



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 10:23 AM EDT

PDB ID : 4LOC / pdb_00004loc
Title : Structure of the carboxyl transferase domain from *Rhizobium etli* pyruvate carboxylase with oxamate and biotin
Authors : Lietzan, A.D.; St.Maurice, M.
Deposited on : 2013-07-12
Resolution : 2.26 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

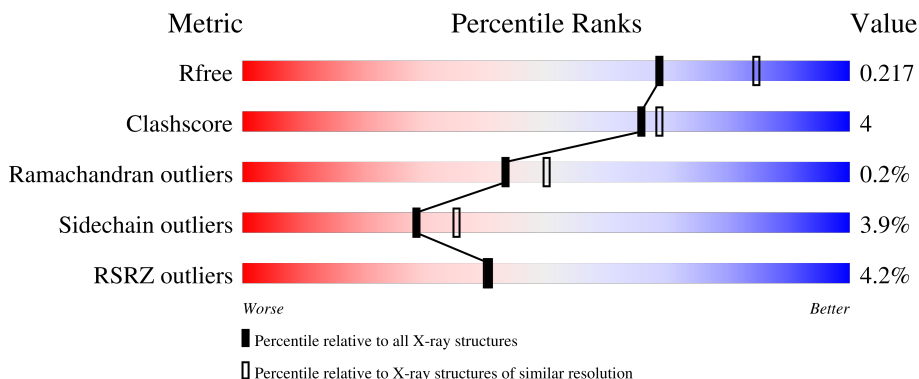
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	632	% 83% 10% • 6%
1	B	632	8% 82% 11% • 6%
1	C	632	5% 84% 9% 6%
1	D	632	2% 82% 12% • 6%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 18570 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	595	Total	C	N	O	S	0	3	0
			4572	2908	771	870	23			
1	B	593	Total	C	N	O	S	0	1	0
			4389	2784	743	839	23			
1	C	595	Total	C	N	O	S	0	1	0
			4456	2841	746	846	23			
1	D	596	Total	C	N	O	S	0	1	0
			4507	2868	761	855	23			

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	436	MET	-	expression tag	UNP Q2K340
A	437	GLY	-	expression tag	UNP Q2K340
A	438	SER	-	expression tag	UNP Q2K340
A	439	SER	-	expression tag	UNP Q2K340
A	440	HIS	-	expression tag	UNP Q2K340
A	441	HIS	-	expression tag	UNP Q2K340
A	442	HIS	-	expression tag	UNP Q2K340
A	443	HIS	-	expression tag	UNP Q2K340
A	444	HIS	-	expression tag	UNP Q2K340
A	445	HIS	-	expression tag	UNP Q2K340
A	446	HIS	-	expression tag	UNP Q2K340
A	447	HIS	-	expression tag	UNP Q2K340
A	448	ASP	-	expression tag	UNP Q2K340
A	449	TYR	-	expression tag	UNP Q2K340
A	450	ASP	-	expression tag	UNP Q2K340
A	451	ILE	-	expression tag	UNP Q2K340
A	452	PRO	-	expression tag	UNP Q2K340
A	453	THR	-	expression tag	UNP Q2K340
A	454	SER	-	expression tag	UNP Q2K340
A	455	GLU	-	expression tag	UNP Q2K340
A	456	ASN	-	expression tag	UNP Q2K340

