



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 09:51 pm BST

PDB ID : 3Q83
Title : Crystal structure of Staphylococcus aureus nucleoside diphosphate kinase
Authors : Srivastava, S.K.; Rajasree, K.; Gopal, B.
Deposited on : 2011-01-06
Resolution : 2.50 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 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	:	2.11
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

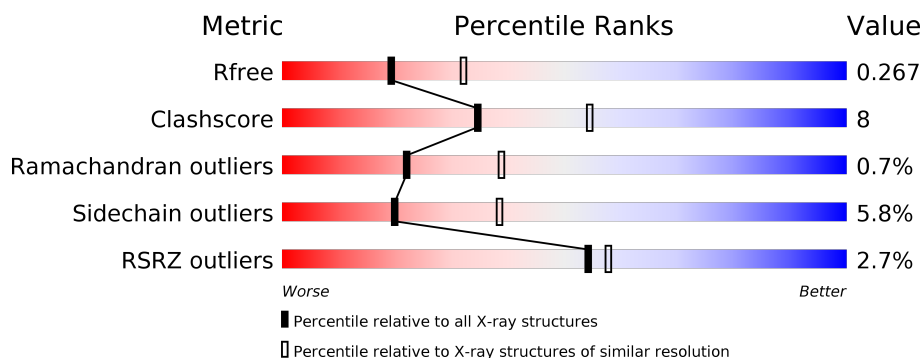
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	157	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>• 5%</div> </div> </div>
1	B	157	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>11%</div> <div>• 5%</div> </div> </div>
1	C	157	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>18%</div> <div>• 5%</div> </div> </div>
1	D	157	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>12%</div> <div>• 5%</div> </div> </div>
1	E	157	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>16%</div> <div>• 5%</div> </div> </div>
1	F	157	<div> <div>7%</div> <div> <div></div> <div>71%</div> <div>20%</div> <div>• 5%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7365 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	149	Total	C	N	O	S	0	0	0
			1161	731	202	223	5			
1	B	149	Total	C	N	O	S	0	0	0
			1155	728	201	221	5			
1	C	149	Total	C	N	O	S	0	0	0
			1152	726	201	220	5			
1	D	149	Total	C	N	O	S	0	0	0
			1161	731	202	223	5			
1	E	149	Total	C	N	O	S	0	0	0
			1157	729	202	221	5			
1	F	149	Total	C	N	O	S	0	0	0
			1150	722	201	222	5			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	150	LEU	-	EXPRESSION TAG	UNP Q5HFBV4
A	151	GLU	-	EXPRESSION TAG	UNP Q5HFBV4
A	152	HIS	-	EXPRESSION TAG	UNP Q5HFBV4
A	153	HIS	-	EXPRESSION TAG	UNP Q5HFBV4
A	154	HIS	-	EXPRESSION TAG	UNP Q5HFBV4
A	155	HIS	-	EXPRESSION TAG	UNP Q5HFBV4
A	156	HIS	-	EXPRESSION TAG	UNP Q5HFBV4
A	157	HIS	-	EXPRESSION TAG	UNP Q5HFBV4
B	150	LEU	-	EXPRESSION TAG	UNP Q5HFBV4
B	151	GLU	-	EXPRESSION TAG	UNP Q5HFBV4
B	152	HIS	-	EXPRESSION TAG	UNP Q5HFBV4
B	153	HIS	-	EXPRESSION TAG	UNP Q5HFBV4
B	154	HIS	-	EXPRESSION TAG	UNP Q5HFBV4
B	155	HIS	-	EXPRESSION TAG	UNP Q5HFBV4
B	156	HIS	-	EXPRESSION TAG	UNP Q5HFBV4
B	157	HIS	-	EXPRESSION TAG	UNP Q5HFBV4
C	150	LEU	-	EXPRESSION TAG	UNP Q5HFBV4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	151	GLU	-	EXPRESSION TAG	UNP Q5HJV4
C	152	HIS	-	EXPRESSION TAG	UNP Q5HJV4
C	153	HIS	-	EXPRESSION TAG	UNP Q5HJV4
C	154	HIS	-	EXPRESSION TAG	UNP Q5HJV4
C	155	HIS	-	EXPRESSION TAG	UNP Q5HJV4
C	156	HIS	-	EXPRESSION TAG	UNP Q5HJV4
C	157	HIS	-	EXPRESSION TAG	UNP Q5HJV4
D	150	LEU	-	EXPRESSION TAG	UNP Q5HJV4
D	151	GLU	-	EXPRESSION TAG	UNP Q5HJV4
D	152	HIS	-	EXPRESSION TAG	UNP Q5HJV4
D	153	HIS	-	EXPRESSION TAG	UNP Q5HJV4
D	154	HIS	-	EXPRESSION TAG	UNP Q5HJV4
D	155	HIS	-	EXPRESSION TAG	UNP Q5HJV4
D	156	HIS	-	EXPRESSION TAG	UNP Q5HJV4
D	157	HIS	-	EXPRESSION TAG	UNP Q5HJV4
E	150	LEU	-	EXPRESSION TAG	UNP Q5HJV4
E	151	GLU	-	EXPRESSION TAG	UNP Q5HJV4
E	152	HIS	-	EXPRESSION TAG	UNP Q5HJV4
E	153	HIS	-	EXPRESSION TAG	UNP Q5HJV4
E	154	HIS	-	EXPRESSION TAG	UNP Q5HJV4
E	155	HIS	-	EXPRESSION TAG	UNP Q5HJV4
E	156	HIS	-	EXPRESSION TAG	UNP Q5HJV4
E	157	HIS	-	EXPRESSION TAG	UNP Q5HJV4
F	150	LEU	-	EXPRESSION TAG	UNP Q5HJV4
F	151	GLU	-	EXPRESSION TAG	UNP Q5HJV4
F	152	HIS	-	EXPRESSION TAG	UNP Q5HJV4
F	153	HIS	-	EXPRESSION TAG	UNP Q5HJV4
F	154	HIS	-	EXPRESSION TAG	UNP Q5HJV4
F	155	HIS	-	EXPRESSION TAG	UNP Q5HJV4
F	156	HIS	-	EXPRESSION TAG	UNP Q5HJV4
F	157	HIS	-	EXPRESSION TAG	UNP Q5HJV4

