



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 06:37 PM BST

PDB ID : 3FXR  
Title : Crystal structure of TsaR in complex with sulfate  
Authors : Monferrer, D.; Tralau, T.; Kertesz, M.A.; Kikhney, A.; Svergun, D.; Uson, I.  
Deposited on : 2009-01-21  
Resolution : 2.50 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.

---

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

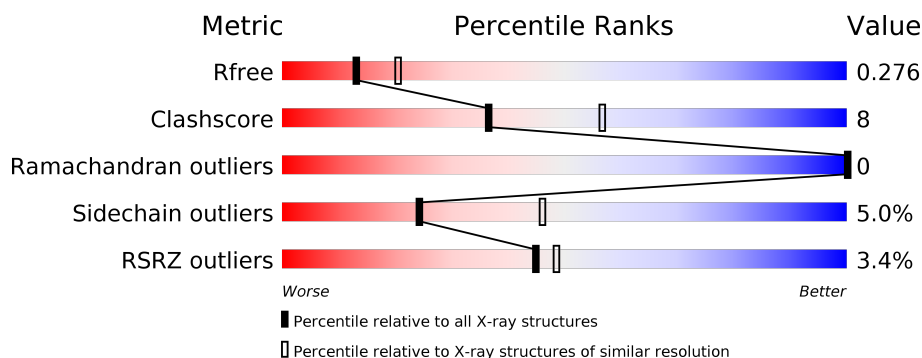
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	305	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>• •</div> </div> </div>
1	B	305	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div>• •</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
4	ASC	A	3001	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4909 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 LysR type regulator of tsaMBCD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	1	0
			2290	1456	416	409	9			
1	B	296	Total	C	N	O	S	0	1	0
			2288	1456	414	409	9			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	LEU	-	SEE REMARK 999	UNP P94678
A	300	HIS	-	expression tag	UNP P94678
A	301	HIS	-	expression tag	UNP P94678
A	302	HIS	-	expression tag	UNP P94678
A	303	HIS	-	expression tag	UNP P94678
A	304	HIS	-	expression tag	UNP P94678
A	305	HIS	-	expression tag	UNP P94678
B	2	LEU	-	SEE REMARK 999	UNP P94678
B	300	HIS	-	expression tag	UNP P94678
B	301	HIS	-	expression tag	UNP P94678
B	302	HIS	-	expression tag	UNP P94678
B	303	HIS	-	expression tag	UNP P94678
B	304	HIS	-	expression tag	UNP P94678
B	305	HIS	-	expression tag	UNP P94678

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



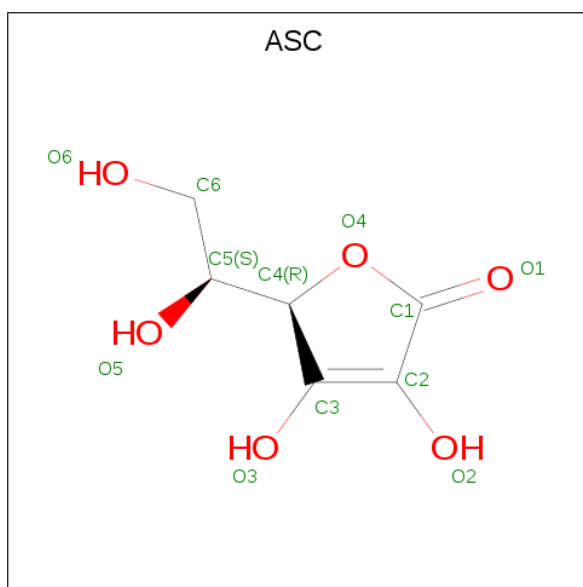
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 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
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		

- Molecule 4 is ASCORBIC ACID (three-letter code: ASC) (formula:  $C_6H_8O_6$ ).



