



wwPDB X-ray Structure Validation Summary Report ⓘ

May 3, 2021 – 12:42 PM EDT

PDB ID : 6DG3
Title : LarE, a sulfur transferase involved in synthesis of the cofactor for lactate racemase, in complex with caesium
Authors : Fellner, M.; Hausinger, R.P.; Hu, J.
Deposited on : 2018-05-16
Resolution : 2.94 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 ⓘ 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 : 2.18
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) : 2.18

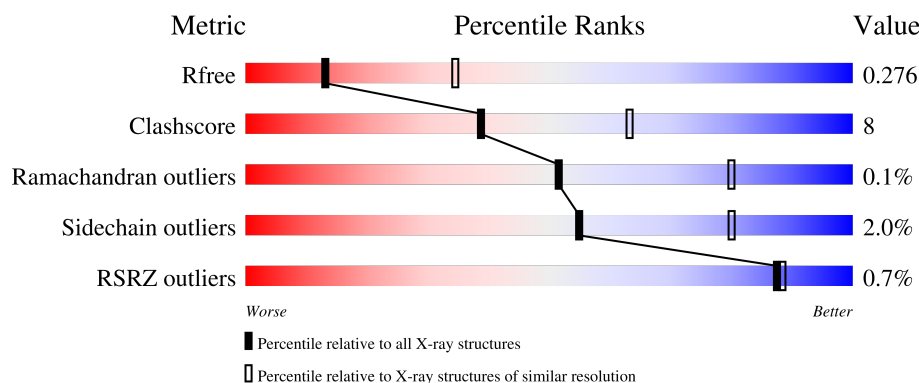
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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 ≥ 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	286	
1	B	286	
1	C	286	
1	D	286	
1	E	286	

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Mol	Chain	Length	Quality of chain
1	F	286	
1	G	286	
1	H	286	
1	I	286	
1	J	286	
1	K	286	
1	L	286	

