



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:52 PM UTC

PDB ID : 1DD9 / pdb_00001dd9
Title : STRUCTURE OF THE DNAG CATALYTIC CORE
Authors : Keck, J.L.; Roche, D.D.; Lynch, A.S.; Berger, J.M.
Deposited on : 1999-11-09
Resolution : 1.60 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

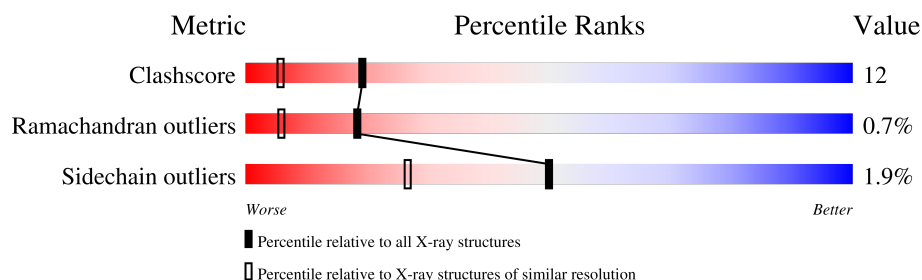
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)

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	338	 72% 19% • 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2693 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 PRIMASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2458	1548	439	460	11			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	MET	GLU	expression tag	UNP P0ABS5
A	97	ARG	VAL	expression tag	UNP P0ABS5
A	98	GLY	PRO	expression tag	UNP P0ABS5
A	99	SER	PHE	expression tag	UNP P0ABS5
A	100	HIS	GLU	expression tag	UNP P0ABS5
A	101	HIS	ALA	expression tag	UNP P0ABS5
A	102	HIS	GLY	expression tag	UNP P0ABS5
A	103	HIS	SER	expression tag	UNP P0ABS5
A	104	HIS	GLY	expression tag	UNP P0ABS5
A	105	HIS	PRO	expression tag	UNP P0ABS5
A	106	GLY	SER	expression tag	UNP P0ABS5
A	107	SER	GLN	expression tag	UNP P0ABS5
A	108	GLY	ILE	expression tag	UNP P0ABS5
A	109	SER	GLU	expression tag	UNP P0ABS5
A	110	MET	ARG	expression tag	UNP P0ABS5

- Molecule 2 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Sr	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	234	Total 234	O 234	0	0

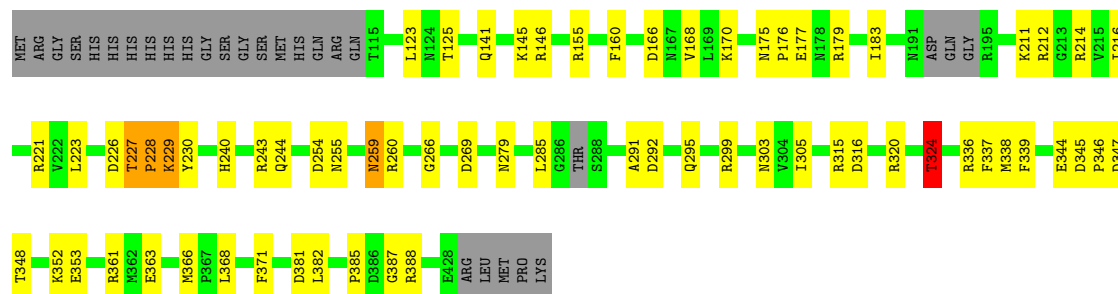
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: DNA PRIMASE

Chain A: 



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 21	Depositor
Cell constants a, b, c, α , β , γ	38.34Å 57.87Å 148.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.60	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-1.60)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.231 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2693	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SR

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	0.45	0/2505	1.17	6/3386 (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	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	THR	CA-C-O	-15.39	99.08	120.16
1	A	228	PRO	CA-N-CD	-7.60	101.37	112.00
1	A	228	PRO	N-CA-CB	6.71	110.30	103.25
1	A	228	PRO	N-CD-CG	6.32	112.68	103.20
1	A	303	ASN	CA-CB-CG	6.30	118.90	112.60
1	A	324	THR	N-CA-CB	5.41	119.22	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	227	THR	Mainchain,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	2458	0	2425	57	0
2	A	1	0	0	0	0
3	A	234	0	0	7	0
All	All	2693	0	2425	57	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 12.

