



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1JDE / pdb_00001jde
Title : K22A mutant of pyruvate, phosphate dikinase
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Deposited on : 2001-06-13
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

<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
Mogul	:	2022.3.0, CSD as543be (2022)
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

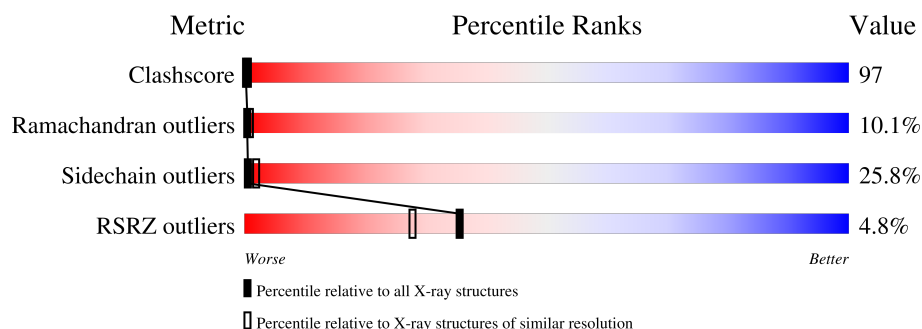
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 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	873	5% 11% 53% 29% 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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	902	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6768 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.

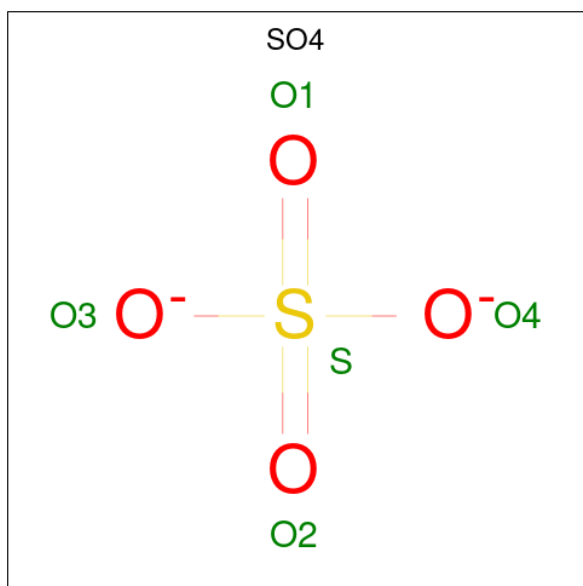
- Molecule 1 is a protein called PYRUVATE, PHOSPHATE DIKINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	868	6717	4226	1138	1302	51	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ALA	LYS	engineered mutation	UNP P22983

