



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 3, 2023 – 08:50 AM EDT

PDB ID : 3SJN  
Title : Crystal structure of enolase Spea\_3858 (target EFI-500646) from *Shewanella pealeana* with magnesium bound  
Authors : Patskovsky, Y.; Kim, J.; Toro, R.; Bhosle, R.; Hillerich, B.; Seidel, R.D.; Washington, E.; Scott Glenn, A.; Chowdhury, S.; Evans, B.; Hammonds, J.; Zencheck, W.D.; Imker, H.J.; Gerlt, J.A.; Almo, S.C.; Enzyme Function Initiative (EFI)  
Deposited on : 2011-06-21  
Resolution : 1.90 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.35  
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)

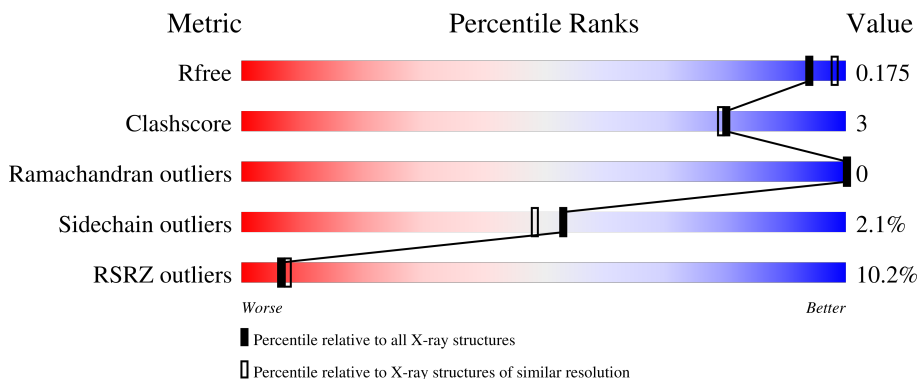
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 of 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	374	 9% 90% 9%
1	B	374	 11% 92% 8%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6121 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 Mandelate racemase/muconate lactonizing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	373	2925	1861	492	555	17	0	8	0
1	B	373	2926	1860	494	554	18	0	7	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP A8H9D1
A	1	VAL	-	expression tag	UNP A8H9D1
B	0	MET	-	expression tag	UNP A8H9D1
B	1	VAL	-	expression tag	UNP A8H9D1

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0

- Molecule 3 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	8	4	2	2	0	0
3	B	1	Total	C	O		0	0
			4	2	2			

- Molecule 4 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
4	A	1	Total C O 6 3 3	0	0

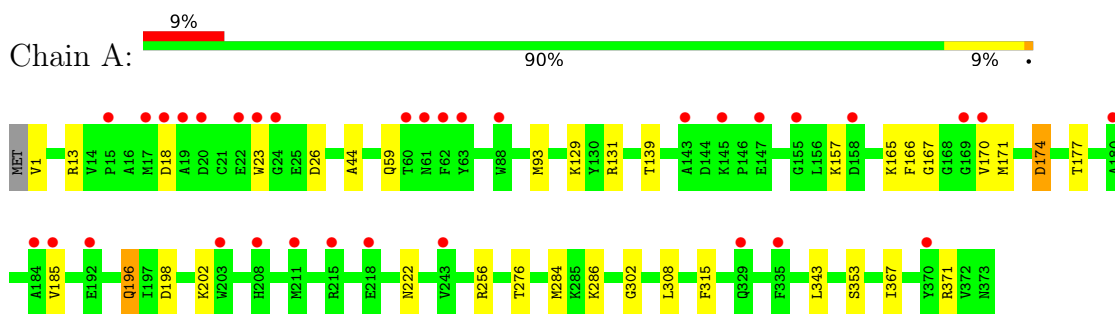
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	130	Total O 130 130	0	0
5	B	120	Total O 120 120	0	0

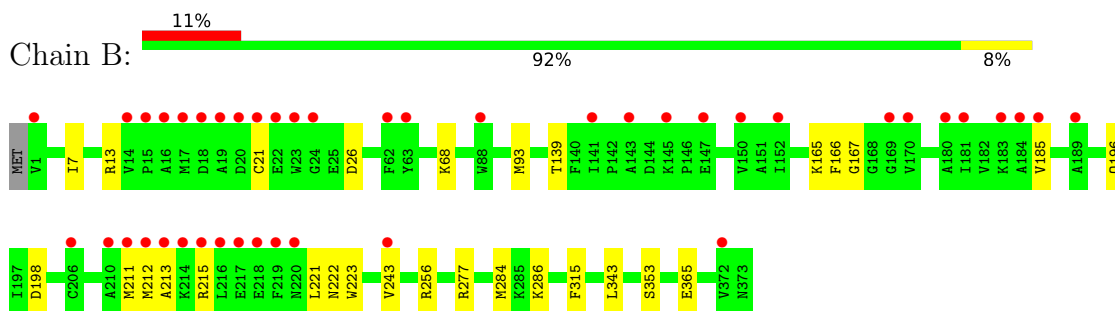
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Mandelate racemase/muconate lactonizing protein