All (57) 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:166:ASP:OD2	1:A:170:LYS:HE3	1.63	0.98
1:A:260:ARG:NH1	1:A:363:GLU:OE2	2.12	0.82
1:A:337:PHE:HE1	1:A:368:LEU:HD12	1.45	0.81
1:A:226:ASP:OD2	3:A:691:HOH:O	1.98	0.79
1:A:366:MET:HE1	1:A:371:PHE:CD1	2.24	0.73
1:A:141:GLN:HG2	1:A:145:LYS:HE3	1.73	0.70
1:A:339:PHE:HE1	1:A:366:MET:HE2	1.57	0.70
1:A:254:ASP:O	1:A:254:ASP:OD1	2.10	0.69
1:A:344:GLU:OE1	1:A:348:THR:OG1	2.05	0.69
1:A:166:ASP:OD2	1:A:170:LYS:CE	2.39	0.69
1:A:123:LEU:HD21	1:A:168:VAL:HG13	1.76	0.68
1:A:269:ASP:OD1	3:A:614:HOH:O	2.12	0.67
1:A:348:THR:O	1:A:352:LYS:HG3	1.97	0.64
1:A:316:ASP:OD1	3:A:692:HOH:O	2.15	0.64
1:A:216:ILE:HD12	1:A:244:GLN:OE1	1.99	0.62
1:A:315:ARG:HG3	3:A:657:HOH:O	1.99	0.62
1:A:339:PHE:HE1	1:A:366:MET:CE	2.14	0.60
1:A:216:ILE:CD1	1:A:244:GLN:OE1	2.48	0.60
1:A:175:ASN:OD1	1:A:177:GLU:HB2	2.01	0.59
1:A:259:ASN:HD22	1:A:259:ASN:H	1.48	0.59
1:A:339:PHE:CE1	1:A:366:MET:HE2	2.37	0.57
1:A:292:ASP:HA	1:A:295:GLN:HE21	1.69	0.56
1:A:337:PHE:CE1	1:A:368:LEU:HD12	2.35	0.55
1:A:320:ARG:O	1:A:324:THR:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:LYS:NZ	1:A:299:ARG:NH2	2.56	0.53
1:A:155:ARG:NH1	1:A:279:ASN:OD1	2.41	0.53
1:A:146:ARG:NH1	1:A:347:ASP:OD2	2.42	0.53
1:A:160:PHE:HE1	1:A:223:LEU:HD12	1.75	0.51
1:A:320:ARG:HD2	3:A:569:HOH:O	2.10	0.51
1:A:179:ARG:O	1:A:183:ILE:HG13	2.09	0.51
1:A:366:MET:HE1	1:A:371:PHE:HD1	1.72	0.51
1:A:291:ALA:O	1:A:295:GLN:HG3	2.11	0.50
1:A:385:PRO:HA	1:A:388:ARG:NH1	2.27	0.50
1:A:254:ASP:OD2	1:A:279:ASN:HB3	2.12	0.49
1:A:345:ASP:HB2	1:A:346:PRO:CD	2.43	0.49
1:A:123:LEU:HD21	1:A:168:VAL:CG1	2.40	0.49
1:A:211:LYS:NZ	1:A:299:ARG:HH22	2.11	0.48
1:A:175:ASN:ND2	1:A:176:PRO:HD2	2.29	0.47
1:A:160:PHE:CE1	1:A:223:LEU:HD12	2.49	0.47
1:A:254:ASP:OD2	1:A:279:ASN:CB	2.63	0.47
1:A:125:THR:OG1	3:A:700:HOH:O	1.96	0.46
1:A:240:HIS:HB2	1:A:243:ARG:HG2	1.96	0.46
1:A:345:ASP:HB2	1:A:346:PRO:HD2	1.98	0.44
1:A:385:PRO:HA	1:A:388:ARG:HH11	1.82	0.44
1:A:366:MET:HE3	1:A:371:PHE:HB2	1.99	0.44
1:A:381:ASP:O	1:A:387:GLY:HA3	2.18	0.43
1:A:353:GLU:OE2	1:A:361:ARG:NH2	2.36	0.42
1:A:229:LYS:HG3	1:A:230:TYR:CD1	2.55	0.42
1:A:259:ASN:H	1:A:259:ASN:ND2	2.16	0.42
1:A:221:ARG:HG3	1:A:230:TYR:CE2	2.54	0.42
1:A:266:GLY:HA2	3:A:708:HOH:O	2.19	0.42
1:A:338:MET:HE3	1:A:361:ARG:HG2	2.01	0.41
1:A:211:LYS:HZ3	1:A:299:ARG:HH22	1.66	0.41
1:A:305:ILE:HD11	1:A:336:ARG:NH2	2.35	0.40
1:A:337:PHE:HE1	1:A:368:LEU:CD1	2.25	0.40
1:A:212:ARG:NH1	1:A:214:ARG:NH1	2.68	0.40
1:A:259:ASN:ND2	1:A:259:ASN:N	2.70	0.40

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	304/338 (90%)	299 (98%)	3 (1%)	2 (1%)	18 6

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	228	PRO
1	A	255	ASN

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	259/283 (92%)	254 (98%)	5 (2%)	50 27

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	229	LYS
1	A	259	ASN
1	A	285	LEU
1	A	324	THR
1	A	382	LEU

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	124	ASN
1	A	128	GLN
1	A	175	ASN
1	A	178	ASN
1	A	225	ASN
1	A	259	ASN
1	A	295	GLN
1	A	374	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.