



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:54 PM GMT

PDB ID : 4GA5
Title : Crystal structure of AMP phosphorylase C-terminal deletion mutant in the apo-form
Authors : Nishitani, Y.; Aono, R.; Nakamura, A.; Sato, T.; Atomi, H.; Imanaka, T.; Miki, K.
Deposited on : 2012-07-25
Resolution : 3.25 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

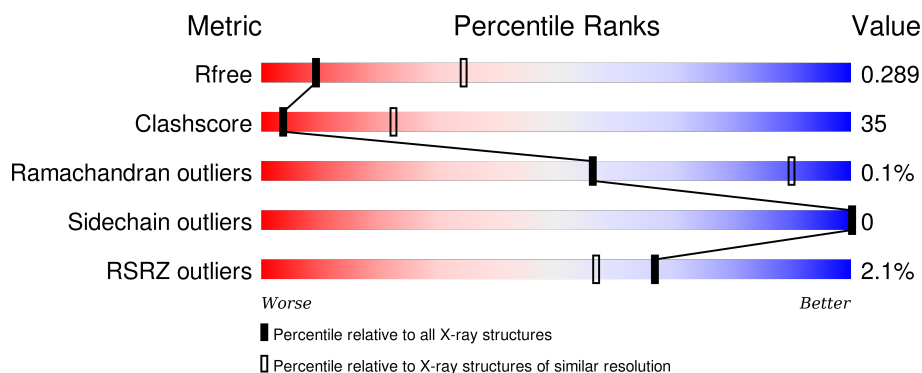
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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}	91344	1624 (3.32-3.20)
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (3.32-3.20)

