



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 12:26 pm BST

PDB ID : 1K3F
Title : Uridine Phosphorylase from E. coli, Refined in the Monoclinic Crystal Lattice
Authors : Morgunova, E.Yu.; Mikhailov, A.M.; Popov, A.N.; Blagova, E.V.; Smirnova, E.A.; Vainshtein, B.K.; Mao, C.; Armstrong, S.R.; Ealick, S.E.; Komissarov, A.A.; Linkova, E.V.; Burlakova, A.A.; Mironov, A.S.; Debabov, V.G.
Deposited on : 2001-10-02
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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

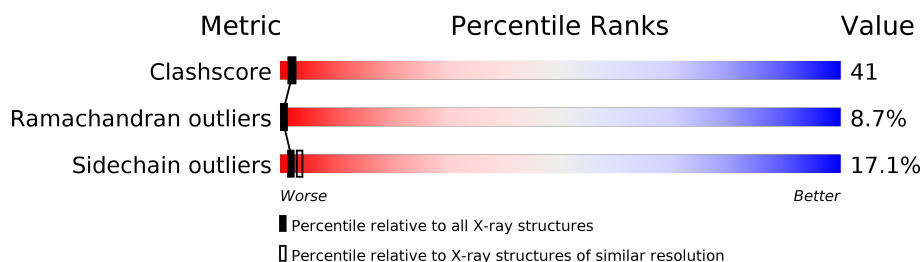
1 Overall quality at a glance

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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	253	<div> <div>45%</div> <div>41%</div> <div>11%</div> <div>.</div> </div>
1	B	253	<div> <div>39%</div> <div>48%</div> <div>13%</div> <div>.</div> </div>
1	C	253	<div> <div>37%</div> <div>50%</div> <div>11%</div> <div>.</div> </div>
1	D	253	<div> <div>38%</div> <div>48%</div> <div>14%</div> </div>
1	E	253	<div> <div>37%</div> <div>46%</div> <div>16%</div> <div>.</div> </div>
1	F	253	<div> <div>33%</div> <div>51%</div> <div>14%</div> <div>.</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11286 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 uridine phosphorylase.

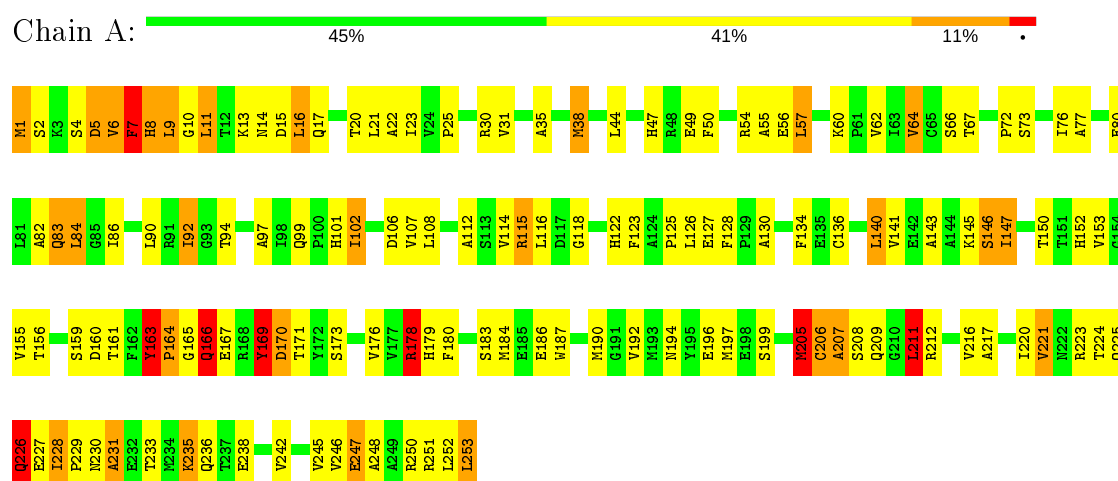
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			1881	1180	322	367	12			
1	B	253	Total	C	N	O	S	0	0	0
			1881	1180	322	367	12			
1	C	253	Total	C	N	O	S	0	0	0
			1881	1180	322	367	12			
1	D	253	Total	C	N	O	S	0	0	0
			1881	1180	322	367	12			
1	E	253	Total	C	N	O	S	0	0	0
			1881	1180	322	367	12			
1	F	253	Total	C	N	O	S	0	0	0
			1881	1180	322	367	12			

