



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:38 PM GMT

PDB ID : 1L8A  
Title : E. COLI PYRUVATE DEHYDROGENASE  
Authors : Furey, W.; Arjunan, P.  
Deposited on : 2002-03-19  
Resolution : 1.85 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

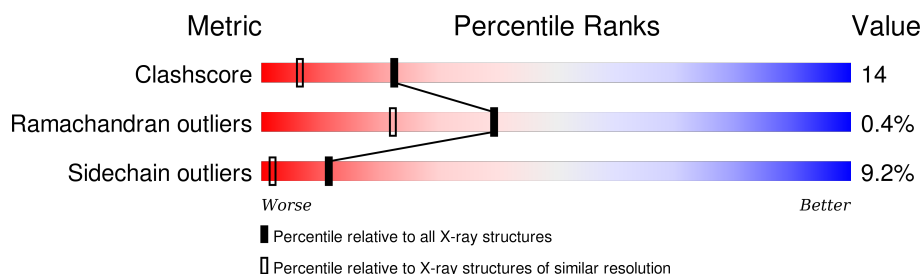
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)

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  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	886	 65% 21% • 10%
1	B	886	 65% 20% 5% 10%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13418 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.

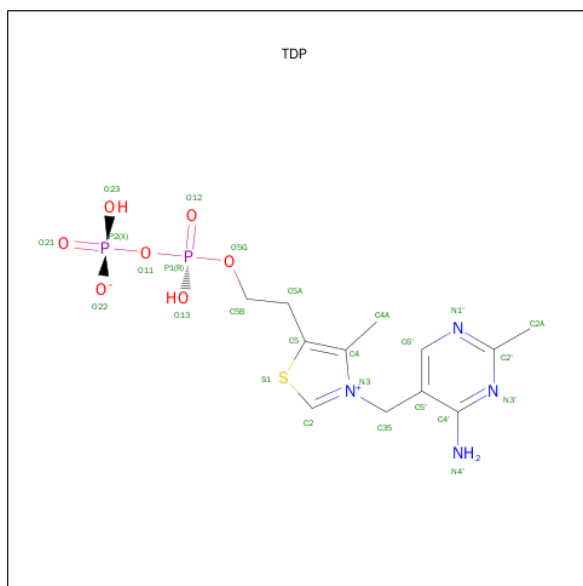
- Molecule 1 is a protein called Pyruvate dehydrogenase E1 component.

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 THIAMIN DIPHOSPHATE (three-letter code: TDP) (formula: C<sub>12</sub>H<sub>18</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 4 is water.

