



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2026 – 08:02 PM UTC

PDB ID : 7MK0 / pdb_00007mk0
Title : Trypanosoma cruzi Nucleoside Diphosphate Kinase 1 form a quinary multi-hexameric structure
Authors : Gomez, J.A.; Aguilar, C.F.
Deposited on : 2021-04-21
Resolution : 3.50 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

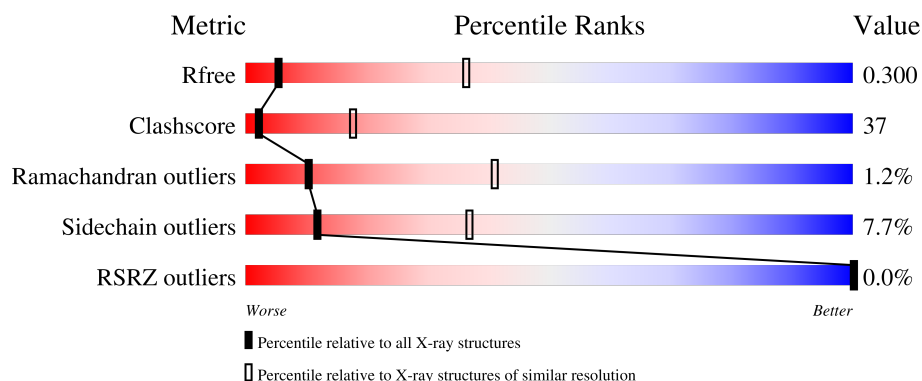
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

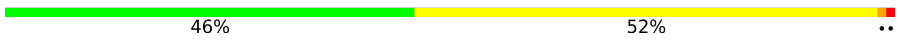
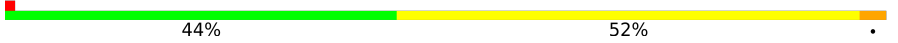
The reported resolution of this entry is 3.50 Å.

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.



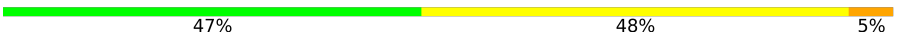
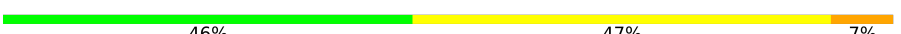
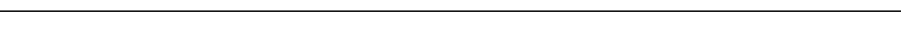
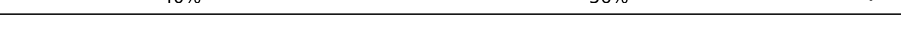
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	151	
1	B	151	
1	C	151	
1	D	151	
1	E	151	

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Mol	Chain	Length	Quality of chain
1	F	151	 56% 39% 5% .
1	G	151	 47% 48% 5%
1	H	151	 41% 54% 5%
1	I	151	 50% 44% 5%
1	J	151	 46% 47% 7%
1	K	151	 49% 46% 5% .
1	L	151	 50% 46% .
1	M	151	 36% 58% 7%
1	N	151	 43% 50% 6% .
1	O	151	 48% 46% 5% .
1	P	151	 46% 50% 5%
1	Q	151	 56% 37% 5% .
1	R	151	 54% 42% . .
1	S	151	 54% 42% .
1	T	151	 40% 56% .
1	U	151	 56% 39% 5%
1	V	151	 50% 46% .
1	W	151	 58% 37% 5% .
1	X	151	 43% 52% . .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 28296 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	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	B	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	C	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	D	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	E	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	F	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	G	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	H	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	I	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	J	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	K	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	L	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	M	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	N	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	O	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	P	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			

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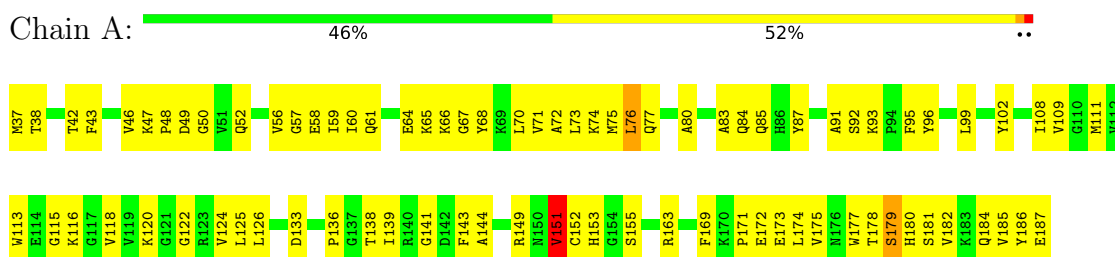
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	R	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	S	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	T	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	U	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	V	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	W	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	X	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			

