

# wwPDB X-ray Structure Validation Summary Report (i)

#### Aug 2, 2023 - 10:48 PM EDT

PDB ID	:	1I7D
Title	:	NONCOVALENT COMPLEX OF E.COLI DNA TOPOISOMERASE III
		WITH AN 8-BASE SINGLE-STRANDED DNA OLIGONUCLEOTIDE
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Deposited on	:	2001-03-08
Resolution	:	2.05  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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.05 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.



Motria	Whole archive	Similar resolution
wietric	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length		Quality of chair	1	
1	В	8	25%	62%		12%
2	А	659		64%	29%	• 6%



## 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5429 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 5'-D(\*CP\*GP\*CP\*AP\*AP\*CP\*TP\*T)-3'.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	В	8	Total 158	C 77	N 28	O 46	Р 7	0	0	0

• Molecule 2 is a protein called DNA TOPOISOMERASE III.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	А	620	Total 4933	C 3119	N 892	O 902	S 20	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual Comment		Reference
А	328	PHE	TYR	engineered mutation	UNP P14294
А	654	HIS	-	expression tag	UNP P14294
А	655	HIS	-	expression tag	UNP P14294
А	656	HIS	-	expression tag	UNP P14294
А	657	HIS	-	expression tag	UNP P14294
А	658	HIS	-	expression tag	UNP P14294
А	659	HIS	-	expression tag	UNP P14294

• Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	5	ZeroOcc	AltConf
3	А	1	Total ( 1	Cl 1	0	0

• Molecule 4 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	А	1	Total 5	0 4	S 1	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	25	Total O 25 25	0	0
5	А	307	Total O 307 307	0	0



## 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. 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: 5'-D(\*CP\*GP\*CP\*AP\*AP\*CP\*TP\*T)-3'





## 4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source	
Space group	C 1 2 1	Depositor	
Cell constants	122.01Å 60.83Å 125.36Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.73^{\circ}$ $90.00^{\circ}$	Depositor	
Resolution (Å)	29.63 - 2.05	Depositor	
% Data completeness	96 1 (29 63-2 05)	Depositor	
(in resolution range)	30.1 (23.03 2.00)	Depositor	
$R_{merge}$	0.10	Depositor	
R <sub>sym</sub>	9.00	Depositor	
Refinement program	CNS 1.0	Depositor	
$R, R_{free}$	0.233 , $0.260$	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	5429	wwPDB-VP	
Average B, all atoms $(Å^2)$	47.0	wwPDB-VP	



# 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: CL,  $\mathrm{SO4}$ 

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).

Mal	Chain	Bond	lengths	Bond angles		
MIOI	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	В	0.49	0/176	1.00	0/269	
2	А	0.32	0/5040	0.57	0/6835	
All	All	0.32	0/5216	0.59	0/7104	

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	В	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	В	705	DA	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.



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	В	158	0	92	17	0
2	А	4933	0	4954	169	0
3	А	1	0	0	0	0
4	А	5	0	0	0	0
5	А	307	0	0	14	0
5	В	25	0	0	3	0
All	All	5429	0	5046	185	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 18.

The worst 5 of 185 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:B:706:DC:C2'	1:B:707:DT:H5"	1.76	1.15	
1:B:707:DT:H5'	1:B:707:DT:H6	1.24	1.03	
1:B:706:DC:H2'	1:B:707:DT:H5"	1.47	0.95	
2:A:612:ARG:HD2	2:A:613:GLN:N	1.84	0.92	
2:A:467:VAL:HG12	2:A:468:ALA:H	1.37	0.89	

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	А	618/659~(94%)	583 (94%)	27~(4%)	8 (1%)	12 4	

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	А	430	ALA
2	А	432	GLY

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Mol	Chain	Res	Type
2	А	452	SER
2	А	270	SER
2	А	544	LYS

#### 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed Rotameric Out		Outliers	Percentiles
2	А	528/555~(95%)	509~(96%)	19 (4%)	35 28

 $5~{\rm of}~19$  residues with a non-rotameric side chain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
2	А	389	ARG
2	А	586	CYS
2	А	599	LEU
2	А	569	ASP
2	А	222	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	$\operatorname{Res}$	Type
2	А	354	HIS
2	А	580	GLN
2	А	382	HIS
2	А	605	GLN
2	А	490	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 monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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 Cha		Chain	Chain Rea		Bond lengths			Bond angles		
IVIOI	Type	Chain	res	LINK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
4	SO4	А	900	-	4,4,4	0.28	0	$6,\!6,\!6$	0.06	0

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 (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 (i)

### 6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

#### 6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