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	77	Total O 77 77	0	0
2	B	66	Total O 66 66	0	0
2	C	75	Total O 75 75	0	0
2	D	75	Total O 75 75	0	0

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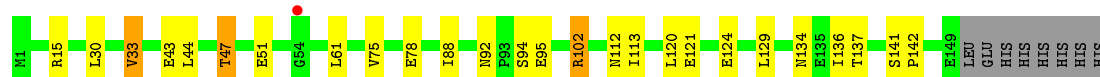
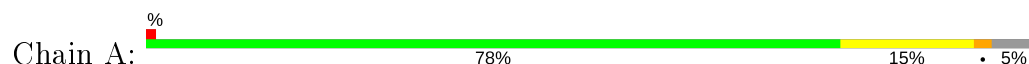
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	75	Total	O	0	0
			75	75		
2	F	61	Total	O	0	0
			61	61		

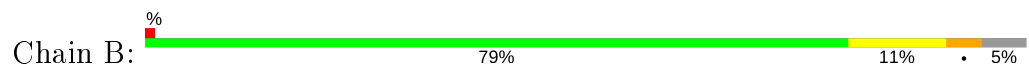
3 Residue-property plots [i](#)

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.

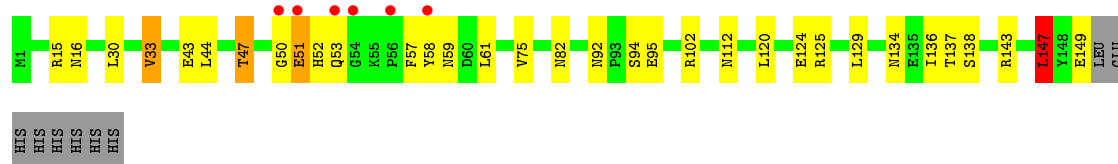
- Molecule 1: Nucleoside diphosphate kinase



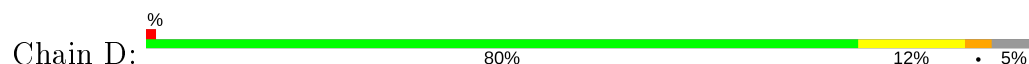
- Molecule 1: Nucleoside diphosphate kinase



- Molecule 1: Nucleoside diphosphate kinase



- Molecule 1: Nucleoside diphosphate kinase

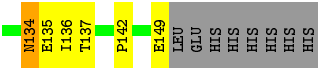
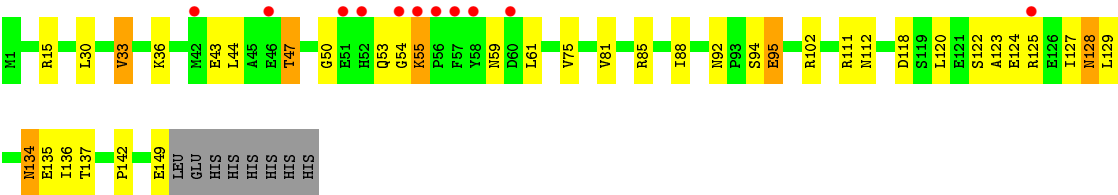


