



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 6J2B / pdb\_00006j2b  
Title : CTX-M-64 beta-lactamase S130T sulbactam complex  
Authors : Cheng, Q.; Chen, S.  
Deposited on : 2018-12-31  
Resolution : 1.44 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)

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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 : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	302	-	-	X	-
3	GOL	B	302	-	X	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4423 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-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	3	0
			1972	1227	357	382	6			
1	B	260	Total	C	N	O	S	0	1	0
			1958	1218	353	381	6			

There are 50 discrepancies between the modelled and reference sequences:

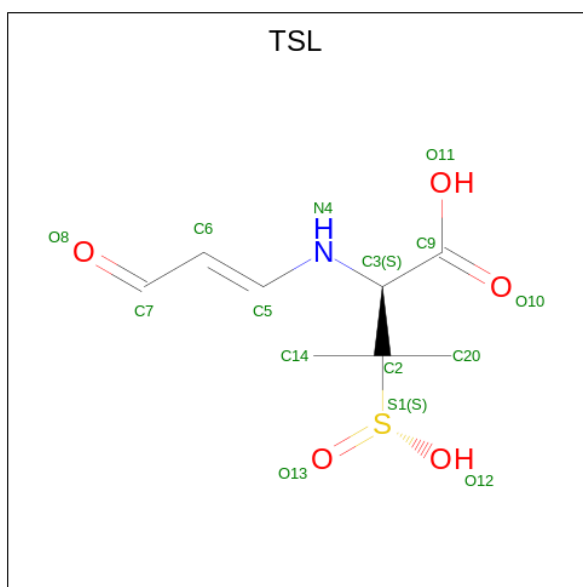
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	HIS	-	expression tag	UNP C8CP57
A	2	HIS	-	expression tag	UNP C8CP57
A	3	HIS	-	expression tag	UNP C8CP57
A	4	HIS	-	expression tag	UNP C8CP57
A	5	HIS	-	expression tag	UNP C8CP57
A	6	HIS	-	expression tag	UNP C8CP57
A	7	SER	-	expression tag	UNP C8CP57
A	8	SER	-	expression tag	UNP C8CP57
A	9	GLY	-	expression tag	UNP C8CP57
A	10	LEU	-	expression tag	UNP C8CP57
A	11	VAL	-	expression tag	UNP C8CP57
A	12	PRO	-	expression tag	UNP C8CP57
A	13	ARG	-	expression tag	UNP C8CP57
A	14	GLY	-	expression tag	UNP C8CP57
A	15	SER	-	expression tag	UNP C8CP57
A	16	HIS	-	expression tag	UNP C8CP57
A	17	MET	-	expression tag	UNP C8CP57
A	18	ALA	-	expression tag	UNP C8CP57
A	19	SER	-	expression tag	UNP C8CP57
A	20	GLY	-	expression tag	UNP C8CP57
A	21	GLY	-	expression tag	UNP C8CP57
A	22	THR	-	expression tag	UNP C8CP57
A	23	GLU	-	expression tag	UNP C8CP57
A	24	LEU	-	expression tag	UNP C8CP57
A	130	THR	SER	engineered mutation	UNP C8CP57

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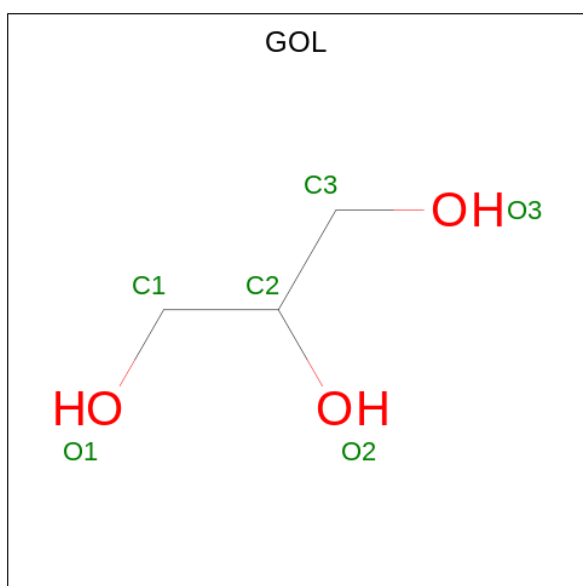
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	HIS	-	expression tag	UNP C8CP57
B	2	HIS	-	expression tag	UNP C8CP57
B	3	HIS	-	expression tag	UNP C8CP57
B	4	HIS	-	expression tag	UNP C8CP57
B	5	HIS	-	expression tag	UNP C8CP57
B	6	HIS	-	expression tag	UNP C8CP57
B	7	SER	-	expression tag	UNP C8CP57
B	8	SER	-	expression tag	UNP C8CP57
B	9	GLY	-	expression tag	UNP C8CP57
B	10	LEU	-	expression tag	UNP C8CP57
B	11	VAL	-	expression tag	UNP C8CP57
B	12	PRO	-	expression tag	UNP C8CP57
B	13	ARG	-	expression tag	UNP C8CP57
B	14	GLY	-	expression tag	UNP C8CP57
B	15	SER	-	expression tag	UNP C8CP57
B	16	HIS	-	expression tag	UNP C8CP57
B	17	MET	-	expression tag	UNP C8CP57
B	18	ALA	-	expression tag	UNP C8CP57
B	19	SER	-	expression tag	UNP C8CP57
B	20	GLY	-	expression tag	UNP C8CP57
B	21	GLY	-	expression tag	UNP C8CP57
B	22	THR	-	expression tag	UNP C8CP57
B	23	GLU	-	expression tag	UNP C8CP57
B	24	LEU	-	expression tag	UNP C8CP57
B	130	THR	SER	engineered mutation	UNP C8CP57

