



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 10:35 PM UTC

PDB ID : 5VYW / pdb_00005vyw
Title : Crystal structure of Lactococcus lactis pyruvate carboxylase
Authors : Choi, P.H.; Tong, L.
Deposited on : 2017-05-26
Resolution : 3.10 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
Mogul : 2022.3.0, CSD as543be (2022)
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

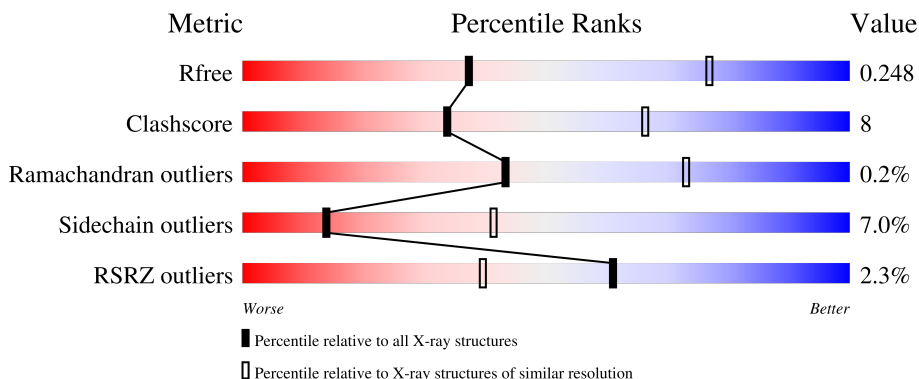
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	1143	
1	B	1143	
1	C	1143	
1	D	1143	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 31425 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 carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	981	Total	C	N	O	S	0	0	0
			7743	4918	1334	1463	28			
1	B	979	Total	C	N	O	S	0	0	0
			7729	4907	1335	1459	28			
1	C	978	Total	C	N	O	S	0	0	0
			7731	4908	1337	1458	28			
1	D	1046	Total	C	N	O	S	0	0	0
			8202	5206	1413	1552	31			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	VAL	-	expression tag	UNP A0A089XIW4
A	-4	PRO	-	expression tag	UNP A0A089XIW4
A	-3	ARG	-	expression tag	UNP A0A089XIW4
A	-2	GLY	-	expression tag	UNP A0A089XIW4
A	-1	SER	-	expression tag	UNP A0A089XIW4
A	0	HIS	-	expression tag	UNP A0A089XIW4
A	1055	ALA	THR	conflict	UNP A0A089XIW4
B	-5	VAL	-	expression tag	UNP A0A089XIW4
B	-4	PRO	-	expression tag	UNP A0A089XIW4
B	-3	ARG	-	expression tag	UNP A0A089XIW4
B	-2	GLY	-	expression tag	UNP A0A089XIW4
B	-1	SER	-	expression tag	UNP A0A089XIW4
B	0	HIS	-	expression tag	UNP A0A089XIW4
B	1055	ALA	THR	conflict	UNP A0A089XIW4
C	-5	VAL	-	expression tag	UNP A0A089XIW4
C	-4	PRO	-	expression tag	UNP A0A089XIW4
C	-3	ARG	-	expression tag	UNP A0A089XIW4
C	-2	GLY	-	expression tag	UNP A0A089XIW4
C	-1	SER	-	expression tag	UNP A0A089XIW4
C	0	HIS	-	expression tag	UNP A0A089XIW4
C	1055	ALA	THR	conflict	UNP A0A089XIW4

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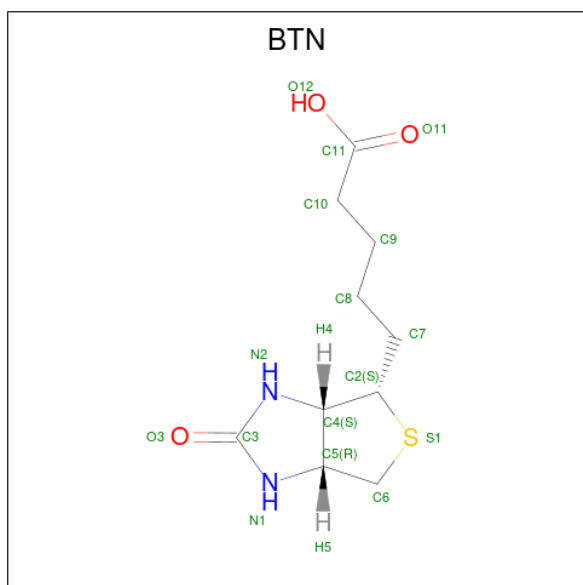
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	VAL	-	expression tag	UNP A0A089XIW4
D	-4	PRO	-	expression tag	UNP A0A089XIW4
D	-3	ARG	-	expression tag	UNP A0A089XIW4
D	-2	GLY	-	expression tag	UNP A0A089XIW4
D	-1	SER	-	expression tag	UNP A0A089XIW4
D	0	HIS	-	expression tag	UNP A0A089XIW4
D	1055	ALA	THR	conflict	UNP A0A089XIW4

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		

- Molecule 3 is BIOTIN (CCD ID: BTN) (formula: C₁₀H₁₆N₂O₃S).