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Chain	Residue	Modelled	Actual	Comment	Reference
A	457	LEU	-	expression tag	UNP Q2K340
A	458	TYR	-	expression tag	UNP Q2K340
A	459	PHE	-	expression tag	UNP Q2K340
A	460	GLN	-	expression tag	UNP Q2K340
A	461	GLY	-	expression tag	UNP Q2K340
A	462	LEU	-	expression tag	UNP Q2K340
A	463	LEU	-	expression tag	UNP Q2K340
A	464	HIS	-	expression tag	UNP Q2K340
B	436	MET	-	expression tag	UNP Q2K340
B	437	GLY	-	expression tag	UNP Q2K340
B	438	SER	-	expression tag	UNP Q2K340
B	439	SER	-	expression tag	UNP Q2K340
B	440	HIS	-	expression tag	UNP Q2K340
B	441	HIS	-	expression tag	UNP Q2K340
B	442	HIS	-	expression tag	UNP Q2K340
B	443	HIS	-	expression tag	UNP Q2K340
B	444	HIS	-	expression tag	UNP Q2K340
B	445	HIS	-	expression tag	UNP Q2K340
B	446	HIS	-	expression tag	UNP Q2K340
B	447	HIS	-	expression tag	UNP Q2K340
B	448	ASP	-	expression tag	UNP Q2K340
B	449	TYR	-	expression tag	UNP Q2K340
B	450	ASP	-	expression tag	UNP Q2K340
B	451	ILE	-	expression tag	UNP Q2K340
B	452	PRO	-	expression tag	UNP Q2K340
B	453	THR	-	expression tag	UNP Q2K340
B	454	SER	-	expression tag	UNP Q2K340
B	455	GLU	-	expression tag	UNP Q2K340
B	456	ASN	-	expression tag	UNP Q2K340
B	457	LEU	-	expression tag	UNP Q2K340
B	458	TYR	-	expression tag	UNP Q2K340
B	459	PHE	-	expression tag	UNP Q2K340
B	460	GLN	-	expression tag	UNP Q2K340
B	461	GLY	-	expression tag	UNP Q2K340
B	462	LEU	-	expression tag	UNP Q2K340
B	463	LEU	-	expression tag	UNP Q2K340
B	464	HIS	-	expression tag	UNP Q2K340
C	436	MET	-	expression tag	UNP Q2K340
C	437	GLY	-	expression tag	UNP Q2K340
C	438	SER	-	expression tag	UNP Q2K340
C	439	SER	-	expression tag	UNP Q2K340
C	440	HIS	-	expression tag	UNP Q2K340

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Chain	Residue	Modelled	Actual	Comment	Reference
C	441	HIS	-	expression tag	UNP Q2K340
C	442	HIS	-	expression tag	UNP Q2K340
C	443	HIS	-	expression tag	UNP Q2K340
C	444	HIS	-	expression tag	UNP Q2K340
C	445	HIS	-	expression tag	UNP Q2K340
C	446	HIS	-	expression tag	UNP Q2K340
C	447	HIS	-	expression tag	UNP Q2K340
C	448	ASP	-	expression tag	UNP Q2K340
C	449	TYR	-	expression tag	UNP Q2K340
C	450	ASP	-	expression tag	UNP Q2K340
C	451	ILE	-	expression tag	UNP Q2K340
C	452	PRO	-	expression tag	UNP Q2K340
C	453	THR	-	expression tag	UNP Q2K340
C	454	SER	-	expression tag	UNP Q2K340
C	455	GLU	-	expression tag	UNP Q2K340
C	456	ASN	-	expression tag	UNP Q2K340
C	457	LEU	-	expression tag	UNP Q2K340
C	458	TYR	-	expression tag	UNP Q2K340
C	459	PHE	-	expression tag	UNP Q2K340
C	460	GLN	-	expression tag	UNP Q2K340
C	461	GLY	-	expression tag	UNP Q2K340
C	462	LEU	-	expression tag	UNP Q2K340
C	463	LEU	-	expression tag	UNP Q2K340
C	464	HIS	-	expression tag	UNP Q2K340
D	436	MET	-	expression tag	UNP Q2K340
D	437	GLY	-	expression tag	UNP Q2K340
D	438	SER	-	expression tag	UNP Q2K340
D	439	SER	-	expression tag	UNP Q2K340
D	440	HIS	-	expression tag	UNP Q2K340
D	441	HIS	-	expression tag	UNP Q2K340
D	442	HIS	-	expression tag	UNP Q2K340
D	443	HIS	-	expression tag	UNP Q2K340
D	444	HIS	-	expression tag	UNP Q2K340
D	445	HIS	-	expression tag	UNP Q2K340
D	446	HIS	-	expression tag	UNP Q2K340
D	447	HIS	-	expression tag	UNP Q2K340
D	448	ASP	-	expression tag	UNP Q2K340
D	449	TYR	-	expression tag	UNP Q2K340
D	450	ASP	-	expression tag	UNP Q2K340
D	451	ILE	-	expression tag	UNP Q2K340
D	452	PRO	-	expression tag	UNP Q2K340
D	453	THR	-	expression tag	UNP Q2K340

