



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 03:14 AM BST

PDB ID : 3SCS
Title : Crystal Structure of Rice BGlu1 E386S Mutant Complexed with alpha-Glucosyl Fluoride
Authors : Pengthaisong, S.; Withers, S.G.; Kuaprasert, B.; Ketudat Cairns, J.R.
Deposited on : 2011-06-08
Resolution : 1.85 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
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)	:	2.13.1

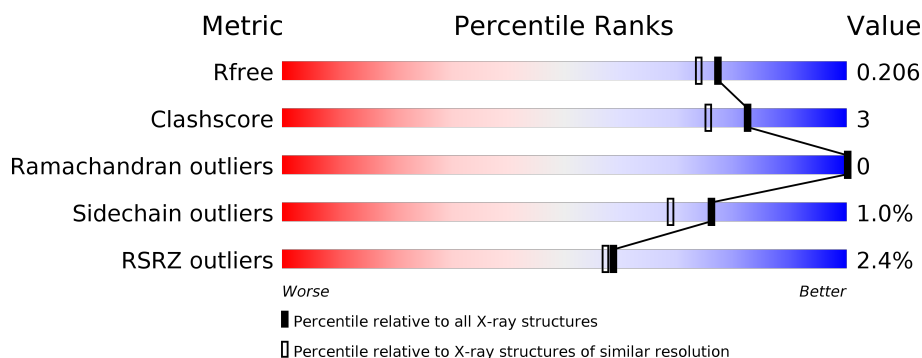
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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 ≥ 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	481	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>5%</div> </div> </div>
1	B	481	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>5%</div> </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8553 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 Beta-glucosidase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	0	0
			3806	2448	655	690	13			
1	B	472	Total	C	N	O	S	0	0	0
			3806	2448	655	690	13			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	ALA	-	expression tag	UNP Q75I93
A	-3	MET	-	expression tag	UNP Q75I93
A	-2	ALA	-	expression tag	UNP Q75I93
A	-1	ASP	-	expression tag	UNP Q75I93
A	0	VAL	-	expression tag	UNP Q75I93
A	24	VAL	ALA	SEE REMARK 999	UNP Q75I93
A	386	SER	GLU	engineered mutation	UNP Q75I93
B	-4	ALA	-	expression tag	UNP Q75I93
B	-3	MET	-	expression tag	UNP Q75I93
B	-2	ALA	-	expression tag	UNP Q75I93
B	-1	ASP	-	expression tag	UNP Q75I93
B	0	VAL	-	expression tag	UNP Q75I93
B	24	VAL	ALA	SEE REMARK 999	UNP Q75I93
B	386	SER	GLU	engineered mutation	UNP Q75I93

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

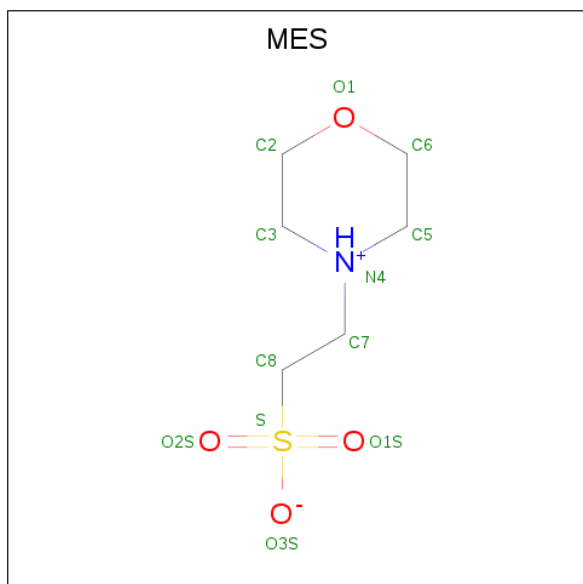
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



