wwPDB X-ray Structure Validation Summary Report (i)

May 15, 2020 – 11:08 pm BST

PDB ID	:	1T94
Title	:	Crystal structure of the catalytic core of human DNA polymerase kappa
Authors	:	Uljon, S.N.; Johnson, R.E.; Edwards, T.A.; Prakash, S.; Prakash, L.; Aggarwal, A.K.
Deposited on	:	2004-05-14
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

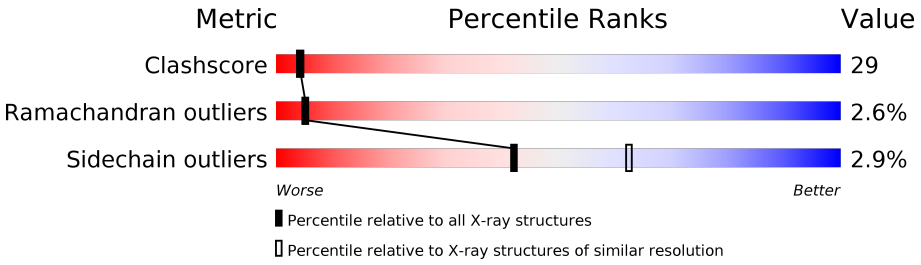
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	459	54% 30% 11%
1	B	459	45% 37% 17%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6532 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 polymerase (DNA directed) kappa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	0	0
			3185	2012	557	597	19			
1	B	382	Total	C	N	O	S	0	0	0
			2987	1889	525	555	18			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	187	Total	O	0	0
			187	187		
2	B	173	Total	O	0	0
			173	173		

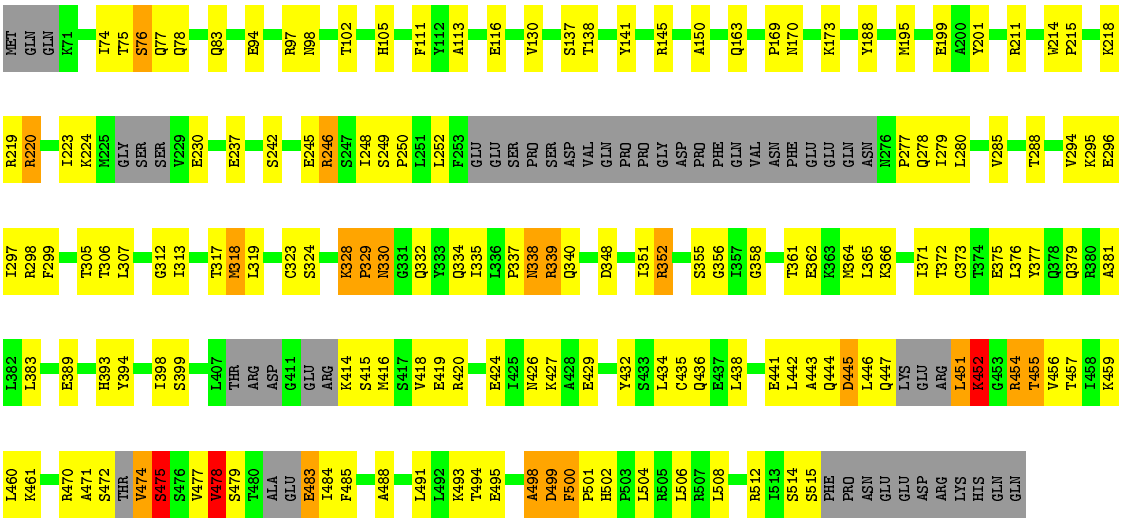
3 Residue-property plots (i)

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. 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.

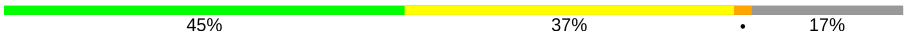
- Molecule 1: polymerase (DNA directed) kappa

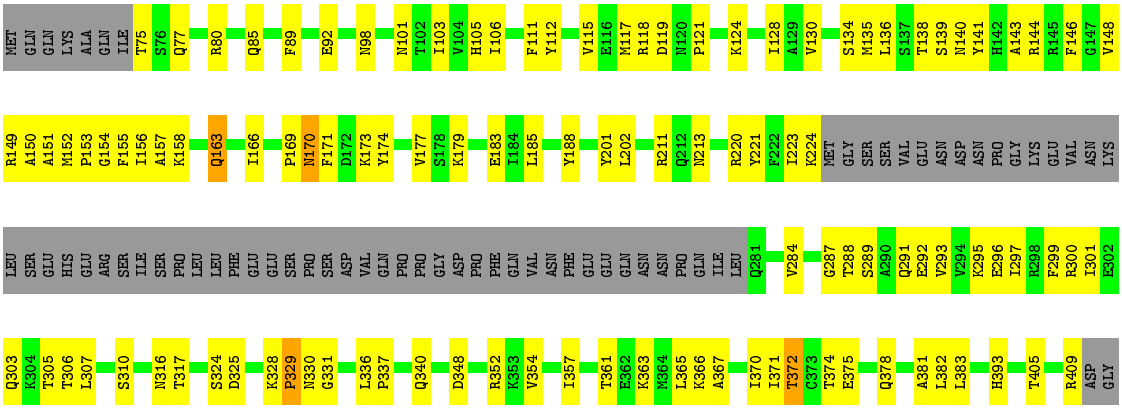
Chain A:

