



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:15 am BST

PDB ID : 6CA1
Title : THE CRYSTAL STRUCTURE OF THE W169Y MUTANT OF ALPHA-GLUCOSIDASE (GH 31) FROM RUMINOCOCCUS OBEUM ATCC 29174 in complex with miglitol
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Deposited on : 2018-01-29
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

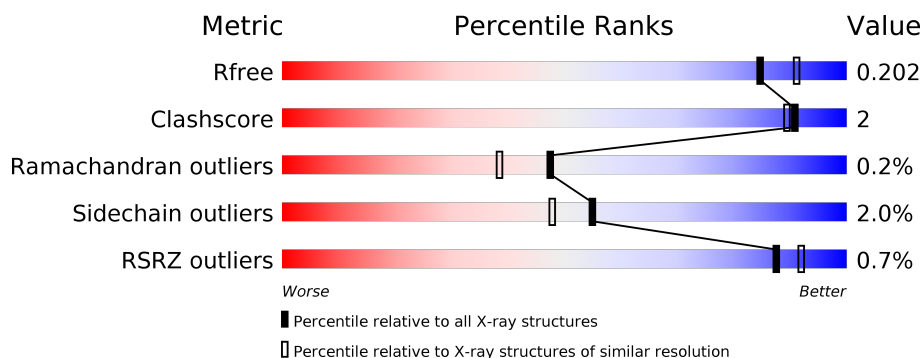
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	666	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 93% 6% </div> </div>
1	B	666	<div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 95% 5% </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11690 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.

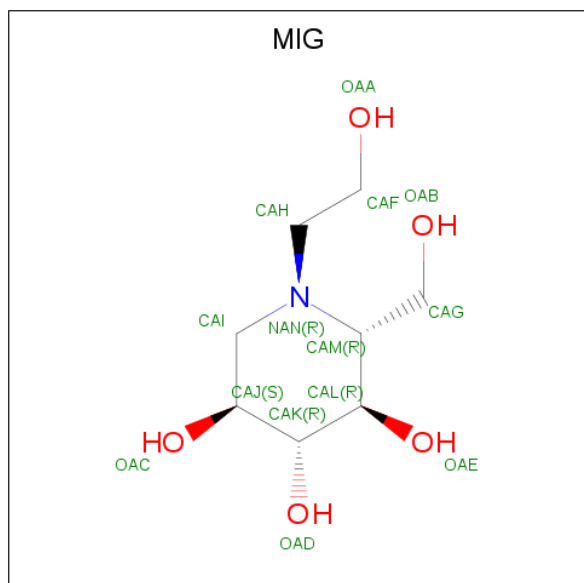
- Molecule 1 is a protein called Glycosyl hydrolase, family 31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	664	Total	C	N	O	S	0	2	0
			5428	3488	886	1019	35			
1	B	665	Total	C	N	O	S	0	0	0
			5416	3478	889	1014	35			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP A5ZY13
A	-1	ASN	-	expression tag	UNP A5ZY13
A	0	ALA	-	expression tag	UNP A5ZY13
B	-2	SER	-	expression tag	UNP A5ZY13
B	-1	ASN	-	expression tag	UNP A5ZY13
B	0	ALA	-	expression tag	UNP A5ZY13

- Molecule 2 is (2R,3R,4R,5S)-1-(2-hydroxyethyl)-2-(hydroxymethyl)piperidine-3,4,5-triol (three-letter code: MIG) (formula: C₈H₁₇NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

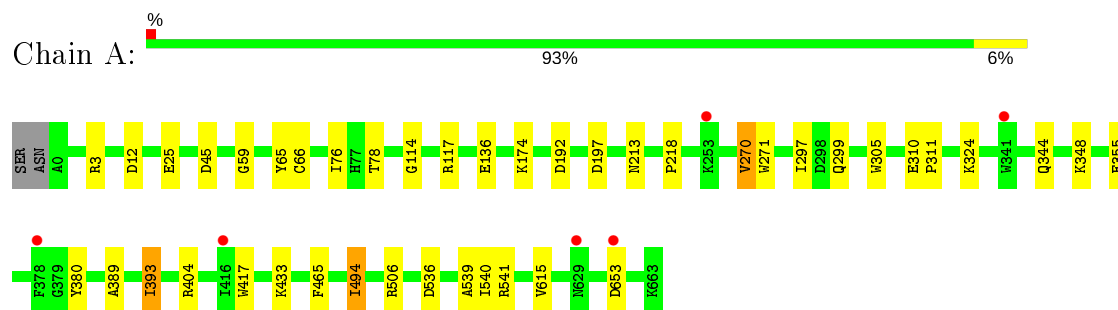
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	402	Total	O	0	0
			402	402		
4	B	404	Total	O	0	0
			404	404		

