wwPDB X-ray Structure Validation Summary Report (i)

Nov 6, 2023 – 02:48 PM EST

PDB ID	:	4JX5
Title	:	Structure of the carboxyl transferase domain from Rhizobium etli pyruvate carboxylase with pyruvate
Authors	:	Lietzan, A.D.; St Maurice, M.
Deposited on	:	2013-03-27
Resolution	:	2.55 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 (i) 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 (1)) were used in the production of this report:

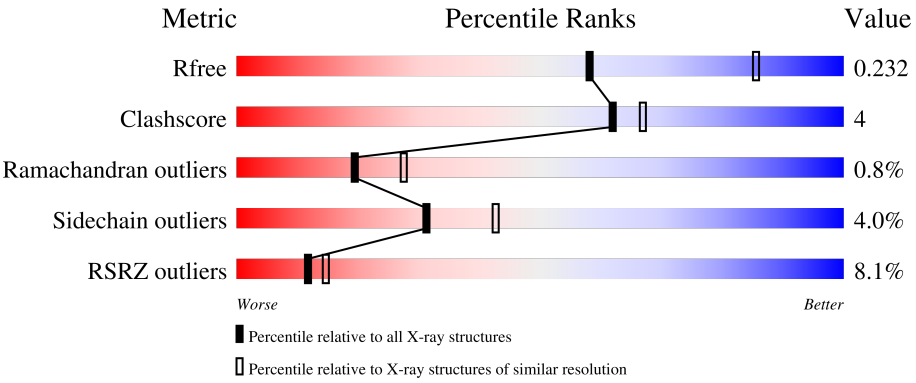
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 <=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	2% 82% 11% • 6%
1	B	632	7% 85% 9% 6%
1	C	632	13% 81% 12% • 6%
1	D	632	8% 81% 11% • 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	C	1102	-	-	X	-
6	GOL	B	1101	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 17941 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	597	Total	C	N	O	S	0	2	0
			4539	2889	758	869	23			
1	B	596	Total	C	N	O	S	0	1	0
			4468	2840	747	858	23			
1	C	591	Total	C	N	O	S	0	0	0
			4357	2758	739	838	22			
1	D	590	Total	C	N	O	S	0	0	0
			4322	2733	733	834	22			

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

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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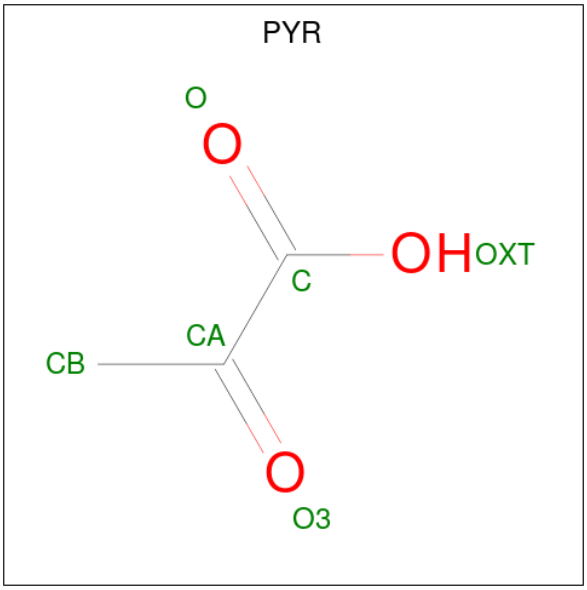
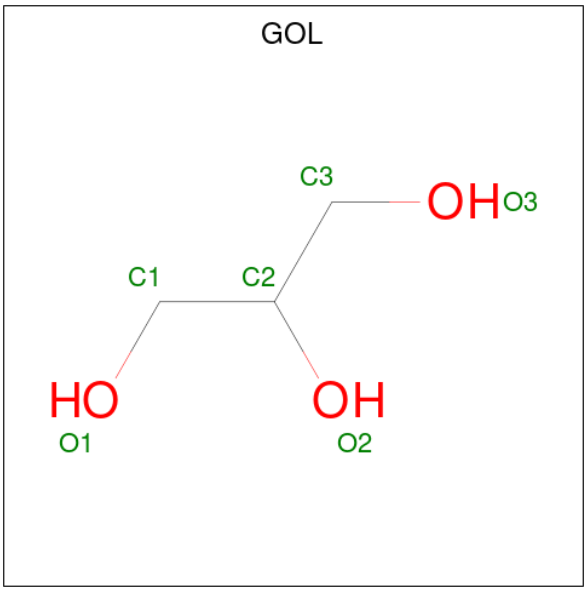
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0