- Molecule 1: Mandelate racemase/muconate lactonizing protein



## 4 Data and refinement statistics i

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.21Å 109.21Å 141.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 38.61 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-1.90) 99.6 (38.61-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 1.81Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.160 , 0.176 0.160 , 0.175	Depositor DCC
$R_{free}$ test set	2283 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.7	Xtrriage
Anisotropy	0.693	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 34.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	0.239 for -h,k,-l	Xtrriage
Reported twinning fraction	0.711 for H, K, L 0.289 for -H, K, -L	Depositor
Outliers	0 of 75778 reflections	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6121	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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: UNL, 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	0.51	0/3008	0.63	0/4070
1	B	0.52	0/3006	0.62	0/4065
All	All	0.51	0/6014	0.62	0/8135

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 [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	2925	0	2917	17	0
1	B	2926	0	2915	16	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	8	0	0	0	0
3	B	4	0	0	0	0
4	A	6	0	8	1	0
5	A	130	0	0	1	0
5	B	120	0	0	1	0
All	All	6121	0	5840	32	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.

All (32) 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:171:MET:O	1:A:202:LYS:HE3	1.89	0.72
1:A:59:GLN:HE21	1:B:21:CYS:H	1.40	0.67
1:B:196:GLN:HG2	1:B:223:TRP:CD2	2.36	0.61
1:B:256[B]:ARG:HD3	1:B:286[B]:LYS:HD2	1.82	0.61
1:A:131:ARG:HE	4:A:376:GOL:H2	1.70	0.56
1:B:196:GLN:HG3	1:B:222:ASN:HB3	1.87	0.56
1:A:196:GLN:HE21	1:A:222:ASN:HB3	1.70	0.56
1:B:284:MET:HG3	1:B:315:PHE:CZ	2.44	0.53
1:B:277:ARG:NH1	5:B:496:HOH:O	2.41	0.52
1:B:167:GLY:HA3	1:B:198:ASP:O	2.10	0.52
1:B:7:ILE:HB	1:B:68:LYS:HG3	1.94	0.50
1:B:213:ALA:CB	1:B:243:VAL:HG22	2.42	0.48
1:A:166:PHE:CE1	1:A:185:VAL:HG21	2.48	0.48
1:A:284:MET:HG3	1:A:315:PHE:CZ	2.48	0.48
1:A:167:GLY:HA3	1:A:198:ASP:O	2.13	0.48
1:A:256[A]:ARG:NH1	5:A:417:HOH:O	2.47	0.48
1:A:256[B]:ARG:HD3	1:A:286[B]:LYS:HD2	1.95	0.47
1:B:7:ILE:HD12	1:B:68:LYS:HA	1.96	0.47
1:B:196:GLN:HG2	1:B:223:TRP:CE3	2.49	0.47
1:A:174:ASP:HB2	1:A:177:THR:HB	1.96	0.47
1:A:343:LEU:HD21	1:A:353:SER:HB2	1.96	0.47
1:B:343:LEU:HD21	1:B:353:SER:HB2	1.97	0.47
1:B:139:THR:HA	1:B:165:LYS:O	2.16	0.45
1:A:174:ASP:HB2	1:A:177:THR:CB	2.48	0.43
1:A:139:THR:HA	1:A:165:LYS:O	2.19	0.43
1:B:212:MET:HA	1:B:215:ARG:HB2	2.01	0.42
1:A:367:ILE:O	1:A:371:ARG:HB2	2.21	0.41
1:B:13:ARG:HG3	1:B:26:ASP:HB3	2.02	0.41
1:A:13:ARG:HG3	1:A:26:ASP:HB3	2.03	0.41
1:B:166:PHE:CE1	1:B:185:VAL:HG21	2.56	0.41
1:A:44:ALA:HA	1:A:276:THR:HB	2.03	0.40
1:A:302:GLY:HA3	1:A:308:LEU:HD21	2.02	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	379/374 (101%)	367 (97%)	12 (3%)	0	100	100
1	B	378/374 (101%)	365 (97%)	13 (3%)	0	100	100
All	All	757/748 (101%)	732 (97%)	25 (3%)	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	316/309 (102%)	307 (97%)	9 (3%)	43	36
1	B	315/309 (102%)	311 (99%)	4 (1%)	69	68
All	All	631/618 (102%)	618 (98%)	13 (2%)	53	48