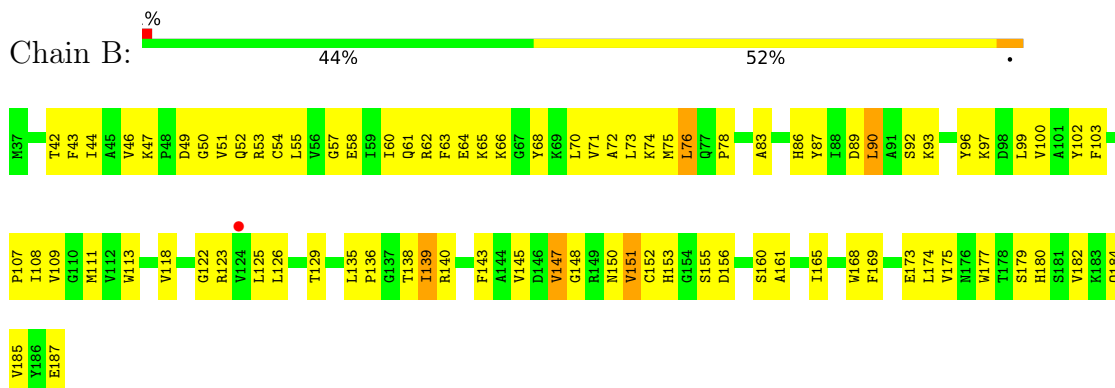
3 Residue-property plots

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.

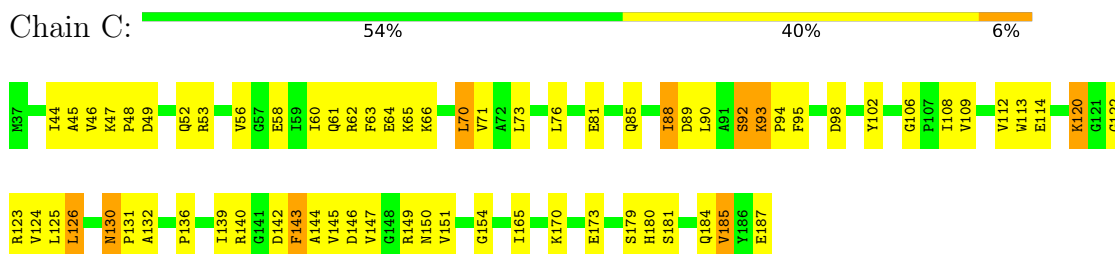
- Molecule 1: Nucleoside diphosphate kinase



