



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 01:44 AM UTC

PDB ID : 1K4S / pdb_00001k4s
Title : HUMAN DNA TOPOISOMERASE I IN COVALENT COMPLEX WITH A
22 BASE PAIR DNA DUPLEX
Authors : Staker, B.L.; Hjerrild, K.; Feese, M.D.; Behnke, C.A.; Burgin Jr., A.B.; Stewart, L.J.
Deposited on : 2001-10-08
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

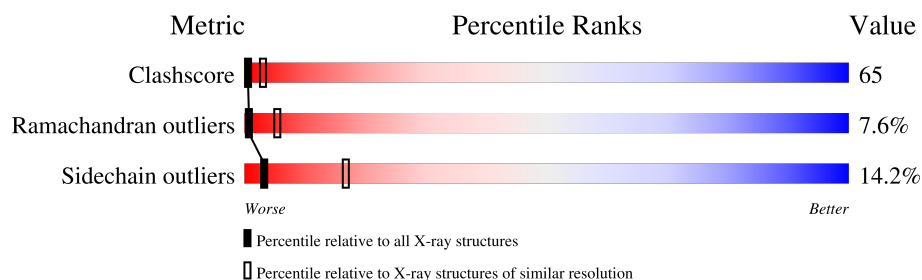
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	10	80% 20%
2	C	12	8% 58% 33%
3	D	22	45% 55%
4	A	592	22% 47% 12% • 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	5IU	B	9	-	-	X	-
2	5IU	C	18	-	-	X	-
2	5IU	C	19	-	-	X	-
2	5IU	C	20	-	-	X	-
3	5IU	D	107	-	-	X	-
3	5IU	D	109	-	-	X	-
3	5IU	D	110	-	-	X	-
3	5IU	D	116	-	-	X	-
3	5IU	D	118	-	-	X	-
3	5IU	D	119	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4858 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 5'-D(*AP*AP*AP*AP*AP*GP*AP*CP*(5IU)P*(5IU))-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	10	Total	C	I	N	O	P	0	0	0
			203	97	2	42	53	9			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	12	Total	C	I	N	O	P	0	0	0
			244	116	4	42	70	11			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D	22	Total	C	I	N	O	P	0	0	0
			445	209	9	73	133	21			

- Molecule 4 is a protein called DNA topoisomerase I.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	A	490	Total	C	N	O	P	S	0	0	0
			3966	2540	689	715	1	21			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	723	PTR	TYR	modified residue	UNP P11387

Note EDS was not executed.

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N745	K746	T747	Q748	R749	E750	K751	F752	A753	W754	A755	T756	D757	M758	A759	D760	E761	Y762	E763	E764	F765																																						
GLU	SER	LYS	LYS	LYS	ALA	VAL	GLN	ARG	LEU	GLU	GLU	GLN	LEU	MET	LYS	LEU	GLU	GLN	ALA	THR	ASP	R708	E709	E710	M711	K712	Q713	I714	I715	L716	G717	T718	S719	K720	L721	M722	Y723	L724	D725	P726	R727	I728	T729	V730	A731	W732	G733	K734	K735	W736	G737	V738	P739	T740	E741	F742	I743	Y744
A625	V626	A627	L628	L629	C630	M631	H632	GLN	ARG	ALA	PRO	PRO	LYS	THR	PHE	GLU	LYS	SER	MET	NET	ASN	LEU	GLN	THR	LYS	ILE	ASP	ALA	LYS	LYS	GLU	GLN	LEU	ALA	ASP	ALA	ARG	ARG	Q601	L602	E604	SER	L605	ALA	LYS	ALA	VAL	MET	LYS	ASP	ALA	LYS	THR	LYS	VAL	VAL		
E561	D562	D563	L564	F565	D566	R567	L568	M569	T570	G571	N574	K575	H576	L577	Q578	D579	L580	M581	E582	G583	L584	T585	V588	F589	R590	T591	Y592	N593	A594	S595	T597	D532	S534	T535	R536	Y537	N538	K540	V541	E544	V547	F548	I549	K549	M550	L551	Q552	L553	F554	M555	E556	N557	Q558	P560				
E495	G496	E497	T498	A499	D500	G503	C504	G505	S506	V509	E510	H511	I512	N513	L514	H515	F516	E517	L518	Q521	V524	V525	E526	F527	D528	F529	L530	G531	K532	D533	S534	T535	R536	Y537	N538	K540	V541	E544	V547	F548	I549	K549	M550	L551	Q552	L553	F554	M555	E556	N557	Q558	P560						
I427	M428	L429	N430	S433	R434	I435	K436	G437	E438	K439	D440	W441	Q442	K443	Y444	E445	T446	A447	R448	R449	L450	K456	I457	R458	M459	Q460	Y461	R462	E463	D464	W465	K466	S467	W470	R473	Q474	V477	A478	L479	Y480	F481	I482	D483	K484	L485	A486	L487	R488	A489	G490	M491	E492	K493	E494				

