



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2024 – 03:31 AM EDT

PDB ID : 3WX8
Title : Purification, characterization and structure of nucleoside diphosphate kinase from *Drosophila* S2 cells
Authors : Qian, L.
Deposited on : 2014-07-25
Resolution : 1.95 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 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

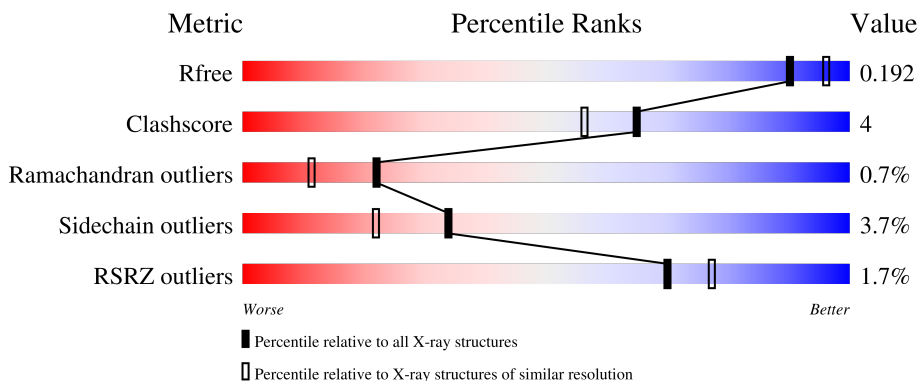
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	153	 90% 8% .
1	B	153	 88% 11% .
1	C	153	 86% 12% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7882 atoms, of which 3618 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 Nucleoside diphosphate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	153	2419	783	1206	210	214	6	0	0	0
1	B	153	2419	783	1206	210	214	6	0	0	0
1	C	152	2411	778	1206	209	213	5	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	ARG	LYS	conflict	UNP P08879
A	101	LYS	LEU	conflict	UNP P08879
A	125	LYS	GLU	conflict	UNP P08879
B	35	ARG	LYS	conflict	UNP P08879
B	101	LYS	LEU	conflict	UNP P08879
B	125	LYS	GLU	conflict	UNP P08879
C	35	ARG	LYS	conflict	UNP P08879
C	101	LYS	LEU	conflict	UNP P08879
C	125	LYS	GLU	conflict	UNP P08879

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	226	Total 226	O 226	0	0
2	B	215	Total 215	O 215	0	0
2	C	192	Total 192	O 192	0	0

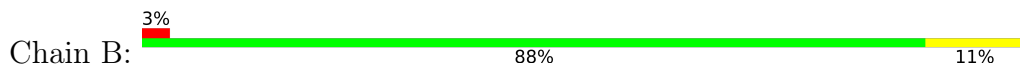
3 Residue-property plots [i](#)

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.

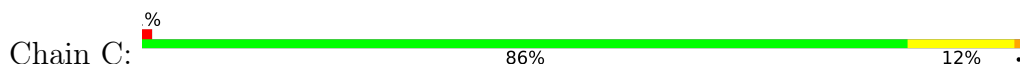
- Molecule 1: Nucleoside diphosphate kinase



- Molecule 1: Nucleoside diphosphate kinase



- Molecule 1: Nucleoside diphosphate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	114.24Å 114.24Å 94.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.47 – 1.95 49.47 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.47-1.95) 94.8 (49.47-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.48 (at 1.95Å)	Xtrriage
Refinement program	CNS, PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.155 , 0.182 0.166 , 0.192	Depositor DCC
R_{free} test set	2572 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	17.1	Xtrriage
Anisotropy	0.493	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7882	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage'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](#)

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	0.51	0/1243	0.63	0/1680
1	B	0.48	0/1243	0.64	2/1680 (0.1%)
1	C	0.54	0/1235	0.62	0/1670
All	All	0.51	0/3721	0.63	2/5030 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	28	ARG	NE-CZ-NH2	-8.17	116.21	120.30
1	B	28	ARG	NE-CZ-NH1	5.19	122.89	120.30

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	1213	1206	1228	6	0
1	B	1213	1206	1228	9	0
1	C	1205	1206	1216	17	0
2	A	226	0	0	1	0
2	B	215	0	0	1	1
2	C	192	0	0	8	1
All	All	4264	3618	3672	30	1

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.

