wwPDB X-ray Structure Validation Summary Report (i)

May 23, 2020 – 02:43 am BST

PDB ID	:	4MIM
Title	:	Structure of the carboxyl transferase domain from Rhizobium etli pyruvate carboxylase with 3-bromopyruvate
Authors	:	Lietzan, A.D.; St.Maurice, M.
Deposited on	:	2013-09-01
Resolution	:	2.65 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 following versions of software and data (see references (1)) were used in the production of this report:

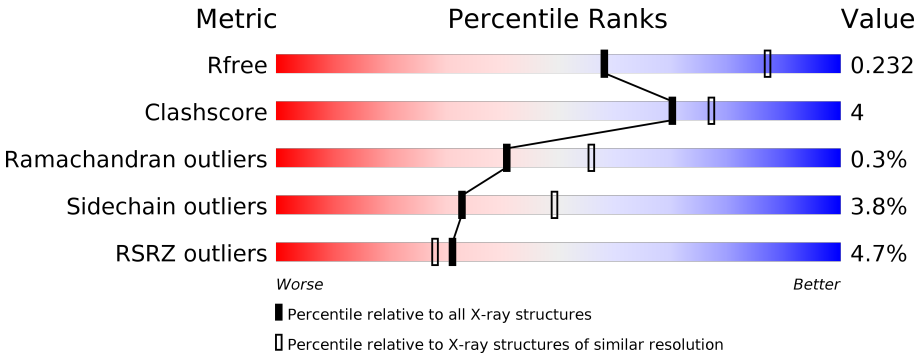
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 on 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% 83% 11% 6%
1	B	632	9% 84% 9% • 6%
1	C	632	2% 86% 9% 6%
1	D	632	6% 84% 9% • 6%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CL	B	1104	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17720 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	1	0
			4515	2868	755	869	23			
1	B	593	Total	C	N	O	S	0	1	0
			4297	2715	727	832	23			
1	C	597	Total	C	N	O	S	0	1	0
			4428	2815	744	846	23			
1	D	592	Total	C	N	O	S	0	1	0
			4288	2716	721	828	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

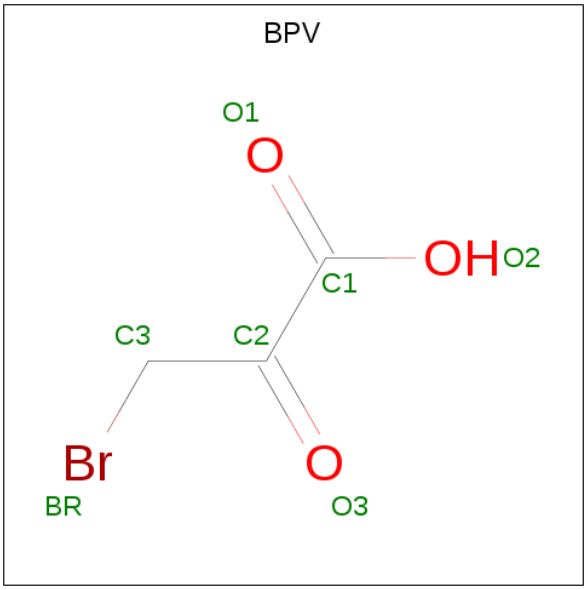
Continued from previous page...

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	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is Bromopyruvate (three-letter code: BPV) (formula: $C_3H_3BrO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Br C O 14 2 6 6	0	1
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

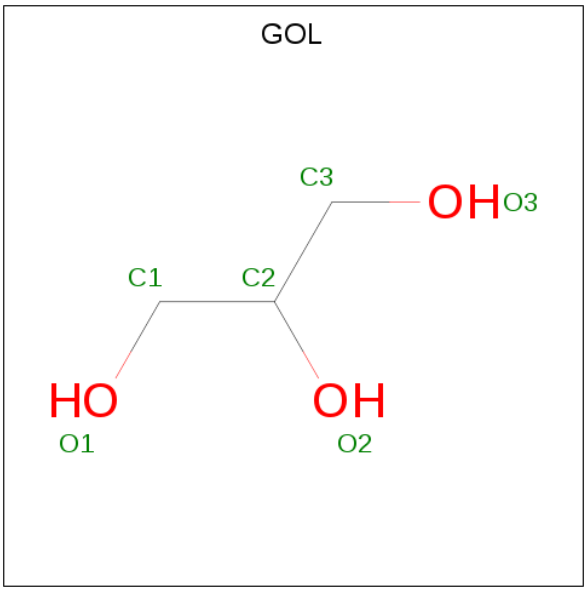
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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