- Molecule 1: Nucleoside diphosphate kinase

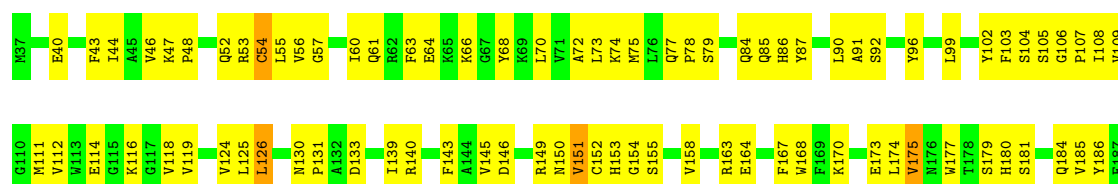


- Molecule 1: Nucleoside diphosphate kinase

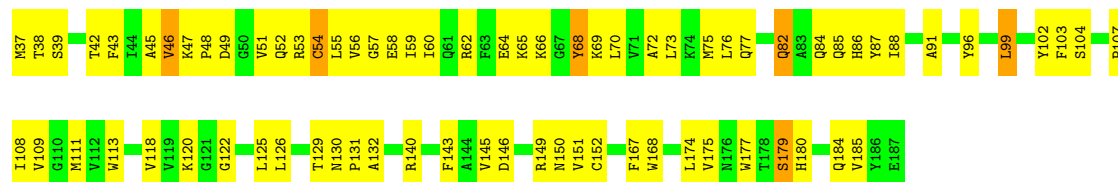


- Molecule 1: Nucleoside diphosphate kinase

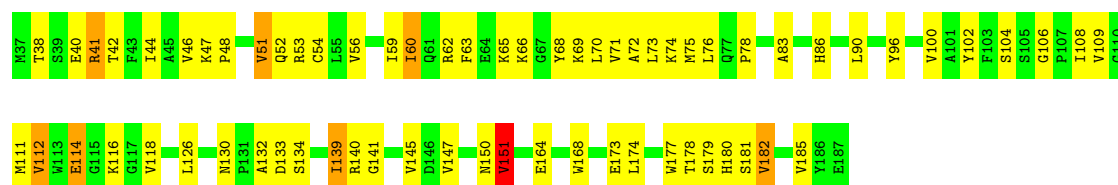




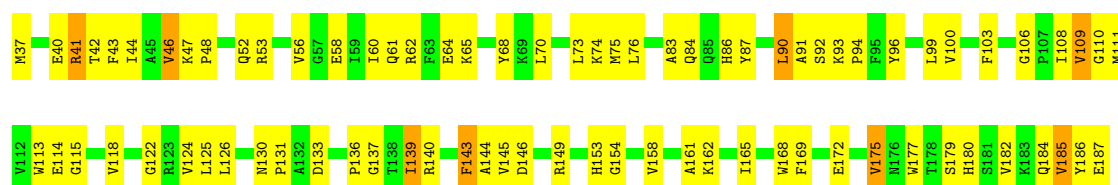
• Molecule 1: Nucleoside diphosphate kinase



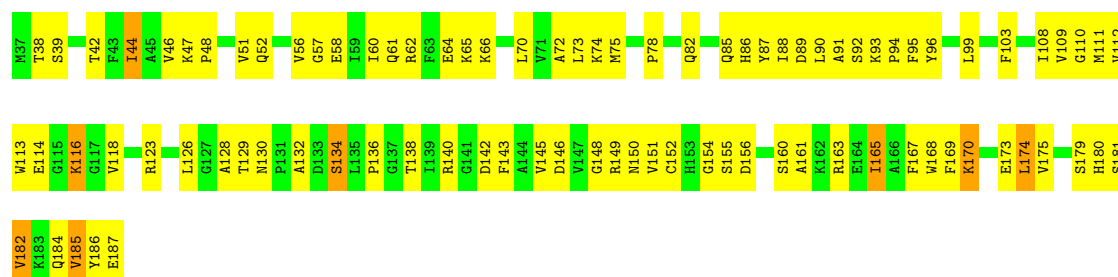
• Molecule 1: Nucleoside diphosphate kinase



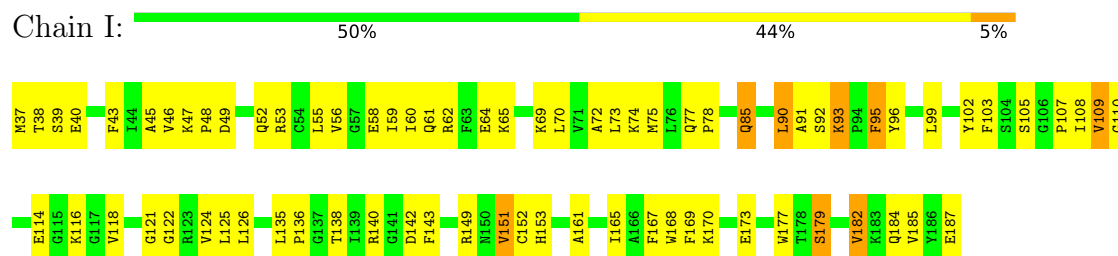
• Molecule 1: Nucleoside diphosphate kinase



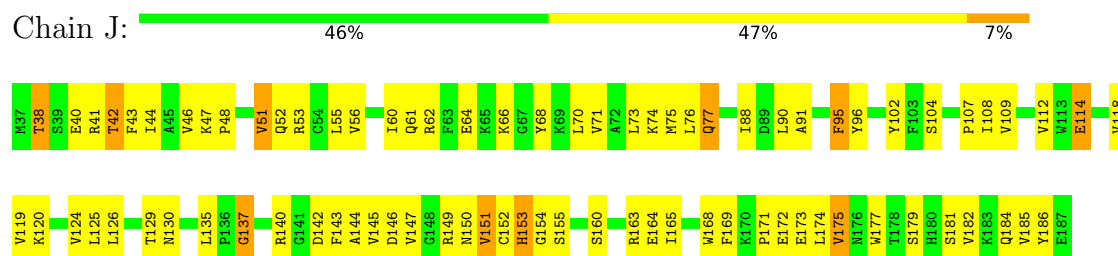
• Molecule 1: Nucleoside diphosphate kinase



