



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 6, 2023 – 07:02 am GMT

PDB ID : 2BYT  
Title : Thermus thermophilus Leucyl-tRNA synthetase complexed with a tRNA<sup>Leu</sup> transcript in the post-editing conformation  
Authors : Cusack, S.; Tukalo, M.; Yaremchuk, A.; Fukunaga, R.; Yokoyama, S.  
Deposited on : 2005-08-04  
Resolution : 3.30 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 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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

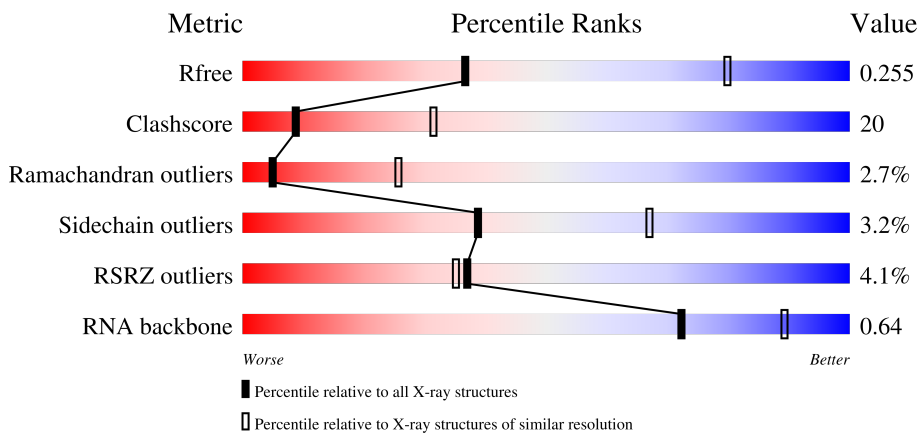
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

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	878	 2% 59% 37%
1	D	878	 6% 58% 39%
2	B	83	 4% 42% 39% 11% 6%
2	E	83	 5% 46% 39% 8% 6%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 17697 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.

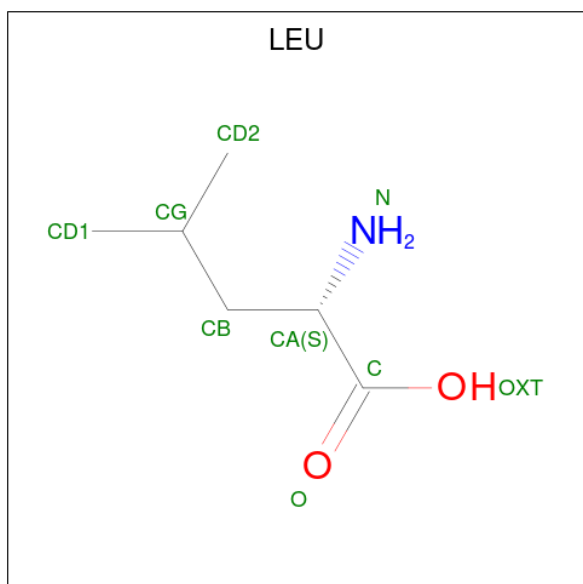
- Molecule 1 is a protein called LEUCYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	876	Total 7122	C 4593	N 1223	O 1275	S 31	0	0	0
1	D	876	Total 7122	C 4593	N 1223	O 1275	S 31	0	0	0

- Molecule 2 is a RNA chain called TRNALEU TRANSCRIPT WITH ANTICODON CAG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	78	Total 1677	C 745	N 309	O 545	P 78	0	0	0
2	E	78	Total 1677	C 745	N 309	O 545	P 78	0	0	0

- Molecule 3 is LEUCINE (three-letter code: LEU) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	6	1	2		
3	D	1	Total	C	N	O	0	0
			9	6	1	2		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		
4	D	2	Total	Zn	0	0
			2	2		

- Molecule 5 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Hg	0	0
			1	1		
5	D	1	Total	Hg	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

