



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 08:50 AM UTC

PDB ID : 4QSL / pdb_00004qsl
Title : Crystal Structure of Listeria Monocytogenes Pyruvate Carboxylase
Authors : Choi, P.H.; Tong, L.
Deposited on : 2014-07-04
Resolution : 3.28 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
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

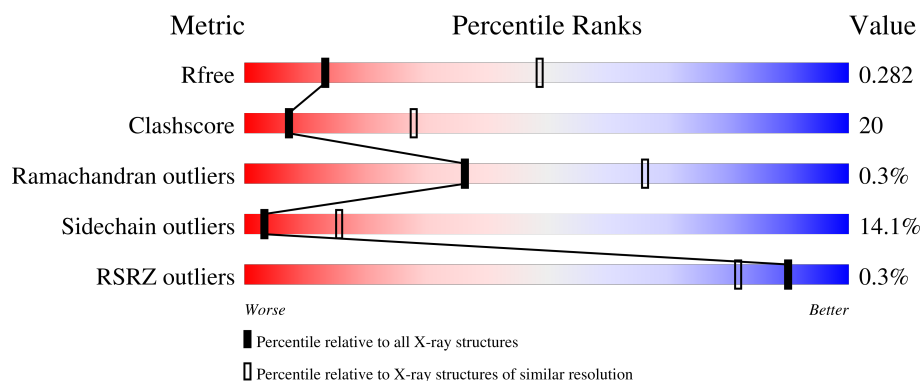
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.28 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	1303 (3.30-3.26)
Clashscore	190562	1354 (3.30-3.26)
Ramachandran outliers	187476	1334 (3.30-3.26)
Sidechain outliers	187428	1333 (3.30-3.26)
RSRZ outliers	180081	1303 (3.30-3.26)

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	1146	
1	B	1146	
1	C	1146	
1	D	1146	
1	E	1146	

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Mol	Chain	Length	Quality of chain
1	F	1146	 57% 29% 5% 8%
1	G	1146	 52% 26% 5% 18%
1	H	1146	 56% 29% 5% 10%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 60495 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.