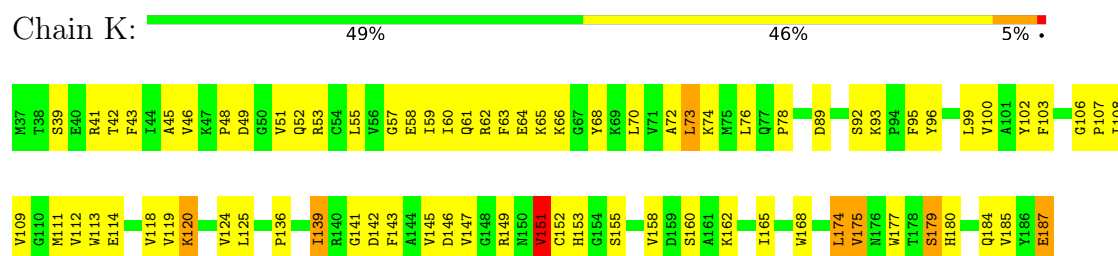
- Molecule 1: Nucleoside diphosphate kinase



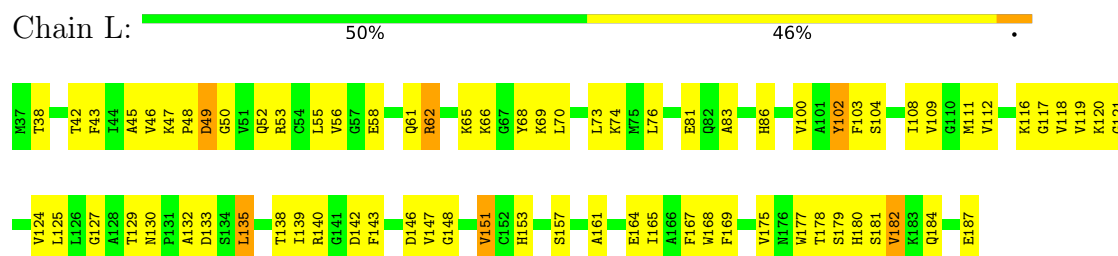
- Molecule 1: Nucleoside diphosphate kinase



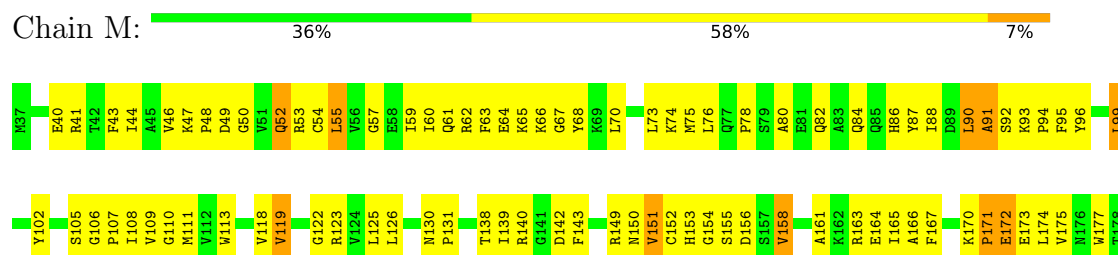
- Molecule 1: Nucleoside diphosphate kinase



- Molecule 1: Nucleoside diphosphate kinase



- Molecule 1: Nucleoside diphosphate kinase



S179
H160
S181
V182
K183
Q184
Y186
E187

• Molecule 1: Nucleoside diphosphate kinase

Chain N: 43% 50% 6% •

K37 R41 T42 T44 V46 K47 F48 D49 G50 V51 Q52 R53 R54 L55 V56 G57 E58 T59 I60 F63 E64 K65 K66 G67 Y68 K69 L70 V71 A72 L73 L74 M75 L76 Q82 A83 H86 Y87 I88 D89 L90 A91 S92 K93 P94 F95 Y96 L99 V100 A101 Y102 F103 S104 S105 G106 P107

I108 V109 M111 V112 V113 E114 G115 K116 G117 V118 V119 K120 R123 V124 L125 T129 N130 P131 A132 I139 R140 G141 D142 F143 A144 V145 V146 V147 G148 R149 N150 V151 C152 G153 D156 S157 A161 I165 A166 F167 W168 E172 V175 N176 W177 T178 S179 H180 S181 V182 K183

Q184 V185 E187

• Molecule 1: Nucleoside diphosphate kinase

Chain O: 48% 46% 5% •

K37 R41 I44 A45 V46 K47 P48 D49 G50 V51 Q52 R53 C54 L55 G56 G57 E58 I59 I60 Q61 E64 K65 K66 L70 V71 A72 L73 K74 M75 L76 Q77 P78 S79 A80 Q82 A83 Q84 Q85 Y87 I88 D89 L90 A91 S92 K93 F95 Y96 K97 D98 L99 V100 A101 Y102

