



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 08:57 pm GMT

PDB ID : 1QHM
Title : ESCHERICHIA COLI PYRUVATE FORMATE LYASE LARGE DOMAIN
Authors : Leppanen, V.-M.; Merckel, M.C.; Ollis, D.L.; Wong, K.K.; Kozarich, J.W.;
Goldman, A.
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

<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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

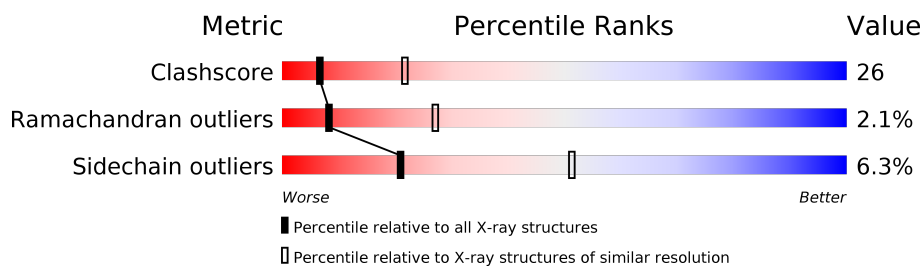
1 Overall quality at a glance

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	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (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 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	624	
1	B	624	

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.

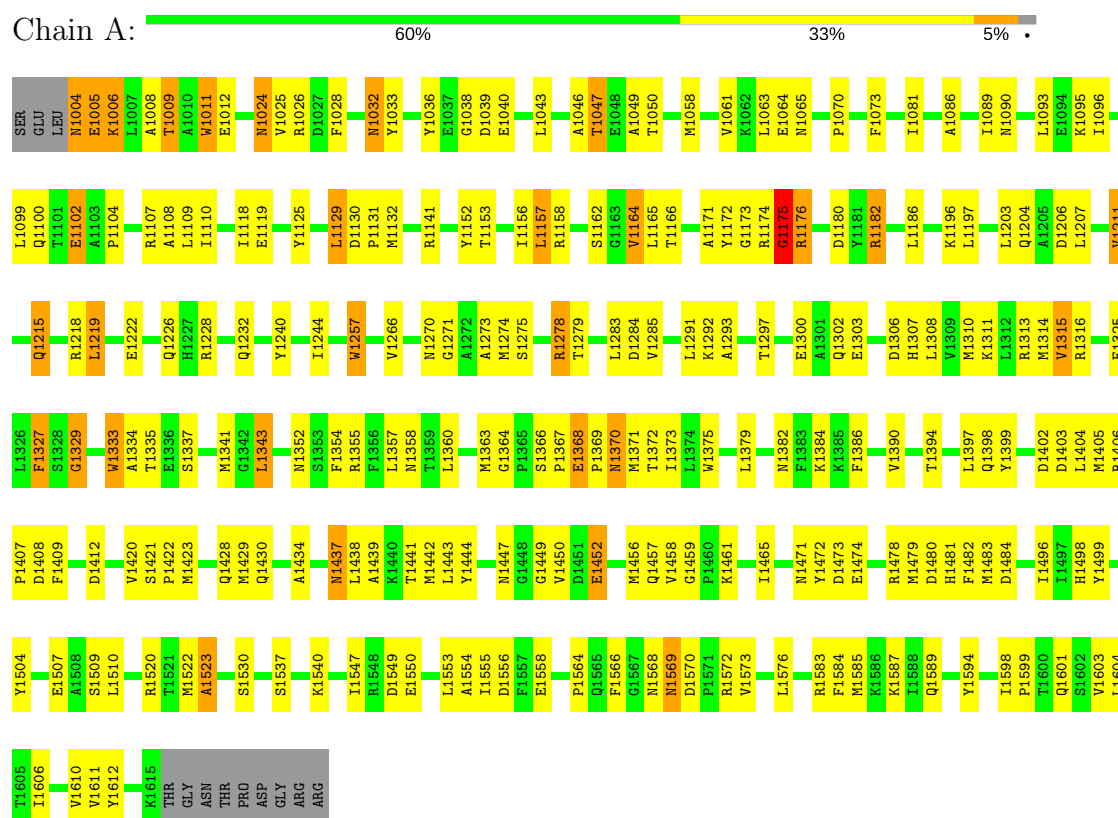
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	125	Total	O	0	0
			125	125		
2	B	109	Total	O	0	0
			109	109		