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0

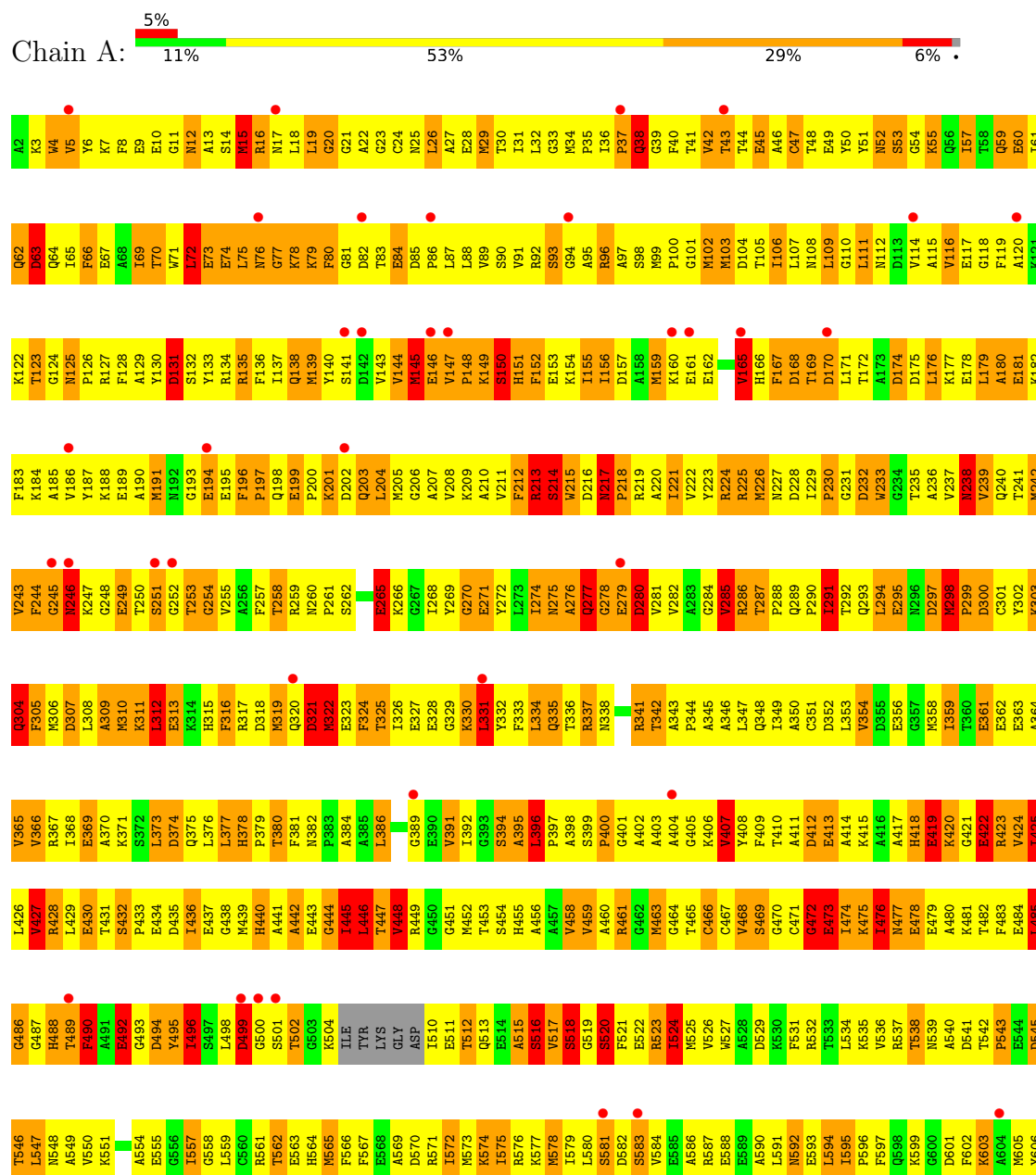
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	41	Total	O	0	0
			41	41		

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, PHOSPHATE DIKINASE



F857	K607	V671	G732	I794
R858	A608	T672	G733	T795
V859	L609	Y673	S734	E796
P860	E610	P674	D735	S797
I861	G611	E675	M736	D798
A862	R612	T676	Q737	P799
R863	F613	A677	Y738	F800
L864	M614	K678	H739	A801
A865	T615	M679	I740	R802
A866	V616	Q680	G741	L803
A867	R617	T681	T742	D804
Q868	Y618	R682	M743	Q805
A869	L619	A683	I744	V806
A870	D620	V684	E745	
L871	P621	M685	I746	
N872	P622	E686	P747	L811
N873	L623	A687	R748	V812
K874	H624	A688	A749	E813
	E625	I689	A750	M814
	F626	E690	L751	A815
	V627	V691	T752	V816
	P628	K692	A753	K817
	H629	E693	D754	K818
	T630	E694	A755	E819
		T695	I756	R820
	E633	G696	A757	Q821
	Q634	I697	E758	R822
	A635	I699		R823
	E636	V700		
	L637	P701	E761	L826
		E702	F762	K827
	M641	I703	S764	C828
		M704	F765	G829
	T644	I705	G766	I830
L645	A646	P706	T767	C831
A646	E647	L707	N768	Q832
E647	V648	V708	D769	E833
K649		G709	L770	H834
A650		E710	I771	G835
K651	V652	K711	Q772	C836
V652	D653	K712	M773	D837
E654	L655	E713	T774	P838
H656	E657	L714	F775	S839
E657	F658	F716	G776	S840
F658	N659	K718	F777	V841
N659	P660	D719	S778	E842
P660	M661	V720	R779	F843
M661	H662	V721	D780	C844
H662	G663	V722	V781	H845
G663	H664	E723	A782	K846
H664	R665	V724	G783	V847
R665	G666	A725	K784	C848
G666	C667		F785	L849
C667	R668	V728	L786	N850
R668	L669	K729	D787	Y851
L669	A670	K730	S788	V852
A670		E731	Y789	S853
			Y790	C854
			K791	S855
				P856

