W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 27, 2014 – 10:07 PM GMT

PDB ID	:	1A36
Title	:	TOPOISOMERASE I/DNA COMPLEX
Authors	:	Stewart, L.; Redinbo, M.R.; Qiu, X.; Champoux, J.J.; Hol, W.G.J.
Deposited on	:	1998-01-29
Resolution	:	2.80 Å(reported)

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 2.80 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	Percentile Ranks	Value
Clashscore		26
Ramachandran outliers		0.6%
Sidechain outliers		4.9%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
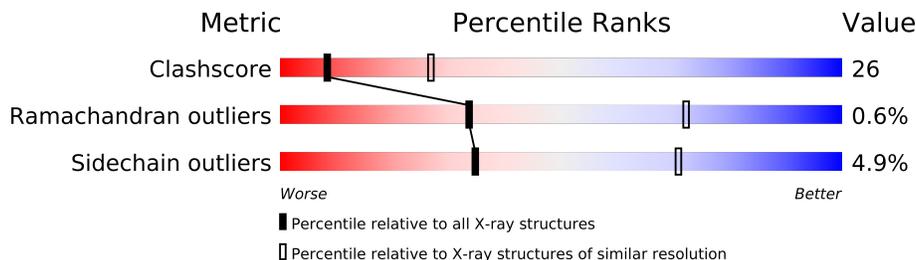
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)

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	B	22	
2	C	22	
3	A	591	

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 5285 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*TP*TP* AP*GP*AP*AP*AP*AP*AP*TP*TP*TP*TP*T)- 3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	22	Total 452	C 219	N 87	O 125	P 21	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	22	Total 444	C 218	N 70	O 135	P 21	0	0	0

- Molecule 3 is a protein called TOPOISOMERASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	544	Total 4332	C 2764	N 761	O 784	S 23	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	723	PHE	TYR	ENGINEERED	UNP P11387

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	49	Total 49	O 49	0	0
4	B	5	Total 5	O 5	0	0
4	C	3	Total 3	O 3	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

• Molecule 1: DNA (5'-D(*AP*AP*AP*AP*AP*GP*AP*CP*TP*TP*AP*GP*AP*AP*AP*AP *AP*TP*TP*TP*TP*T)- 3')
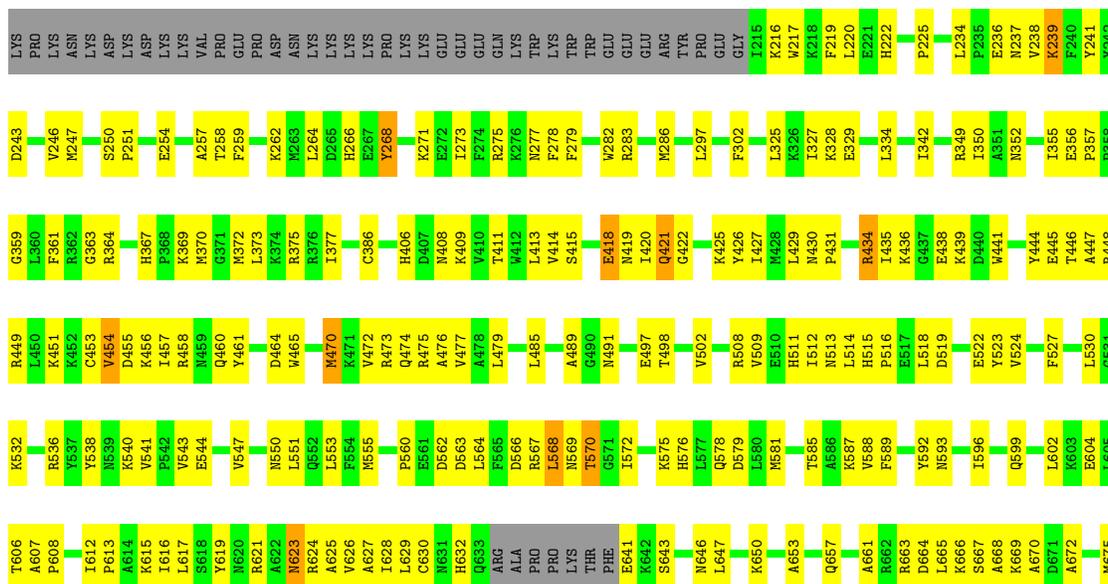
Chain B:
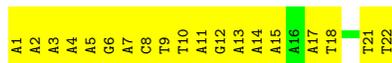
• Molecule 2: DNA (5'-D(*AP*AP*AP*AP*AP*TP*TP*TP*TP*TP*CP*TP*AP*AP*GP*TP *CP*TP*TP*TP*TP*T)- 3')