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	PO4	L	302	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21737 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 Pyridinium-3,5-biscarboxylic acid mononucleotide sulfurtransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	0	0
			1847	1164	319	358	6			
1	B	204	Total	C	N	O	S	0	0	0
			1513	955	264	289	5			
1	C	246	Total	C	N	O	S	0	0	0
			1894	1195	330	363	6			
1	D	244	Total	C	N	O	S	0	0	0
			1795	1130	309	350	6			
1	E	221	Total	C	N	O	S	0	0	0
			1593	1005	279	304	5			
1	F	247	Total	C	N	O	S	0	0	0
			1892	1193	327	366	6			
1	G	250	Total	C	N	O	S	0	0	0
			1903	1198	329	370	6			
1	H	245	Total	C	N	O	S	0	0	0
			1868	1178	323	361	6			
1	I	247	Total	C	N	O	S	0	0	0
			1883	1183	326	368	6			
1	J	249	Total	C	N	O	S	0	0	0
			1902	1198	330	368	6			
1	K	235	Total	C	N	O	S	0	0	0
			1711	1074	297	334	6			
1	L	241	Total	C	N	O	S	0	0	0
			1857	1171	321	359	6			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	277	ALA	-	SEE REMARK 999	UNP F9UST4
A	278	SER	-	SEE REMARK 999	UNP F9UST4
A	279	TRP	-	SEE REMARK 999	UNP F9UST4
A	280	SER	-	SEE REMARK 999	UNP F9UST4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	281	HIS	-	SEE REMARK 999	UNP F9UST4
A	282	PRO	-	SEE REMARK 999	UNP F9UST4
A	283	GLN	-	SEE REMARK 999	UNP F9UST4
A	284	PHE	-	SEE REMARK 999	UNP F9UST4
A	285	GLU	-	SEE REMARK 999	UNP F9UST4
A	286	LYS	-	SEE REMARK 999	UNP F9UST4
B	277	ALA	-	SEE REMARK 999	UNP F9UST4
B	278	SER	-	SEE REMARK 999	UNP F9UST4
B	279	TRP	-	SEE REMARK 999	UNP F9UST4
B	280	SER	-	SEE REMARK 999	UNP F9UST4
B	281	HIS	-	SEE REMARK 999	UNP F9UST4
B	282	PRO	-	SEE REMARK 999	UNP F9UST4
B	283	GLN	-	SEE REMARK 999	UNP F9UST4
B	284	PHE	-	SEE REMARK 999	UNP F9UST4
B	285	GLU	-	SEE REMARK 999	UNP F9UST4
B	286	LYS	-	SEE REMARK 999	UNP F9UST4
C	277	ALA	-	SEE REMARK 999	UNP F9UST4
C	278	SER	-	SEE REMARK 999	UNP F9UST4
C	279	TRP	-	SEE REMARK 999	UNP F9UST4
C	280	SER	-	SEE REMARK 999	UNP F9UST4
C	281	HIS	-	SEE REMARK 999	UNP F9UST4
C	282	PRO	-	SEE REMARK 999	UNP F9UST4
C	283	GLN	-	SEE REMARK 999	UNP F9UST4
C	284	PHE	-	SEE REMARK 999	UNP F9UST4
C	285	GLU	-	SEE REMARK 999	UNP F9UST4
C	286	LYS	-	SEE REMARK 999	UNP F9UST4
D	277	ALA	-	SEE REMARK 999	UNP F9UST4
D	278	SER	-	SEE REMARK 999	UNP F9UST4
D	279	TRP	-	SEE REMARK 999	UNP F9UST4
D	280	SER	-	SEE REMARK 999	UNP F9UST4
D	281	HIS	-	SEE REMARK 999	UNP F9UST4
D	282	PRO	-	SEE REMARK 999	UNP F9UST4
D	283	GLN	-	SEE REMARK 999	UNP F9UST4
D	284	PHE	-	SEE REMARK 999	UNP F9UST4
D	285	GLU	-	SEE REMARK 999	UNP F9UST4
D	286	LYS	-	SEE REMARK 999	UNP F9UST4
E	277	ALA	-	SEE REMARK 999	UNP F9UST4
E	278	SER	-	SEE REMARK 999	UNP F9UST4
E	279	TRP	-	SEE REMARK 999	UNP F9UST4
E	280	SER	-	SEE REMARK 999	UNP F9UST4
E	281	HIS	-	SEE REMARK 999	UNP F9UST4
E	282	PRO	-	SEE REMARK 999	UNP F9UST4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	283	GLN	-	SEE REMARK 999	UNP F9UST4
E	284	PHE	-	SEE REMARK 999	UNP F9UST4
E	285	GLU	-	SEE REMARK 999	UNP F9UST4
E	286	LYS	-	SEE REMARK 999	UNP F9UST4
F	277	ALA	-	SEE REMARK 999	UNP F9UST4
F	278	SER	-	SEE REMARK 999	UNP F9UST4
F	279	TRP	-	SEE REMARK 999	UNP F9UST4
F	280	SER	-	SEE REMARK 999	UNP F9UST4
F	281	HIS	-	SEE REMARK 999	UNP F9UST4
F	282	PRO	-	SEE REMARK 999	UNP F9UST4
F	283	GLN	-	SEE REMARK 999	UNP F9UST4
F	284	PHE	-	SEE REMARK 999	UNP F9UST4
F	285	GLU	-	SEE REMARK 999	UNP F9UST4
F	286	LYS	-	SEE REMARK 999	UNP F9UST4
G	277	ALA	-	SEE REMARK 999	UNP F9UST4
G	278	SER	-	SEE REMARK 999	UNP F9UST4
G	279	TRP	-	SEE REMARK 999	UNP F9UST4
G	280	SER	-	SEE REMARK 999	UNP F9UST4
G	281	HIS	-	SEE REMARK 999	UNP F9UST4
G	282	PRO	-	SEE REMARK 999	UNP F9UST4
G	283	GLN	-	SEE REMARK 999	UNP F9UST4
G	284	PHE	-	SEE REMARK 999	UNP F9UST4
G	285	GLU	-	SEE REMARK 999	UNP F9UST4
G	286	LYS	-	SEE REMARK 999	UNP F9UST4
H	277	ALA	-	SEE REMARK 999	UNP F9UST4
H	278	SER	-	SEE REMARK 999	UNP F9UST4
H	279	TRP	-	SEE REMARK 999	UNP F9UST4
H	280	SER	-	SEE REMARK 999	UNP F9UST4
H	281	HIS	-	SEE REMARK 999	UNP F9UST4
H	282	PRO	-	SEE REMARK 999	UNP F9UST4
H	283	GLN	-	SEE REMARK 999	UNP F9UST4
H	284	PHE	-	SEE REMARK 999	UNP F9UST4
H	285	GLU	-	SEE REMARK 999	UNP F9UST4
H	286	LYS	-	SEE REMARK 999	UNP F9UST4
I	277	ALA	-	SEE REMARK 999	UNP F9UST4
I	278	SER	-	SEE REMARK 999	UNP F9UST4
I	279	TRP	-	SEE REMARK 999	UNP F9UST4
I	280	SER	-	SEE REMARK 999	UNP F9UST4
I	281	HIS	-	SEE REMARK 999	UNP F9UST4
I	282	PRO	-	SEE REMARK 999	UNP F9UST4
I	283	GLN	-	SEE REMARK 999	UNP F9UST4
I	284	PHE	-	SEE REMARK 999	UNP F9UST4

