



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:00 AM GMT

PDB ID : 1SC7  
Title : Human DNA Topoisomerase I (70 Kda) In Complex With The Indenoisoquinoline MJ-II-38 and Covalent Complex With A 22 Base Pair DNA Duplex  
Authors : Staker, B.L.; Feese, M.D.; Cushman, M.; Pommier, Y.; Zembower, D.; Stewart, L.; Burgin, A.B.  
Deposited on : 2004-02-11  
Resolution : 3.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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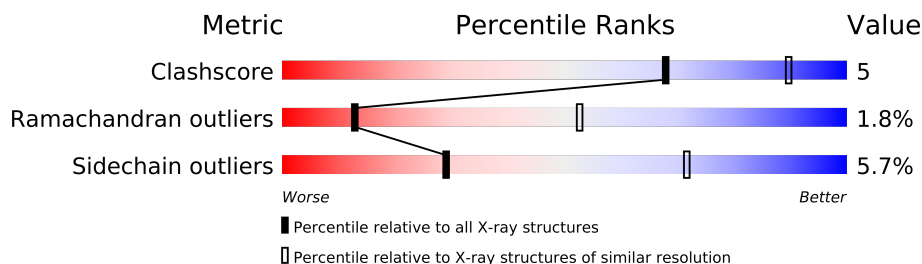
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	10	
2	C	12	
3	D	22	
4	A	592	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5629 atoms, of which 0 are hydrogen and 0 are deuterium.

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(\*AP\*AP\*AP\*AP\*AP\*GP\*AP\*CP\*TP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	10	Total	C	N	O	P	0	0	0
			203	99	42	53	9			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	12	Total	C	N	O	P	S	0	0	0
			246	120	45	69	11	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	22	Total	C	N	O	P	0	0	0
			443	217	71	134	21			

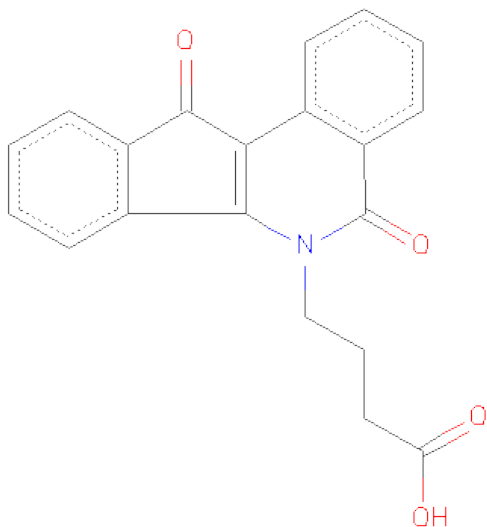
- Molecule 4 is a protein called DNA topoisomerase I.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	A	567	Total	C	N	O	P	S	0	0	0
			4699	2990	822	860	1	26			

There is a discrepancy between the modelled and reference sequences:

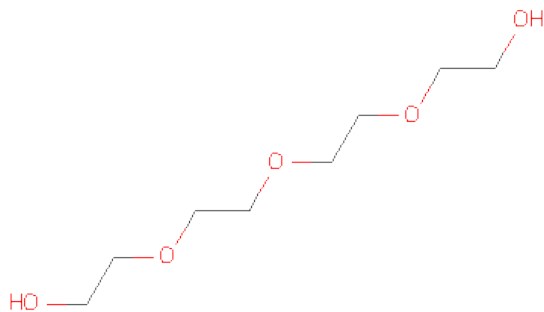
Chain	Residue	Modelled	Actual	Comment	Reference
A	723	PTR	TYR	MODIFIED RESIDUE	UNP P11387

- Molecule 5 is 4-(5,11-DIOXO-5H-INDENO[1,2-C]ISOQUINOLIN-6(11H)-YL)BUTANOATE (three-letter code: M38) (formula: C<sub>20</sub>H<sub>15</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	C	1	25	20	1	4	0	0

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	13	8	5	0	0



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	260.94Å 74.66Å 57.49Å 90.00° 96.94° 90.00°	Depositor
Resolution (Å)	19.85 – 3.00	Depositor
% Data completeness (in resolution range)	87.9 (19.85-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
Refinement program	CNX 2002	Depositor
R, $R_{free}$	0.233 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5629	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	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: PG4, M38, PTR, TGP

