



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:55 PM GMT

PDB ID : 1D6M
Title : CRYSTAL STRUCTURE OF E. COLI DNA TOPOISOMERASE III
Authors : Mondragon, A.; DiGate, R.
Deposited on : 1999-10-14
Resolution : 3.00 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

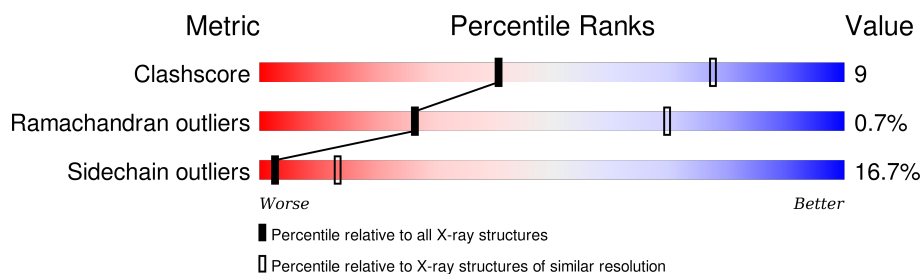
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (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 ≥ 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 $\leq 5\%$. 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	653	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4798 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 protein called DNA TOPOISOMERASE III.

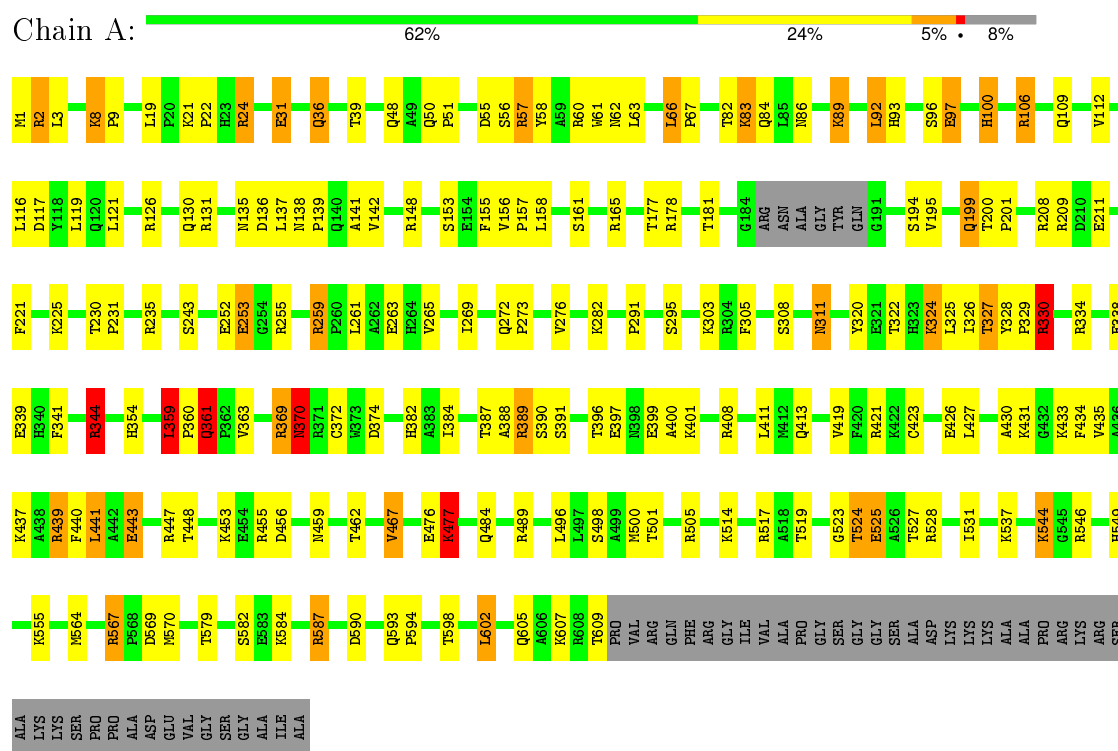
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	603	4798	3033	863	882	20	0	0	0

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 TOPOISOMERASE III



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	236.00Å 236.00Å 108.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 3.00	Depositor
% Data completeness (in resolution range)	93.6 (10.00-3.00)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC, X-PLOR	Depositor
R, R_{free}	0.237 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4798	wwPDB-VP
Average B, all atoms (Å ²)	51.0	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	A	0.39	0/4900	1.16	20/6644 (0.3%)

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	A	0	2

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	546	ARG	CD-NE-CZ	7.42	133.99	123.60
1	A	2	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	A	165	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	A	2	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	A	369	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	A	259	ARG	CD-NE-CZ	6.01	132.02	123.60
1	A	359	LEU	N-CA-C	5.99	127.17	111.00
1	A	374	ASP	CB-CG-OD1	5.96	123.67	118.30
1	A	344	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	546	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	A	126	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	A	439	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	A	178	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	408	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	361	GLN	N-CA-C	5.35	125.45	111.00
1	A	567	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	330	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	A	58	TYR	CB-CG-CD1	5.14	124.09	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	A	165	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	221	PHE	Mainchain
1	A	338	GLU	Mainchain

5.2 Too-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 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	4798	0	4815	83	0
All	All	4798	0	4815	83	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 9.