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. 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	513	<div> <div></div> <div>65%31%.</div> </div>
1	B	513	<div> <div>%</div> <div>62%34%.</div> </div>
1	C	513	<div> <div>%</div> <div>55%41%.</div> </div>
1	D	513	<div> <div>%</div> <div>58%38%.</div> </div>
1	E	513	<div> <div>%</div> <div>59%37%.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	513	 62%34%6%
1	G	513	 6%53%43%6%
1	H	513	 6%55%41%6%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 26752 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 Putative thymidine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	493	Total	C	N	O	S	0	0	0
			3344	2123	560	647	14			
1	A	493	Total	C	N	O	S	0	0	0
			3344	2123	560	647	14			
1	C	493	Total	C	N	O	S	0	0	0
			3344	2123	560	647	14			
1	D	493	Total	C	N	O	S	0	0	0
			3344	2123	560	647	14			
1	E	493	Total	C	N	O	S	0	0	0
			3344	2123	560	647	14			
1	F	493	Total	C	N	O	S	0	0	0
			3344	2123	560	647	14			
1	G	493	Total	C	N	O	S	0	0	0
			3344	2123	560	647	14			
1	H	493	Total	C	N	O	S	0	0	0
			3344	2123	560	647	14			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	494	GLY	-	EXPRESSION TAG	UNP Q5JCX3
B	495	ASN	-	EXPRESSION TAG	UNP Q5JCX3
B	496	SER	-	EXPRESSION TAG	UNP Q5JCX3
B	497	SER	-	EXPRESSION TAG	UNP Q5JCX3
B	498	SER	-	EXPRESSION TAG	UNP Q5JCX3
B	499	VAL	-	EXPRESSION TAG	UNP Q5JCX3
B	500	ASP	-	EXPRESSION TAG	UNP Q5JCX3
B	501	LYS	-	EXPRESSION TAG	UNP Q5JCX3
B	502	LEU	-	EXPRESSION TAG	UNP Q5JCX3
B	503	ALA	-	EXPRESSION TAG	UNP Q5JCX3
B	504	ALA	-	EXPRESSION TAG	UNP Q5JCX3
B	505	ALA	-	EXPRESSION TAG	UNP Q5JCX3
B	506	LEU	-	EXPRESSION TAG	UNP Q5JCX3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	507	GLU	-	EXPRESSION TAG	UNP Q5JCX3
B	508	HIS	-	EXPRESSION TAG	UNP Q5JCX3
B	509	HIS	-	EXPRESSION TAG	UNP Q5JCX3
B	510	HIS	-	EXPRESSION TAG	UNP Q5JCX3
B	511	HIS	-	EXPRESSION TAG	UNP Q5JCX3
B	512	HIS	-	EXPRESSION TAG	UNP Q5JCX3
B	513	HIS	-	EXPRESSION TAG	UNP Q5JCX3
A	494	GLY	-	EXPRESSION TAG	UNP Q5JCX3
A	495	ASN	-	EXPRESSION TAG	UNP Q5JCX3
A	496	SER	-	EXPRESSION TAG	UNP Q5JCX3
A	497	SER	-	EXPRESSION TAG	UNP Q5JCX3
A	498	SER	-	EXPRESSION TAG	UNP Q5JCX3
A	499	VAL	-	EXPRESSION TAG	UNP Q5JCX3
A	500	ASP	-	EXPRESSION TAG	UNP Q5JCX3
A	501	LYS	-	EXPRESSION TAG	UNP Q5JCX3
A	502	LEU	-	EXPRESSION TAG	UNP Q5JCX3
A	503	ALA	-	EXPRESSION TAG	UNP Q5JCX3
A	504	ALA	-	EXPRESSION TAG	UNP Q5JCX3
A	505	ALA	-	EXPRESSION TAG	UNP Q5JCX3
A	506	LEU	-	EXPRESSION TAG	UNP Q5JCX3
A	507	GLU	-	EXPRESSION TAG	UNP Q5JCX3