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Chain	Residue	Modelled	Actual	Comment	Reference
I	285	GLU	-	SEE REMARK 999	UNP F9UST4
I	286	LYS	-	SEE REMARK 999	UNP F9UST4
J	277	ALA	-	SEE REMARK 999	UNP F9UST4
J	278	SER	-	SEE REMARK 999	UNP F9UST4
J	279	TRP	-	SEE REMARK 999	UNP F9UST4
J	280	SER	-	SEE REMARK 999	UNP F9UST4
J	281	HIS	-	SEE REMARK 999	UNP F9UST4
J	282	PRO	-	SEE REMARK 999	UNP F9UST4
J	283	GLN	-	SEE REMARK 999	UNP F9UST4
J	284	PHE	-	SEE REMARK 999	UNP F9UST4
J	285	GLU	-	SEE REMARK 999	UNP F9UST4
J	286	LYS	-	SEE REMARK 999	UNP F9UST4
K	277	ALA	-	SEE REMARK 999	UNP F9UST4
K	278	SER	-	SEE REMARK 999	UNP F9UST4
K	279	TRP	-	SEE REMARK 999	UNP F9UST4
K	280	SER	-	SEE REMARK 999	UNP F9UST4
K	281	HIS	-	SEE REMARK 999	UNP F9UST4
K	282	PRO	-	SEE REMARK 999	UNP F9UST4
K	283	GLN	-	SEE REMARK 999	UNP F9UST4
K	284	PHE	-	SEE REMARK 999	UNP F9UST4
K	285	GLU	-	SEE REMARK 999	UNP F9UST4
K	286	LYS	-	SEE REMARK 999	UNP F9UST4
L	277	ALA	-	SEE REMARK 999	UNP F9UST4
L	278	SER	-	SEE REMARK 999	UNP F9UST4
L	279	TRP	-	SEE REMARK 999	UNP F9UST4
L	280	SER	-	SEE REMARK 999	UNP F9UST4
L	281	HIS	-	SEE REMARK 999	UNP F9UST4
L	282	PRO	-	SEE REMARK 999	UNP F9UST4
L	283	GLN	-	SEE REMARK 999	UNP F9UST4
L	284	PHE	-	SEE REMARK 999	UNP F9UST4
L	285	GLU	-	SEE REMARK 999	UNP F9UST4
L	286	LYS	-	SEE REMARK 999	UNP F9UST4

- Molecule 2 is CESIUM ION (three-letter code: CS) (formula: Cs).

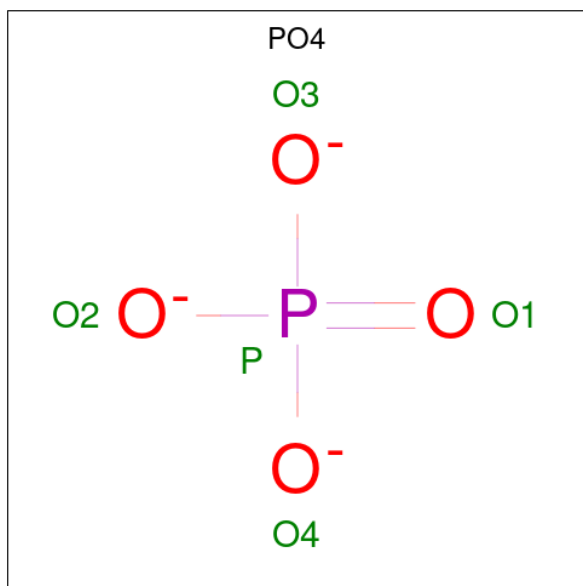
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cs 1 1	0	0
2	B	1	Total Cs 1 1	0	0
2	C	1	Total Cs 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Cs	0	0
			1	1		
2	E	1	Total	Cs	0	0
			1	1		
2	F	1	Total	Cs	0	0
			1	1		
2	G	1	Total	Cs	0	0
			1	1		
2	H	1	Total	Cs	0	0
			1	1		
2	I	1	Total	Cs	0	0
			1	1		
2	J	1	Total	Cs	0	0
			1	1		
2	K	1	Total	Cs	0	0
			1	1		
2	L	1	Total	Cs	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