- Molecule 5 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is water.

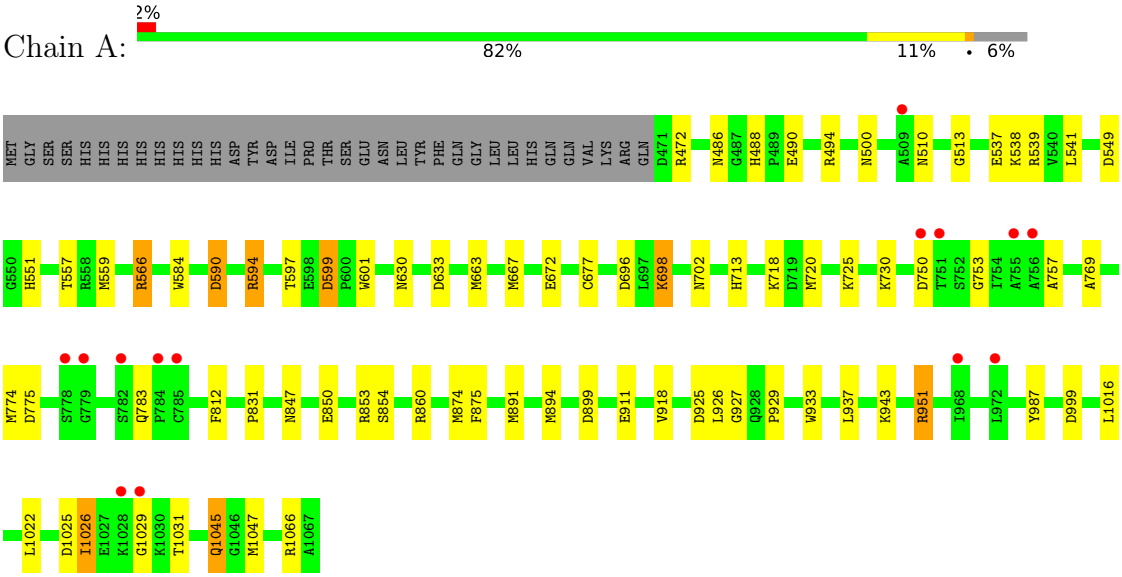
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	86	Total O 86 86	0	0
7	B	46	Total O 46 46	0	0
7	C	42	Total O 42 42	0	0
7	D	33	Total O 33 33	0	0

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.

