



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 12, 2023 – 04:55 AM EDT

PDB ID : 4MFE  
Title : Structure of the carboxyl transferase domain from *Rhizobium etli* pyruvate carboxylase with 3-hydroxypyruvate  
Authors : Lietzan, A.D.; St.Maurice, M.  
Deposited on : 2013-08-27  
Resolution : 2.61 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

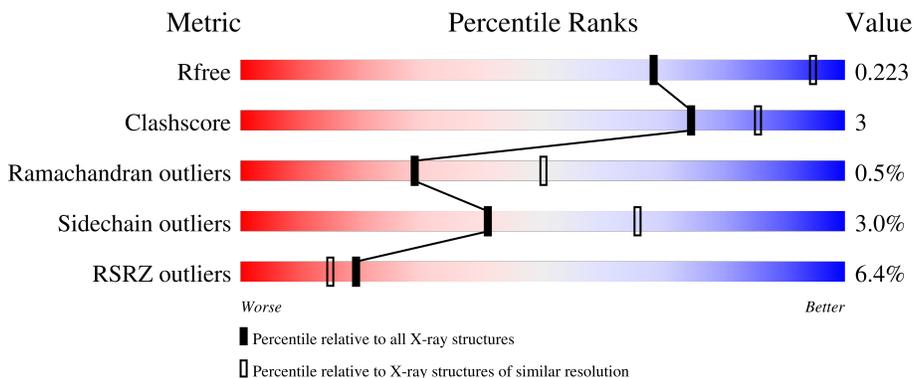
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 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))
$R_{free}$	130704	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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  $\geq 3$ , 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	 10% 83% 11% 6%
1	B	632	 4% 87% 7% 6%
1	C	632	 10% 86% 9% 6%
1	D	632	 10% 83% 11% 6%

## 2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 17744 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
			Total	C	N	O	S			
1	A	597	4497	2859	752	863	23	0	1	0
1	B	594	4295	2720	720	832	23	0	1	0
1	C	597	4416	2807	743	843	23	0	2	0
1	D	594	4278	2708	727	820	23	0	1	0

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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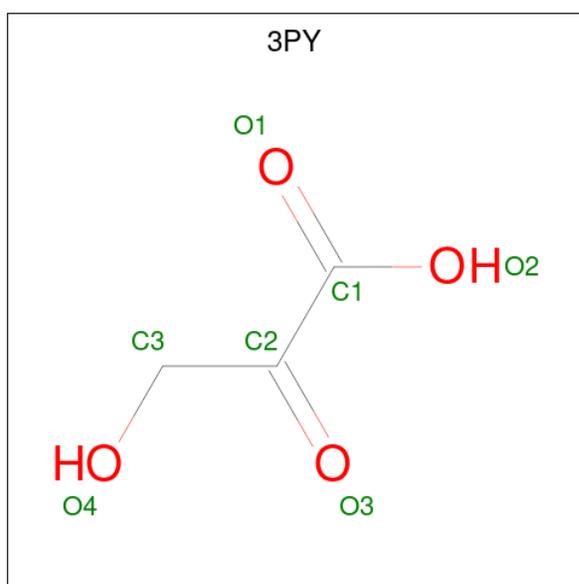
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Chain	Residue	Modelled	Actual	Comment	Reference
D	454	SER	-	expression tag	UNP Q2K340
D	455	GLU	-	expression tag	UNP Q2K340
D	456	ASN	-	expression tag	UNP Q2K340
D	457	LEU	-	expression tag	UNP Q2K340
D	458	TYR	-	expression tag	UNP Q2K340
D	459	PHE	-	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 (three-letter code: ZN) (formula: Zn).