S105 G106 P107 V109 G110 M111 V112 E114 V118 V119 K120 G121 L122 G123 V124 L125 L126 G127 A128 N129 P131 A132 D133 S134 L135 P136 T139 R140 A144 V145 D146 R149 N150 V151 V154 G154 S160 F167 E172 V175 Q184 V185 Y186 E187

• Molecule 1: Nucleoside diphosphate kinase

Chain P: 46% 50% 5% •

K37 R41 T42 T44 A45 V46 K47 P48 D49 G50 V51 Q52 R53 C54 L55 V56 G57 E58 I59 I60 F63 E64 K65 K66 G67 Y68 A72 L73 K74 M75 A80 Q82 A83 Q84 H86 Y87 I88 D89 L90 K93 Y96 L99 P107 I108 V109 G110 M111 W113

E114 G115 K120 V124 L125 L126 G127 A128 N129 P131 I139 R140 F143 A144 V145 D146 V147 N150 V151 C152 H153 D156 S157 A161 A162 R163 E164 I165 A166 F167 W168 F169 E173 L174 V175 W176 W177 S179 H180 S181 Q184 V185 Y186 E187

• Molecule 1: Nucleoside diphosphate kinase

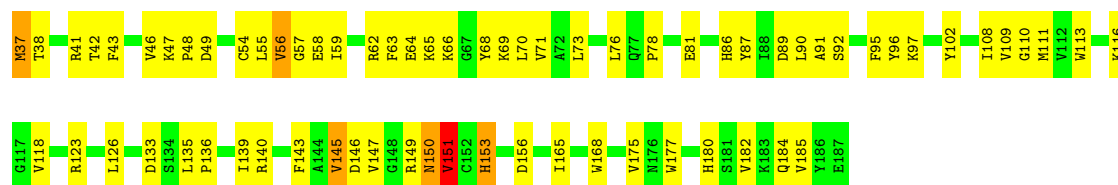
Chain Q: 56% 37% 5% •

K37 R41 V46 P48 D49 G50 V51 Q52 R53 C54 L55 I59 I60 Q61 R62 F63 E64 K65 K66 G67 Y68 V71 A72 L73 K74 M75 L76 Q84 Y87 L90 Y96 A101 Y102 S105 G106 P107 I108 V109 G110 M111 V112 W113 G114 G115 V118 G122

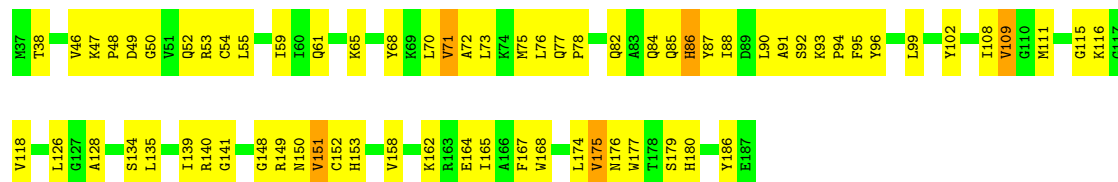
L125 L126 N130 P131 L135 T139 R140 G141 D142 F143 A144 V145 G148 R149 N150 V151 C152 H153 S157 S160 I165 K170 P171 E172 E173 W177 T178 S179 V182 K183 Q184 V185 Y186 E187

• Molecule 1: Nucleoside diphosphate kinase

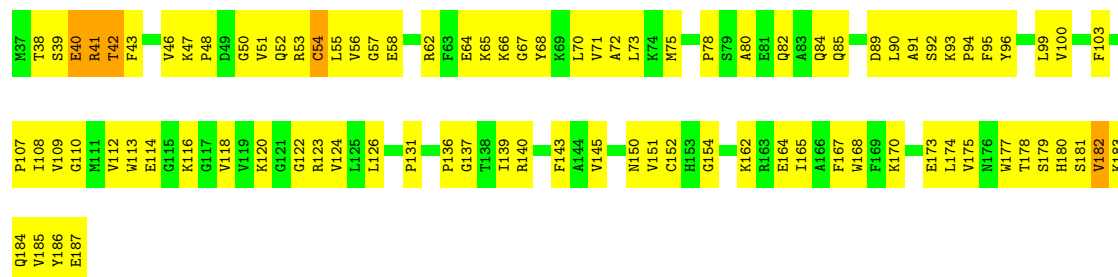
Chain R: 54% 42% • •



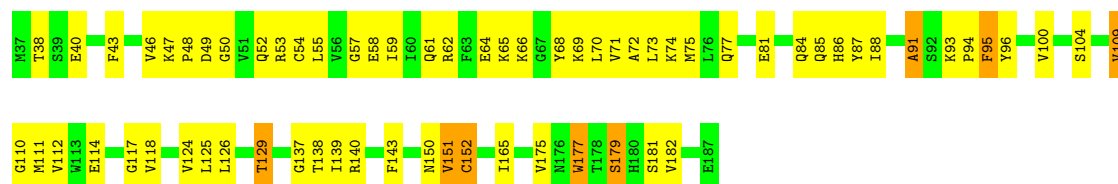
- Molecule 1: Nucleoside diphosphate kinase



