wwPDB X-ray Structure Validation Summary Report (i)

Oct 5, 2023 – 08:23 AM EDT

PDB ID	:	6UWE
Title	:	Crystal structure of recombinant thiocyanate dehydrogenase from Thioalkalivibrio paradoxus saturated with copper
Authors	:	Shabalin, I.G.; Osipov, E.; Tikhonova, T.V.; Rakitina, T.V.; Boyko, K.M.; Popov, V.O.
Deposited on	:	2019-11-05
Resolution	:	1.60 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
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 1.60 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 4 unique types of molecules in this entry. The entry contains 17147 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 thiocyanate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	13	0
			3689	2363	610	696	20			
1	B	467	Total	C	N	O	S	0	14	0
			3692	2365	610	697	20			
1	C	467	Total	C	N	O	S	0	11	0
			3684	2355	615	694	20			
1	D	467	Total	C	N	O	S	0	11	0
			3683	2357	612	694	20			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	GLY	-	expression tag	UNP W0DP94
A	79	ALA	-	expression tag	UNP W0DP94
A	80	MET	-	expression tag	UNP W0DP94
A	81	GLY	-	expression tag	UNP W0DP94
B	78	GLY	-	expression tag	UNP W0DP94
B	79	ALA	-	expression tag	UNP W0DP94
B	80	MET	-	expression tag	UNP W0DP94
B	81	GLY	-	expression tag	UNP W0DP94
C	78	GLY	-	expression tag	UNP W0DP94
C	79	ALA	-	expression tag	UNP W0DP94
C	80	MET	-	expression tag	UNP W0DP94
C	81	GLY	-	expression tag	UNP W0DP94
D	78	GLY	-	expression tag	UNP W0DP94
D	79	ALA	-	expression tag	UNP W0DP94
D	80	MET	-	expression tag	UNP W0DP94
D	81	GLY	-	expression tag	UNP W0DP94

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	6	Total Cu 6 6	0	0
2	B	6	Total Cu 6 6	0	0
2	C	6	Total Cu 6 6	0	0
2	D	6	Total Cu 6 6	0	0

- Molecule 3 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total X 1 1	0	0
3	B	2	Total X 2 2	0	0
3	C	1	Total X 1 1	0	0
3	D	2	Total X 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	565	Total O 575 575	0	14
4	B	570	Total O 583 583	0	14
4	C	584	Total O 597 597	0	14
4	D	600	Total O 614 614	0	16

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 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.42Å 163.15Å 90.63Å 90.00° 119.29° 90.00°	Depositor
Resolution (Å)	44.80 – 1.60	Depositor
% Data completeness (in resolution range)	91.0 (44.80-1.60)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 1.59Å)	Xtriage
Refinement program	REFMAC 5.8.0257, Coot	Depositor
R, R_{free}	0.141 , 0.160	Depositor
Wilson B-factor (Å^2)	13.3	Xtriage
Anisotropy	0.133	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.044 for -h-l,k,h 0.044 for l,k,-h-l 0.045 for h,-k,-h-l 0.044 for -h-l,-k,l 0.358 for l,-k,h	Xtriage
Reported twinning fraction	0.688 for H, K, L 0.312 for -L, -K, -H	Depositor
Outliers	0 of 276564 reflections	Xtriage
Total number of atoms	17147	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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 30 ligands modelled in this entry, 24 are monoatomic and 6 are unknown - leaving 0 for Mogul analysis.

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.

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.