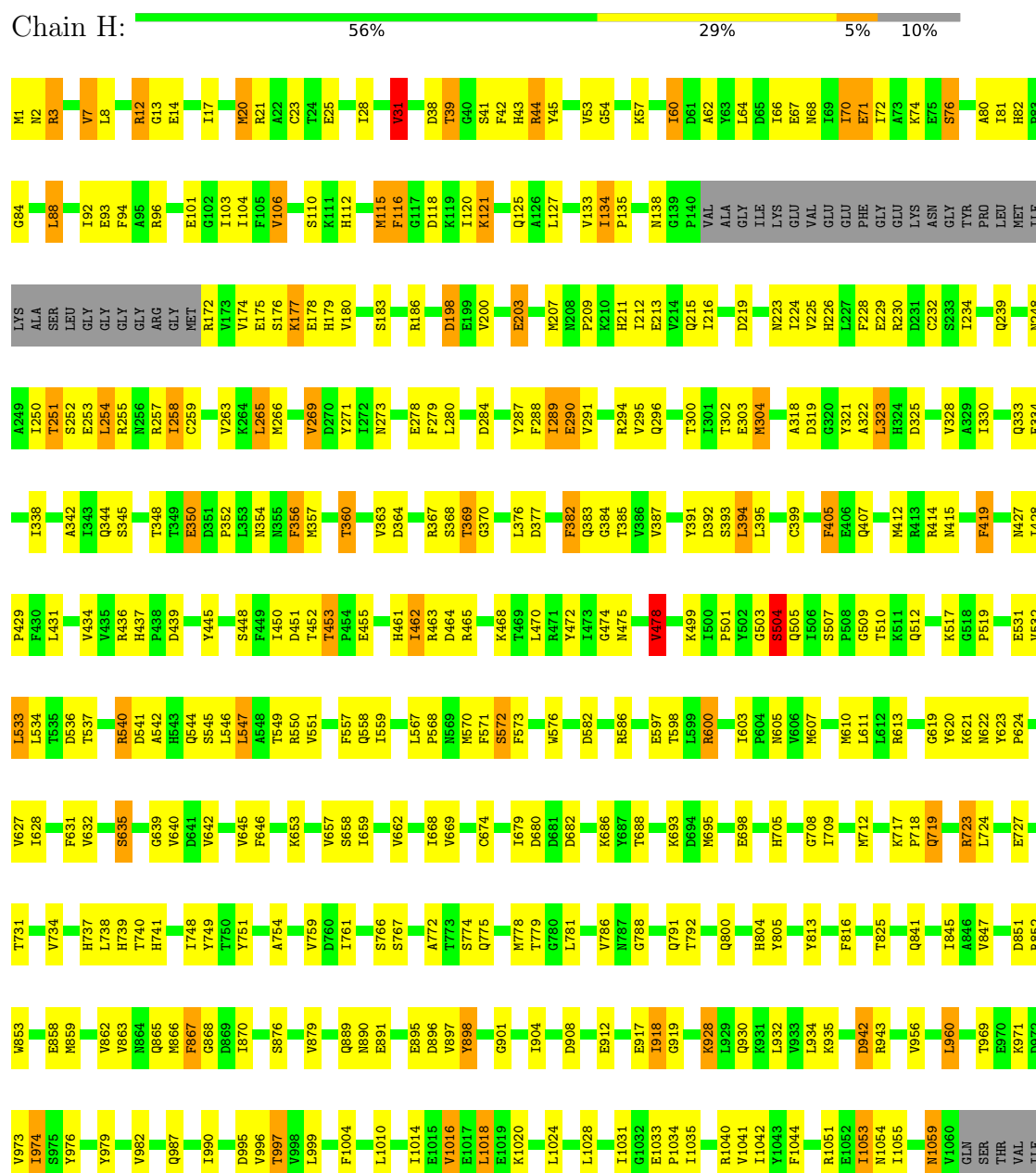
- Molecule 1 is a protein called Pyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	1029	Total	C	N	O	S	0	0	0
			7881	4992	1351	1504	34			
1	F	1052	Total	C	N	O	S	0	0	0
			7969	5063	1353	1518	35			
1	E	1031	Total	C	N	O	S	0	0	0
			7492	4716	1292	1459	25			
1	G	942	Total	C	N	O	S	0	0	0
			6909	4338	1202	1341	28			
1	D	1029	Total	C	N	O	S	0	0	0
			7881	4992	1351	1504	34			
1	A	1052	Total	C	N	O	S	0	0	0
			7969	5063	1353	1518	35			
1	B	1031	Total	C	N	O	S	0	0	0
			7492	4716	1292	1459	25			
1	C	941	Total	C	N	O	S	0	0	0
			6902	4333	1201	1340	28			

