



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 07:33 AM EDT

PDB ID : 1QHM
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	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
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)	:	2.36.2

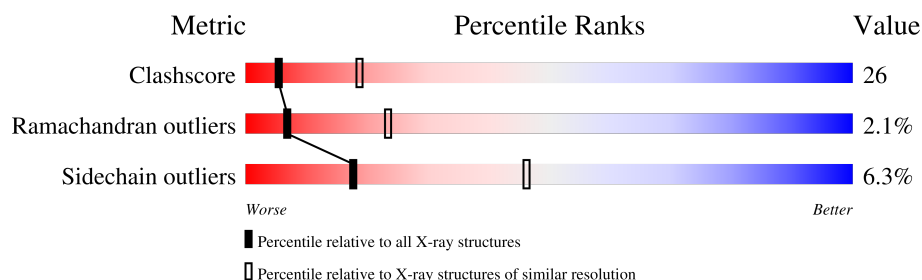
1 Overall quality at a glance

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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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	
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.

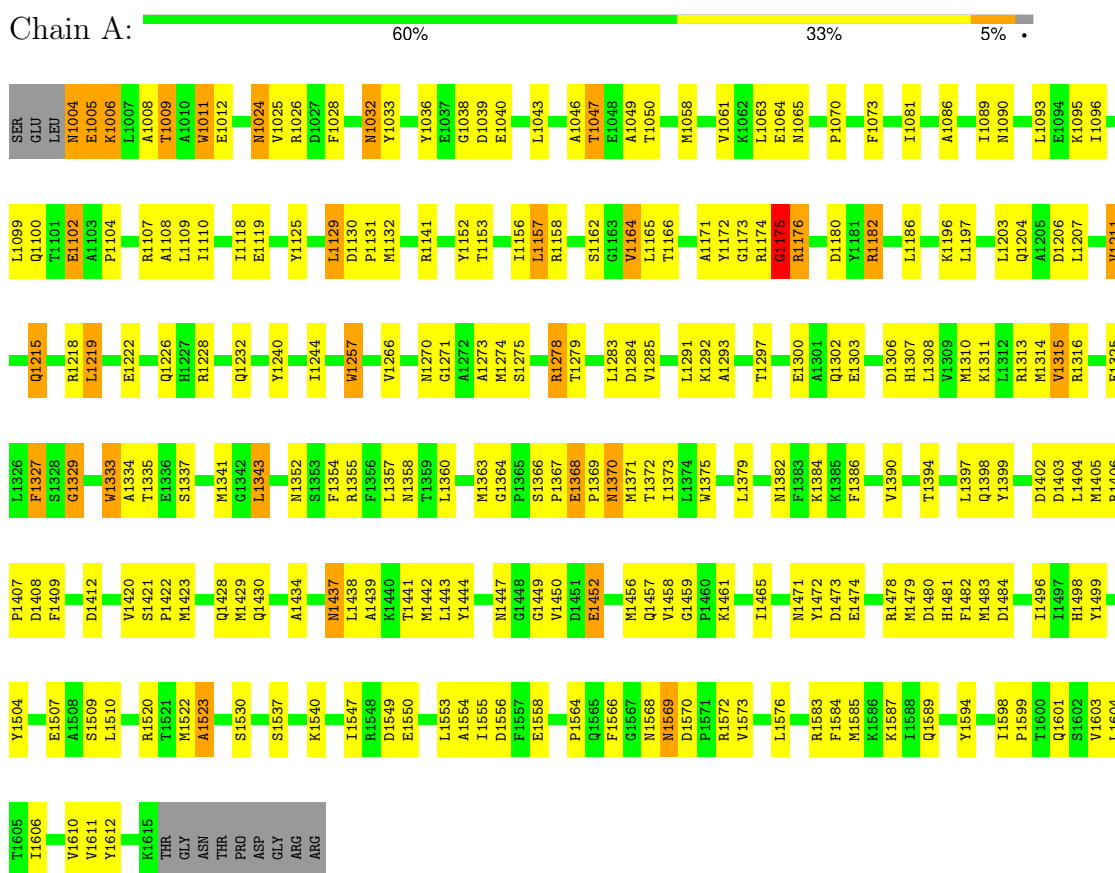
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	125	Total	O	0	0
			125	125		
2	B	109	Total	O	0	0
			109	109		