A	508	HIS	-	EXPRESSION TAG	UNP Q5JCX3
A	509	HIS	-	EXPRESSION TAG	UNP Q5JCX3
A	510	HIS	-	EXPRESSION TAG	UNP Q5JCX3
A	511	HIS	-	EXPRESSION TAG	UNP Q5JCX3
A	512	HIS	-	EXPRESSION TAG	UNP Q5JCX3
A	513	HIS	-	EXPRESSION TAG	UNP Q5JCX3
C	494	GLY	-	EXPRESSION TAG	UNP Q5JCX3
C	495	ASN	-	EXPRESSION TAG	UNP Q5JCX3
C	496	SER	-	EXPRESSION TAG	UNP Q5JCX3
C	497	SER	-	EXPRESSION TAG	UNP Q5JCX3
C	498	SER	-	EXPRESSION TAG	UNP Q5JCX3
C	499	VAL	-	EXPRESSION TAG	UNP Q5JCX3
C	500	ASP	-	EXPRESSION TAG	UNP Q5JCX3
C	501	LYS	-	EXPRESSION TAG	UNP Q5JCX3
C	502	LEU	-	EXPRESSION TAG	UNP Q5JCX3
C	503	ALA	-	EXPRESSION TAG	UNP Q5JCX3
C	504	ALA	-	EXPRESSION TAG	UNP Q5JCX3
C	505	ALA	-	EXPRESSION TAG	UNP Q5JCX3
C	506	LEU	-	EXPRESSION TAG	UNP Q5JCX3
C	507	GLU	-	EXPRESSION TAG	UNP Q5JCX3
C	508	HIS	-	EXPRESSION TAG	UNP Q5JCX3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	509	HIS	-	EXPRESSION TAG	UNP Q5JCX3
C	510	HIS	-	EXPRESSION TAG	UNP Q5JCX3
C	511	HIS	-	EXPRESSION TAG	UNP Q5JCX3
C	512	HIS	-	EXPRESSION TAG	UNP Q5JCX3
C	513	HIS	-	EXPRESSION TAG	UNP Q5JCX3
D	494	GLY	-	EXPRESSION TAG	UNP Q5JCX3
D	495	ASN	-	EXPRESSION TAG	UNP Q5JCX3
D	496	SER	-	EXPRESSION TAG	UNP Q5JCX3
D	497	SER	-	EXPRESSION TAG	UNP Q5JCX3
D	498	SER	-	EXPRESSION TAG	UNP Q5JCX3
D	499	VAL	-	EXPRESSION TAG	UNP Q5JCX3
D	500	ASP	-	EXPRESSION TAG	UNP Q5JCX3
D	501	LYS	-	EXPRESSION TAG	UNP Q5JCX3
D	502	LEU	-	EXPRESSION TAG	UNP Q5JCX3
D	503	ALA	-	EXPRESSION TAG	UNP Q5JCX3
D	504	ALA	-	EXPRESSION TAG	UNP Q5JCX3
D	505	ALA	-	EXPRESSION TAG	UNP Q5JCX3
D	506	LEU	-	EXPRESSION TAG	UNP Q5JCX3
D	507	GLU	-	EXPRESSION TAG	UNP Q5JCX3
D	508	HIS	-	EXPRESSION TAG	UNP Q5JCX3
D	509	HIS	-	EXPRESSION TAG	UNP Q5JCX3
D	510	HIS	-	EXPRESSION TAG	UNP Q5JCX3
D	511	HIS	-	EXPRESSION TAG	UNP Q5JCX3
D	512	HIS	-	EXPRESSION TAG	UNP Q5JCX3
D	513	HIS	-	EXPRESSION TAG	UNP Q5JCX3
E	494	GLY	-	EXPRESSION TAG	UNP Q5JCX3
E	495	ASN	-	EXPRESSION TAG	UNP Q5JCX3
E	496	SER	-	EXPRESSION TAG	UNP Q5JCX3
E	497	SER	-	EXPRESSION TAG	UNP Q5JCX3
E	498	SER	-	EXPRESSION TAG	UNP Q5JCX3
E	499	VAL	-	EXPRESSION TAG	UNP Q5JCX3
E	500	ASP	-	EXPRESSION TAG	UNP Q5JCX3
E	501	LYS	-	EXPRESSION TAG	UNP Q5JCX3
E	502	LEU	-	EXPRESSION TAG	UNP Q5JCX3
E	503	ALA	-	EXPRESSION TAG	UNP Q5JCX3
E	504	ALA	-	EXPRESSION TAG	UNP Q5JCX3
E	505	ALA	-	EXPRESSION TAG	UNP Q5JCX3
E	506	LEU	-	EXPRESSION TAG	UNP Q5JCX3
E	507	GLU	-	EXPRESSION TAG	UNP Q5JCX3
E	508	HIS	-	EXPRESSION TAG	UNP Q5JCX3
E	509	HIS	-	EXPRESSION TAG	UNP Q5JCX3
E	510	HIS	-	EXPRESSION TAG	UNP Q5JCX3

