



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:21 PM GMT

PDB ID : 1F3X
Title : S402P MUTANT OF RABBIT MUSCLE PYRUVATE KINASE
Authors : Wooll, J.O.; Friesen, R.H.E.; White, M.A.; Watowich, S.J.; Fox, R.O.; Lee, J.C.; Czerwinski, E.W.
Deposited on : 2000-06-06
Resolution : 2.80 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

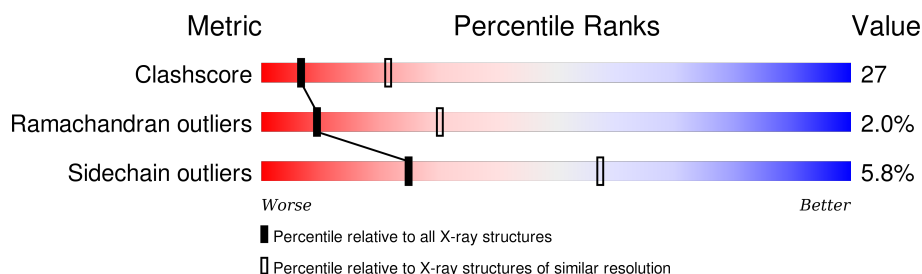
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)


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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	530	
1	B	530	
1	C	530	
1	D	530	
1	E	530	
1	F	530	
1	G	530	

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Mol	Chain	Length	Quality of chain
1	H	530	 A horizontal bar chart showing the quality of chain H. The bar is divided into three segments: green (56%), yellow (37%), and orange (5%). The segments are labeled with their respective percentages: 56%, 37%, and 5%.

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32060 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 KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	0	0
			3974	2497	707	742	28			
1	B	519	Total	C	N	O	S	0	0	0
			3974	2497	707	742	28			
1	C	519	Total	C	N	O	S	0	0	0
			3974	2497	707	742	28			
1	D	519	Total	C	N	O	S	0	0	0
			3974	2497	707	742	28			
1	E	519	Total	C	N	O	S	0	0	0
			3974	2497	707	742	28			
1	F	519	Total	C	N	O	S	0	0	0
			3974	2497	707	742	28			
1	G	519	Total	C	N	O	S	0	0	0
			3974	2497	707	742	28			
1	H	519	Total	C	N	O	S	0	0	0
			3974	2497	707	742	28			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	402	PRO	SER	ENGINEERED	UNP P11974
B	402	PRO	SER	ENGINEERED	UNP P11974
C	402	PRO	SER	ENGINEERED	UNP P11974
D	402	PRO	SER	ENGINEERED	UNP P11974
E	402	PRO	SER	ENGINEERED	UNP P11974
F	402	PRO	SER	ENGINEERED	UNP P11974
G	402	PRO	SER	ENGINEERED	UNP P11974
H	402	PRO	SER	ENGINEERED	UNP P11974

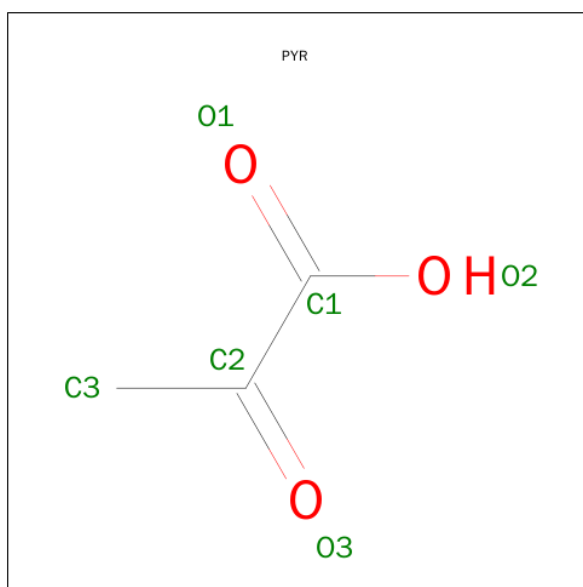
- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total K 1 1	0	0
2	D	1	Total K 1 1	0	0
2	E	1	Total K 1 1	0	0
2	H	1	Total K 1 1	0	0
2	B	1	Total K 1 1	0	0
2	C	1	Total K 1 1	0	0
2	A	1	Total K 1 1	0	0
2	F	1	Total K 1 1	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Mn 1 1	0	0
3	D	1	Total Mn 1 1	0	0
3	E	1	Total Mn 1 1	0	0
3	H	1	Total Mn 1 1	0	0
3	B	1	Total Mn 1 1	0	0
3	C	1	Total Mn 1 1	0	0
3	A	1	Total Mn 1 1	0	0
3	F	1	Total Mn 1 1	0	0