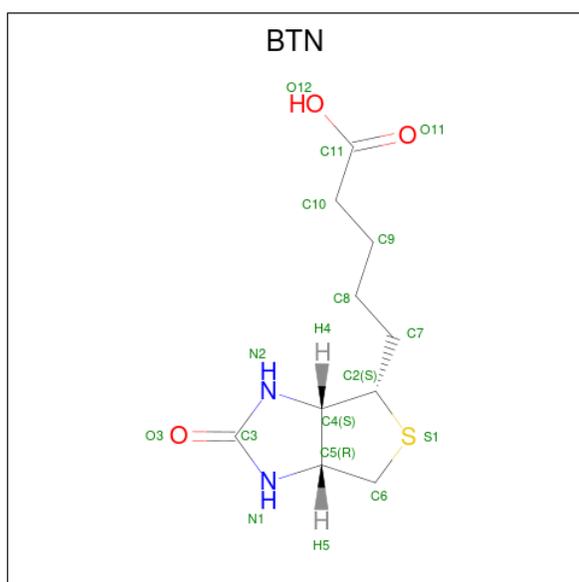
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is 3-HYDROXYPYRUVIC ACID (three-letter code: 3PY) (formula: C<sub>3</sub>H<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	3	4		
3	B	1	Total	C	O	0	0
			7	3	4		
3	C	1	Total	C	O	0	0
			7	3	4		
3	D	1	Total	C	O	0	0
			7	3	4		

- Molecule 4 is BIOTIN (three-letter code: BTN) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>2</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			9	5	2	1	1		
4	B	1	Total	C	N	O	S	0	0
			10	6	2	1	1		
4	C	1	Total	C	N	O	S	0	0
			10	6	2	1	1		
4	D	1	Total	C	N	O	S	0	0
			9	5	2	1	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		

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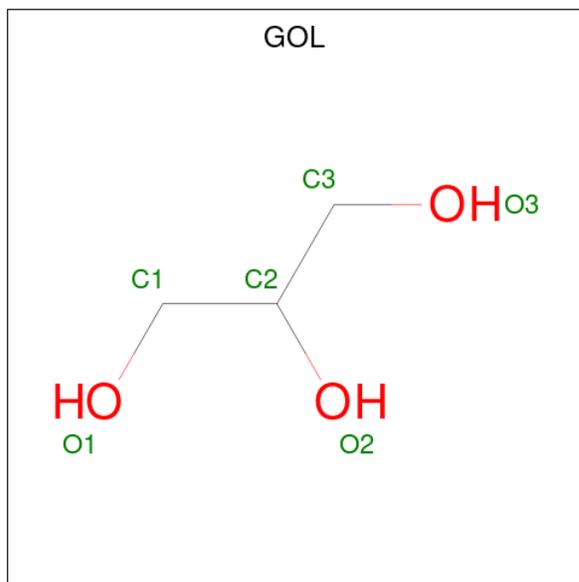
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Mg 1 1	0	0
5	D	1	Total Mg 1 1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0
6	B	1	Total Cl 1 1	0	0
6	C	1	Total Cl 1 1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 8 is water.

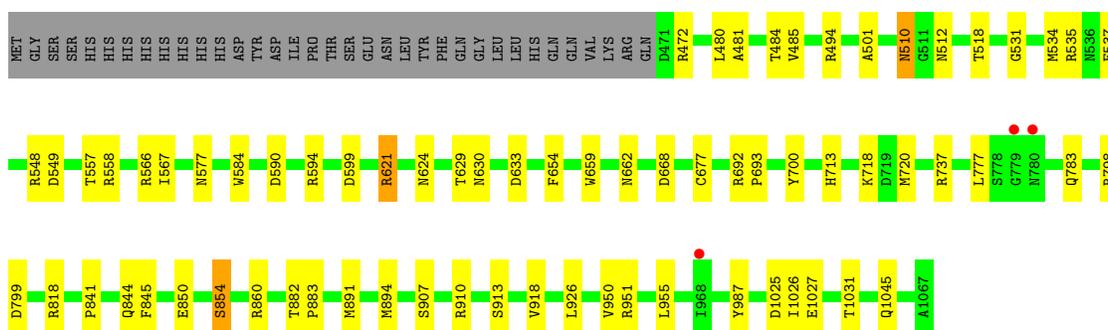
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	62	Total O 62 62	0	0
8	B	35	Total O 35 35	0	0
8	C	40	Total O 40 40	0	0
8	D	32	Total O 32 32	0	0

