



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 23, 2026 – 04:06 PM EDT

PDB ID : 11KB / pdb\_000011kb  
Title : E.Coli DNA Topoisomerase 3 in complex with an 8mer ssDNA oligo AACT-GTTG  
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Deposited on : 2026-02-27  
Resolution : 1.90 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](mailto:validation@mail.wwpdb.org)

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<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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

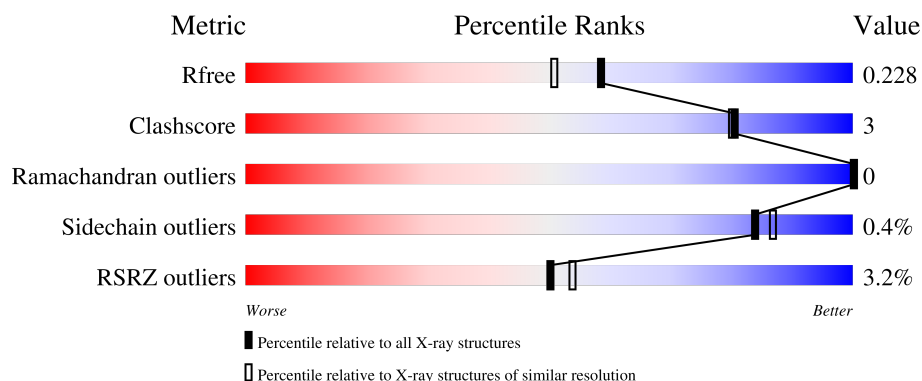
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


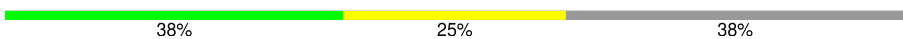
The reported resolution of this entry is 1.90 Å.

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))
$R_{free}$	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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  $\geq 3$ , 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  $\leq 5\%$ . 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.

Mol	Chain	Length	Quality of chain
1	A	646	 3% 90% 6%
2	B	8	 38% 25% 38%

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5542 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 topoisomerase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	620	Total	C	N	O	S	0	10	0
			5015	3166	913	915	21			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	641	GLU	-	expression tag	UNP P14294
A	642	ASN	-	expression tag	UNP P14294
A	643	LEU	-	expression tag	UNP P14294
A	644	TYR	-	expression tag	UNP P14294
A	645	PHE	-	expression tag	UNP P14294
A	646	GLN	-	expression tag	UNP P14294

- Molecule 2 is a DNA chain called DNA (5'-D(\*CP\*GP\*CP\*AP\*AP\*CP\*TP\*T)-3').

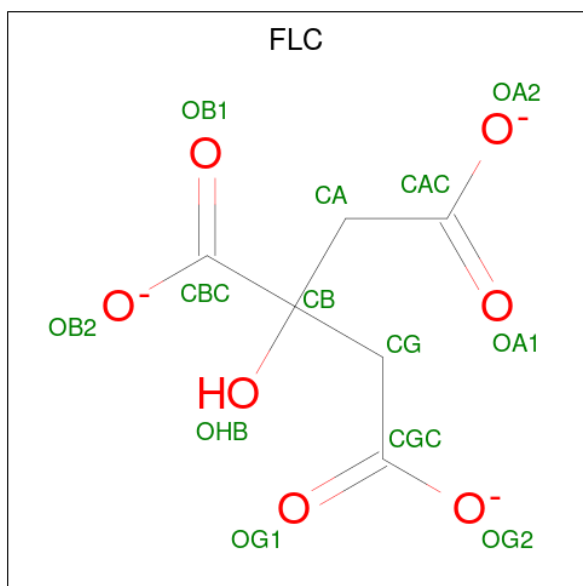
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	5	Total	C	N	O	P	0	0	0
			104	50	16	33	5			

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is CITRATE ANION (CCD ID: FLC) (formula:  $C_6H_5O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		