- Molecule 4 is PYRUVIC ACID (three-letter code: PYR) (formula: C₃H₄O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	42	Total	O	0	0
			42	42		
5	B	18	Total	O	0	0
			18	18		
5	C	31	Total	O	0	0
			31	31		
5	D	11	Total	O	0	0
			11	11		

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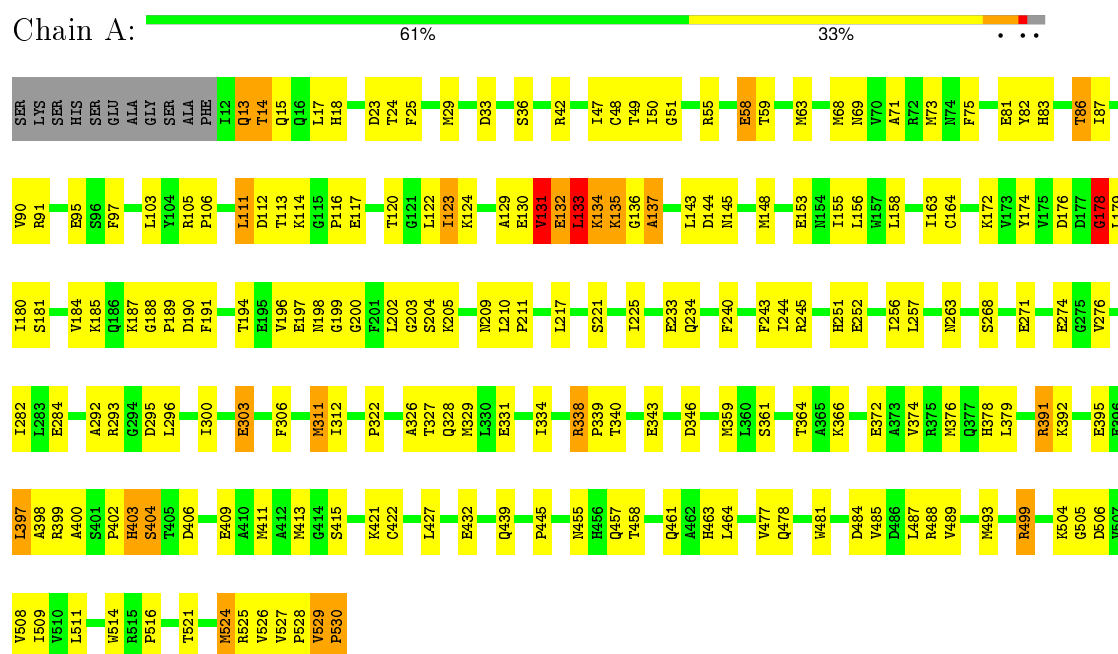
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	42	Total 42	O 42	0	0
5	F	18	Total 18	O 18	0	0
5	G	31	Total 31	O 31	0	0
5	H	11	Total 11	O 11	0	0

