



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:28 am BST

PDB ID : 5JVJ
Title : C4-type pyruvate phosphate dikinase: different conformational states of the nucleotide binding domain in the dimer
Authors : Minges, A.; Hoepfner, A.; Groth, G.
Deposited on : 2016-05-11
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 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 : 2.11
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

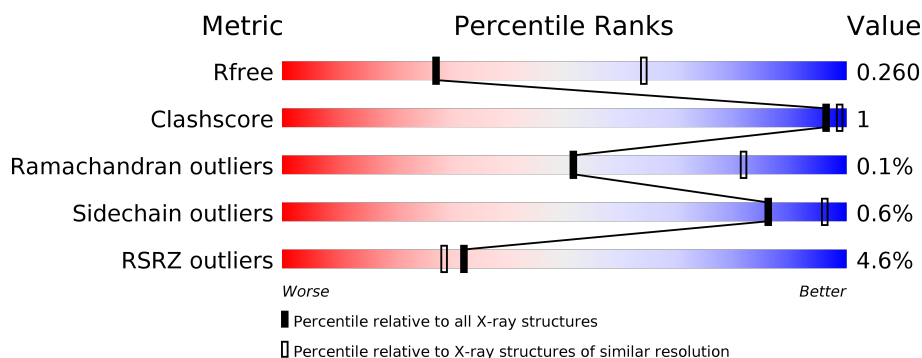
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 $\leq 5\%$. 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	874	<div> <div>3%</div> <div>95%</div> <div>••</div> </div>
1	B	874	<div> <div>6%</div> <div>89%</div> <div>• 9%</div> </div>

2 Entry composition [i](#)

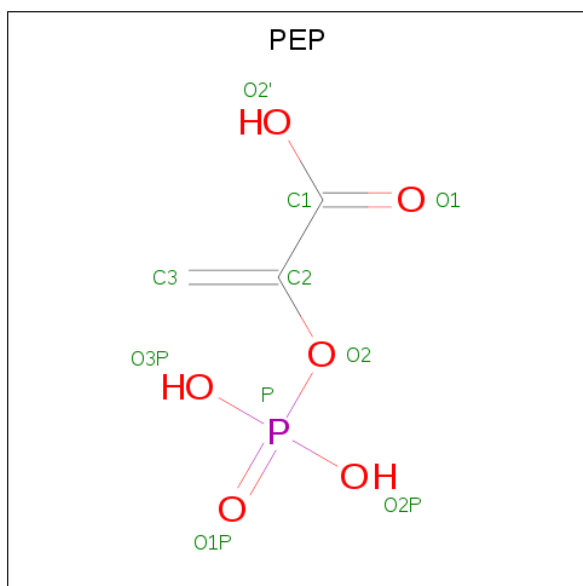
There are 3 unique types of molecules in this entry. The entry contains 11950 atoms, of which 0 are hydrogens and 0 are deuteriums.

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, phosphate dikinase, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	865	Total	C	N	O	S	0	2	0
			6504	4084	1127	1249	44			
1	B	797	Total	C	N	O	S	0	0	0
			5424	3386	942	1057	39			

- Molecule 2 is PHOSPHOENOLPYRUVATE (three-letter code: PEP) (formula: $C_3H_5O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			10	3	6	1		
2	B	1	Total	C	O	P	0	0
			10	3	6	1		

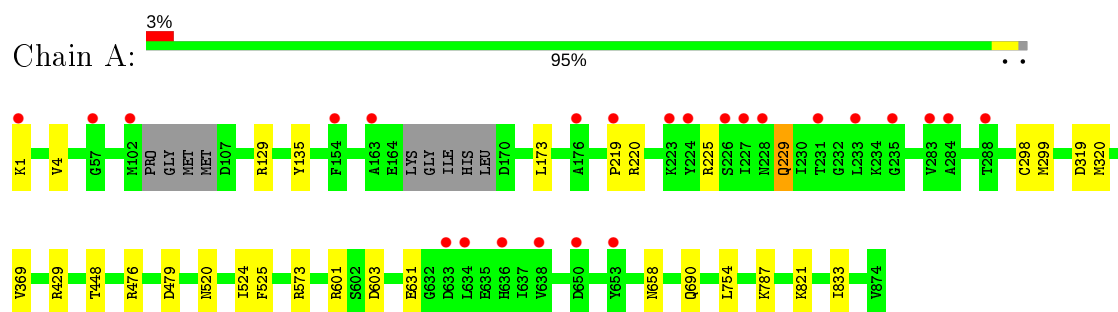
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