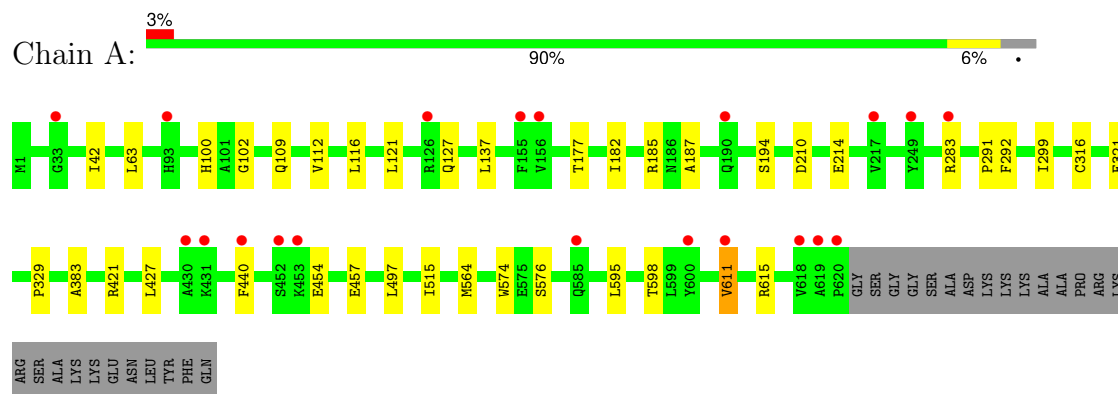
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	381	Total	O	0	0
			381	381		
7	B	20	Total	O	0	0
			20	20		

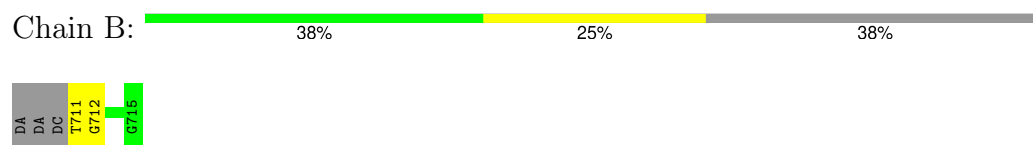
### 3 Residue-property plots [i](#)

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 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.

#### • Molecule 1: DNA topoisomerase 3



#### • Molecule 2: DNA (5'-D(\*CP\*GP\*CP\*AP\*AP\*CP\*TP\*T)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	38.97Å 123.12Å 86.25Å 90.00° 98.67° 90.00°	Depositor
Resolution (Å)	42.64 – 1.90 42.64 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (42.64-1.90) 99.4 (42.64-1.90)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.189 , 0.228 0.189 , 0.228	Depositor DCC
$R_{free}$ test set	3011 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.4	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 37.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5542	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, FLC, EDO, NA

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	0.37	0/5128	0.52	0/6949
2	B	0.67	0/115	0.72	0/176
All	All	0.38	0/5243	0.53	0/7125

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	292	PHE	Peptide

### 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	A	5015	0	5042	26	0
2	B	104	0	59	3	0
3	A	4	0	3	0	0
4	A	13	0	5	0	0
5	A	4	0	6	0	0
6	A	1	0	0	0	0
7	A	381	0	0	0	0
7	B	20	0	0	0	0
All	All	5542	0	5115	27	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 3.