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

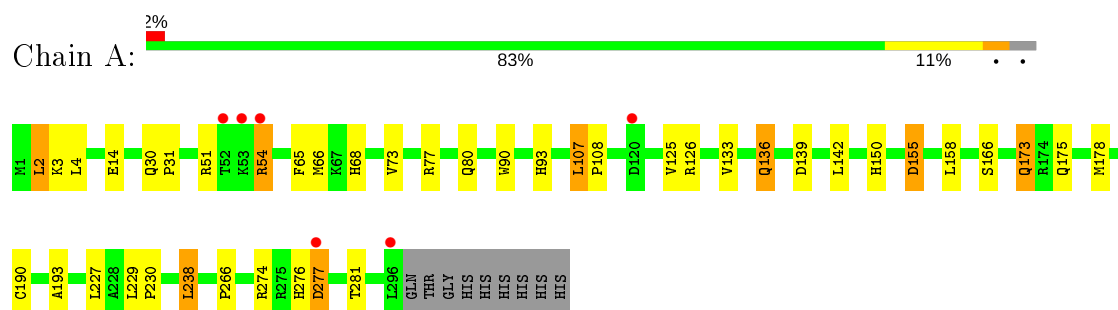
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	126	Total 126	O 126	0	0
5	B	125	Total 125	O 125	0	0

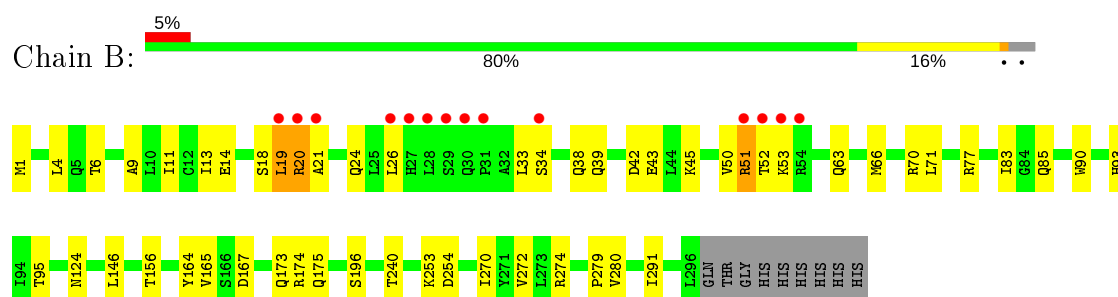
### 3 Residue-property plots [i](#)

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: LysR type regulator of tsaMBCD



- Molecule 1: LysR type regulator of tsaMBCD





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.11Å 51.83Å 107.99Å 90.00° 110.52° 90.00°	Depositor
Resolution (Å)	19.90 – 2.50 19.86 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.90-2.50) 99.8 (19.86-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.01	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.65 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.5.0046	Depositor
R, $R_{free}$	0.204 , 0.269 0.205 , 0.276	Depositor DCC
$R_{free}$ test set	1251 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.9	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4909	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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: ASC, GOL, 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	0.46	0/2345	0.63	1/3194 (0.0%)
1	B	0.50	0/2338	0.68	0/3184
All	All	0.48	0/4683	0.65	1/6378 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	LEU	CA-CB-CG	5.27	127.43	115.30

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	2290	0	2335	41	0
1	B	2288	0	2335	39	0
2	A	35	0	0	1	0
2	B	15	0	0	0	0
3	A	6	0	8	3	0
3	B	12	0	16	5	0
4	A	12	0	6	6	0
5	A	126	0	0	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	125	0	0	4	0
All	All	4909	0	4700	74	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 8.

The worst 5 of 74 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:227:LEU:O	3:A:2001:GOL:H32	1.53	1.09
1:A:150:HIS:HE1	4:A:3001:ASC:H5	1.33	0.91
1:A:150:HIS:CE1	4:A:3001:ASC:H5	2.16	0.79
1:B:274:ARG:HH21	3:B:2002:GOL:H2	1.53	0.72
1:A:227:LEU:O	3:A:2001:GOL:C3	2.36	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	295/305 (97%)	284 (96%)	11 (4%)	0	100	100
1	B	294/305 (96%)	281 (96%)	13 (4%)	0	100	100
All	All	589/610 (97%)	565 (96%)	24 (4%)	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	240/248 (97%)	228 (95%)	12 (5%)	24	46
1	B	240/248 (97%)	228 (95%)	12 (5%)	24	46
All	All	480/496 (97%)	456 (95%)	24 (5%)	24	46