3 Residue-property plots

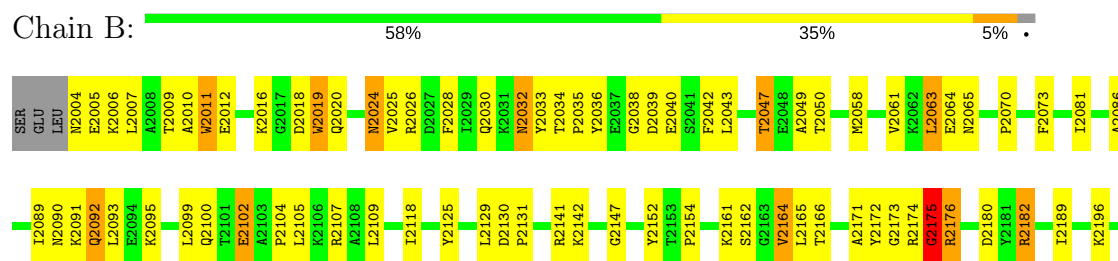
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

• Molecule 1: PYRUVATE FORMATE-LYASE



• Molecule 1: PYRUVATE FORMATE-LYASE



A2577	R2478	Y2399	M2314	L2203
R2583	M2479	E2400	V2315	
F2584	D2480	N2401	R2316	D2206
M2585	H2481	D2402		L2207
K2586	F2482	D2403	E2322	
K2587	M2483	L2404		V2211
I2588	D2484	M2405	E2325	
Q2589		R2406	L2326	Q2215
Y2594	I2491	P2407	F2327	
	I2496	D2408	S2328	R2218
Q2601	I2497	F2409	G2329	L2219
S2602		D2412	M2333	
V2603	H2498		A2334	E2222
L2604	Y2499	V2420	T2335	
	Y2504	S2421	E2336	Q2226
N2609		P2422	S2337	
V2610	E2507	M2423		K2234
K2615	A2508	Q2428	M2341	Y2240
THR	S2509	M2429	G2342	
GLY	L2510	Q2430	L2343	I2244
ASN			R2346	
THR	R2520	A2434		P2247
PRO	A2523		K2351	
ASP	S2535	N2437	N2352	W2257
GLY	I2539	L2438	S2353	
ARG	K2540	A2439	F2354	V2266
		T2441	R2355	
	V2544	M2442	F2356	A2272
K2645	R2645	L2443	L2357	A2273
P2546	I2546		N2358	M2274
R2548	I2547	N2447	I2359	S2275
D2549	R2548	G2448	L2360	
E2550	D2549			R2278
		D2451	S2366	T2279
L2553	L2553	E2452	P2367	
A2554	A2554	R2453	E2368	L2283
I2555	I2555	L2454	P2369	D2284
D2556	D2556	K2455	N2370	V2285
F2557	F2557	M2456	M2371	
E2558	F2557	Q2457	T2372	L2291
I2559	E2558	V2458	I2373	K2292
		G2459	L2374	A2293
		P2460	W2375	
P2564	P2564	K2461		T2297
Q2565	Q2565	S2462	L2379	
F2566	F2566	E2463	N2382	E2300
G2567	G2567	P2464	F2383	A2301
N2568	N2568	I2465	K2384	Q2302
N2569	N2569		K2385	E2303
D2570	D2570	D2468	F2386	
P2571	P2571	V2469		D2306
R2572	R2572	L2470	V2390	H2307
V2573	V2573	N2471		L2308
D2574	D2574	Y2472	T2394	V2309
D2575	D2575	E2474		M2310
L2576	L2576		L2397	K2311
			Q2398	L2312
				R2313

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	0.46	0/4891	0.66	2/6623 (0.0%)
1	B	0.46	0/4879	0.67	2/6610 (0.0%)
All	All	0.46	0/9770	0.67	4/13233 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1175	GLY	N-CA-C	6.33	128.93	113.10
1	B	2175	GLY	N-CA-C	6.09	128.32	113.10
1	A	1176	ARG	N-CA-C	-5.68	95.66	111.00
1	B	2176	ARG	N-CA-C	-5.52	96.09	111.00

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	235	0
1	B	4782	0	4636	261	0
2	A	125	0	0	3	0
2	B	109	0	0	5	0
All	All	9810	0	9295	493	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 26.

The worst 5 of 493 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%)	10	32
1	B	610/624 (98%)	539 (88%)	56 (9%)	15 (2%)	6	22
All	All	1220/1248 (98%)	1084 (89%)	110 (9%)	26 (2%)	8	27

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 ⓘ

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%)	470 (94%)	32 (6%)	20	50
1	B	499/528 (94%)	468 (94%)	31 (6%)	21	52
All	All	1001/1056 (95%)	938 (94%)	63 (6%)	21	51

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1443	LEU
1	B	2047	THR
1	B	2473	ASP
1	A	1452	GLU
1	A	1550	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1457	GLN
1	B	2024	ASN
1	B	2457	GLN
1	A	1471	ASN
1	A	1498	HIS

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 [i](#)

There are no carbohydrates 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.