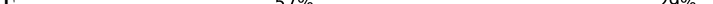
3 Residue-property plots

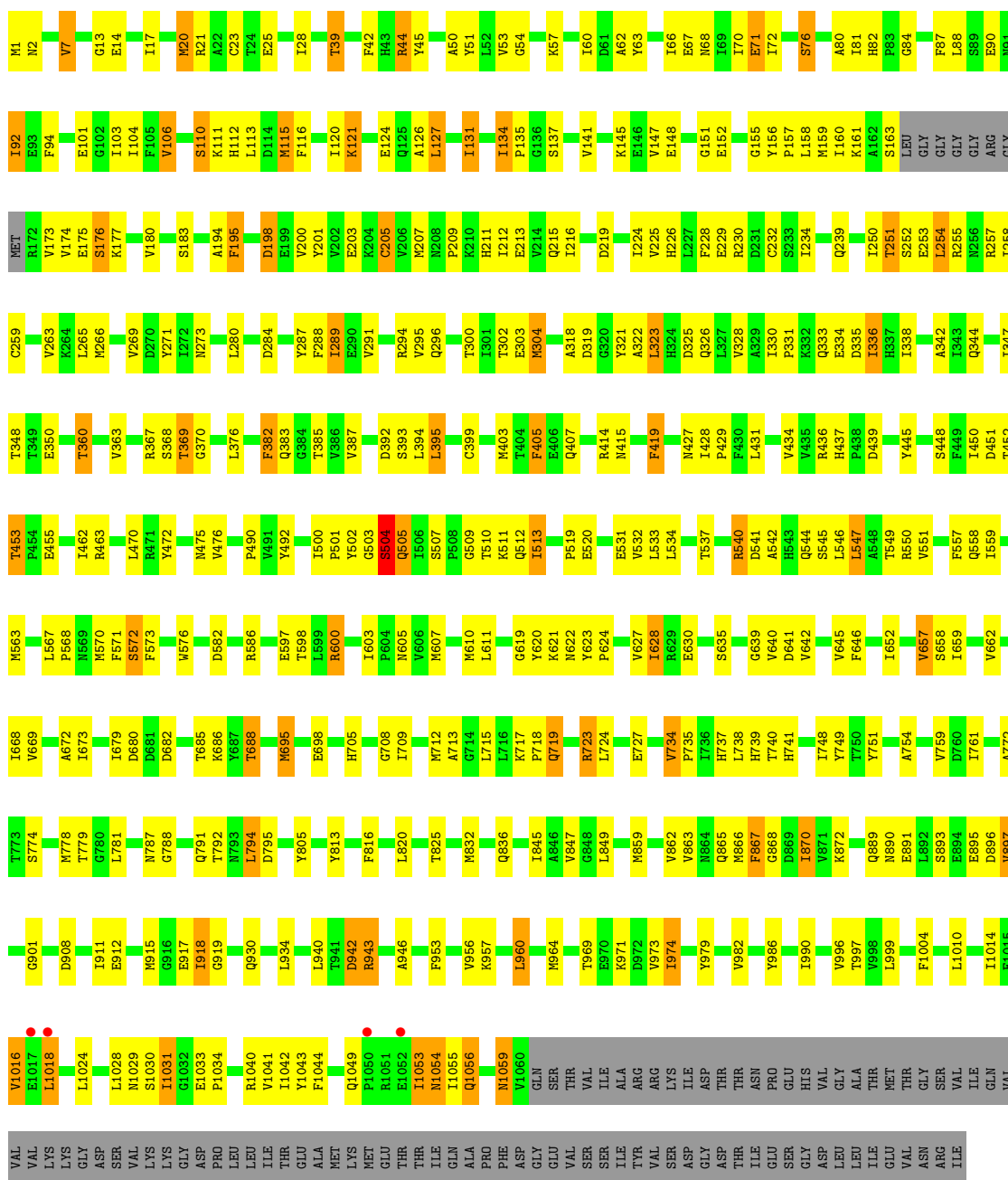
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Pyruvate carboxylase



- Molecule 1: Pyruvate carboxylase

Chain F:  57% 29% 5% 8%



- Molecule 1: Pyruvate carboxylase





Response	Percentage
Yes, the current government is responsible	52%
No, the crisis is the result of the economic situation	26%
Yes, but the crisis is also the result of the economic situation	5%
Don't know	18%