- Molecule 2 is TRANS-ENAMINE INTERMEDIATE OF SULBACTAM (CCD ID: TSL)  
(formula: C<sub>8</sub>H<sub>13</sub>NO<sub>5</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	S	0	0
			15	8	1	5	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



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		

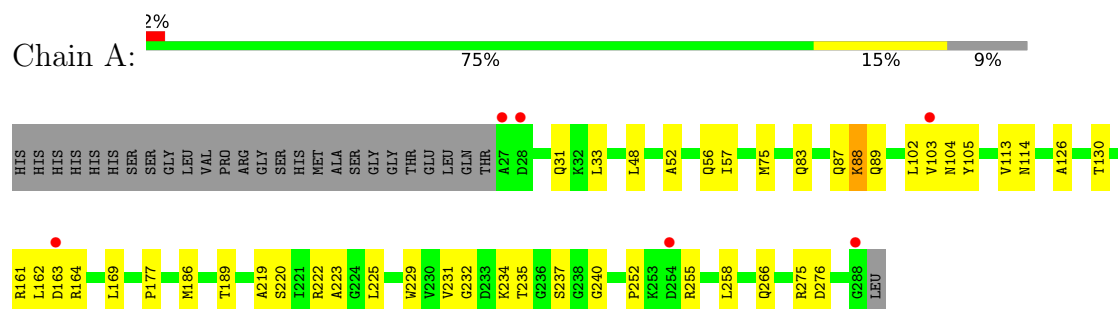
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	225	Total 225	O 225	0	0
4	B	226	Total 226	O 226	0	0

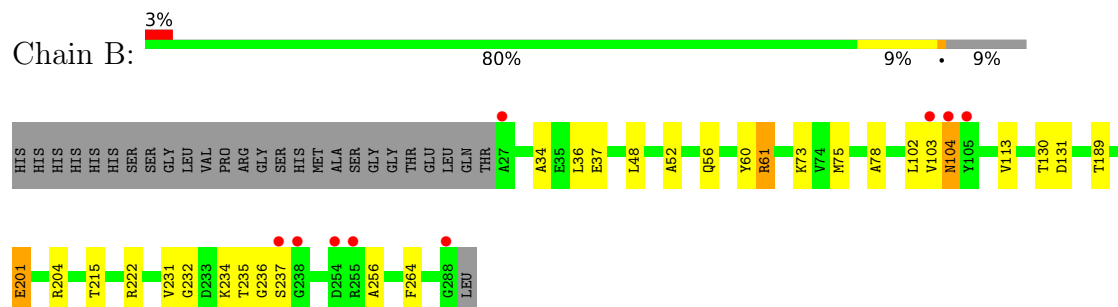
### 3 Residue-property plots [i](#)

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: Beta-lactamase



#### • Molecule 1: Beta-lactamase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.84Å 105.88Å 47.44Å 90.00° 101.16° 90.00°	Depositor
Resolution (Å)	46.54 – 1.44 46.54 – 1.44	Depositor EDS
% Data completeness (in resolution range)	97.6 (46.54-1.44) 97.6 (46.54-1.44)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.96 (at 1.44Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, $R_{free}$	0.153 , 0.187 0.164 , 0.195	Depositor DCC
$R_{free}$ test set	3797 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.8	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 34.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4423	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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, TSL

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	1.49	15/2008 (0.7%)	1.30	4/2730 (0.1%)
1	B	1.47	9/1988 (0.5%)	1.28	9/2704 (0.3%)
All	All	1.48	24/3996 (0.6%)	1.29	13/5434 (0.2%)

