



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 04:07 AM UTC

PDB ID : 6JOH / pdb_00006joh
Title : The crystal of nucleoside diphosphate kinase from *Aspergillus flavus*
Authors : Wang, Y.; Wang, S.; Wang, S.H.
Deposited on : 2019-03-21
Resolution : 2.40 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

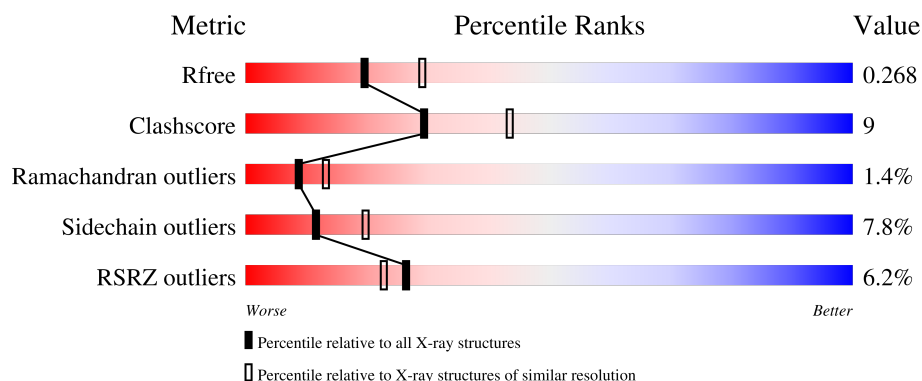
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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.



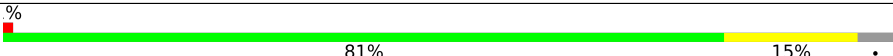
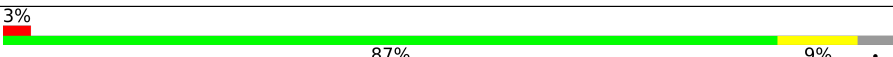
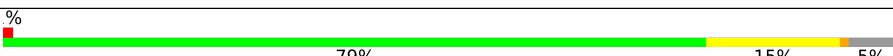
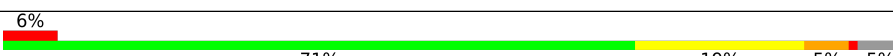
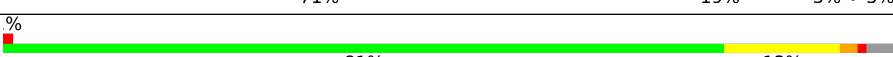
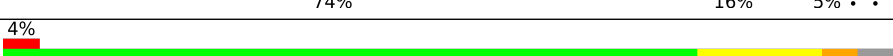
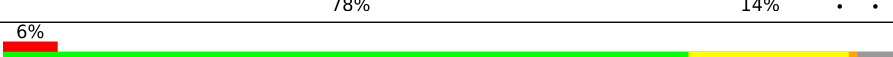
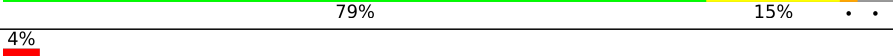
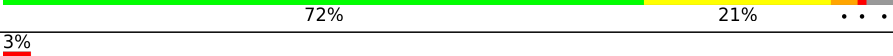
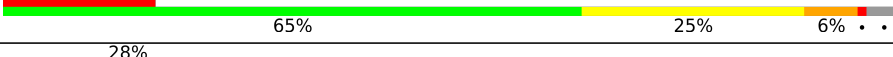
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	155	
1	B	155	
1	C	155	
1	D	155	
1	E	155	

