



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:49 AM UTC

PDB ID : 1T8I / pdb_00001t8i
Title : Human DNA Topoisomerase I (70 Kda) In Complex With The Poison Camptothecin and Covalent Complex With A 22 Base Pair DNA Duplex
Authors : Staker, B.L.; Feese, M.D.; Cushman, M.; Pommier, Y.; Zembower, D.; Stewart, L.; Burgin, A.B.
Deposited on : 2004-05-12
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

<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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

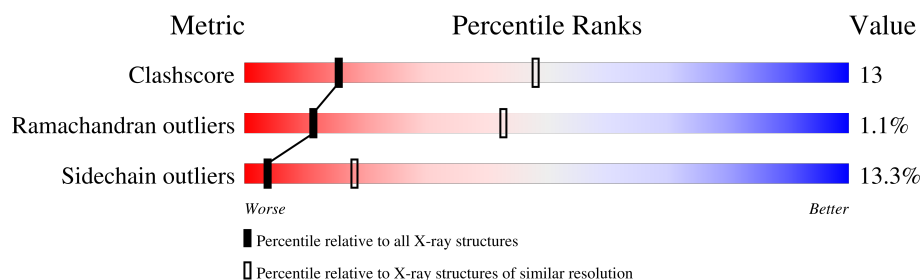
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (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 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	10% 70% 20%
2	C	12	17% 75% 8%
3	D	22	18% 77% 5%
4	A	592	65% 26% 5% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5605 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*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	10	Total	C	N	O	P	0	0	0
			203	99	42	53	9			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	12	Total	C	N	O	P	S	0	0	0
			246	120	45	69	11	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	22	Total	C	N	O	P	0	0	0
			443	217	71	134	21			

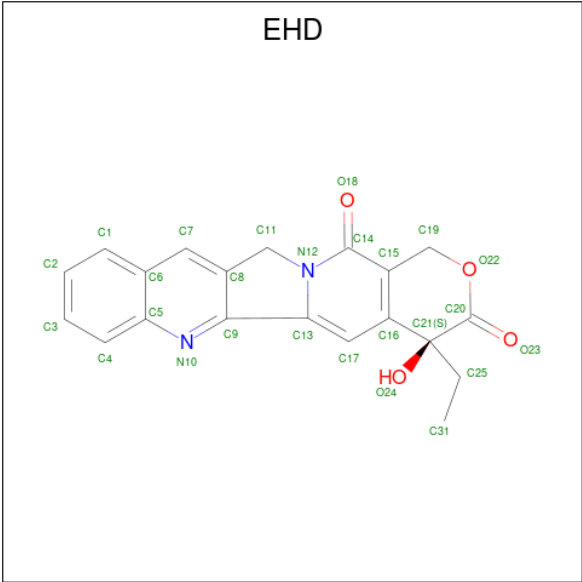
- Molecule 4 is a protein called DNA topoisomerase I.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	A	565	Total	C	N	O	P	S	0	0	0
			4687	2980	823	857	1	26			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 5 is 4-ETHYL-4-HYDROXY-1,12-DIHYDRO-4H-2-OXA-6,12A-DIAZA-DIBENZ O[B,H]FLUORENE-3,13-DIONE (CCD ID: EHD) (formula: C₂₀H₁₆N₂O₄).



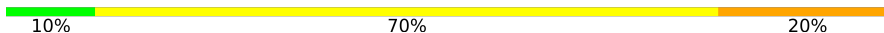
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	N	O	0	0
			26	20	2	4		

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. 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. 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.