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

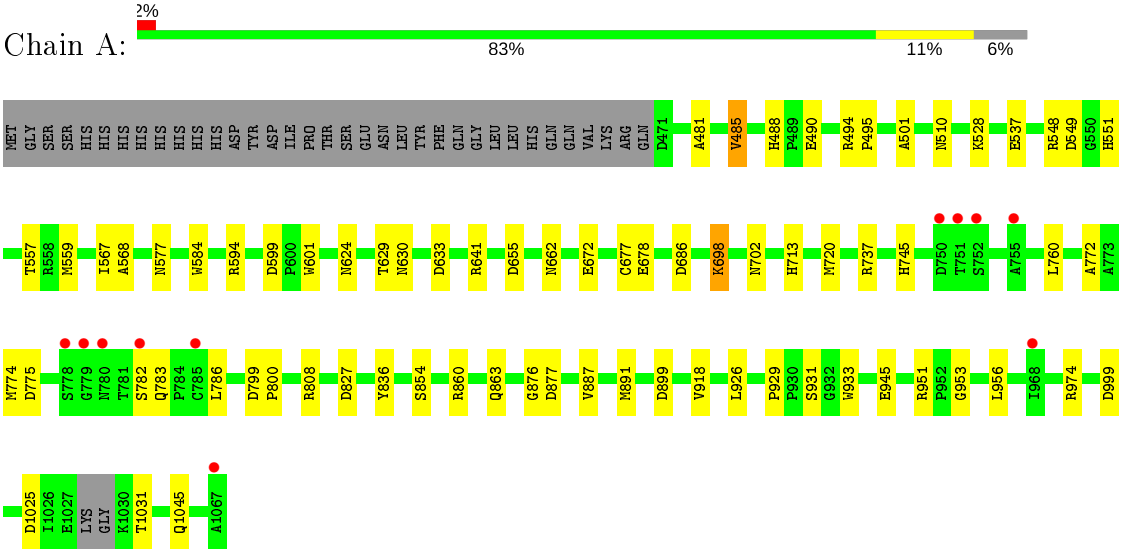
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	54	Total O 54 54	0	0
7	B	29	Total O 29 29	0	0
7	C	33	Total O 33 33	0	0
7	D	20	Total O 20 20	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

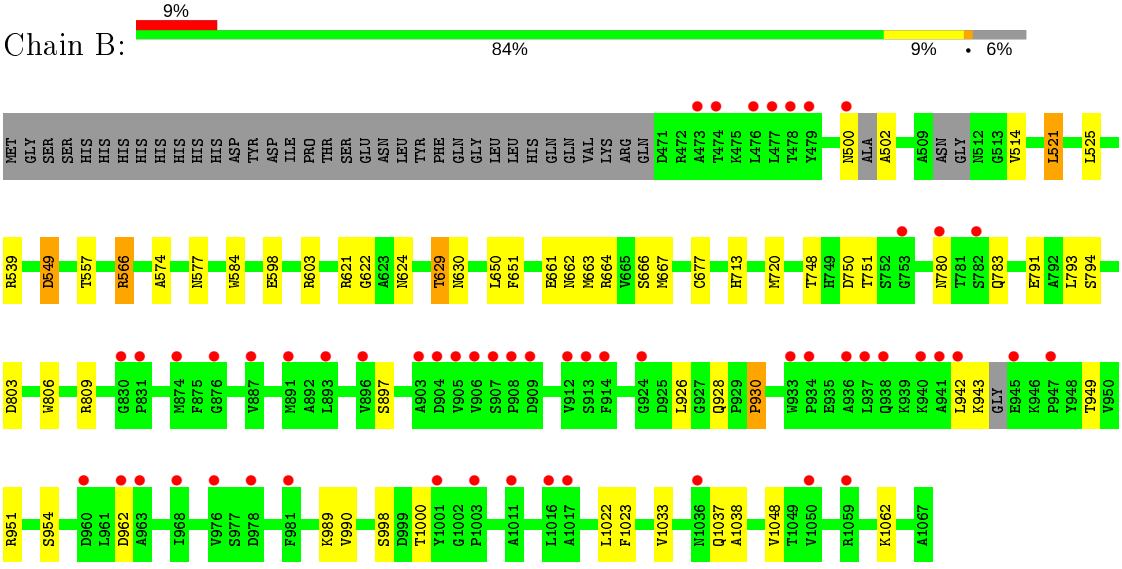
- Molecule 1: PYRUVATE CARBOXYLASE

Chain A:



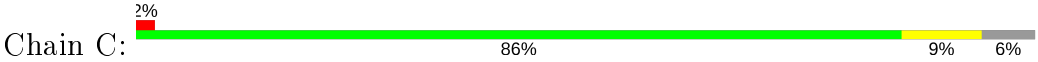
- Molecule 1: PYRUVATE CARBOXYLASE

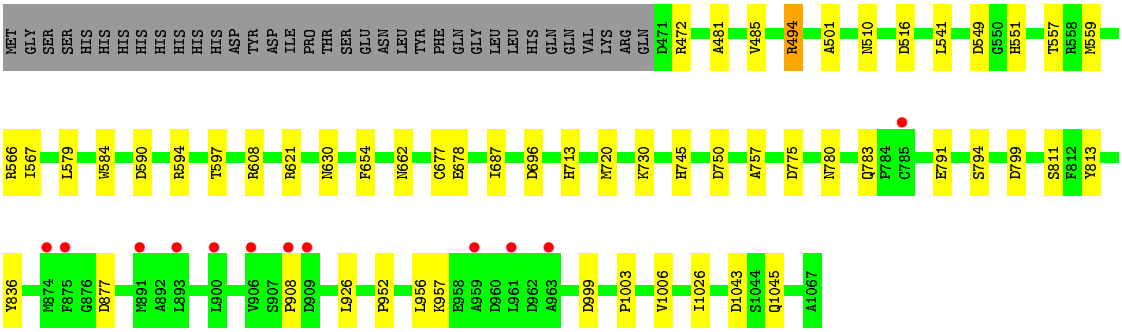
Chain B:



- Molecule 1: PYRUVATE CARBOXYLASE

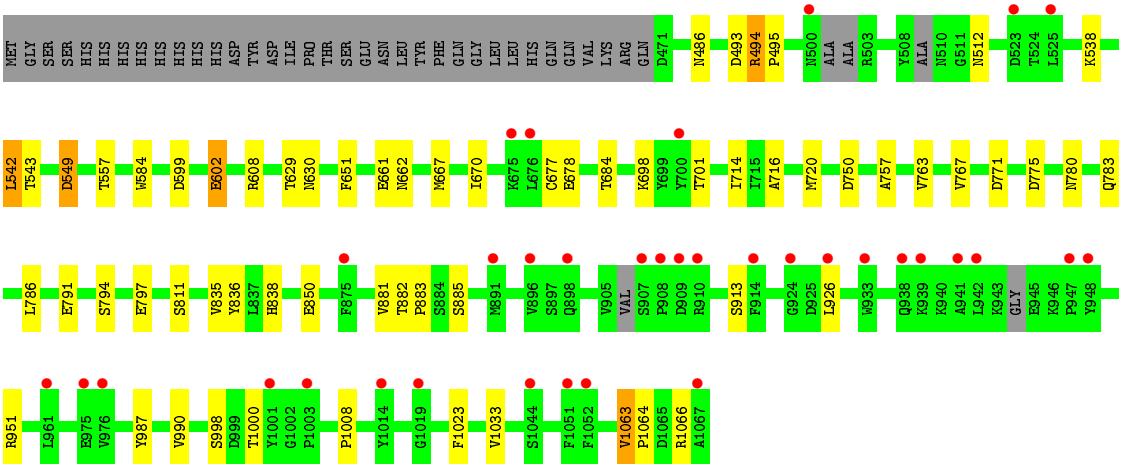
Chain C:





- 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	85.59Å 157.06Å 243.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.13 – 2.65 48.08 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.13-2.65) 99.3 (48.08-2.65)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.75 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.186 , 0.235 0.190 , 0.232	Depositor DCC
R_{free} test set	4756 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	64.3	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 42.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17720	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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: GOL, ZN, CL, MG, BPV, KCX