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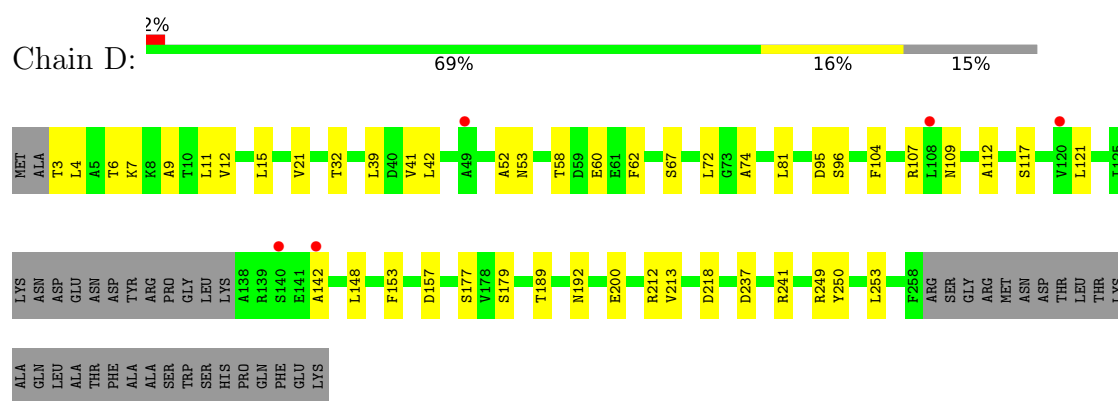
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		
3	G	1	Total	O	P	0	0
			5	4	1		
3	H	1	Total	O	P	0	0
			5	4	1		
3	I	1	Total	O	P	0	0
			5	4	1		
3	J	1	Total	O	P	0	0
			5	4	1		
3	K	1	Total	O	P	0	0
			5	4	1		
3	L	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

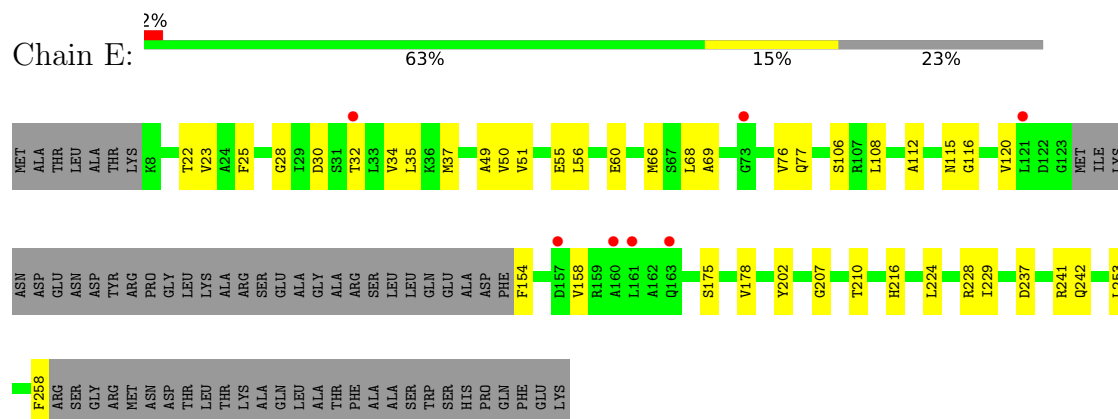
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	1	Total	O	0	0
			1	1		
4	C	1	Total	O	0	0
			1	1		
4	E	1	Total	O	0	0
			1	1		
4	F	2	Total	O	0	0
			2	2		
4	L	1	Total	O	0	0
			1	1		

- Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide sulfurtransferase

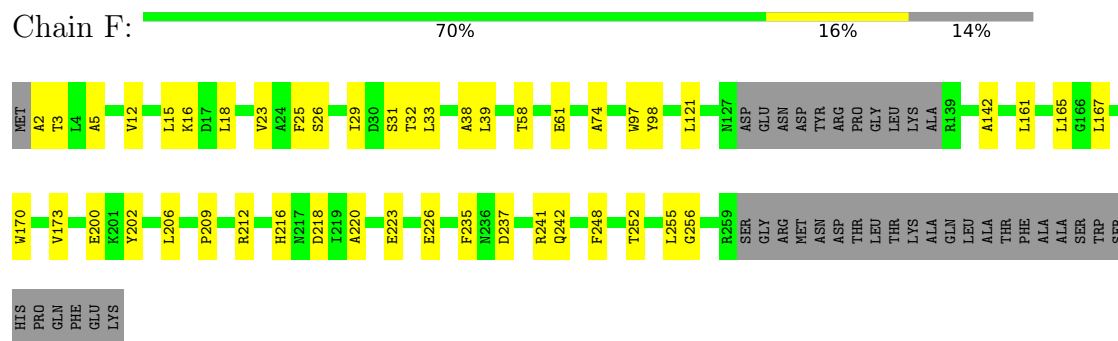




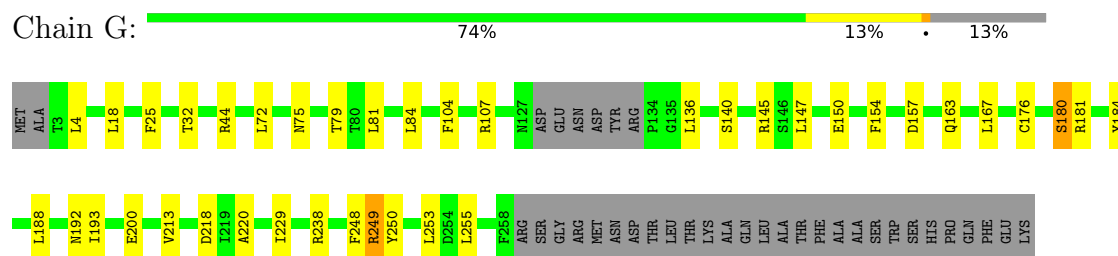
- Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide sulfurtransferase



- Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide sulfurtransferase

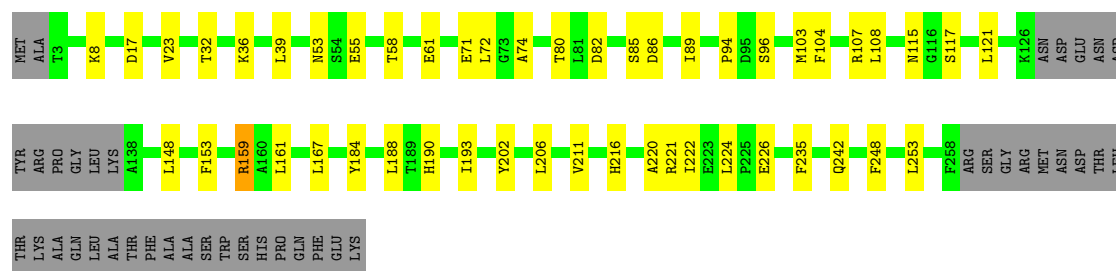


- Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide sulfurtransferase



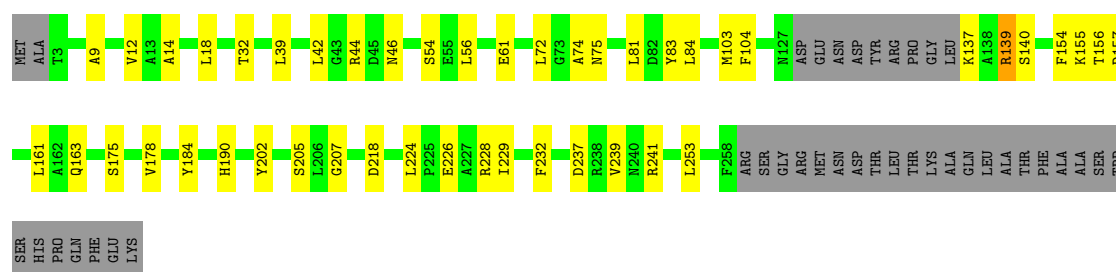
- Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide sulfurtransferase

Chain H: 