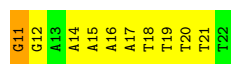
- Molecule 1: 5'-D(*AP*AP*AP*AP*AP*GP*AP*CP*TP*T)-3'

Chain B: 

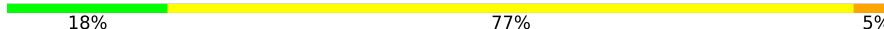


- Molecule 2: 5'-D(*(TGP)P*GP*AP*AP*AP*AP*AP*TP*TP*TP*TP*T)-3'

Chain C: 



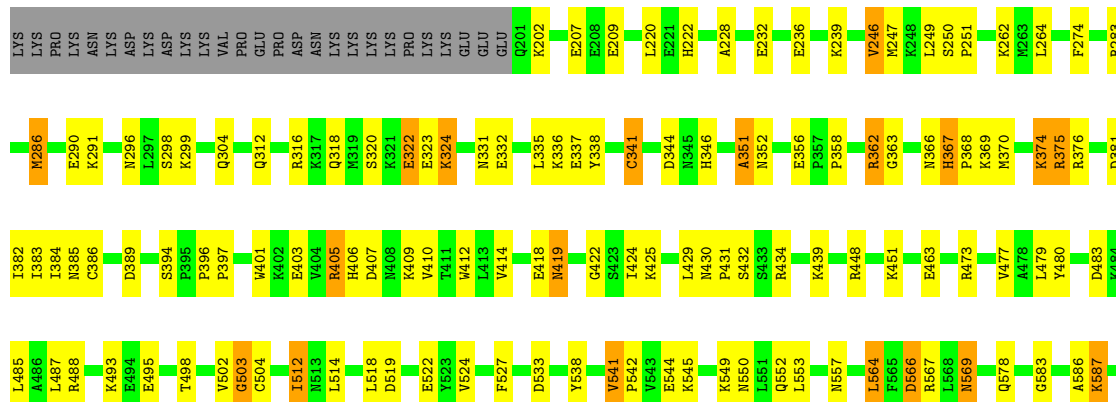
- Molecule 3: 5'-D(*AP*AP*AP*AP*AP*TP*TP*TP*TP*TP*CP*CP*AP*AP*GP*TP*CP*TP*TP*TP*TP*T)-3'

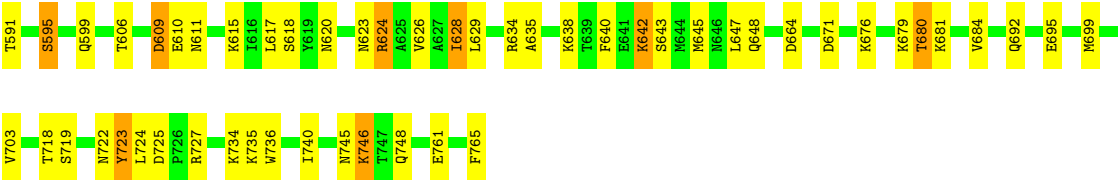
Chain D: 



- Molecule 4: DNA topoisomerase I

Chain A: 





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.36 Å 114.42 Å 74.12 Å 90.00° 93.49° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	90.9 (20.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.241 , 0.292	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5605	wwPDB-VP
Average B, all atoms (Å ²)	70.0	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: EHD, PTR, TGP

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	0.56	0/229	0.81	0/351
2	C	0.49	0/254	0.85	0/390
3	D	0.56	0/494	0.99	0/760
4	A	0.80	2/4770 (0.0%)	1.25	36/6401 (0.6%)
All	All	0.76	2/5747 (0.0%)	1.19	36/7902 (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
1	B	0	2
3	D	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	286	MET	SD-CE	-5.44	1.66	1.79
4	A	541	VAL	CA-CB	5.38	1.59	1.54

