



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:44 AM UTC

PDB ID : 2H7G / pdb_00002h7g
Title : Structure of variola topoisomerase non-covalently bound to DNA
Authors : Perry, K.; Hwang, Y.; Bushman, F.D.; Van Duyne, G.D.
Deposited on : 2006-06-02
Resolution : 1.90 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

<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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

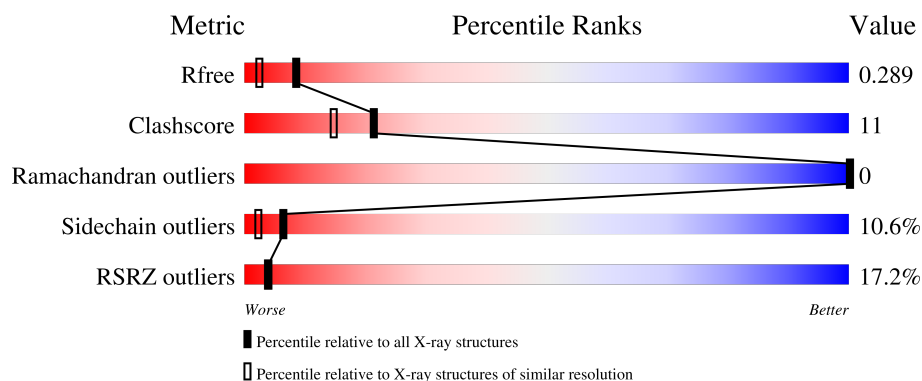
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	Y	12	8% 67% 33%
2	Z	14	71% 21% 7%
3	X	314	18% 71% 25% ••

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3547 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(*TP*TP*GP*TP*CP*GP*CP*CP*CP*TP*TP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Y	12	Total	C	N	O	P	0	0	0
			221	106	32	72	11			

- Molecule 2 is a DNA chain called 5'-D(*TP*AP*AP*TP*AP*AP*GP*GP*GP*CP*GP*AP*CP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Z	14	Total	C	N	O	P	0	1	0
			310	148	65	83	14			

- Molecule 3 is a protein called DNA topoisomerase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	312	Total	C	N	O	S	0	7	0
			2621	1694	446	472	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	100	SER	CYS	engineered mutation	UNP P32989
X	211	SER	CYS	engineered mutation	UNP P32989

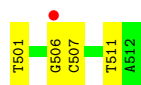
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Y	30	Total	O	0	0
			30	30		
4	Z	51	Total	O	0	0
			51	51		
4	X	314	Total	O	0	0
			314	314		

3 Residue-property plots [i](#)

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

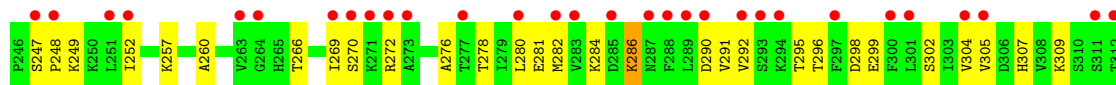
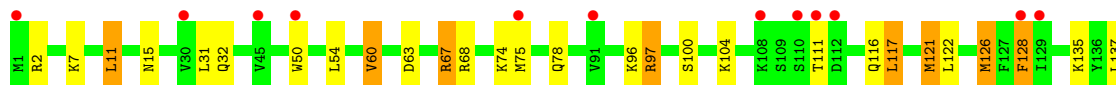
- Molecule 1: 5'-D(*TP*TP*GP*TP*CP*GP*CP*CP*TP*TP*A)-3'



- Molecule 2: 5'-D(*TP*AP*AP*TP*AP*AP*GP*GP*GP*CP*GP*AP*CP*A)-3'



- Molecule 3: DNA topoisomerase 1



ASP
GLY

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	66.18Å 133.65Å 112.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 50.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.2 (50.00-1.90) 96.2 (50.00-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 1.89Å)	Xtriage
Refinement program	REFMAC refmac_5.2.0005	Depositor
R, R_{free}	0.197 , 0.243 0.245 , 0.289	Depositor DCC
R_{free} test set	1915 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 29.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3547	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	Y	0.72	0/244	1.54	3/375 (0.8%)
2	Z	0.66	1/350 (0.3%)	1.32	1/539 (0.2%)
3	X	0.75	0/2677	0.92	0/3606
All	All	0.74	1/3271 (0.0%)	1.04	4/4520 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	527	DC	O3'-P	-5.62	1.52	1.61

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	501	DT	O4'-C1'-N1	-6.86	98.11	108.40
1	Y	511	DT	P-O3'-C3'	5.56	128.53	120.20
1	Y	507	DC	O5'-C5'-C4'	-5.36	102.76	110.80
2	Z	516	DA	C4'-C3'-O3'	5.13	117.70	110.00

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	Y	221	0	127	2	0
2	Z	310	0	169	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	X	2621	0	2688	62	0
4	X	314	0	0	11	0
4	Y	30	0	0	0	0
4	Z	51	0	0	1	0
All	All	3547	0	2984	67	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 11.

