



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 02:26 AM UTC

PDB ID : 1UAA / pdb_00001uaa
Title : E. COLI REP HELICASE/DNA COMPLEX
Authors : Korolev, S.; Waksman, G.
Deposited on : 1997-06-30
Resolution : 3.00 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 ⓘ 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

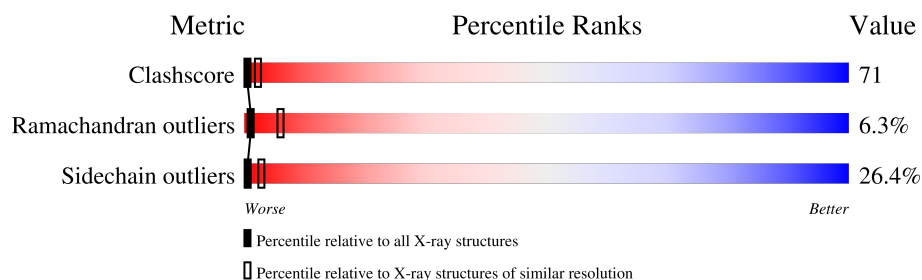
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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	C	16	
2	A	673	
2	B	673	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10404 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 DNA chain called DNA (5'-D(*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	16	Total	C	N	O	P	0	0	0
			317	160	32	110	15			

- Molecule 2 is a protein called PROTEIN (ATP-DEPENDENT DNA HELICASE REP.).

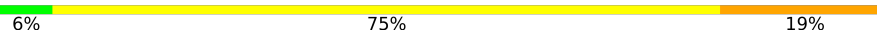
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	636	Total	C	N	O	S	0	0	0
			5032	3186	881	942	23			
2	B	633	Total	C	N	O	S	0	0	0
			5055	3203	886	945	21			

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.

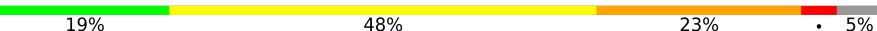
Note EDS was not executed.

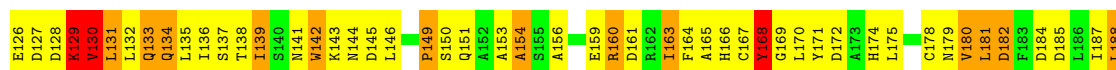
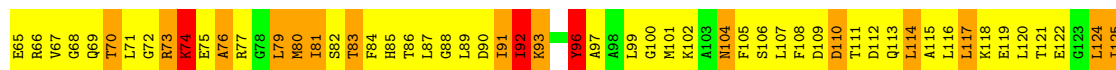
- Molecule 1: DNA (5'-D(*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3')

Chain C: 



- Molecule 2: PROTEIN (ATP-DEPENDENT DNA HELICASE REP.)

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 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	141.80 Å 141.80 Å 284.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00	Depositor
% Data completeness (in resolution range)	88.0 (15.00-3.00)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.228 , 0.328	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10404	wwPDB-VP
Average B, all atoms (Å ²)	43.0	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	C	0.61	0/348	1.23	4/536 (0.7%)
2	A	1.07	10/5127 (0.2%)	1.37	83/6932 (1.2%)
2	B	1.14	15/5151 (0.3%)	1.37	72/6961 (1.0%)
All	All	1.10	25/10626 (0.2%)	1.37	159/14429 (1.1%)

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
2	A	0	2

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	620	GLU	CA-C	8.95	1.57	1.52
2	B	570	MET	SD-CE	-8.90	1.57	1.79
2	B	327	VAL	CA-CB	-7.70	1.45	1.54
2	A	475	VAL	CA-CB	-7.34	1.46	1.54
2	B	555	MET	SD-CE	-6.78	1.62	1.79

The worst 5 of 159 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	374	GLY	N-CA-C	12.24	123.92	111.56
2	A	410	LYS	N-CA-C	10.86	133.94	110.80
2	B	444	THR	N-CA-C	-9.79	100.47	111.82
2	B	535	THR	N-CA-C	9.78	122.84	111.11
2	B	3	LEU	N-CA-C	9.66	123.65	108.67

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	308	TYR	Sidechain
2	A	569	TYR	Sidechain

5.2 Too-close contacts [i](#)

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	C	317	0	194	68	0
2	A	5032	0	4953	704	0
2	B	5055	0	5014	710	0
All	All	10404	0	10161	1457	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 71.

The worst 5 of 1457 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:C:10:DT:H5'	1:C:10:DT:C6	1.73	1.24
1:C:10:DT:OP1	1:C:10:DT:H3'	1.41	1.20
1:C:4:DT:H2''	1:C:5:DT:C5'	1.79	1.12
1:C:11:DT:H2'	1:C:11:DT:OP2	1.49	1.11
1:C:10:DT:H6	1:C:10:DT:C5'	1.66	1.09

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	
2	A	632/673 (94%)	449 (71%)	142 (22%)	41 (6%)	1	5
2	B	629/673 (94%)	443 (70%)	148 (24%)	38 (6%)	1	7
All	All	1261/1346 (94%)	892 (71%)	290 (23%)	79 (6%)	1	6

5 of 79 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	127	ASP
2	A	341	GLN
2	A	357	VAL
2	A	372	SER
2	A	375	THR

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	
2	A	528/580 (91%)	396 (75%)	132 (25%)	0	3
2	B	536/580 (92%)	387 (72%)	149 (28%)	0	2
All	All	1064/1160 (92%)	783 (74%)	281 (26%)	0	3

5 of 281 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	411	ARG
2	B	430	LYS
2	B	551	GLN
2	A	431	SER
2	A	421	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	174	HIS
2	B	245	GLN
2	B	195	GLN
2	B	217	GLN
2	B	354	GLN

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.