wwPDB X-ray Structure Validation Summary Report (i)

Oct 5, 2023 – 01:59 AM EDT

PDB ID	:	6UTR
Title	:	LarE, a sulfur transferase involved in synthesis of the cofactor for lactate racemase in complex with copper
Authors	:	Fellner, M.; Huizenga, K.; Hausinger, R.P.; Hu, J.
Deposited on	:	2019-10-29
Resolution	:	2.41 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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 5 unique types of molecules in this entry. The entry contains 11580 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 ATP-dependent sacrificial sulfur transferase LarE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			1993	1253	348	385	7			
1	B	245	Total	C	N	O	S	0	0	0
			1876	1184	327	359	6			
1	C	249	Total	C	N	O	S	0	0	0
			1919	1210	337	366	6			
1	D	233	Total	C	N	O	S	0	0	0
			1735	1096	303	330	6			
1	E	262	Total	C	N	O	S	0	0	0
			1970	1250	337	376	7			
1	F	247	Total	C	N	O	S	0	0	0
			1908	1200	333	369	6			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	277	ALA	-	expression tag	UNP A0A0G9FES3
A	278	SER	-	expression tag	UNP A0A0G9FES3
A	279	TRP	-	expression tag	UNP A0A0G9FES3
A	280	SER	-	expression tag	UNP A0A0G9FES3
A	281	HIS	-	expression tag	UNP A0A0G9FES3
A	282	PRO	-	expression tag	UNP A0A0G9FES3
A	283	GLN	-	expression tag	UNP A0A0G9FES3
A	284	PHE	-	expression tag	UNP A0A0G9FES3
A	285	GLU	-	expression tag	UNP A0A0G9FES3
A	286	LYS	-	expression tag	UNP A0A0G9FES3
B	277	ALA	-	expression tag	UNP A0A0G9FES3
B	278	SER	-	expression tag	UNP A0A0G9FES3
B	279	TRP	-	expression tag	UNP A0A0G9FES3
B	280	SER	-	expression tag	UNP A0A0G9FES3
B	281	HIS	-	expression tag	UNP A0A0G9FES3
B	282	PRO	-	expression tag	UNP A0A0G9FES3
B	283	GLN	-	expression tag	UNP A0A0G9FES3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	284	PHE	-	expression tag	UNP A0A0G9FES3
B	285	GLU	-	expression tag	UNP A0A0G9FES3
B	286	LYS	-	expression tag	UNP A0A0G9FES3
C	277	ALA	-	expression tag	UNP A0A0G9FES3
C	278	SER	-	expression tag	UNP A0A0G9FES3
C	279	TRP	-	expression tag	UNP A0A0G9FES3
C	280	SER	-	expression tag	UNP A0A0G9FES3
C	281	HIS	-	expression tag	UNP A0A0G9FES3
C	282	PRO	-	expression tag	UNP A0A0G9FES3
C	283	GLN	-	expression tag	UNP A0A0G9FES3
C	284	PHE	-	expression tag	UNP A0A0G9FES3
C	285	GLU	-	expression tag	UNP A0A0G9FES3
C	286	LYS	-	expression tag	UNP A0A0G9FES3
D	277	ALA	-	expression tag	UNP A0A0G9FES3
D	278	SER	-	expression tag	UNP A0A0G9FES3
D	279	TRP	-	expression tag	UNP A0A0G9FES3
D	280	SER	-	expression tag	UNP A0A0G9FES3
D	281	HIS	-	expression tag	UNP A0A0G9FES3
D	282	PRO	-	expression tag	UNP A0A0G9FES3
D	283	GLN	-	expression tag	UNP A0A0G9FES3
D	284	PHE	-	expression tag	UNP A0A0G9FES3
D	285	GLU	-	expression tag	UNP A0A0G9FES3
D	286	LYS	-	expression tag	UNP A0A0G9FES3
E	277	ALA	-	expression tag	UNP A0A0G9FES3
E	278	SER	-	expression tag	UNP A0A0G9FES3
E	279	TRP	-	expression tag	UNP A0A0G9FES3
E	280	SER	-	expression tag	UNP A0A0G9FES3
E	281	HIS	-	expression tag	UNP A0A0G9FES3
E	282	PRO	-	expression tag	UNP A0A0G9FES3
E	283	GLN	-	expression tag	UNP A0A0G9FES3
E	284	PHE	-	expression tag	UNP A0A0G9FES3
E	285	GLU	-	expression tag	UNP A0A0G9FES3
E	286	LYS	-	expression tag	UNP A0A0G9FES3
F	277	ALA	-	expression tag	UNP A0A0G9FES3
F	278	SER	-	expression tag	UNP A0A0G9FES3
F	279	TRP	-	expression tag	UNP A0A0G9FES3
F	280	SER	-	expression tag	UNP A0A0G9FES3
F	281	HIS	-	expression tag	UNP A0A0G9FES3
F	282	PRO	-	expression tag	UNP A0A0G9FES3
F	283	GLN	-	expression tag	UNP A0A0G9FES3
F	284	PHE	-	expression tag	UNP A0A0G9FES3
F	285	GLU	-	expression tag	UNP A0A0G9FES3