3 Residue-property plots

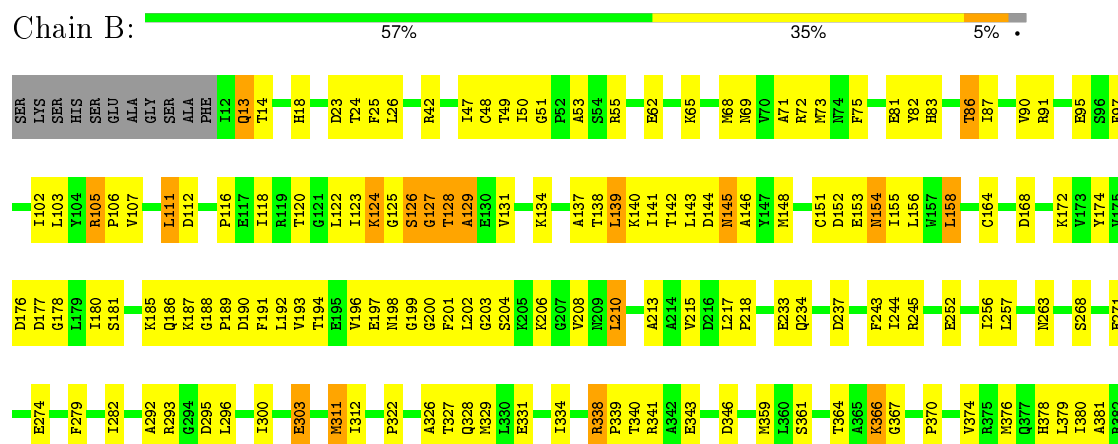
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

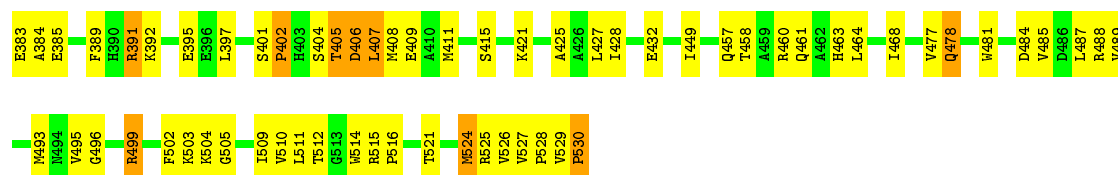
Note EDS was not executed.