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	367	HIS	CA-C-N	9.27	129.48	119.28
4	A	367	HIS	C-N-CA	9.27	129.48	119.28
4	A	504	CYS	N-CA-C	8.46	121.34	111.02
4	A	564	LEU	N-CA-C	-8.37	100.45	111.24
4	A	746	LYS	N-CA-C	8.07	120.07	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	642	LYS	N-CA-C	-7.83	101.91	112.94
4	A	541	VAL	N-CA-C	7.62	119.74	107.71
4	A	566	ASP	N-CA-C	-7.57	99.27	110.48
4	A	643	SER	N-CA-C	-7.41	104.24	113.28
4	A	246	VAL	N-CA-C	7.37	118.96	109.30
4	A	609	ASP	N-CA-C	7.29	118.86	111.07
4	A	419	ASN	N-CA-C	7.04	121.62	112.89
4	A	635	ALA	N-CA-C	-6.92	101.08	109.72
4	A	647	LEU	N-CA-C	-6.65	105.79	114.04
4	A	412	TRP	N-CA-C	6.60	120.25	110.48
4	A	401	TRP	N-CA-C	-6.60	101.64	110.55
4	A	351	ALA	N-CA-C	6.54	118.29	111.03
4	A	374	LYS	N-CA-C	-6.53	97.03	108.20
4	A	586	ALA	N-CA-C	6.43	120.74	113.02
4	A	381	ASP	N-CA-C	-6.15	106.37	114.31
4	A	422	GLY	N-CA-C	-6.14	105.63	115.08
4	A	545	LYS	N-CA-C	6.09	117.59	111.07
4	A	409	LYS	N-CA-C	-6.02	105.59	113.17
4	A	322	GLU	N-CA-C	-5.94	105.12	112.72
4	A	692	GLN	N-CA-C	5.82	117.70	111.36
4	A	228	ALA	CA-C-N	5.80	126.35	120.38
4	A	228	ALA	C-N-CA	5.80	126.35	120.38
4	A	610	GLU	N-CA-C	5.74	118.38	110.35
4	A	671	ASP	N-CA-C	-5.39	107.07	113.97
4	A	338	TYR	N-CA-C	5.37	120.85	113.97
4	A	664	ASP	N-CA-C	-5.35	105.02	112.45
4	A	503	GLY	N-CA-C	-5.33	100.52	110.66
4	A	645	MET	N-CA-C	-5.17	105.83	111.82
4	A	250	SER	CA-C-N	5.10	126.22	119.84
4	A	250	SER	C-N-CA	5.10	126.22	119.84
4	A	346	HIS	N-CA-C	5.04	116.86	109.24

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	8	DC	Sidechain
1	B	9	DT	Sidechain
3	D	112	DC	Sidechain

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	B	203	0	112	21	0
2	C	246	0	138	29	0
3	D	443	0	255	38	0
4	A	4687	0	4721	69	0
5	D	26	0	15	3	0
All	All	5605	0	5241	142	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 13.