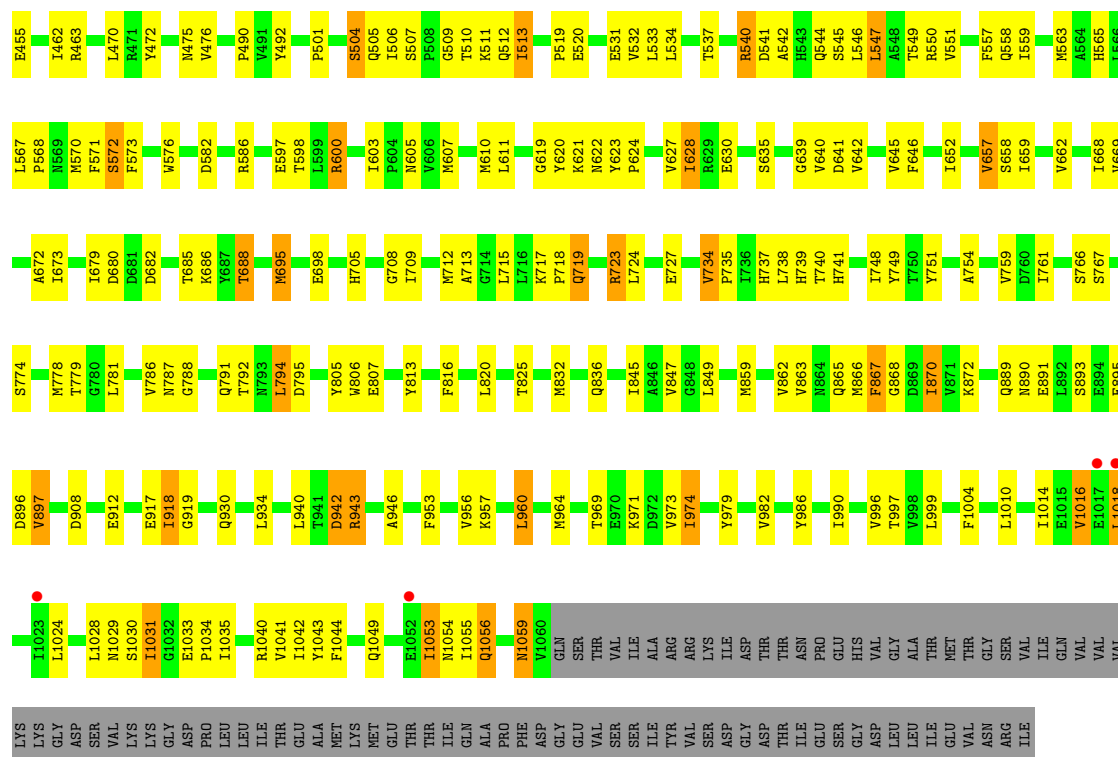


ILE	ALA	K971	D851	L724	M622	E520	D335	N248
	ARG	D972	R852	ARG	P623	E531		
VAL	ARG	V973	W853	E727	P624	E531	H337	I250
SER	LYS	I974	S858	T731	V627	L533	I338	T251
ASP	ILE	S975	M859	V734	L628	L534	H339	S252
GLY	ASP	Y976	M859	V734	L628	L535	A342	E253
ASP	THR	Y979						
THR	THR	Y979	V862	H737	P631	D536	I343	L294
ILE	ASN	V982	V863	L738	V632	T537	Q344	R255
GLU	PRO	V982	M864	L738	V632	T537	S345	R257
SER	GLU	Q987	Q865	H739	S635	R540	H437	I258
GLY	HIS	Q987	M866	T740				
ASP	VAL	Q987	F867	H741	D541	D541	T348	C759
GLY	VAL	Q987	F867	H741	D541	D541	T348	C759
ASP	VAL	Q987	F867	H741	D541	D541	T348	C759
LEU	GLY	I990	D868	I748	V640	H543	E350	K263
LEU	ALA	D995	D869	I748	V640	H543	D351	K263
ILE	ILE	D995	I870	T750	V642	S545	L265	L265
GLU	MET	V996	S876	T750	V642	S545	L265	L265
THR	THR	V997	S876	T751	V645	L547	N354	V289
GLY	GLY	V998	V998	T751	P646	A548	N355	V289
ASN	SER	L999	V879	A754	K653	V551	M357	Y271
ARG	VAL	F1004	Q889	V759	V657	F557	T360	N273
ILE	ILE	F1004	N890	D760	V657	F557	T360	N273
VAL	VAL	L1010	E891	I761	S658	Q558	V363	E278
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VAL	VAL	L1010	E891	I761	S658	Q558	D364	F279
VAL	VAL	L1010	E					