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Mol	Chain	Length	Quality of chain
1	F	155	
1	G	155	
1	H	155	
1	I	155	
1	J	155	
1	K	155	
1	L	155	
1	M	155	
1	N	155	
1	O	155	
1	P	155	
1	Q	155	
1	R	155	
1	S	155	
1	T	155	
1	U	155	
1	V	155	
1	W	155	
1	X	155	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 28040 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 Nucleoside diphosphate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	148	Total	C	N	O	S	0	0	0
			1162	748	200	210	4			
1	B	149	Total	C	N	O	S	0	0	0
			1169	750	201	214	4			
1	C	149	Total	C	N	O	S	0	0	0
			1171	752	201	214	4			
1	D	149	Total	C	N	O	S	0	0	0
			1171	752	201	214	4			
1	E	149	Total	C	N	O	S	0	0	0
			1171	752	201	214	4			
1	F	149	Total	C	N	O	S	0	0	0
			1171	752	201	214	4			
1	G	148	Total	C	N	O	S	0	0	0
			1159	745	200	210	4			
1	H	148	Total	C	N	O	S	0	0	0
			1162	748	200	210	4			
1	I	149	Total	C	N	O	S	0	0	0
			1171	752	201	214	4			
1	J	149	Total	C	N	O	S	0	0	0
			1171	752	201	214	4			
1	K	148	Total	C	N	O	S	0	0	0
			1159	745	200	210	4			
1	L	148	Total	C	N	O	S	0	0	0
			1162	748	200	210	4			
1	M	149	Total	C	N	O	S	0	0	0
			1171	752	201	214	4			
1	N	149	Total	C	N	O	S	0	0	0
			1171	752	201	214	4			
1	Q	149	Total	C	N	O	S	0	0	0
			1171	752	201	214	4			
1	R	149	Total	C	N	O	S	0	0	0
			1171	752	201	214	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	U	148	Total	C	N	O	S	0	0	0
			1162	748	200	210	4			
1	V	149	Total	C	N	O	S	0	0	0
			1169	750	201	214	4			
1	W	149	Total	C	N	O	S	0	0	0
			1171	752	201	214	4			
1	X	149	Total	C	N	O	S	0	0	0
			1171	752	201	214	4			
1	O	149	Total	C	N	O	S	0	0	0
			1171	752	201	214	4			
1	P	149	Total	C	N	O	S	0	0	0
			1171	752	201	214	4			
1	S	149	Total	C	N	O	S	0	0	0
			1171	752	201	214	4			
1	T	149	Total	C	N	O	S	0	0	0
			1171	752	201	214	4			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP B8NQF0
A	0	PRO	-	expression tag	UNP B8NQF0
B	-1	GLY	-	expression tag	UNP B8NQF0
B	0	PRO	-	expression tag	UNP B8NQF0
C	-1	GLY	-	expression tag	UNP B8NQF0
C	0	PRO	-	expression tag	UNP B8NQF0
D	-1	GLY	-	expression tag	UNP B8NQF0
D	0	PRO	-	expression tag	UNP B8NQF0
E	-1	GLY	-	expression tag	UNP B8NQF0
E	0	PRO	-	expression tag	UNP B8NQF0
F	-1	GLY	-	expression tag	UNP B8NQF0
F	0	PRO	-	expression tag	UNP B8NQF0
G	-1	GLY	-	expression tag	UNP B8NQF0
G	0	PRO	-	expression tag	UNP B8NQF0
H	-1	GLY	-	expression tag	UNP B8NQF0
H	0	PRO	-	expression tag	UNP B8NQF0
I	-1	GLY	-	expression tag	UNP B8NQF0
I	0	PRO	-	expression tag	UNP B8NQF0
J	-1	GLY	-	expression tag	UNP B8NQF0
J	0	PRO	-	expression tag	UNP B8NQF0
K	-1	GLY	-	expression tag	UNP B8NQF0
K	0	PRO	-	expression tag	UNP B8NQF0
L	-1	GLY	-	expression tag	UNP B8NQF0

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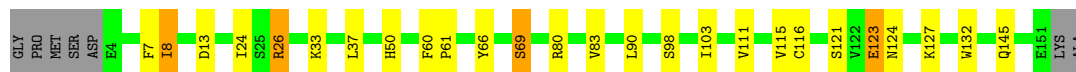
Chain	Residue	Modelled	Actual	Comment	Reference
L	0	PRO	-	expression tag	UNP B8NQF0
M	-1	GLY	-	expression tag	UNP B8NQF0
M	0	PRO	-	expression tag	UNP B8NQF0
N	-1	GLY	-	expression tag	UNP B8NQF0
N	0	PRO	-	expression tag	UNP B8NQF0
Q	-1	GLY	-	expression tag	UNP B8NQF0
Q	0	PRO	-	expression tag	UNP B8NQF0
R	-1	GLY	-	expression tag	UNP B8NQF0
R	0	PRO	-	expression tag	UNP B8NQF0
U	-1	GLY	-	expression tag	UNP B8NQF0
U	0	PRO	-	expression tag	UNP B8NQF0
V	-1	GLY	-	expression tag	UNP B8NQF0
V	0	PRO	-	expression tag	UNP B8NQF0
W	-1	GLY	-	expression tag	UNP B8NQF0
W	0	PRO	-	expression tag	UNP B8NQF0
X	-1	GLY	-	expression tag	UNP B8NQF0
X	0	PRO	-	expression tag	UNP B8NQF0
O	-1	GLY	-	expression tag	UNP B8NQF0
O	0	PRO	-	expression tag	UNP B8NQF0
P	-1	GLY	-	expression tag	UNP B8NQF0
P	0	PRO	-	expression tag	UNP B8NQF0
S	-1	GLY	-	expression tag	UNP B8NQF0
S	0	PRO	-	expression tag	UNP B8NQF0
T	-1	GLY	-	expression tag	UNP B8NQF0
T	0	PRO	-	expression tag	UNP B8NQF0

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.