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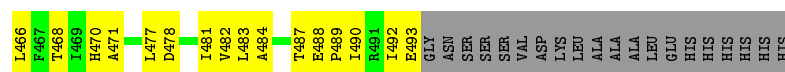
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Chain	Residue	Modelled	Actual	Comment	Reference
E	511	HIS	-	EXPRESSION TAG	UNP Q5JCX3
E	512	HIS	-	EXPRESSION TAG	UNP Q5JCX3
E	513	HIS	-	EXPRESSION TAG	UNP Q5JCX3
F	494	GLY	-	EXPRESSION TAG	UNP Q5JCX3
F	495	ASN	-	EXPRESSION TAG	UNP Q5JCX3
F	496	SER	-	EXPRESSION TAG	UNP Q5JCX3
F	497	SER	-	EXPRESSION TAG	UNP Q5JCX3
F	498	SER	-	EXPRESSION TAG	UNP Q5JCX3
F	499	VAL	-	EXPRESSION TAG	UNP Q5JCX3
F	500	ASP	-	EXPRESSION TAG	UNP Q5JCX3
F	501	LYS	-	EXPRESSION TAG	UNP Q5JCX3
F	502	LEU	-	EXPRESSION TAG	UNP Q5JCX3
F	503	ALA	-	EXPRESSION TAG	UNP Q5JCX3
F	504	ALA	-	EXPRESSION TAG	UNP Q5JCX3
F	505	ALA	-	EXPRESSION TAG	UNP Q5JCX3
F	506	LEU	-	EXPRESSION TAG	UNP Q5JCX3
F	507	GLU	-	EXPRESSION TAG	UNP Q5JCX3
F	508	HIS	-	EXPRESSION TAG	UNP Q5JCX3
F	509	HIS	-	EXPRESSION TAG	UNP Q5JCX3
F	510	HIS	-	EXPRESSION TAG	UNP Q5JCX3
F	511	HIS	-	EXPRESSION TAG	UNP Q5JCX3
F	512	HIS	-	EXPRESSION TAG	UNP Q5JCX3
F	513	HIS	-	EXPRESSION TAG	UNP Q5JCX3
G	494	GLY	-	EXPRESSION TAG	UNP Q5JCX3
G	495	ASN	-	EXPRESSION TAG	UNP Q5JCX3
G	496	SER	-	EXPRESSION TAG	UNP Q5JCX3
G	497	SER	-	EXPRESSION TAG	UNP Q5JCX3
G	498	SER	-	EXPRESSION TAG	UNP Q5JCX3
G	499	VAL	-	EXPRESSION TAG	UNP Q5JCX3
G	500	ASP	-	EXPRESSION TAG	UNP Q5JCX3
G	501	LYS	-	EXPRESSION TAG	UNP Q5JCX3
G	502	LEU	-	EXPRESSION TAG	UNP Q5JCX3
G	503	ALA	-	EXPRESSION TAG	UNP Q5JCX3
G	504	ALA	-	EXPRESSION TAG	UNP Q5JCX3
G	505	ALA	-	EXPRESSION TAG	UNP Q5JCX3
G	506	LEU	-	EXPRESSION TAG	UNP Q5JCX3
G	507	GLU	-	EXPRESSION TAG	UNP Q5JCX3
G	508	HIS	-	EXPRESSION TAG	UNP Q5JCX3
G	509	HIS	-	EXPRESSION TAG	UNP Q5JCX3
G	510	HIS	-	EXPRESSION TAG	UNP Q5JCX3
G	511	HIS	-	EXPRESSION TAG	UNP Q5JCX3
G	512	HIS	-	EXPRESSION TAG	UNP Q5JCX3