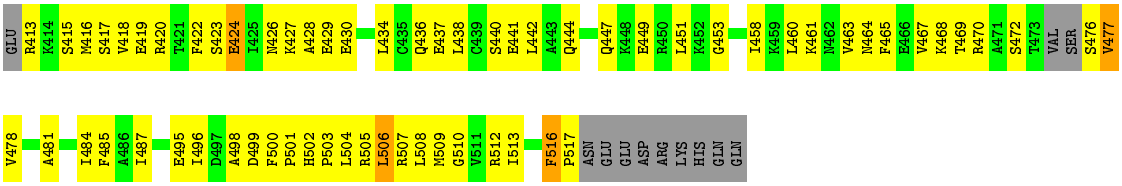


- Molecule 1: polymerase (DNA directed) kappa

Chain B:






GLU R413 K414 S415 M416 S417 V418 E419 R420 T421 F422 S423 E424 I425 N426 K427 A428 E429 E430 L434 C435 Q436 E437 L438 C439 S440 E441 L442 A443 Q444 Q447 K448 E449 R450 L451 K452 G453 I458 K459 L460 K461 N462 V463 M464 F465 E466 V467 K468 T469 R470 A471 S472 T473 VAL SER S476 V477
V478 A481 I484 F485 A486 I487 E495 I496 D497 A498 D499 F500 P501 H502 P503 L504 R505 L506 R507 L508 M509 G510 V511 R512 I513 F516 P517 ASN GLU GLU ASP ARG LYS HIS GLN GLN

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	85.21Å 109.46Å 111.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.03 – 2.40	Depositor
% Data completeness (in resolution range)	91.2 (20.03-2.40)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.246 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6532	wwPDB-VP
Average B, all atoms (Å^2)	40.0	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	0.48	2/3232 (0.1%)	0.82	12/4358 (0.3%)
1	B	0.39	0/3036	0.70	2/4097 (0.0%)
All	All	0.44	2/6268 (0.0%)	0.76	14/8455 (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	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	389	GLU	CD-OE2	7.28	1.33	1.25
1	A	455	THR	N-CA	6.36	1.59	1.46

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	516	PHE	C-N-CD	-10.41	97.70	120.60
1	A	475	SER	N-CA-C	8.00	132.59	111.00
1	A	451	LEU	N-CA-C	7.27	130.64	111.00
1	A	452	LYS	N-CA-C	6.66	128.99	111.00
1	B	449	GLU	N-CA-C	-6.58	93.23	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	474	VAL	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	3185	0	3153	159	0
1	B	2987	0	2961	198	0
2	A	187	0	0	19	0
2	B	173	0	0	20	0
All	All	6532	0	6114	357	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 29.

The worst 5 of 357 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:B:416:MET:HB2	1:B:513:ILE:HG22	1.28	1.14
1:B:305:THR:HG22	1:B:306:THR:H	1.11	1.13
1:A:451:LEU:O	1:A:452:LYS:CB	1.96	1.09
1:A:470:ARG:NH2	1:A:494:THR:HB	1.75	1.00
1:A:461:LYS:HB2	1:A:508:LEU:HB3	1.45	0.98

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	394/459 (86%)	356 (90%)	24 (6%)	14 (4%)	3 3
1	B	374/459 (82%)	340 (91%)	28 (8%)	6 (2%)	9 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	768/918 (84%)	696 (91%)	52 (7%)	20 (3%)	5 5

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	LYS
1	A	444	GLN
1	A	452	LYS
1	A	454	ARG
1	A	475	SER

5.3.2 Protein sidechains (i)

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	341/412 (83%)	331 (97%)	10 (3%)	42 62
1	B	317/412 (77%)	308 (97%)	9 (3%)	43 63
All	All	658/824 (80%)	639 (97%)	19 (3%)	42 62

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	352	ARG
1	B	85	GLN
1	B	382	LEU
1	A	340	GLN
1	B	383	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	330	ASN
1	A	397	HIS
1	B	303	GLN

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Mol	Chain	Res	Type
1	A	278	GLN
1	B	406	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.