All (67) 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)
3:X:149[A]:LYS:H	3:X:152:HIS:HD2	1.06	0.95
3:X:11[B]:LEU:HD21	3:X:31:LEU:HD11	1.54	0.90
3:X:149[B]:LYS:H	3:X:152:HIS:HD2	1.07	0.89
3:X:155:ILE:HD11	3:X:190:THR:HG21	1.65	0.77
3:X:149[A]:LYS:H	3:X:152:HIS:CD2	1.98	0.77
3:X:282:MET:HE1	3:X:304:VAL:HG22	1.67	0.76
3:X:149[B]:LYS:H	3:X:152:HIS:CD2	1.98	0.76
3:X:116:GLN:HE22	3:X:202:LYS:H	1.38	0.70
3:X:298:ASP:HB3	4:X:422:HOH:O	1.92	0.69
3:X:239:VAL:HG21	3:X:292:VAL:CG1	2.25	0.67
3:X:295:THR:HB	3:X:299:GLU:HG3	1.78	0.64
3:X:239:VAL:HG21	3:X:292:VAL:HG12	1.81	0.62
3:X:291:VAL:O	3:X:295:THR:HG23	1.99	0.61
3:X:11[B]:LEU:HD21	3:X:31:LEU:CD1	2.29	0.60
3:X:260:ALA:HB2	3:X:270:SER:HB2	1.83	0.60
3:X:296:THR:HG22	3:X:299:GLU:HG2	1.86	0.57
3:X:206:ARG:O	3:X:210:GLU:HG2	2.05	0.56
3:X:260:ALA:HB2	3:X:270:SER:CB	2.35	0.56
3:X:296:THR:HG23	3:X:299:GLU:H	1.70	0.56
3:X:128:PHE:CD2	3:X:226:GLY:HA3	2.42	0.54
3:X:252:ILE:HD13	3:X:280:LEU:HD21	1.88	0.54
3:X:286:LYS:O	3:X:286:LYS:HE3	2.07	0.54
2:Z:516:DA:H4'	2:Z:517[B]:DA:OP1	2.07	0.54
3:X:60:VAL:HG22	3:X:68:ARG:NH2	2.23	0.54
1:Y:506:DG:O5'	1:Y:506:DG:H2'	2.08	0.53
3:X:252:ILE:HD13	3:X:280:LEU:CD2	2.38	0.53
2:Z:516:DA:H4'	2:Z:517[A]:DA:OP1	2.07	0.53
3:X:117:LEU:O	3:X:121:MET:HG2	2.09	0.53
3:X:210:GLU:HG3	4:X:359:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:235:PHE:HD2	4:X:558:HOH:O	1.92	0.52
3:X:269:ILE:HG21	4:X:575:HOH:O	2.10	0.52
3:X:266:THR:OG1	3:X:269:ILE:HG22	2.10	0.52
3:X:97:ARG:HG2	3:X:97:ARG:HH11	1.76	0.50
3:X:239:VAL:HG21	3:X:292:VAL:HG11	1.92	0.50
3:X:247:SER:HB2	3:X:248:PRO:HD2	1.93	0.50
3:X:156:SER:O	3:X:157:PRO:C	2.54	0.49
3:X:122:LEU:HG	3:X:182:LEU:HG	1.93	0.49
3:X:163:LYS:HD2	4:X:471:HOH:O	2.13	0.48
3:X:236:TRP:HA	4:X:558:HOH:O	2.13	0.48
3:X:243:SER:HB3	3:X:244:PRO:HD3	1.95	0.47
3:X:100:SER:O	3:X:104:LYS:HD3	2.14	0.47
3:X:75:MET:HG2	4:X:443:HOH:O	2.13	0.47
3:X:126:MET:HE3	4:X:397:HOH:O	2.14	0.47
3:X:150:ASN:HA	3:X:153:ILE:HD12	1.96	0.47
3:X:281:GLU:O	3:X:284:LYS:HB2	2.15	0.47
3:X:50:TRP:CZ2	3:X:54:LEU:HD13	2.51	0.46
4:Z:118:HOH:O	3:X:135:LYS:HE3	2.15	0.46
3:X:172:HIS:HE1	4:X:336:HOH:O	1.98	0.45
3:X:201:ASN:N	3:X:201:ASN:HD22	2.14	0.45
3:X:209:TYR:OH	4:X:526:HOH:O	2.21	0.44
3:X:243:SER:CB	3:X:244:PRO:HD3	2.48	0.44
3:X:276:ALA:O	3:X:280:LEU:HD23	2.19	0.43
3:X:156:SER:HB2	3:X:157:PRO:CD	2.49	0.43
3:X:201:ASN:HD22	3:X:201:ASN:H	1.67	0.43
3:X:278:THR:HG22	3:X:282:MET:HE2	2.01	0.43
3:X:281:GLU:OE2	3:X:307:HIS:HE1	2.03	0.42
2:Z:515:DT:H2'	2:Z:516:DA:C5	2.54	0.42
3:X:219:ILE:O	3:X:222:LEU:HB2	2.19	0.42
3:X:305:VAL:O	3:X:309:LYS:HG3	2.20	0.42
3:X:121:MET:HE1	3:X:212:ILE:HD13	2.02	0.41
3:X:235:PHE:CD2	4:X:558:HOH:O	2.57	0.41
1:Y:506:DG:O5'	1:Y:506:DG:C2'	2.68	0.41
3:X:63:ASP:OD2	3:X:67:ARG:CD	2.69	0.41
3:X:63:ASP:OD2	3:X:67:ARG:HD3	2.21	0.41
3:X:156:SER:HB2	3:X:157:PRO:HD2	2.03	0.40
3:X:194:SER:HB3	3:X:197:GLU:HG3	2.03	0.40
3:X:296:THR:HG22	3:X:299:GLU:CG	2.52	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	
3	X	317/314 (101%)	309 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	X	299/293 (102%)	265 (89%)	34 (11%)	5	2