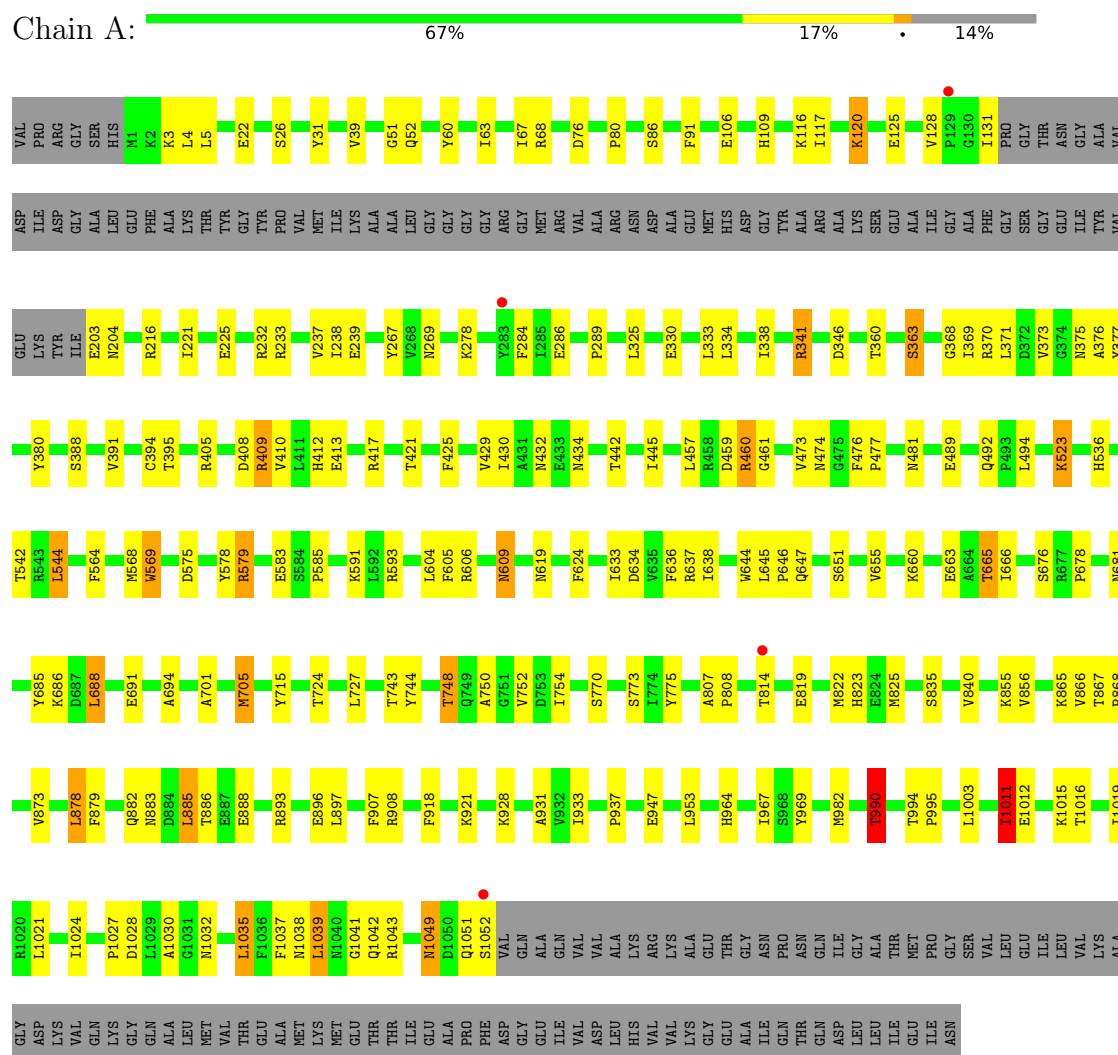


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			16	10	2	3	1		

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 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.

