



# wwPDB X-ray Structure Validation Summary Report

Oct 3, 2023 – 09:03 AM EDT

PDB ID : 6P24  
Title : Escherichia coli tRNA synthetase  
Authors : Kahne, D.; Baidin, V.; Owens, T.W.  
Deposited on : 2019-05-20  
Resolution : 2.12 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 : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : **FAILED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

## 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 2.12 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 17272 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 Phenylalanine-tRNA ligase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	241	Total	C	N	O	S	0	1	0
			1925	1227	337	352	9			
1	C	323	Total	C	N	O	S	0	0	0
			2447	1542	441	455	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P08312
A	-3	SER	-	expression tag	UNP P08312
A	-2	HIS	-	expression tag	UNP P08312
A	-1	MET	-	expression tag	UNP P08312
A	0	ALA	-	expression tag	UNP P08312
A	1	SER	-	expression tag	UNP P08312
C	-4	GLY	-	expression tag	UNP P08312
C	-3	SER	-	expression tag	UNP P08312
C	-2	HIS	-	expression tag	UNP P08312
C	-1	MET	-	expression tag	UNP P08312
C	0	ALA	-	expression tag	UNP P08312
C	1	SER	-	expression tag	UNP P08312

- Molecule 2 is a protein called Phenylalanine-tRNA ligase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	793	Total	C	N	O	S	0	0	0
			6041	3797	1061	1156	27			
2	D	794	Total	C	N	O	S	0	0	0
			6088	3832	1076	1153	27			

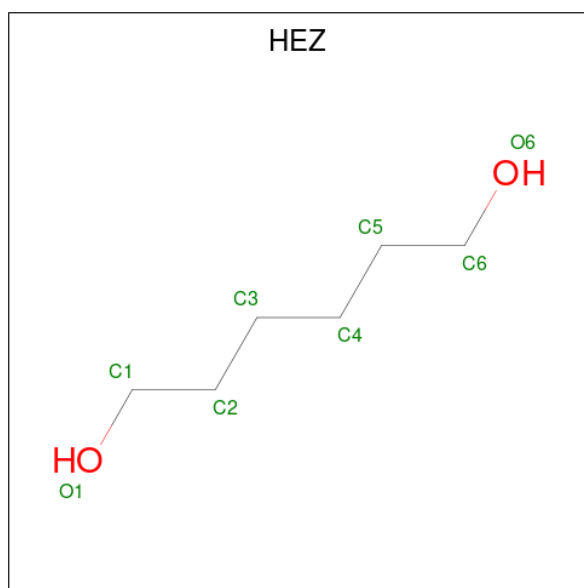
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total Mg 5 5	0	0
3	B	4	Total Mg 4 4	0	0
3	C	2	Total Mg 2 2	0	0
3	D	2	Total Mg 2 2	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

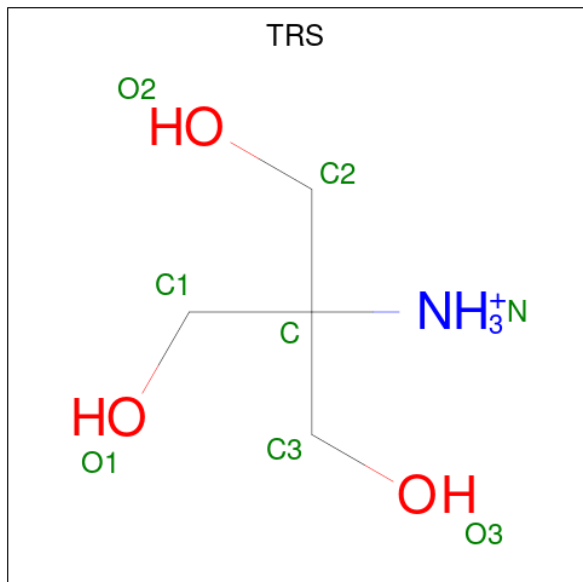
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0

- Molecule 5 is HEXANE-1,6-DIOL (three-letter code: HEZ) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 8 6 2	0	0
5	D	1	Total C O 8 6 2	0	0
5	D	1	Total C O 8 6 2	0	0
5	D	1	Total C O 8 6 2	0	0
5	D	1	Total C O 8 6 2	0	0