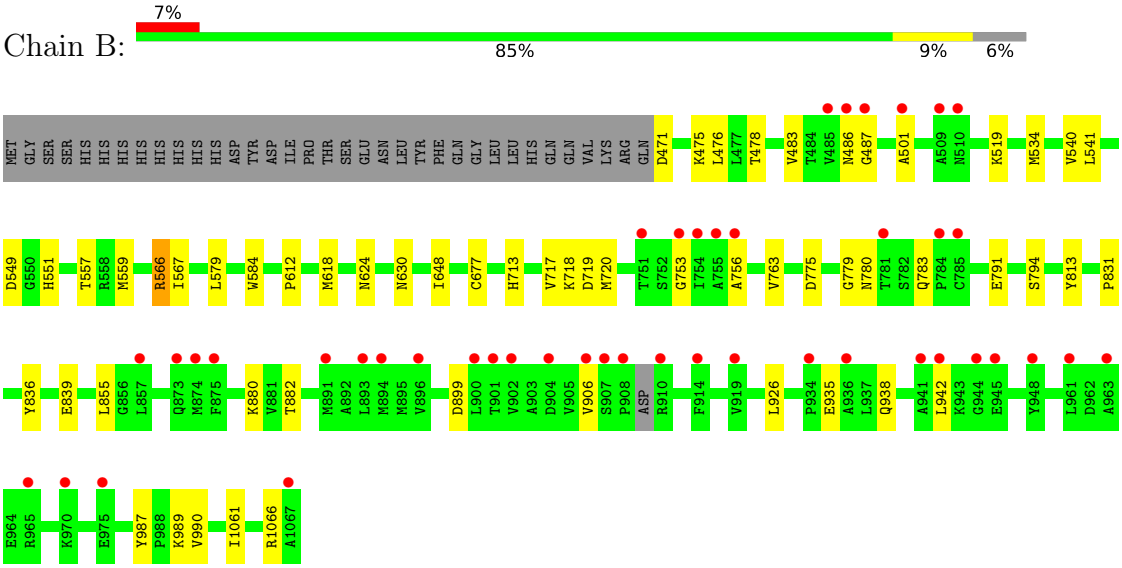
• Molecule 1: Pyruvate carboxylase

Chain A:



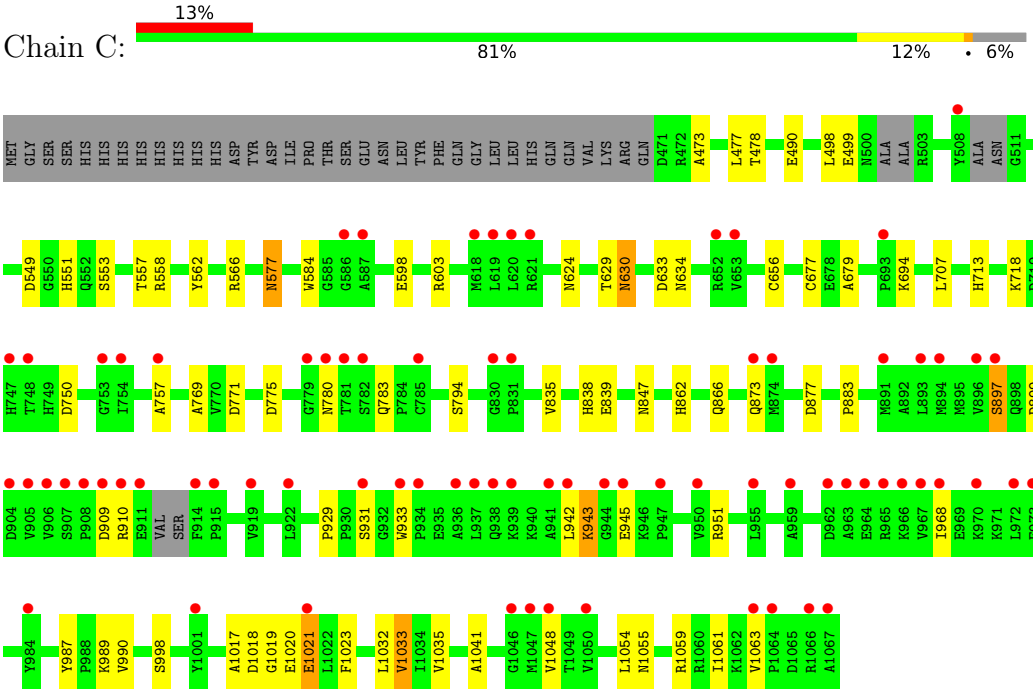
• Molecule 1: Pyruvate carboxylase

Chain B:



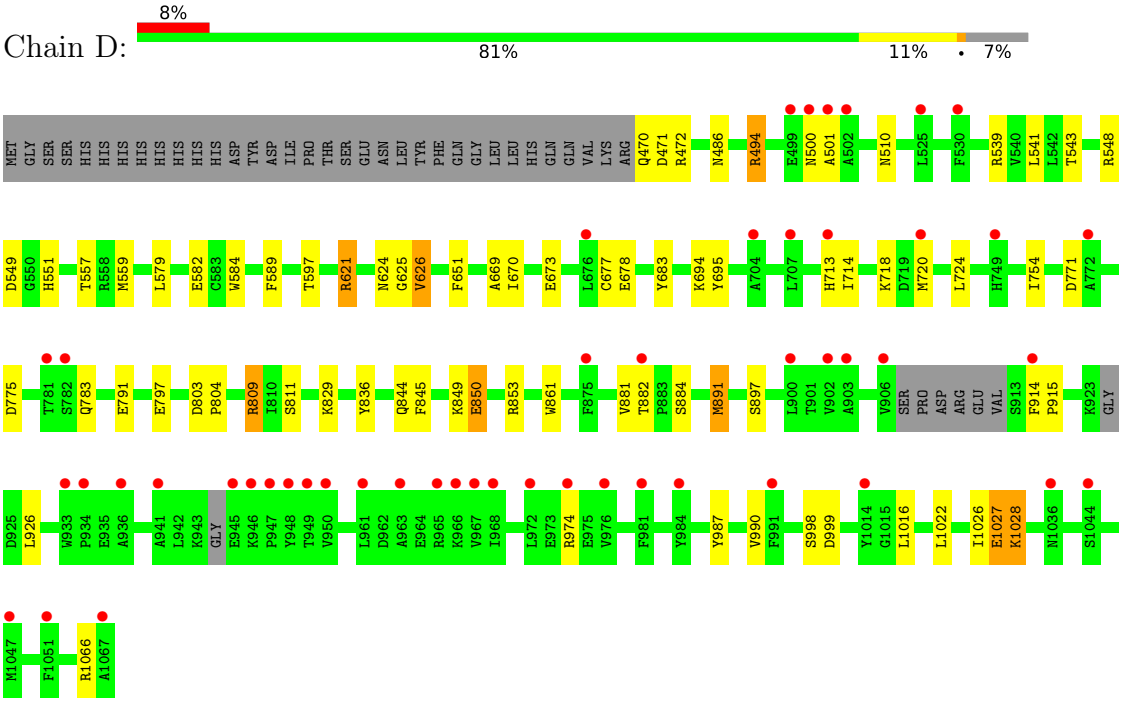
• Molecule 1: Pyruvate carboxylase

Chain C:



• Molecule 1: Pyruvate carboxylase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	85.13Å 157.25Å 245.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.88 – 2.55 46.84 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.88-2.55) 99.5 (46.84-2.55)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.38 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.187 , 0.232 0.188 , 0.232	Depositor DCC
R_{free} test set	5384 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	55.9	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17941	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PYR, MG, CL, KCX, GOL

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	0.70	0/4630	0.81	5/6301 (0.1%)
1	B	0.58	0/4554	0.73	1/6210 (0.0%)
1	C	0.67	4/4438 (0.1%)	0.75	3/6056 (0.0%)
1	D	0.50	0/4402	0.66	0/6013
All	All	0.62	4/18024 (0.0%)	0.74	9/24580 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1063	VAL	C-O	10.64	1.43	1.23
1	C	910	ARG	CZ-NH1	7.20	1.42	1.33
1	C	1059	ARG	CZ-NH1	6.77	1.41	1.33
1	C	1048	VAL	C-O	6.47	1.35	1.23

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	750	ASP	CB-CG-OD1	7.65	125.18	118.30
1	C	910	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	A	599	ASP	CB-CG-OD1	6.18	123.86	118.30
1	C	910	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	B	719	ASP	CB-CG-OD1	5.59	123.33	118.30