All (142) 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:1:DA:H2''	1:B:2:DA:H5'	1.11	1.10
3:D:119:DT:H2''	3:D:120:DT:H5''	1.31	1.10
1:B:1:DA:C2'	1:B:2:DA:H5'	1.95	0.95
4:A:745:ASN:H	4:A:748:GLN:HE21	1.03	0.95
2:C:11:TGP:H2''	2:C:12:DG:C8	2.04	0.92
2:C:12:DG:H5'	5:D:990:EHD:H311	1.49	0.91
2:C:17:DA:H2''	2:C:18:DT:H5''	1.50	0.90
4:A:599:GLN:HE22	4:A:765:PHE:H	1.15	0.89
4:A:375:ARG:H	4:A:419:ASN:HD21	1.20	0.88
2:C:15:DA:H8	2:C:15:DA:H5'	1.40	0.86
3:D:119:DT:C2'	3:D:120:DT:H5''	2.07	0.84
4:A:578:GLN:HE22	4:A:583:GLY:H	1.24	0.83
2:C:15:DA:H5'	2:C:15:DA:C8	2.13	0.83
1:B:4:DA:H1'	1:B:5:DA:H5''	1.59	0.82
4:A:745:ASN:H	4:A:748:GLN:NE2	1.78	0.81
1:B:1:DA:H2''	1:B:2:DA:C5'	2.04	0.80
3:D:106:DT:H2'	3:D:107:DT:H72	1.68	0.76
3:D:111:DC:H2''	3:D:112:DC:O5'	1.87	0.75
4:A:578:GLN:NE2	4:A:583:GLY:H	1.87	0.72
3:D:120:DT:C5'	3:D:120:DT:H6	2.05	0.70
2:C:15:DA:H2''	2:C:16:DA:O5'	1.93	0.69
4:A:375:ARG:HD2	4:A:419:ASN:HD22	1.56	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:430:ASN:HD22	4:A:432:SER:H	1.41	0.68
3:D:120:DT:H6	3:D:120:DT:H5'	1.59	0.68
2:C:17:DA:C2'	2:C:18:DT:H5''	2.24	0.66
1:B:2:DA:H1'	1:B:3:DA:C8	2.31	0.66
4:A:549:LYS:O	4:A:553:LEU:HD13	1.95	0.65
3:D:119:DT:H2''	3:D:120:DT:C5'	2.19	0.65
4:A:367:HIS:HD2	4:A:369:LYS:H	1.44	0.64
4:A:599:GLN:NE2	4:A:765:PHE:H	1.93	0.64
1:B:10:DT:H4'	4:A:723:PTR:O2P	1.97	0.64
1:B:1:DA:H61	3:D:122:DT:H3	1.47	0.63
1:B:2:DA:H4'	1:B:3:DA:OP1	1.99	0.62
2:C:18:DT:H3	3:D:105:DA:H61	1.46	0.62
3:D:114:DA:H2''	3:D:115:DG:OP2	2.00	0.62
3:D:120:DT:H2'	3:D:121:DT:H72	1.82	0.62
3:D:121:DT:H2'	3:D:122:DT:H71	1.82	0.61
4:A:375:ARG:H	4:A:419:ASN:ND2	1.95	0.61
1:B:3:DA:H61	3:D:120:DT:H3	1.47	0.61
4:A:626:VAL:HG11	4:A:724:LEU:HD21	1.84	0.60
4:A:745:ASN:N	4:A:748:GLN:HE21	1.87	0.59
2:C:18:DT:C2'	2:C:19:DT:C6	2.86	0.59
4:A:488:ARG:NH2	4:A:723:PTR:O1P	2.36	0.58
2:C:11:TGP:C2'	2:C:12:DG:C8	2.82	0.58
3:D:109:DT:H6	3:D:109:DT:H5'	1.69	0.58
4:A:624:ARG:O	4:A:628:ILE:HG13	2.03	0.58
3:D:111:DC:C6	3:D:111:DC:H5'	2.39	0.58