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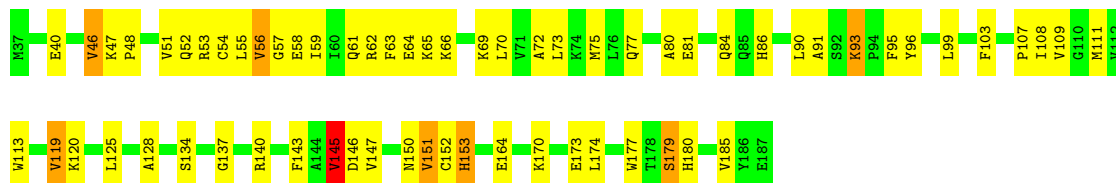


- Molecule 1: Nucleoside diphosphate kinase

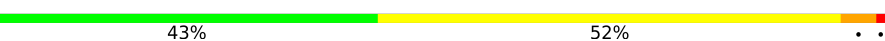


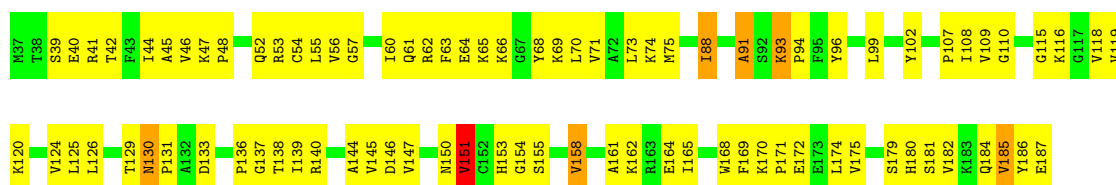
- Molecule 1: Nucleoside diphosphate kinase

Chain W:  58% 37% 5%



- Molecule 1: Nucleoside diphosphate kinase

Chain X:  43% 52%



4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	127.84Å 127.84Å 275.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 3.50 10.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (10.00-3.50) 99.4 (10.00-3.50)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.269 , 0.278 0.280 , 0.300	Depositor DCC
R_{free} test set	3156 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.27$, $\langle L^2 \rangle = 0.11$	Xtriage
Estimated twinning fraction	0.309 for -h,-k,l 0.318 for h,-h-k,-l 0.317 for -k,-h,-l	Xtriage
Reported twinning fraction	0.291 for H, K, L 0.237 for -K, -H, -L 0.240 for K, H, -L 0.232 for -h,-k,l	Depositor
Outliers	0 of 63155 reflections	Xtriage
F_o, F_c correlation	0.62	EDS
Total number of atoms	28296	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.58% 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	0.74	0/1206	1.08	3/1628 (0.2%)
1	B	0.74	0/1206	1.01	2/1628 (0.1%)
1	C	0.74	0/1206	1.07	7/1628 (0.4%)
1	D	0.73	0/1206	1.04	0/1628
1	E	0.73	0/1206	1.08	1/1628 (0.1%)
1	F	0.71	0/1206	1.06	6/1628 (0.4%)
1	G	0.75	0/1206	1.09	3/1628 (0.2%)
1	H	0.70	0/1206	1.03	0/1628
1	I	0.71	0/1206	1.07	2/1628 (0.1%)
1	J	0.73	0/1206	1.07	6/1628 (0.4%)
1	K	0.71	0/1206	1.05	3/1628 (0.2%)
1	L	0.74	0/1206	1.05	0/1628
1	M	0.77	0/1206	1.09	2/1628 (0.1%)
1	N	0.73	0/1206	1.01	2/1628 (0.1%)
1	O	0.72	0/1206	1.04	1/1628 (0.1%)
1	P	0.72	0/1206	1.07	4/1628 (0.2%)
1	Q	0.72	0/1206	1.03	6/1628 (0.4%)
1	R	0.76	0/1206	1.05	2/1628 (0.1%)
1	S	0.72	0/1206	1.03	0/1628
1	T	0.72	0/1206	1.02	1/1628 (0.1%)
1	U	0.72	0/1206	1.05	2/1628 (0.1%)
1	V	0.74	0/1206	1.07	3/1628 (0.2%)
1	W	0.72	0/1206	1.12	4/1628 (0.2%)
1	X	0.75	0/1206	1.11	6/1628 (0.4%)
All	All	0.73	0/28944	1.06	66/39072 (0.2%)

There are no bond length outliers.