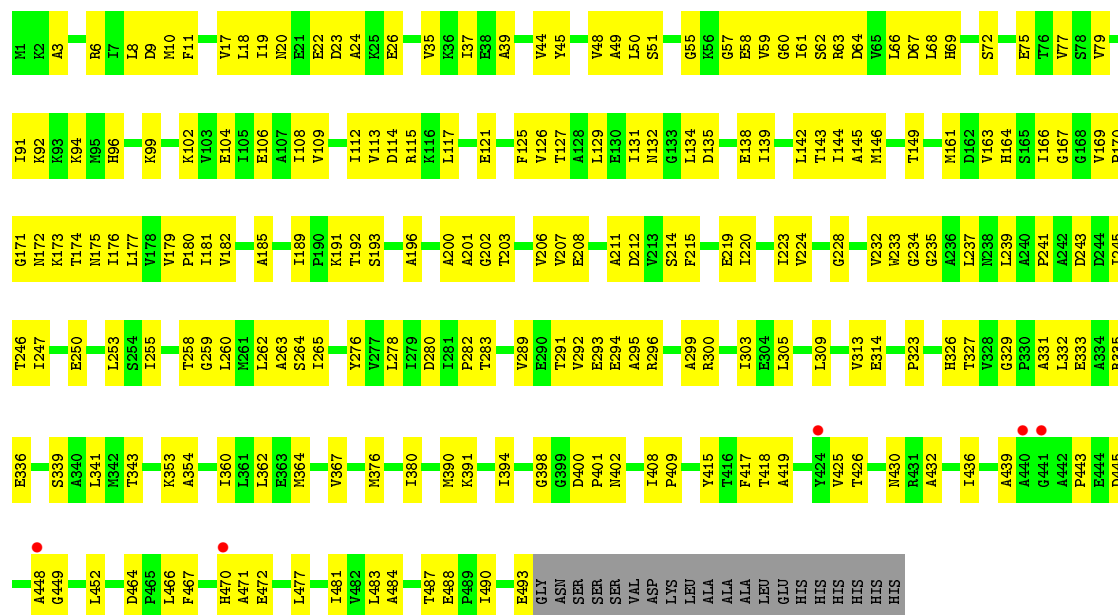
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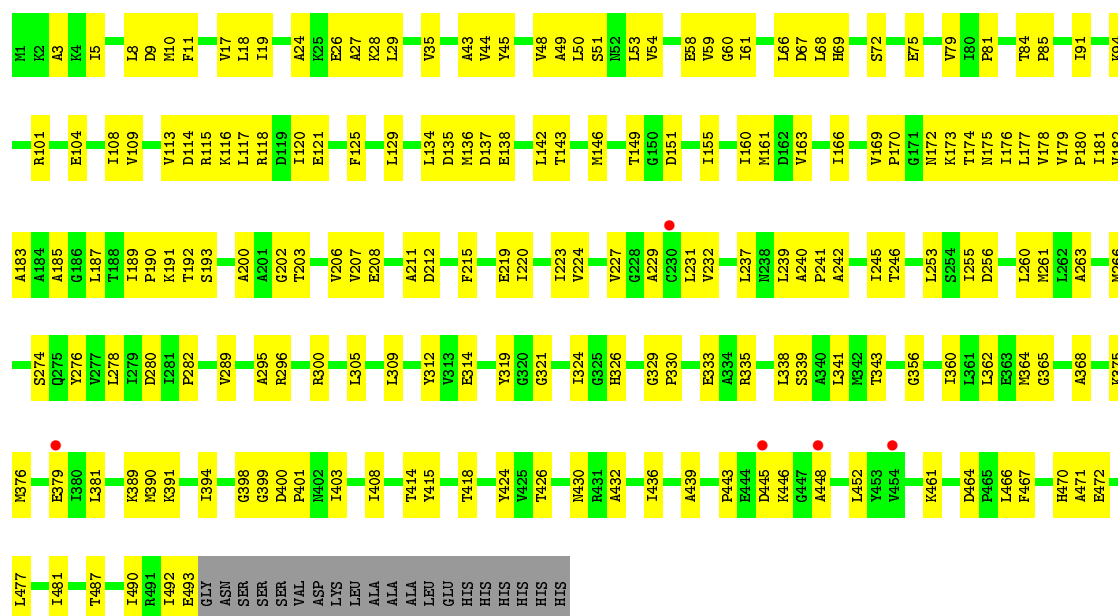
Chain	Residue	Modelled	Actual	Comment	Reference
G	513	HIS	-	EXPRESSION TAG	UNP Q5JCX3
H	494	GLY	-	EXPRESSION TAG	UNP Q5JCX3
H	495	ASN	-	EXPRESSION TAG	UNP Q5JCX3
H	496	SER	-	EXPRESSION TAG	UNP Q5JCX3
H	497	SER	-	EXPRESSION TAG	UNP Q5JCX3
H	498	SER	-	EXPRESSION TAG	UNP Q5JCX3
H	499	VAL	-	EXPRESSION TAG	UNP Q5JCX3
H	500	ASP	-	EXPRESSION TAG	UNP Q5JCX3
H	501	LYS	-	EXPRESSION TAG	UNP Q5JCX3
H	502	LEU	-	EXPRESSION TAG	UNP Q5JCX3
H	503	ALA	-	EXPRESSION TAG	UNP Q5JCX3
H	504	ALA	-	EXPRESSION TAG	UNP Q5JCX3
H	505	ALA	-	EXPRESSION TAG	UNP Q5JCX3
H	506	LEU	-	EXPRESSION TAG	UNP Q5JCX3
H	507	GLU	-	EXPRESSION TAG	UNP Q5JCX3
H	508	HIS	-	EXPRESSION TAG	UNP Q5JCX3
H	509	HIS	-	EXPRESSION TAG	UNP Q5JCX3
H	510	HIS	-	EXPRESSION TAG	UNP Q5JCX3
H	511	HIS	-	EXPRESSION TAG	UNP Q5JCX3
H	512	HIS	-	EXPRESSION TAG	UNP Q5JCX3
H	513	HIS	-	EXPRESSION TAG	UNP Q5JCX3