3 Residue-property plots

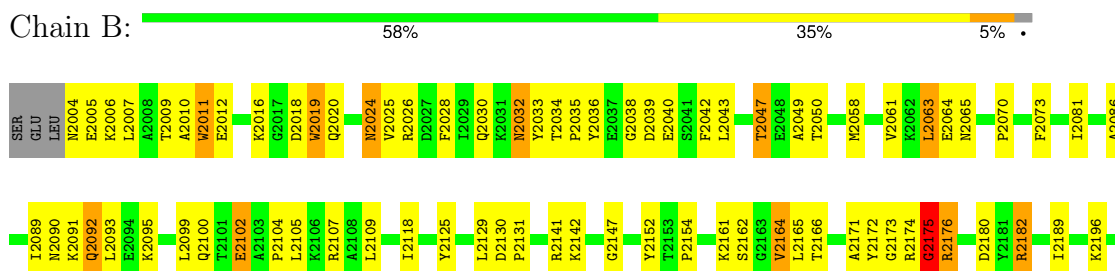
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



A2577	R2478	Y2399	M2314	L2203
R2583	M2479	E2400	V2315	
F2584	D2480	N2401	R2316	D2206
M2585	H2481	D2402		L2207
K2586	F2482	L2403	E2322	V2211
K2587	M2483	L2404	E2325	Q2215
I2588	D2484	N2405	L2326	F2327
Q2589	I2491	R2406	S2328	L2218
	I2496	P2407	G2329	L2219
Y2594	I2497	F2409		E2222
Q2601	H2498	D2412	W2333	Q2226
S2602	Y2499		A2334	K2234
V2603	Y2504	V2420	T2335	Y2240
L2604	Y2504	S2421	E2336	T2244
		P2422	S2337	P2247
N2609	E2507	N2423		
V2610	A2508	Q2428	M2341	
K2615	S2509	M2429	G2342	
THR	L2510	Q2430	L2343	
GLY	R2520		R2346	
ASN		A2434		V2257
THR	A2523		K2351	
PRO		N2437	N2352	
ASP	S2535	L2438	S2353	V2266
GLY	I2539	A2439	F2354	
ARG	K2540	K2440	R2355	G2271
		T2441	F2356	A2272
V2544		N2442	L2357	A2273
K2545		L2443	N2358	H2274
R2546			I2359	S2275
I2547		N2447	L2360	
R2548		G2448		R2278
D2549			S2366	T2279
E2550		D2451	P2367	
		E2452	E2368	L2283
L2553		K2453	P2369	D2284
A2554		L2454	N2370	V2285
I2555		N2455	M2371	
D2556		K2456	T2372	L2291
F2557		Q2457	I2373	K2292
E2558		V2458	I2374	A2293
I2559		G2459	W2375	
		P2460		T2297
P2564		K2461		
Q2565		S2462		E2300
F2566		E2463	N2382	A2301
G2567		P2464	F2383	Q2302
		I2465	K2384	E2303
N2568			K2385	
N2569		D2468		D2306
D2570		V2469	F2386	H2307
P2571		L2470		L2308
R2572		N2471	V2390	V2309
V2573		Y2472	T2394	H2310
D2574		E2473		K2311
D2575			L2397	L2312
L2576			Q2398	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	140.80 Å 140.80 Å 215.90 Å 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%)	8	28
1	B	610/624 (98%)	539 (88%)	56 (9%)	15 (2%)	5	19
All	All	1220/1248 (98%)	1084 (89%)	110 (9%)	26 (2%)	7	23

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%)	470 (94%)	32 (6%)	17	45
1	B	499/528 (94%)	468 (94%)	31 (6%)	18	47
All	All	1001/1056 (95%)	938 (94%)	63 (6%)	18	46

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

Mol	Chain	Res	Type
1	A	1443	LEU
1	B	2382	ASN
1	B	2047	THR
1	B	2368	GLU
1	B	2559	ILE

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

Mol	Chain	Res	Type
1	B	2215	GLN
1	B	2447	ASN
1	B	2226	GLN
1	B	2428	GLN
1	B	2471	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 monosaccharides 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.