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	130	ASN	CA-C-N	8.10	129.97	119.84
1	X	130	ASN	C-N-CA	8.10	129.97	119.84
1	X	93	LYS	CA-C-N	7.61	129.35	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	93	LYS	C-N-CA	7.61	129.35	119.84
1	J	130	ASN	CA-C-N	7.25	127.88	119.47

There are no chirality outliers.

There are no planarity outliers.

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	1179	0	1178	210	0
1	B	1179	0	1178	128	0
1	C	1179	0	1178	150	0
1	D	1179	0	1178	154	0
1	E	1179	0	1178	116	0
1	F	1179	0	1178	63	0
1	G	1179	0	1178	127	0
1	H	1179	0	1178	142	0
1	I	1179	0	1178	98	0
1	J	1179	0	1178	119	0
1	K	1179	0	1178	93	0
1	L	1179	0	1178	99	0
1	M	1179	0	1178	158	1
1	N	1179	0	1178	111	0
1	O	1179	0	1178	110	1
1	P	1179	0	1178	127	0
1	Q	1179	0	1178	86	0
1	R	1179	0	1178	82	0
1	S	1179	0	1178	122	0
1	T	1179	0	1178	175	0
1	U	1179	0	1178	90	0
1	V	1179	0	1178	123	0
1	W	1179	0	1178	95	0
1	X	1179	0	1178	118	0
All	All	28296	0	28272	2082	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 37.

The worst 5 of 2082 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:180:HIS:NE2	1:P:184:GLN:HG3	1.28	1.44
1:C:93:LYS:CA	1:M:92:SER:HB2	1.46	1.42
1:C:93:LYS:HA	1:M:92:SER:CB	1.54	1.38
1:B:92:SER:O	1:N:92:SER:HB3	1.29	1.32
1:G:184:GLN:HG3	1:L:180:HIS:CD2	1.65	1.31

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)
1:M:172:GLU:OE1	1:O:78:PRO:O[3_555]	2.07	0.13

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	149/151 (99%)	139 (93%)	8 (5%)	2 (1%)	9	39
1	B	149/151 (99%)	141 (95%)	7 (5%)	1 (1%)	18	51
1	C	149/151 (99%)	145 (97%)	3 (2%)	1 (1%)	18	51
1	D	149/151 (99%)	142 (95%)	5 (3%)	2 (1%)	9	39
1	E	149/151 (99%)	141 (95%)	6 (4%)	2 (1%)	9	39
1	F	149/151 (99%)	145 (97%)	3 (2%)	1 (1%)	18	51
1	G	149/151 (99%)	139 (93%)	10 (7%)	0	100	100
1	H	149/151 (99%)	139 (93%)	8 (5%)	2 (1%)	9	39
1	I	149/151 (99%)	142 (95%)	5 (3%)	2 (1%)	9	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
1	K	149/151 (99%)	141 (95%)	7 (5%)	1 (1%)	18	51
1	L	149/151 (99%)	139 (93%)	8 (5%)	2 (1%)	9	39
1	M	149/151 (99%)	138 (93%)	10 (7%)	1 (1%)	18	51
1	N	149/151 (99%)	132 (89%)	13 (9%)	4 (3%)	4	27
1	O	149/151 (99%)	135 (91%)	12 (8%)	2 (1%)	9	39
1	P	149/151 (99%)	139 (93%)	8 (5%)	2 (1%)	9	39
1	Q	149/151 (99%)	138 (93%)	9 (6%)	2 (1%)	9	39
1	R	149/151 (99%)	136 (91%)	10 (7%)	3 (2%)	6	32
1	S	149/151 (99%)	142 (95%)	5 (3%)	2 (1%)	9	39
1	T	149/151 (99%)	137 (92%)	8 (5%)	4 (3%)	4	27
1	U	149/151 (99%)	138 (93%)	8 (5%)	3 (2%)	6	32
1	V	149/151 (99%)	132 (89%)	15 (10%)	2 (1%)	9	39
1	W	149/151 (99%)	143 (96%)	4 (3%)	2 (1%)	9	39
1	X	149/151 (99%)	135 (91%)	13 (9%)	1 (1%)	18	51
All	All	3576/3624 (99%)	3343 (94%)	189 (5%)	44 (1%)	10	41