• Molecule 1: Putative thymidine phosphorylase

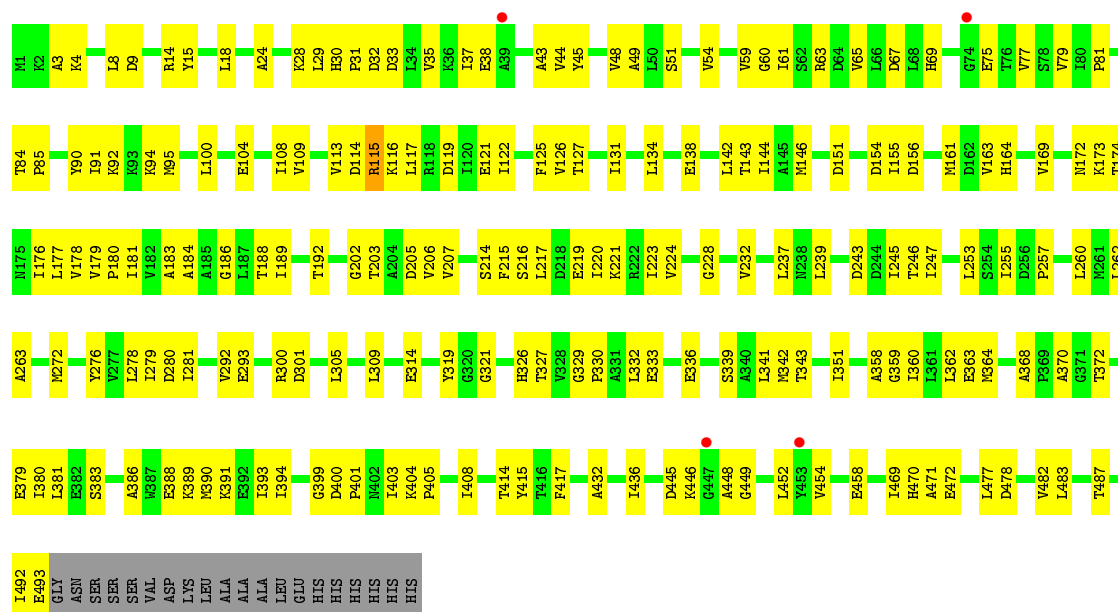


• Molecule 1: Putative thymidine phosphorylase

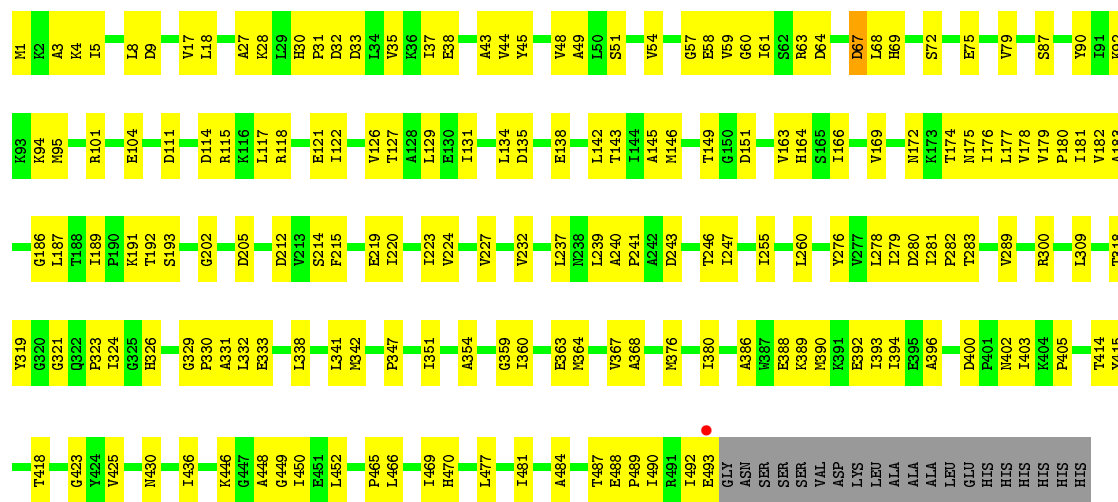


• Molecule 1: Putative thymidine phosphorylase

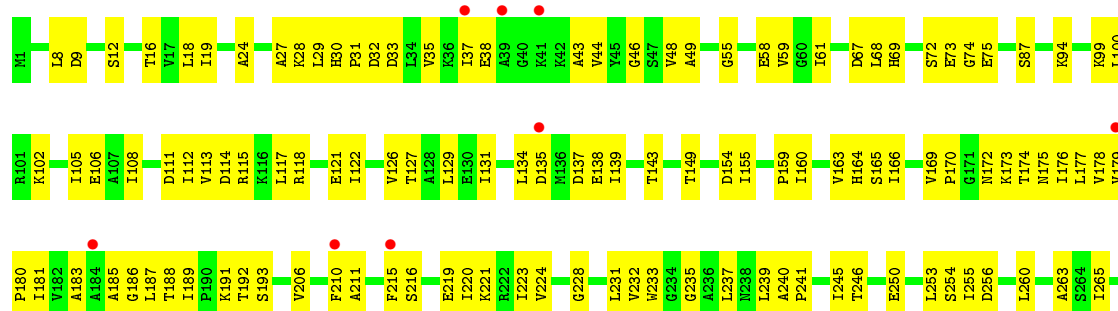


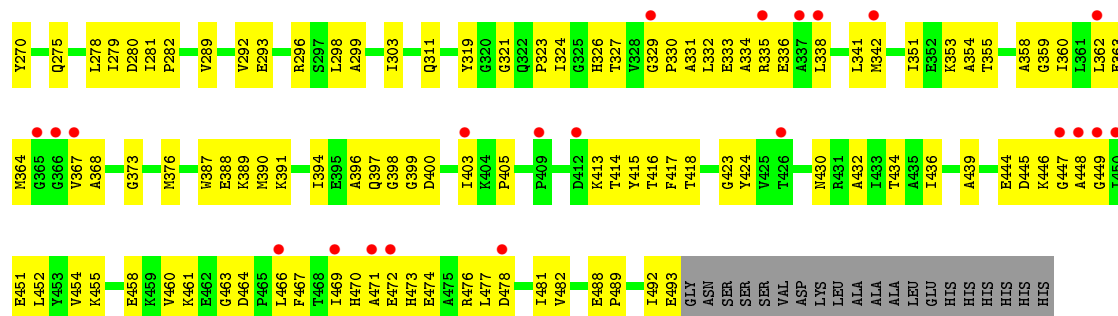


• Molecule 1: Putative thymidine phosphorylase

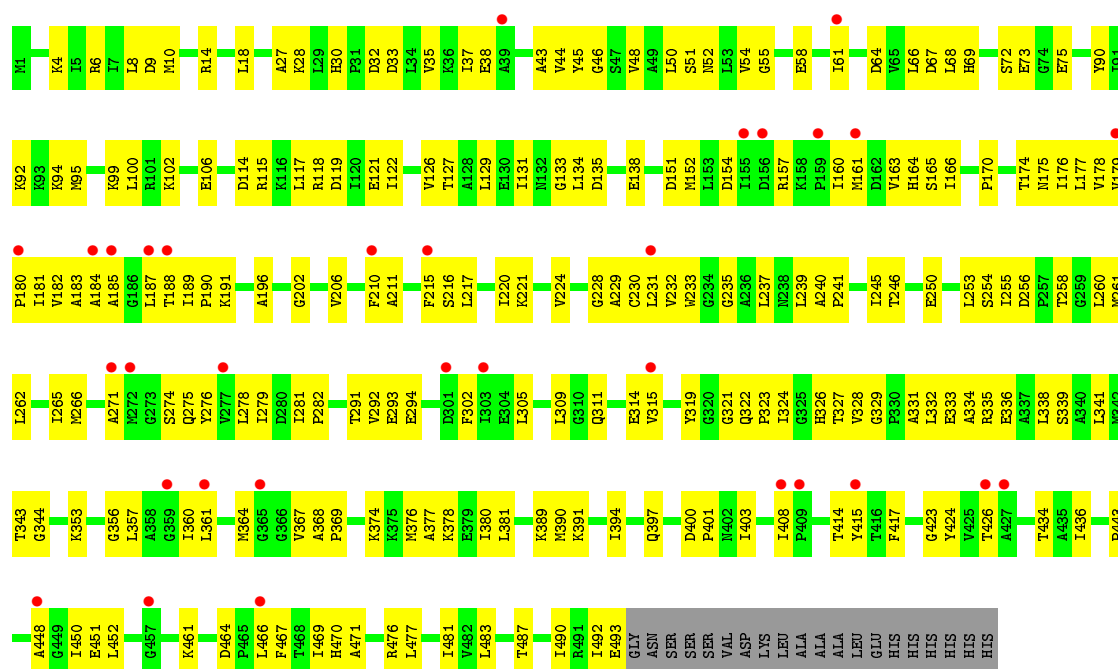


• Molecule 1: Putative thymidine phosphorylase





• Molecule 1: Putative thymidine phosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	124.33Å 249.48Å 162.37Å 90.00° 110.44° 90.00°	Depositor
Resolution (Å)	50.00 – 3.25 48.99 – 3.24	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.25) 99.3 (48.99-3.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 3.25Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.261 , 0.289 0.261 , 0.289	Depositor DCC
R_{free} test set	3649 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	65.6	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 84.0	EDS
Estimated twinning fraction	0.055 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 72994 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	26752	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 6.21% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.52	0/3391	0.61	0/4637
1	B	0.47	0/3391	0.60	0/4637
1	C	0.50	0/3391	0.61	0/4637
1	D	0.49	0/3391	0.61	0/4637
1	E	0.48	0/3391	0.61	0/4637