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	4539	0	4406	36	0
1	B	4468	0	4278	32	0
1	C	4357	0	4067	44	0
1	D	4322	0	3993	46	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	2	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	6	0	0	0	0
5	B	6	0	0	0	0
5	C	6	0	0	0	0
5	D	6	0	0	1	0
6	B	6	0	8	5	0
6	C	6	0	8	0	0
7	A	86	0	0	4	0
7	B	46	0	0	0	0
7	C	42	0	0	1	0
7	D	33	0	0	1	0
All	All	17941	0	16760	153	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 153 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:D:809:ARG:HG2	1:D:809:ARG:HH11	1.17	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:470:GLN:HG3	1:D:472:ARG:HB2	1.43	1.01
1:C:677:CYS:H	1:C:713:HIS:HD2	1.10	0.99
1:B:566:ARG:HH11	1:B:566:ARG:HG3	1.27	0.99
1:D:677:CYS:H	1:D:713:HIS:HD2	1.00	0.97

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	596/632 (94%)	577 (97%)	16 (3%)	3 (0%)	29	40
1	B	592/632 (94%)	563 (95%)	26 (4%)	3 (0%)	29	40
1	C	582/632 (92%)	541 (93%)	33 (6%)	8 (1%)	11	15
1	D	581/632 (92%)	540 (93%)	36 (6%)	5 (1%)	17	24
All	All	2351/2528 (93%)	2221 (94%)	111 (5%)	19 (1%)	19	27

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1041	ALA
1	D	500	ASN
1	D	510	ASN
1	D	1028	LYS
1	A	1029	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	462/519 (89%)	441 (96%)	21 (4%)	27	37
1	B	447/519 (86%)	433 (97%)	14 (3%)	40	54
1	C	422/519 (81%)	406 (96%)	16 (4%)	33	45
1	D	412/519 (79%)	393 (95%)	19 (5%)	27	36
All	All	1743/2076 (84%)	1673 (96%)	70 (4%)	31	43

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	720	MET
1	D	809	ARG
1	D	926	LEU
1	B	566	ARG
1	B	557	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	702	ASN
1	D	470	GLN
1	C	783	GLN
1	D	486	ASN
1	B	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	B	718	2,1	9,11,12	0.40	0	5,12,14	3.82	2 (40%)
1	KCX	D	718	2,1	9,11,12	0.51	0	5,12,14	3.26	2 (40%)
1	KCX	C	718	2,1	9,11,12	0.75	0	5,12,14	1.48	1 (20%)
1	KCX	A	718	2,1	9,11,12	1.05	0	5,12,14	2.50	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	B	718	2,1	-	6/9/10/12	-
1	KCX	D	718	2,1	-	4/9/10/12	-
1	KCX	C	718	2,1	-	0/9/10/12	-
1	KCX	A	718	2,1	-	1/9/10/12	-

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	718	KCX	CE-NZ-CX	8.00	134.72	121.89
1	D	718	KCX	CE-NZ-CX	6.06	131.61	121.89
1	A	718	KCX	CE-NZ-CX	4.27	128.73	121.89
1	D	718	KCX	OQ1-CX-NZ	-3.55	119.45	124.96
1	A	718	KCX	OQ1-CX-NZ	3.32	130.10	124.96

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	718	KCX	O-C-CA-CB
1	B	718	KCX	N-CA-CB-CG
1	B	718	KCX	C-CA-CB-CG
1	B	718	KCX	O-C-CA-CB
1	B	718	KCX	CD-CE-NZ-CX

