



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:30 AM UTC

PDB ID : 1RPL / pdb_00001rpl
Title : 2.3 ANGSTROMS CRYSTAL STRUCTURE OF THE CATALYTIC DOMAIN OF DNA POLYMERASE BETA
Authors : Davies II, J.F.; Almassy, R.J.
Deposited on : 1994-10-25
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

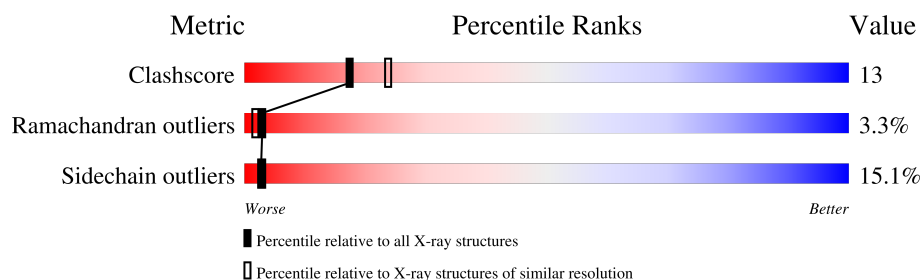
1 Overall quality at a glance

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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (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 of 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	251	47% 31% 13% . .

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		

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	120.80Å 63.40Å 38.70Å 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

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	1.60	16/2004 (0.8%)	2.16	98/2699 (3.6%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150	ILE	CA-C	10.15	1.61	1.53
1	A	150	ILE	CA-CB	9.03	1.64	1.54
1	A	231	GLY	N-CA	7.51	1.51	1.44
1	A	260	ILE	CA-CB	7.42	1.63	1.54
1	A	285	HIS	ND1-CE1	5.93	1.38	1.32
1	A	304	THR	CA-CB	5.86	1.63	1.53
1	A	214	VAL	CA-CB	5.72	1.60	1.54
1	A	303	VAL	CA-CB	5.67	1.62	1.54
1	A	98	ASN	N-CA	5.41	1.53	1.46
1	A	207	GLN	CA-C	5.38	1.59	1.52
1	A	293	ILE	CA-C	5.35	1.58	1.52
1	A	212	HIS	CE1-NE2	5.34	1.37	1.32
1	A	210	LEU	N-CA	5.32	1.52	1.46
1	A	238	VAL	CA-CB	5.32	1.64	1.55
1	A	273	THR	N-CA	5.30	1.53	1.46
1	A	134	HIS	ND1-CE1	5.01	1.37	1.32

