



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1QHM / pdb_00001qhm
Title : ESCHERICHIA COLI PYRUVATE FORMATE LYASE LARGE DOMAIN
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Deposited on : 1999-05-19
Resolution : 2.80 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

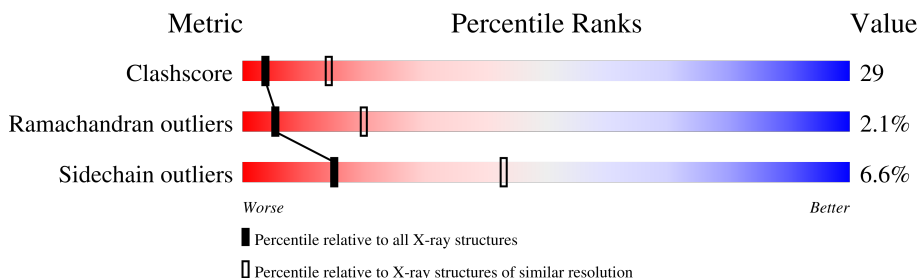
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	624	 55% 37% 6% •
1	B	624	 53% 39% 6% •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9810 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 FORMATE-LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	612	Total	C	N	O	S	0	0	1
			4794	3034	810	920	30			
1	B	612	Total	C	N	O	S	0	0	1
			4782	3026	809	917	30			

- Molecule 2 is water.

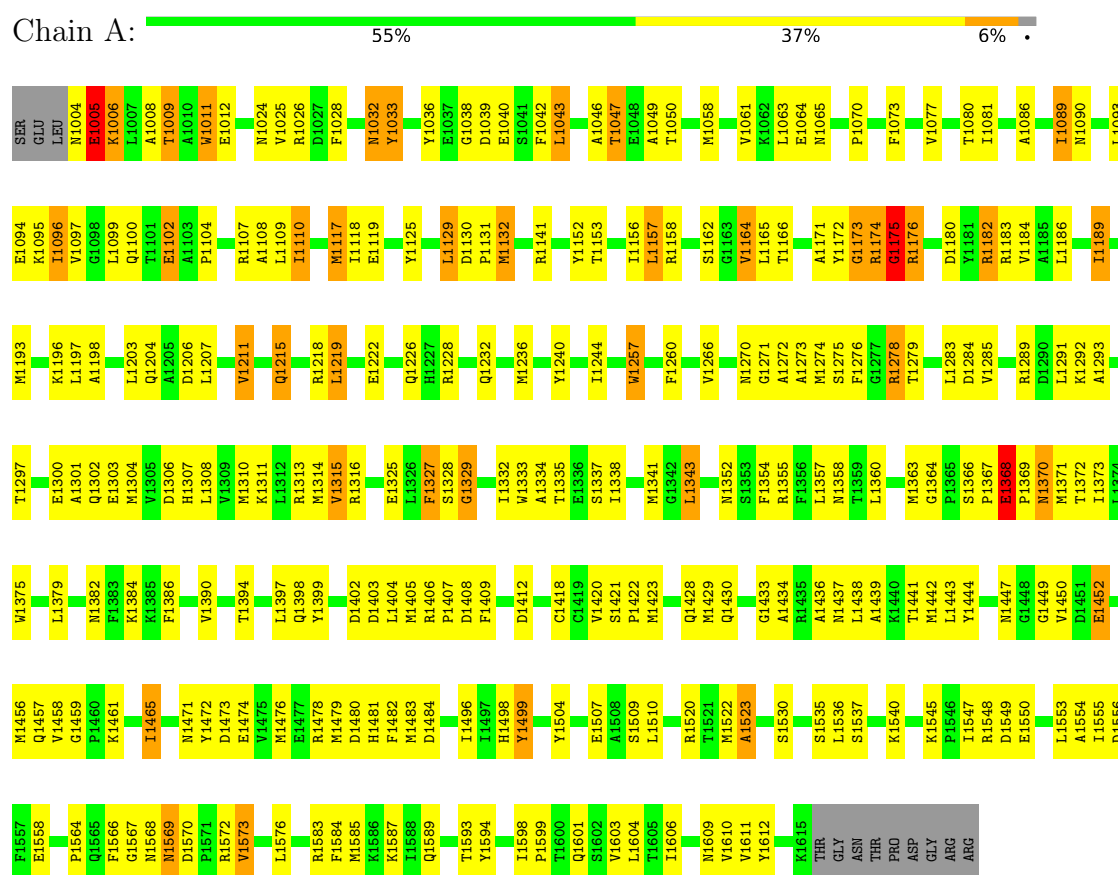
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	125	Total	O	0	0
			125	125		
2	B	109	Total	O	0	0
			109	109		