All (83) 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:A:361:GLN:HE21	1:A:363:VAL:H	1.12	0.91
1:A:109:GLN:HE22	1:A:131:ARG:HE	1.02	0.90
1:A:177:THR:HG22	1:A:195:VAL:H	1.40	0.87
1:A:109:GLN:NE2	1:A:131:ARG:HE	1.79	0.77
1:A:19:LEU:HD22	1:A:36:GLN:HG2	1.71	0.73
1:A:370:ASN:ND2	1:A:372:CYS:H	1.92	0.67
1:A:523:GLY:HA3	1:A:528:ARG:HG2	1.78	0.66
1:A:156:VAL:HB	1:A:157:PRO:HD3	1.81	0.62
1:A:63:LEU:HA	1:A:66:LEU:HD22	1.81	0.61
1:A:387:THR:HG22	1:A:388:ALA:H	1.66	0.60
1:A:116:LEU:HD22	1:A:121:LEU:HD22	1.85	0.59
1:A:441:LEU:H	1:A:459:ASN:HD21	1.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LEU:HD11	1:A:39:THR:HG22	1.85	0.58
1:A:153:SER:O	1:A:156:VAL:HG23	2.06	0.56
1:A:523:GLY:H	1:A:528:ARG:HE	1.54	0.55
1:A:55:ASP:OD2	1:A:57:ARG:HD3	2.06	0.55
1:A:135:ASN:O	1:A:327:THR:HG22	2.06	0.55
1:A:89:LYS:HG3	1:A:119:LEU:HD22	1.88	0.54
1:A:544:LYS:HB2	1:A:549:HIS:HD1	1.73	0.54
1:A:106:ARG:HH22	1:A:579:THR:HA	1.72	0.53
1:A:441:LEU:H	1:A:459:ASN:ND2	2.06	0.53
1:A:430:ALA:O	1:A:431:LYS:HB2	2.07	0.53
1:A:397:GLU:O	1:A:401:LYS:HG2	2.09	0.52
1:A:524:THR:HG23	1:A:525:GLU:HG2	1.91	0.52
1:A:370:ASN:C	1:A:370:ASN:HD22	2.12	0.51
1:A:496:LEU:HG	1:A:500:MET:CE	2.41	0.51
1:A:564:MET:HG2	1:A:605:GLN:HE22	1.75	0.51
1:A:455:ARG:HD2	1:A:456:ASP:OD1	2.11	0.51
1:A:276:VAL:HG21	1:A:467:VAL:HG13	1.94	0.50
1:A:200:THR:N	1:A:201:PRO:HD2	2.26	0.50
1:A:419:VAL:HB	1:A:443:GLU:HB2	1.92	0.49
1:A:21:LYS:HB2	1:A:22:PRO:HD3	1.94	0.48
1:A:109:GLN:HE22	1:A:131:ARG:NE	1.87	0.48
1:A:359:LEU:O	1:A:359:LEU:HD12	2.13	0.48
1:A:66:LEU:HB3	1:A:67:PRO:HD3	1.96	0.48
1:A:322:THR:O	1:A:324:LYS:HD2	2.14	0.47
1:A:426:GLU:HG2	1:A:435:VAL:HG22	1.96	0.47
1:A:476:GLU:O	1:A:477:LYS:HB3	2.16	0.46
1:A:92:LEU:HG	1:A:121:LEU:HD13	1.97	0.46
1:A:305:PHE:CE2	1:A:401:LYS:HB3	2.49	0.46
1:A:272:GLN:HB3	1:A:273:PRO:HD2	1.96	0.46
1:A:253:GLU:HG3	1:A:255:ARG:NH2	2.31	0.46
1:A:359:LEU:O	1:A:360:PRO:C	2.54	0.46
1:A:161:SER:CB	1:A:582:SER:HB3	2.46	0.46
1:A:155:PHE:HB3	1:A:158:LEU:HD12	1.97	0.46
1:A:328:TYR:CZ	1:A:330:ARG:HG3	2.51	0.46
1:A:63:LEU:O	1:A:66:LEU:HB2	2.17	0.45
1:A:341:PHE:O	1:A:344:ARG:HB3	2.17	0.45
1:A:24:ARG:HB2	1:A:31:GLU:HB2	1.98	0.45
1:A:100:HIS:CE1	1:A:112:VAL:HB	2.52	0.44
1:A:587:ARG:HG3	1:A:590:ASP:OD2	2.17	0.44
1:A:593:GLN:N	1:A:594:PRO:HD2	2.32	0.44
1:A:208:ARG:NH2	1:A:567:ARG:HG2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ASN:ND2	1:A:387:THR:HG21	2.33	0.44
1:A:354:HIS:HE1	1:A:389:ARG:O	2.00	0.43
1:A:137:LEU:HD12	1:A:320:TYR:O	2.18	0.43
1:A:598:THR:O	1:A:602:LEU:HB2	2.18	0.43
1:A:199:GLN:HG3	1:A:199:GLN:H	1.60	0.43
1:A:421:ARG:HG2	1:A:440:PHE:CZ	2.53	0.43
1:A:61:TRP:HZ3	1:A:181:THR:HG21	1.84	0.43
1:A:291:PRO:HD2	1:A:334:ARG:O	2.19	0.43
1:A:230:THR:HB	1:A:231:PRO:HD2	2.01	0.43
1:A:8:LYS:HB2	1:A:9:PRO:HD2	2.00	0.43
1:A:138:ASN:HA	1:A:139:PRO:HD3	1.87	0.42
1:A:400:ALA:O	1:A:401:LYS:C	2.58	0.42
1:A:253:GLU:HG3	1:A:255:ARG:CZ	2.48	0.42
1:A:2:ARG:HG3	1:A:97:GLU:OE1	2.19	0.42
1:A:269:ILE:HD13	1:A:430:ALA:HB3	2.01	0.42
1:A:269:ILE:HG13	1:A:434:PHE:HZ	1.84	0.42
1:A:329:PRO:HA	1:A:384:ILE:HG12	2.02	0.42
1:A:359:LEU:HD13	1:A:411:LEU:HD13	2.02	0.42
1:A:327:THR:HG21	1:A:382:HIS:NE2	2.34	0.41
1:A:305:PHE:CE1	1:A:401:LYS:HD2	2.55	0.41
1:A:136:ASP:HB3	1:A:141:ALA:HB1	2.01	0.41
1:A:359:LEU:HD13	1:A:411:LEU:CD1	2.51	0.41
1:A:265:VAL:O	1:A:269:ILE:HG12	2.21	0.41
1:A:396:THR:HG23	1:A:399:GLU:OE1	2.20	0.41
1:A:523:GLY:N	1:A:528:ARG:HE	2.18	0.41
1:A:308:SER:OG	1:A:311:ASN:HB2	2.19	0.41
1:A:199:GLN:HB3	1:A:531:ILE:HG23	2.02	0.41
1:A:50:GLN:HB3	1:A:51:PRO:HD2	2.03	0.41
1:A:83:LYS:HD3	1:A:84:GLN:H	1.86	0.40
1:A:138:ASN:O	1:A:142:VAL:HG23	2.21	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
1	A	599/653 (92%)	545 (91%)	50 (8%)	4 (1%)	26 70