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	89.90Å 58.60Å 102.30Å 90.00° 95.10° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80 10.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.80) 88.8 (10.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.77Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.193 , (Not available) 0.260 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.56 , 166.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	6768	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.30% 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: SO4

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	1.46	22/6839 (0.3%)	1.96	184/9217 (2.0%)

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	798	ASP	CA-C	6.24	1.60	1.52
1	A	547	LEU	N-CA	-5.96	1.40	1.46
1	A	146	GLU	CD-OE2	5.92	1.36	1.25
1	A	70	THR	C-N	-5.90	1.26	1.33
1	A	473	GLU	C-N	-5.76	1.28	1.33

The worst 5 of 184 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	474	ILE	N-CA-C	10.17	117.10	106.21
1	A	672	THR	CA-C-N	9.87	130.97	122.28
1	A	672	THR	C-N-CA	9.87	130.97	122.28
1	A	300	ASP	N-CA-C	-9.59	103.69	114.62
1	A	575	ILE	N-CA-C	-9.40	103.56	112.96

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	6717	0	6632	1290	0
2	A	10	0	0	6	0
3	A	41	0	0	5	0
All	All	6768	0	6632	1290	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 97.

The worst 5 of 1290 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:219:ARG:NH2	1:A:437:GLU:H	1.41	1.18
1:A:276:ALA:HB1	1:A:281:VAL:HG21	1.27	1.14
1:A:219:ARG:HH21	1:A:437:GLU:N	1.46	1.13
1:A:574:LYS:HD3	1:A:593:GLU:HB2	1.20	1.13
1:A:5:VAL:HG22	1:A:42:VAL:HA	1.27	1.12

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	864/873 (99%)	628 (73%)	149 (17%)	87 (10%)	0 1

5 of 87 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	55	LYS
1	A	59	GLN
1	A	60	GLU
1	A	96	ARG

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	709/713 (99%)	526 (74%)	183 (26%)	0 2

5 of 183 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	477	ASN
1	A	653	ASP
1	A	489	THR
1	A	538	THR
1	A	708	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	564	HIS
1	A	659	ASN
1	A	624	HIS
1	A	680	GLN
1	A	238	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](#)

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](#)

2 ligands 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	$\# Z > 2$
2	SO4	A	901	-	4,4,4	0.80	0	6,6,6	0.46	0
2	SO4	A	902	-	4,4,4	1.26	1 (25%)	6,6,6	0.20	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	902	SO4	O2-S	2.18	1.57	1.44

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	SO4	1	0
2	A	902	SO4	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 [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	868/873 (99%)	0.50	42 (4%) 35 28	8, 28, 41, 53	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	76	ASN	4.5
1	A	501	SER	3.7
1	A	146	GLU	3.4
1	A	389	GLY	3.4
1	A	120	ALA	3.3

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 [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	SO4	A	902	5/5	0.88	0.17	59,61,63,64	0
2	SO4	A	901	5/5	0.94	0.08	45,45,54,56	5

6.5 Other polymers [i](#)

There are no such residues in this entry.