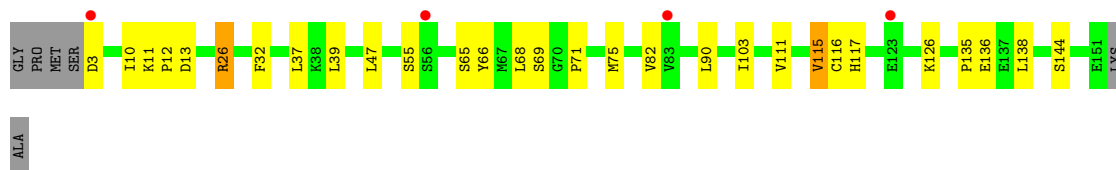
- Molecule 1: Nucleoside diphosphate kinase

Chain A: 



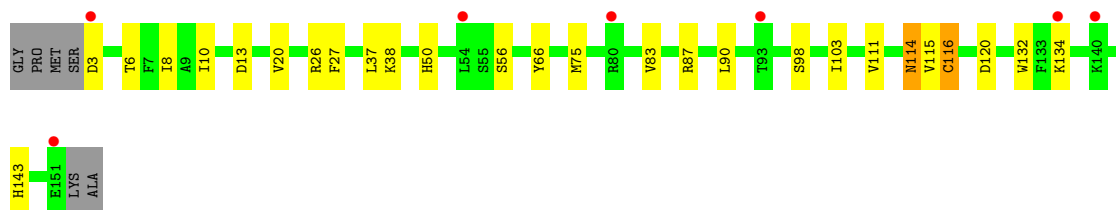
- Molecule 1: Nucleoside diphosphate kinase

Chain B: 



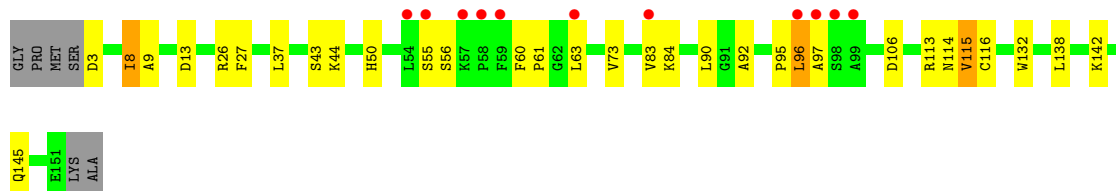
- Molecule 1: Nucleoside diphosphate kinase

Chain C: 

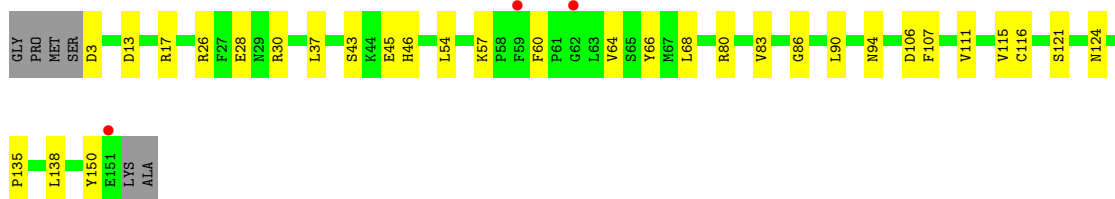
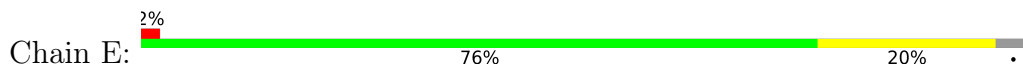


- Molecule 1: Nucleoside diphosphate kinase

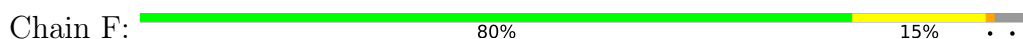
Chain D: 



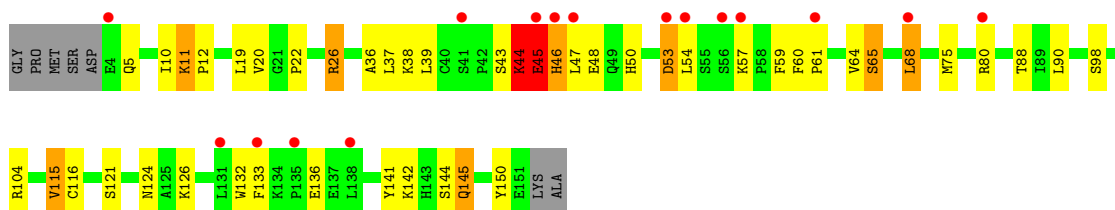
• Molecule 1: Nucleoside diphosphate kinase