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	73.23Å 73.23Å 186.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.20	Depositor
% Data completeness (in resolution range)	96.8 (50.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
Refinement program	CNX	Depositor
R, R_{free}	0.217 , 0.222	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4858	wwPDB-VP
Average B, all atoms (Å ²)	41.0	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: PTR, 5IU, SPT

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	0.37	0/186	0.77	0/285
2	C	0.35	0/165	0.69	0/250
3	D	0.37	0/296	0.78	0/447
4	A	0.56	0/4046	1.12	30/5464 (0.5%)
All	All	0.54	0/4693	1.07	30/6446 (0.5%)

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	3

There are no bond length outliers.

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	396	PRO	CA-C-N	8.91	130.98	119.84
4	A	396	PRO	C-N-CA	8.91	130.98	119.84
4	A	541	VAL	N-CA-C	7.80	116.89	107.61
4	A	541	VAL	CA-C-N	7.67	127.95	119.90
4	A	541	VAL	C-N-CA	7.67	127.95	119.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	111	DC	Sidechain

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Mol	Chain	Res	Type	Group
3	D	114	DA	Sidechain
3	D	117	DC	Sidechain

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	B	203	0	106	44	0
2	C	244	0	127	28	0
3	D	445	0	228	94	0
4	A	3966	0	3841	460	0
All	All	4858	0	4302	585	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 65.

The worst 5 of 585 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:B:8:DC:H2''	1:B:9:5IU:I5	1.95	1.35
3:D:115:DG:H2'	3:D:116:5IU:I5	2.10	1.20
1:B:8:DC:H2'	4:A:428:MET:HE1	1.30	1.11
3:D:118:5IU:H2''	3:D:119:5IU:H5'	1.21	1.11
3:D:118:5IU:C2'	3:D:119:5IU:H5'	1.88	1.03

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	485/592 (82%)	367 (76%)	81 (17%)	37 (8%)	1 5

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	344	ASP
4	A	387	SER
4	A	388	LYS
4	A	389	ASP
4	A	495	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
4	A	408/535 (76%)	350 (86%)	58 (14%)	3 17

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	402	LYS
4	A	713	GLN
4	A	446	THR
4	A	709	GLU
4	A	628	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
4	A	511	HIS
4	A	593	ASN
4	A	559	GLN
4	A	632	HIS
4	A	331	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