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	274	ARG
1	B	19	LEU
1	B	240	THR
1	A	277	ASP
1	B	14	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	150	HIS
1	B	292	GLN
1	B	173	GLN
1	A	188	GLN
1	B	267	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry

14 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	$\# Z  > 2$
3	GOL	B	2003	-	5,5,5	0.29	0	5,5,5	0.51	0
3	GOL	A	2001	-	5,5,5	0.50	0	5,5,5	0.58	0
2	SO4	B	1007	-	4,4,4	0.14	0	6,6,6	0.11	0
2	SO4	A	1009	-	4,4,4	0.15	0	6,6,6	0.18	0
2	SO4	A	1010	-	4,4,4	0.16	0	6,6,6	0.13	0
2	SO4	A	1008	-	4,4,4	0.15	0	6,6,6	0.15	0
2	SO4	B	1005	-	4,4,4	0.16	0	6,6,6	0.16	0
2	SO4	A	1003	-	4,4,4	0.16	0	6,6,6	0.16	0
2	SO4	A	1004	-	4,4,4	0.13	0	6,6,6	0.29	0
2	SO4	B	1001	-	4,4,4	0.13	0	6,6,6	0.37	0
2	SO4	A	1006	-	4,4,4	0.15	0	6,6,6	0.09	0
3	GOL	B	2002	-	5,5,5	0.38	0	5,5,5	0.63	0
2	SO4	A	1002	-	4,4,4	0.12	0	6,6,6	0.47	0
4	ASC	A	3001	-	12,12,12	1.93	1 (8%)	17,17,17	1.63	4 (23%)

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	B	2002	-	-	2/4/4/4	-
3	GOL	B	2003	-	-	4/4/4/4	-
3	GOL	A	2001	-	-	2/4/4/4	-
4	ASC	A	3001	-	-	1/6/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3001	ASC	O4-C1	6.29	1.45	1.36

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3001	ASC	C4-O4-C1	-3.72	105.05	109.25
4	A	3001	ASC	O3-C3-C2	-3.20	123.88	132.29
4	A	3001	ASC	O3-C3-C4	2.78	125.34	118.08
4	A	3001	ASC	O4-C1-O1	2.12	123.75	121.25

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2003	GOL	O1-C1-C2-C3
3	B	2003	GOL	C1-C2-C3-O3
3	A	2001	GOL	O1-C1-C2-O2
3	A	2001	GOL	O1-C1-C2-C3
3	B	2003	GOL	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2003	GOL	3	0
3	A	2001	GOL	3	0
2	A	1004	SO4	1	0
3	B	2002	GOL	2	0
4	A	3001	ASC	6	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	296/305 (97%)	-0.10	6 (2%) 65 68	8, 16, 25, 35	9 (3%)
1	B	296/305 (97%)	0.00	14 (4%) 31 33	6, 15, 33, 43	3 (1%)
All	All	592/610 (97%)	-0.05	20 (3%) 45 48	6, 15, 30, 43	12 (2%)

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	28	LEU	10.2
1	B	29	SER	7.2
1	B	54	ARG	4.4
1	B	52	THR	4.2
1	B	51	ARG	4.0

### 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
3	GOL	A	2001	6/6	0.79	0.33	35,37,38,40	0
4	ASC	A	3001	12/12	0.82	0.29	45,48,49,49	0
2	SO4	A	1006	5/5	0.85	0.34	90,90,90,90	0
3	GOL	B	2003	6/6	0.88	0.44	38,40,41,41	0
2	SO4	B	1007	5/5	0.90	0.23	89,89,89,89	0
3	GOL	B	2002	6/6	0.93	0.21	40,41,41,42	0
2	SO4	A	1009	5/5	0.94	0.28	66,66,67,67	0
2	SO4	A	1010	5/5	0.96	0.24	55,55,55,56	0
2	SO4	A	1003	5/5	0.97	0.12	48,48,49,49	0
2	SO4	B	1005	5/5	0.97	0.13	47,47,47,48	0
2	SO4	A	1008	5/5	0.98	0.10	33,33,34,34	0
2	SO4	B	1001	5/5	0.99	0.08	26,27,28,28	0
2	SO4	A	1002	5/5	0.99	0.09	21,22,23,23	0
2	SO4	A	1004	5/5	0.99	0.17	29,29,30,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.