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



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

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 7 4 3	0	0
7	B	1	Total C O 7 4 3	0	0
7	B	1	Total C O 7 4 3	0	0
7	B	1	Total C O 7 4 3	0	0
7	B	1	Total C O 7 4 3	0	0
7	B	1	Total C O 7 4 3	0	0
7	C	1	Total C O 7 4 3	0	0
7	C	1	Total C O 7 4 3	0	0
7	D	1	Total C O 7 4 3	0	0
7	D	1	Total C O 7 4 3	0	0

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



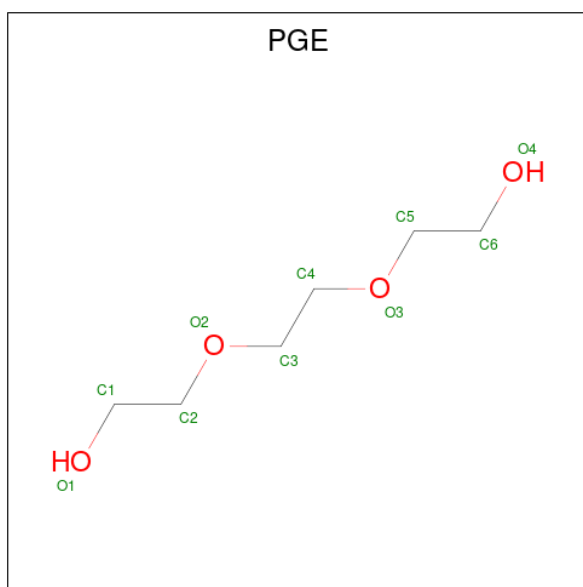
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	C	1	Total C O 4 2 2	0	0
8	C	1	Total C O 4 2 2	0	0
8	C	1	Total C O 4 2 2	0	0
8	D	1	Total C O 4 2 2	0	0
8	D	1	Total C O 4 2 2	0	0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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			4	2	2		
8	D	1	Total	C	O	0	0
			4	2	2		
8	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			10	6	4		
9	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	56	Total	O	0	0
			56	56		
10	B	169	Total	O	0	0
			169	169		
10	C	46	Total	O	0	0
			46	46		
10	D	256	Total	O	0	0
			256	256		



MolProbity and EDS failed to run properly - this section is therefore empty.

### 3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.27Å 173.58Å 251.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.04 – 2.12	Depositor
% Data completeness (in resolution range)	99.1 (82.04-2.12)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.09 (at 2.12Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.229 , 0.265	Depositor
Wilson B-factor (Å <sup>2</sup> )	50.9	Xtrriage
Anisotropy	0.148	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	17272	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.23% 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.

