



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2017 – 03:35 PM EST

PDB ID : 1RPL
Title : 2.3 ANGSTROMS CRYSTAL STRUCTURE OF THE CATALYTIC DOMAIN OF DNA POLYMERASE BETA
Authors : Davies II, J.F.; Almasy, R.J.
Deposited on : unknown
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

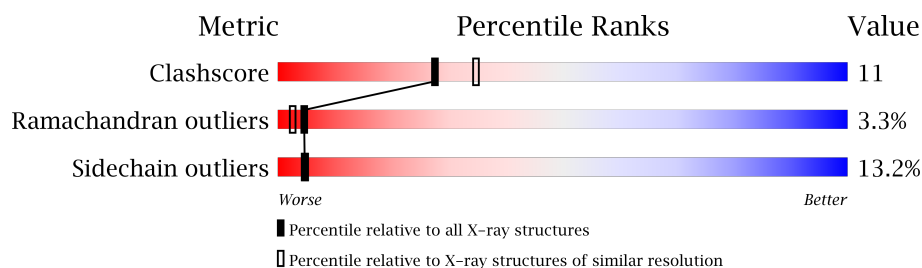
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	251	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2024 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 DNA POLYMERASE BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	0
			1965	1236	345	376	8			

- Molecule 2 is water.

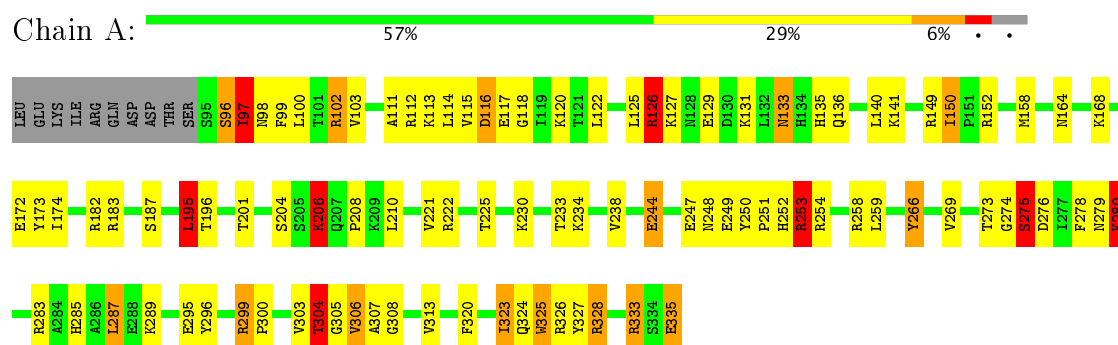
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	59	Total	O	0	0
			59	59		

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.

Note EDS was not executed.

• Molecule 1: DNA POLYMERASE BETA



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	120.80 Å 63.40 Å 38.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.220 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2024	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

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	1.17	2/2004 (0.1%)	1.79	45/2699 (1.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	296	TYR	CB-CG	-5.51	1.43	1.51
1	A	173	TYR	CB-CG	-5.48	1.43	1.51

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	ARG	NE-CZ-NH1	15.83	128.22	120.30
1	A	254	ARG	NE-CZ-NH2	-15.67	112.46	120.30
1	A	253	ARG	NE-CZ-NH2	-11.69	114.46	120.30
1	A	152	ARG	NE-CZ-NH1	10.04	125.32	120.30
1	A	253	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	A	274	GLY	CA-C-N	-9.35	96.63	117.20
1	A	274	GLY	C-N-CA	9.00	144.19	121.70
1	A	299	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	A	328	ARG	CA-CB-CG	-8.21	95.33	113.40
1	A	195	LEU	CA-CB-CG	7.92	133.52	115.30
1	A	274	GLY	O-C-N	7.68	134.98	122.70
1	A	258	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	A	173	TYR	CB-CG-CD2	-7.33	116.60	121.00
1	A	126	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	A	326	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	A	222	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	A	206	LYS	N-CA-C	6.71	129.11	111.00
1	A	266	TYR	CA-CB-CG	-6.51	101.02	113.40
1	A	250	TYR	CA-CB-CG	-6.16	101.70	113.40
1	A	333	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	141	LYS	CA-CB-CG	6.03	126.66	113.40
1	A	158	MET	CG-SD-CE	6.00	109.80	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	ARG	CG-CD-NE	-5.84	99.54	111.80
1	A	172	GLU	CA-CB-CG	-5.74	100.77	113.40
1	A	275	SER	N-CA-CB	5.65	118.98	110.50
1	A	152	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	183	ARG	CB-CG-CD	-5.54	97.19	111.60
1	A	296	TYR	CB-CG-CD2	-5.46	117.72	121.00
1	A	244	GLU	N-CA-C	5.40	125.58	111.00
1	A	98	ASN	N-CA-CB	5.39	120.30	110.60
1	A	125	LEU	CA-CB-CG	5.38	127.67	115.30
1	A	280	LYS	CB-CG-CD	5.37	125.56	111.60
1	A	296	TYR	CD1-CG-CD2	5.37	123.80	117.90
1	A	102	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	275	SER	N-CA-C	-5.31	96.67	111.00
1	A	306	VAL	CA-C-N	-5.30	105.53	117.20
1	A	230	LYS	CA-CB-CG	5.30	125.06	113.40
1	A	182	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	234	LYS	CB-CG-CD	5.25	125.25	111.60
1	A	131	LYS	CA-CB-CG	-5.19	101.98	113.40
1	A	258	ARG	CB-CG-CD	-5.19	98.12	111.60
1	A	324	GLN	CA-CB-CG	-5.15	102.06	113.40
1	A	280	LYS	CG-CD-CE	5.13	127.30	111.90
1	A	98	ASN	CB-CA-C	-5.12	100.16	110.40
1	A	149	ARG	NE-CZ-NH2	-5.05	117.78	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	1965	0	1944	44	0
2	A	59	0	0	4	0
All	All	2024	0	1944	44	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 11.