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	B	0	1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	232	GLY	CA-C	-10.41	1.44	1.52
1	A	57	ILE	C-N	7.97	1.45	1.33
1	A	266	GLN	N-CA	7.24	1.51	1.45
1	B	37	GLU	CA-C	7.14	1.61	1.52
1	B	34	ALA	C-O	-7.05	1.15	1.24

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	36	LEU	CA-C-O	5.62	126.72	120.82
1	A	52	ALA	N-CA-C	-5.41	105.39	111.28
1	B	131	ASP	N-CA-C	5.28	122.03	110.80
1	B	104	ASN	CA-C-N	5.24	131.12	121.70
1	B	104	ASN	C-N-CA	5.24	131.12	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	104	ASN	Peptide

## 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	1972	0	2006	29	0
1	B	1958	0	1985	16	0
2	A	15	0	11	1	0
2	B	15	0	11	1	0
3	A	6	0	7	9	0
3	B	6	0	7	9	0
4	A	225	0	0	2	0
4	B	226	0	0	1	0
All	All	4423	0	4027	45	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 6.

The worst 5 of 45 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:234[A]:LYS:HZ1	3:B:302:GOL:C1	1.74	0.99
1:B:201:GLU:OE1	1:B:204:ARG:NH2	2.14	0.80
1:A:234[A]:LYS:NZ	3:A:302:GOL:H31	1.97	0.79
1:B:234[A]:LYS:HZ1	3:B:302:GOL:H12	1.50	0.76
1:A:234[A]:LYS:HZ1	3:A:302:GOL:C3	2.02	0.73

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	261/287 (91%)	257 (98%)	4 (2%)	0	100	100
1	B	259/287 (90%)	253 (98%)	6 (2%)	0	100	100
All	All	520/574 (91%)	510 (98%)	10 (2%)	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	207/226 (92%)	206 (100%)	1 (0%)	86	72
1	B	205/226 (91%)	204 (100%)	1 (0%)	86	72
All	All	412/452 (91%)	410 (100%)	2 (0%)	86	72

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	B	103	VAL

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	30	GLN

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Mol	Chain	Res	Type
1	A	56	GLN
1	A	268	GLN
1	B	93	GLN
1	B	206	GLN

### 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 oligosaccharides in this entry.

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

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	TSL	A	301	1	9,14,14	1.38	1 (11%)	9,19,19	0.40	0
2	TSL	B	301	1	9,14,14	1.39	1 (11%)	9,19,19	0.40	0
3	GOL	B	302	-	5,5,5	1.84	1 (20%)	5,5,5	3.21	5 (100%)
3	GOL	A	302	-	5,5,5	1.36	1 (20%)	5,5,5	2.27	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	TSL	A	301	1	-	2/17/21/21	-
2	TSL	B	301	1	-	2/17/21/21	-
3	GOL	B	302	-	-	3/4/4/4	-
3	GOL	A	302	-	-	1/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	GOL	O2-C2	-3.83	1.32	1.43
2	B	301	TSL	C6-C7	-3.40	1.34	1.44
2	A	301	TSL	C6-C7	-3.39	1.34	1.44
3	A	302	GOL	O2-C2	-2.03	1.37	1.43

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	GOL	O1-C1-C2	3.98	129.29	110.20
3	B	302	GOL	O2-C2-C1	-3.93	91.82	109.12
3	A	302	GOL	O2-C2-C3	-3.84	92.19	109.12
3	B	302	GOL	C3-C2-C1	-2.88	100.50	111.70
3	B	302	GOL	O2-C2-C3	2.62	120.65	109.12

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	TSL	C5-C6-C7-O8
2	B	301	TSL	C5-C6-C7-O8
3	B	302	GOL	O2-C2-C3-O3
3	B	302	GOL	O1-C1-C2-O2
2	B	301	TSL	C9-C3-N4-C5

There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	TSL	1	0
2	B	301	TSL	1	0
3	B	302	GOL	9	0
3	A	302	GOL	9	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	260/287 (90%)	-0.02	6 (2%) 61 62	6, 16, 28, 52	3 (1%)
1	B	260/287 (90%)	0.07	9 (3%) 47 48	6, 17, 30, 54	1 (0%)
All	All	520/574 (90%)	0.03	15 (2%) 54 54	6, 16, 30, 54	4 (0%)

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	237	SER	3.7
1	B	104	ASN	3.5
1	A	27	ALA	3.4
1	A	288	GLY	3.1
1	B	288	GLY	3.0

### 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( $\text{\AA}^2$ )	Q<0.9
2	TSL	B	301	15/15	0.89	0.12	15,23,27,29	0
2	TSL	A	301	15/15	0.91	0.10	14,20,25,26	0
3	GOL	B	302	6/6	0.92	0.12	18,33,34,35	0
3	GOL	A	302	6/6	0.93	0.10	17,28,31,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.