3	A	2787	GOL	1	0
3	B	2791	GOL	7	0
3	A	2795	GOL	2	0
3	A	2802	GOL	7	0
3	A	2791	GOL	2	0
3	A	2777	GOL	1	0
3	A	2803	GOL	2	0
3	A	2799	GOL	4	0
3	A	2778	GOL	5	0
3	A	2773	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	1028/1039 (98%)	-0.40	18 (1%) 68 66	7, 13, 31, 79	0
1	B	1027/1039 (98%)	-0.34	15 (1%) 73 72	9, 17, 34, 54	0
All	All	2055/2078 (98%)	-0.37	33 (1%) 72 70	7, 15, 33, 79	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1693	GLY	7.8
1	A	1692	ASN	6.2
1	A	790	THR	4.5
1	A	1765	PRO	4.5
1	A	1647	ASN	4.5

### 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( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	2797	6/6	0.60	0.28	53,56,58,59	0
3	GOL	B	2789	6/6	0.62	0.37	44,45,46,51	0
3	GOL	A	2791	6/6	0.66	0.26	31,33,35,35	0
3	GOL	A	2799	6/6	0.67	0.27	38,45,47,49	0
3	GOL	A	2793	6/6	0.72	0.29	50,54,56,60	0
3	GOL	B	2787	6/6	0.73	0.28	44,54,55,57	0
3	GOL	A	2803	6/6	0.73	0.31	35,37,38,42	0
3	GOL	B	2790	6/6	0.73	0.26	55,57,59,61	0
3	GOL	A	2798	6/6	0.75	0.25	52,54,55,55	0
3	GOL	A	2795	6/6	0.77	0.34	39,46,46,46	0
3	GOL	B	2793	6/6	0.77	0.31	31,38,41,44	0
3	GOL	B	2788	6/6	0.78	0.30	46,52,56,56	0
6	IPA	B	2810	4/4	0.78	0.18	30,34,35,36	0
4	SO4	A	2812	5/5	0.79	0.34	55,58,66,68	0
3	GOL	B	2785[B]	6/6	0.80	0.48	27,30,30,32	6
3	GOL	B	2777	6/6	0.80	0.23	25,27,32,34	0
3	GOL	A	2782	6/6	0.80	0.30	28,29,33,36	0
3	GOL	B	2792	6/6	0.80	0.17	34,41,42,44	0
3	GOL	B	2794	6/6	0.80	0.24	32,40,41,42	0
3	GOL	B	2785[A]	6/6	0.80	0.48	14,15,15,15	6
3	GOL	A	2779	6/6	0.81	0.32	33,40,43,45	0
3	GOL	A	2801	6/6	0.81	0.26	29,35,38,44	0
5	ACY	B	2809	4/4	0.82	0.18	36,39,42,43	0
3	GOL	A	2786	6/6	0.82	0.21	31,35,38,44	0
3	GOL	A	2802	6/6	0.83	0.24	27,33,39,44	0
3	GOL	B	2781	6/6	0.83	0.32	33,42,43,45	0
3	GOL	A	2783	6/6	0.84	0.15	39,46,48,48	0
5	ACY	A	2815	4/4	0.84	0.18	53,54,57,57	0
3	GOL	B	2791	6/6	0.84	0.34	32,37,43,44	0
3	GOL	A	2792	6/6	0.84	0.24	28,37,39,41	0
3	GOL	B	2773	6/6	0.84	0.25	25,25,27,29	0
3	GOL	A	2776	6/6	0.85	0.17	34,37,42,42	0
4	SO4	A	2823	5/5	0.85	0.29	53,59,65,66	0
3	GOL	A	2775	6/6	0.85	0.22	28,33,37,41	0
5	ACY	B	2805	4/4	0.85	0.13	52,53,54,55	0
3	GOL	A	2796	6/6	0.86	0.29	32,38,43,47	0
3	GOL	A	2800	6/6	0.86	0.29	23,25,29,36	0
3	GOL	B	2783	6/6	0.86	0.17	31,35,39,41	0
4	SO4	B	2800	5/5	0.86	0.23	56,61,68,68	0
3	GOL	A	2788	6/6	0.87	0.28	21,29,35,35	0
3	GOL	B	2779	6/6	0.87	0.22	33,39,40,40	0