• Molecule 1: PYRUVATE KINASE

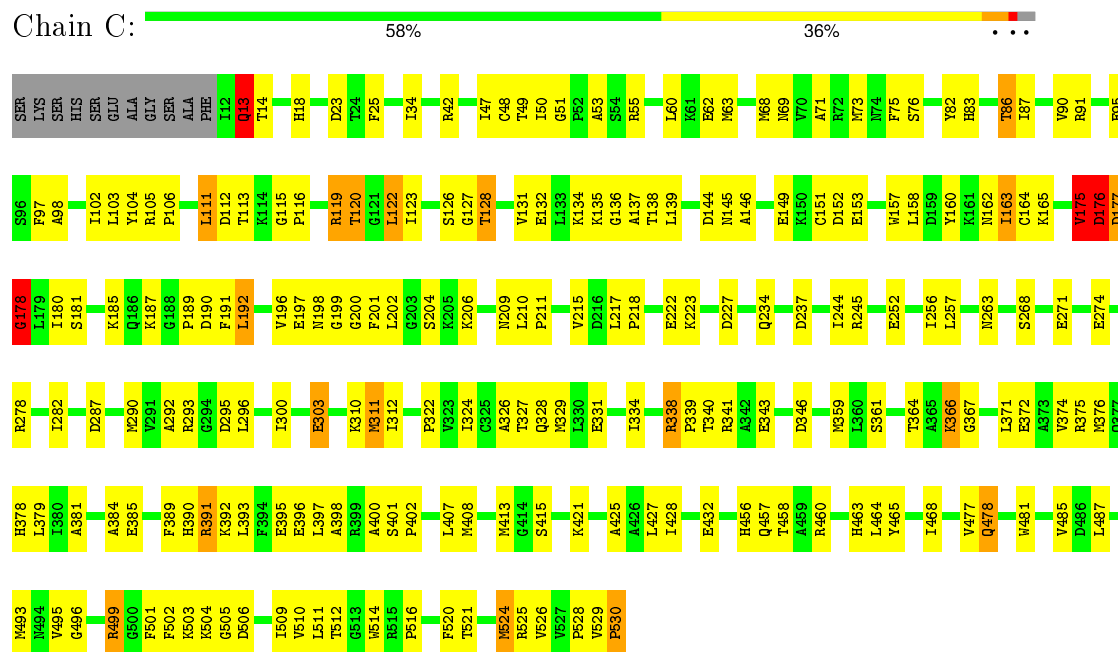


• Molecule 1: PYRUVATE KINASE

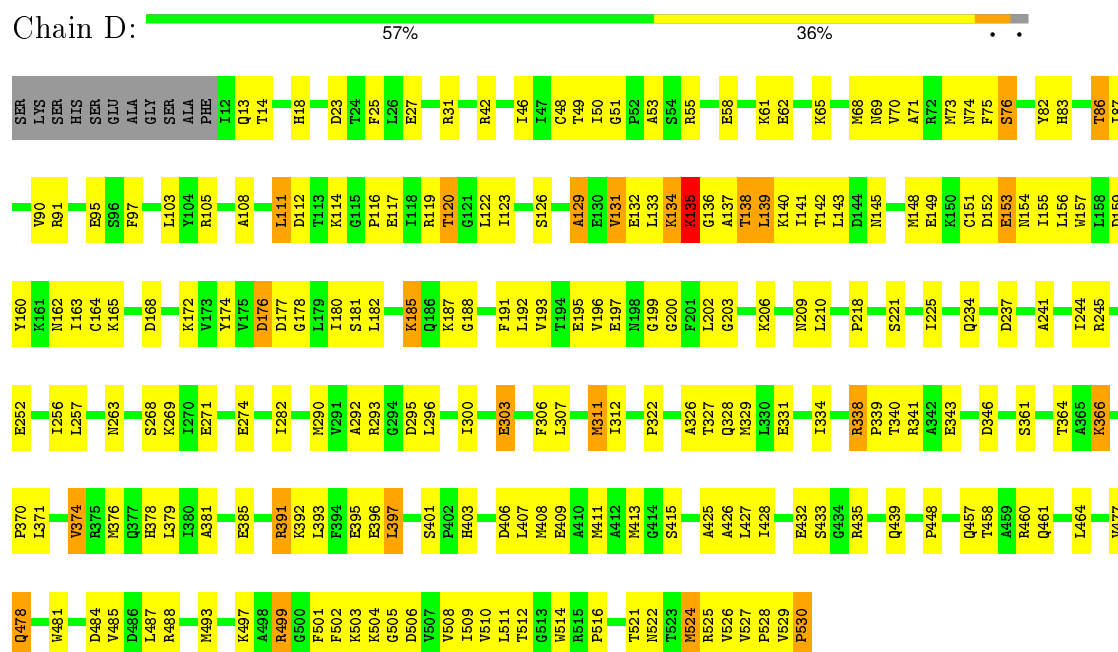




• Molecule 1: PYRUVATE KINASE