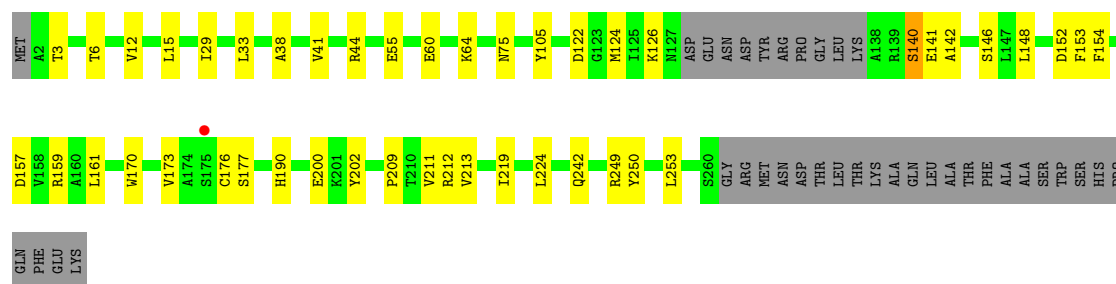
- Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide sulfurtransferase

Chain I: 



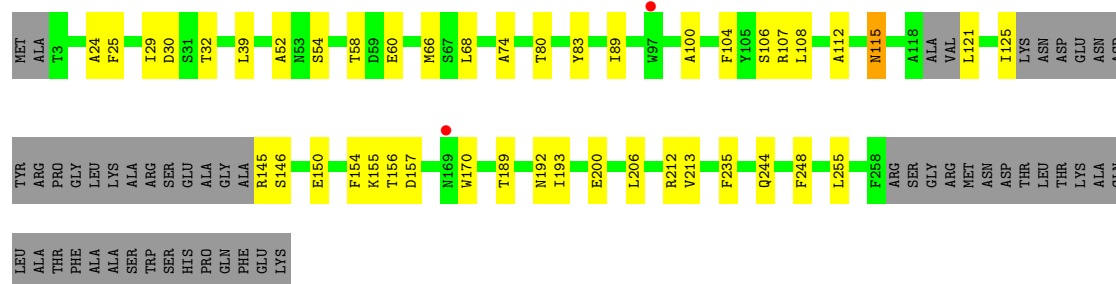
- Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide sulfurtransferase

Chain J: 

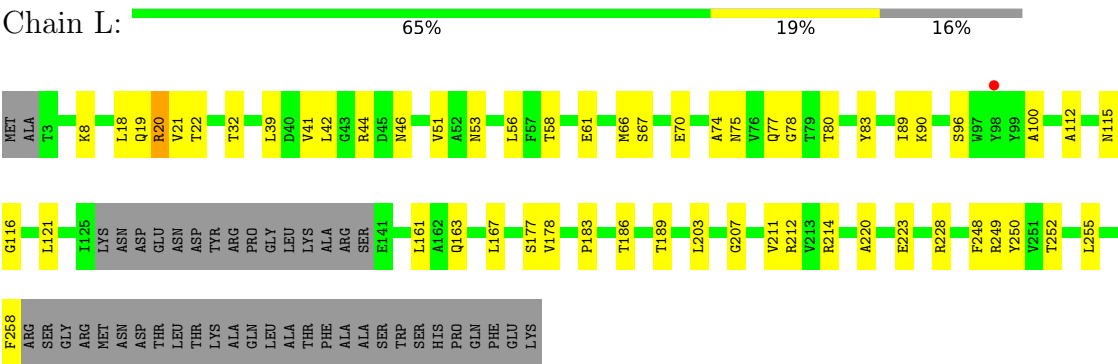


- Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide sulfurtransferase

Chain K: 



● Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide sulfurtransferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	152.37Å 154.16Å 328.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 – 2.94 48.91 – 2.94	Depositor EDS
% Data completeness (in resolution range)	96.9 (48.91-2.94) 96.2 (48.91-2.94)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.50 (at 2.96Å)	Xtriage
Refinement program	PHENIX dev-3092	Depositor
R, R_{free}	0.196 , 0.274 0.197 , 0.276	Depositor DCC
R_{free} test set	4126 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 17.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.210 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	21737	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PO4, CS

