



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3PQE / pdb_00003pqe
Title : Crystal structure of L-lactate dehydrogenase from Bacillus subtilis with H171C mutation
Authors : Zhang, Y.; Garavito, R.M.
Deposited on : 2010-11-26
Resolution : 2.20 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

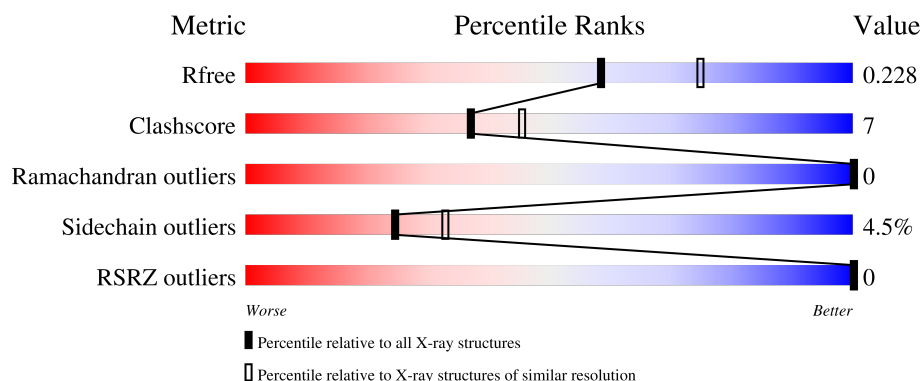
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	326	
1	B	326	
1	C	326	
1	D	326	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9845 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 L-lactate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2397	1527	401	460	9			
1	B	314	Total	C	N	O	S	0	0	0
			2397	1527	401	460	9			
1	C	305	Total	C	N	O	S	0	0	0
			2331	1488	387	447	9			
1	D	306	Total	C	N	O	S	0	0	0
			2342	1494	391	448	9			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	CYS	HIS	engineered mutation	UNP P13714
A	321	HIS	-	expression tag	UNP P13714
A	322	HIS	-	expression tag	UNP P13714
A	323	HIS	-	expression tag	UNP P13714
A	324	HIS	-	expression tag	UNP P13714
A	325	HIS	-	expression tag	UNP P13714
A	326	HIS	-	expression tag	UNP P13714
B	171	CYS	HIS	engineered mutation	UNP P13714
B	321	HIS	-	expression tag	UNP P13714
B	322	HIS	-	expression tag	UNP P13714
B	323	HIS	-	expression tag	UNP P13714
B	324	HIS	-	expression tag	UNP P13714
B	325	HIS	-	expression tag	UNP P13714
B	326	HIS	-	expression tag	UNP P13714
C	171	CYS	HIS	engineered mutation	UNP P13714
C	321	HIS	-	expression tag	UNP P13714
C	322	HIS	-	expression tag	UNP P13714
C	323	HIS	-	expression tag	UNP P13714
C	324	HIS	-	expression tag	UNP P13714
C	325	HIS	-	expression tag	UNP P13714
C	326	HIS	-	expression tag	UNP P13714

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Chain	Residue	Modelled	Actual	Comment	Reference
D	171	CYS	HIS	engineered mutation	UNP P13714
D	321	HIS	-	expression tag	UNP P13714
D	322	HIS	-	expression tag	UNP P13714
D	323	HIS	-	expression tag	UNP P13714
D	324	HIS	-	expression tag	UNP P13714
D	325	HIS	-	expression tag	UNP P13714
D	326	HIS	-	expression tag	UNP P13714

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	157	Total 157	O 157	0	0
2	B	154	Total 154	O 154	0	0
2	C	29	Total 29	O 29	0	0
2	D	38	Total 38	O 38	0	0