1	F	0.50	0/3391	0.62	1/4637 (0.0%)
1	G	0.43	0/3391	0.60	0/4637
1	H	0.43	0/3391	0.59	0/4637
All	All	0.48	0/27128	0.61	1/37096 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	67	ASP	CB-CG-OD2	5.18	122.97	118.30

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	3344	0	3133	158	0
1	B	3344	0	3133	180	0
1	C	3344	0	3133	233	0
1	D	3344	0	3133	234	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3344	0	3133	230	0
1	F	3344	0	3133	191	0
1	G	3344	0	3133	337	0
1	H	3344	0	3133	301	0
All	All	26752	0	25064	1837	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 35.

The worst 5 of 1837 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:G:237:LEU:CD1	1:G:239:LEU:HG	1.42	1.46
1:H:237:LEU:HD13	1:H:239:LEU:CG	1.57	1.32
1:B:237:LEU:CD1	1:B:239:LEU:HG	1.61	1.31
1:H:237:LEU:CD1	1:H:239:LEU:HG	1.64	1.28
1:G:415:TYR:CE2	1:G:417:PHE:CZ	2.22	1.26

There are no symmetry-related clashes.

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	491/513 (96%)	482 (98%)	9 (2%)	0	100	100
1	B	491/513 (96%)	485 (99%)	6 (1%)	0	100	100
1	C	491/513 (96%)	482 (98%)	8 (2%)	1 (0%)	52	87
1	D	491/513 (96%)	479 (98%)	12 (2%)	0	100	100
1	E	491/513 (96%)	484 (99%)	6 (1%)	1 (0%)	52	87
1	F	491/513 (96%)	481 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	491/513 (96%)	480 (98%)	11 (2%)	0	100	100
1	H	491/513 (96%)	482 (98%)	9 (2%)	0	100	100
All	All	3928/4104 (96%)	3855 (98%)	71 (2%)	2 (0%)	56	90