Chain C:

• Molecule 3: TOPOISOMERASE I

Chain A:

K676 D677 A678 K679 T680 K681 K682 V683 V684 E685 S686　K689 A690 V691　L694 E695 E696 Q697 L698 M699　E702 V703 Q704 A705 T706 D707 R708 E709 E710 N711　I714 A715 L716 G717 T718　L721 N722 F723 L724 D725 P726 R727 I728 T729 V730 A731 W732 C733 K734 K735 W736 G737 V738　N745

K746 T747 Q748　K751　A759　Y763 E764 F765
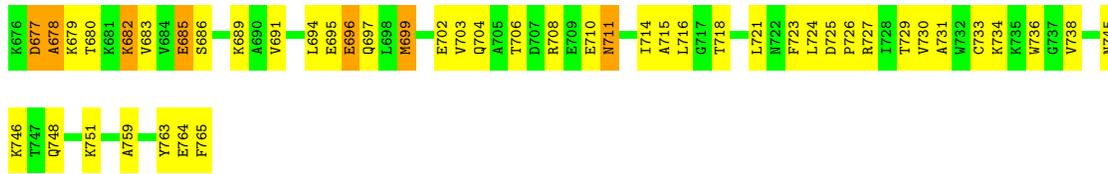
4 Data and refinement statistics ⓘ

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	56.50Å 118.40Å 71.50Å 90.00° 101.20° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	94.7 (8.00-2.80)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.224 , 0.312	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5285	wwPDB-VP
Average B, all atoms (Å^2)	41.0	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	B	0.80	0/509	0.86	0/784
2	C	0.86	0/495	0.97	1/762 (0.1%)
3	A	0.65	0/4422	0.78	0/5960
All	All	0.69	0/5426	0.81	1/7506 (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
2	C	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	103	DA	C1'-O4'-C4'	-5.14	104.96	110.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	108	DT	Sidechain
2	C	115	DG	Sidechain
2	C	121	DT	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	452	0	251	37	0
2	C	444	0	256	40	0
3	A	4332	0	4261	207	0
4	A	49	0	0	2	0
4	B	5	0	0	0	0
4	C	3	0	0	0	0
All	All	5285	0	4768	260	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 26.

The worst 5 of 260 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:121:DT:H2"	2:C:122:DT:C5	1.96	0.99
2:C:121:DT:H2"	2:C:122:DT:C7	1.93	0.99
1:B:13:DA:H5'	3:A:364:ARG:NH1	1.82	0.92
2:C:121:DT:H2"	2:C:122:DT:H71	1.53	0.88
3:A:626:VAL:HG11	3:A:724:LEU:HD21	1.55	0.88

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	540/591 (91%)	491 (91%)	46 (8%)	3 (1%)	33 72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	677	ASP

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Mol	Chain	Res	Type
3	A	678	ALA
3	A	696	GLU

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
3	A	446/535 (83%)	424 (95%)	22 (5%)	35 71

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	438	GLU
3	A	568	LEU
3	A	702	GLU
3	A	454	VAL
3	A	470	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	430	ASN
3	A	460	GLN
3	A	599	GLN
3	A	421	GLN
3	A	578	GLN

5.3.3 RNA (i)

There are no RNA chains 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 ⓘ

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.