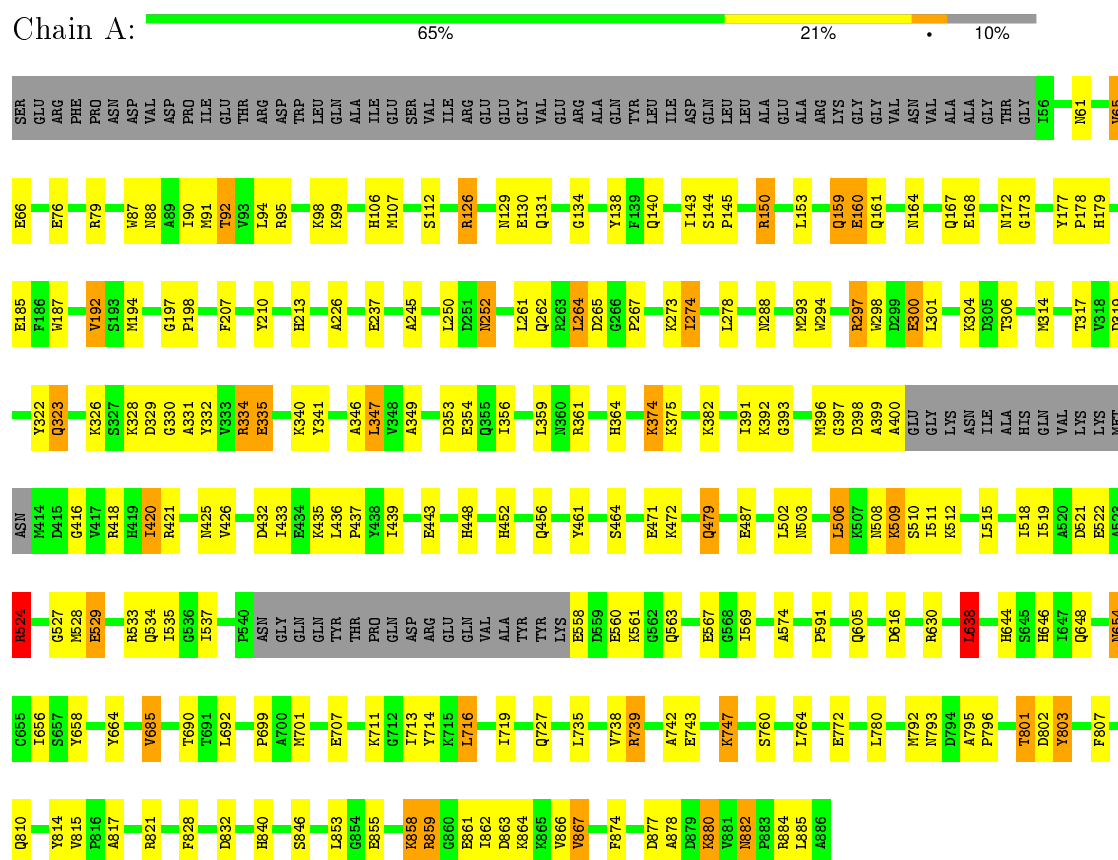
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	330	Total	O	0	0
			330	330		
4	B	352	Total	O	0	0
			352	352		

### 3 Residue-property plots

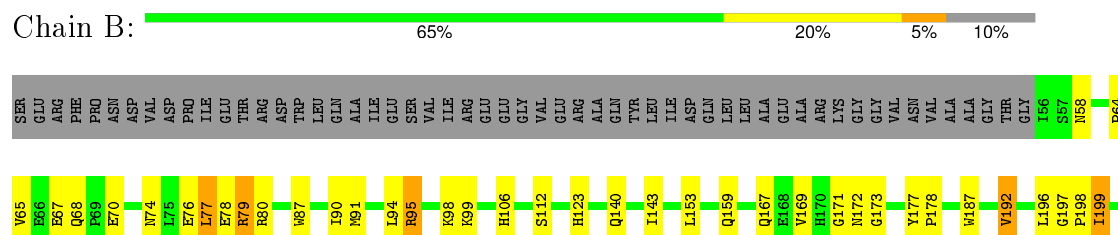
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

- Molecule 1: Pyruvate dehydrogenase E1 component



- Molecule 1: Pyruvate dehydrogenase E1 component



Y820	R821	F828	D832	V843	S846	L853	E855	L856	A857	R858	R859	G860	E861	I862	D863	K864	K865	F874	A886																													
R654	Y658	V664	R676	Q682	V685	V686	V687	T690	H701	I713	L716	K723	G724	K725	V726	Q727	H737	V738	R739	D754	V758	T759	S760	L764	D770	M776	L777	H778	P779	L780	E781	M793	S800	Y803	M804	R812	D818	D819										
R524	E529	F532	R533	Q534	I537	Y538	S539	P540	ASN	GLY	GLN	D432	I433	TYR	E434	THR	K435	L436	P437	Y438	I439	G440	S445	LYS	E558	D559	E560	K561	E567	G568	I569	L572	G573	A574	P591	L610	R620	L633	N634	G635	E636	G637	L638	Q639	H644	S645	H646	
R418	H419	I420	R421	D422	R423	F424	H425	V426	P427	S429	D430	A431	D432	I433	TYR	E434	THR	K435	L436	P437	Y438	I439	G440	S445	LYS	E446	E447	H452	A453	Q454	K457	Y461	Q466	F469	T470	E471	L475	L506	K507	M508	K509	S510	L515	L519	A520	D521	E522	A523
K328	Y332	V333	R334	Y341	F342	T344	T352	Q355	N360	R361	H364	K368	K374	K375	A376	Q377	G381	K382	V385	T390	I391	K392	G393	Y394	G395	K396	D397	A399	A400	GLU	GLY	LYS	ASN	ILE	ALA	HIS	GLN	VAL	LYS	LYS	MET	ASN	M414	D415	G416	V417		
H213	K221	D234	E237	T244	A245	T246	R247	L250	D251	N252	N260	L261	Q262	R263	L264	D265	G266	P267	T274	L278	E279	E283	G286	W287	N288	V289	I290	W294	R297	W298	D299	E300	R303	ASN	ILE	ALA	HIS	GLN	VAL	LYS	LYS	MET	ASN	M414	D415	G416	V417	