• Molecule 1: Pyruvate carboxylase



• Molecule 1: Pyruvate carboxylase

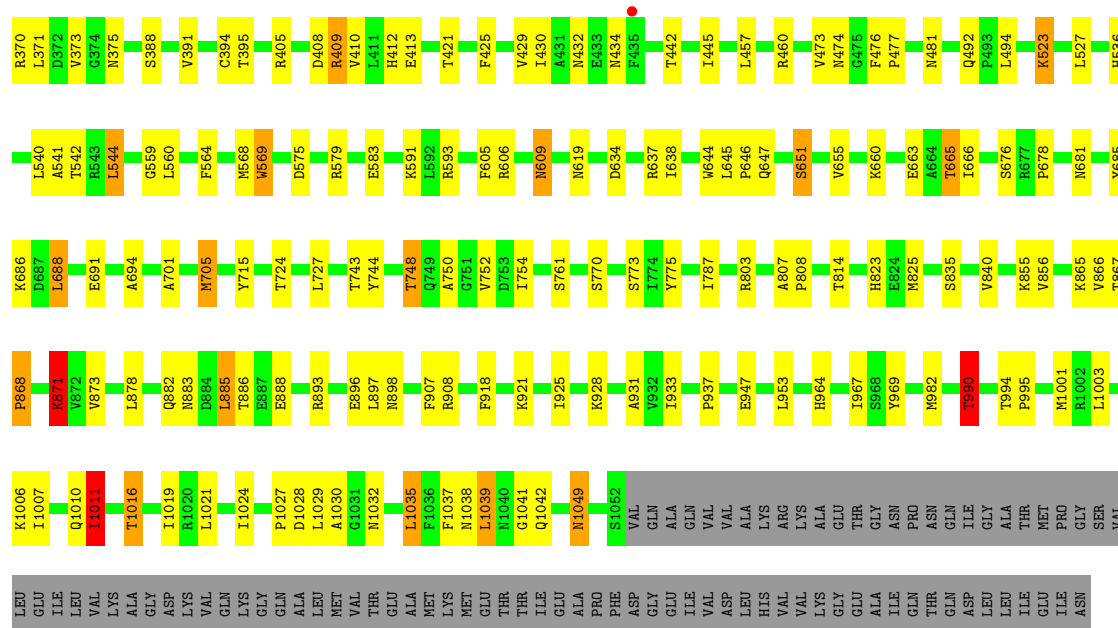


ILE	GLU	ILE	ASN	THR	MET	PRO	GLY	SER	VAL	LEU	GLU	ILE	LEU	VAL	LYS	ALA	GLY	ALA	GLY	LEU	VAL	LYS	THR	ILE	GLU	GLY	ILE	ALA	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY	THR	ASN	GLY	ILE	GLY</
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• Molecule 1: Pyruvate carboxylase