3 Residue-property plots

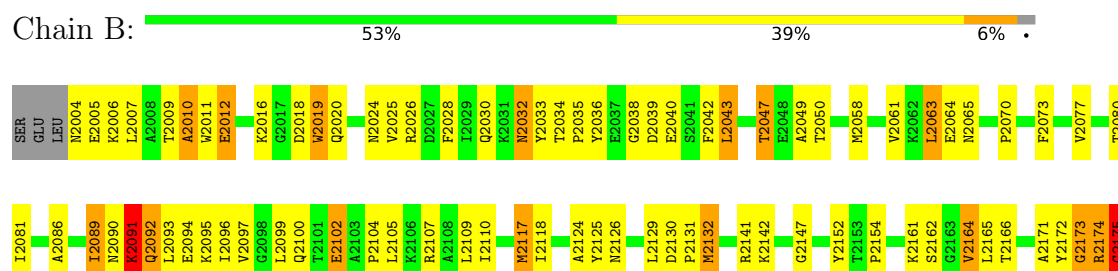
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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 FORMATE-LYASE



• Molecule 1: PYRUVATE FORMATE-LYASE





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	140.80Å 140.80Å 215.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	99.0 (20.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	5.20	Depositor
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.228 , 0.253	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9810	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.54	0/4891	1.02	28/6623 (0.4%)
1	B	0.54	0/4879	1.05	27/6610 (0.4%)
All	All	0.54	0/9770	1.04	55/13233 (0.4%)

There are no bond length outliers.

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2089	ILE	N-CA-C	-13.61	98.74	111.67
1	A	1089	ILE	N-CA-C	-12.18	100.10	111.67
1	B	2368	GLU	CA-C-N	-10.05	107.28	119.84
1	B	2368	GLU	C-N-CA	-10.05	107.28	119.84
1	A	1368	GLU	CA-C-N	-9.97	107.37	119.84

There are no chirality outliers.

There are no planarity outliers.

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	4794	0	4659	260	0
1	B	4782	0	4636	287	0
2	A	125	0	0	5	0
2	B	109	0	0	5	0
All	All	9810	0	9295	544	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 29.

The worst 5 of 544 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:2465:ILE:CA	1:B:2478:ARG:HH12	1.42	1.33
1:B:2465:ILE:CG1	1:B:2478:ARG:NH1	1.96	1.28
1:B:2465:ILE:HG13	1:B:2478:ARG:NH1	1.57	1.14
1:B:2465:ILE:CA	1:B:2478:ARG:NH1	2.11	1.14
1:B:2465:ILE:N	1:B:2478:ARG:HH12	1.49	1.11

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	610/624 (98%)	545 (89%)	54 (9%)	11 (2%)	6	23
1	B	610/624 (98%)	539 (88%)	56 (9%)	15 (2%)	4	16
All	All	1220/1248 (98%)	1084 (89%)	110 (9%)	26 (2%)	5	20

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1175	GLY
1	A	1569	ASN
1	B	2175	GLY
1	B	2327	PHE
1	B	2329	GLY

5.3.2 Protein sidechains [i](#)

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	502/528 (95%)	468 (93%)	34 (7%)	14	42
1	B	499/528 (94%)	467 (94%)	32 (6%)	16	44
All	All	1001/1056 (95%)	935 (93%)	66 (7%)	15	43

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2322	GLU
1	B	2368	GLU
1	B	2609	ASN
1	A	1315	VAL
1	A	1308	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2215	GLN
1	B	2457	GLN
1	B	2226	GLN
1	B	2430	GLN
1	B	2609	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.