



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:54 PM UTC

PDB ID : 1TL8 / pdb_00001tl8
Title : Human DNA topoisomerase I (70 kDa) in complex with the indenoisoquinoline AI-III-52 and covalent complex with a 22 base pair DNA duplex
Authors : Ioanoviciu, A.; Antony, S.; Pommier, Y.; Staker, B.L.; Stewart, L.; Cushman, M.
Deposited on : 2004-06-09
Resolution : 3.10 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

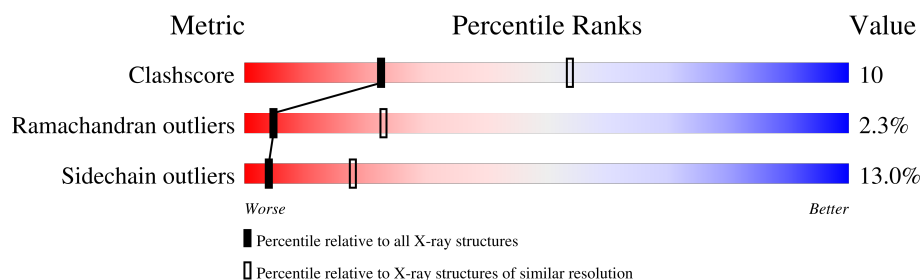
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)

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	8% 83% 8%
3	D	22	32% 64% 5%
4	A	592	66% 25% 5% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5619 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(*(TPC)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
			243	119	43	69	11	1			

- Molecule 3 is a DNA chain called 5'-D(*AP*AP*AP*AP*AP*TP*TP*TP*TP*TP*CP*GP*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
			446	218	73	134	21			

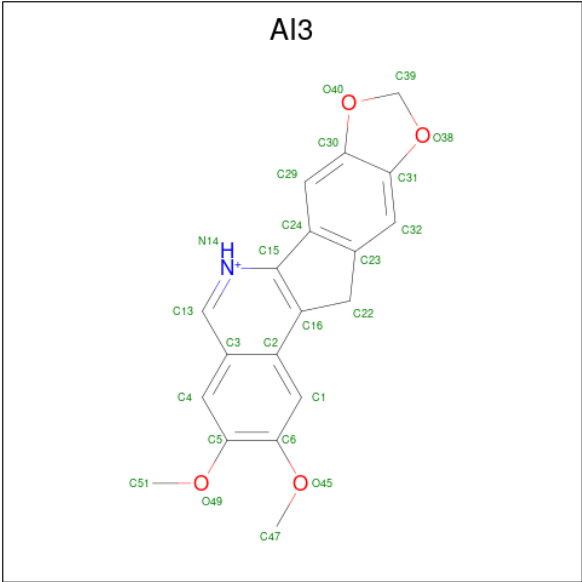
- Molecule 4 is a protein called DNA topoisomerase I.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	A	565	Total	C	N	O	P	S	0	0	0
			4703	2992	825	859	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 2,3-DIMETHOXY-12H-[1,3]DIOXOLO[5,6]INDENO[1,2-C]ISOQUINOLIN-6-IUM (CCD ID: AI3) (formula: C₁₉H₁₆NO₄).



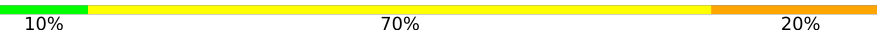
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	N	O	0	0
			24	19	1	4		

3 Residue-property plots

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.

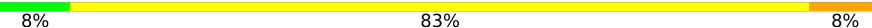
Note EDS was not executed.