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	VAL
1	F	151	VAL
1	L	151	VAL
1	R	56	VAL
1	R	151	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	126/126 (100%)	120 (95%)	6 (5%)	23	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	126/126 (100%)	119 (94%)	7 (6%)	19	46
1	C	126/126 (100%)	116 (92%)	10 (8%)	11	36
1	D	126/126 (100%)	114 (90%)	12 (10%)	8	31
1	E	126/126 (100%)	117 (93%)	9 (7%)	13	38
1	F	126/126 (100%)	117 (93%)	9 (7%)	13	38
1	G	126/126 (100%)	119 (94%)	7 (6%)	19	46
1	H	126/126 (100%)	115 (91%)	11 (9%)	9	33
1	I	126/126 (100%)	119 (94%)	7 (6%)	19	46
1	J	126/126 (100%)	116 (92%)	10 (8%)	11	36
1	K	126/126 (100%)	112 (89%)	14 (11%)	6	25
1	L	126/126 (100%)	118 (94%)	8 (6%)	16	42
1	M	126/126 (100%)	110 (87%)	16 (13%)	4	21
1	N	126/126 (100%)	111 (88%)	15 (12%)	5	23
1	O	126/126 (100%)	110 (87%)	16 (13%)	4	21
1	P	126/126 (100%)	118 (94%)	8 (6%)	16	42
1	Q	126/126 (100%)	119 (94%)	7 (6%)	19	46
1	R	126/126 (100%)	116 (92%)	10 (8%)	11	36
1	S	126/126 (100%)	115 (91%)	11 (9%)	9	33
1	T	126/126 (100%)	120 (95%)	6 (5%)	23	49
1	U	126/126 (100%)	117 (93%)	9 (7%)	13	38
1	V	126/126 (100%)	117 (93%)	9 (7%)	13	38
1	W	126/126 (100%)	118 (94%)	8 (6%)	16	42
1	X	126/126 (100%)	117 (93%)	9 (7%)	13	38
All	All	3024/3024 (100%)	2790 (92%)	234 (8%)	12	37

5 of 234 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	99	LEU
1	W	145	VAL
1	O	79	SER
1	W	119	VAL
1	U	74	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	153	HIS
1	W	86	HIS
1	N	85	GLN
1	V	180	HIS
1	X	180	HIS

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](#)

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 ⓘ

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	151/151 (100%)	-0.98	0	100	100	4, 7, 57, 141	0
1	B	151/151 (100%)	-0.93	1 (0%)	84	63	4, 7, 48, 105	0
1	C	151/151 (100%)	-0.87	0	100	100	4, 7, 51, 107	0
1	D	151/151 (100%)	-1.04	0	100	100	2, 7, 46, 95	0
1	E	151/151 (100%)	-0.91	0	100	100	4, 7, 41, 74	0
1	F	151/151 (100%)	-1.09	0	100	100	4, 7, 48, 78	0
1	G	151/151 (100%)	-1.00	0	100	100	4, 7, 53, 95	0
1	H	151/151 (100%)	-0.85	0	100	100	4, 7, 54, 97	0
1	I	151/151 (100%)	-0.92	0	100	100	4, 7, 54, 105	0
1	J	151/151 (100%)	-0.99	0	100	100	4, 7, 54, 91	0
1	K	151/151 (100%)	-0.91	0	100	100	4, 7, 46, 84	0
1	L	151/151 (100%)	-0.90	0	100	100	4, 7, 43, 79	0
1	M	151/151 (100%)	-1.02	0	100	100	4, 7, 60, 93	0
1	N	151/151 (100%)	-0.95	0	100	100	4, 7, 47, 105	0
1	O	151/151 (100%)	-0.94	0	100	100	4, 7, 52, 96	0
1	P	151/151 (100%)	-1.02	0	100	100	4, 7, 51, 89	0
1	Q	151/151 (100%)	-0.89	0	100	100	4, 7, 42, 73	0
1	R	151/151 (100%)	-1.03	0	100	100	4, 7, 45, 90	0
1	S	151/151 (100%)	-0.95	0	100	100	4, 7, 49, 88	0
1	T	151/151 (100%)	-0.95	0	100	100	4, 7, 52, 118	0
1	U	151/151 (100%)	-1.05	0	100	100	4, 7, 53, 98	0
1	V	151/151 (100%)	-0.82	0	100	100	4, 7, 47, 98	0
1	W	151/151 (100%)	-1.01	0	100	100	4, 7, 42, 68	0
1	X	151/151 (100%)	-0.98	0	100	100	4, 7, 44, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3624/3624 (100%)	-0.96	1 (0%) 100 100	2, 7, 51, 141	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	124	VAL	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 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.