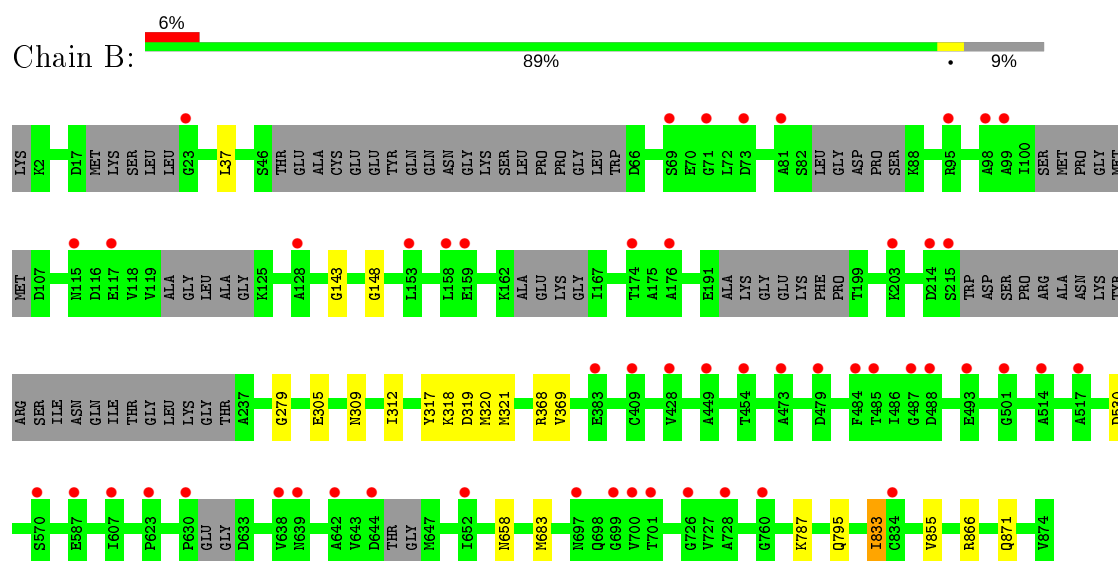
3 Residue-property plots [i](#)

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, phosphate dikinase, chloroplastic



- Molecule 1: Pyruvate, phosphate dikinase, chloroplastic



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	208.74Å 69.04Å 166.76Å 90.00° 112.84° 90.00°	Depositor
Resolution (Å)	38.42 – 2.90 38.42 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.1 (38.42-2.90) 98.1 (38.42-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.90Å)	Xtriage
Refinement program	PHENIX dev_2386	Depositor
R, R_{free}	0.237 , 0.261 0.235 , 0.260	Depositor DCC
R_{free} test set	1227 reflections (2.55%)	wwPDB-VP
Wilson B-factor (Å ²)	39.7	Xtriage
Anisotropy	0.903	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	11950	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PEP

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	0.26	0/6623	0.41	0/8961
1	B	0.25	0/5503	0.41	0/7492
All	All	0.25	0/12126	0.41	0/16453

There are no bond length outliers.

There are no bond angle outliers.

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	6504	0	6370	15	0
1	B	5424	0	4761	11	0
2	A	10	0	2	0	0
2	B	10	0	2	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	11950	0	11135	24	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 1.

All (24) 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:658:ASN:O	1:B:787:LYS:NZ	2.22	0.73
1:A:601:ARG:NH1	1:A:690:GLN:OE1	2.27	0.66
1:A:319:ASP:OD1	1:A:320:MET:N	2.34	0.60
1:B:305:GLU:O	1:B:309:ASN:ND2	2.34	0.58
1:A:129:ARG:NH1	1:A:173:LEU:O	2.36	0.58
1:B:369:VAL:O	1:B:871:GLN:NE2	2.37	0.58
1:A:787:LYS:NZ	1:B:658:ASN:O	2.34	0.57
1:B:143:GLY:O	1:B:148:GLY:N	2.39	0.52
1:B:318:LYS:O	1:B:368:ARG:NH1	2.41	0.52
1:A:479:ASP:N	1:A:479:ASP:OD1	2.45	0.49
1:A:754:LEU:O	1:A:821:LYS:NZ	2.45	0.49
1:B:319:ASP:OD1	1:B:320:MET:N	2.46	0.48
1:A:573:ARG:NH1	1:A:603:ASP:OD2	2.41	0.47
1:B:317:TYR:HB2	1:B:321:MET:HE3	1.96	0.46
1:A:225:ARG:O	1:A:229:GLN:N	2.44	0.45
1:B:37:LEU:HD21	1:B:312:ILE:HG21	2.00	0.44
1:A:1:LYS:N	1:A:4:VAL:O	2.52	0.43
1:B:833:ILE:HG23	1:B:855:VAL:HA	2.02	0.42
1:A:298:CYS:HB2	1:A:299:MET:HE2	2.02	0.41
1:A:219:PRO:O	1:A:220:ARG:CB	2.68	0.41
1:A:520:ASN:O	1:A:524:ILE:HG12	2.21	0.41
1:B:530:ASP:OD1	1:B:866:ARG:HD2	2.21	0.41
1:A:369:VAL:HB	1:A:525:PHE:CZ	2.56	0.40
1:A:429:ARG:O	1:A:448:THR:HA	2.21	0.40