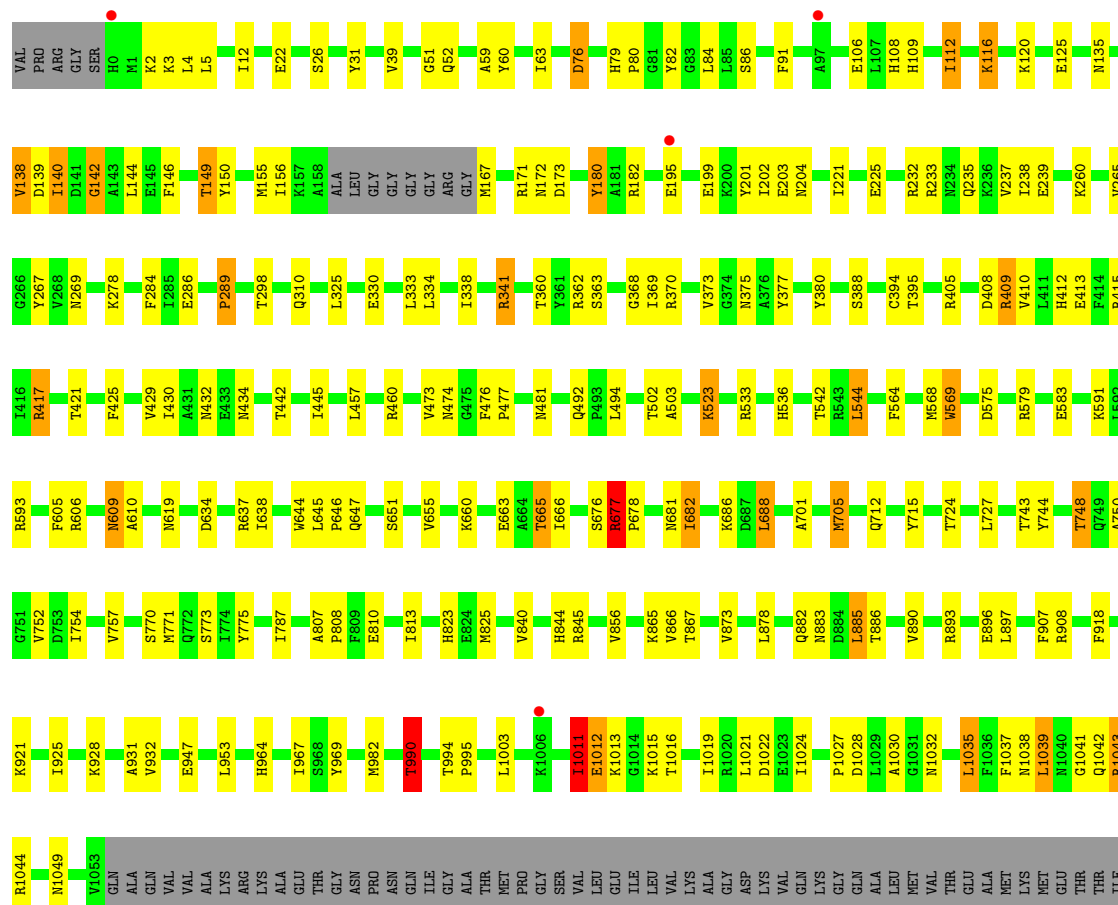


VAL	PRO	ARG	GLY	SER	HIS	M1	K2	K3	L4	L5	I12	E22	S26	Y31	V39	G51	Q52	Y60	I63	D76	A77	P80	G81	Y82	L85	S86	F91	R96	L100	V101	F102	G104	P105	E106	L107	H108	H109	I112	K116	K120												
E125			P129	GLY	ILE	PRO	THR	ASN	GLY	ALA	VAL	ASP	ILE	GLY	ALA	LEU	PHE	ALA	LYS	THR	TYR	TYR	GLY	GLY	GLY	GLY	ARG	GLY	MET	VAL	ALA	ARG	ASN	ASP	ALA	GLU	HIS	ASP	GLY	TYR	ALA	ARG	ALA	LYS	SER	GLU						
ALA	ILE	GLY	ALA	PHE	GLY	SER	GLY	GLY	ILE	TYR	VAL	GLU	LYS	TYR	ILE	GLU	N204	P205	K206	H207	I208	Q211	I212	L213	G218	I221	H222	L223	H224	E225	G226	D227	R232	R233	N234	V237	I238	E239	P242	A243	V244	G245	L246	S247	P248	D249	F250	I254	C255	E256	A257	A258
K260	L261	C262	V265	G266	Y267	N269	V273	E274	F275	L276	V277	V283	E284	I285	E286	P289	R290	V291	L300	V304	R321	E322	I323	G324	L325	P326	A327	E330	I331	P332	L333	L334	I338	R341	D346	L352	P353	T360	Y361	R362	S363	G368	I369									



• Molecule 1: Pyruvate carboxylase

Chain D: 71% 18% 8%



GLU	ALA	PRO	PHE	ASP	GLY	GLU	TLE	VAL	ASP	LEU	HIS	VAL	VAL	LYS	GLY	GLU	ALA	TLE	GLN	THR	GLN	ASP	LEU	LEU	TLE	GLU	TLE	ASN
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4 Data and refinement statistics

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α , β , γ	139.66Å 139.66Å 610.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.75 – 3.10 49.75 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.75-3.10) 99.6 (49.75-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.200 , 0.248 0.203 , 0.248	Depositor DCC
R_{free} test set	6234 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	77.3	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.049 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	31425	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, BTN

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	0.93	3/7899 (0.0%)	1.04	8/10693 (0.1%)
1	B	0.89	1/7885 (0.0%)	1.02	7/10673 (0.1%)
1	C	0.89	0/7887	1.03	4/10675 (0.0%)
1	D	0.96	3/8367 (0.0%)	1.07	9/11329 (0.1%)
All	All	0.92	7/32038 (0.0%)	1.04	28/43370 (0.1%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	ASN	N-CA	8.13	1.52	1.46
1	D	204	ASN	N-CA	7.76	1.51	1.46
1	D	289	PRO	N-CA	-5.71	1.43	1.47
1	B	576	VAL	C-O	-5.55	1.17	1.24
1	D	204	ASN	C-O	5.26	1.26	1.23