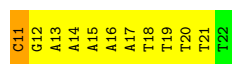
- Molecule 1: 5'-D(*AP*AP*AP*AP*AP*GP*AP*CP*TP*T)-3'

Chain B: 

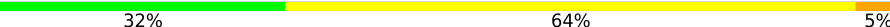


- Molecule 2: 5'-D(*(TPC)P*GP*AP*AP*AP*AP*AP*TP*TP*TP*TP*T)-3'

Chain C: 



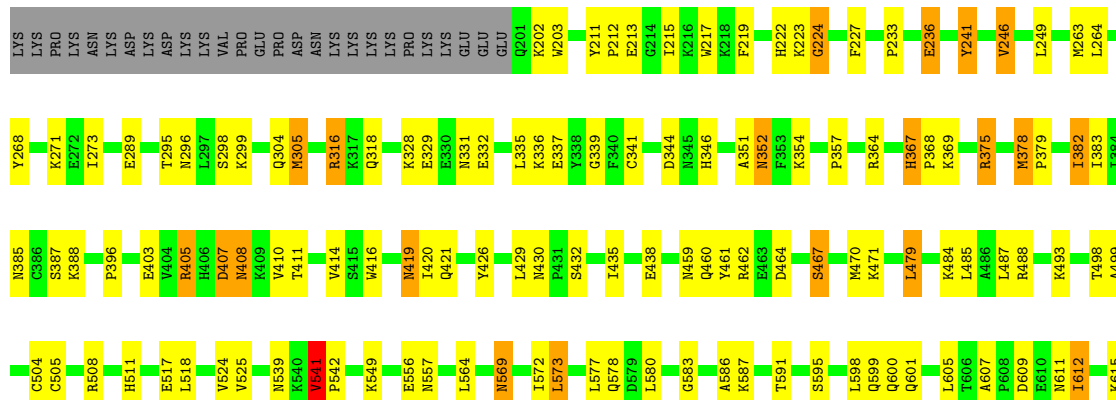
- Molecule 3: 5'-D(*AP*AP*AP*AP*AP*TP*TP*TP*TP*TP*CP*GP*AP*AP*GP*TP*CP*TP*TP*TP*TP*T)-3'

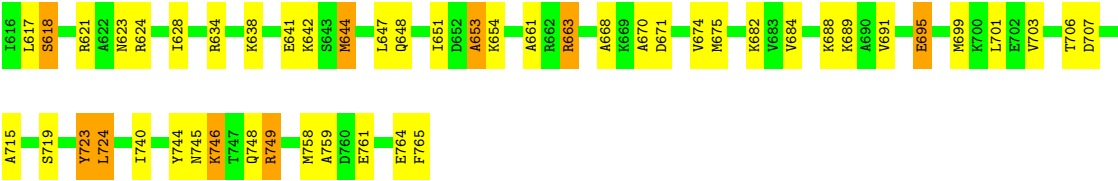
Chain D: 



- 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	56.95Å 114.14Å 73.50Å 90.00° 94.18° 90.00°	Depositor
Resolution (Å)	46.57 – 3.10	Depositor
% Data completeness (in resolution range)	97.8 (46.57-3.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	CNX 2002	Depositor
R, R_{free}	0.229 , 0.305	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5619	wwPDB-VP
Average B, all atoms (Å ²)	60.0	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: AI3, TPC, PTR

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	0.55	0/229	0.86	0/351
2	C	0.43	0/254	0.89	0/390
3	D	0.53	0/498	0.96	0/767
4	A	0.99	5/4787 (0.1%)	1.37	45/6422 (0.7%)
All	All	0.92	5/5768 (0.1%)	1.29	45/7930 (0.6%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	612	ILE	CA-CB	9.66	1.58	1.54
4	A	541	VAL	CA-CB	7.67	1.61	1.54
4	A	305	MET	SD-CE	-5.64	1.65	1.79
4	A	378	MET	SD-CE	5.35	1.93	1.79
4	A	357	PRO	CA-C	5.10	1.55	1.52