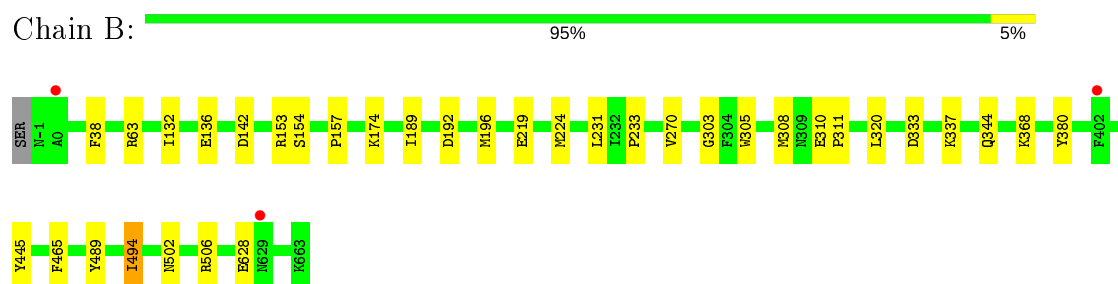
3 Residue-property plots [i](#)

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: Glycosyl hydrolase, family 31



- Molecule 1: Glycosyl hydrolase, family 31



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	64.75Å 70.06Å 88.16Å 111.32° 107.59° 97.67°	Depositor
Resolution (Å)	31.55 – 1.95 31.54 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.3 (31.55-1.95) 96.3 (31.54-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.8.1 _1168	Depositor
R, R_{free}	0.152 , 0.201 0.152 , 0.202	Depositor DCC
R_{free} test set	4668 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.513	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for -h,-k,h+k+l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11690	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MIG

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	0.36	0/5577	0.54	0/7523
1	B	0.36	0/5559	0.52	0/7499
All	All	0.36	0/11136	0.53	0/15022

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	5428	0	5175	22	0
1	B	5416	0	5162	17	0
2	A	14	0	16	1	0
2	B	14	0	16	1	0
3	A	6	0	8	1	0
3	B	6	0	8	0	0
4	A	402	0	0	2	0
4	B	404	0	0	2	0
All	All	11690	0	10385	36	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 2.

All (36) 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:219:GLU:OE2	4:B:801:HOH:O	2.15	0.64
1:A:3:ARG:NH2	1:A:136:GLU:OE2	2.33	0.61
1:B:174:LYS:NZ	4:B:803:HOH:O	2.37	0.57
1:A:297:ILE:HG21	1:A:393:ILE:HD11	1.87	0.55
1:A:389:ALA:O	1:A:393:ILE:HG23	2.09	0.52
1:A:348:LYS:HG2	1:B:344:GLN:NE2	2.25	0.51
1:B:38:PHE:CZ	1:B:132:ILE:HD11	2.47	0.50
1:A:218:PRO:HG3	1:A:299:GLN:HG2	1.93	0.49
1:A:348:LYS:HG2	1:B:344:GLN:HE21	1.78	0.47
1:A:270:VAL:HG12	1:A:271:TRP:H	1.78	0.47
1:A:59:GLY:HA2	1:A:433:LYS:HD3	1.97	0.47
1:B:310:GLU:N	1:B:311:PRO:HA	2.29	0.46
1:A:310:GLU:N	1:A:311:PRO:HA	2.31	0.45
1:A:404:ARG:HB2	1:A:417:TRP:CH2	2.52	0.45
1:B:308:MET:SD	2:B:701:MIG:HAHA	2.57	0.45
1:A:114:GLY:HA2	1:A:117:ARG:O	2.18	0.43
1:A:174:LYS:HD3	1:A:213:ASN:O	2.18	0.43
1:A:536:ASP:HB3	1:A:539:ALA:HB3	1.99	0.43
1:B:233:PRO:HD2	1:B:303:GLY:O	2.18	0.43
1:A:271:TRP:HZ2	2:A:701:MIG:HOAA	1.65	0.43
1:A:344:GLN:HG2	1:A:348:LYS:HE2	2.01	0.43
1:B:196:MET:HB2	1:B:233:PRO:HA	2.01	0.43
1:A:65:TYR:CG	1:A:66:CYS:N	2.85	0.42
1:A:324:LYS:NZ	1:B:333:ASP:O	2.44	0.42
1:A:76:ILE:HG22	1:A:78:THR:HG23	2.01	0.42
1:B:153:ARG:HG2	1:B:154:SER:N	2.35	0.42
1:A:197:ASP:HB3	4:A:813:HOH:O	2.20	0.42
1:B:489:TYR:HA	1:B:494:ILE:HD12	2.02	0.42
1:A:540:ILE:HG13	1:A:541:ARG:HG2	2.02	0.41
1:A:506:ARG:HB3	1:A:615:VAL:HG13	2.02	0.41
1:A:494:ILE:HG23	4:A:1018:HOH:O	2.21	0.40
3:A:702:GOL:H2	1:B:63:ARG:CZ	2.51	0.40
1:B:189:ILE:HD11	1:B:494:ILE:HD11	2.02	0.40
1:B:224:MET:HG3	1:B:231:LEU:HD11	2.02	0.40
1:B:157:PRO:HG3	1:B:445:TYR:CD1	2.56	0.40
1:B:502:ASN:O	1:B:506:ARG:HG3	2.21	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	664/666 (100%)	638 (96%)	25 (4%)	1 (0%)	47	38
1	B	663/666 (100%)	634 (96%)	28 (4%)	1 (0%)	47	38
All	All	1327/1332 (100%)	1272 (96%)	53 (4%)	2 (0%)	47	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	VAL
1	B	270	VAL