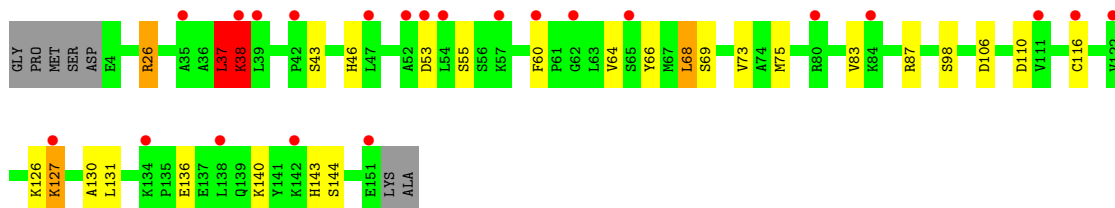
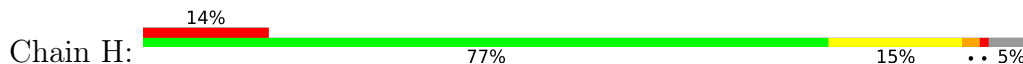
• Molecule 1: Nucleoside diphosphate kinase



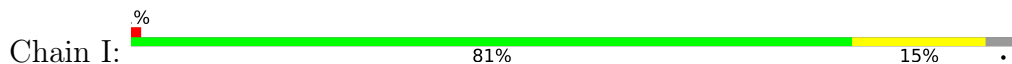
• Molecule 1: Nucleoside diphosphate kinase



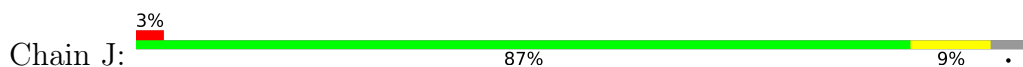
• Molecule 1: Nucleoside diphosphate kinase



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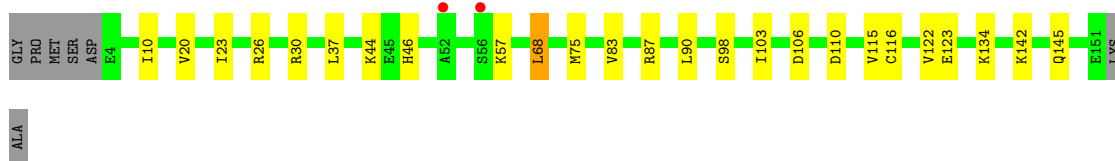
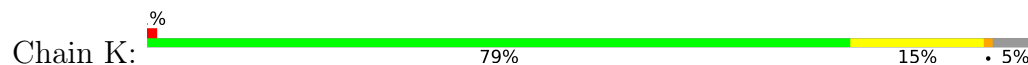


• Molecule 1: Nucleoside diphosphate kinase

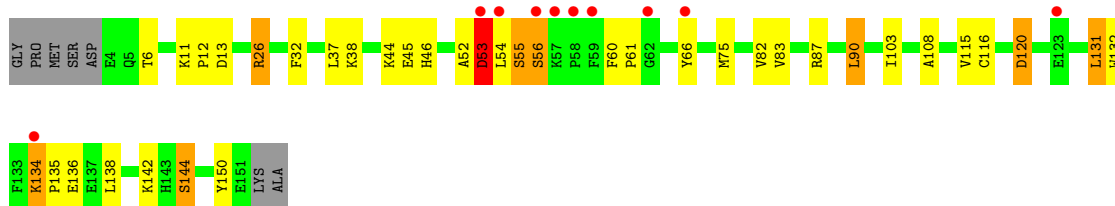




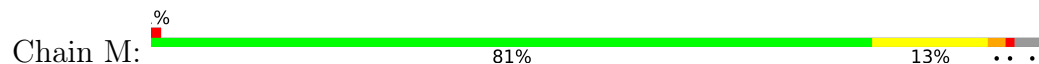
- Molecule 1: Nucleoside diphosphate kinase



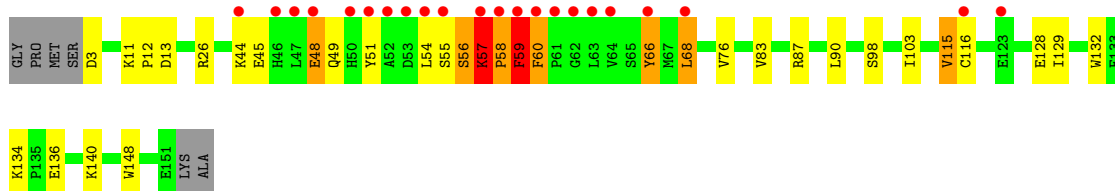
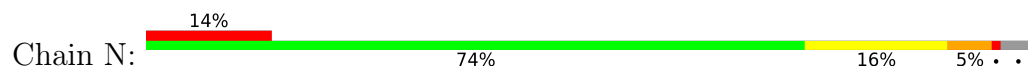
- Molecule 1: Nucleoside diphosphate kinase