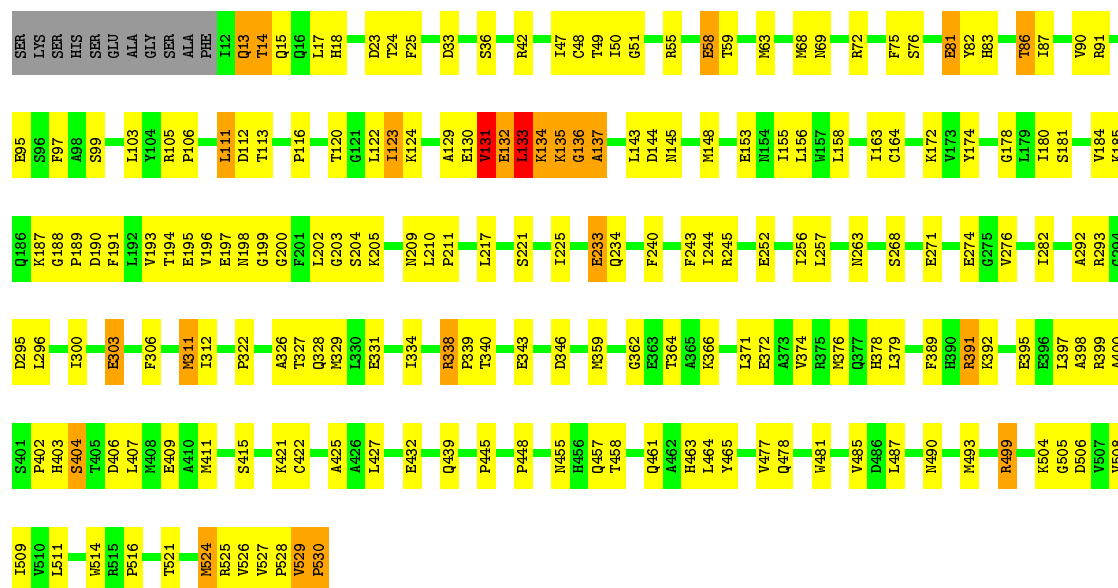


• Molecule 1: PYRUVATE KINASE



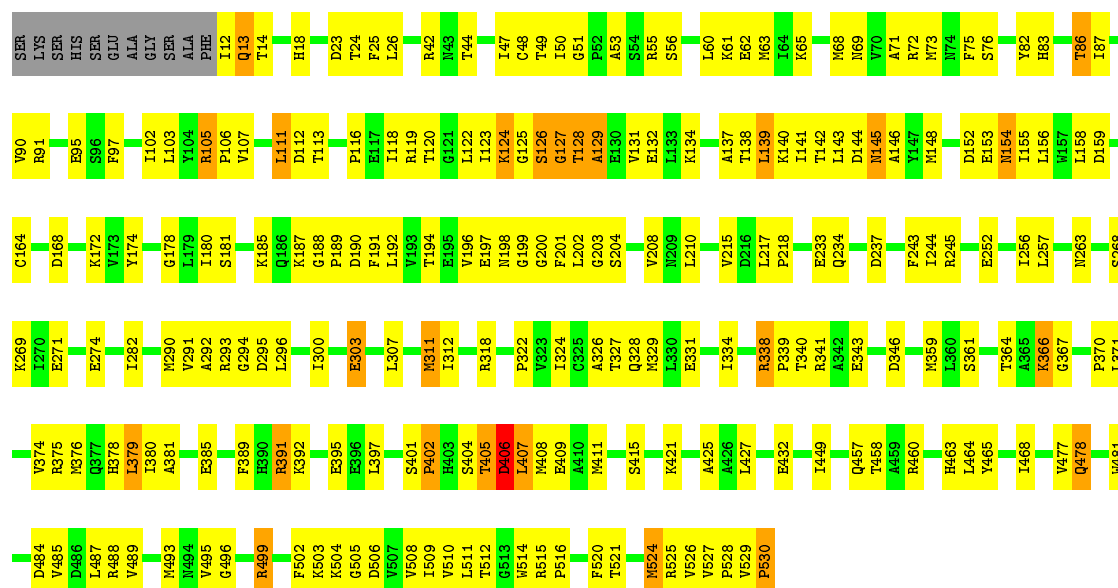
• Molecule 1: PYRUVATE KINASE

Chain E: 