3 Residue-property plots

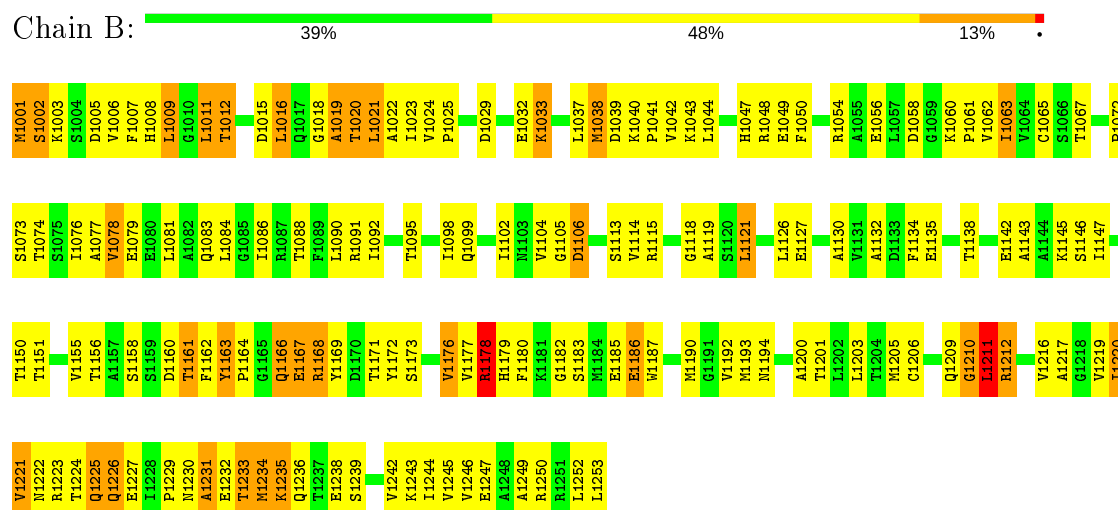
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