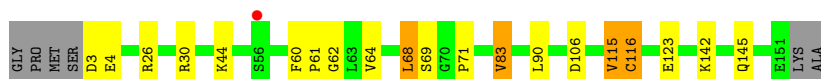
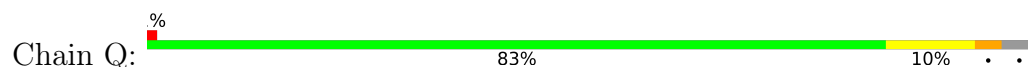
- Molecule 1: Nucleoside diphosphate kinase



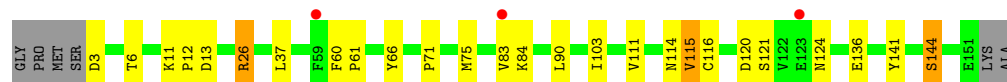
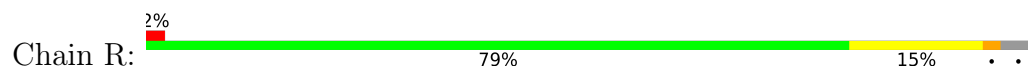
- Molecule 1: Nucleoside diphosphate kinase



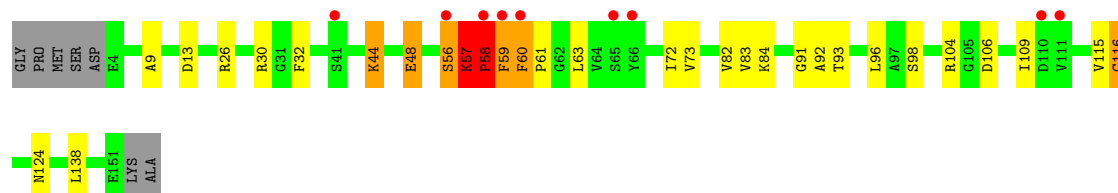
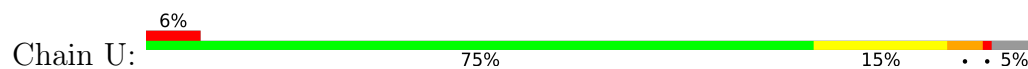
- Molecule 1: Nucleoside diphosphate kinase



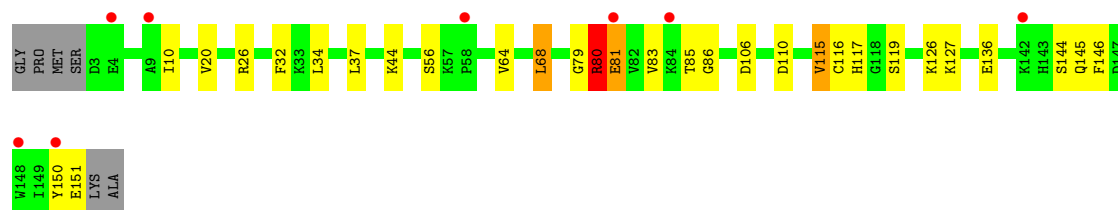
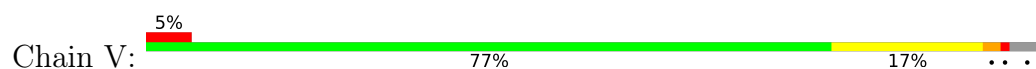
- Molecule 1: Nucleoside diphosphate kinase



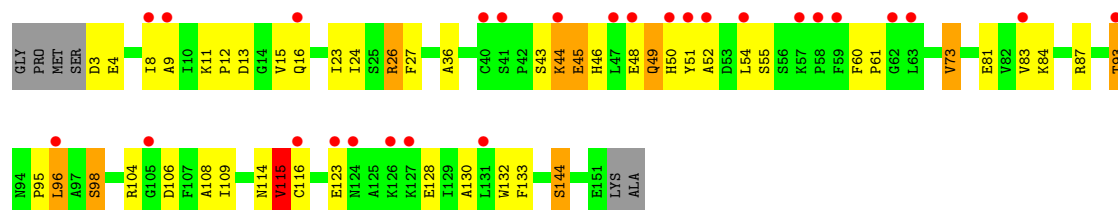
- Molecule 1: Nucleoside diphosphate kinase



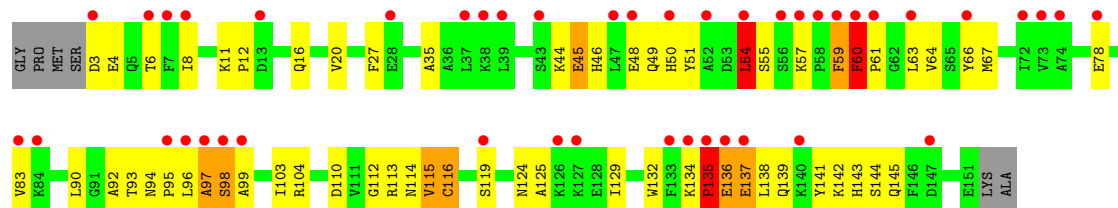
- Molecule 1: Nucleoside diphosphate kinase