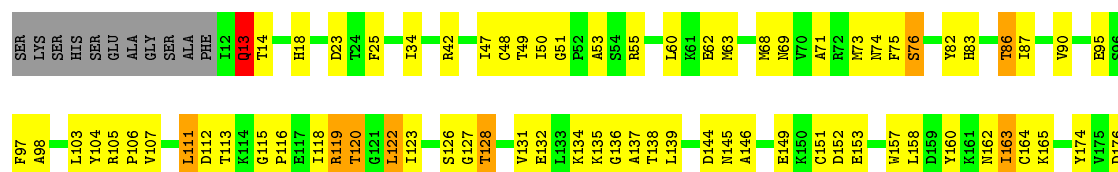
• Molecule 1: PYRUVATE KINASE

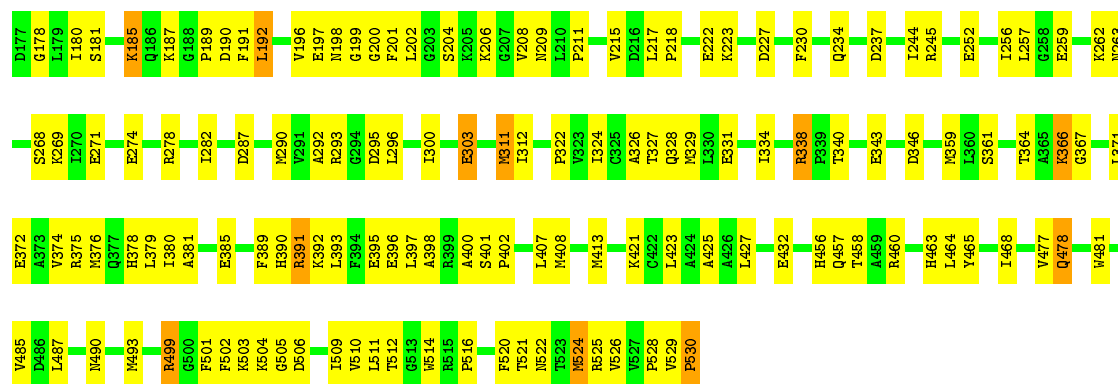
Chain F: 



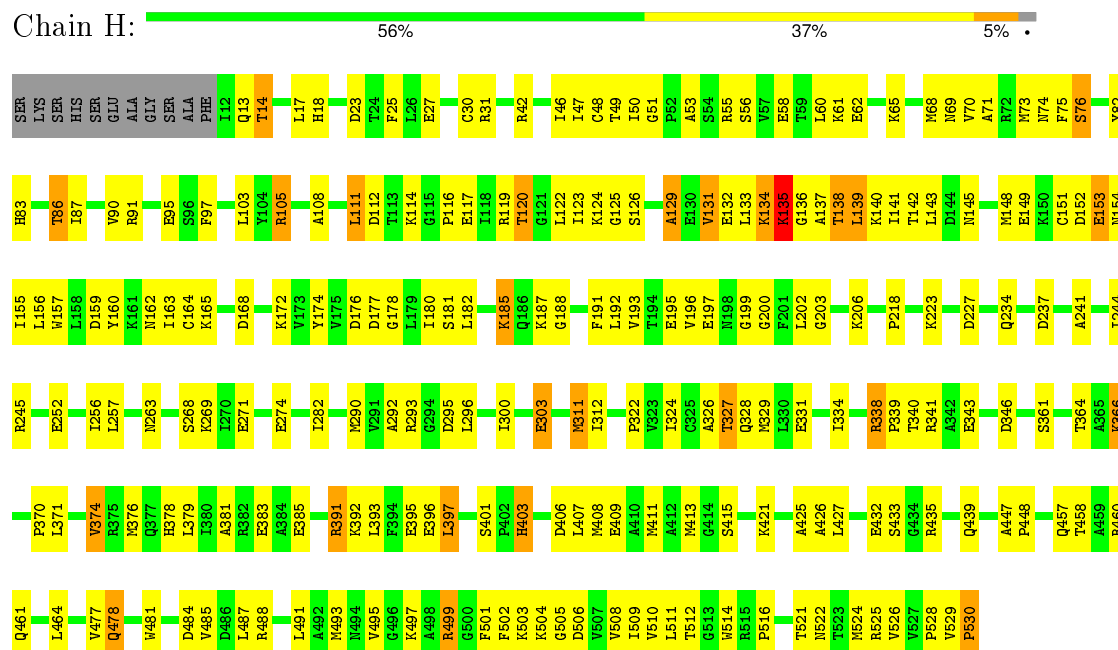
• Molecule 1: PYRUVATE KINASE

Chain G: 