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	586	ALA	N-CA-C	9.57	124.22	112.54
4	A	642	LYS	N-CA-C	-9.12	101.08	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	316	ARG	N-CA-C	-8.15	102.34	113.18
4	A	420	ILE	N-CA-C	-8.06	104.88	111.81
4	A	289	GLU	N-CA-C	-7.93	102.63	111.82
4	A	541	VAL	N-CA-C	7.62	119.74	107.71
4	A	688	LYS	N-CA-C	-7.59	104.15	113.41
4	A	524	VAL	N-CA-C	7.21	120.15	108.97
4	A	644	MET	N-CA-C	-7.14	104.70	113.41
4	A	419	ASN	N-CA-C	6.95	121.67	111.87
4	A	346	HIS	N-CA-C	6.80	120.63	109.06
4	A	504	CYS	N-CA-C	6.79	118.37	110.97
4	A	746	LYS	N-CA-C	6.72	118.39	111.14
4	A	382	ILE	N-CA-C	6.54	118.24	108.23
4	A	691	VAL	N-CA-C	-6.53	103.88	111.00
4	A	758	MET	N-CA-C	6.34	120.87	111.04
4	A	367	HIS	CA-C-N	6.34	126.02	119.56
4	A	367	HIS	C-N-CA	6.34	126.02	119.56
4	A	707	ASP	N-CA-C	-6.22	105.18	112.89
4	A	426	TYR	N-CA-C	6.05	118.16	109.14
4	A	661	ALA	N-CA-C	-5.96	105.50	112.89
4	A	653	ALA	N-CA-C	-5.93	105.13	112.72
4	A	459	ASN	N-CA-C	-5.90	105.74	113.12
4	A	249	LEU	N-CA-C	5.87	119.66	110.32
4	A	759	ALA	N-CA-C	5.87	118.85	110.10
4	A	467	SER	N-CA-C	5.82	123.20	110.80
4	A	429	LEU	N-CA-C	5.79	118.18	110.53
4	A	595	SER	N-CA-C	5.72	117.19	111.07
4	A	337	GLU	N-CA-C	5.57	117.43	111.36
4	A	295	THR	N-CA-C	5.53	118.49	111.69
4	A	241	TYR	N-CA-C	5.49	117.91	109.07
4	A	203	TRP	N-CA-C	5.47	117.21	108.41
4	A	224	GLY	CA-C-N	5.45	126.66	119.84
4	A	224	GLY	C-N-CA	5.45	126.66	119.84
4	A	539	ASN	N-CA-C	5.38	116.80	107.93
4	A	689	LYS	N-CA-C	-5.36	106.00	112.54
4	A	670	ALA	N-CA-C	-5.32	106.73	114.12
4	A	268	TYR	N-CA-C	5.27	118.81	112.38
4	A	564	LEU	N-CA-C	-5.20	105.69	111.36
4	A	615	LYS	N-CA-C	-5.17	105.54	111.07
4	A	339	GLY	N-CA-C	5.08	123.81	115.73
4	A	695	GLU	N-CA-C	-5.07	105.22	111.40
4	A	405	ARG	CB-CG-CD	-5.02	99.74	111.30
4	A	607	ALA	CA-C-N	5.02	124.62	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	607	ALA	C-N-CA	5.02	124.62	119.05

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	10	DT	Sidechain
1	B	8	DC	Sidechain
3	D	102	DA	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	10	0
2	C	243	0	138	20	0
3	D	446	0	255	28	0
4	A	4703	0	4750	63	0
5	D	24	0	16	0	0
All	All	5619	0	5271	113	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 10.