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Chain	Residue	Modelled	Actual	Comment	Reference
D	454	SER	-	expression tag	UNP Q2K340
D	455	GLU	-	expression tag	UNP Q2K340
D	456	ASN	-	expression tag	UNP Q2K340
D	457	LEU	-	expression tag	UNP Q2K340
D	458	TYR	-	expression tag	UNP Q2K340
D	459	PHE	-	expression tag	UNP Q2K340
D	460	GLN	-	expression tag	UNP Q2K340
D	461	GLY	-	expression tag	UNP Q2K340
D	462	LEU	-	expression tag	UNP Q2K340
D	463	LEU	-	expression tag	UNP Q2K340
D	464	HIS	-	expression tag	UNP Q2K340

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

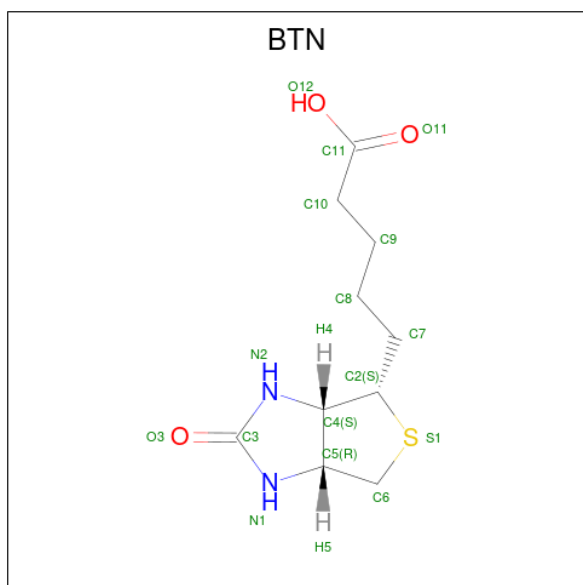
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0

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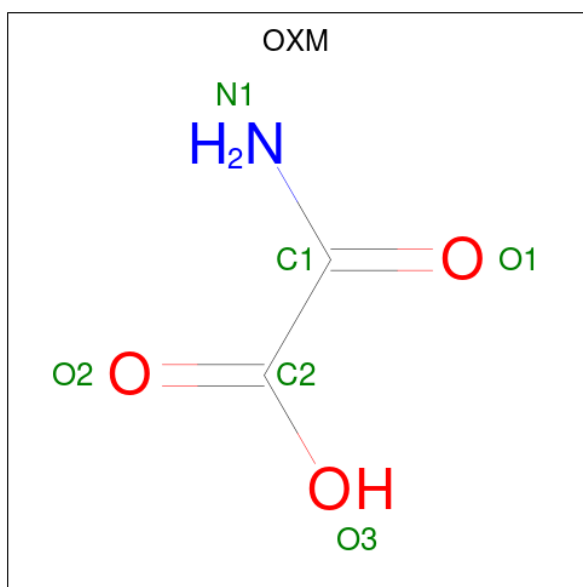
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		

- Molecule 5 is BIOTIN (CCD ID: BTN) (formula: $C_{10}H_{16}N_2O_3S$).