• Molecule 1: PYRUVATE KINASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	82.14Å 108.71Å 144.39Å 95.26° 93.47° 112.24°	Depositor
Resolution (Å)	36.00 – 2.80	Depositor
% Data completeness (in resolution range)	81.8 (36.00-2.80)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.241 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	32060	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PYR, MN, K

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	0.44	0/4038	0.77	3/5451 (0.1%)
1	B	0.41	0/4038	0.67	1/5451 (0.0%)
1	C	0.59	2/4038 (0.0%)	0.75	6/5451 (0.1%)
1	D	0.39	0/4038	0.66	4/5451 (0.1%)
1	E	0.43	0/4038	0.67	0/5451
1	F	0.42	0/4038	0.66	1/5451 (0.0%)
1	G	0.42	0/4038	0.66	1/5451 (0.0%)
1	H	0.38	0/4038	0.62	0/5451
All	All	0.44	2/32304 (0.0%)	0.68	16/43608 (0.0%)

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	A	0	1
1	C	0	3
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	175	VAL	C-N	-25.13	0.76	1.34
1	C	178	GLY	C-O	-5.15	1.15	1.23

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	GLY	O-C-N	-21.66	88.05	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	175	VAL	C-N-CA	15.30	159.94	121.70
1	C	175	VAL	O-C-N	-13.74	100.71	122.70
1	A	178	GLY	CA-C-O	12.95	143.90	120.60
1	C	175	VAL	CA-C-N	9.19	137.42	117.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	GLY	Mainchain
1	C	175	VAL	Peptide
1	C	176	ASP	Mainchain
1	C	178	GLY	Mainchain

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	3974	0	4047	230	0
1	B	3974	0	4047	223	0
1	C	3974	0	4045	207	0
1	D	3974	0	4046	240	0
1	E	3974	0	4046	236	0
1	F	3974	0	4047	232	0
1	G	3974	0	4046	224	0
1	H	3974	0	4046	260	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
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	6	0	3	1	0
4	B	6	0	3	1	0
4	C	6	0	3	1	0
4	D	6	0	3	1	0
4	E	6	0	3	1	0
4	F	6	0	3	1	0
4	G	6	0	3	1	0
4	H	6	0	3	1	0
5	A	42	0	0	4	0
5	B	18	0	0	0	0
5	C	31	0	0	1	0
5	D	11	0	0	0	0
5	E	42	0	0	7	0
5	F	18	0	0	3	0
5	G	31	0	0	1	0
5	H	11	0	0	1	0
All	All	32060	0	32394	1735	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 27.

The worst 5 of 1735 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:C:175:VAL:O	1:C:176:ASP:N	1.57	1.31
1:E:511:LEU:HB3	1:E:521:THR:HG21	1.20	1.17
1:A:511:LEU:HB3	1:A:521:THR:HG21	1.19	1.16
1:D:511:LEU:HB3	1:D:521:THR:HG21	1.17	1.14
1:C:511:LEU:HB3	1:C:521:THR:HG21	1.18	1.14

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	517/530 (98%)	470 (91%)	36 (7%)	11 (2%)	9	29
1	B	517/530 (98%)	479 (93%)	28 (5%)	10 (2%)	10	32
1	C	517/530 (98%)	482 (93%)	26 (5%)	9 (2%)	11	36
1	D	517/530 (98%)	470 (91%)	36 (7%)	11 (2%)	9	29
1	E	517/530 (98%)	468 (90%)	39 (8%)	10 (2%)	10	32
1	F	517/530 (98%)	474 (92%)	32 (6%)	11 (2%)	9	29
1	G	517/530 (98%)	481 (93%)	29 (6%)	7 (1%)	14	42
1	H	517/530 (98%)	469 (91%)	36 (7%)	12 (2%)	8	26
All	All	4136/4240 (98%)	3793 (92%)	262 (6%)	81 (2%)	9	30