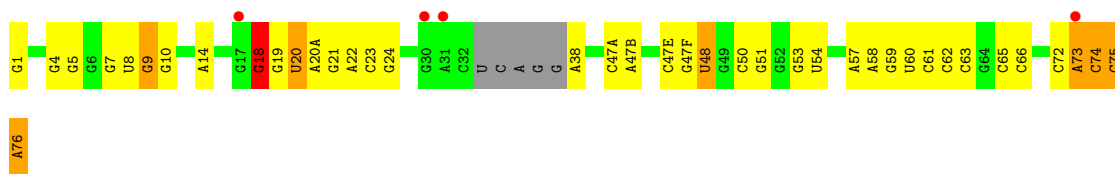
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 5	O 4	S 1	0	0
6	A	1	Total 5	O 4	S 1	0	0
6	A	1	Total 5	O 4	S 1	0	0
6	A	1	Total 5	O 4	S 1	0	0
6	A	1	Total 5	O 4	S 1	0	0
6	A	1	Total 5	O 4	S 1	0	0
6	A	1	Total 5	O 4	S 1	0	0
6	A	1	Total 5	O 4	S 1	0	0
6	D	1	Total 5	O 4	S 1	0	0
6	D	1	Total 5	O 4	S 1	0	0
6	D	1	Total 5	O 4	S 1	0	0
6	D	1	Total 5	O 4	S 1	0	0
6	D	1	Total 5	O 4	S 1	0	0
6	D	1	Total 5	O 4	S 1	0	0









## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	203.87Å 125.58Å 172.98Å 90.00° 118.44° 90.00°	Depositor
Resolution (Å)	24.45 – 3.30 24.45 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (24.45-3.30) 99.3 (24.45-3.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.65 (at 3.30Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.243 , 0.282 0.225 , 0.255	Depositor DCC
$R_{free}$ test set	2289 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	83.7	Xtrriage
Anisotropy	0.197	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 76.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	17697	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: HG, SO4, ZN

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	0.48	0/7327	0.60	0/9945
1	D	0.40	0/7327	0.57	0/9945
2	B	0.64	2/1874 (0.1%)	0.80	3/2917 (0.1%)
2	E	0.58	2/1874 (0.1%)	0.79	2/2917 (0.1%)
All	All	0.48	4/18402 (0.0%)	0.64	5/25724 (0.0%)

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
2	B	1	0
2	E	1	0
All	All	2	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	38	A	OP3-P	-7.26	1.52	1.61
2	B	38	A	OP3-P	-7.17	1.52	1.61
2	B	1	G	OP3-P	-7.15	1.52	1.61
2	E	1	G	OP3-P	-7.03	1.52	1.61

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	9	G	C2'-C3'-O3'	10.45	132.48	109.50
2	B	9	G	C2'-C3'-O3'	10.35	132.26	109.50
2	B	18	G	C2'-C3'-O3'	5.61	122.67	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	18	G	C2'-C3'-O3'	5.44	122.41	113.70
2	B	48	U	C5'-C4'-C3'	-5.22	107.64	116.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	9	G	C3'
2	E	9	G	C3'

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	7122	0	7031	311	0
1	D	7122	0	7031	316	0
2	B	1677	0	849	34	0
2	E	1677	0	849	40	0
3	A	9	0	10	0	0
3	D	9	0	10	1	0
4	A	2	0	0	0	0
4	D	2	0	0	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	A	45	0	0	0	0
6	D	30	0	0	0	0
All	All	17697	0	15780	686	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 20.

The worst 5 of 686 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:D:826:ARG:HD2	1:D:828:ARG:HH22	1.07	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:826:ARG:HD2	1:A:828:ARG:HH22	1.09	1.16
1:D:826:ARG:HD2	1:D:828:ARG:NH2	1.68	1.07
1:A:826:ARG:HD2	1:A:828:ARG:NH2	1.69	1.05
1:A:346:ARG:HH22	2:B:76:A:H1'	1.21	1.02

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	874/878 (100%)	728 (83%)	121 (14%)	25 (3%)	4	24
1	D	874/878 (100%)	734 (84%)	117 (13%)	23 (3%)	5	27
All	All	1748/1756 (100%)	1462 (84%)	238 (14%)	48 (3%)	5	26

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	796	PRO
1	A	861	VAL
1	D	856	LEU
1	D	861	VAL
1	A	847	LEU

### 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	741/742 (100%)	717 (97%)	24 (3%)	39	67
1	D	741/742 (100%)	717 (97%)	24 (3%)	39	67
All	All	1482/1484 (100%)	1434 (97%)	48 (3%)	39	67

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	74	LEU
1	D	327	TYR
1	D	82	PHE
1	D	189	LEU
1	D	430	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	574	GLN
1	D	824	ASN
1	D	726	HIS
1	A	792	HIS
1	D	163	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	76/83 (91%)	11 (14%)	4 (5%)
2	E	76/83 (91%)	8 (10%)	4 (5%)
All	All	152/166 (91%)	19 (12%)	8 (5%)

5 of 19 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	10	G
2	B	18	G
2	B	19	G
2	B	20	U
2	B	47(B)	A