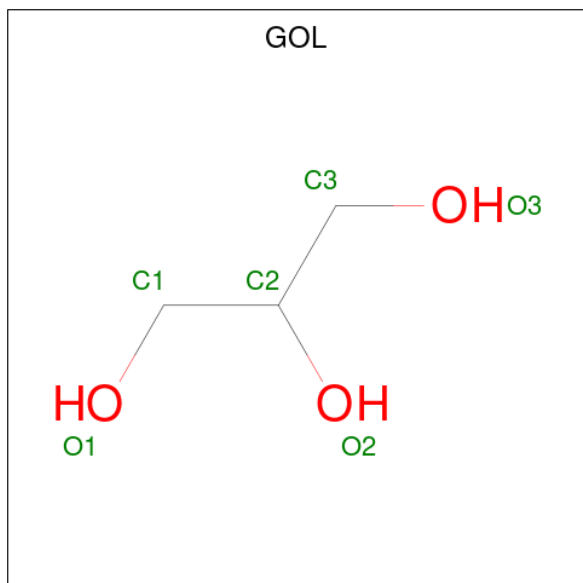
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
5	B	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
5	C	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
5	D	1	Total	C	N	O	S	0	0
			16	10	2	3	1		

- Molecule 6 is OXAMIC ACID (CCD ID: OXM) (formula: $C_2H_3NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			6	2	1	3		
6	B	1	Total	C	N	O	0	0
			6	2	1	3		
6	C	1	Total	C	N	O	0	0
			6	2	1	3		
6	D	1	Total	C	N	O	0	0
			6	2	1	3		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		

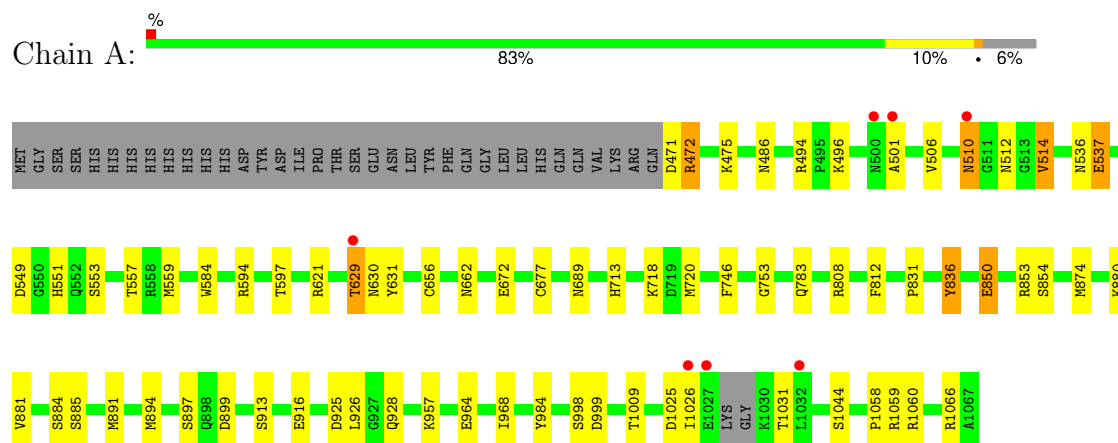
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	213	Total	O	0	0
			213	213		
8	B	97	Total	O	0	0
			97	97		
8	C	79	Total	O	0	0
			79	79		
8	D	146	Total	O	0	0
			146	146		

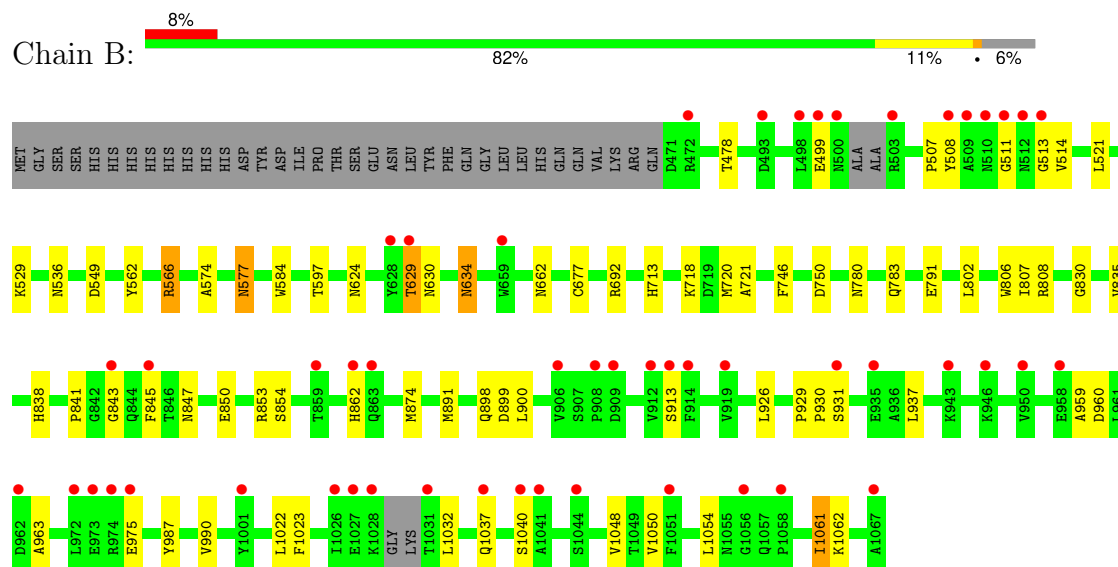
3 Residue-property plots [i](#)

