



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 04:52 pm BST

PDB ID : 1RP7
Title : E. COLI PYRUVATE DEHYDROGENASE INHIBITOR COMPLEX
Authors : Arjunan, P.; Chandrasekhar, K.; Furey, W.
Deposited on : 2003-12-03
Resolution : 2.09 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
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) : 2.11

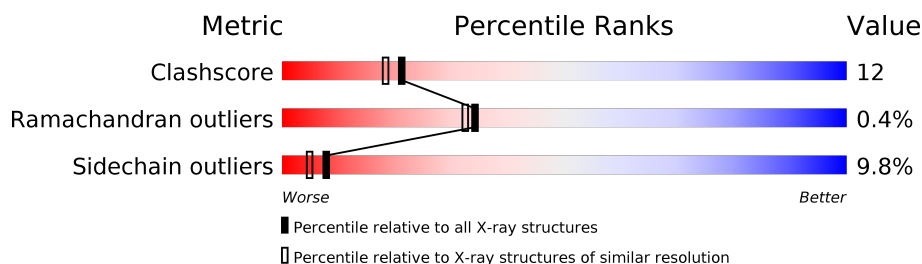
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	886	
1	B	886	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13237 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.

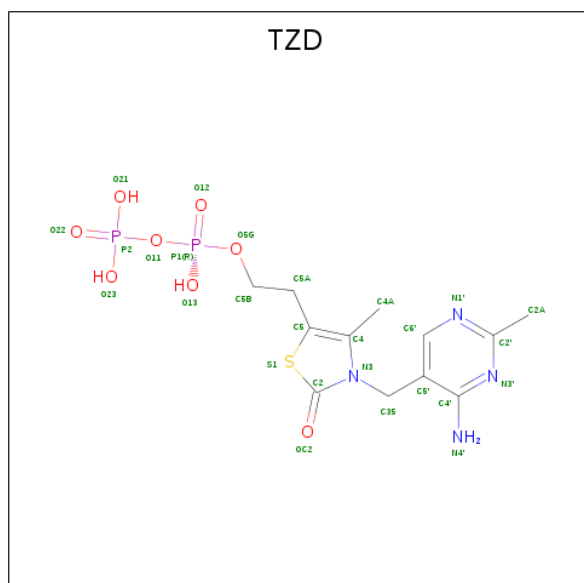
- Molecule 1 is a protein called Pyruvate dehydrogenase E1 component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	801	Total	C	N	O	S	0	0	0
			6341	4018	1093	1204	26			
1	B	801	Total	C	N	O	S	0	0	0
			6341	4018	1093	1204	26			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is 2-{3-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-4-METHYL-2-OXO-2,3-DIHYDRO-1,3-THIAZOL-5-YL}ETHYL TRIHYDROGEN DIPHOSPHATE (three-letter code: TZD) (formula: C₁₂H₁₈N₄O₈P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			27	12	4	8	2	1		
3	B	1	Total	C	N	O	P	S	0	0
			27	12	4	8	2	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	223	Total	O	0	0
			223	223		
4	B	276	Total	O	0	0
			276	276		



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.55Å 141.84Å 82.17Å 90.00° 102.61° 90.00°	Depositor
Resolution (Å)	8.00 – 2.09	Depositor
% Data completeness (in resolution range)	84.5 (8.00-2.09)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.192 , 0.252	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13237	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

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: MG, TZD

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	0.36	0/6484	0.60	1/8766 (0.0%)
1	B	0.37	0/6484	0.61	1/8766 (0.0%)
All	All	0.36	0/12968	0.61	2/17532 (0.0%)

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	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	171	GLY	N-CA-C	5.40	126.61	113.10
1	B	638	LEU	CA-CB-CG	5.35	127.61	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	803	TYR	Sidechain

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	6341	0	6179	162	0
1	B	6341	0	6179	154	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	15	0	0
3	B	27	0	15	1	0
4	A	223	0	0	2	0
4	B	276	0	0	10	0
All	All	13237	0	12388	304	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 304 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:309:LYS:HG3	1:B:343:GLU:HG3	1.34	1.09
1:B:90:ILE:HG12	1:B:107:MET:HE3	1.37	1.01
1:A:64:PRO:HG2	1:A:67:GLU:HG3	1.47	0.96
1:B:509:LYS:HD2	1:B:509:LYS:H	1.30	0.95
1:B:198:PRO:HG3	1:B:228:LEU:HD22	1.52	0.91

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	795/886 (90%)	752 (95%)	40 (5%)	3 (0%)	34 32
1	B	795/886 (90%)	755 (95%)	37 (5%)	3 (0%)	34 32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1590/1772 (90%)	1507 (95%)	77 (5%)	6 (0%)	34	32

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	397	GLY
1	A	305	ASP
1	B	627	THR
1	B	398	ASP
1	A	399	ALA

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	665/735 (90%)	605 (91%)	60 (9%)	9	6
1	B	665/735 (90%)	595 (90%)	70 (10%)	7	4
All	All	1330/1470 (90%)	1200 (90%)	130 (10%)	8	5

5 of 130 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	867	VAL
1	B	211	LEU
1	B	723	LYS
1	B	65	VAL
1	B	175	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	737	HIS
1	B	737	HIS
1	B	106	HIS