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	GLY	O-C-N	11.91	134.98	122.60
1	A	274	GLY	CA-C-N	11.86	144.19	121.54
1	A	274	GLY	C-N-CA	11.86	144.19	121.54
1	A	99	PHE	CA-CB-CG	-9.53	104.27	113.80
1	A	328	ARG	CA-CB-CG	-9.38	95.33	114.10
1	A	206	LYS	N-CA-C	8.60	129.11	110.80
1	A	307	ALA	N-CA-C	8.42	122.53	111.75
1	A	317	GLN	OE1-CD-NE2	-8.05	114.55	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	SER	N-CA-C	8.01	121.11	111.82
1	A	234	LYS	N-CA-C	7.80	120.80	107.93
1	A	116	ASP	CA-CB-CG	7.73	120.33	112.60
1	A	150	ILE	CA-C-O	7.62	124.76	119.20
1	A	150	ILE	O-C-N	-7.51	115.60	121.46
1	A	254	ARG	NE-CZ-NH2	-7.49	112.46	119.20
1	A	199	ASN	OD1-CG-ND2	-7.32	115.28	122.60
1	A	159	GLN	OE1-CD-NE2	-7.28	115.32	122.60
1	A	266	TYR	CA-CB-CG	-7.15	101.02	113.90
1	A	297	THR	N-CA-C	7.11	119.55	108.96
1	A	133	ASN	OD1-CG-ND2	-7.08	115.52	122.60
1	A	279	ASN	OD1-CG-ND2	-6.98	115.62	122.60
1	A	128	ASN	OD1-CG-ND2	-6.97	115.63	122.60
1	A	280	LYS	CG-CD-CE	6.96	127.30	111.30
1	A	244	GLU	N-CA-C	6.94	125.58	110.80
1	A	273	THR	CA-C-O	6.84	127.80	119.38
1	A	250	TYR	CA-CB-CG	-6.78	101.70	113.90
1	A	254	ARG	NE-CZ-NH1	6.72	128.22	121.50
1	A	172	GLU	CA-CB-CG	-6.67	100.77	114.10
1	A	265	TYR	N-CA-C	6.63	118.59	111.36
1	A	275	SER	N-CA-C	-6.63	96.67	110.80
1	A	278	PHE	CA-CB-CG	-6.48	107.32	113.80
1	A	121	THR	O-C-N	-6.38	115.76	123.10
1	A	143	PHE	CA-CB-CG	-6.36	107.44	113.80
1	A	306	VAL	CA-C-O	6.32	128.68	120.78
1	A	141	LYS	CA-CB-CG	6.28	126.66	114.10
1	A	207	GLN	N-CA-C	6.27	123.67	109.81
1	A	106	ILE	N-CA-C	6.22	116.20	107.37
1	A	280	LYS	CB-CG-CD	6.20	125.56	111.30
1	A	136	GLN	OE1-CD-NE2	-6.18	116.42	122.60
1	A	150	ILE	CB-CA-C	6.17	117.87	110.78
1	A	183	ARG	CB-CG-CD	-6.14	97.19	111.30
1	A	164	ASN	OD1-CG-ND2	-6.07	116.53	122.60
1	A	234	LYS	CB-CG-CD	6.06	125.25	111.30
1	A	219	GLN	OE1-CD-NE2	-6.06	116.54	122.60
1	A	131	LYS	CA-CB-CG	-6.06	101.98	114.10
1	A	212	HIS	N-CA-C	6.03	118.64	111.71
1	A	324	GLN	CA-CB-CG	-6.02	102.06	114.10
1	A	232	GLU	CB-CG-CD	-6.01	102.38	112.60
1	A	120	LYS	N-CA-C	5.93	119.74	111.56
1	A	293	ILE	N-CA-C	5.93	117.12	108.53
1	A	296	TYR	CB-CA-C	-5.92	100.79	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	GLU	N-CA-C	5.91	118.87	110.24
1	A	306	VAL	CA-C-N	5.84	128.91	120.38
1	A	306	VAL	C-N-CA	5.84	128.91	120.38
1	A	98	ASN	N-CA-CB	5.81	120.30	110.49
1	A	233	THR	N-CA-CB	-5.75	101.82	110.73
1	A	258	ARG	CB-CG-CD	-5.73	98.12	111.30
1	A	133	ASN	CA-CB-CG	5.73	118.33	112.60
1	A	254	ARG	CG-CD-NE	-5.66	99.54	112.00
1	A	194	LEU	O-C-N	-5.66	116.77	123.22
1	A	207	GLN	O-C-N	-5.63	114.85	121.32
1	A	124	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	249	GLU	CA-C-N	-5.62	113.42	123.08
1	A	249	GLU	C-N-CA	-5.62	113.42	123.08
1	A	150	ILE	CA-CB-CG2	5.58	119.99	110.50
1	A	310	PRO	N-CA-C	5.56	119.59	111.03
1	A	96	SER	N-CA-C	-5.50	105.36	111.36
1	A	230	LYS	CA-CB-CG	5.48	125.06	114.10
1	A	214	VAL	CA-C-N	5.46	127.64	120.60
1	A	214	VAL	C-N-CA	5.46	127.64	120.60
1	A	197	HIS	CB-CG-CD2	-5.46	124.10	131.20
1	A	249	GLU	CB-CG-CD	5.43	121.83	112.60
1	A	245	ASN	OD1-CG-ND2	-5.34	117.26	122.60
1	A	157	GLN	CB-CG-CD	-5.34	103.53	112.60
1	A	334	SER	CA-C-N	5.30	131.25	121.70
1	A	334	SER	C-N-CA	5.30	131.25	121.70
1	A	97	ILE	CA-C-N	5.28	131.63	121.54
1	A	97	ILE	C-N-CA	5.28	131.63	121.54
1	A	253	ARG	NE-CZ-NH2	-5.27	114.46	119.20
1	A	103	VAL	CA-C-O	5.25	126.84	120.85
1	A	221	VAL	CA-C-N	5.24	130.00	122.40
1	A	221	VAL	C-N-CA	5.24	130.00	122.40
1	A	206	LYS	O-C-N	-5.17	115.71	122.59
1	A	98	ASN	CB-CA-C	-5.16	100.16	110.42
1	A	150	ILE	N-CA-C	5.15	113.54	107.77
1	A	106	ILE	N-CA-CB	-5.15	106.34	111.90
1	A	127	LYS	CA-C-O	5.13	126.16	119.95
1	A	226	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	150	ILE	N-CA-CB	-5.10	104.96	111.23
1	A	231	GLY	O-C-N	-5.10	117.11	123.12
1	A	135	HIS	CB-CG-CD2	-5.08	124.59	131.20
1	A	173	TYR	CB-CA-C	-5.08	101.77	109.89
1	A	300	PRO	O-C-N	-5.07	118.01	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	LYS	N-CA-CB	-5.06	104.20	111.54
1	A	162	VAL	N-CA-C	5.06	115.28	110.42
1	A	313	VAL	O-C-N	-5.03	118.44	122.97
1	A	273	THR	N-CA-C	-5.03	106.41	112.54
1	A	275	SER	N-CA-CB	5.02	118.98	110.49
1	A	103	VAL	N-CA-CB	5.02	116.00	110.53

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	49	0
2	A	59	0	0	4	0
All	All	2024	0	1944	49	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 13.

All (49) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:155:MET:HE2	1:A:188:SER:CB	2.43	0.48
1:A:295:GLU:H	1:A:295:GLU:CD	2.22	0.48
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:O	1:A:97:ILE:HD13	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:133:ASN:C	1:A:133:ASN:HD22	2.25	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:116:ASP:C	1:A:118:GLY:H	2.26	0.43
1:A:287:LEU:HD22	1:A:287:LEU:HA	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
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:294:ASN:OD1	1:A:294:ASN:C	2.62	0.41
1:A:116:ASP:O	1:A:118:GLY:N	2.53	0.41
1:A:282:MET:HE2	1:A:319:ILE:HG22	2.02	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

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

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%)	186 (85%)	33 (15%)	3 3

All (33) 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

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Mol	Chain	Res	Type
1	A	103	VAL
1	A	116	ASP
1	A	121	THR
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	234	LYS
1	A	238	VAL
1	A	253	ARG
1	A	254	ARG
1	A	280	LYS
1	A	282	MET
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	133	ASN
1	A	135	HIS
1	A	164	ASN
1	A	199	ASN
1	A	212	HIS
1	A	217	GLN
1	A	252	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 oligosaccharides 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.