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.69 Å   141.60 Å   82.46 Å 90.00°   102.40°   90.00°	Depositor
Resolution (Å)	8.00 – 1.85	Depositor
% Data completeness (in resolution range)	85.4 (8.00-1.85)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.189 , 0.236	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13418	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	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, TDP

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	0.62	2/8766 (0.0%)
1	B	0.38	0/6484	0.67	9/8766 (0.1%)
All	All	0.37	0/12968	0.65	11/17532 (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
1	B	0	1
All	All	0	2

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	394	TYR	O-C-N	-13.41	100.41	123.20
1	B	394	TYR	CA-C-N	11.27	138.73	116.20
1	B	400	ALA	N-CA-CB	-8.41	98.32	110.10
1	A	524	ARG	NE-CZ-NH2	8.27	124.43	120.30
1	B	303	ARG	NE-CZ-NH2	8.20	124.40	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	803	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	B	803	TYR	Sidechain

## 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	6341	0	6179	178	0
1	B	6341	0	6179	178	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	26	0	16	4	0
3	B	26	0	16	4	0
4	A	330	0	0	11	0
4	B	352	0	0	9	0
All	All	13418	0	12390	345	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 14.

The worst 5 of 345 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)
3:B:887:TDP:H2	3:B:887:TDP:C2	0.97	1.49
3:A:887:TDP:H2	3:A:887:TDP:C2	0.97	1.49
1:A:801:THR:HG22	1:A:803:TYR:H	1.13	1.08
1:A:61:ASN:HD21	1:A:294:TRP:H	1.06	0.92
1:A:364:HIS:HE1	1:A:391:ILE:H	1.16	0.88

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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%)	756 (95%)	38 (5%)	1 (0%)	56	39
1	B	795/886 (90%)	754 (95%)	36 (4%)	5 (1%)	30	13
All	All	1590/1772 (90%)	1510 (95%)	74 (5%)	6 (0%)	39	22

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	172	ASN
1	B	397	GLY
1	A	397	GLY
1	B	394	TYR
1	B	521	ASP

### 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%)	606 (91%)	59 (9%)	12	2
1	B	665/735 (90%)	602 (90%)	63 (10%)	11	1
All	All	1330/1470 (90%)	1208 (91%)	122 (9%)	11	2

5 of 122 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	867	VAL
1	B	234	ASP
1	B	725	LYS
1	A	880	LYS
1	B	79	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	737	HIS
1	B	68	GLN
1	B	727	GLN
1	A	790	GLN
1	A	840	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	TDP	A	887	2	21,27,27	1.48	4 (19%)	31,40,40	0.97	1 (3%)
3	TDP	B	887	2	21,27,27	1.47	5 (23%)	31,40,40	0.98	1 (3%)

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	TDP	A	887	2	-	0/16/17/17	0/2/2/2
3	TDP	B	887	2	-	0/16/17/17	0/2/2/2

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	887	TDP	P2-O21	2.14	1.56	1.50
3	B	887	TDP	C4-N3	2.15	1.41	1.39
3	B	887	TDP	C2'-N1'	2.36	1.38	1.34
3	B	887	TDP	C5'-C4'	2.37	1.48	1.42
3	A	887	TDP	C2'-N1'	2.39	1.38	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	887	TDP	C6'-N1'-C2'	2.53	120.20	115.77
3	A	887	TDP	C6'-N1'-C2'	2.58	120.28	115.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	887	TDP	4	0
3	B	887	TDP	4	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](#)

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.