### 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.

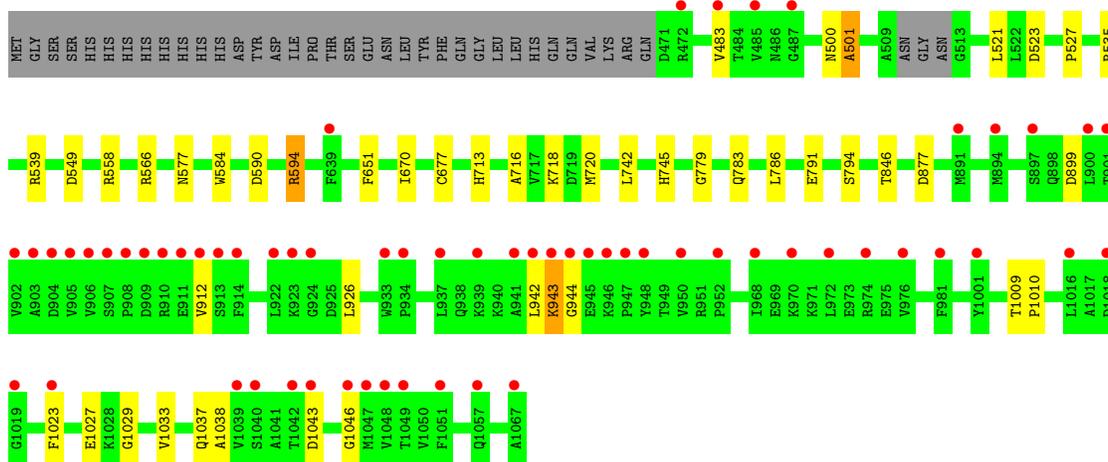
#### • Molecule 1: PYRUVATE CARBOXYLASE

Chain A: 



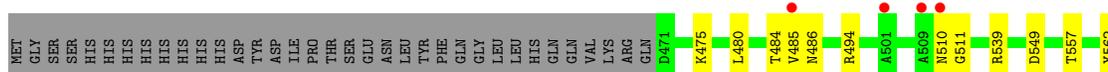
#### • Molecule 1: PYRUVATE CARBOXYLASE

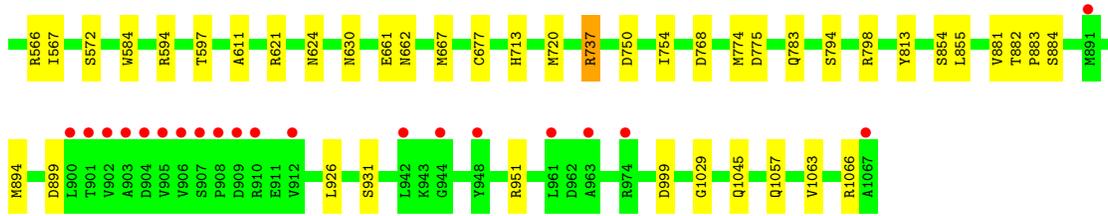
Chain B: 