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	0.82	0/4600	0.90	9/6261 (0.1%)
1	B	0.69	0/4380	0.81	4/5985 (0.1%)
1	C	0.67	0/4515	0.81	3/6162 (0.0%)
1	D	0.60	0/4371	0.73	1/5973 (0.0%)
All	All	0.70	0/17866	0.81	17/24381 (0.1%)

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	539	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	B	549	ASP	CB-CG-OD1	6.88	124.49	118.30
1	C	516	ASP	CB-CG-OD1	6.43	124.09	118.30
1	A	974	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	B	577	ASN	CB-CA-C	-5.55	99.29	110.40

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	4515	0	4362	30	0
1	B	4297	0	3912	34	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4428	0	4203	29	0
1	D	4288	0	3900	34	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	14	0	0	2	0
3	B	6	0	0	0	0
3	C	6	0	0	0	0
3	D	6	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	2	0
4	C	1	0	0	0	0
4	D	1	0	0	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	B	6	0	8	1	0
6	C	6	0	8	3	0
7	A	54	0	0	0	0
7	B	29	0	0	0	0
7	C	33	0	0	0	0
7	D	20	0	0	0	0
All	All	17720	0	16393	123	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 123 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:677:CYS:H	1:B:713:HIS:HD2	1.17	0.92
1:C:481:ALA:O	1:C:485:VAL:HG13	1.81	0.81
1:A:677:CYS:H	1:A:713:HIS:HD2	1.30	0.77
1:A:481:ALA:O	1:A:485:VAL:HG13	1.87	0.74
1:A:481:ALA:O	1:A:485:VAL:CG1	2.37	0.72

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	591/632 (94%)	578 (98%)	12 (2%)	1 (0%)	47	64
1	B	585/632 (93%)	555 (95%)	29 (5%)	1 (0%)	47	64
1	C	595/632 (94%)	570 (96%)	22 (4%)	3 (0%)	29	43
1	D	582/632 (92%)	552 (95%)	29 (5%)	1 (0%)	47	64
All	All	2353/2528 (93%)	2255 (96%)	92 (4%)	6 (0%)	41	56

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	501	ALA
1	D	512	ASN
1	A	501	ALA
1	B	930	PRO
1	C	877	ASP

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	457/519 (88%)	437 (96%)	20 (4%)	28	43
1	B	400/519 (77%)	384 (96%)	16 (4%)	31	47
1	C	435/519 (84%)	425 (98%)	10 (2%)	50	68
1	D	399/519 (77%)	381 (96%)	18 (4%)	27	42
All	All	1691/2076 (82%)	1627 (96%)	64 (4%)	33	49

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	794	SER
1	B	1022	LEU
1	D	926	LEU
1	B	897	SER
1	B	962	ASP

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

Mol	Chain	Res	Type
1	B	783	GLN
1	C	577	ASN
1	D	713	HIS
1	C	486	ASN
1	C	624	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	1,2	7,11,12	0.49	0	4,12,14	1.33	0
1	KCX	A	718	1,2	7,11,12	0.58	0	4,12,14	0.78	0
1	KCX	D	718	1,2	7,11,12	0.56	0	4,12,14	0.78	0
1	KCX	C	718	1,2	7,11,12	0.80	0	4,12,14	0.80	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
1	KCX	B	718	1,2	-	2/7/10/12	-
1	KCX	A	718	1,2	-	1/7/10/12	-
1	KCX	D	718	1,2	-	1/7/10/12	-
1	KCX	C	718	1,2	-	1/7/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	718	KCX	O-C-CA-CB
1	A	718	KCX	O-C-CA-CB
1	D	718	KCX	O-C-CA-CB
1	C	718	KCX	O-C-CA-CB
1	B	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 12 are monoatomic - leaving 7 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	BPV	C	1102	-	2,5,6	0.64	0	2,6,7	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BPV	D	1102	-	2,5,6	0.62	0	2,6,7	1.64	1 (50%)
3	BPV	A	1102[B]	-	3,6,6	3.64	2 (66%)	2,7,7	3.26	1 (50%)
3	BPV	A	1102[A]	-	3,6,6	1.60	1 (33%)	2,7,7	3.78	2 (100%)
6	GOL	B	1101	-	5,5,5	0.49	0	5,5,5	1.07	0
3	BPV	B	1103	-	2,5,6	0.69	0	2,6,7	0.14	0
6	GOL	C	1105	-	5,5,5	0.33	0	5,5,5	0.76	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
3	BPV	C	1102	-	-	0/0/4/6	-
3	BPV	D	1102	-	-	0/0/4/6	-
3	BPV	A	1102[B]	-	-	0/2/6/6	-
3	BPV	A	1102[A]	-	-	0/2/6/6	-
6	GOL	B	1101	-	-	2/4/4/4	-
3	BPV	B	1103	-	-	0/0/4/6	-
6	GOL	C	1105	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1102[B]	BPV	BR-C3	4.63	2.10	1.94
3	A	1102[B]	BPV	C3-C2	3.95	1.58	1.51
3	A	1102[A]	BPV	BR-C3	2.57	2.03	1.94