All (113) 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)
2:C:17:DA:H2''	2:C:18:DT:H5''	1.28	1.12
3:D:119:DT:H2''	3:D:120:DT:H5''	1.15	1.10
3:D:120:DT:H2'	3:D:121:DT:H71	1.47	0.92
3:D:119:DT:C2'	3:D:120:DT:H5''	2.00	0.91
2:C:17:DA:C2'	2:C:18:DT:H5''	2.03	0.87
4:A:578:GLN:HE22	4:A:583:GLY:H	1.27	0.81
1:B:2:DA:H1'	1:B:3:DA:C8	2.16	0.80
3:D:105:DA:H1'	3:D:106:DT:H5''	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:598:LEU:HD22	4:A:724:LEU:HD13	1.66	0.78
4:A:367:HIS:HD2	4:A:369:LYS:H	1.31	0.78
4:A:375:ARG:NH1	4:A:419:ASN:HD22	1.86	0.73
4:A:505:CYS:SG	4:A:573:LEU:HD12	2.31	0.70
4:A:375:ARG:HH11	4:A:419:ASN:ND2	1.90	0.70
3:D:119:DT:H2''	3:D:120:DT:C5'	2.08	0.69
3:D:120:DT:H5'	3:D:120:DT:H6	1.57	0.69
3:D:112:DG:H21	4:A:364:ARG:HH12	1.41	0.69
4:A:430:ASN:HD22	4:A:432:SER:H	1.39	0.68
4:A:215:ILE:HG23	4:A:408:ASN:HD21	1.59	0.67
4:A:352:ASN:HD22	4:A:352:ASN:N	1.93	0.66
4:A:296:ASN:HD21	4:A:299:LYS:HD2	1.59	0.66
4:A:745:ASN:H	4:A:748:GLN:NE2	1.93	0.66
2:C:17:DA:H2''	2:C:18:DT:C5'	2.18	0.64
3:D:120:DT:H2'	3:D:121:DT:C7	2.24	0.64
4:A:599:GLN:HE22	4:A:765:PHE:H	1.45	0.63
4:A:578:GLN:NE2	4:A:583:GLY:H	1.97	0.62
4:A:375:ARG:NH1	4:A:419:ASN:ND2	2.46	0.62
2:C:20:DT:H3	3:D:104:DA:H2	1.46	0.62
3:D:120:DT:C5'	3:D:120:DT:H6	2.13	0.61
3:D:115:DG:H2'	3:D:116:DT:H71	1.85	0.59
1:B:3:DA:H61	3:D:120:DT:H3	1.51	0.58
4:A:745:ASN:H	4:A:748:GLN:HE21	1.51	0.58
4:A:485:LEU:HD11	4:A:541:VAL:HG11	1.84	0.58
1:B:5:DA:H2''	1:B:6:DG:O5'	2.05	0.57
1:B:4:DA:H2''	1:B:5:DA:H5''	1.87	0.57
2:C:20:DT:N3	3:D:104:DA:H2	2.03	0.57
2:C:16:DA:H2	3:D:108:DT:O2	1.86	0.56
4:A:488:ARG:NH2	4:A:723:PTR:O1P	2.38	0.56
3:D:105:DA:C1'	3:D:106:DT:H5''	2.35	0.56
2:C:15:DA:C2	2:C:16:DA:C2	2.94	0.56
1:B:10:DT:H4'	4:A:723:PTR:O2P	2.05	0.56
2:C:15:DA:C8	2:C:15:DA:H5'	2.41	0.55
4:A:569:ASN:HD21	4:A:572:ILE:HG13	1.71	0.55
3:D:109:DT:C6	3:D:109:DT:H5'	2.42	0.54
2:C:13:DA:C6	2:C:14:DA:C6	2.95	0.54
2:C:11:TPC:H2'1	2:C:12:DG:C8	2.42	0.54
4:A:222:HIS:HB3	4:A:341:CYS:HB2	1.89	0.54
4:A:273:ILE:H	4:A:273:ILE:HD12	1.72	0.53
2:C:20:DT:H1'	2:C:21:DT:H5'	1.90	0.53
2:C:20:DT:C6	2:C:21:DT:H72	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:651:ILE:C	4:A:653:ALA:H	2.17	0.53
4:A:383:ILE:HG23	4:A:403:GLU:HB3	1.92	0.52
3:D:101:DA:H2''	3:D:102:DA:C8	2.45	0.51