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	X	2	ARG
3	X	7	LYS
3	X	11[A]	LEU
3	X	11[B]	LEU
3	X	15	ASN
3	X	32	GLN
3	X	60	VAL
3	X	67	ARG
3	X	74	LYS
3	X	78	GLN
3	X	96	LYS
3	X	97	ARG
3	X	111	THR

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Mol	Chain	Res	Type
3	X	117	LEU
3	X	121	MET
3	X	126	MET
3	X	128	PHE
3	X	137	LEU
3	X	145	LEU
3	X	146	LEU
3	X	148	LEU
3	X	154[A]	GLU
3	X	154[B]	GLU
3	X	182	LEU
3	X	188	LYS
3	X	201	ASN
3	X	222	LEU
3	X	249	LYS
3	X	257	LYS
3	X	272	ARG
3	X	286	LYS
3	X	290	ASP
3	X	302[A]	SER
3	X	302[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
3	X	15	ASN
3	X	78	GLN
3	X	93	ASN
3	X	116	GLN
3	X	152	HIS
3	X	172	HIS
3	X	201	ASN
3	X	234	ASN
3	X	307	HIS

5.3.3 RNA ⓘ

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 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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Y	12/12 (100%)	0.55	1 (8%) 17 18	39, 40, 51, 54	0
2	Z	14/14 (100%)	0.63	0 100 100	24, 40, 52, 54	1 (7%)
3	X	312/314 (99%)	1.31	57 (18%) 3 3	18, 42, 54, 60	7 (2%)
All	All	338/340 (99%)	1.26	58 (17%) 4 4	18, 42, 54, 60	8 (2%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	X	243	SER	5.6
3	X	111	THR	5.5
3	X	1	MET	4.6
3	X	244	PRO	4.4
3	X	294	LYS	4.4
3	X	248	PRO	3.8
3	X	269	ILE	3.8
3	X	288	PHE	3.7
3	X	271	LYS	3.6
3	X	297	PHE	3.6
3	X	239	VAL	3.5
3	X	110	SER	3.5
3	X	273	ALA	3.3
3	X	272	ARG	3.2
3	X	304	VAL	3.2
3	X	242	ILE	3.2
3	X	300	PHE	3.2
3	X	283	VAL	3.1
3	X	112	ASP	3.1
3	X	290	ASP	3.1
3	X	280	LEU	3.0
3	X	289	LEU	3.0
3	X	245	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
3	X	247	SER	2.9
3	X	141	GLU	2.9
3	X	301	LEU	2.8
3	X	270	SER	2.8
3	X	311	SER	2.7
3	X	312	THR	2.7
3	X	287	ASN	2.6
3	X	236	TRP	2.5
3	X	285	ASP	2.5
3	X	128	PHE	2.4
3	X	50	TRP	2.4
3	X	282	MET	2.4
3	X	263	VAL	2.4
3	X	45	VAL	2.4
3	X	293	SER	2.4
3	X	222	LEU	2.3
3	X	209	TYR	2.3
3	X	264	GLY	2.3
3	X	91	VAL	2.3
3	X	277	THR	2.3
3	X	233	TYR	2.3
3	X	292	VAL	2.3
3	X	108	LYS	2.3
3	X	210	GLU	2.2
3	X	129	ILE	2.2
1	Y	506	DG	2.2
3	X	30	VAL	2.2
3	X	157	PRO	2.2
3	X	145	LEU	2.1
3	X	138	LYS	2.1
3	X	305	VAL	2.1
3	X	251	LEU	2.1
3	X	158	ASP	2.1
3	X	75	MET	2.0
3	X	252	ILE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.