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.

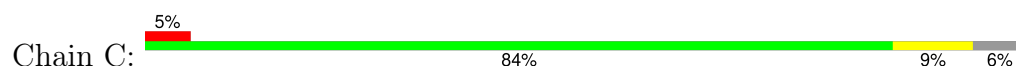
- Molecule 1: Pyruvate carboxylase

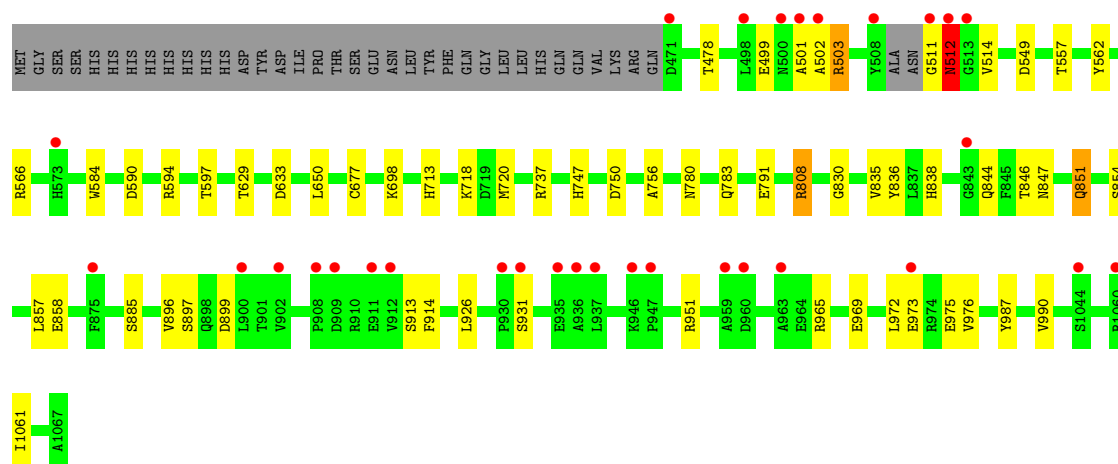


- Molecule 1: Pyruvate carboxylase

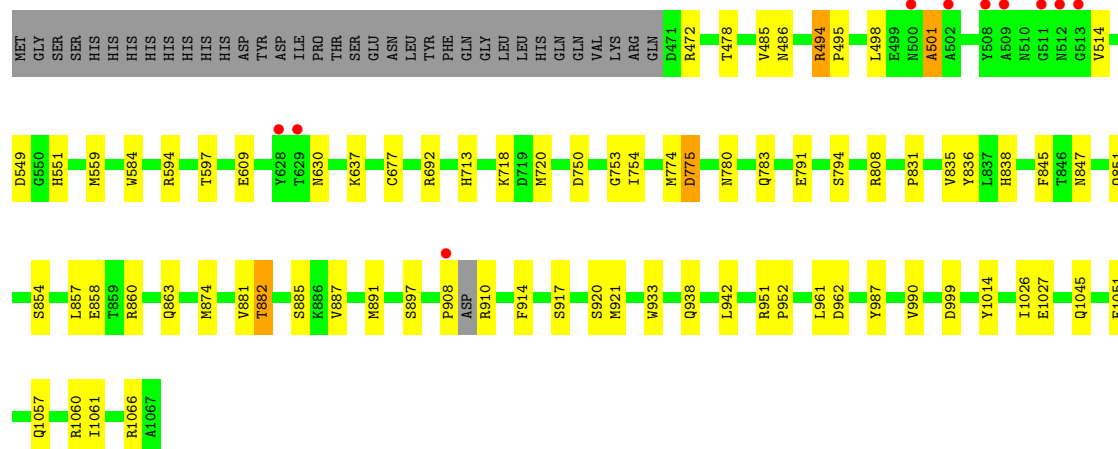
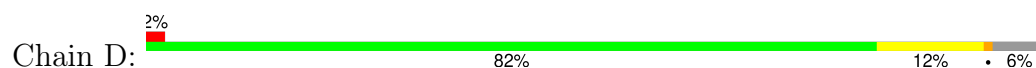


- Molecule 1: Pyruvate carboxylase





• Molecule 1: Pyruvate carboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.87Å 157.12Å 244.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.75 – 2.26 43.75 – 2.26	Depositor EDS
% Data completeness (in resolution range)	98.0 (43.75-2.26) 98.0 (43.75-2.26)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.74 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.176 , 0.216 0.184 , 0.217	Depositor DCC
R_{free} test set	7592 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18570	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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: MG, GOL, ZN, CL, KCX, OXM, 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	1.34	9/4665 (0.2%)	1.19	14/6338 (0.2%)
1	B	1.09	6/4474 (0.1%)	1.12	14/6103 (0.2%)
1	C	1.03	1/4542 (0.0%)	1.08	5/6189 (0.1%)
1	D	1.20	3/4593 (0.1%)	1.10	4/6251 (0.1%)