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Mol	Chain	Res	Type
1	A	466	GLN
1	B	466	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 ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	TZD	A	889	2	23,28,28	1.56	6 (26%)	28,42,42	1.09	2 (7%)
3	TZD	B	887	2	23,28,28	1.65	5 (21%)	28,42,42	1.10	2 (7%)

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
3	TZD	A	889	2	-	3/16/17/17	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TZD	B	887	2	-	5/16/17/17	0/2/2/2

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	887	TZD	C4'-N3'	3.86	1.40	1.35
3	A	889	TZD	C4'-N3'	3.69	1.40	1.35
3	B	887	TZD	C5'-C4'	3.61	1.49	1.42
3	A	889	TZD	C5'-C4'	3.31	1.48	1.42
3	B	887	TZD	C2'-N1'	2.65	1.38	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	887	TZD	C6'-N1'-C2'	2.59	120.37	115.96
3	A	889	TZD	C6'-N1'-C2'	2.54	120.28	115.96
3	B	887	TZD	C5-C4-N3	2.17	112.20	107.66
3	A	889	TZD	C5-C4-N3	2.01	111.87	107.66

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	889	TZD	P1-O11-P2-O21
3	B	887	TZD	C4-C5-C5A-C5B
3	B	887	TZD	P1-O11-P2-O21
3	B	887	TZD	P1-O11-P2-O23
3	A	889	TZD	C4-C5-C5A-C5B

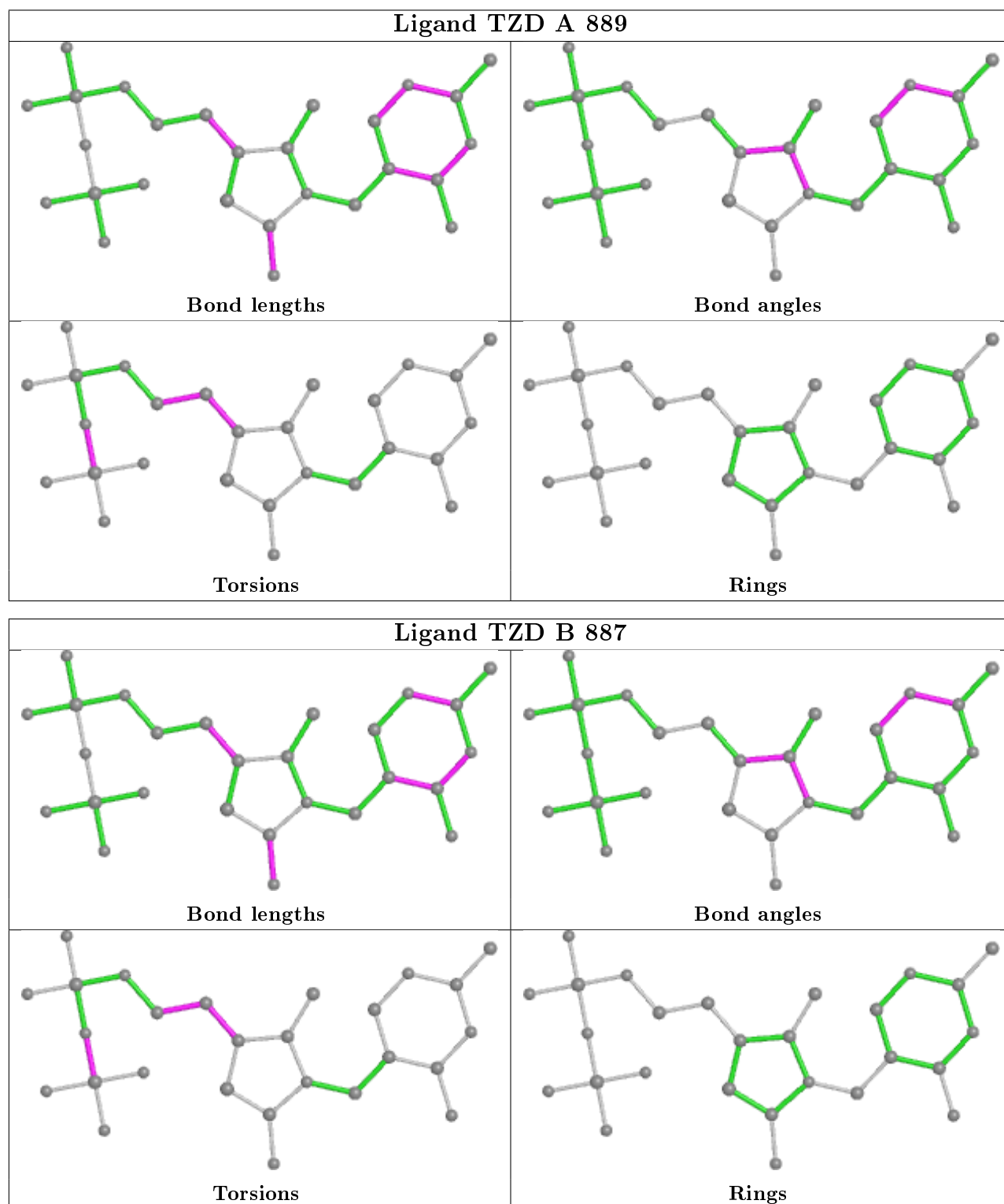
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	887	TZD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.