Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:57 PM GMT

PDB ID	:	1DD9
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
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:

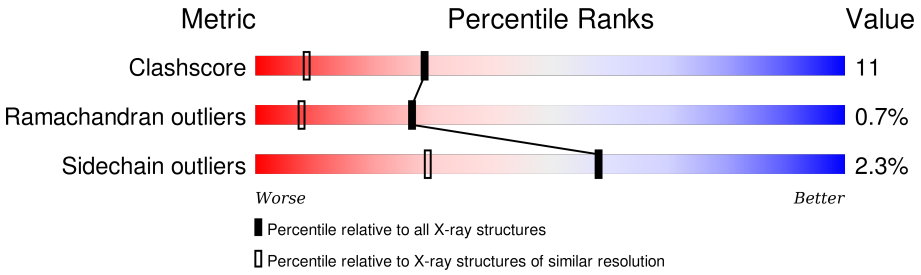
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (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 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 <=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	338	71% 18% • 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 (three-letter code: 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	O	0	0
			234	234		

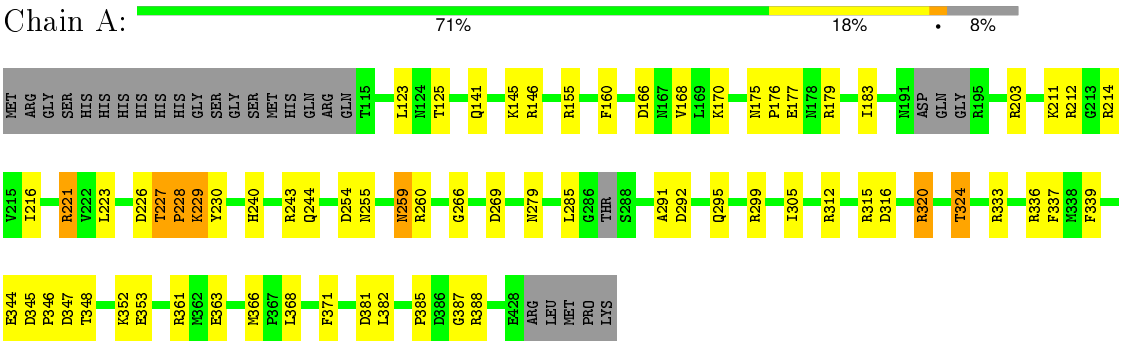
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 PRIMASE

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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	0.36	0/2505	0.96	10/3386 (0.3%)

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 (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	227	THR	CA-C-O	-10.01	99.08	120.10
1	A	228	PRO	CA-N-CD	-7.24	101.37	111.50
1	A	320	ARG	NE-CZ-NH2	-7.09	116.76	120.30
1	A	333	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	A	333	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	228	PRO	N-CD-CG	6.32	112.68	103.20
1	A	203	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	A	228	PRO	N-CA-CB	5.83	110.30	103.30
1	A	221	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	221	ARG	CD-NE-CZ	5.13	130.79	123.60

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	56	0
2	A	1	0	0	0	0
3	A	234	0	0	7	0
All	All	2693	0	2425	56	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 (56) 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:141:GLN:HG2	1:A:145:LYS:HE3	1.73	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:366:MET:HE3	1:A:371:PHE:HB2	1.75	0.66
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:292:ASP:HA	1:A:295:GLN:HE21	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:MET:HE1	1:A:371:PHE:CD1	2.41	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
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:339:PHE:HE1	1:A:366:MET:HE2	1.75	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:240:HIS:HB2	1:A:243:ARG:HG2	1.96	0.46
1:A:125:THR:OG1	3:A:700:HOH:O	1.96	0.46
1:A:385:PRO:HA	1:A:388:ARG:HH11	1.82	0.44
1:A:345:ASP:HB2	1:A:346:PRO:HD2	1.98	0.44
1:A:339:PHE:HE1	1:A:366:MET:HE1	1.82	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:211:LYS:HZ3	1:A:299:ARG:HH22	1.66	0.41
1:A:339:PHE:CE1	1:A:366:MET:HE2	2.55	0.41
1:A:337:PHE:HE1	1:A:368:LEU:CD1	2.25	0.40
1:A:305:ILE:HD11	1:A:336:ARG:NH2	2.35	0.40
1:A:259:ASN:N	1:A:259:ASN:ND2	2.70	0.40
1:A:212:ARG:NH1	1:A:214:ARG:NH1	2.68	0.40

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	304/338 (90%)	299 (98%)	3 (1%)	2 (1%)	26 8

All (2) Ramachandran outliers are listed below:

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

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	259/283 (92%)	253 (98%)	6 (2%)	58 29

All (6) 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	312	ARG
1	A	324	THR
1	A	382	LEU

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	124	ASN
1	A	178	ASN
1	A	232	ASN
1	A	259	ASN
1	A	295	GLN
1	A	374	ASN
1	A	417	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 carbohydrates 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 will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.