2:C:11:TGP:H2''	2:C:12:DG:N7	2.18	0.57
4:A:296:ASN:HD21	4:A:299:LYS:HD2	1.69	0.57
1:B:3:DA:H2''	1:B:4:DA:O5'	2.05	0.56
1:B:1:DA:H2'	1:B:2:DA:C8	2.41	0.56
1:B:8:DC:H2''	1:B:9:DT:O5'	2.06	0.56
3:D:103:DA:H2''	3:D:104:DA:O5'	2.07	0.55
4:A:220:LEU:O	4:A:386:CYS:HB2	2.08	0.54
4:A:320:SER:C	4:A:322:GLU:H	2.16	0.54
3:D:112:DC:H5	4:A:356:GLU:OE2	1.91	0.54
2:C:11:TGP:H1'	5:D:990:EHD:H252	1.90	0.53
4:A:578:GLN:HE22	4:A:583:GLY:N	2.00	0.53
2:C:18:DT:H2'	2:C:19:DT:C6	2.44	0.53
4:A:362:ARG:HD3	4:A:363:GLY:O	2.09	0.53
4:A:383:ILE:HG23	4:A:403:GLU:HB3	1.91	0.53
2:C:18:DT:H2''	2:C:19:DT:C6	2.44	0.53
3:D:112:DC:H2''	5:D:990:EHD:H3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:106:DT:H2''	3:D:107:DT:O5'	2.08	0.52
3:D:118:DT:H2'	3:D:119:DT:H71	1.91	0.52
4:A:407:ASP:O	4:A:410:VAL:HG22	2.10	0.52
3:D:114:DA:H4'	4:A:533:ASP:OD1	2.09	0.52
3:D:120:DT:H2'	3:D:121:DT:C7	2.38	0.52
2:C:17:DA:H3'	4:A:324:LYS:NZ	2.23	0.52
2:C:19:DT:H2''	2:C:20:DT:H72	1.93	0.51
3:D:109:DT:H5'	3:D:109:DT:C6	2.46	0.51
1:B:6:DG:P	4:A:424:ILE:HD11	2.51	0.51
4:A:332:GLU:O	4:A:336:LYS:HG2	2.10	0.51
4:A:680:THR:O	4:A:684:VAL:HG23	2.11	0.50
4:A:341:CYS:SG	4:A:429:LEU:HD21	2.52	0.50
4:A:283:ARG:HA	4:A:286:MET:HE2	1.93	0.50
4:A:418:GLU:HG2	4:A:425:LYS:HE2	1.94	0.49
1:B:10:DT:OP1	4:A:587:LYS:NZ	2.45	0.49
2:C:15:DA:C2	2:C:16:DA:C2	3.01	0.49
2:C:20:DT:H2''	2:C:21:DT:C6	2.47	0.49
4:A:569:ASN:C	4:A:569:ASN:HD22	2.20	0.49
4:A:367:HIS:CD2	4:A:369:LYS:H	2.29	0.49
4:A:761:GLU:H	4:A:761:GLU:CD	2.20	0.49
4:A:249:LEU:HD23	4:A:290:GLU:OE1	2.13	0.49
4:A:405:ARG:HG3	4:A:406:HIS:H	1.75	0.49
1:B:1:DA:H2'	1:B:2:DA:H8	1.78	0.48
3:D:120:DT:C5'	3:D:120:DT:C6	2.91	0.48
4:A:718:THR:O	4:A:722:ASN:HB2	2.13	0.48
4:A:448:ARG:HE	4:A:765:PHE:HA	1.78	0.48
4:A:527:PHE:O	4:A:538:TYR:HA	2.13	0.48
1:B:3:DA:N6	3:D:120:DT:H3	2.12	0.48
2:C:19:DT:C2'	2:C:20:DT:H72	2.45	0.47
3:D:113:DA:H2''	3:D:114:DA:C8	2.50	0.47
4:A:566:ASP:O	4:A:567:ARG:HB2	2.14	0.47
2:C:19:DT:H2''	2:C:20:DT:C7	2.45	0.47
2:C:19:DT:H2''	2:C:20:DT:OP2	2.13	0.47