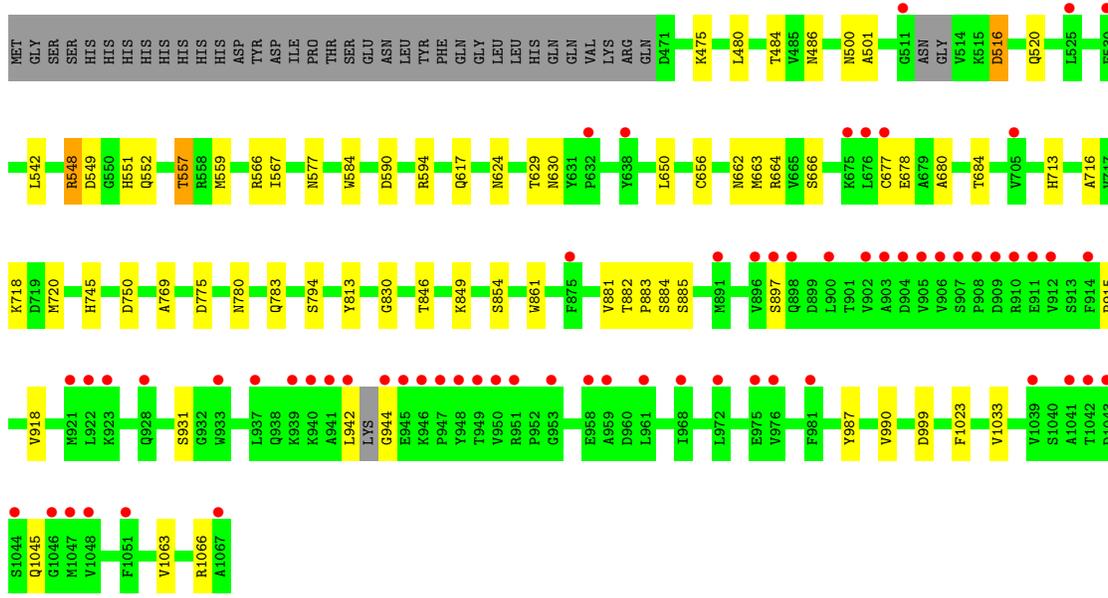
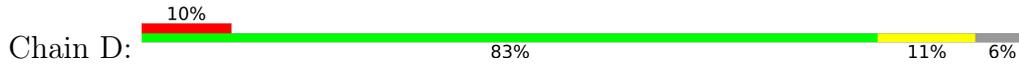
#### • Molecule 1: PYRUVATE CARBOXYLASE

Chain C: 





• Molecule 1: PYRUVATE CARBOXYLASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.25Å 157.85Å 243.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.37 – 2.61 49.32 – 2.61	Depositor EDS
% Data completeness (in resolution range)	95.7 (49.37-2.61) 95.7 (49.32-2.61)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.81 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.177 , 0.225 0.180 , 0.223	Depositor DCC
$R_{free}$ test set	4797 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.5	Xtrriage
Anisotropy	0.140	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 45.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17744	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ZN, MG, BTN, KCX, GOL, 3PY, CL

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	0.89	4/4583 (0.1%)	0.94	9/6245 (0.1%)
1	B	0.71	1/4380 (0.0%)	0.82	6/5991 (0.1%)
1	C	0.74	0/4507	0.88	8/6156 (0.1%)
1	D	0.65	0/4362	0.76	1/5967 (0.0%)
All	All	0.75	5/17832 (0.0%)	0.85	24/24359 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	854	SER	CB-OG	-5.64	1.34	1.42
1	A	700	TYR	CE1-CZ	-5.62	1.31	1.38
1	B	791	GLU	CD-OE2	5.50	1.31	1.25
1	A	845	PHE	CB-CG	-5.46	1.42	1.51
1	A	659	TRP	CZ3-CH2	5.25	1.48	1.40

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	737	ARG	NE-CZ-NH2	12.93	126.77	120.30
1	A	737	ARG	NE-CZ-NH1	-8.58	116.01	120.30
1	C	737	ARG	NE-CZ-NH1	-7.68	116.46	120.30
1	C	594	ARG	NE-CZ-NH2	7.09	123.85	120.30
1	A	737	ARG	NE-CZ-NH2	6.75	123.67	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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	4497	0	4328	35	0
1	B	4295	0	3918	21	0
1	C	4416	0	4162	24	0
1	D	4278	0	3903	29	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	7	0	3	0	0
3	B	7	0	3	0	0
3	C	7	0	3	1	0
3	D	7	0	3	0	0
4	A	9	0	6	0	0
4	B	10	0	7	0	0
4	C	10	0	7	0	0
4	D	9	0	6	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	6	0	8	3	0
7	D	6	0	8	1	0
8	A	62	0	0	0	0
8	B	35	0	0	2	0
8	C	40	0	0	0	0
8	D	32	0	0	0	0
All	All	17744	0	16365	110	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 3.