• Molecule 1: Pyruvate carboxylase

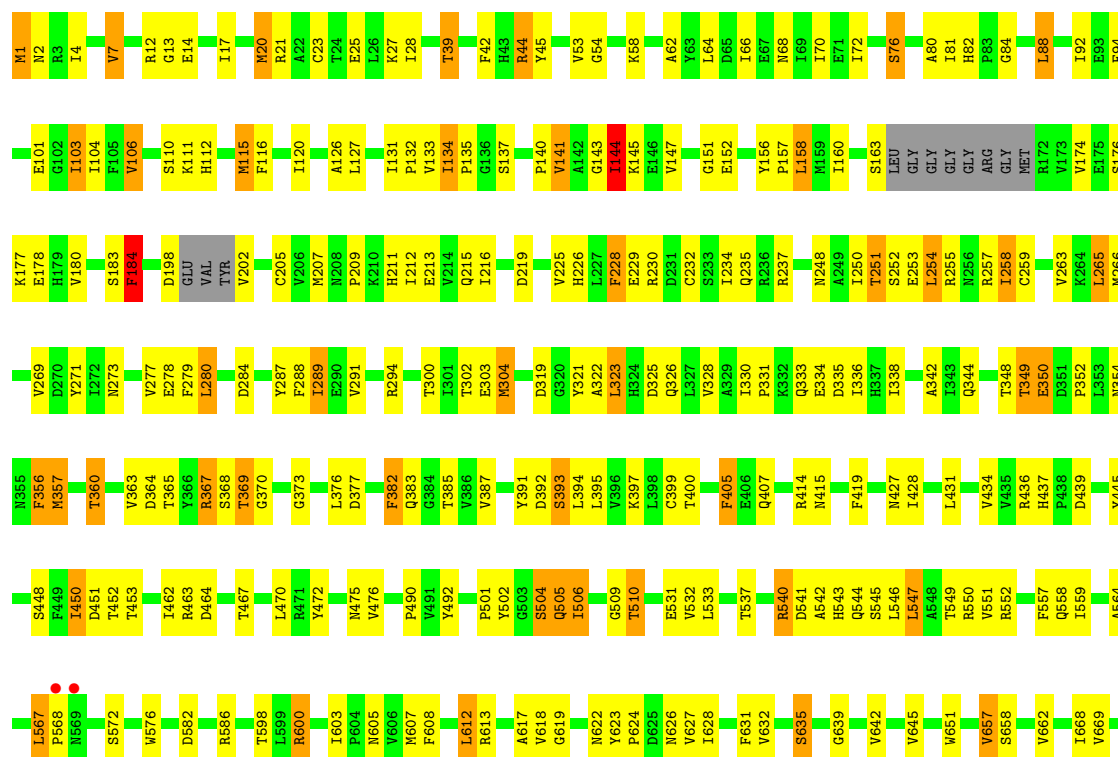
Chain A:  58% 29% 5% 8%

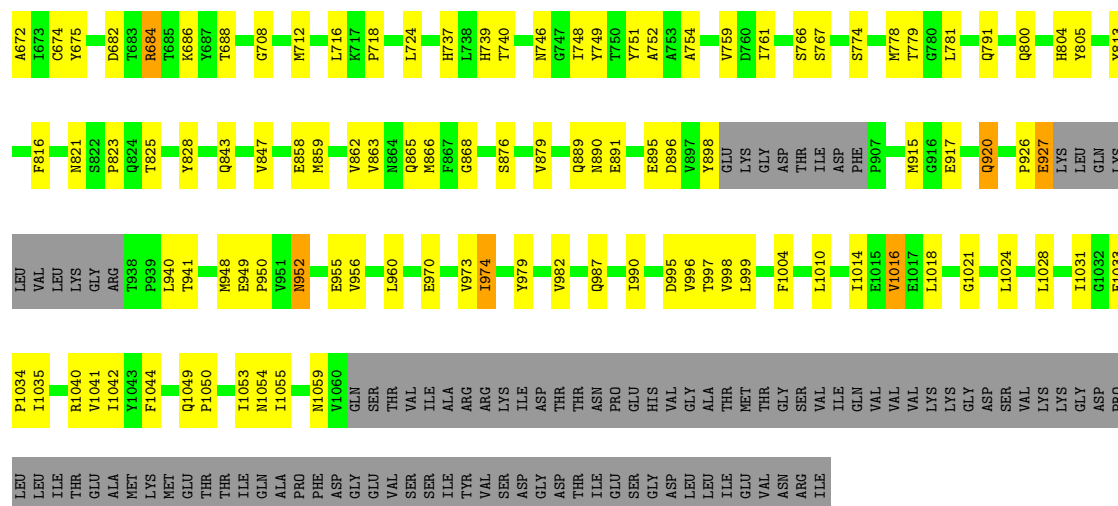