3:D:105:DA:H1'	3:D:106:DT:H5''	1.97	0.47
4:A:403:GLU:OE2	4:A:405:ARG:HD3	2.15	0.47
1:B:6:DG:OP2	4:A:424:ILE:HD11	2.15	0.46
3:D:102:DA:C2	3:D:103:DA:C6	3.03	0.46
3:D:113:DA:H2''	3:D:114:DA:H8	1.80	0.46
2:C:20:DT:H2''	2:C:21:DT:H6	1.79	0.46
3:D:120:DT:H5'	3:D:120:DT:C6	2.46	0.46
3:D:118:DT:C2'	3:D:119:DT:H71	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:18:DT:H3	3:D:105:DA:N6	2.13	0.46
2:C:15:DA:C2	3:D:109:DT:O2	2.69	0.45
2:C:14:DA:H1'	2:C:15:DA:H5''	1.97	0.45
4:A:405:ARG:HG3	4:A:406:HIS:N	2.31	0.45
4:A:615:LYS:NZ	4:A:736:TRP:HB3	2.31	0.45
1:B:2:DA:C2	1:B:3:DA:C4	3.04	0.45
2:C:11:TGP:C2'	2:C:12:DG:N7	2.79	0.45
4:A:541:VAL:HA	4:A:542:PRO:HD3	1.86	0.44
4:A:725:ASP:OD2	4:A:727:ARG:NH2	2.43	0.44
4:A:485:LEU:HD11	4:A:541:VAL:HG11	1.99	0.44
1:B:6:DG:H2'	4:A:424:ILE:HD12	1.99	0.43
4:A:514:LEU:HD13	4:A:552:GLN:HG2	1.99	0.43
2:C:18:DT:H2'	2:C:19:DT:C7	2.49	0.43
4:A:591:THR:O	4:A:595:SER:HB2	2.19	0.43
1:B:4:DA:C2	1:B:5:DA:C4	3.07	0.43
3:D:103:DA:H1'	3:D:104:DA:H5'	2.01	0.42
4:A:640:PHE:C	4:A:642:LYS:H	2.27	0.42
2:C:15:DA:H2''	2:C:16:DA:C5'	2.48	0.42
4:A:473:ARG:HD3	4:A:550:ASN:OD1	2.19	0.42
4:A:676:LYS:HZ2	4:A:681:LYS:HB2	1.85	0.42
3:D:110:DT:H1'	3:D:111:DC:H5''	2.02	0.42
4:A:358:PRO:HG3	4:A:376:ARG:HE	1.85	0.42
4:A:620:ASN:HB3	4:A:624:ARG:NH2	2.34	0.42
3:D:104:DA:H2''	3:D:105:DA:OP2	2.20	0.42
4:A:222:HIS:HB3	4:A:341:CYS:HB2	2.02	0.41
4:A:316:ARG:C	4:A:318:GLN:H	2.28	0.41
4:A:502:VAL:HB	4:A:503:GLY:H	1.71	0.41
3:D:113:DA:OP2	4:A:374:LYS:NZ	2.49	0.41
4:A:274:PHE:HA	4:A:370:MET:O	2.21	0.41
1:B:4:DA:H2''	1:B:5:DA:OP2	2.21	0.41
4:A:312:GLN:O	4:A:316:ARG:HB2	2.21	0.41
4:A:384:ILE:HG22	4:A:385:ASN:N	2.35	0.41
4:A:477:VAL:O	4:A:480:TYR:HB3	2.21	0.41
4:A:512:ILE:HD11	4:A:564:LEU:HD13	2.02	0.40
4:A:382:ILE:HG23	4:A:414:VAL:HG13	2.01	0.40
4:A:351:ALA:C	4:A:352:ASN:HD22	2.29	0.40
3:D:120:DT:H5''	3:D:120:DT:H6	1.84	0.40
2:C:14:DA:H2''	2:C:15:DA:C5'	2.51	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	
4	A	562/592 (95%)	508 (90%)	48 (8%)	6 (1%)	11	43