- Molecule 1: uridine phosphorylase

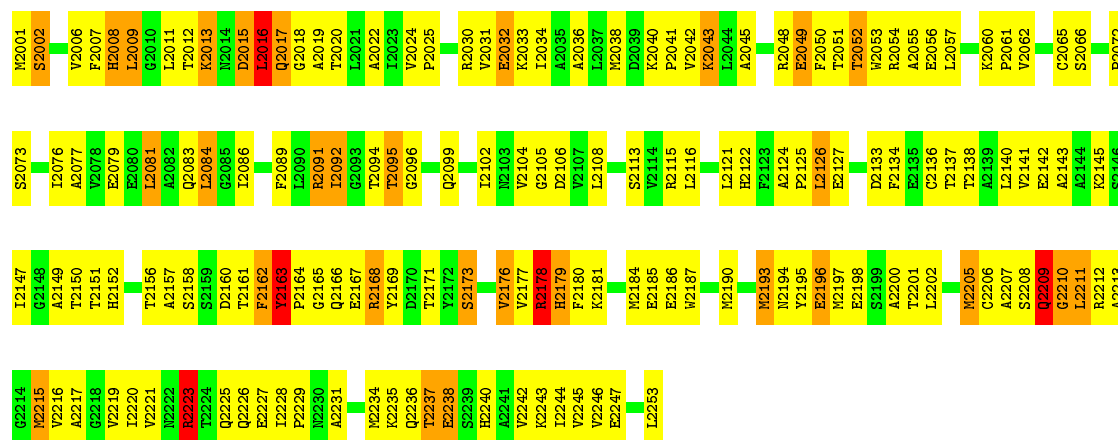


- Molecule 1: uridine phosphorylase

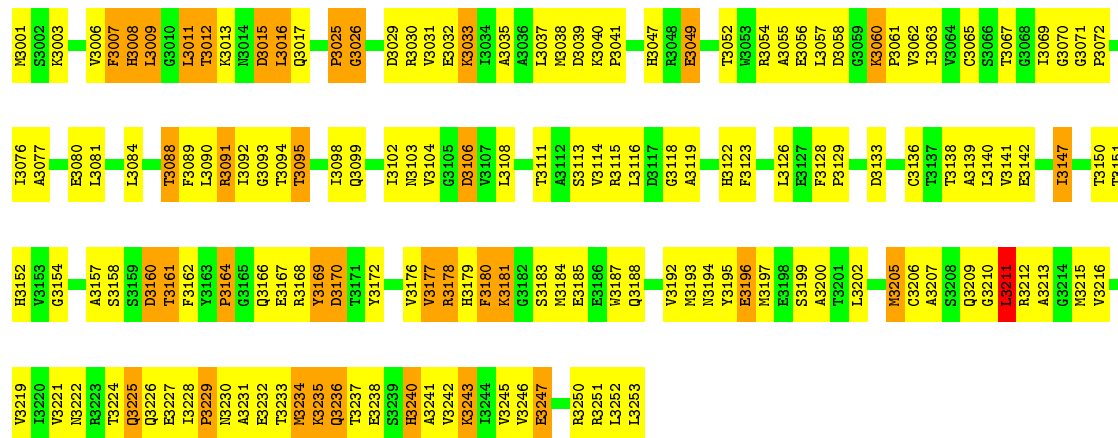


- Molecule 1: uridine phosphorylase

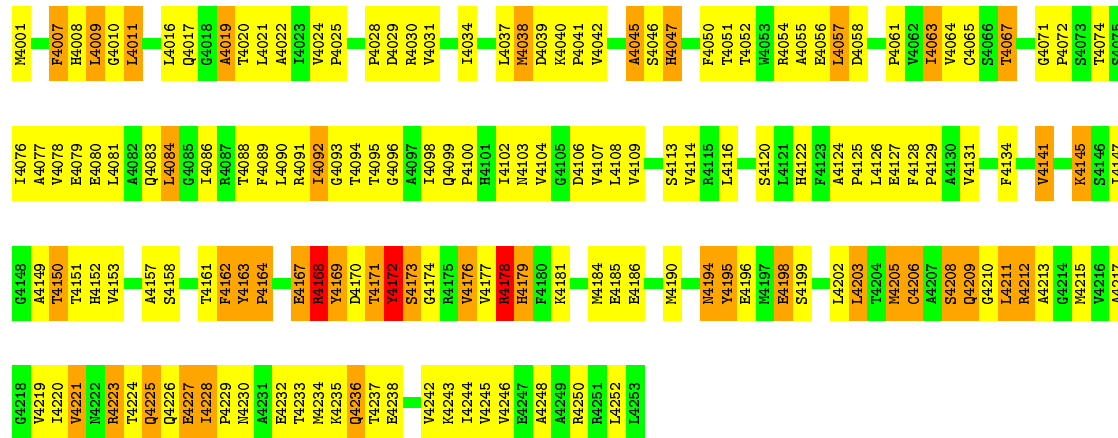




• Molecule 1: uridine phosphorylase

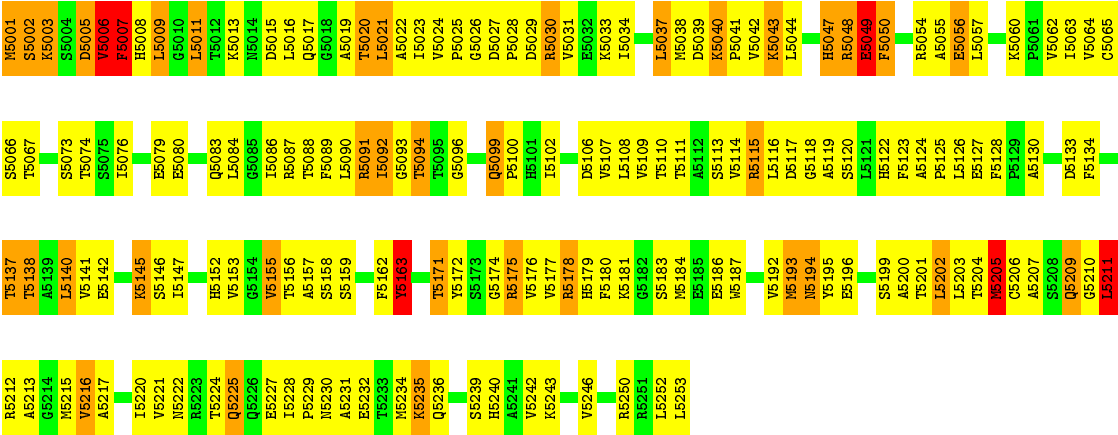


• Molecule 1: uridine phosphorylase



• Molecule 1: uridine phosphorylase

Chain F: 33% 51% 14% .