5 of 81 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	VAL
1	A	133	LEU
1	A	134	LYS
1	A	135	LYS
1	B	126	SER

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	424/433 (98%)	398 (94%)	26 (6%)	23	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	424/433 (98%)	399 (94%)	25 (6%)	24	57
1	C	424/433 (98%)	399 (94%)	25 (6%)	24	57
1	D	424/433 (98%)	404 (95%)	20 (5%)	32	67
1	E	424/433 (98%)	395 (93%)	29 (7%)	20	49
1	F	424/433 (98%)	396 (93%)	28 (7%)	21	51
1	G	424/433 (98%)	402 (95%)	22 (5%)	29	62
1	H	424/433 (98%)	403 (95%)	21 (5%)	30	64
All	All	3392/3464 (98%)	3196 (94%)	196 (6%)	25	57

5 of 196 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	374	VAL
1	E	233	GLU
1	H	135	LYS
1	D	477	VAL
1	E	76	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 88 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	463	HIS
1	E	463	HIS
1	H	317	ASN
1	D	478	GLN
1	E	198	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 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	$\# Z > 2$
4	PYR	A	541	3	2,5,5	5.09	2 (100%)	2,6,6	5.99	2 (100%)
4	PYR	B	542	3	2,5,5	5.28	2 (100%)	2,6,6	6.02	2 (100%)
4	PYR	C	543	3	2,5,5	5.19	2 (100%)	2,6,6	5.66	2 (100%)
4	PYR	D	544	3	2,5,5	5.34	2 (100%)	2,6,6	5.72	2 (100%)
4	PYR	E	545	3	2,5,5	4.93	2 (100%)	2,6,6	5.92	2 (100%)
4	PYR	F	546	3	2,5,5	5.09	2 (100%)	2,6,6	5.97	2 (100%)
4	PYR	G	547	3	2,5,5	5.42	2 (100%)	2,6,6	5.59	2 (100%)
4	PYR	H	548	3	2,5,5	5.10	2 (100%)	2,6,6	5.99	2 (100%)

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
4	PYR	A	541	3	-	0/0/4/4	0/0/0/0
4	PYR	B	542	3	-	0/0/4/4	0/0/0/0
4	PYR	C	543	3	-	0/0/4/4	0/0/0/0
4	PYR	D	544	3	-	0/0/4/4	0/0/0/0
4	PYR	E	545	3	-	0/0/4/4	0/0/0/0
4	PYR	F	546	3	-	0/0/4/4	0/0/0/0
4	PYR	G	547	3	-	0/0/4/4	0/0/0/0
4	PYR	H	548	3	-	0/0/4/4	0/0/0/0

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	548	PYR	O3-C2	4.44	1.38	1.22
4	E	545	PYR	O3-C2	4.46	1.38	1.22
4	F	546	PYR	O3-C2	4.47	1.38	1.22
4	A	541	PYR	O3-C2	4.67	1.38	1.22
4	C	543	PYR	O3-C2	4.68	1.38	1.22

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	542	PYR	O3-C2-C3	-7.79	101.47	120.13
4	F	546	PYR	O3-C2-C3	-7.67	101.74	120.13
4	A	541	PYR	O3-C2-C3	-7.67	101.75	120.13
4	H	548	PYR	O3-C2-C3	-7.60	101.91	120.13
4	E	545	PYR	O3-C2-C3	-7.56	102.00	120.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	541	PYR	1	0
4	B	542	PYR	1	0
4	C	543	PYR	1	0
4	D	544	PYR	1	0
4	E	545	PYR	1	0
4	F	546	PYR	1	0
4	G	547	PYR	1	0
4	H	548	PYR	1	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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.