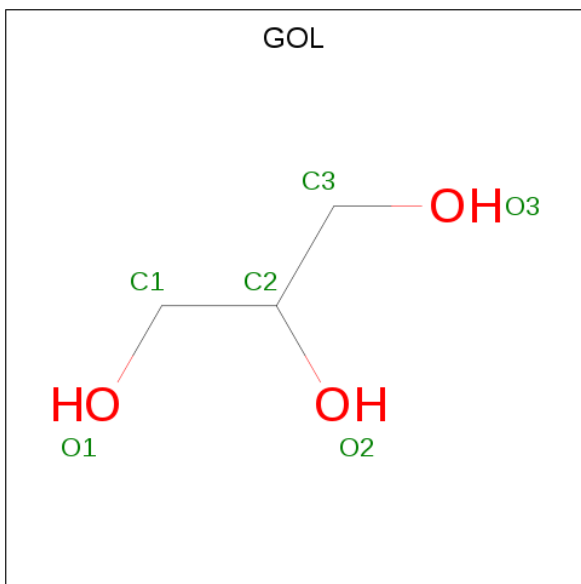
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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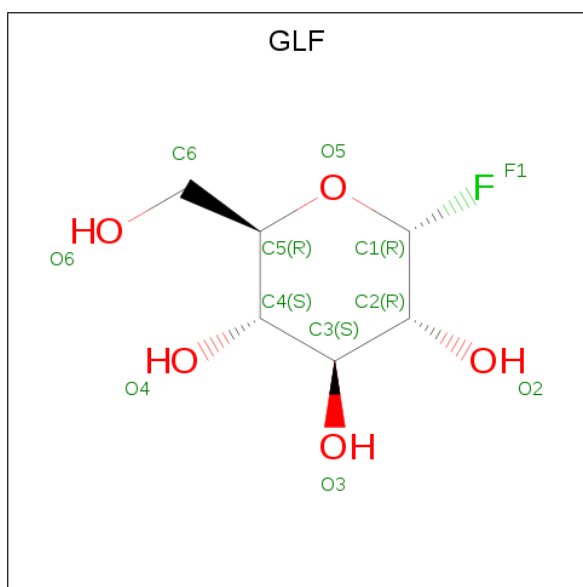
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is alpha-D-glucopyranosyl fluoride (three-letter code: GLF) (formula: $C_6H_{11}FO_5$).

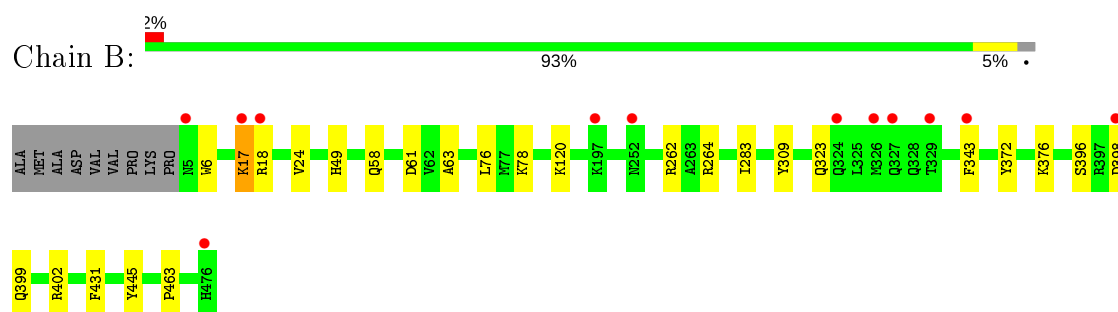


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	F	O	0	0
			12	6	1	5		
6	B	1	Total	C	F	O	0	0
			12	6	1	5		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	441	Total	O	0	0
			441	441		
7	B	429	Total	O	0	0
			429	429		

- Molecule 1: Beta-glucosidase 7



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.13Å 100.86Å 127.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.30 – 1.85 25.30 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (25.30-1.85) 99.9 (25.30-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.36 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.174 , 0.205 0.175 , 0.206	Depositor DCC
R_{free} test set	4328 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	10.4	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8553	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.03 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.9431e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GOL, ZN, SO4, GLF, MES

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	0.61	0/3922	0.62	1/5331 (0.0%)
1	B	0.63	0/3922	0.63	1/5331 (0.0%)
All	All	0.62	0/7844	0.63	2/10662 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	264	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	264	ARG	NE-CZ-NH2	-5.03	117.79	120.30

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	3806	0	3643	18	0
1	B	3806	0	3643	19	0
2	A	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	12	0	12	0	0
4	B	12	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	6	0	8	1	0
5	B	6	0	8	0	0
6	A	12	0	11	0	0
6	B	12	0	11	0	0
7	A	441	0	0	6	0
7	B	429	0	0	5	0
All	All	8553	0	7348	38	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 3.

