



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:44 PM GMT

PDB ID : 4Y7M  
Title : T6SS protein TssM C-terminal domain (835-1129) from EAEC  
Authors : Nguyen, V.S.; Spinelli, S.; Durand, E.; Roussel, A.; Cambillau, C.  
Deposited on : 2015-02-15  
Resolution : 1.92 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

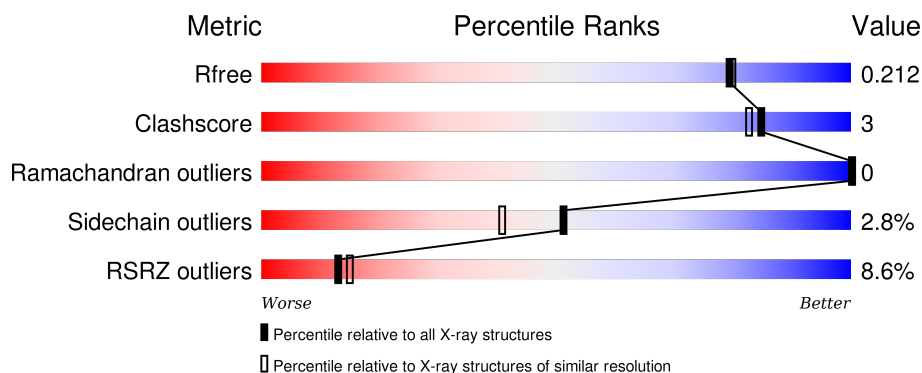
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.92 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))
$R_{free}$	91344	5832 (1.94-1.90)
Clashscore	102246	6540 (1.94-1.90)
Ramachandran outliers	100387	6464 (1.94-1.90)
Sidechain outliers	100360	6465 (1.94-1.90)
RSRZ outliers	91569	5846 (1.94-1.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	129	<div> <div>4%</div> <div>96%</div> <div>.</div> </div>
1	B	129	<div> <div>2%</div> <div>98%</div> <div>.</div> </div>
2	C	295	<div> <div>2%</div> <div>74%</div> <div>7%</div> <div>18%</div> </div>
2	D	295	<div> <div>16%</div> <div>64%</div> <div>12%</div> <div>23%</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
3	SO4	C	1201	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6337 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 Hi113 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	0
			959	604	158	190	7			
1	B	129	Total	C	N	O	S	0	0	0
			963	607	159	190	7			

- Molecule 2 is a protein called Type VI secretion protein IcmF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	241	Total	C	N	O	S	0	0	0
			1856	1185	326	341	4			
2	D	226	Total	C	N	O	S	0	0	0
			1740	1111	311	314	4			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

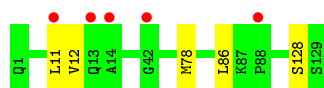
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	164	Total O 164 164	0	0
4	B	163	Total O 163 163	0	0
4	C	300	Total O 300 300	0	0
4	D	177	Total O 177 177	0	0

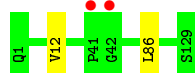
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