All (44) 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:A:99:PHE:HZ	1:A:122:LEU:HD13	1.58	0.68
1:A:99:PHE:CZ	1:A:122:LEU:HD13	2.30	0.66
1:A:303:VAL:HB	1:A:306:VAL:HG11	1.78	0.66
1:A:320:PHE:O	1:A:323:ILE:HG22	1.95	0.65
1:A:269:VAL:O	1:A:273:THR:HG22	1.99	0.62
1:A:328:ARG:NH1	1:A:335:GLU:HB3	2.17	0.60
1:A:206:LYS:HE3	1:A:208:PRO:HD2	1.85	0.59
1:A:303:VAL:HB	1:A:306:VAL:CG1	2.33	0.59
1:A:299:ARG:HG2	1:A:308:GLY:O	2.05	0.56
1:A:320:PHE:CD2	1:A:327:TYR:HD1	2.24	0.55
1:A:150:ILE:HD13	1:A:253:ARG:HD3	1.90	0.54
1:A:113:LYS:HE3	1:A:114:LEU:HG	1.90	0.54
1:A:273:THR:HG23	2:A:446:HOH:O	2.08	0.53
1:A:97:ILE:HG12	1:A:111:ALA:HB1	1.91	0.52
1:A:96:SER:HB2	1:A:120:LYS:HB2	1.92	0.52
1:A:112:ARG:O	1:A:115:VAL:HG12	2.11	0.51
1:A:285:HIS:CE1	1:A:289:LYS:HE2	2.45	0.51
1:A:252:HIS:HE1	2:A:454:HOH:O	1.94	0.50
1:A:249:GLU:O	1:A:251:PRO:HD2	2.12	0.49
1:A:122:LEU:O	1:A:126:ARG:HB2	2.13	0.49
1:A:266:TYR:HB2	1:A:313:VAL:HG12	1.95	0.49
1:A:323:ILE:HG23	1:A:325:TRP:HB2	1.95	0.48
1:A:275:SER:HB3	1:A:278:PHE:HB3	1.96	0.48
1:A:304:THR:H	1:A:306:VAL:HG12	1.79	0.46
1:A:174:ILE:HB	1:A:196:THR:HG22	1.96	0.46
1:A:279:ASN:HB2	1:A:280:LYS:HE2	1.97	0.46
1:A:97:ILE:HD13	1:A:97:ILE:O	2.16	0.46
1:A:328:ARG:HH12	1:A:335:GLU:HB3	1.79	0.45
1:A:99:PHE:O	1:A:102:ARG:HB2	2.17	0.45
1:A:252:HIS:CE1	2:A:454:HOH:O	2.68	0.45
1:A:305:GLY:HA2	2:A:451:HOH:O	2.17	0.45
1:A:195:LEU:HD13	1:A:259:LEU:HD13	1.99	0.44
1:A:323:ILE:HD13	1:A:323:ILE:HG21	1.66	0.44
1:A:225:THR:OG1	1:A:238:VAL:HG22	2.17	0.43
1:A:133:ASN:HD21	1:A:135:HIS:HB3	1.82	0.43
1:A:295:GLU:H	1:A:295:GLU:CD	2.22	0.43
1:A:287:LEU:HA	1:A:287:LEU:HD22	1.88	0.43
1:A:299:ARG:HB3	1:A:307:ALA:O	2.19	0.42
1:A:133:ASN:ND2	1:A:136:GLN:H	2.18	0.42
1:A:275:SER:HB3	1:A:278:PHE:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:THR:O	1:A:204:SER:HB3	2.20	0.41
1:A:306:VAL:O	1:A:306:VAL:HG13	2.20	0.41
1:A:116:ASP:O	1:A:118:GLY:N	2.53	0.41
1:A:275:SER:HB2	1:A:333:ARG:O	2.21	0.41

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	239/251 (95%)	214 (90%)	17 (7%)	8 (3%)	4 2

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	275	SER
1	A	117	GLU
1	A	248	ASN
1	A	304	THR
1	A	206	LYS
1	A	97	ILE
1	A	244	GLU
1	A	247	GLU

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	219/229 (96%)	190 (87%)	29 (13%)	5 5

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	SER
1	A	97	ILE
1	A	100	LEU
1	A	103	VAL
1	A	116	ASP
1	A	126	ARG
1	A	127	LYS
1	A	129	GLU
1	A	133	ASN
1	A	140	LEU
1	A	150	ILE
1	A	164	ASN
1	A	168	LYS
1	A	187	SER
1	A	195	LEU
1	A	206	LYS
1	A	210	LEU
1	A	221	VAL
1	A	233	THR
1	A	253	ARG
1	A	276	ASP
1	A	280	LYS
1	A	283	ARG
1	A	287	LEU
1	A	300	PRO
1	A	304	THR
1	A	323	ILE
1	A	325	TRP
1	A	335	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	ASN
1	A	164	ASN
1	A	199	ASN
1	A	212	HIS

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Mol	Chain	Res	Type
1	A	217	GLN
1	A	252	HIS
1	A	285	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 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.