MET	R2	K3	F15	S18	K42	A43	M44	G45	D46	V47	M48	H52	V61	E69	V77	H84	GLN	LYS	PRO	GLY	GLU	THR	R91	L92	E93	K97	S107	M110	F114	A121	L138	P139	K140	G145	L150	S160	A165	Q168	N169	
E177	E182	L183	P184	V185	N190	V194	P195	E198	E201	D204	ALA	Y206	K207	Q208	E209	E210	L211	D212	I225	K228	T232	Y233	L240	N250	L254	S258	T259	Y260	L261	D262	G263	Q264	D268	D269	V270	Y271	N279	L289	K294	Q298
H301	V305	L306	I309	K311	P312	H313	F314	ALA	GLU	GLN	LYS	VAL	ASN	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	133.41Å 133.41Å 99.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.93 – 2.20 26.93 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (26.93-2.20) 99.5 (26.93-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.56 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6 _289)	Depositor
R, R_{free}	0.201 , 0.235 0.197 , 0.228	Depositor DCC
R_{free} test set	2993 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å ²)	44.3	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.487 for -h,-k,l 0.027 for h,-h-k,-l 0.027 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9845	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.64	0/2443	0.83	2/3311 (0.1%)
1	B	0.63	0/2443	0.81	0/3311
1	C	0.42	0/2374	0.76	1/3215 (0.0%)
1	D	0.42	0/2385	0.77	1/3229 (0.0%)
All	All	0.54	0/9645	0.79	4/13066 (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	D	194	VAL	N-CA-C	5.99	113.01	107.56
1	C	194	VAL	N-CA-C	5.94	112.96	107.56
1	A	156	ARG	N-CA-C	5.85	117.73	111.36
1	A	155	PHE	N-CA-C	-5.50	104.93	111.69

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	2397	0	2384	32	0
1	B	2397	0	2384	35	0
1	C	2331	0	2315	41	0
1	D	2342	0	2328	42	0
2	A	157	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	154	0	0	3	0
2	C	29	0	0	1	0
2	D	38	0	0	0	0
All	All	9845	0	9411	133	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 7.

The worst 5 of 133 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:156:ARG:HH11	1:B:156:ARG:HG2	1.12	1.13
1:A:48:MET:HE1	1:D:228:LYS:HD2	1.36	1.02
1:B:85:GLN:HB3	1:B:94:LEU:HD22	1.43	1.00
1:B:156:ARG:HG2	1:B:156:ARG:NH1	1.82	0.90
1:B:48:MET:HE1	1:C:228:LYS:HD2	1.52	0.88

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	312/326 (96%)	301 (96%)	11 (4%)	0	100	100
1	B	312/326 (96%)	301 (96%)	11 (4%)	0	100	100
1	C	299/326 (92%)	284 (95%)	15 (5%)	0	100	100
1	D	300/326 (92%)	291 (97%)	9 (3%)	0	100	100
All	All	1223/1304 (94%)	1177 (96%)	46 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	255/267 (96%)	246 (96%)	9 (4%)	32	43
1	B	255/267 (96%)	244 (96%)	11 (4%)	26	35
1	C	249/267 (93%)	237 (95%)	12 (5%)	23	30
1	D	250/267 (94%)	237 (95%)	13 (5%)	21	26
All	All	1009/1068 (94%)	964 (96%)	45 (4%)	24	33

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	210	GLU
1	D	69	GLU
1	C	232	THR
1	D	18	SER
1	D	168	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	313	HIS
1	D	203	ASN
1	D	298	GLN
1	D	208	GLN
1	D	178	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 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	314/326 (96%)	-1.31	0 100 100	27, 40, 65, 81	0
1	B	314/326 (96%)	-1.31	0 100 100	27, 40, 66, 81	0
1	C	305/326 (93%)	-1.09	0 100 100	39, 63, 92, 103	0
1	D	306/326 (93%)	-1.08	0 100 100	39, 64, 93, 110	0
All	All	1239/1304 (95%)	-1.20	0 100 100	27, 51, 86, 110	0

There are no RSRZ outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.