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 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
5	PYR	C	1105	-	5,5,5	1.42	1 (20%)	3,6,6	1.29	0
5	PYR	D	1104	-	5,5,5	1.36	0	3,6,6	1.29	0
6	GOL	C	1101	-	5,5,5	0.42	0	5,5,5	1.55	1 (20%)
5	PYR	B	1105	-	5,5,5	1.35	1 (20%)	3,6,6	1.88	1 (33%)
5	PYR	A	1104	-	5,5,5	1.17	0	3,6,6	1.95	2 (66%)
6	GOL	B	1101	-	5,5,5	0.25	0	5,5,5	1.22	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
5	PYR	C	1105	-	-	0/4/4/4	-
5	PYR	D	1104	-	-	2/4/4/4	-
6	GOL	C	1101	-	-	2/4/4/4	-
5	PYR	B	1105	-	-	2/4/4/4	-
5	PYR	A	1104	-	-	3/4/4/4	-
6	GOL	B	1101	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1105	PYR	CA-C	-2.51	1.45	1.54
5	C	1105	PYR	CA-C	-2.26	1.46	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1105	PYR	OXT-C-CA	3.17	122.64	113.97
5	A	1104	PYR	OXT-C-CA	2.44	120.65	113.97
5	A	1104	PYR	OXT-C-O	-2.23	118.52	123.61
6	C	1101	GOL	O1-C1-C2	-2.01	100.54	110.20

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1105	PYR	OXT-C-CA-CB
5	D	1104	PYR	OXT-C-CA-CB
6	C	1101	GOL	O1-C1-C2-C3
5	B	1105	PYR	O-C-CA-CB
5	D	1104	PYR	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1104	PYR	1	0
6	B	1101	GOL	5	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

6.1 Protein, DNA and RNA chains

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^{th} 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	596/632 (94%)	0.01	14 (2%) 60 67	31, 48, 72, 130	19 (3%)
1	B	595/632 (94%)	0.25	45 (7%) 13 17	42, 63, 108, 149	17 (2%)
1	C	590/632 (93%)	0.73	84 (14%) 2 3	34, 81, 162, 211	14 (2%)
1	D	589/632 (93%)	0.43	50 (8%) 10 12	49, 81, 123, 140	14 (2%)
All	All	2370/2528 (93%)	0.35	193 (8%) 12 15	31, 65, 130, 211	64 (2%)

The worst 5 of 193 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	968	ILE	7.0
1	C	963	ALA	6.2
1	D	501	ALA	6.1
1	B	891[A]	MET	5.4
1	C	914	PHE	5.4

6.2 Non-standard residues in protein, DNA, RNA chains

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^{th} 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	D	718	12/13	0.95	0.28	62,66,73,74	0
1	KCX	C	718	12/13	0.97	0.28	54,59,66,70	0
1	KCX	A	718	12/13	0.98	0.22	37,40,46,47	0
1	KCX	B	718	12/13	0.98	0.23	55,57,60,61	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^{th} 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
4	MG	D	1102	1/1	0.80	0.26	57,57,57,57	0
4	MG	B	1103	1/1	0.84	0.06	52,52,52,52	0
5	PYR	D	1104	6/6	0.88	0.44	46,51,60,60	3
3	CL	B	1102	1/1	0.90	0.09	66,66,66,66	0
4	MG	C	1103	1/1	0.92	0.16	41,41,41,41	0
3	CL	D	1101	1/1	0.95	0.11	79,79,79,79	0
5	PYR	C	1105	6/6	0.96	0.78	30,32,35,38	6
6	GOL	B	1101	6/6	0.96	0.24	49,56,59,64	0
6	GOL	C	1101	6/6	0.97	0.35	45,47,51,51	0
3	CL	C	1102	1/1	0.98	0.10	76,76,76,76	0
5	PYR	B	1105	6/6	0.98	0.39	34,41,44,48	3
2	ZN	D	1103	1/1	0.98	0.17	60,60,60,60	0
5	PYR	A	1104	6/6	0.99	0.22	44,51,52,54	0
2	ZN	A	1101	1/1	0.99	0.13	43,43,43,43	0
4	MG	A	1103	1/1	0.99	0.17	45,45,45,45	0
3	CL	A	1102	1/1	0.99	0.09	53,53,53,53	0
2	ZN	B	1104	1/1	0.99	0.14	51,51,51,51	0
2	ZN	C	1104	1/1	0.99	0.15	54,54,54,54	0

6.5 Other polymers (i)

There are no such residues in this entry.