



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 24, 2017 – 05:12 AM EDT

PDB ID : 3GZ4
Title : Crystal structure of putative short chain dehydrogenase FROM ES-
CHERICHIA COLI CFT073 complexed with NADPH
Authors : Malashkevich, V.N.; Toro, R.; Morano, C.; Sauder, J.M.; Burley, S.K.; Almo,
S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : unknown
Resolution : 2.10 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

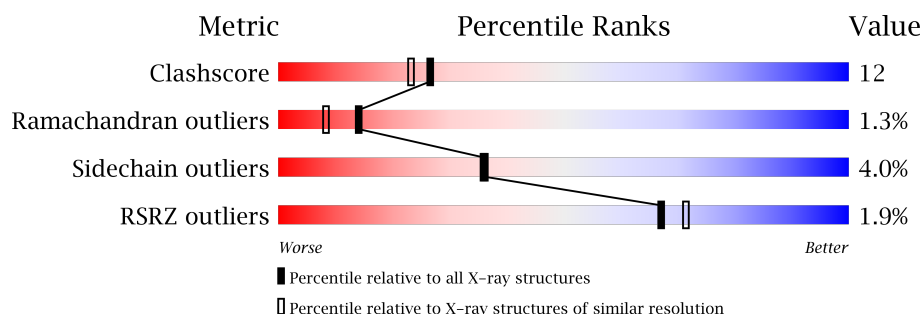
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	262	 3% 68% 21% • 8%
1	B	262	 68% 22% • 8%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3959 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.

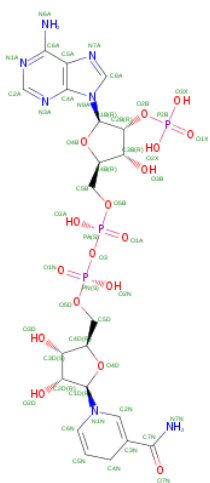
- Molecule 1 is a protein called Hypothetical oxidoreductase yciK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	1	0
			1881	1172	337	358	14			
1	B	240	Total	C	N	O	S	0	1	0
			1866	1164	334	354	14			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	MET	-	expression tag	UNP Q8FHV3
A	-2	SER	-	expression tag	UNP Q8FHV3
A	-1	LEU	-	expression tag	UNP Q8FHV3
A	251	GLU	-	expression tag	UNP Q8FHV3
A	252	GLY	-	expression tag	UNP Q8FHV3
A	253	HIS	-	expression tag	UNP Q8FHV3
A	254	HIS	-	expression tag	UNP Q8FHV3
A	255	HIS	-	expression tag	UNP Q8FHV3
A	256	HIS	-	expression tag	UNP Q8FHV3
A	257	HIS	-	expression tag	UNP Q8FHV3
A	258	HIS	-	expression tag	UNP Q8FHV3
B	-3	MET	-	expression tag	UNP Q8FHV3
B	-2	SER	-	expression tag	UNP Q8FHV3
B	-1	LEU	-	expression tag	UNP Q8FHV3
B	251	GLU	-	expression tag	UNP Q8FHV3
B	252	GLY	-	expression tag	UNP Q8FHV3
B	253	HIS	-	expression tag	UNP Q8FHV3
B	254	HIS	-	expression tag	UNP Q8FHV3
B	255	HIS	-	expression tag	UNP Q8FHV3
B	256	HIS	-	expression tag	UNP Q8FHV3
B	257	HIS	-	expression tag	UNP Q8FHV3
B	258	HIS	-	expression tag	UNP Q8FHV3

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

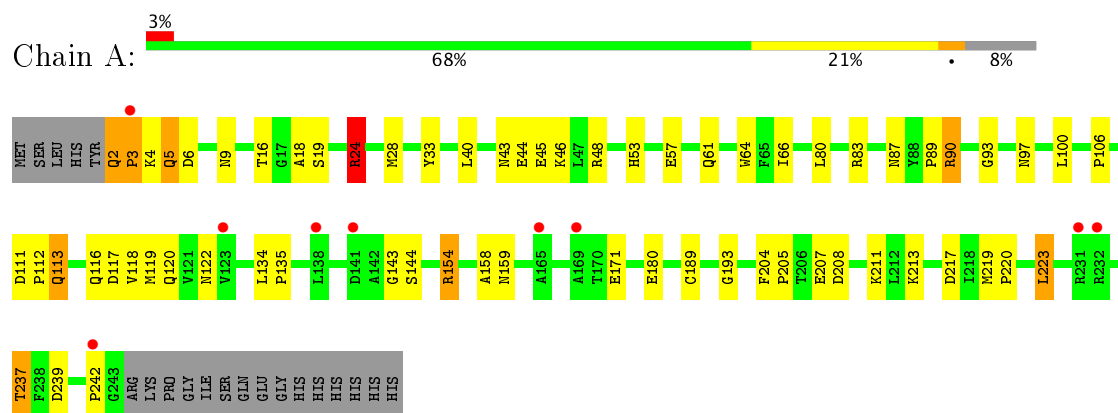
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	116	Total O 116 116	0	0