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1011	ILE	CB-CA-C	-8.31	103.32	111.30
1	D	677	ARG	NE-CZ-NH2	7.44	125.90	119.20
1	D	138	VAL	N-CA-C	6.48	116.91	108.35
1	C	1011	ILE	CB-CA-C	-6.44	104.60	110.91
1	A	128	VAL	CA-C-N	6.27	126.23	120.03

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	7743	0	7699	121	0
1	B	7729	0	7684	119	0
1	C	7731	0	7692	117	0
1	D	8202	0	8122	139	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	16	0	15	0	0
All	All	31425	0	31212	482	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 8.

The worst 5 of 482 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:A:116:LYS:O	1:A:120:LYS:HG2	1.62	0.98
1:A:819:GLU:HG2	1:A:822:MET:HE3	1.45	0.98
1:D:682:ILE:HD12	1:D:682:ILE:H	1.38	0.86
1:C:523:LYS:HE3	1:C:523:LYS:HA	1.57	0.86
1:A:523:LYS:HA	1:A:523:LYS:HE3	1.60	0.83

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	977/1143 (86%)	919 (94%)	56 (6%)	2 (0%)	43	73
1	B	975/1143 (85%)	922 (95%)	52 (5%)	1 (0%)	48	78
1	C	974/1143 (85%)	917 (94%)	56 (6%)	1 (0%)	48	78
1	D	1042/1143 (91%)	983 (94%)	56 (5%)	3 (0%)	36	67
All	All	3968/4572 (87%)	3741 (94%)	220 (6%)	7 (0%)	43	73

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	460	ARG
1	B	269	ASN
1	C	269	ASN
1	D	269	ASN
1	A	269	ASN

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	832/955 (87%)	774 (93%)	58 (7%)	14	41
1	B	830/955 (87%)	774 (93%)	56 (7%)	15	43
1	C	831/955 (87%)	773 (93%)	58 (7%)	14	41
1	D	872/955 (91%)	809 (93%)	63 (7%)	13	40
All	All	3365/3820 (88%)	3130 (93%)	235 (7%)	14	41

5 of 235 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	125	GLU
1	D	885	LEU
1	C	681	ASN
1	D	748	THR
1	D	481	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 104 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	412	HIS
1	C	794	GLN
1	D	964	HIS
1	C	439	GLN
1	C	619	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](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	BTN	A	1202	-	17,17,17	1.22	2 (11%)	23,23,23	1.66	6 (26%)

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	BTN	A	1202	-	-	1/7/28/28	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1202	BTN	C2-S1	-2.66	1.78	1.82
3	A	1202	BTN	C6-S1	-2.02	1.75	1.81

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1202	BTN	C6-C5-N1	-3.24	109.01	113.18
3	A	1202	BTN	O12-C11-C10	2.91	123.19	114.00
3	A	1202	BTN	O3-C3-N1	-2.62	122.12	125.89
3	A	1202	BTN	C6-S1-C2	2.48	95.15	89.98
3	A	1202	BTN	O12-C11-O11	-2.25	117.55	123.33

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1202	BTN	C2-C7-C8-C9

There are no ring outliers.

No monomer is involved in short contacts.

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	981/1143 (85%)	-0.28	4 (0%) 88 76	40, 71, 108, 160	0
1	B	979/1143 (85%)	-0.01	20 (2%) 65 44	36, 86, 149, 219	0
1	C	978/1143 (85%)	0.27	62 (6%) 26 14	37, 90, 168, 255	0
1	D	1046/1143 (91%)	-0.34	4 (0%) 88 76	40, 70, 108, 177	0
All	All	3984/4572 (87%)	-0.09	90 (2%) 61 39	36, 76, 144, 255	0

The worst 5 of 90 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	284	PHE	4.7
1	C	284	PHE	4.6
1	C	105	PRO	4.4
1	C	262	CYS	4.4
1	C	283	TYR	4.2

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BTN	A	1202	16/16	0.90	0.15	88,114,121,123	0
2	MN	C	2000	1/1	0.93	0.08	99,99,99,99	0
2	MN	B	2000	1/1	0.96	0.06	90,90,90,90	0
2	MN	D	2000	1/1	0.97	0.05	88,88,88,88	0
2	MN	A	1201	1/1	0.97	0.05	98,98,98,98	0

6.5 Other polymers [i](#)

There are no such residues in this entry.