The worst 5 of 38 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:B:343:PHE:HE1	7:B:547:HOH:O	1.46	0.96
1:A:396:SER:H	1:A:399:GLN:HE21	1.21	0.88
1:B:396:SER:H	1:B:399:GLN:HE21	1.17	0.88
1:B:343:PHE:HB3	7:B:799:HOH:O	1.86	0.75
5:A:1007:GOL:H11	7:A:591:HOH:O	1.90	0.71

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	470/481 (98%)	458 (97%)	12 (3%)	0	100	100
1	B	470/481 (98%)	457 (97%)	13 (3%)	0	100	100
All	All	940/962 (98%)	915 (97%)	25 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	390/397 (98%)	386 (99%)	4 (1%)	76	69
1	B	390/397 (98%)	386 (99%)	4 (1%)	76	69
All	All	780/794 (98%)	772 (99%)	8 (1%)	76	69

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	323	GLN
1	B	323	GLN
1	B	17	LYS
1	A	127	ASN
1	B	6	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	399	GLN
1	A	462	HIS
1	B	371	ASN
1	A	327	GLN
1	B	323	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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	SO4	B	1004	-	4,4,4	0.20	0	6,6,6	0.23	0
5	GOL	A	1007	-	5,5,5	0.33	0	5,5,5	0.48	0
5	GOL	B	1008	-	5,5,5	0.49	0	5,5,5	0.39	0
4	MES	A	1005	-	12,12,12	1.53	1 (8%)	14,16,16	6.24	8 (57%)
6	GLF	A	477	-	12,12,12	1.28	1 (8%)	16,17,17	1.00	0
4	MES	B	1006	-	12,12,12	1.49	1 (8%)	14,16,16	5.33	8 (57%)
3	SO4	A	1003	-	4,4,4	0.23	0	6,6,6	0.20	0
6	GLF	B	1002	-	12,12,12	1.35	2 (16%)	16,17,17	0.93	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
5	GOL	A	1007	-	-	1/4/4/4	-
5	GOL	B	1008	-	-	2/4/4/4	-
4	MES	A	1005	-	-	2/6/14/14	0/1/1/1
4	MES	B	1006	-	-	1/6/14/14	0/1/1/1
6	GLF	A	477	-	-	0/2/22/22	0/1/1/1
6	GLF	B	1002	-	-	0/2/22/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1006	MES	C8-S	-4.61	1.71	1.77
4	A	1005	MES	C8-S	-4.60	1.71	1.77
6	A	477	GLF	O5-C1	3.74	1.43	1.40
6	B	1002	GLF	C2-C1	2.97	1.54	1.52
6	B	1002	GLF	O5-C1	2.81	1.42	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1005	MES	O1S-S-C8	-15.00	88.86	106.92
4	B	1006	MES	O1S-S-C8	-12.77	91.54	106.92
4	A	1005	MES	O2S-S-C8	-12.20	92.23	106.92
4	B	1006	MES	O2S-S-C8	-8.51	96.66	106.92
4	A	1005	MES	O3S-S-C8	-8.07	92.72	105.77

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1008	GOL	C1-C2-C3-O3
4	A	1005	MES	C8-C7-N4-C5
4	B	1006	MES	C8-C7-N4-C5
5	B	1008	GOL	O2-C2-C3-O3
5	A	1007	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1007	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, 95th 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 ²)	Q<0.9
1	A	472/481 (98%)	-0.36	11 (2%) 60 59	4, 8, 19, 33	0
1	B	472/481 (98%)	-0.35	12 (2%) 57 56	4, 8, 19, 33	0
All	All	944/962 (98%)	-0.35	23 (2%) 59 57	4, 8, 19, 33	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	324	GLN	4.1
1	B	476	HIS	4.0
1	A	5	ASN	3.9
1	A	327	GLN	3.6
1	A	476	HIS	3.4

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 monosaccharides 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, 95th 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(\AA^2)	Q<0.9
5	GOL	A	1007	6/6	0.79	0.31	27,30,31,32	0
5	GOL	B	1008	6/6	0.79	0.26	31,33,33,34	0
4	MES	A	1005	12/12	0.94	0.14	16,20,21,22	0
4	MES	B	1006	12/12	0.95	0.11	12,13,15,16	0
3	SO4	B	1004	5/5	0.98	0.11	22,22,23,24	0
6	GLF	B	1002	12/12	0.98	0.07	3,5,7,9	0
3	SO4	A	1003	5/5	0.99	0.11	20,21,22,23	0
6	GLF	A	477	12/12	0.99	0.07	4,5,7,8	0
2	ZN	A	1001	1/1	1.00	0.03	6,6,6,6	0

6.5 Other polymers [i](#)

There are no such residues in this entry.