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	344	ASP
4	A	638	LYS
4	A	740	ILE
4	A	202	LYS
4	A	483	ASP
4	A	519	ASP

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	504/535 (94%)	437 (87%)	67 (13%)	4	18

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	207	GLU
4	A	209	GLU
4	A	232	GLU
4	A	236	GLU
4	A	239	LYS

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Mol	Chain	Res	Type
4	A	246	VAL
4	A	247	MET
4	A	251	PRO
4	A	262	LYS
4	A	264	LEU
4	A	291	LYS
4	A	298	SER
4	A	304	GLN
4	A	323	GLU
4	A	324	LYS
4	A	331	ASN
4	A	335	LEU
4	A	337	GLU
4	A	341	CYS
4	A	362	ARG
4	A	366	ASN
4	A	368	PRO
4	A	375	ARG
4	A	389	ASP
4	A	394	SER
4	A	396	PRO
4	A	397	PRO
4	A	405	ARG
4	A	431	PRO
4	A	434	ARG
4	A	439	LYS
4	A	451	LYS
4	A	463	GLU
4	A	479	LEU
4	A	487	LEU
4	A	493	LYS
4	A	495	GLU
4	A	498	THR
4	A	512	ILE
4	A	518	LEU
4	A	522	GLU
4	A	524	VAL
4	A	544	GLU
4	A	557	ASN
4	A	569	ASN
4	A	587	LYS
4	A	595	SER

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Mol	Chain	Res	Type
4	A	606	THR
4	A	609	ASP
4	A	611	ASN
4	A	617	LEU
4	A	618	SER
4	A	623	ASN
4	A	624	ARG
4	A	628	ILE
4	A	629	LEU
4	A	634	ARG
4	A	648	GLN
4	A	679	LYS
4	A	680	THR
4	A	695	GLU
4	A	699	MET
4	A	703	VAL
4	A	719	SER
4	A	734	LYS
4	A	735	LYS
4	A	746	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	277	ASN
4	A	304	GLN
4	A	331	ASN
4	A	352	ASN
4	A	367	HIS
4	A	399	HIS
4	A	419	ASN
4	A	430	ASN
4	A	459	ASN
4	A	460	GLN
4	A	557	ASN
4	A	559	GLN
4	A	569	ASN
4	A	576	HIS
4	A	578	GLN
4	A	593	ASN
4	A	599	GLN
4	A	601	GLN

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Mol	Chain	Res	Type
4	A	620	ASN
4	A	623	ASN
4	A	631	ASN
4	A	633	GLN
4	A	657	GLN
4	A	697	GLN
4	A	704	GLN
4	A	711	ASN
4	A	722	ASN
4	A	748	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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$
2	TGP	C	11	3,2	21,21,25	0.97	1 (4%)	30,31,38	0.54	1 (3%)
4	PTR	A	723	1,4	15,16,17	1.07	0	17,22,24	1.10	1 (5%)

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	TGP	C	11	3,2	-	2/6/18/22	0/3/3/3
4	PTR	A	723	1,4	-	1/10/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	11	TGP	C5'-S5'	3.77	1.89	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	723	PTR	O2P-P-O1P	2.31	119.82	110.83
2	C	11	TGP	C5'-C4'-C3'	2.11	120.20	115.02

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	11	TGP	O4'-C4'-C5'-S5'
2	C	11	TGP	C3'-C4'-C5'-S5'
4	A	723	PTR	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	11	TGP	5	0
4	A	723	PTR	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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
5	EHD	D	990	-	26,30,30	3.36	14 (53%)	27,47,47	2.29	10 (37%)

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
5	EHD	D	990	-	-	3/3/28/28	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	990	EHD	C9-C13	-6.87	1.38	1.46
5	D	990	EHD	O18-C14	6.16	1.35	1.23
5	D	990	EHD	C15-C16	5.97	1.46	1.36
5	D	990	EHD	O22-C20	5.47	1.41	1.34
5	D	990	EHD	C5-N10	5.12	1.45	1.37
5	D	990	EHD	O23-C20	4.87	1.31	1.20
5	D	990	EHD	O24-C21	-4.66	1.34	1.42
5	D	990	EHD	C3-C4	3.84	1.44	1.36
5	D	990	EHD	C14-C15	-3.40	1.36	1.44
5	D	990	EHD	C13-N12	-2.75	1.34	1.40
5	D	990	EHD	C4-C5	-2.61	1.37	1.41
5	D	990	EHD	C17-C13	2.56	1.42	1.37
5	D	990	EHD	C6-C5	2.14	1.45	1.42
5	D	990	EHD	C3-C2	2.08	1.42	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	990	EHD	C17-C16-C15	-7.07	112.70	120.25
5	D	990	EHD	C13-N12-C14	-3.99	120.85	124.57
5	D	990	EHD	C11-N12-C13	3.70	114.82	113.10
5	D	990	EHD	C11-C8-C9	-3.31	107.10	109.56
5	D	990	EHD	C9-C13-N12	3.07	108.80	107.06
5	D	990	EHD	C11-C8-C7	2.28	134.05	130.34
5	D	990	EHD	C4-C5-C6	2.24	121.28	119.04
5	D	990	EHD	O18-C14-C15	-2.21	120.86	125.06
5	D	990	EHD	C15-C14-N12	2.12	118.85	115.16
5	D	990	EHD	C4-C5-N10	-2.09	115.64	118.69