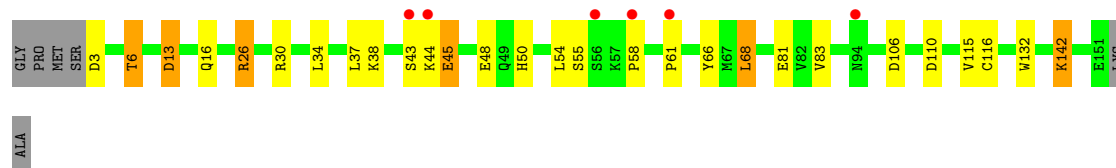
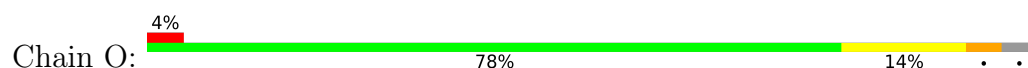
- Molecule 1: Nucleoside diphosphate kinase



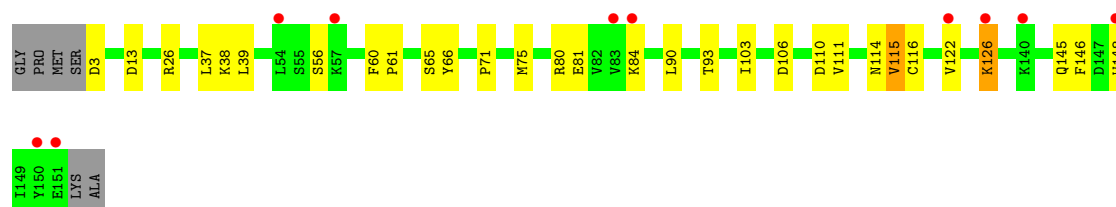
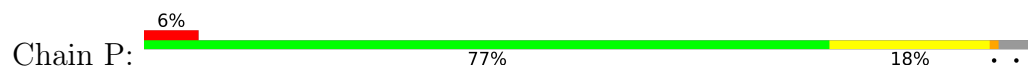
- Molecule 1: Nucleoside diphosphate kinase



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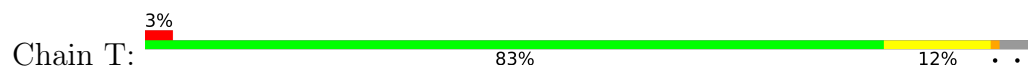
- Molecule 1: Nucleoside diphosphate kinase



- Molecule 1: Nucleoside diphosphate kinase



- Molecule 1: Nucleoside diphosphate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	190.84Å 169.47Å 146.94Å 90.00° 92.92° 90.00°	Depositor
Resolution (Å)	33.69 – 2.40 33.69 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (33.69-2.40) 98.8 (33.69-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.16 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.222 , 0.268 0.225 , 0.268	Depositor DCC
R_{free} test set	8979 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	48.2	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 29.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28040	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 2.54% 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	1.05	0/1192	1.46	3/1612 (0.2%)
1	B	1.02	0/1198	1.45	6/1619 (0.4%)
1	C	1.08	0/1201	1.48	4/1624 (0.2%)
1	D	1.06	0/1201	1.47	2/1624 (0.1%)
1	E	1.08	0/1201	1.43	2/1624 (0.1%)
1	F	1.04	0/1201	1.41	3/1624 (0.2%)
1	G	1.10	0/1189	1.56	5/1608 (0.3%)
1	H	1.06	0/1192	1.52	5/1612 (0.3%)
1	I	1.08	0/1201	1.49	2/1624 (0.1%)
1	J	1.07	0/1201	1.45	0/1624
1	K	1.07	0/1189	1.44	2/1608 (0.1%)
1	L	1.09	0/1192	1.46	3/1612 (0.2%)
1	M	1.10	0/1201	1.43	4/1624 (0.2%)
1	N	1.06	0/1201	1.44	0/1624
1	O	1.09	0/1201	1.46	2/1624 (0.1%)
1	P	1.06	0/1201	1.49	3/1624 (0.2%)
1	Q	1.07	0/1201	1.45	4/1624 (0.2%)
1	R	1.03	0/1201	1.41	1/1624 (0.1%)
1	S	1.03	0/1201	1.45	3/1624 (0.2%)
1	T	1.07	0/1201	1.46	2/1624 (0.1%)
1	U	1.13	1/1192 (0.1%)	1.49	8/1612 (0.5%)
1	V	1.11	0/1198	1.50	5/1619 (0.3%)
1	W	1.12	0/1201	1.53	6/1624 (0.4%)
1	X	1.14	0/1201	1.58	6/1624 (0.4%)
All	All	1.08	1/28758 (0.0%)	1.47	81/38886 (0.2%)