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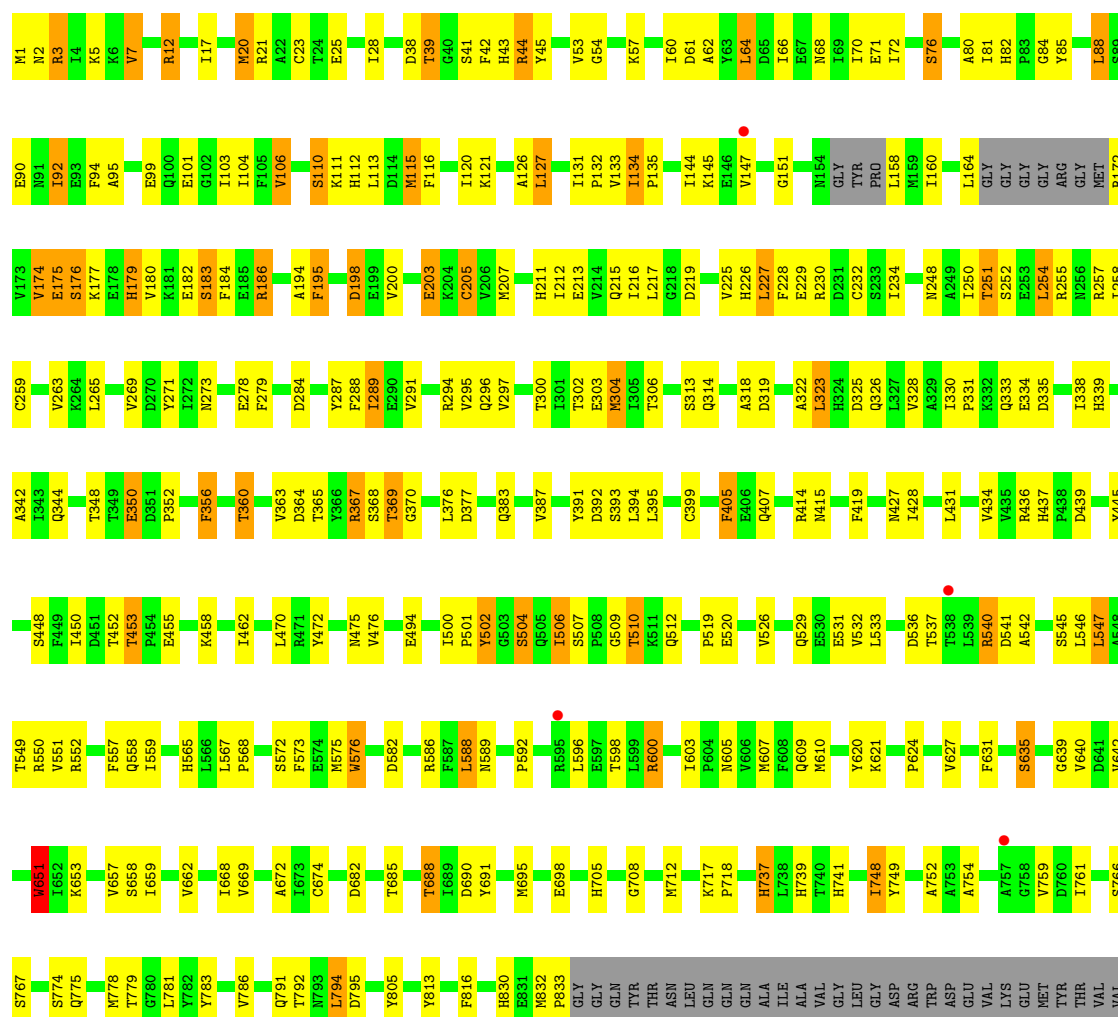
• Molecule 1: Pyruvate carboxylase