3	GOL	B	2786	6/6	0.88	0.23	28,30,31,33	0
3	GOL	A	2778	6/6	0.88	0.18	20,22,24,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	B	2803	5/5	0.89	0.17	62,63,68,69	0
3	GOL	A	2774	6/6	0.89	0.29	26,27,31,33	0
3	GOL	B	2776	6/6	0.89	0.23	26,30,32,36	0
3	GOL	A	2784	6/6	0.90	0.17	25,33,35,38	0
3	GOL	B	2780	6/6	0.90	0.21	27,33,34,42	0
3	GOL	B	2782	6/6	0.90	0.15	34,39,39,45	0
3	GOL	A	2780	6/6	0.90	0.17	22,26,29,29	0
3	GOL	A	2785	6/6	0.90	0.15	33,41,45,49	0
3	GOL	A	2787	6/6	0.90	0.19	47,48,49,52	0
5	ACY	A	2816	4/4	0.91	0.17	43,44,44,47	0
3	GOL	A	2777	6/6	0.91	0.18	33,38,41,42	0
5	ACY	B	2806	4/4	0.91	0.13	33,35,36,36	0
5	ACY	B	2808	4/4	0.91	0.21	31,32,33,34	0
5	ACY	A	2817	4/4	0.92	0.12	43,44,45,45	0
4	SO4	B	2804	5/5	0.92	0.29	59,59,61,61	0
3	GOL	A	2794	6/6	0.92	0.14	17,19,20,20	0
3	GOL	A	2781	6/6	0.92	0.17	18,19,20,21	0
5	ACY	A	2820	4/4	0.92	0.14	37,38,39,40	0
3	GOL	A	2789	6/6	0.92	0.14	25,26,27,28	0
4	SO4	A	2808	5/5	0.93	0.23	45,49,52,53	0
4	SO4	A	2813	5/5	0.93	0.34	64,65,68,71	0
3	GOL	B	2784	6/6	0.93	0.15	33,35,40,42	0
5	ACY	A	2814	4/4	0.93	0.10	27,28,28,29	0
5	ACY	A	2821	4/4	0.93	0.12	31,34,35,36	0
3	GOL	B	2778	6/6	0.94	0.11	23,24,26,28	0
4	SO4	B	2801	5/5	0.94	0.33	63,66,68,71	0
3	GOL	A	2790	6/6	0.94	0.33	32,33,33,35	0
5	ACY	A	2819	4/4	0.94	0.15	39,40,41,41	0
4	SO4	A	2810	5/5	0.94	0.15	43,47,50,52	0
6	IPA	A	2822	4/4	0.94	0.15	34,35,35,38	0
4	SO4	B	2798	5/5	0.94	0.21	42,43,48,48	0
5	ACY	A	2818	4/4	0.95	0.25	34,34,36,36	0
4	SO4	B	2797	5/5	0.95	0.21	39,39,43,44	0
3	GOL	B	2775	6/6	0.95	0.11	20,21,22,23	0
5	ACY	B	2807	4/4	0.95	0.14	42,43,44,44	0
4	SO4	B	2802	5/5	0.95	0.17	48,53,55,56	0
4	SO4	A	2807	5/5	0.95	0.23	44,45,47,48	0
4	SO4	B	2799	5/5	0.96	0.19	42,44,46,47	0
4	SO4	A	2806	5/5	0.96	0.24	38,40,43,44	0
3	GOL	A	2772	6/6	0.97	0.09	13,14,15,15	0
4	SO4	A	2811	5/5	0.97	0.16	35,38,40,42	0
3	GOL	A	2773	6/6	0.97	0.10	12,13,15,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	2771	6/6	0.98	0.08	11,12,13,15	0
3	GOL	B	2774	6/6	0.98	0.13	12,15,15,17	0
4	SO4	A	2809	5/5	0.98	0.12	37,37,40,41	0
4	SO4	B	2796	5/5	0.99	0.14	28,28,30,33	0
4	SO4	B	2795	5/5	0.99	0.09	29,30,31,32	0
4	SO4	A	2804	5/5	0.99	0.09	34,34,36,36	0
2	CA	B	2772	1/1	1.00	0.09	13,13,13,13	0
2	CA	A	2770	1/1	1.00	0.07	8,8,8,8	0
4	SO4	A	2805	5/5	1.00	0.06	16,16,17,17	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.