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	B	0.57	0/229	0.83	0/351
2	C	0.43	0/254	0.74	0/390
3	D	0.52	0/494	0.83	0/760
4	A	0.63	0/4783	0.74	2/6420 (0.0%)
All	All	0.61	0/5760	0.75	2/7921 (0.0%)

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
3	D	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	A	617	LEU	CA-CB-CG	5.83	128.70	115.30
4	A	335	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	112	DC	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	203	0	112	10	0
2	C	246	0	138	7	0
3	D	443	0	255	18	0
4	A	4699	0	4726	21	0
5	C	25	0	14	1	0
6	A	13	0	18	1	0
All	All	5629	0	5263	53	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (53) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:17:DA:H2''	2:C:18:DT:H5''	1.44	0.96
4:A:599:GLN:HE22	4:A:765:PHE:H	1.02	0.92
1:B:1:DA:H2'	1:B:2:DA:C8	2.03	0.92
4:A:419:ASN:H	4:A:419:ASN:HD22	1.35	0.74
3:D:121:DT:H2'	3:D:122:DT:H72	1.73	0.71
1:B:7:DA:H2''	1:B:8:DC:O5'	1.92	0.69
3:D:101:DA:H2'	3:D:102:DA:C8	2.26	0.69
1:B:8:DC:H2'	1:B:9:DT:C7	2.24	0.68
2:C:18:DT:H2'	2:C:19:DT:H72	1.75	0.67
2:C:17:DA:C2'	2:C:18:DT:H5''	2.23	0.67
4:A:599:GLN:NE2	4:A:765:PHE:H	1.85	0.66
4:A:740:ILE:HD13	4:A:740:ILE:H	1.61	0.64
4:A:419:ASN:H	4:A:419:ASN:ND2	1.99	0.60
1:B:6:DG:OP2	4:A:424:ILE:HD11	2.03	0.59
4:A:599:GLN:HE22	4:A:765:PHE:N	1.87	0.58
3:D:121:DT:H2''	3:D:122:DT:C6	2.39	0.57
2:C:13:DA:OP2	4:A:636:PRO:HD3	2.05	0.56
2:C:18:DT:H2''	2:C:19:DT:C6	2.40	0.56
3:D:121:DT:H2'	3:D:122:DT:C7	2.37	0.55
1:B:8:DC:H2'	1:B:9:DT:H72	1.88	0.54
3:D:106:DT:H6	3:D:106:DT:H5'	1.72	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:18:DT:H2'	2:C:19:DT:C7	2.39	0.53
4:A:296:ASN:HD21	4:A:299:LYS:HD2	1.74	0.52
2:C:11:TGP:H2'	2:C:12:DG:N7	2.25	0.51
3:D:105:DA:H2''	3:D:106:DT:C5'	2.41	0.51
3:D:115:DG:H2'	3:D:116:DT:C7	2.41	0.51
4:A:505:CYS:SG	4:A:573:LEU:HD12	2.52	0.50
4:A:626:VAL:HG11	4:A:724:LEU:HD21	1.94	0.50
4:A:383:ILE:HG23	4:A:403:GLU:HG3	1.93	0.49
1:B:5:DA:H2''	1:B:6:DG:O5'	2.14	0.48
4:A:511:HIS:HE2	6:A:911:PG4:H81	1.80	0.47
1:B:5:DA:H5'	1:B:5:DA:C8	2.50	0.47
3:D:105:DA:H2''	3:D:106:DT:H5'	1.97	0.47
1:B:5:DA:H5'	1:B:5:DA:H8	1.79	0.47
3:D:118:DT:C6	3:D:119:DT:H72	2.50	0.47
3:D:116:DT:OP1	4:A:488:ARG:HB3	2.15	0.46
4:A:485:LEU:HD21	4:A:541:VAL:HG11	1.96	0.46
3:D:102:DA:H2''	3:D:103:DA:OP2	2.15	0.45
3:D:109:DT:H2''	3:D:110:DT:O5'	2.15	0.45
3:D:115:DG:H2'	3:D:116:DT:H72	1.99	0.45
3:D:112:DC:H2''	3:D:113:DA:H5''	1.97	0.45
4:A:273:ILE:H	4:A:273:ILE:HD12	1.82	0.44
3:D:120:DT:H5'	3:D:120:DT:H6	1.84	0.43
3:D:120:DT:H2''	3:D:121:DT:OP2	2.18	0.43
1:B:4:DA:H1'	1:B:5:DA:H5''	2.00	0.43
5:C:990:M38:H17	5:C:990:M38:H222	2.01	0.43
4:A:254:GLU:O	4:A:258:THR:HG23	2.19	0.42
1:B:8:DC:H5''	4:A:428:MET:SD	2.60	0.42
4:A:541:VAL:HA	4:A:542:PRO:HD3	1.94	0.41
3:D:111:DC:C6	3:D:111:DC:H5'	2.56	0.41
4:A:341:CYS:SG	4:A:429:LEU:HD21	2.60	0.41
4:A:216:LYS:HB3	4:A:435:ILE:HD11	2.03	0.40
3:D:106:DT:C6	3:D:106:DT:H5'	2.53	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	
4	A	564/592 (95%)	521 (92%)	33 (6%)	10 (2%)	13	53