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	566/575 (98%)	555 (98%)	11 (2%)	57	50
1	B	564/575 (98%)	553 (98%)	11 (2%)	55	48
All	All	1130/1150 (98%)	1108 (98%)	22 (2%)	55	50

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	A	25	GLU
1	A	45	ASP
1	A	192	ASP

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Mol	Chain	Res	Type
1	A	305	TRP
1	A	355	GLU
1	A	380	TYR
1	A	393	ILE
1	A	465	PHE
1	A	494	ILE
1	A	653	ASP
1	B	136	GLU
1	B	142	ASP
1	B	192	ASP
1	B	305	TRP
1	B	320	LEU
1	B	337	LYS
1	B	368	LYS
1	B	380	TYR
1	B	465	PHE
1	B	494	ILE
1	B	628	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	344	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 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	MIG	A	701	-	14,14,14	1.22	1 (7%)	17,19,19	1.46	2 (11%)
3	GOL	B	702	-	5,5,5	0.34	0	5,5,5	0.32	0
2	MIG	B	701	-	14,14,14	1.38	1 (7%)	17,19,19	1.35	3 (17%)
3	GOL	A	702	-	5,5,5	0.30	0	5,5,5	0.35	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	MIG	A	701	-	-	0/5/25/25	0/1/1/1
3	GOL	B	702	-	-	4/4/4/4	-
2	MIG	B	701	-	-	1/5/25/25	0/1/1/1
3	GOL	A	702	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	MIG	CAJ-CAK	-3.81	1.46	1.52
2	A	701	MIG	CAJ-CAK	-3.28	1.47	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	MIG	CAH-NAN-CAM	3.24	121.97	113.29
2	B	701	MIG	CAH-NAN-CAM	2.89	121.03	113.29
2	B	701	MIG	CAI-NAN-CAM	2.32	115.08	109.69
2	A	701	MIG	OAA-CAF-CAH	2.21	120.37	111.19
2	B	701	MIG	OAB-CAG-CAM	2.18	116.10	111.42

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	702	GOL	C1-C2-C3-O3
3	A	702	GOL	O1-C1-C2-C3
3	B	702	GOL	O1-C1-C2-C3
3	A	702	GOL	O1-C1-C2-O2
3	B	702	GOL	O2-C2-C3-O3
2	B	701	MIG	OAA-CAF-CAH-NAN
3	B	702	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	MIG	1	0
2	B	701	MIG	1	0
3	A	702	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	664/666 (99%)	-0.26	6 (0%) 84 89	16, 27, 49, 65	0
1	B	665/666 (99%)	-0.34	3 (0%) 91 94	18, 29, 47, 67	0
All	All	1329/1332 (99%)	-0.30	9 (0%) 87 92	16, 28, 48, 67	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	629	ASN	3.6
1	A	629	ASN	2.6
1	A	416	ILE	2.5
1	B	0	ALA	2.4
1	B	402	PHE	2.4
1	A	653	ASP	2.2
1	A	341	TRP	2.1
1	A	378	PHE	2.1
1	A	253	LYS	2.0

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, 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
3	GOL	A	702	6/6	0.93	0.13	32,46,50,50	0
3	GOL	B	702	6/6	0.95	0.11	37,45,47,57	0
2	MIG	B	701	14/14	0.96	0.08	22,26,31,37	0
2	MIG	A	701	14/14	0.96	0.08	23,27,34,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.