All	All	1.17	19/18274 (0.1%)	1.12	37/24881 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1009	THR	C-O	-6.93	1.18	1.24
1	B	1050	VAL	C-O	6.89	1.31	1.24
1	A	746	PHE	N-CA	6.53	1.54	1.46
1	A	998	SER	CA-C	-6.32	1.44	1.52
1	B	1040	SER	CB-OG	6.24	1.54	1.42

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	501	ALA	N-CA-C	10.11	123.66	111.02
1	B	692	ARG	CA-C-N	7.11	126.82	119.64
1	B	692	ARG	C-N-CA	7.11	126.82	119.64
1	A	631	TYR	N-CA-C	6.90	118.59	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1037	GLN	N-CA-C	6.81	118.78	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	512	ASN	Peptide

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	4572	0	4488	35	0
1	B	4389	0	4132	32	0
1	C	4456	0	4274	30	0
1	D	4507	0	4379	42	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	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	16	0	15	0	0
5	B	16	0	15	1	0
5	C	16	0	15	0	0
5	D	16	0	15	1	0
6	A	6	0	2	0	0
6	B	6	0	2	0	0
6	C	6	0	2	0	0
6	D	6	0	2	0	0
7	B	6	0	8	1	0
7	C	6	0	8	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	213	0	0	10	0
8	B	97	0	0	3	0
8	C	79	0	0	1	0
8	D	146	0	0	7	0
All	All	18570	0	17357	134	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 4.