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	C	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	2
1	H	0	2
1	L	0	2
1	N	0	2
1	S	0	1
1	U	0	2
1	W	0	2
1	X	0	6
All	All	0	20

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	U	72	ILE	C-O	6.37	1.30	1.24

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	140	LYS	CB-CA-C	6.90	121.82	110.78
1	T	59	PHE	CA-CB-CG	6.53	120.33	113.80
1	C	143	HIS	CA-C-N	6.51	129.89	120.38
1	C	143	HIS	C-N-CA	6.51	129.89	120.38
1	P	3	ASP	CA-C-N	6.42	130.26	120.82

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	56	SER	Peptide
1	G	44	LYS	Peptide
1	G	45	GLU	Peptide
1	H	127	LYS	Peptide
1	H	37	LEU	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	1162	0	1157	10	0
1	B	1169	0	1158	16	0
1	C	1171	0	1164	12	0
1	D	1171	0	1164	17	0
1	E	1171	0	1164	14	0
1	F	1171	0	1164	12	0
1	G	1159	0	1148	58	0
1	H	1162	0	1157	60	0
1	I	1171	0	1164	12	0
1	J	1171	0	1164	6	0
1	K	1159	0	1148	9	0
1	L	1162	0	1157	23	0
1	M	1171	0	1164	10	0
1	N	1171	0	1163	86	0
1	O	1171	0	1164	17	0
1	P	1171	0	1164	18	0
1	Q	1171	0	1164	7	0
1	R	1171	0	1164	13	0
1	S	1171	0	1164	19	0
1	T	1171	0	1164	11	0
1	U	1162	0	1157	80	0
1	V	1169	0	1158	21	0
1	W	1171	0	1164	31	0
1	X	1171	0	1164	45	0
All	All	28040	0	27863	481	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 9.

The worst 5 of 481 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:N:56:SER:N	1:U:58:PRO:HA	1.30	1.45
1:G:38:LYS:HA	1:H:38:LYS:CG	1.50	1.41
1:N:57:LYS:CB	1:U:58:PRO:CD	1.98	1.40
1:N:57:LYS:CG	1:U:58:PRO:HD3	1.58	1.33
1:N:56:SER:OG	1:U:59:PHE:C	1.86	1.19

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	146/155 (94%)	142 (97%)	3 (2%)	1 (1%)	18	28
1	B	147/155 (95%)	141 (96%)	5 (3%)	1 (1%)	18	28
1	C	147/155 (95%)	140 (95%)	6 (4%)	1 (1%)	18	28
1	D	147/155 (95%)	134 (91%)	11 (8%)	2 (1%)	9	13
1	E	147/155 (95%)	143 (97%)	3 (2%)	1 (1%)	18	28
1	F	147/155 (95%)	140 (95%)	5 (3%)	2 (1%)	9	13
1	G	146/155 (94%)	131 (90%)	11 (8%)	4 (3%)	4	4
1	H	146/155 (94%)	136 (93%)	9 (6%)	1 (1%)	18	28
1	I	147/155 (95%)	142 (97%)	3 (2%)	2 (1%)	9	13
1	J	147/155 (95%)	142 (97%)	4 (3%)	1 (1%)	18	28
1	K	146/155 (94%)	140 (96%)	5 (3%)	1 (1%)	18	28
1	L	146/155 (94%)	133 (91%)	9 (6%)	4 (3%)	4	4
1	M	147/155 (95%)	141 (96%)	5 (3%)	1 (1%)	18	28
1	N	147/155 (95%)	132 (90%)	9 (6%)	6 (4%)	2	2
1	O	147/155 (95%)	141 (96%)	5 (3%)	1 (1%)	18	28
1	P	147/155 (95%)	135 (92%)	11 (8%)	1 (1%)	18	28
1	Q	147/155 (95%)	140 (95%)	6 (4%)	1 (1%)	18	28
1	R	147/155 (95%)	143 (97%)	3 (2%)	1 (1%)	18	28
1	S	147/155 (95%)	139 (95%)	6 (4%)	2 (1%)	9	13
1	T	147/155 (95%)	136 (92%)	9 (6%)	2 (1%)	9	13
1	U	146/155 (94%)	136 (93%)	7 (5%)	3 (2%)	5	7
1	V	147/155 (95%)	138 (94%)	7 (5%)	2 (1%)	9	13
1	W	147/155 (95%)	130 (88%)	13 (9%)	4 (3%)	4	4
1	X	147/155 (95%)	126 (86%)	15 (10%)	6 (4%)	2	2
All	All	3522/3720 (95%)	3301 (94%)	170 (5%)	51 (1%)	9	13

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	115	VAL
1	C	115	VAL
1	G	45	GLU
1	G	115	VAL
1	I	115	VAL

