Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:36 PM GMT

PDB ID	:	465D
Title	:	STRUCTURE OF THE TOPOISOMERASE II POISON BOUND TO DNA
Authors	:	Adams, A.; Guss, J.M.; Collyer, C.A.; Denny, W.A.; Wakelin, L.P.
Deposited on	:	1999-04-14
Resolution	:	1.60 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

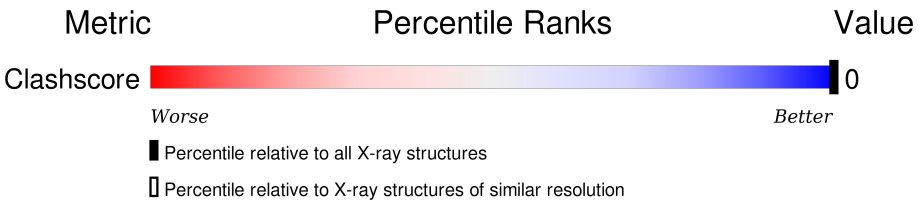
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	102246	2732 (1.60-1.60)

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. 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% 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	6	100%

2 Entry composition (i)

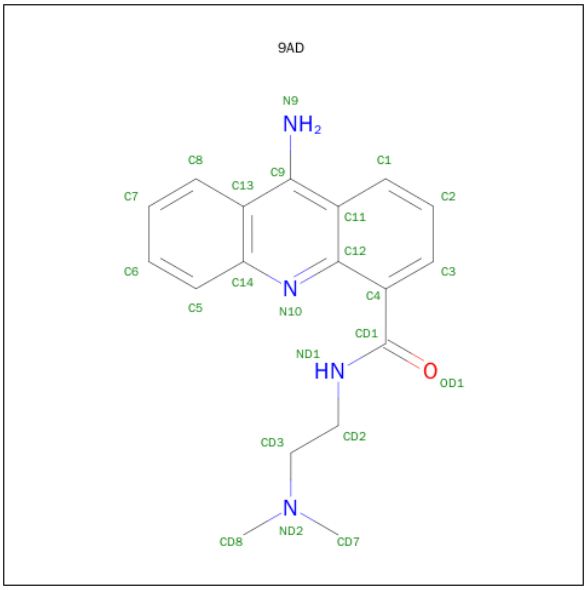
There are 3 unique types of molecules in this entry. The entry contains 195 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DNA (5'-D(*CP*GP*TP*AP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	6	120	58	23	34	5	0	0	0

- Molecule 2 is 9-AMINO-(N-(2-DIMETHYLAMINO)ETHYL)ACRIDINE-4-CARBOXAMIDE (three-letter code: 9AD) (formula: $C_{18}H_{20}N_4O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	23	18	4	1	0	0
			Total	C	N	O		
2	A	1	23	18	4	1	0	1

- Molecule 3 is water.

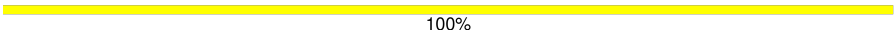
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	29	29	29	0	0

3 Residue-property plots (i)

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(*CP*GP*TP*AP*CP*G)-3')

Chain A: 

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α, β, γ	30.16Å 30.16Å 39.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	16.00 – 1.60	Depositor
% Data completeness (in resolution range)	98.5 (16.00-1.60)	Depositor
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.193 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	195	wwPDB-VP
Average B, all atoms (Å^2)	24.0	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: 9AD

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	4.05	27/134 (20.1%)	3.63	24/205 (11.7%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1003	DT	O4'-C1'	10.40	1.54	1.42
1	A	1001	DC	O4'-C1'	10.27	1.54	1.42
1	A	1004	DA	O4'-C1'	10.18	1.54	1.42
1	A	1002	DG	C4'-C3'	9.22	1.62	1.53
1	A	1003	DT	C2'-C1'	9.12	1.61	1.52
1	A	1006	DG	C4'-C3'	9.00	1.62	1.53
1	A	1003	DT	C4'-C3'	8.83	1.62	1.53
1	A	1002	DG	O4'-C1'	8.62	1.52	1.42
1	A	1005	DC	C4'-C3'	8.60	1.61	1.53
1	A	1005	DC	C2'-C1'	8.54	1.60	1.52
1	A	1002	DG	C2'-C1'	8.25	1.60	1.52
1	A	1001	DC	C4'-C3'	8.00	1.61	1.53
1	A	1006	DG	C2'-C1'	7.87	1.60	1.52
1	A	1006	DG	O4'-C1'	7.80	1.51	1.42
1	A	1004	DA	C2'-C1'	6.79	1.59	1.52
1	A	1004	DA	C4'-C3'	6.70	1.60	1.53
1	A	1001	DC	C2'-C1'	6.37	1.58	1.52
1	A	1005	DC	O4'-C1'	6.08	1.49	1.42
1	A	1002	DG	O3'-P	6.06	1.68	1.61
1	A	1001	DC	C3'-C2'	5.93	1.59	1.52
1	A	1003	DT	C1'-N1	-5.83	1.39	1.47
1	A	1005	DC	C1'-N1	-5.65	1.39	1.47
1	A	1004	DA	C3'-O3'	5.56	1.51	1.44
1	A	1002	DG	C1'-N9	5.52	1.56	1.49
1	A	1001	DC	C3'-O3'	5.46	1.51	1.44
1	A	1005	DC	O3'-P	5.26	1.67	1.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1006	DG	C1'-N9	5.21	1.56	1.49