The worst 5 of 134 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:885:SER:N	8:A:1355:HOH:O	1.76	1.18
1:D:630:ASN:HB2	8:D:1268:HOH:O	1.64	0.97
1:A:677:CYS:H	1:A:713:HIS:HD2	1.19	0.90
1:C:780:ASN:H	7:C:1103:GOL:H12	1.36	0.90
1:C:677:CYS:H	1:C:713:HIS:HD2	1.22	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	593/632 (94%)	577 (97%)	15 (2%)	1 (0%)	43	50
1	B	587/632 (93%)	567 (97%)	18 (3%)	2 (0%)	36	40
1	C	591/632 (94%)	563 (95%)	27 (5%)	1 (0%)	43	50
1	D	592/632 (94%)	573 (97%)	18 (3%)	1 (0%)	43	50
All	All	2363/2528 (94%)	2280 (96%)	78 (3%)	5 (0%)	43	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	501	ALA
1	C	512	ASN
1	D	501	ALA
1	B	930	PRO
1	B	843	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	472/519 (91%)	452 (96%)	20 (4%)	26	31
1	B	427/519 (82%)	409 (96%)	18 (4%)	26	31
1	C	439/519 (85%)	421 (96%)	18 (4%)	27	33
1	D	455/519 (88%)	442 (97%)	13 (3%)	37	47
All	All	1793/2076 (86%)	1724 (96%)	69 (4%)	28	36

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	514	VAL
1	D	720	MET
1	D	897	SER
1	B	577	ASN
1	B	566	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	486	ASN
1	D	510	ASN
1	D	783	GLN
1	B	630	ASN
1	B	624	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	KCX	D	718	1,2	10,11,12	0.94	0	6,12,14	1.60	2 (33%)
1	KCX	A	718	1,2	10,11,12	1.14	0	6,12,14	2.76	3 (50%)
1	KCX	B	718	1,2	10,11,12	0.88	0	6,12,14	2.89	2 (33%)
1	KCX	C	718	1,2	10,11,12	1.03	1 (10%)	6,12,14	2.51	2 (33%)

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
1	KCX	D	718	1,2	-	1/9/10/12	-
1	KCX	A	718	1,2	-	1/9/10/12	-
1	KCX	B	718	1,2	-	1/9/10/12	-
1	KCX	C	718	1,2	-	1/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	718	KCX	OQ1-CX	-2.25	1.17	1.21

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	718	KCX	CE-NZ-CX	5.92	132.02	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	718	KCX	CE-NZ-CX	4.96	130.39	121.98
1	A	718	KCX	CE-NZ-CX	4.71	129.98	121.98
1	A	718	KCX	OQ1-CX-NZ	-3.41	119.74	124.92
1	C	718	KCX	CD-CE-NZ	3.02	120.66	112.20

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	718	KCX	O-C-CA-CB
1	B	718	KCX	O-C-CA-CB
1	C	718	KCX	O-C-CA-CB
1	D	718	KCX	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 11 are monoatomic - leaving 10 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	$\# Z > 2$
7	GOL	C	1103	-	5,5,5	0.70	0	5,5,5	1.68	2 (40%)
6	OXM	B	1105	-	5,5,5	3.12	1 (20%)	2,6,6	1.19	0
5	BTN	B	1104	-	17,17,17	1.03	0	23,23,23	1.89	5 (21%)
6	OXM	A	1105	-	5,5,5	4.53	3 (60%)	2,6,6	0.53	0
6	OXM	D	1105	-	5,5,5	4.33	2 (40%)	2,6,6	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	B	1101	-	5,5,5	0.52	0	5,5,5	2.08	2 (40%)
5	BTN	D	1104	-	17,17,17	0.90	0	23,23,23	1.54	5 (21%)
5	BTN	A	1104	-	17,17,17	1.30	2 (11%)	23,23,23	2.01	9 (39%)
5	BTN	C	1105	-	17,17,17	0.85	0	23,23,23	1.54	4 (17%)
6	OXM	C	1106	-	5,5,5	3.29	1 (20%)	2,6,6	0.41	0

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
7	GOL	C	1103	-	-	1/4/4/4	-
6	OXM	B	1105	-	-	0/4/4/4	-
5	BTN	B	1104	-	-	7/7/28/28	0/2/2/2
6	OXM	A	1105	-	-	0/4/4/4	-
6	OXM	D	1105	-	-	0/4/4/4	-
7	GOL	B	1101	-	-	0/4/4/4	-
5	BTN	D	1104	-	-	6/7/28/28	0/2/2/2
5	BTN	A	1104	-	-	7/7/28/28	0/2/2/2
5	BTN	C	1105	-	-	6/7/28/28	0/2/2/2
6	OXM	C	1106	-	-	0/4/4/4	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1105	OXM	C1-C2	-9.33	1.44	1.55
6	D	1105	OXM	C1-C2	-9.32	1.44	1.55
6	C	1106	OXM	C1-C2	-6.96	1.47	1.55
6	B	1105	OXM	C1-C2	-6.67	1.47	1.55
5	A	1104	BTN	C10-C11	2.71	1.56	1.50