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

Mol	Chain	Res	Type
1	A	1	VAL
1	A	18	ASP
1	A	23	TRP
1	A	93	MET
1	A	129	LYS
1	A	157	LYS
1	A	170	VAL
1	A	174	ASP

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Mol	Chain	Res	Type
1	A	196	GLN
1	B	93	MET
1	B	211	MET
1	B	221	LEU
1	B	365	GLU

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

Mol	Chain	Res	Type
1	A	59	GLN
1	A	196	GLN
1	B	196	GLN
1	B	208	HIS
1	B	222	ASN

### 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](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic and 2 are unknown - leaving 1 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
4	GOL	A	376	-	5,5,5	0.37	0	5,5,5	0.29	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
4	GOL	A	376	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	376	GOL	O1-C1-C2-C3
4	A	376	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	376	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

### 6.1 Protein, DNA and RNA chains

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	373/374 (99%)	0.53	33 (8%) 10 11	17, 40, 81, 102	0
1	B	373/374 (99%)	0.58	43 (11%) 4 5	19, 40, 86, 105	0
All	All	746/748 (99%)	0.56	76 (10%) 6 8	17, 40, 82, 105	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	23	TRP	6.6
1	A	15	PRO	6.0
1	A	62	PHE	6.0
1	A	169	GLY	5.8
1	B	20	ASP	5.5
1	B	22	GLU	5.5
1	B	23	TRP	5.5
1	B	18	ASP	5.3
1	B	211	MET	4.5
1	B	145	LYS	4.3
1	B	16	ALA	4.2
1	A	184	ALA	4.0
1	A	22	GLU	4.0
1	B	21	CYS	3.9
1	A	145	LYS	3.9
1	A	88	TRP	3.7
1	A	170	VAL	3.7
1	A	24	GLY	3.7
1	A	211	MET	3.6
1	B	152	ILE	3.6
1	B	17	MET	3.6
1	B	19	ALA	3.6
1	A	17	MET	3.5
1	A	180	ALA	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	61	ASN	3.5
1	B	184	ALA	3.4
1	A	20	ASP	3.4
1	B	15	PRO	3.4
1	B	185	VAL	3.4
1	B	62	PHE	3.3
1	B	88	TRP	3.3
1	B	183	LYS	3.2
1	B	216	LEU	3.1
1	B	170	VAL	3.1
1	A	215	ARG	3.1
1	A	63	TYR	3.0
1	B	219	PHE	3.0
1	B	1	VAL	2.9
1	A	19	ALA	2.9
1	B	24	GLY	2.9
1	A	185	VAL	2.9
1	B	180	ALA	2.9
1	A	158	ASP	2.7
1	A	143	ALA	2.6
1	B	181	ILE	2.6
1	A	329	GLN	2.6
1	B	141	ILE	2.6
1	B	213	ALA	2.6
1	A	243	VAL	2.5
1	B	147	GLU	2.5
1	A	370	TYR	2.5
1	B	143	ALA	2.5
1	B	215	ARG	2.5
1	A	60	THR	2.5
1	A	335	PHE	2.4
1	B	63	TYR	2.4
1	A	208	HIS	2.4
1	B	210	ALA	2.3
1	B	206	CYS	2.3
1	B	169	GLY	2.3
1	B	217	GLU	2.3
1	A	155	GLY	2.2
1	B	372	VAL	2.2
1	A	147	GLU	2.1
1	B	243	VAL	2.1
1	B	218	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	214	LYS	2.1
1	A	18	ASP	2.1
1	A	218	GLU	2.1
1	B	150	VAL	2.1
1	B	220	ASN	2.1
1	B	14	VAL	2.0
1	A	203	TRP	2.0
1	B	189	ALA	2.0
1	B	212	MET	2.0
1	A	192	GLU	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 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, 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
4	GOL	A	376	6/6	0.81	0.33	55,67,71,77	0
3	UNL	A	375	8/-	0.88	0.23	65,73,80,80	0
2	MG	B	374	1/1	0.93	0.10	43,43,43,43	0
3	UNL	B	375	4/-	0.95	0.07	35,36,38,39	0
2	MG	A	374	1/1	0.95	0.08	40,40,40,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.