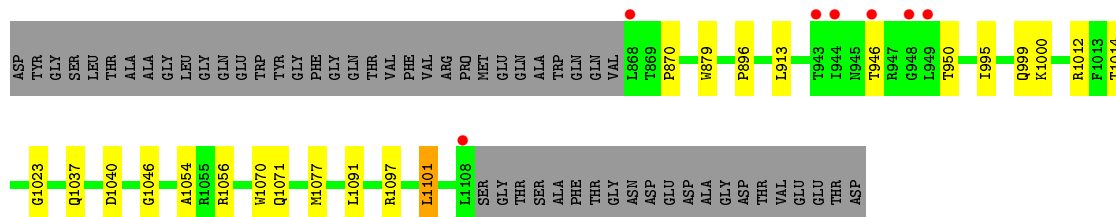
- Molecule 1: Hi113 protein



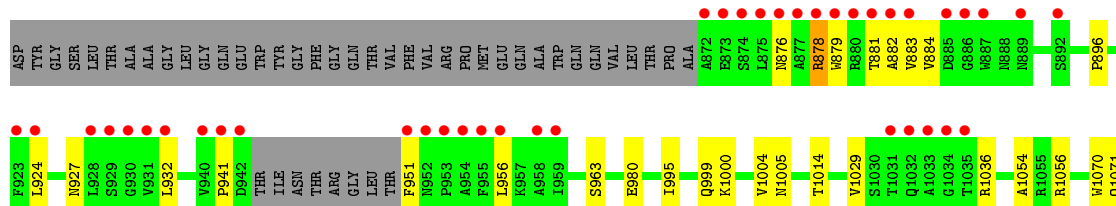
- Molecule 1: Hi113 protein

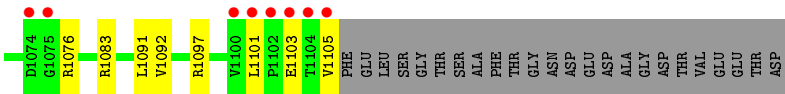


- Molecule 2: Type VI secretion protein IcmF



- Molecule 2: Type VI secretion protein IcmF





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.23Å 95.23Å 172.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.61 – 1.92 47.62 – 1.92	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.61-1.92) 100.0 (47.62-1.92)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 1.92Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, $R_{free}$	0.183 , 0.210 0.184 , 0.212	Depositor DCC
$R_{free}$ test set	3356 reflections (5.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.4	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 52.4	EDS
Estimated twinning fraction	0.047 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 67557 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6337	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.45	0/980	0.64	0/1330
1	B	0.50	0/984	0.64	0/1334
2	C	0.48	0/1903	0.63	0/2600
2	D	0.45	0/1784	0.68	0/2433
All	All	0.47	0/5651	0.65	0/7697

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	959	0	898	2	0
1	B	963	0	909	1	0
2	C	1856	0	1821	10	0
2	D	1740	0	1706	18	0
3	B	5	0	0	0	0
3	C	10	0	0	0	0
4	A	164	0	0	0	0
4	B	163	0	0	0	0
4	C	300	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	177	0	0	0	0
All	All	6337	0	5334	31	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 (31) 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)
2:C:999:GLN:HE22	2:C:1014:THR:H	1.27	0.79
2:D:999:GLN:HE22	2:D:1014:THR:H	1.26	0.78
1:A:11:LEU:HD11	1:A:128:SER:HB3	1.72	0.70
2:D:1004:VAL:HG12	2:D:1005:ASN:N	2.07	0.69
2:D:980:GLU:OE1	2:D:1083:ARG:HD2	1.98	0.63
2:C:995:ILE:HG12	2:C:1000:LYS:HG2	1.85	0.59
2:D:995:ILE:HG12	2:D:1000:LYS:HG2	1.85	0.58
2:D:1056:ARG:HD2	2:D:1091:LEU:HD22	1.86	0.57
2:D:932:LEU:HD13	2:D:941:PRO:HB3	1.87	0.57
2:C:1056:ARG:HD2	2:C:1091:LEU:HD22	1.88	0.54
2:D:883:VAL:HG23	2:D:884:VAL:H	1.72	0.54
2:D:951:PHE:HB3	2:D:956:LEU:HD11	1.90	0.53
2:C:896:PRO:O	2:C:1097:ARG:HD2	2.09	0.52
2:C:1037:GLN:HE21	2:C:1040:ASP:HB2	1.75	0.52
2:D:1004:VAL:CG1	2:D:1005:ASN:N	2.73	0.50
2:D:1054:ALA:HB2	2:D:1070:TRP:CE2	2.48	0.49
2:C:1071:GLN:HG3	2:C:1077:MET:HE1	1.95	0.49
2:D:896:PRO:O	2:D:1097:ARG:HD2	2.13	0.48
2:D:884:VAL:HG11	2:D:1103:GLU:HG2	1.95	0.48
2:D:879:TRP:CD1	2:D:1105:VAL:HG23	2.47	0.48
2:D:879:TRP:O	2:D:879:TRP:CG	2.67	0.48
2:D:876:ASN:C	2:D:878:ARG:H	2.17	0.47
2:D:980:GLU:OE1	2:D:1083:ARG:CD	2.65	0.44
2:C:1054:ALA:HB2	2:C:1070:TRP:CE2	2.53	0.44
1:A:12:VAL:HG11	1:A:86:LEU:HD13	2.01	0.43
2:C:870:PRO:HD2	4:C:1597:HOH:O	2.19	0.42
2:C:1023:GLY:HA2	2:C:1046:GLY:HA3	2.02	0.42
2:C:879:TRP:HZ2	2:C:1101:LEU:HD22	1.85	0.41
2:D:881:THR:HA	2:D:882:ALA:HA	1.81	0.41
2:D:1004:VAL:HG12	2:D:1005:ASN:CG	2.41	0.41
1:B:12:VAL:HG11	1:B:86:LEU:HD13	2.03	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	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
1	B	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
2	C	239/295 (81%)	233 (98%)	6 (2%)	0	100	100
2	D	222/295 (75%)	212 (96%)	10 (4%)	0	100	100
All	All	715/848 (84%)	695 (97%)	20 (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	98/102 (96%)	97 (99%)	1 (1%)	82	80
1	B	99/102 (97%)	99 (100%)	0	100	100
2	C	190/237 (80%)	185 (97%)	5 (3%)	54	44
2	D	176/237 (74%)	166 (94%)	10 (6%)	25	13
All	All	563/678 (83%)	547 (97%)	16 (3%)	51	41

