



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 11:47 PM GMT

PDB ID : 1A31
Title : HUMAN RECONSTITUTED DNA TOPOISOMERASE I IN COVALENT
COMPLEX WITH A 22 BASE PAIR DNA DUPLEX
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Deposited on : 1998-01-27
Resolution : 2.10 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

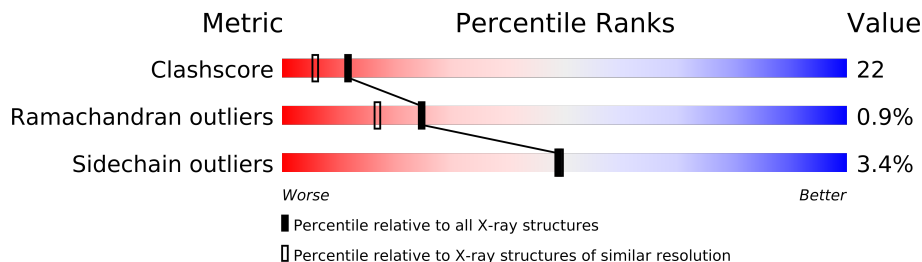
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.10 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	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)

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. 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	C	22	
2	D	22	
3	A	591	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4991 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 DNA (5'-D(*AP*AP*AP*AP*AP*GP*AP*CP*5IUP*5IU*TP*GP*AP*AP*AP*AP*AP*5IUP*5IUP*5IUP*5IUP*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	22	Total	C	I	N	O	P	0	0	0
			447	213	6	84	124	20			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	22	Total	C	I	N	O	P	0	0	0
			445	214	4	73	133	21			

- Molecule 3 is a protein called PROTEIN (TOPOISOMERASE I).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	A	458	Total	C	N	O	P	S	0	0	0
			3690	2365	640	664	1	20			

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 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	296	Total	O	0	0
			296	296		
4	C	47	Total	O	0	0
			47	47		
4	D	66	Total	O	0	0
			66	66		

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.00Å 66.60Å 71.80Å 90.00° 98.30° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	97.2 (20.00-2.10)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.247 , 0.310	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4991	wwPDB-VP
Average B, all atoms (Å ²)	49.0	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: 5IU, PTR

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	0.96	0/370	0.91	0/565
2	D	0.92	0/408	0.92	0/625
3	A	0.64	0/3761	0.77	0/5077
All	All	0.70	0/4539	0.80	0/6267

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	C	0	2
2	D	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	13	DA	Sidechain
1	C	8	DC	Sidechain
2	D	112	DA	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	C	447	0	234	17	0
2	D	445	0	243	23	0
3	A	3690	0	3588	151	0
4	A	296	0	0	30	0
4	C	47	0	0	2	0
4	D	66	0	0	7	0
All	All	4991	0	4065	187	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 22.

The worst 5 of 187 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1:DA:H2''	1:C:2:DA:H5'	1.13	1.12
2:D:101:DA:H2''	2:D:102:DA:H5'	1.15	1.10
1:C:1:DA:H2''	1:C:2:DA:C5'	1.87	1.05
2:D:107:5IU:H5''	4:D:1230:HOH:O	1.59	1.02
1:C:8:DC:H2'	1:C:9:5IU:I5	2.30	1.01

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
3	A	453/591 (77%)	426 (94%)	23 (5%)	4 (1%)	25 17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	561	GLU
3	A	721	LEU
3	A	495	GLU
3	A	761	GLU

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	
3	A	381/534 (71%)	368 (97%)	13 (3%)	49	49

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	418	GLU
3	A	434	ARG
3	A	568	LEU
3	A	408	ASN
3	A	561	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	459	ASN
3	A	748	GLN
3	A	599	GLN
3	A	430	ASN
3	A	576	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

11 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$
3	PTR	A	723	1,3	16,16,17	4.52	2 (12%)	20,22,24	1.08	1 (5%)
1	5IU	C	10	1,3,2	18,20,22	2.18	2 (11%)	17,28,33	3.11	4 (23%)
1	5IU	C	18	1,2	19,21,22	2.00	3 (15%)	22,30,33	2.07	3 (13%)
1	5IU	C	19	1,2	19,21,22	1.94	3 (15%)	22,30,33	1.70	3 (13%)
1	5IU	C	20	1,2	19,21,22	1.99	2 (10%)	22,30,33	2.79	3 (13%)
1	5IU	C	21	1,2	19,21,22	1.91	2 (10%)	22,30,33	2.33	3 (13%)
1	5IU	C	9	1,2	19,21,22	2.23	3 (15%)	22,30,33	2.32	3 (13%)
2	5IU	D	107	1,2	19,21,22	2.09	2 (10%)	22,30,33	2.80	3 (13%)
2	5IU	D	108	1,2	19,21,22	2.15	3 (15%)	22,30,33	2.18	3 (13%)
2	5IU	D	109	1,2	19,21,22	2.28	2 (10%)	22,30,33	3.37	5 (22%)
2	5IU	D	110	1,2	19,21,22	2.15	3 (15%)	22,30,33	2.19	3 (13%)

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
3	PTR	A	723	1,3	-	0/9/11/13	0/1/1/1
1	5IU	C	10	1,3,2	-	0/5/18/22	0/2/2/2
1	5IU	C	18	1,2	-	0/5/21/22	0/2/2/2
1	5IU	C	19	1,2	-	0/5/21/22	0/2/2/2
1	5IU	C	20	1,2	-	0/5/21/22	0/2/2/2
1	5IU	C	21	1,2	-	0/5/21/22	0/2/2/2
1	5IU	C	9	1,2	-	0/5/21/22	0/2/2/2
2	5IU	D	107	1,2	-	0/5/21/22	0/2/2/2
2	5IU	D	108	1,2	-	0/5/21/22	0/2/2/2
2	5IU	D	109	1,2	-	0/5/21/22	0/2/2/2
2	5IU	D	110	1,2	-	0/5/21/22	0/2/2/2

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	723	PTR	O-C	16.24	1.22	1.11
2	D	109	5IU	C5-I5	-9.19	1.92	2.10
1	C	9	5IU	C5-I5	-8.65	1.93	2.10
2	D	110	5IU	C5-I5	-8.38	1.93	2.10
2	D	108	5IU	C5-I5	-8.21	1.94	2.10

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	109	5IU	C4-C5-I5	-13.80	116.97	121.31
1	C	20	5IU	C4-C5-I5	-10.59	117.98	121.31
2	D	107	5IU	C4-C5-I5	-10.32	118.06	121.31
1	C	9	5IU	C4-C5-I5	-8.43	118.66	121.31
1	C	10	5IU	C4-C5-I5	-8.36	118.68	121.31

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 ⓘ

There are no ligands in this entry.

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.