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1004	DA	O4'-C1'-N9	-16.61	96.37	108.00
1	A	1002	DG	O4'-C1'-N9	-13.40	98.62	108.00
1	A	1006	DG	O4'-C1'-N9	-11.60	99.88	108.00
1	A	1003	DT	O4'-C1'-C2'	-11.10	97.02	105.90
1	A	1005	DC	O4'-C1'-N1	8.63	114.04	108.00
1	A	1006	DG	C5-C6-O6	-8.52	123.49	128.60
1	A	1002	DG	C6-N1-C2	-7.70	120.48	125.10
1	A	1002	DG	O4'-C1'-C2'	-7.53	99.88	105.90
1	A	1002	DG	C5-C6-O6	-7.26	124.24	128.60
1	A	1004	DA	O4'-C1'-C2'	-6.94	100.35	105.90
1	A	1006	DG	P-O5'-C5'	-6.83	109.98	120.90
1	A	1005	DC	O4'-C1'-C2'	-6.71	100.53	105.90
1	A	1001	DC	N1-C1'-C2'	6.67	125.27	112.60
1	A	1005	DC	C6-N1-C2	6.53	122.91	120.30
1	A	1002	DG	P-O5'-C5'	-6.40	110.66	120.90
1	A	1006	DG	N9-C4-C5	-6.09	102.96	105.40
1	A	1006	DG	O4'-C1'-C2'	-6.07	101.04	105.90
1	A	1003	DT	P-O3'-C3'	6.07	126.98	119.70
1	A	1006	DG	N1-C6-O6	5.88	123.43	119.90
1	A	1006	DG	C8-N9-C4	5.81	108.72	106.40
1	A	1001	DC	C6-N1-C2	5.78	122.61	120.30
1	A	1006	DG	N1-C2-N3	-5.65	120.51	123.90
1	A	1006	DG	C4-N9-C1'	-5.28	119.64	126.50
1	A	1006	DG	N3-C2-N2	5.05	123.44	119.90

There are no chirality outliers.

There are no planarity outliers.

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	120	0	69	0	0
2	A	46	0	40	0	0
3	A	29	0	0	0	0
All	All	195	0	109	0	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 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein molecules in this entry.

5.3.2 Protein sidechains (i)

There are no protein molecules in this entry.

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
2	9AD	A	3014	-	25,25,25	1.15	2 (8%)	31,35,35	1.46	4 (12%)
2	9AD	A	3015[A]	-	25,25,25	1.24	3 (12%)	31,35,35	1.64	7 (22%)

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
2	9AD	A	3014	-	-	0/10/10/10	0/3/3/3
2	9AD	A	3015[A]	-	-	0/10/10/10	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3015[A]	9AD	C14-N10	-2.65	1.31	1.35
2	A	3014	9AD	C3-C4	2.01	1.41	1.37
2	A	3015[A]	9AD	C3-C4	2.02	1.41	1.37
2	A	3014	9AD	C4-CD1	2.70	1.54	1.50
2	A	3015[A]	9AD	C4-CD1	3.13	1.55	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	3015[A]	9AD	C11-C12-N10	-3.37	118.84	123.38
2	A	3014	9AD	C13-C14-N10	-2.88	120.82	123.45
2	A	3015[A]	9AD	C3-C4-C12	-2.87	115.51	118.71
2	A	3015[A]	9AD	OD1-CD1-ND1	-2.87	116.55	122.58
2	A	3014	9AD	OD1-CD1-C4	-2.80	117.47	121.59
2	A	3015[A]	9AD	C13-C9-N9	-2.18	118.17	120.56
2	A	3015[A]	9AD	C13-C14-N10	-2.17	121.46	123.45
2	A	3014	9AD	C2-C3-C4	2.36	123.91	119.56
2	A	3015[A]	9AD	C11-C9-N9	2.64	123.44	120.56
2	A	3014	9AD	C12-N10-C14	4.65	122.15	117.14
2	A	3015[A]	9AD	C12-N10-C14	5.03	122.56	117.14

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.