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	861/874 (98%)	832 (97%)	28 (3%)	1 (0%)	51 82

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	775/874 (89%)	752 (97%)	22 (3%)	1 (0%)	51 82
All	All	1636/1748 (94%)	1584 (97%)	50 (3%)	2 (0%)	51 82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	279	GLY
1	A	229	GLN

5.3.2 Protein sidechains ⓘ

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	675/715 (94%)	671 (99%)	4 (1%)	86 96
1	B	467/715 (65%)	464 (99%)	3 (1%)	86 96
All	All	1142/1430 (80%)	1135 (99%)	7 (1%)	86 96

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	TYR
1	A	476	ARG
1	A	631	GLU
1	A	833	ILE
1	B	683	MET
1	B	795	GLN
1	B	833	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
2	PEP	B	901	3	6,9,9	0.72	0	8,13,13	0.92	0
2	PEP	A	901	3	6,9,9	0.79	0	8,13,13	0.91	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
2	PEP	B	901	3	-	0/5/9/9	-
2	PEP	A	901	3	-	2/5/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	PEP	C1-C2-O2-P
2	A	901	PEP	C3-C2-O2-P

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	865/874 (98%)	-0.07	24 (2%)	53 49	11, 34, 100, 133	0
1	B	797/874 (91%)	0.52	52 (6%)	18 14	32, 80, 118, 156	0
All	All	1662/1748 (95%)	0.21	76 (4%)	32 29	11, 61, 114, 156	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	473	ALA	4.7
1	B	215	SER	4.6
1	B	176	ALA	4.2
1	A	57	GLY	4.1
1	A	231	THR	3.9
1	B	214	ASP	3.7
1	B	697	ASN	3.6
1	A	219	PRO	3.6
1	B	487	GLY	3.6
1	B	69	SER	3.5
1	B	570	SER	3.5
1	B	642	ALA	3.4
1	A	284	ALA	3.4
1	B	488	ASP	3.4
1	B	128	ALA	3.3
1	A	233	LEU	3.3
1	B	493	GLU	3.3
1	A	224	TYR	3.3
1	A	634	LEU	3.2
1	B	81	ALA	3.1
1	B	98	ALA	3.1
1	A	653	TYR	3.1
1	B	174	THR	3.0
1	B	153	LEU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	409	CYS	3.0
1	B	203	LYS	2.9
1	A	226	SER	2.9
1	B	454	THR	2.8
1	B	587	GLU	2.7
1	B	700	VAL	2.7
1	B	607	ILE	2.7
1	A	163	ALA	2.6
1	B	95	ARG	2.6
1	B	834	CYS	2.6
1	B	728	ALA	2.6
1	B	652	ILE	2.6
1	B	630	PRO	2.6
1	B	158	LEU	2.6
1	A	283	VAL	2.5
1	B	639	ASN	2.5
1	A	176	ALA	2.5
1	B	73	ASP	2.5
1	A	228	ASN	2.4
1	A	227	ILE	2.4
1	A	636	HIS	2.4
1	A	1	LYS	2.4
1	A	102	MET	2.4
1	B	117	GLU	2.4
1	B	699	GLY	2.4
1	B	23	GLY	2.3
1	B	428	VAL	2.3
1	A	650	ASP	2.3
1	A	154	PHE	2.3
1	B	71	GLY	2.3
1	B	514	ALA	2.3
1	B	726	GLY	2.3
1	B	485	THR	2.3
1	B	517	ALA	2.2
1	B	701	THR	2.2
1	B	99	ALA	2.2
1	A	223	LYS	2.2
1	A	633	ASP	2.2
1	B	383	GLU	2.2
1	B	159	GLU	2.2
1	B	115	ASN	2.2
1	B	638	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	638	VAL	2.1
1	B	484	PHE	2.1
1	A	235	GLY	2.1
1	B	501	GLY	2.1
1	B	760	GLY	2.1
1	A	288	THR	2.0
1	B	449	ALA	2.0
1	B	479	ASP	2.0
1	B	644	ASP	2.0
1	B	623	PRO	2.0

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 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, 95th 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
2	PEP	B	901	10/10	0.95	0.27	39,41,43,44	0
3	MG	A	902	1/1	0.97	0.21	23,23,23,23	0
2	PEP	A	901	10/10	0.97	0.18	13,19,23,24	0
3	MG	B	902	1/1	0.98	0.20	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.