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.60 Å 98.80 Å 93.70 Å 90.00° 120.20° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.50)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.186 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11286	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

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	0.68	1/1913 (0.1%)	0.95	3/2599 (0.1%)
1	B	0.62	0/1913	0.92	2/2599 (0.1%)
1	C	0.69	1/1913 (0.1%)	0.91	0/2599
1	D	0.65	0/1913	0.94	1/2599 (0.0%)
1	E	0.67	0/1913	0.92	5/2599 (0.2%)
1	F	2.39	8/1913 (0.4%)	1.02	5/2599 (0.2%)
All	All	1.15	10/11478 (0.1%)	0.94	16/15594 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	5007	PHE	CE1-CZ	45.72	2.24	1.37
1	F	5007	PHE	CE2-CZ	45.69	2.24	1.37
1	F	5007	PHE	CD2-CE2	44.49	2.28	1.39
1	F	5007	PHE	CD1-CE1	44.03	2.27	1.39
1	F	5007	PHE	CG-CD2	29.57	1.83	1.38

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	5001	MET	C-N-CA	15.24	159.80	121.70
1	F	5007	PHE	CB-CG-CD1	-9.44	114.19	120.80
1	A	211	LEU	CA-CB-CG	6.32	129.84	115.30
1	E	4170	ASP	N-CA-C	6.25	127.87	111.00
1	A	16	LEU	CA-CB-CG	6.14	129.42	115.30

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	1881	0	1871	155	0
1	B	1881	0	1868	145	0
1	C	1881	0	1868	180	0
1	D	1881	0	1868	151	0
1	E	1881	0	1868	154	0
1	F	1881	0	1868	214	0
All	All	11286	0	11211	929	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 41.

The worst 5 of 929 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:F:5007:PHE:CG	1:F:5007:PHE:CD1	1.82	1.67
1:F:5007:PHE:CD2	1:F:5007:PHE:CG	1.83	1.60
1:F:5002:SER:CA	1:F:5002:SER:N	1.75	1.48
1:F:5007:PHE:CZ	1:F:5007:PHE:CE1	2.24	1.26
1:F:5007:PHE:CE2	1:F:5007:PHE:CZ	2.24	1.25

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	251/253 (99%)	189 (75%)	37 (15%)	25 (10%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	251/253 (99%)	180 (72%)	47 (19%)	24 (10%)	0	0
1	C	251/253 (99%)	193 (77%)	35 (14%)	23 (9%)	1	0
1	D	251/253 (99%)	194 (77%)	40 (16%)	17 (7%)	1	1
1	E	251/253 (99%)	187 (74%)	41 (16%)	23 (9%)	1	0
1	F	251/253 (99%)	193 (77%)	39 (16%)	19 (8%)	1	1
All	All	1506/1518 (99%)	1136 (75%)	239 (16%)	131 (9%)	1	0

5 of 131 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	7	PHE
1	A	13	LYS
1	A	30	ARG
1	A	163	TYR

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	200/204 (98%)	170 (85%)	30 (15%)	3	5
1	B	200/204 (98%)	166 (83%)	34 (17%)	2	3
1	C	200/204 (98%)	168 (84%)	32 (16%)	2	4
1	D	200/204 (98%)	158 (79%)	42 (21%)	1	2
1	E	200/204 (98%)	165 (82%)	35 (18%)	2	3
1	F	200/204 (98%)	168 (84%)	32 (16%)	2	4
All	All	1200/1224 (98%)	995 (83%)	205 (17%)	2	3

5 of 205 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2215	MET

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Mol	Chain	Res	Type
1	D	3113	SER
1	F	5137	THR
1	C	2238	GLU
1	D	3052	THR

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

Mol	Chain	Res	Type
1	C	2240	HIS
1	D	3194	ASN
1	F	5152	HIS
1	D	3099	GLN
1	D	3166	GLN

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 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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.