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	0.41	0/1874	0.63	0/2543
1	B	0.40	0/1540	0.57	0/2095
1	C	0.43	0/1923	0.69	4/2604 (0.2%)
1	D	0.38	0/1821	0.60	0/2476
1	E	0.39	0/1620	0.58	0/2207
1	F	0.45	0/1921	0.67	1/2604 (0.0%)
1	G	0.41	0/1931	0.59	0/2615
1	H	0.42	0/1897	0.62	0/2574
1	I	0.43	0/1910	0.65	0/2588
1	J	0.49	0/1931	0.66	0/2616
1	K	0.39	0/1739	0.59	0/2367
1	L	0.41	0/1886	0.63	0/2556
All	All	0.42	0/21993	0.63	5/29845 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	20	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	C	20	ARG	CA-CB-CG	-7.72	96.41	113.40
1	C	20	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	C	20	ARG	CB-CG-CD	5.63	126.25	111.60
1	F	256	GLY	C-N-CA	5.10	133.01	122.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1847	0	1789	22	0
1	B	1513	0	1405	40	0
1	C	1894	0	1864	25	0
1	D	1795	0	1702	28	0
1	E	1593	0	1439	26	0
1	F	1892	0	1852	28	0
1	G	1903	0	1870	23	0
1	H	1868	0	1817	29	0
1	I	1883	0	1837	26	0
1	J	1902	0	1853	24	0
1	K	1711	0	1532	33	0
1	L	1857	0	1823	32	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
3	C	5	0	0	1	0
3	D	5	0	0	1	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	1	0
3	H	5	0	0	0	0
3	I	5	0	0	0	0
3	J	5	0	0	1	0
3	K	5	0	0	0	0
3	L	5	0	0	2	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	F	2	0	0	0	0
4	L	1	0	0	0	0
All	All	21737	0	20783	319	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 319 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:E:23:VAL:HG21	1:E:35:LEU:HD13	1.54	0.88
1:I:14:ALA:O	1:I:18:LEU:HD12	1.73	0.88
1:A:32:THR:HG23	1:A:72:LEU:HD11	1.61	0.81
1:L:212:ARG:NH1	3:L:302:PO4:O1	2.13	0.81
1:L:214:ARG:NH2	3:L:302:PO4:O3	2.17	0.78

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	241/286 (84%)	235 (98%)	6 (2%)	0	100	100
1	B	200/286 (70%)	184 (92%)	15 (8%)	1 (0%)	29	60
1	C	242/286 (85%)	238 (98%)	3 (1%)	1 (0%)	34	64
1	D	240/286 (84%)	232 (97%)	8 (3%)	0	100	100
1	E	217/286 (76%)	210 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	243/286 (85%)	238 (98%)	5 (2%)	0	100	100
1	G	246/286 (86%)	241 (98%)	5 (2%)	0	100	100
1	H	241/286 (84%)	235 (98%)	6 (2%)	0	100	100
1	I	243/286 (85%)	237 (98%)	5 (2%)	1 (0%)	34	64
1	J	245/286 (86%)	235 (96%)	10 (4%)	0	100	100
1	K	229/286 (80%)	219 (96%)	10 (4%)	0	100	100
1	L	237/286 (83%)	229 (97%)	8 (3%)	0	100	100
All	All	2824/3432 (82%)	2733 (97%)	88 (3%)	3 (0%)	51	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	233	LEU
1	I	155	LYS
1	C	126	LYS

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	189/236 (80%)	187 (99%)	2 (1%)	73	90
1	B	147/236 (62%)	139 (95%)	8 (5%)	22	51
1	C	197/236 (84%)	195 (99%)	2 (1%)	76	91
1	D	177/236 (75%)	173 (98%)	4 (2%)	50	78
1	E	144/236 (61%)	140 (97%)	4 (3%)	43	73
1	F	197/236 (84%)	196 (100%)	1 (0%)	88	96
1	G	199/236 (84%)	195 (98%)	4 (2%)	55	80
1	H	193/236 (82%)	191 (99%)	2 (1%)	76	91
1	I	196/236 (83%)	192 (98%)	4 (2%)	55	80
1	J	196/236 (83%)	191 (97%)	5 (3%)	46	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	K	158/236 (67%)	154 (98%)	4 (2%)	47 76
1	L	195/236 (83%)	191 (98%)	4 (2%)	53 79
All	All	2188/2832 (77%)	2144 (98%)	44 (2%)	55 80

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	139	ARG
1	J	159	ARG
1	I	163	GLN
1	J	64	LYS
1	K	66	MET