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1104	BTN	C8-C7-C2	5.14	125.86	114.04
5	A	1104	BTN	O12-C11-C10	4.77	129.08	114.00
5	C	1105	BTN	C6-C5-N1	-4.04	107.98	113.18
7	B	1101	GOL	C3-C2-C1	-3.37	99.45	111.80
5	B	1104	BTN	C5-C4-N2	-3.29	98.96	102.68

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1104	BTN	C4-C2-C7-C8
5	B	1104	BTN	S1-C2-C7-C8
5	B	1104	BTN	C4-C2-C7-C8
5	C	1105	BTN	S1-C2-C7-C8
5	C	1105	BTN	C4-C2-C7-C8

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1103	GOL	3	0
5	B	1104	BTN	1	0
7	B	1101	GOL	1	0
5	D	1104	BTN	1	0

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	594/632 (93%)	-0.38	7 (1%) 76 77	18, 34, 57, 82	15 (2%)
1	B	592/632 (93%)	0.38	51 (8%) 16 15	26, 61, 122, 160	8 (1%)
1	C	594/632 (93%)	0.28	31 (5%) 33 31	33, 59, 96, 129	7 (1%)
1	D	595/632 (94%)	-0.08	10 (1%) 69 70	28, 44, 79, 106	4 (0%)
All	All	2375/2528 (93%)	0.05	99 (4%) 40 40	18, 46, 100, 160	34 (1%)

The worst 5 of 99 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	500	ASN	6.3
1	B	512	ASN	5.2
1	C	502	ALA	4.7
1	D	512	ASN	4.6
1	B	510	ASN	4.4

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	KCX	B	718	12/13	0.95	0.08	38,41,48,48	0
1	KCX	C	718	12/13	0.95	0.09	40,41,43,46	0
1	KCX	A	718	12/13	0.98	0.04	21,23,25,26	0
1	KCX	D	718	12/13	0.98	0.04	31,32,34,35	0

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
5	BTN	B	1104	16/16	0.67	0.23	55,71,80,82	0
5	BTN	A	1104	16/16	0.84	0.16	44,55,73,74	0
5	BTN	D	1104	16/16	0.86	0.17	51,57,81,87	0
5	BTN	C	1105	16/16	0.87	0.14	53,62,72,78	0
7	GOL	B	1101	6/6	0.88	0.14	42,45,49,51	0
3	MG	B	1103	1/1	0.90	0.12	32,32,32,32	0
7	GOL	C	1103	6/6	0.91	0.15	42,50,54,55	0
6	OXM	B	1105	6/6	0.94	0.10	40,43,45,45	0
6	OXM	C	1106	6/6	0.95	0.09	42,44,48,49	0
6	OXM	D	1105	6/6	0.95	0.10	33,38,41,41	0
6	OXM	A	1105	6/6	0.96	0.07	30,36,37,42	0
3	MG	D	1102	1/1	0.96	0.07	33,33,33,33	0
4	CL	C	1104	1/1	0.96	0.09	58,58,58,58	0
4	CL	D	1103	1/1	0.97	0.15	49,49,49,49	0
3	MG	C	1102	1/1	0.98	0.13	41,41,41,41	0
2	ZN	B	1102	1/1	0.99	0.04	41,41,41,41	0
2	ZN	C	1101	1/1	0.99	0.04	41,41,41,41	0
3	MG	A	1102	1/1	0.99	0.06	34,34,34,34	0
4	CL	A	1103	1/1	0.99	0.05	45,45,45,45	0
2	ZN	D	1101	1/1	1.00	0.03	34,34,34,34	0
2	ZN	A	1101	1/1	1.00	0.02	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.