The worst 5 of 110 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:481:ALA:O	1:A:485:VAL:HG23	1.46	1.15
1:B:500:ASN:OD1	1:B:501:ALA:N	1.94	1.00
1:A:480:LEU:O	1:A:484:THR:OG1	1.79	0.99
1:C:480:LEU:O	1:C:484:THR:OG1	1.91	0.88
1:D:942:LEU:C	1:D:944:GLY:N	2.26	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	595/632 (94%)	573 (96%)	21 (4%)	1 (0%)	47 69
1	B	590/632 (93%)	556 (94%)	29 (5%)	5 (1%)	19 36
1	C	596/632 (94%)	557 (94%)	35 (6%)	4 (1%)	22 41
1	D	588/632 (93%)	558 (95%)	28 (5%)	2 (0%)	41 62
All	All	2369/2528 (94%)	2244 (95%)	113 (5%)	12 (0%)	29 50

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	510	ASN
1	D	501	ALA
1	A	501	ALA
1	B	501	ALA
1	C	511	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	451/519 (87%)	440 (98%)	11 (2%)	49	72
1	B	401/519 (77%)	392 (98%)	9 (2%)	52	74
1	C	430/519 (83%)	417 (97%)	13 (3%)	41	66
1	D	397/519 (76%)	379 (96%)	18 (4%)	27	50
All	All	1679/2076 (81%)	1628 (97%)	51 (3%)	41	66

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	855	LEU
1	D	542	LEU
1	D	931	SER
1	C	899	ASP
1	C	1057	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	873	GLN
1	D	783	GLN
1	C	624	ASN
1	D	624	ASN
1	C	577	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](#)

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	A	718	1,2	9,11,12	1.27	1 (11%)	5,12,14	2.62	2 (40%)
1	KCX	C	718	1,2	9,11,12	0.79	0	5,12,14	0.87	0
1	KCX	D	718	1,2	9,11,12	0.76	0	5,12,14	5.10	3 (60%)
1	KCX	B	718	1,2	9,11,12	1.19	1 (11%)	5,12,14	2.56	2 (40%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	718	KCX	OQ1-CX	3.25	1.27	1.21
1	A	718	KCX	OQ1-CX	-3.03	1.16	1.21

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	718	KCX	OQ1-CX-NZ	-8.09	112.42	124.96
1	D	718	KCX	CE-NZ-CX	6.99	133.11	121.89
1	A	718	KCX	CE-NZ-CX	5.08	130.05	121.89
1	B	718	KCX	OQ1-CX-NZ	5.02	132.74	124.96
1	D	718	KCX	CD-CE-NZ	3.91	123.38	112.21

There are no chirality outliers.

All (5) 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

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Mol	Chain	Res	Type	Atoms
1	C	718	KCX	OQ1-CX-NZ-CE
1	C	718	KCX	OQ2-CX-NZ-CE
1	D	718	KCX	CG-CD-CE-NZ

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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	D	1101	-	5,5,5	0.49	0	5,5,5	1.51	2 (40%)
3	3PY	A	1102	-	5,6,6	3.03	1 (20%)	6,7,7	1.78	2 (33%)
3	3PY	D	1103	-	5,6,6	2.32	1 (20%)	6,7,7	1.90	2 (33%)
4	BTN	B	1103	-	10,11,17	0.53	0	15,16,23	2.00	2 (13%)
3	3PY	C	1102	-	5,6,6	3.18	1 (20%)	6,7,7	2.72	3 (50%)
4	BTN	C	1103	-	10,11,17	0.80	0	15,16,23	1.78	3 (20%)
7	GOL	A	1106	-	5,5,5	0.28	0	5,5,5	1.02	0
3	3PY	B	1102	-	5,6,6	2.38	1 (20%)	6,7,7	2.15	3 (50%)
4	BTN	A	1103	-	10,10,17	0.77	0	11,14,23	1.44	2 (18%)
4	BTN	D	1104	-	10,10,17	0.59	0	11,14,23	2.25	3 (27%)