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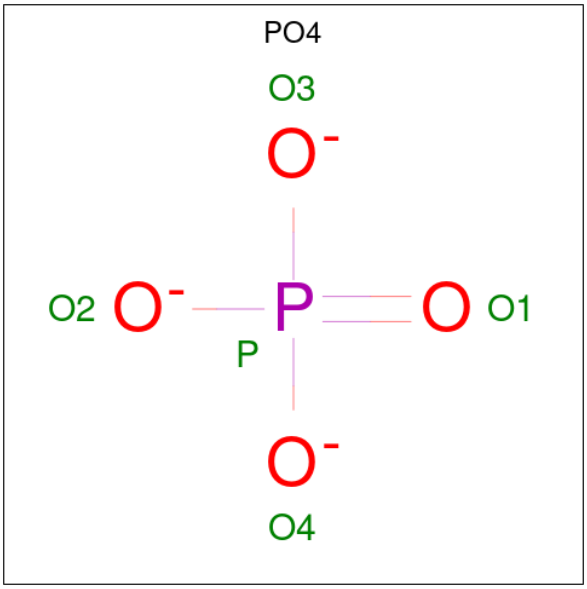
Chain	Residue	Modelled	Actual	Comment	Reference
F	286	LYS	-	expression tag	UNP A0A0G9FES3

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

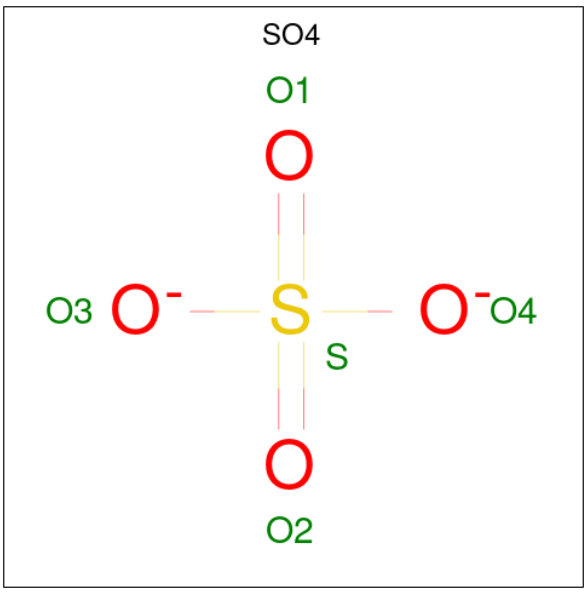


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cu 1 1	0	0
3	D	1	Total Cu 1 1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	24	Total O 24 24	0	0
5	B	26	Total O 26 26	0	0
5	C	16	Total O 16 16	0	0
5	D	13	Total O 13 13	0	0
5	E	21	Total O 21 21	0	0
5	F	22	Total O 22 22	0	0

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

3 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	108.98Å 108.98Å 323.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.35 – 2.41	Depositor
% Data completeness (in resolution range)	99.5 (48.35-2.41)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.17-3644	Depositor
R, R_{free}	0.208 , 0.254	Depositor
Wilson B-factor (Å^2)	59.5	Xtriage
Anisotropy	0.321	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11580	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
2	PO4	A	301	-	4,4,4	1.20	0	6,6,6	0.42	0
2	PO4	B	301	-	4,4,4	2.09	3 (75%)	6,6,6	1.13	0
4	SO4	C	302	-	4,4,4	0.10	0	6,6,6	0.12	0
4	SO4	A	303	-	4,4,4	0.11	0	6,6,6	0.19	0
4	SO4	E	302	-	4,4,4	0.17	0	6,6,6	0.07	0
2	PO4	D	301	-	4,4,4	1.07	0	6,6,6	0.51	0
2	PO4	C	301	-	4,4,4	1.06	0	6,6,6	1.73	2 (33%)
2	PO4	F	301	-	4,4,4	1.01	0	6,6,6	0.71	0
4	SO4	B	302	-	4,4,4	0.19	0	6,6,6	0.34	0
2	PO4	E	301	-	4,4,4	0.84	0	6,6,6	0.74	0
4	SO4	F	302	-	4,4,4	0.13	0	6,6,6	0.20	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	PO4	P-O2	-2.35	1.47	1.54
2	B	301	PO4	P-O1	-2.17	1.45	1.50
2	B	301	PO4	P-O3	-2.16	1.48	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	PO4	O4-P-O2	3.01	117.63	107.97
2	C	301	PO4	O4-P-O1	-2.17	102.95	110.89

There are no chirality outliers.

There are no torsion outliers.

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.