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	123/129 (95%)	110 (89%)	13 (11%)	6	10
1	B	124/129 (96%)	117 (94%)	7 (6%)	19	33
1	C	125/129 (97%)	119 (95%)	6 (5%)	23	40
1	D	125/129 (97%)	115 (92%)	10 (8%)	11	19
1	E	125/129 (97%)	116 (93%)	9 (7%)	13	23
1	F	125/129 (97%)	118 (94%)	7 (6%)	19	33
1	G	122/129 (95%)	106 (87%)	16 (13%)	4	5
1	H	123/129 (95%)	115 (94%)	8 (6%)	15	27
1	I	125/129 (97%)	115 (92%)	10 (8%)	11	19
1	J	125/129 (97%)	122 (98%)	3 (2%)	43	65
1	K	122/129 (95%)	113 (93%)	9 (7%)	13	22
1	L	123/129 (95%)	112 (91%)	11 (9%)	9	15
1	M	125/129 (97%)	118 (94%)	7 (6%)	19	33
1	N	125/129 (97%)	112 (90%)	13 (10%)	7	10
1	O	125/129 (97%)	113 (90%)	12 (10%)	8	12
1	P	125/129 (97%)	119 (95%)	6 (5%)	23	40
1	Q	125/129 (97%)	116 (93%)	9 (7%)	13	23
1	R	125/129 (97%)	118 (94%)	7 (6%)	19	33
1	S	125/129 (97%)	113 (90%)	12 (10%)	8	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	T	125/129 (97%)	116 (93%)	9 (7%)	13	23
1	U	123/129 (95%)	113 (92%)	10 (8%)	11	18
1	V	124/129 (96%)	112 (90%)	12 (10%)	8	12
1	W	125/129 (97%)	112 (90%)	13 (10%)	7	10
1	X	125/129 (97%)	111 (89%)	14 (11%)	6	9
All	All	2984/3096 (96%)	2751 (92%)	233 (8%)	11	20

5 of 233 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	140	LYS
1	S	136	GLU
1	R	136	GLU
1	S	119	SER
1	O	45	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	29	ASN
1	T	124	ASN
1	R	46	HIS
1	T	117	HIS
1	O	50	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 ⓘ

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	148/155 (95%)	0.08	0 100 100	37, 49, 66, 84	0
1	B	149/155 (96%)	0.06	4 (2%) 56 52	34, 49, 80, 96	0
1	C	149/155 (96%)	0.23	7 (4%) 36 32	38, 53, 79, 93	0
1	D	149/155 (96%)	0.44	11 (7%) 20 17	39, 55, 97, 131	0
1	E	149/155 (96%)	0.10	3 (2%) 65 60	33, 49, 67, 90	0
1	F	149/155 (96%)	-0.01	0 100 100	31, 48, 70, 84	0
1	G	148/155 (95%)	0.90	16 (10%) 11 8	41, 63, 96, 131	0
1	H	148/155 (95%)	0.99	22 (14%) 5 4	47, 66, 108, 127	0
1	I	149/155 (96%)	0.09	1 (0%) 84 81	37, 52, 68, 79	0
1	J	149/155 (96%)	0.15	4 (2%) 56 52	37, 52, 79, 118	0
1	K	148/155 (95%)	0.20	2 (1%) 73 69	36, 51, 69, 85	0
1	L	148/155 (95%)	0.49	10 (6%) 23 20	36, 56, 99, 155	0
1	M	149/155 (96%)	0.11	2 (1%) 75 71	36, 48, 65, 79	0
1	N	149/155 (96%)	0.75	22 (14%) 5 4	38, 58, 148, 247	0
1	O	149/155 (96%)	0.39	6 (4%) 42 38	36, 53, 83, 98	0
1	P	149/155 (96%)	0.53	10 (6%) 24 20	34, 62, 92, 115	0
1	Q	149/155 (96%)	0.03	1 (0%) 84 81	33, 47, 66, 86	0
1	R	149/155 (96%)	0.16	3 (2%) 65 60	35, 52, 75, 102	0
1	S	149/155 (96%)	0.17	6 (4%) 42 38	36, 53, 77, 96	0
1	T	149/155 (96%)	0.26	4 (2%) 56 52	36, 53, 75, 114	0
1	U	148/155 (95%)	0.39	9 (6%) 27 23	36, 53, 79, 176	0
1	V	149/155 (96%)	0.54	8 (5%) 31 28	41, 63, 90, 114	0
1	W	149/155 (96%)	1.22	27 (18%) 3 3	50, 71, 122, 156	0
1	X	149/155 (96%)	1.49	44 (29%) 1 1	50, 72, 117, 148	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
All	All	3570/3720 (95%)	0.41	222 (6%)	26	23	31, 55, 92, 247	0

The worst 5 of 222 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	54	LEU	8.4
1	N	68	LEU	7.0
1	N	52	ALA	6.0
1	N	51	TYR	5.5
1	G	68	LEU	5.5

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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.