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	D	1101	-	-	2/4/4/4	-
3	3PY	A	1102	-	-	2/5/6/6	-
3	3PY	D	1103	-	-	3/5/6/6	-
4	BTN	B	1103	-	-	-	0/2/2/2
3	3PY	C	1102	-	-	0/5/6/6	-
4	BTN	C	1103	-	-	-	0/2/2/2
7	GOL	A	1106	-	-	2/4/4/4	-
3	3PY	B	1102	-	-	3/5/6/6	-
4	BTN	A	1103	-	-	-	0/2/2/2
4	BTN	D	1104	-	-	-	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1102	3PY	C2-C1	-6.89	1.44	1.53
3	A	1102	3PY	C2-C1	-6.29	1.45	1.53
3	B	1102	3PY	C2-C1	-4.95	1.46	1.53
3	D	1103	3PY	C2-C1	-4.82	1.47	1.53

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1103	BTN	C2-C4-N2	6.42	118.78	113.11
4	C	1103	BTN	C2-C4-N2	5.37	117.86	113.11
3	C	1102	3PY	O1-C1-C2	-5.37	114.56	121.72
4	D	1104	BTN	C4-C2-S1	-4.58	102.63	106.33
4	D	1104	BTN	C2-C4-C5	4.07	113.34	108.28

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1102	3PY	C1-C2-C3-O4
3	B	1102	3PY	O3-C2-C3-O4
3	D	1103	3PY	O1-C1-C2-O3
3	D	1103	3PY	O1-C1-C2-C3
3	D	1103	3PY	O3-C2-C3-O4

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	1101	GOL	1	0
3	C	1102	3PY	1	0
7	A	1106	GOL	3	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	596/632 (94%)	-0.24	3 (0%) 91   89	34, 56, 84, 138	13 (2%)
1	B	593/632 (93%)	0.37	62 (10%) 6   4	40, 86, 160, 212	5 (0%)
1	C	596/632 (94%)	-0.00	24 (4%) 38   32	45, 70, 120, 158	10 (1%)
1	D	593/632 (93%)	0.34	64 (10%) 5   3	45, 88, 146, 188	8 (1%)
All	All	2378/2528 (94%)	0.12	153 (6%) 19   15	34, 72, 140, 212	36 (1%)

The worst 5 of 153 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	912	VAL	7.3
1	D	944	GLY	6.8
1	D	907	SER	6.0
1	D	941	ALA	5.7
1	D	908	PRO	5.4

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	KCX	B	718	12/13	0.96	0.17	59,60,65,68	0
1	KCX	D	718	12/13	0.96	0.19	68,72,87,90	0
1	KCX	C	718	12/13	0.97	0.22	48,51,61,62	0
1	KCX	A	718	12/13	0.99	0.18	40,42,44,46	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	MG	D	1105	1/1	0.78	0.21	66,66,66,66	0
5	MG	C	1104	1/1	0.84	0.07	61,61,61,61	0
6	CL	C	1105	1/1	0.87	0.18	80,80,80,80	0
4	BTN	B	1103	10/16	0.89	0.29	82,94,104,106	0
4	BTN	D	1104	9/16	0.91	0.22	76,81,86,89	0
5	MG	B	1104	1/1	0.92	0.18	60,60,60,60	0
7	GOL	D	1101	6/6	0.92	0.28	53,62,68,68	0
5	MG	A	1104	1/1	0.93	0.05	58,58,58,58	0
3	3PY	B	1102	7/7	0.94	0.14	64,70,72,78	0
6	CL	B	1105	1/1	0.94	0.06	89,89,89,89	0
7	GOL	A	1106	6/6	0.95	0.31	58,63,67,72	0
4	BTN	A	1103	9/16	0.96	0.16	58,70,73,77	0
2	ZN	D	1102	1/1	0.96	0.17	69,69,69,69	0
4	BTN	C	1103	10/16	0.96	0.15	67,77,81,87	0
3	3PY	D	1103	7/7	0.97	0.17	74,82,88,92	0
3	3PY	A	1102	7/7	0.97	0.21	44,48,52,62	0
3	3PY	C	1102	7/7	0.97	0.20	53,59,60,68	0
6	CL	A	1105	1/1	0.97	0.16	61,61,61,61	0
2	ZN	A	1101	1/1	0.99	0.17	44,44,44,44	0
2	ZN	B	1101	1/1	1.00	0.13	61,61,61,61	0
2	ZN	C	1101	1/1	1.00	0.17	54,54,54,54	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.