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

Mol	Chain	Res	Type
1	A	192	ASN
1	D	88	HIS
1	D	114	ASN
1	E	77	GLN
1	J	53	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 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	$\# Z > 2$
3	PO4	F	302	-	4,4,4	0.93	0	6,6,6	0.46	0
3	PO4	A	302	-	4,4,4	0.90	0	6,6,6	0.92	0
3	PO4	I	302	-	4,4,4	0.94	0	6,6,6	0.67	0
3	PO4	D	302	-	4,4,4	0.88	0	6,6,6	0.70	0
3	PO4	H	302	-	4,4,4	0.96	0	6,6,6	0.52	0
3	PO4	L	302	-	4,4,4	0.85	0	6,6,6	0.91	0
3	PO4	K	302	-	4,4,4	0.86	0	6,6,6	0.57	0
3	PO4	B	302	-	4,4,4	0.81	0	6,6,6	0.75	0
3	PO4	E	302	-	4,4,4	0.86	0	6,6,6	0.64	0
3	PO4	J	302	-	4,4,4	0.83	0	6,6,6	0.61	0
3	PO4	C	302	-	4,4,4	1.04	0	6,6,6	0.74	0
3	PO4	G	302	-	4,4,4	1.04	0	6,6,6	0.62	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.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	302	PO4	1	0
3	L	302	PO4	2	0
3	B	302	PO4	1	0
3	J	302	PO4	1	0
3	C	302	PO4	1	0
3	G	302	PO4	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th 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 ²)	Q<0.9
1	A	245/286 (85%)	-0.09	0 100 100	23, 41, 66, 101	0
1	B	204/286 (71%)	0.03	1 (0%) 91 91	20, 56, 95, 117	0
1	C	246/286 (86%)	-0.12	2 (0%) 86 87	22, 36, 67, 98	0
1	D	244/286 (85%)	0.02	5 (2%) 65 66	20, 50, 86, 105	0
1	E	221/286 (77%)	0.15	7 (3%) 47 46	26, 61, 103, 129	0
1	F	247/286 (86%)	-0.24	0 100 100	17, 27, 47, 76	0
1	G	250/286 (87%)	-0.06	0 100 100	24, 38, 68, 94	0
1	H	245/286 (85%)	-0.10	0 100 100	24, 40, 60, 96	0
1	I	247/286 (86%)	-0.10	0 100 100	22, 38, 64, 99	0
1	J	249/286 (87%)	-0.22	1 (0%) 92 93	17, 27, 51, 87	0
1	K	235/286 (82%)	0.13	2 (0%) 84 85	20, 60, 96, 117	0
1	L	241/286 (84%)	-0.10	1 (0%) 92 93	23, 39, 64, 91	0
All	All	2874/3432 (83%)	-0.06	19 (0%) 87 88	17, 39, 85, 129	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	160	ALA	3.5
1	E	121	LEU	2.9
1	E	163	GLN	2.9
1	J	175	SER	2.6
1	E	161	LEU	2.4

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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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, 95th 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(Å ²)	Q<0.9
2	CS	E	301	1/1	0.85	0.11	139,139,139,139	0
2	CS	B	301	1/1	0.94	0.12	138,138,138,138	0
3	PO4	A	302	5/5	0.96	0.17	30,31,49,54	0
3	PO4	E	302	5/5	0.96	0.17	32,39,48,58	0
2	CS	C	301	1/1	0.97	0.09	79,79,79,79	1
3	PO4	D	302	5/5	0.97	0.18	28,32,57,59	0
2	CS	L	301	1/1	0.97	0.06	99,99,99,99	1
3	PO4	H	302	5/5	0.97	0.16	41,44,49,54	0
3	PO4	K	302	5/5	0.97	0.16	37,37,54,56	0
3	PO4	L	302	5/5	0.97	0.12	24,36,46,46	0
3	PO4	C	302	5/5	0.98	0.17	27,29,45,54	0
2	CS	I	301	1/1	0.98	0.09	98,98,98,98	0
2	CS	J	301	1/1	0.98	0.15	114,114,114,114	0
3	PO4	F	302	5/5	0.98	0.22	19,28,47,51	0
3	PO4	G	302	5/5	0.98	0.15	42,45,49,51	0
2	CS	A	301	1/1	0.98	0.11	100,100,100,100	0
3	PO4	I	302	5/5	0.98	0.15	17,27,34,44	0
2	CS	H	301	1/1	0.98	0.09	99,99,99,99	0
3	PO4	B	302	5/5	0.98	0.13	22,34,46,51	0
2	CS	D	301	1/1	0.99	0.10	87,87,87,87	0
2	CS	F	301	1/1	0.99	0.09	74,74,74,74	1
3	PO4	J	302	5/5	0.99	0.14	15,19,23,25	0
2	CS	G	301	1/1	0.99	0.11	88,88,88,88	0
2	CS	K	301	1/1	0.99	0.11	97,97,97,97	0

6.5 Other polymers ⓘ

There are no such residues in this entry.