17 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	$\# Z > 2$
1	5IU	B	10	4,1,3	17,20,22	1.07	1 (5%)	22,28,33	0.92	1 (4%)
2	5IU	C	19	3,2	18,21,22	0.79	1 (5%)	25,30,33	0.31	0
3	5IU	D	116	1,3	18,21,22	1.12	2 (11%)	25,30,33	0.43	0
3	5IU	D	118	1,3	18,21,22	0.95	1 (5%)	25,30,33	0.43	0
2	5IU	C	20	3,2	18,21,22	1.25	1 (5%)	25,30,33	0.62	0
3	5IU	D	108	3,2	18,21,22	0.85	1 (5%)	25,30,33	0.41	0
3	5IU	D	107	3,2	18,21,22	0.81	1 (5%)	25,30,33	0.38	0
2	5IU	C	18	3,2	18,21,22	0.80	1 (5%)	25,30,33	0.51	0
1	5IU	B	9	1,3	18,21,22	1.03	1 (5%)	25,30,33	0.37	0
3	5IU	D	119	1,3	18,21,22	1.04	1 (5%)	25,30,33	0.46	0
2	SPT	C	11	3,2	18,18,22	0.37	0	25,26,33	0.34	0
3	5IU	D	121	1,3	18,21,22	0.83	1 (5%)	25,30,33	0.42	0
3	5IU	D	110	3,2	18,21,22	0.83	1 (5%)	25,30,33	0.39	0
3	5IU	D	120	1,3	18,21,22	0.69	1 (5%)	25,30,33	0.42	0
3	5IU	D	109	3,2	18,21,22	0.86	1 (5%)	25,30,33	0.39	0
2	5IU	C	21	3,2	18,21,22	0.87	1 (5%)	25,30,33	0.38	0
4	PTR	A	723	4,1	15,16,17	0.83	0	17,22,24	0.77	0

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
1	5IU	B	10	4,1,3	-	0/7/18/22	0/2/2/2
2	5IU	C	19	3,2	-	0/7/21/22	0/2/2/2
3	5IU	D	116	1,3	-	0/7/21/22	0/2/2/2
3	5IU	D	118	1,3	-	0/7/21/22	0/2/2/2
2	5IU	C	20	3,2	-	1/7/21/22	0/2/2/2
3	5IU	D	108	3,2	-	0/7/21/22	0/2/2/2
3	5IU	D	107	3,2	-	0/7/21/22	0/2/2/2
2	5IU	C	18	3,2	-	1/7/21/22	0/2/2/2
1	5IU	B	9	1,3	-	0/7/21/22	0/2/2/2
3	5IU	D	119	1,3	-	3/7/21/22	0/2/2/2
2	SPT	C	11	3,2	-	2/6/18/22	0/2/2/2
3	5IU	D	121	1,3	-	0/7/21/22	0/2/2/2
3	5IU	D	110	3,2	-	0/7/21/22	0/2/2/2
3	5IU	D	120	1,3	-	0/7/21/22	0/2/2/2
3	5IU	D	109	3,2	-	1/7/21/22	0/2/2/2
2	5IU	C	21	3,2	-	0/7/21/22	0/2/2/2
4	PTR	A	723	4,1	-	2/10/11/13	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	20	5IU	C5-I5	-4.29	1.96	2.08
3	D	116	5IU	C5-I5	-3.60	1.98	2.08
3	D	119	5IU	C5-I5	-3.58	1.98	2.08
1	B	10	5IU	C5-I5	-3.49	1.98	2.08
1	B	9	5IU	C5-I5	-3.38	1.98	2.08

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	10	5IU	C2'-C1'-N1	3.37	118.79	112.40

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	11	SPT	O4'-C4'-C5'-S5'
2	C	11	SPT	C3'-C4'-C5'-S5'
4	A	723	PTR	C-CA-CB-CG
3	D	119	5IU	C4'-C5'-O5'-P
3	D	119	5IU	C3'-C4'-C5'-O5'

There are no ring outliers.

17 monomers are involved in 95 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	10	5IU	4	0
2	C	19	5IU	7	0
3	D	116	5IU	16	0
3	D	118	5IU	8	0
2	C	20	5IU	10	0
3	D	108	5IU	4	0
3	D	107	5IU	13	0
2	C	18	5IU	8	0
1	B	9	5IU	10	0
3	D	119	5IU	13	0
2	C	11	SPT	5	0
3	D	121	5IU	1	0
3	D	110	5IU	8	0
3	D	120	5IU	3	0
3	D	109	5IU	9	0
2	C	21	5IU	5	0
4	A	723	PTR	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.