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

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

Of 52 ligands modelled in this entry, 14 are monoatomic - leaving 38 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
8	EDO	B	808	-	3,3,3	0.45	0	2,2,2	0.36	0
7	PEG	D	815	-	6,6,6	0.71	0	5,5,5	0.56	0
7	PEG	B	809	-	6,6,6	0.70	0	5,5,5	0.57	0
7	PEG	B	812	-	6,6,6	0.71	0	5,5,5	0.55	0
8	EDO	D	814	-	3,3,3	0.47	0	2,2,2	0.34	0
8	EDO	D	817	-	3,3,3	0.46	0	2,2,2	0.34	0
5	HEZ	D	804	-	7,7,7	0.34	0	6,6,6	0.89	0
8	EDO	C	403	-	3,3,3	0.45	0	2,2,2	0.30	0
8	EDO	A	410	-	3,3,3	0.45	0	2,2,2	0.37	0
8	EDO	B	815	-	3,3,3	0.45	0	2,2,2	0.35	0
6	TRS	A	408	-	7,7,7	0.29	0	9,9,9	0.25	0
8	EDO	D	816	-	3,3,3	0.47	0	2,2,2	0.29	0
7	PEG	B	805	-	6,6,6	0.68	0	5,5,5	0.55	0
8	EDO	D	810	-	3,3,3	0.47	0	2,2,2	0.32	0
8	EDO	D	818	-	3,3,3	0.46	0	2,2,2	0.36	0
5	HEZ	D	803	-	7,7,7	0.31	0	6,6,6	0.88	0
8	EDO	C	408	-	3,3,3	0.48	0	2,2,2	0.33	0
8	EDO	C	406	3	3,3,3	0.47	0	2,2,2	0.32	0
7	PEG	A	409	-	6,6,6	0.69	0	5,5,5	0.58	0
5	HEZ	D	805	-	7,7,7	0.32	0	6,6,6	0.91	0
8	EDO	D	812	-	3,3,3	0.46	0	2,2,2	0.31	0
8	EDO	B	814	-	3,3,3	0.47	0	2,2,2	0.24	0
7	PEG	B	811	-	6,6,6	0.68	0	5,5,5	0.59	0
5	HEZ	D	806	-	7,7,7	0.35	0	6,6,6	0.86	0
8	EDO	B	807	-	3,3,3	0.44	0	2,2,2	0.37	0
7	PEG	C	405	-	6,6,6	0.70	0	5,5,5	0.55	0
5	HEZ	A	407	-	7,7,7	0.33	0	6,6,6	0.89	0
8	EDO	D	811	-	3,3,3	0.48	0	2,2,2	0.27	0
7	PEG	C	404	-	6,6,6	0.71	0	5,5,5	0.56	0
9	PGE	B	806	-	9,9,9	0.32	0	8,8,8	0.25	0
7	PEG	B	810	-	6,6,6	0.70	0	5,5,5	0.59	0
6	TRS	D	807	-	7,7,7	0.31	0	9,9,9	0.29	0
6	TRS	A	411	-	7,7,7	0.30	0	9,9,9	0.27	0
9	PGE	B	813	-	9,9,9	0.31	0	8,8,8	0.28	0
8	EDO	D	808	-	3,3,3	0.44	0	2,2,2	0.42	0
8	EDO	D	809	-	3,3,3	0.45	0	2,2,2	0.38	0
6	TRS	C	407	-	7,7,7	0.30	0	9,9,9	0.31	0
7	PEG	D	813	-	6,6,6	0.70	0	5,5,5	0.54	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
8	EDO	B	808	-	-	0/1/1/1	-
7	PEG	D	815	-	-	0/4/4/4	-
7	PEG	B	809	-	-	2/4/4/4	-
7	PEG	B	812	-	-	1/4/4/4	-
8	EDO	D	814	-	-	0/1/1/1	-
8	EDO	D	817	-	-	0/1/1/1	-
5	HEZ	D	804	-	-	4/5/5/5	-
8	EDO	C	403	-	-	0/1/1/1	-
8	EDO	A	410	-	-	0/1/1/1	-
8	EDO	B	815	-	-	0/1/1/1	-
6	TRS	A	408	-	-	2/9/9/9	-
8	EDO	D	816	-	-	0/1/1/1	-
7	PEG	B	805	-	-	3/4/4/4	-
8	EDO	D	810	-	-	0/1/1/1	-
8	EDO	D	818	-	-	0/1/1/1	-
5	HEZ	D	803	-	-	0/5/5/5	-
8	EDO	C	408	-	-	0/1/1/1	-
8	EDO	C	406	3	-	1/1/1/1	-
7	PEG	A	409	-	-	1/4/4/4	-
5	HEZ	D	805	-	-	1/5/5/5	-
8	EDO	D	812	-	-	0/1/1/1	-
8	EDO	B	814	-	-	0/1/1/1	-
7	PEG	B	811	-	-	1/4/4/4	-
5	HEZ	D	806	-	-	3/5/5/5	-
8	EDO	B	807	-	-	0/1/1/1	-
7	PEG	C	405	-	-	2/4/4/4	-
5	HEZ	A	407	-	-	4/5/5/5	-
8	EDO	D	811	-	-	0/1/1/1	-
7	PEG	C	404	-	-	1/4/4/4	-
9	PGE	B	806	-	-	1/7/7/7	-
7	PEG	B	810	-	-	0/4/4/4	-
6	TRS	D	807	-	-	0/9/9/9	-
6	TRS	A	411	-	-	0/9/9/9	-
9	PGE	B	813	-	-	4/7/7/7	-
8	EDO	D	808	-	-	0/1/1/1	-
8	EDO	D	809	-	-	0/1/1/1	-
6	TRS	C	407	-	-	0/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PEG	D	813	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	408	TRS	N-C-C2-O2
7	C	405	PEG	O2-C3-C4-O4
5	D	804	HEZ	C2-C3-C4-C5
5	A	407	HEZ	C1-C2-C3-C4
5	D	806	HEZ	C1-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

#### 4.7 Other polymers [i](#)

There are no such residues in this entry.

#### 4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 5 Fit of model and data

### 5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

### 5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

### 5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

### 5.4 Ligands

EDS failed to run properly - this section is therefore empty.

### 5.5 Other polymers

EDS failed to run properly - this section is therefore empty.