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	375	ARG
4	A	636	PRO
4	A	676	LYS
4	A	759	ALA
4	A	213	GLU
4	A	518	LEU
4	A	629	LEU
4	A	641	GLU
4	A	634	ARG
4	A	397	PRO

### 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	
4	A	505/535 (94%)	476 (94%)	29 (6%)	29	71

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	207	GLU
4	A	210	ARG
4	A	236	GLU
4	A	284	LYS
4	A	288	ASN
4	A	304	GLN
4	A	325	LEU
4	A	328	LYS
4	A	335	LEU
4	A	397	PRO

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Mol	Chain	Res	Type
4	A	418	GLU
4	A	419	ASN
4	A	430	ASN
4	A	439	LYS
4	A	461	TYR
4	A	498	THR
4	A	557	ASN
4	A	573	LEU
4	A	623	ASN
4	A	629	LEU
4	A	636	PRO
4	A	648	GLN
4	A	696	GLU
4	A	702	GLU
4	A	708	ARG
4	A	718	THR
4	A	721	LEU
4	A	740	ILE
4	A	760	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	277	ASN
4	A	367	HIS
4	A	419	ASN
4	A	442	GLN
4	A	459	ASN
4	A	460	GLN
4	A	491	ASN
4	A	599	GLN
4	A	611	ASN
4	A	623	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
4	PTR	A	723	1,4	16,16,17	4.64	2 (12%)	20,22,24	1.74	2 (10%)
2	TGP	C	11	3,2	21,21,25	0.74	0	27,31,38	5.99	3 (11%)

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
4	PTR	A	723	1,4	-	0/9/11/13	0/1/1/1
2	TGP	C	11	3,2	-	0/4/18/22	0/1/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	723	PTR	O-C	17.94	1.23	1.11
4	A	723	PTR	CA-C	2.06	1.52	1.48

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	11	TGP	C6-C5-N7	-30.60	130.02	134.14
4	A	723	PTR	C-CA-N	6.79	120.61	113.83
2	C	11	TGP	C6-N1-C2	3.10	124.94	119.51
4	A	723	PTR	O2P-P-O1P	2.39	118.24	110.44
2	C	11	TGP	C2-N3-C4	-2.37	111.76	115.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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	$\# Z  > 2$
6	PG4	A	911	-	12,12,12	0.47	0	11,11,11	0.24	0
5	M38	C	990	-	28,28,28	2.60	9 (32%)	37,41,41	1.17	4 (10%)

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
6	PG4	A	911	-	-	0/10/10/10	0/0/0/0
5	M38	C	990	-	-	0/6/18/18	0/0/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	990	M38	C8-N10	6.77	1.52	1.37
5	C	990	M38	C7-C6	6.20	1.54	1.43
5	C	990	M38	C9-C5	4.38	1.56	1.39
5	C	990	M38	C17-C13	3.87	1.46	1.40
5	C	990	M38	C13-C8	3.00	1.52	1.47
5	C	990	M38	C2-C1	2.71	1.42	1.36
5	C	990	M38	C3-C4	2.68	1.42	1.36
5	C	990	M38	C14-C12	2.64	1.44	1.39
5	C	990	M38	C9-N10	2.56	1.42	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	990	M38	C22-N10-C8	3.51	121.73	119.22
5	C	990	M38	C12-C11-C7	-2.69	103.98	105.66
5	C	990	M38	C13-C8-C7	-2.68	106.48	109.25
5	C	990	M38	C23-C22-N10	2.49	114.33	112.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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.