All (27) 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:187:ALA:HB2	1:A:611:VAL:HG13	1.69	0.73
1:A:100:HIS:HD2	1:A:102:GLY:H	1.44	0.66
1:A:564:MET:HE1	1:A:598:THR:HG21	1.85	0.59
1:A:185:ARG:HH12	2:B:711:DT:H3	1.51	0.58
1:A:316:CYS:HB3	1:A:329:PRO:HB3	1.88	0.56
1:A:100:HIS:CD2	1:A:102:GLY:H	2.24	0.55
1:A:515:ILE:HD13	1:A:576:SER:HB2	1.89	0.54
1:A:177:THR:HG23	1:A:194:SER:HA	1.89	0.54
1:A:187:ALA:HB1	1:A:615:ARG:HG2	1.91	0.53
1:A:185:ARG:NH1	2:B:711:DT:H3	2.09	0.51
1:A:283[A]:ARG:HH21	1:A:421:ARG:HE	1.57	0.51
1:A:210:ASP:O	1:A:214:GLU:HG3	2.12	0.49
1:A:100:HIS:CE1	1:A:112:VAL:HB	2.50	0.46
2:B:711:DT:H2''	2:B:712:DG:H5''	1.99	0.45
1:A:299:ILE:HG13	1:A:497:LEU:HD23	1.98	0.45
1:A:100:HIS:HE1	1:A:109:GLN:O	1.99	0.44
1:A:291:PRO:HB2	1:A:383:ALA:CB	2.48	0.43
1:A:137:LEU:HD12	1:A:321:GLU:HA	1.99	0.43
1:A:63:LEU:HG	1:A:182:ILE:HG21	2.01	0.42
1:A:116:LEU:HD22	1:A:121:LEU:HD22	2.02	0.42
1:A:421:ARG:HB2	1:A:440:PHE:CE1	2.55	0.42
1:A:454:GLU:O	1:A:457:GLU:HG2	2.19	0.41
1:A:42:ILE:HD13	1:A:42:ILE:HG21	1.87	0.41
1:A:574:TRP:CZ2	1:A:595:LEU:HD11	2.55	0.41
1:A:100:HIS:CD2	1:A:100:HIS:C	2.98	0.40
1:A:127:GLN:O	1:A:127:GLN:HG3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:PRO:HB2	1:A:383:ALA:HB1	2.03	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	628/646 (97%)	618 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	538/547 (98%)	536 (100%)	2 (0%)	84	87

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	427	LEU
1	A	611	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	100	HIS
1	A	140	GLN
1	A	264	HIS
1	A	370	ASN
1	A	413	GLN
1	A	580	GLN
1	A	585	GLN
1	A	593	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](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	EDO	A	703	-	3,3,3	0.24	0	2,2,2	0.37	0
3	ACT	A	701	-	3,3,3	1.01	0	3,3,3	1.31	0
4	FLC	A	702	-	12,12,12	1.20	1 (8%)	17,17,17	1.23	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	703	-	-	0/1/1/1	-
4	FLC	A	702	-	-	0/16/16/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	702	FLC	CB-CBC	2.29	1.55	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	702	FLC	OB1-CBC-CB	-2.99	116.31	122.09

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 [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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	620/646 (95%)	0.19	20 (3%)	50	54	13, 35, 59, 90	10 (1%)
2	B	5/8 (62%)	-0.55	0	100	100	23, 23, 35, 61	0
All	All	625/654 (95%)	0.18	20 (3%)	50	54	13, 35, 59, 90	10 (1%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	618	VAL	6.0
1	A	155	PHE	4.7
1	A	600	TYR	4.5
1	A	619	ALA	3.3
1	A	620	PRO	3.1
1	A	156	VAL	2.9
1	A	283[A]	ARG	2.8
1	A	440	PHE	2.7
1	A	452	SER	2.6
1	A	431	LYS	2.5
1	A	33	GLY	2.3
1	A	453	LYS	2.3
1	A	430	ALA	2.2
1	A	249	TYR	2.2
1	A	93	HIS	2.2
1	A	217	VAL	2.2
1	A	126	ARG	2.2
1	A	585	GLN	2.1
1	A	190	GLN	2.1
1	A	611	VAL	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	A	703	4/4	0.79	0.24	45,45,46,47	0
4	FLC	A	702	13/13	0.88	0.10	35,42,49,50	0
3	ACT	A	701	4/4	0.96	0.08	28,30,33,38	0
6	NA	A	704	1/1	0.99	0.04	25,25,25,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.