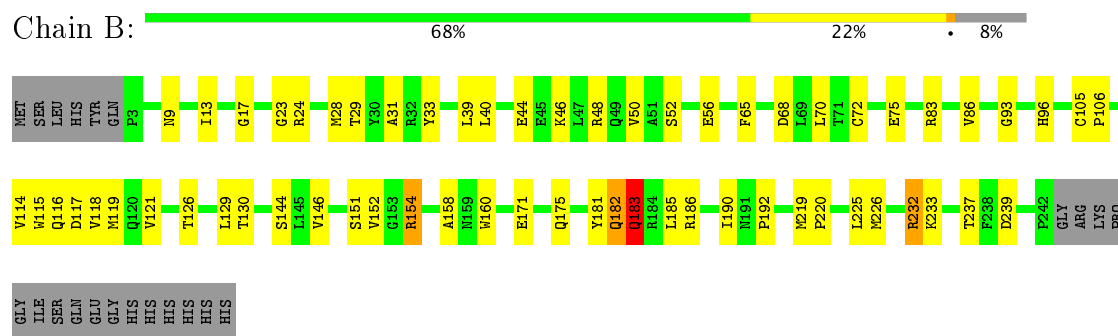
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Hypothetical oxidoreductase yciK



- Molecule 1: Hypothetical oxidoreductase yciK



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	43.79Å 130.51Å 47.93Å 90.00° 115.06° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 33.90 – 1.98	Depositor EDS
% Data completeness (in resolution range)	72.8 (20.00-2.10) 59.4 (33.90-1.98)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 1.98Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.226 , 0.252 0.218 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	39.7	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.946 for H, K, L 0.054 for -H, -K, H+L	Depositor
Outliers	0 of 20117 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3959	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.29% 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: NDP

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	0.57	0/1915	0.76	2/2597 (0.1%)
1	B	0.58	0/1902	0.77	1/2578 (0.0%)
All	All	0.57	0/3817	0.77	3/5175 (0.1%)

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
1	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	70	LEU	CA-CB-CG	5.48	127.90	115.30
1	A	223	LEU	CA-CB-CG	5.22	127.31	115.30
1	A	24	ARG	NE-CZ-NH1	5.21	122.90	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	GLN	Peptide

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	1881	0	1862	53	0
1	B	1866	0	1859	42	0
2	A	48	0	26	2	0
2	B	48	0	26	1	0
3	A	116	0	0	6	0
All	All	3959	0	3773	88	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 12.

The worst 5 of 88 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:B:171:GLU:O	1:B:175:GLN:HG3	1.71	0.90
1:A:4:LYS:HD2	1:A:5:GLN:H	1.44	0.81
1:A:24:ARG:HH11	1:A:24:ARG:HG2	1.43	0.81
1:A:3:PRO:HG3	1:A:223:LEU:HD13	1.65	0.78
1:A:189:CYS:CB	1:A:237:THR:HG23	2.15	0.77

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	241/262 (92%)	221 (92%)	15 (6%)	5 (2%)	8 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	239/262 (91%)	229 (96%)	9 (4%)	1 (0%)	38	35
All	All	480/524 (92%)	450 (94%)	24 (5%)	6 (1%)	14	8

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	ARG
1	B	183	GLN
1	A	3	PRO
1	A	242	PRO
1	A	143	GLY

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	201/218 (92%)	193 (96%)	8 (4%)	36	36
1	B	200/218 (92%)	192 (96%)	8 (4%)	36	36
All	All	401/436 (92%)	385 (96%)	16 (4%)	36	36

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	237	THR
1	B	9	ASN
1	B	154	ARG
1	A	205	PRO
1	B	182	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	GLN
1	B	9	ASN

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Mol	Chain	Res	Type
1	B	155	GLN
1	A	183	GLN
1	B	116	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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	NDP	A	500	-	43,52,52	1.75	7 (16%)	49,80,80	1.92	6 (12%)
2	NDP	B	500	-	43,52,52	1.65	5 (11%)	49,80,80	1.98	4 (8%)

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
2	NDP	A	500	-	-	0/30/77/77	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDP	B	500	-	-	0/30/77/77	0/5/5/5

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	NDP	C4N-C5N	-3.67	1.41	1.49
2	B	500	NDP	C4N-C5N	-3.49	1.41	1.49
2	A	500	NDP	O4D-C4D	-2.07	1.40	1.45
2	B	500	NDP	C2A-N1A	2.39	1.38	1.33
2	A	500	NDP	C6N-C5N	2.57	1.38	1.33

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	NDP	N3A-C2A-N1A	-11.05	119.24	128.86
2	A	500	NDP	N3A-C2A-N1A	-10.46	119.75	128.86
2	B	500	NDP	C1B-N9A-C4A	-4.03	119.68	126.64
2	A	500	NDP	C1B-N9A-C4A	-3.19	121.12	126.64
2	B	500	NDP	O3B-C3B-C2B	-2.40	104.36	111.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	NDP	2	0
2	B	500	NDP	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, 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	242/262 (92%)	0.15	9 (3%) 42 49	23, 35, 51, 57	0
1	B	240/262 (91%)	-0.05	0 100 100	21, 33, 47, 56	0
All	All	482/524 (91%)	0.05	9 (1%) 67 71	21, 34, 50, 57	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	232	ARG	3.0
1	A	165	ALA	2.7
1	A	3	PRO	2.6
1	A	242	PRO	2.4
1	A	123	VAL	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 [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	NDP	A	500	48/48	0.95	0.11	-0.35	26,29,33,36	0
2	NDP	B	500	48/48	0.95	0.09	-0.71	23,30,36,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.