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	115	ARG
1	C	409	PRO

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	292/404 (72%)	292 (100%)	0	100	100
1	B	292/404 (72%)	292 (100%)	0	100	100
1	C	292/404 (72%)	292 (100%)	0	100	100
1	D	292/404 (72%)	292 (100%)	0	100	100
1	E	292/404 (72%)	292 (100%)	0	100	100
1	F	292/404 (72%)	292 (100%)	0	100	100
1	G	292/404 (72%)	292 (100%)	0	100	100
1	H	292/404 (72%)	292 (100%)	0	100	100
All	All	2336/3232 (72%)	2336 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	164	HIS
1	E	275	GLN
1	H	30	HIS

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Mol	Chain	Res	Type
1	D	275	GLN
1	A	275	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 [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	493/513 (96%)	-0.28	1 (0%) 95 94	11, 41, 74, 100	0
1	B	493/513 (96%)	-0.15	5 (1%) 84 78	6, 46, 85, 121	0
1	C	493/513 (96%)	-0.08	5 (1%) 84 78	15, 47, 87, 124	0
1	D	493/513 (96%)	-0.07	5 (1%) 84 78	19, 52, 87, 132	0
1	E	493/513 (96%)	-0.09	4 (0%) 87 82	11, 52, 98, 145	0
1	F	493/513 (96%)	-0.19	1 (0%) 95 94	16, 47, 80, 153	0
1	G	493/513 (96%)	0.40	30 (6%) 25 18	28, 76, 141, 252	0
1	H	493/513 (96%)	0.40	32 (6%) 22 16	26, 86, 148, 225	0
All	All	3944/4104 (96%)	-0.01	83 (2%) 67 57	6, 53, 112, 252	0

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	448	ALA	7.1
1	G	471	ALA	6.1
1	H	426	THR	4.6
1	G	466	LEU	4.2
1	H	415	TYR	4.1

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.