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1102[A]	BPV	BR-C3-C2	4.86	125.19	112.53
3	A	1102[B]	BPV	BR-C3-C2	4.34	123.85	112.53
3	D	1102	BPV	O3-C2-C3	-2.31	114.96	120.17
3	A	1102[A]	BPV	O3-C2-C3	2.25	125.50	121.13

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1101	GOL	C1-C2-C3-O3
6	C	1105	GOL	O1-C1-C2-C3
6	B	1101	GOL	O2-C2-C3-O3
6	C	1105	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1102[A]	BPV	2	0
6	B	1101	GOL	1	0
6	C	1105	GOL	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	594/632 (93%)	-0.20	11 (1%) 66 63	37, 53, 79, 120	13 (2%)
1	B	592/632 (93%)	0.34	54 (9%) 9 7	38, 86, 159, 198	6 (1%)
1	C	596/632 (94%)	-0.02	12 (2%) 65 60	48, 69, 111, 145	8 (1%)
1	D	591/632 (93%)	0.20	35 (5%) 22 19	51, 89, 132, 163	8 (1%)
All	All	2373/2528 (93%)	0.08	112 (4%) 31 28	37, 71, 135, 198	35 (1%)

The worst 5 of 112 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	914	PHE	6.7
1	D	961	LEU	5.0
1	D	907	SER	5.0
1	D	941	ALA	5.0
1	B	912	VAL	5.0

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	B	718	12/13	0.97	0.17	57,60,65,68	0
1	KCX	D	718	12/13	0.97	0.20	66,68,71,73	0
1	KCX	C	718	12/13	0.98	0.20	50,55,58,59	0
1	KCX	A	718	12/13	0.99	0.19	39,42,44,47	0

6.3 Carbohydrates (i)

There are no carbohydrates 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
5	MG	D	1104	1/1	0.78	0.10	69,69,69,69	0
5	MG	C	1104	1/1	0.84	0.09	66,66,66,66	0
4	CL	C	1103	1/1	0.88	0.11	74,74,74,74	0
3	BPV	A	1102[B]	7/7	0.93	0.24	48,53,67,108	7
3	BPV	D	1102	6/7	0.93	0.22	72,73,77,81	0
3	BPV	A	1102[A]	7/7	0.93	0.24	33,34,35,38	7
6	GOL	B	1101	6/6	0.93	0.42	52,55,57,60	0
4	CL	B	1104	1/1	0.93	0.13	87,87,87,87	0
3	BPV	B	1103	6/7	0.94	0.23	52,67,75,75	0
3	BPV	C	1102	6/7	0.94	0.27	55,63,66,67	0
4	CL	D	1103	1/1	0.94	0.18	80,80,80,80	0
6	GOL	C	1105	6/6	0.96	0.25	55,61,63,65	0
4	CL	A	1103	1/1	0.97	0.13	55,55,55,55	0
2	ZN	B	1102	1/1	0.97	0.21	64,64,64,64	0
5	MG	A	1104	1/1	0.98	0.12	59,59,59,59	0
2	ZN	C	1101	1/1	0.98	0.24	61,61,61,61	0
5	MG	B	1105	1/1	0.98	0.05	52,52,52,52	0
2	ZN	D	1101	1/1	0.99	0.20	68,68,68,68	0
2	ZN	A	1101	1/1	0.99	0.19	47,47,47,47	0

6.5 Other polymers (i)

There are no such residues in this entry.