All (30) 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:153:GLU:OE1	2:C:366:HOH:O	1.85	0.93
1:B:90:GLN:OE1	2:B:362:HOH:O	1.98	0.80
1:C:35:ARG:NH2	1:C:80:GLU:OE2	2.31	0.64
1:B:115:ARG:NH1	1:C:153:GLU:HG2	2.15	0.62
1:A:35:ARG:NH2	1:A:80:GLU:OE2	2.32	0.61
1:B:28:ARG:NH2	1:B:103:GLY:O	2.34	0.59
1:C:153:GLU:HB2	2:C:366:HOH:O	2.05	0.56
1:C:153:GLU:CB	2:C:366:HOH:O	2.55	0.54
1:B:35:ARG:NH2	1:B:80:GLU:OE2	2.41	0.54
1:C:35:ARG:NH2	2:C:329:HOH:O	2.40	0.54
1:A:39:LEU:HD23	1:A:77:MET:HG2	1.91	0.52
1:C:48:LEU:HD11	1:C:133:LEU:HG	1.93	0.50
1:B:62:PHE:HB3	1:B:63:PRO:HD3	1.97	0.47
1:C:35:ARG:NH1	2:C:294:HOH:O	2.47	0.46
1:C:51:LYS:NZ	2:C:380:HOH:O	2.50	0.45
1:C:40:LYS:NZ	2:C:352:HOH:O	2.33	0.45
1:B:43:TRP:CZ2	1:B:70:ASN:ND2	2.85	0.45
1:B:97:PRO:HA	1:B:100:SER:OG	2.18	0.44
1:A:101:LYS:NZ	2:A:332:HOH:O	2.40	0.43
1:A:112:GLN:OE1	1:B:153:GLU:HG3	2.18	0.42
1:C:46:LYS:NZ	1:C:67:ASN:OD1	2.41	0.42
1:C:89:ARG:HD3	1:C:121:SER:O	2.20	0.41
1:C:143:TRP:HA	1:C:143:TRP:CE3	2.54	0.41
1:C:62:PHE:HB3	1:C:63:PRO:HD3	2.02	0.41
1:B:89:ARG:HD3	1:B:121:SER:O	2.20	0.41
1:C:48:LEU:CD1	1:C:133:LEU:HG	2.51	0.41
1:C:144:THR:HB	2:C:300:HOH:O	2.21	0.41
1:A:138:LYS:HB3	1:A:138:LYS:HE3	1.79	0.40
1:C:144:THR:HA	1:C:145:PRO:HD3	1.80	0.40
1:A:62:PHE:HB3	1:A:63:PRO:HD3	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:391:HOH:O	2:C:365:HOH:O[3_565]	2.14	0.06

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	151/153 (99%)	148 (98%)	2 (1%)	1 (1%)	22	11
1	B	151/153 (99%)	146 (97%)	4 (3%)	1 (1%)	22	11
1	C	150/153 (98%)	146 (97%)	3 (2%)	1 (1%)	22	11
All	All	452/459 (98%)	440 (97%)	9 (2%)	3 (1%)	22	11

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	ILE
1	B	117	ILE
1	C	117	ILE

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	127/127 (100%)	120 (94%)	7 (6%)	21	9
1	B	127/127 (100%)	125 (98%)	2 (2%)	62	58
1	C	126/127 (99%)	121 (96%)	5 (4%)	31	19
All	All	380/381 (100%)	366 (96%)	14 (4%)	34	22

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	39	LEU
1	A	48	LEU
1	A	86	LYS
1	A	125	LYS
1	A	138	LYS
1	A	142	THR
1	B	1	MET
1	B	47	GLU
1	C	49	LEU
1	C	141	VAL
1	C	142	THR
1	C	143	TRP
1	C	144	THR

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

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 monosaccharides 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

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	153/153 (100%)	-0.08	1 (0%) 87 92	11, 15, 25, 36	0
1	B	153/153 (100%)	0.06	5 (3%) 46 56	12, 18, 31, 45	0
1	C	152/153 (99%)	-0.03	2 (1%) 77 83	10, 17, 31, 44	0
All	All	458/459 (99%)	-0.02	8 (1%) 70 77	10, 17, 30, 45	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	15.9
1	A	1	MET	12.6
1	C	143	TRP	7.3
1	B	43	TRP	4.4
1	B	2	ALA	2.6
1	B	138	LYS	2.5
1	C	43	TRP	2.3
1	B	125	LYS	2.2

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 monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.