Chain B: 58% 27% 10%





• Molecule 1: Pyruvate carboxylase



VAL	GLY	ASN
LYS	PHE	GLN
LYS	PRO	MET
GLY	GLU	PHE
ASP	LYS	GLY
PRO	LEU	ASP
LEU	GLN	ILE
LEU	LYS	VAL
ILE	LEU	LYS
THR	VAL	THR
GLU	LEU	THR
ALA	LYS	PRO
MET	GLY	SER
LYS	ARG	SER
MET	THR	LYS
GLU	PRO	VAL
THR	LEU	VAL
THR	THR	GLY
ILE	ASP	ASP
GLN	R943	LEU
ALA		ALA
PRO	V956	LEU
PHE		PHE
ASP	E959	MET
GLY	L960	VAL
GLU	K961	GLN
VAL	E962	ASN
SER	K963	GLU
ILE		LEU
ILE	P968	SER
TYR		GLU
VAL	L978	GLU
SER	Y979	ASP
ASP		VAL
GLY	V982	TYR
ASP		GLU
THR	M989	LYS
THR		GLY
ILE		GLY
GLU	K992	ASP
SER	Y993	THR
GLY		ILE
ASP	V996	ASP
LEU	T997	PHE
LEU	V998	PRO
ILE	L999	ASP
GLU		SER
VAL	F1004	VAL
ASN		ILE
ARG	L1010	GLU
ILE		PHE
	I1014	
	E1015	MET
	V1016	GLY
	E1017	GLU
	L1018	ILE
		GLY
	L1024	GLN
		PRO
	L1028	TYR
		GLY

I1031	GLY
G1032	PHE
E1033	PRO
P1034	GLU
I1035	LYS
	LEU
R1040	GLN
V1041	LYS
I1042	LEU
Y1043	VAL
F1044	LEU
	LYS
M1047	GLY
G1048	ARG
Q1049	THR
P1050	PRO
R1051	VAL
E1052	LEU
I1053	THR
N1054	ASP
I1055	ASP
	R943
N1059	
V1060	
GLN	
SER	
THR	
VAL	
ILE	
ALA	
ARG	
ARG	
LYS	
ILE	
ASP	
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THR	
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ASP
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GLU
VAL
ASN
ARG
ILE

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	91.36Å 132.62Å 257.54Å 86.65° 79.84° 70.07°	Depositor
Resolution (Å)	47.16 – 3.28 47.16 – 3.29	Depositor EDS
% Data completeness (in resolution range)	88.9 (47.16-3.28) 88.4 (47.16-3.29)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.238 , 0.284 0.235 , 0.282	Depositor DCC
R_{free} test set	7628 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å ²)	116.2	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 138.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.398 for h,h-k,h-l 0.007 for -h,-h+k,-l 0.007 for -h,-k,-h+l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	60495	wwPDB-VP
Average B, all atoms (Å ²)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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

5.1 Standard geometry

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	0.64	0/8136	0.98	9/11083 (0.1%)
1	B	0.64	0/7639	0.99	19/10443 (0.2%)
1	C	0.66	0/7031	0.97	7/9586 (0.1%)
1	D	0.66	0/8042	1.00	19/10933 (0.2%)
1	E	0.65	0/7639	0.99	19/10443 (0.2%)
1	F	0.64	0/8136	0.98	11/11083 (0.1%)
1	G	0.67	0/7039	0.97	8/9597 (0.1%)
1	H	0.68	1/8042 (0.0%)	1.00	16/10933 (0.1%)
All	All	0.65	1/61704 (0.0%)	0.99	108/84101 (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	D	0	1
1	F	0	1
1	H	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	464	ASP	C-O	-5.00	1.18	1.23

The worst 5 of 108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	478	VAL	CB-CA-C	-12.99	96.61	111.55
1	D	478	VAL	CB-CA-C	-12.14	97.59	111.55
1	E	143	GLY	N-CA-C	9.16	125.77	110.56
1	B	184	PHE	N-CA-CB	8.48	122.31	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	184	PHE	N-CA-CB	8.47	122.29	110.01

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	504	SER	Peptide
1	F	504	SER	Peptide
1	H	504	SER	Peptide

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	7969	0	7573	300	0
1	B	7492	0	6807	339	0
1	C	6902	0	6371	301	0
1	D	7881	0	7579	302	0
1	E	7492	0	6807	324	0
1	F	7969	0	7573	309	0
1	G	6909	0	6379	296	0
1	H	7881	0	7579	311	0
All	All	60495	0	56668	2401	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 20.