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	E	75	C
2	E	74	C
2	E	9	G
2	B	75	C
2	E	18	G

## 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 23 ligands modelled in this entry, 6 are monoatomic - leaving 17 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
6	SO4	D	1710	-	4,4,4	0.28	0	6,6,6	0.05	0
6	SO4	A	1501	-	4,4,4	0.29	0	6,6,6	0.09	0
6	SO4	A	1505	-	4,4,4	0.27	0	6,6,6	0.10	0
3	LEU	D	1601	-	7,8,8	0.72	0	9,10,10	0.69	0
6	SO4	A	1509	-	4,4,4	0.26	0	6,6,6	0.09	0
6	SO4	A	1510	-	4,4,4	0.27	0	6,6,6	0.07	0
6	SO4	D	1702	-	4,4,4	0.24	0	6,6,6	0.11	0
6	SO4	D	1708	-	4,4,4	0.25	0	6,6,6	0.07	0
6	SO4	D	1703	-	4,4,4	0.30	0	6,6,6	0.06	0
6	SO4	A	1502	-	4,4,4	0.31	0	6,6,6	0.19	0
6	SO4	D	1704	-	4,4,4	0.27	0	6,6,6	0.07	0
6	SO4	A	1506	-	4,4,4	0.24	0	6,6,6	0.08	0
6	SO4	A	1511	-	4,4,4	0.29	0	6,6,6	0.12	0
6	SO4	A	1503	-	4,4,4	0.27	0	6,6,6	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	LEU	A	1301	-	7,8,8	0.77	0	9,10,10	0.73	0
6	SO4	D	1701	-	4,4,4	0.29	0	6,6,6	0.06	0
6	SO4	A	1504	-	4,4,4	0.27	0	6,6,6	0.13	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	LEU	A	1301	-	-	1/8/8/8	-
3	LEU	D	1601	-	-	0/8/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1301	LEU	OXT-C-CA-N

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1601	LEU	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, 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	876/878 (99%)	-0.17	16 (1%) 68 67	10, 65, 121, 159	0
1	D	876/878 (99%)	0.19	55 (6%) 20 20	46, 101, 144, 160	0
2	B	78/83 (93%)	0.27	3 (3%) 40 37	28, 83, 173, 202	0
2	E	78/83 (93%)	0.46	4 (5%) 28 26	51, 95, 187, 202	0
All	All	1908/1922 (99%)	0.04	78 (4%) 37 35	10, 84, 143, 202	0

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	180	GLU	5.5
1	D	587	GLU	5.0
1	D	172	VAL	4.9
1	D	624	PRO	4.8
1	D	93	PHE	4.7

### 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
4	ZN	D	1602	1/1	0.80	0.08	147,147,147,147	0
6	SO4	D	1701	5/5	0.81	0.30	194,194,194,195	0
6	SO4	A	1511	5/5	0.82	0.20	162,162,163,163	0
6	SO4	A	1501	5/5	0.85	0.28	150,150,152,152	0
6	SO4	A	1509	5/5	0.86	0.26	159,159,160,160	0
6	SO4	A	1505	5/5	0.87	0.15	143,143,145,145	0
4	ZN	A	1302	1/1	0.88	0.03	120,120,120,120	0
6	SO4	D	1703	5/5	0.88	0.18	168,168,168,169	0
6	SO4	D	1704	5/5	0.88	0.13	163,165,165,165	0
6	SO4	D	1710	5/5	0.88	0.50	173,173,173,174	0
4	ZN	D	1603	1/1	0.90	0.05	137,137,137,137	0
6	SO4	D	1708	5/5	0.91	0.30	163,163,164,165	0
6	SO4	A	1506	5/5	0.91	0.41	107,109,111,111	0
3	LEU	D	1601	9/9	0.92	0.21	92,95,96,96	0
6	SO4	A	1510	5/5	0.92	0.25	154,155,156,156	0
6	SO4	A	1504	5/5	0.93	0.13	118,119,120,120	0
6	SO4	D	1702	5/5	0.93	0.11	126,127,129,129	0
4	ZN	A	1303	1/1	0.95	0.09	85,85,85,85	0
3	LEU	A	1301	9/9	0.96	0.19	45,50,56,57	0
6	SO4	A	1503	5/5	0.96	0.11	77,78,83,84	0
6	SO4	A	1502	5/5	0.97	0.13	55,57,58,58	0
5	HG	D	1604	1/1	0.99	0.05	140,140,140,140	0
5	HG	A	1304	1/1	0.99	0.07	86,86,86,86	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.