- Molecule 1: Nucleoside diphosphate kinase



HIS
HIS
HIS
HIS

● 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	91.61Å 91.61Å 176.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.81 – 2.50 45.81 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.81-2.50) 99.7 (45.81-2.50)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.34 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.213 , 0.269 0.212 , 0.267	Depositor DCC
R_{free} test set	1529 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7365	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.05% 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	0.70	1/1184 (0.1%)	0.77	2/1602 (0.1%)
1	B	0.75	0/1178	0.79	2/1595 (0.1%)
1	C	0.71	0/1175	0.81	3/1590 (0.2%)
1	D	0.71	0/1184	0.79	2/1602 (0.1%)
1	E	0.69	0/1180	0.76	0/1597
1	F	0.72	0/1171	0.79	1/1584 (0.1%)
All	All	0.71	1/7072 (0.0%)	0.78	10/9570 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	124	GLU	CG-CD	5.05	1.59	1.51

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	ARG	NE-CZ-NH1	-7.56	116.52	120.30
1	D	15	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	D	120	LEU	CB-CG-CD1	5.82	120.90	111.00
1	B	102	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	B	15	ARG	NE-CZ-NH2	5.55	123.08	120.30

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	1161	0	1145	19	1
1	B	1155	0	1134	16	0
1	C	1152	0	1130	25	0
1	D	1161	0	1145	15	0
1	E	1157	0	1141	17	9
1	F	1150	0	1126	29	8
2	A	77	0	0	2	0
2	B	66	0	0	6	0
2	C	75	0	0	11	0
2	D	75	0	0	4	0
2	E	75	0	0	5	0
2	F	61	0	0	9	0
All	All	7365	0	6821	114	9

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 8.

The worst 5 of 114 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:82:ASN:CB	2:C:409:HOH:O	1.81	1.23
1:C:82:ASN:HB3	2:C:409:HOH:O	1.32	1.22
1:C:52:HIS:CE1	2:C:427:HOH:O	1.97	1.14
1:F:94:SER:HB3	2:F:244:HOH:O	1.50	1.11
1:E:32:LEU:HB2	2:E:419:HOH:O	1.58	1.03

The worst 5 of 9 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:E:46:GLU:OE2	1:F:125:ARG:CZ[2_544]	0.94	1.26
1:E:46:GLU:CD	1:F:125:ARG:NH2[2_544]	1.28	0.92
1:E:46:GLU:CG	1:F:125:ARG:NH2[2_544]	1.29	0.91
1:E:46:GLU:OE2	1:F:125:ARG:NH2[2_544]	1.34	0.86
1:E:46:GLU:OE2	1:F:125:ARG:NH1[2_544]	1.44	0.76

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	147/157 (94%)	141 (96%)	6 (4%)	0	100	100
1	B	147/157 (94%)	140 (95%)	6 (4%)	1 (1%)	22	39
1	C	147/157 (94%)	142 (97%)	4 (3%)	1 (1%)	22	39
1	D	147/157 (94%)	141 (96%)	5 (3%)	1 (1%)	22	39
1	E	147/157 (94%)	140 (95%)	5 (3%)	2 (1%)	11	20
1	F	147/157 (94%)	142 (97%)	4 (3%)	1 (1%)	22	39
All	All	882/942 (94%)	846 (96%)	30 (3%)	6 (1%)	22	39

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	53	GLN
1	D	54	GLY
1	E	50	GLY
1	B	50	GLY
1	C	51	GLU

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	126/135 (93%)	120 (95%)	6 (5%)	25	48
1	B	124/135 (92%)	116 (94%)	8 (6%)	17	33
1	C	123/135 (91%)	116 (94%)	7 (6%)	20	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	126/135 (93%)	120 (95%)	6 (5%)	25	48
1	E	125/135 (93%)	116 (93%)	9 (7%)	14	28
1	F	123/135 (91%)	116 (94%)	7 (6%)	20	39
All	All	747/810 (92%)	704 (94%)	43 (6%)	20	38

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	138	SER
1	D	95	GLU
1	F	95	GLU
1	C	147	LEU
1	D	33	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	16	ASN
1	F	134	ASN
1	E	53	GLN
1	C	134	ASN
1	D	134	ASN

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 [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	149/157 (94%)	-0.25	1 (0%) 87 89	6, 15, 31, 39	0
1	B	149/157 (94%)	-0.22	1 (0%) 87 89	6, 15, 29, 37	0
1	C	149/157 (94%)	-0.14	6 (4%) 38 41	6, 14, 29, 39	0
1	D	149/157 (94%)	-0.28	2 (1%) 77 79	6, 15, 30, 38	0
1	E	149/157 (94%)	-0.18	3 (2%) 65 68	6, 15, 31, 40	0
1	F	149/157 (94%)	0.12	11 (7%) 14 15	6, 15, 30, 38	0
All	All	894/942 (94%)	-0.16	24 (2%) 54 58	6, 15, 31, 40	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	54	GLY	6.4
1	F	56	PRO	5.6
1	C	54	GLY	5.2
1	F	58	TYR	4.4
1	F	125	ARG	4.3

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 carbohydrates 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.