There are no chirality outliers.

All (3) torsion outliers are listed below:

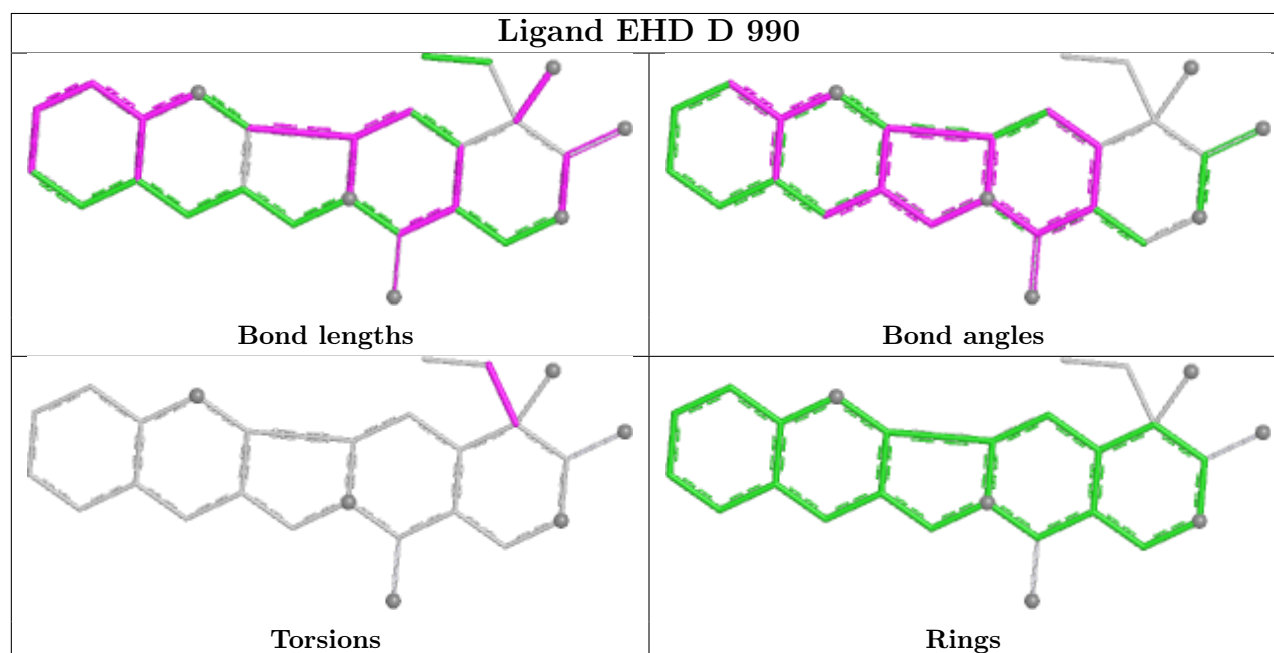
Mol	Chain	Res	Type	Atoms
5	D	990	EHD	C20-C21-C25-C31
5	D	990	EHD	C16-C21-C25-C31
5	D	990	EHD	O24-C21-C25-C31

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	990	EHD	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.