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	GLN
1	A	370	ASN
1	A	477	LYS
1	A	525	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
1	A	515/549 (94%)	429 (83%)	86 (17%)	3 13

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	8	LYS
1	A	24	ARG
1	A	31	GLU
1	A	36	GLN
1	A	48	GLN
1	A	56	SER
1	A	57	ARG
1	A	60	ARG
1	A	62	ASN
1	A	66	LEU
1	A	82	THR
1	A	83	LYS
1	A	86	ASN
1	A	89	LYS

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Mol	Chain	Res	Type
1	A	92	LEU
1	A	93	HIS
1	A	96	SER
1	A	97	GLU
1	A	100	HIS
1	A	106	ARG
1	A	117	ASP
1	A	130	GLN
1	A	148	ARG
1	A	194	SER
1	A	199	GLN
1	A	209	ARG
1	A	211	GLU
1	A	225	LYS
1	A	243	SER
1	A	252	GLU
1	A	253	GLU
1	A	259	ARG
1	A	261	LEU
1	A	263	GLU
1	A	282	LYS
1	A	295	SER
1	A	303	LYS
1	A	311	ASN
1	A	324	LYS
1	A	325	LEU
1	A	326	ILE
1	A	327	THR
1	A	330	ARG
1	A	339	GLU
1	A	344	ARG
1	A	359	LEU
1	A	369	ARG
1	A	370	ASN
1	A	389	ARG
1	A	390	SER
1	A	391	SER
1	A	413	GLN
1	A	423	CYS
1	A	427	LEU
1	A	433	LYS
1	A	437	LYS

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Mol	Chain	Res	Type
1	A	439	ARG
1	A	441	LEU
1	A	443	GLU
1	A	447	ARG
1	A	448	THR
1	A	453	LYS
1	A	462	THR
1	A	467	VAL
1	A	477	LYS
1	A	484	GLN
1	A	489	ARG
1	A	498	SER
1	A	501	THR
1	A	505	ARG
1	A	514	LYS
1	A	517	ARG
1	A	519	THR
1	A	524	THR
1	A	527	THR
1	A	537	LYS
1	A	544	LYS
1	A	555	LYS
1	A	569	ASP
1	A	570	MET
1	A	584	LYS
1	A	587	ARG
1	A	602	LEU
1	A	607	LYS
1	A	609	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	86	ASN
1	A	109	GLN
1	A	354	HIS
1	A	361	GLN
1	A	370	ASN
1	A	459	ASN
1	A	605	GLN

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](#)

There are no ligands in this entry.

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 ⓘ

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.