The worst 5 of 2401 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:345:SER:OG	1:D:412:MET:CE	1.67	1.40
1:H:345:SER:OG	1:H:412:MET:CE	1.68	1.39
1:E:280:LEU:HD12	1:E:289:ILE:CG2	1.54	1.37
1:B:280:LEU:HD12	1:B:289:ILE:CG2	1.55	1.37
1:B:279:PHE:N	1:B:289:ILE:HD11	1.37	1.36

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	1048/1146 (91%)	988 (94%)	57 (5%)	3 (0%)	36	66
1	B	1021/1146 (89%)	966 (95%)	53 (5%)	2 (0%)	43	71
1	C	933/1146 (81%)	882 (94%)	47 (5%)	4 (0%)	30	60
1	D	1025/1146 (89%)	967 (94%)	55 (5%)	3 (0%)	36	66
1	E	1021/1146 (89%)	962 (94%)	56 (6%)	3 (0%)	36	66
1	F	1048/1146 (91%)	992 (95%)	54 (5%)	2 (0%)	43	71
1	G	934/1146 (82%)	881 (94%)	49 (5%)	4 (0%)	30	60
1	H	1025/1146 (89%)	966 (94%)	56 (6%)	3 (0%)	36	66
All	All	8055/9168 (88%)	7604 (94%)	427 (5%)	24 (0%)	36	66

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	273	ASN
1	F	273	ASN
1	E	273	ASN
1	G	176	SER
1	G	273	ASN

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	814/981 (83%)	699 (86%)	115 (14%)	3	16
1	B	719/981 (73%)	617 (86%)	102 (14%)	3	15
1	C	676/981 (69%)	579 (86%)	97 (14%)	3	15
1	D	819/981 (84%)	705 (86%)	114 (14%)	3	16
1	E	719/981 (73%)	618 (86%)	101 (14%)	3	16
1	F	814/981 (83%)	700 (86%)	114 (14%)	3	16
1	G	677/981 (69%)	581 (86%)	96 (14%)	3	15
1	H	819/981 (84%)	706 (86%)	113 (14%)	3	16
All	All	6057/7848 (77%)	5205 (86%)	852 (14%)	3	16

5 of 852 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	334	GLU
1	A	323	LEU
1	C	356	PHE
1	D	407	GLN
1	D	323	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 167 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	415	ASN
1	B	842	GLN
1	A	602	GLN
1	B	226	HIS
1	C	112	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	1052/1146 (91%)	-1.14	4 (0%) 88 78	74, 124, 168, 201	0
1	B	1031/1146 (89%)	-0.97	2 (0%) 91 85	72, 153, 205, 246	0
1	C	941/1146 (82%)	-0.93	4 (0%) 88 78	72, 147, 212, 265	0
1	D	1029/1146 (89%)	-1.13	1 (0%) 92 90	58, 118, 188, 231	0
1	E	1031/1146 (89%)	-0.98	6 (0%) 85 72	68, 149, 205, 248	0
1	F	1052/1146 (91%)	-1.16	4 (0%) 88 78	72, 123, 168, 204	0
1	G	942/1146 (82%)	-1.00	4 (0%) 88 78	70, 141, 208, 267	0
1	H	1029/1146 (89%)	-1.13	0 100 100	59, 114, 185, 232	0
All	All	8107/9168 (88%)	-1.06	25 (0%) 90 82	58, 132, 199, 267	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	569	ASN	3.3
1	A	1017	GLU	2.8
1	E	575	MET	2.7
1	C	757	ALA	2.7
1	A	1018	LEU	2.5

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.