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	MET
2	C	913	LEU
2	C	946	THR
2	C	950	THR
2	C	1012	ARG
2	C	1101	LEU
2	D	878	ARG
2	D	924	LEU
2	D	927	ASN
2	D	963	SER
2	D	1029	VAL
2	D	1036	ARG
2	D	1071	GLN
2	D	1076	ARG
2	D	1092	VAL
2	D	1101	LEU

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

Mol	Chain	Res	Type
2	C	999	GLN
2	C	1037	GLN
2	C	1071	GLN
2	D	927	ASN
2	D	999	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 [i](#)

3 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	SO4	B	201	-	4,4,4	0.44	0	6,6,6	0.28	0
3	SO4	C	1201	-	4,4,4	0.47	0	6,6,6	0.42	0
3	SO4	C	1202	-	4,4,4	0.32	0	6,6,6	0.08	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
3	SO4	B	201	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1201	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1202	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	129/129 (100%)	0.07	5 (3%) 43 47	26, 37, 55, 72	0
1	B	129/129 (100%)	0.02	2 (1%) 74 78	27, 33, 51, 75	0
2	C	241/295 (81%)	-0.09	7 (2%) 55 59	26, 34, 58, 75	0
2	D	226/295 (76%)	0.98	48 (21%) 1 1	27, 45, 100, 126	0
All	All	725/848 (85%)	0.29	62 (8%) 13 15	26, 36, 81, 126	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	879	TRP	9.6
2	D	872	ALA	8.0
2	C	949	LEU	7.0
2	D	881	THR	6.9
2	D	882	ALA	6.8
2	D	955	PHE	6.0
2	D	953	PRO	5.8
2	D	931	VAL	5.8
2	D	951	PHE	5.6
2	D	923	PHE	5.3
2	D	877	ALA	5.2
2	D	875	LEU	5.2
2	D	956	LEU	5.2
2	D	929	SER	5.1
2	D	1032	GLN	5.0
2	D	928	LEU	5.0
2	D	1104	THR	5.0
2	D	940	VAL	4.9
2	C	948	GLY	4.8
2	D	1105	VAL	4.7
2	D	941	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
2	D	954	ALA	4.2
1	B	41	PRO	4.1
2	D	942	ASP	4.0
2	D	930	GLY	3.9
2	D	1031	THR	3.6
2	D	1102	PRO	3.6
2	D	878	ARG	3.6
2	C	946	THR	3.6
2	D	932	LEU	3.6
1	A	42	GLY	3.6
2	C	943	THR	3.6
2	D	889	ASN	3.5
2	D	952	ASN	3.4
2	D	887	TRP	3.4
1	A	11	LEU	3.4
2	D	1075	GLY	3.4
2	D	1034	GLY	3.3
1	A	14	ALA	3.3
2	C	868	LEU	3.3
2	D	886	GLY	3.2
2	D	1101	LEU	3.1
1	B	42	GLY	3.1
2	C	1108	LEU	2.9
2	D	892	SER	2.8
2	D	880	ARG	2.8
1	A	88	PRO	2.8
2	D	1033	ALA	2.7
2	D	1100	VAL	2.7
2	D	883	VAL	2.7
2	D	874	SER	2.7
2	D	924	LEU	2.6
2	C	944	ILE	2.6
2	D	1103	GLU	2.5
2	D	1074	ASP	2.5
1	A	13	GLN	2.5
2	D	959	ILE	2.4
2	D	873	GLU	2.3
2	D	876	ASN	2.1
2	D	958	ALA	2.1
2	D	1035	THR	2.0
2	D	885	ASP	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	C	1201	5/5	0.96	0.19	5.88	93,93,94,94	0
3	SO4	B	201	5/5	0.93	0.22	-	105,105,106,107	0
3	SO4	C	1202	5/5	0.91	0.18	-	103,104,104,106	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.