4:A:367:HIS:CD2	4:A:369:LYS:H	2.20	0.51
4:A:485:LEU:HD21	4:A:541:VAL:HG21	1.92	0.51
3:D:114:DA:C2	3:D:115:DG:C4	2.98	0.51
4:A:382:ILE:HD13	4:A:416:TRP:HB3	1.92	0.50
4:A:460:GLN:HE22	4:A:580:LEU:HD21	1.76	0.50
4:A:215:ILE:HG23	4:A:408:ASN:ND2	2.27	0.49
2:C:11:TPC:H6	2:C:11:TPC:H5'1	1.93	0.49
4:A:479:LEU:HD21	4:A:577:LEU:HD21	1.95	0.49
1:B:1:DA:N1	1:B:2:DA:C6	2.81	0.49
4:A:217:TRP:HZ3	4:A:387:SER:HB3	1.78	0.49
4:A:382:ILE:HG23	4:A:414:VAL:HG13	1.95	0.48
3:D:109:DT:H5'	3:D:109:DT:H6	1.78	0.48
3:D:101:DA:C6	3:D:102:DA:N6	2.81	0.48
4:A:668:ALA:HB1	4:A:684:VAL:HG22	1.96	0.48
2:C:13:DA:OP1	4:A:634:ARG:HG3	2.13	0.48
4:A:407:ASP:O	4:A:410:VAL:HG22	2.13	0.47
3:D:105:DA:C2'	3:D:106:DT:H5''	2.43	0.47
2:C:13:DA:P	4:A:634:ARG:HG3	2.53	0.47
3:D:120:DT:C5'	3:D:120:DT:C6	2.95	0.47
1:B:1:DA:H2'	1:B:2:DA:C8	2.50	0.47
4:A:352:ASN:HD22	4:A:352:ASN:H	1.63	0.46
4:A:605:LEU:HB3	4:A:618:SER:OG	2.16	0.46
2:C:15:DA:H5'	2:C:15:DA:H8	1.78	0.46
4:A:744:TYR:O	4:A:749:ARG:HD3	2.15	0.46
3:D:105:DA:H2''	3:D:106:DT:H5''	1.98	0.46
3:D:111:DC:H2''	3:D:112:DG:C8	2.50	0.46
1:B:4:DA:C2'	1:B:5:DA:H5''	2.46	0.45
2:C:11:TPC:H2'1	2:C:12:DG:N7	2.30	0.45
4:A:241:TYR:HE2	4:A:246:VAL:HG22	1.80	0.45
4:A:385:ASN:HA	4:A:405:ARG:O	2.17	0.45
4:A:498:THR:HG22	4:A:499:ALA:N	2.31	0.45
4:A:745:ASN:N	4:A:748:GLN:HE21	2.15	0.45
4:A:217:TRP:CZ3	4:A:387:SER:HB3	2.51	0.45
3:D:115:DG:H2'	3:D:116:DT:C6	2.52	0.44
4:A:219:PHE:N	4:A:344:ASP:OD1	2.46	0.44
4:A:498:THR:HG22	4:A:499:ALA:H	1.82	0.44
4:A:634:ARG:HB2	4:A:715:ALA:HB2	1.99	0.44
3:D:115:DG:H5''	3:D:115:DG:H8	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:DA:H8	1:B:5:DA:H5'	1.81	0.44
4:A:316:ARG:C	4:A:318:GLN:H	2.26	0.44
4:A:222:HIS:C	4:A:224:GLY:H	2.25	0.43
4:A:663:ARG:HG3	4:A:663:ARG:HH11	1.84	0.43
4:A:569:ASN:ND2	4:A:572:ILE:HG13	2.33	0.43
1:B:8:DC:H2''	1:B:9:DT:O5'	2.19	0.43
4:A:621:ARG:HG2	4:A:624:ARG:NH1	2.34	0.43
2:C:19:DT:H2''	2:C:20:DT:OP2	2.18	0.43
4:A:332:GLU:O	4:A:336:LYS:HG2	2.18	0.43
4:A:641:GLU:OE2	4:A:644:MET:HE2	2.18	0.42
4:A:227:PHE:CZ	4:A:379:PRO:HG3	2.55	0.42
4:A:296:ASN:ND2	4:A:299:LYS:HD2	2.30	0.42
2:C:20:DT:H1'	2:C:21:DT:C5'	2.50	0.42
3:D:105:DA:H2''	3:D:106:DT:OP2	2.19	0.41
4:A:296:ASN:OD1	4:A:299:LYS:N	2.54	0.41
4:A:624:ARG:O	4:A:628:ILE:HG13	2.19	0.41
4:A:461:TYR:HA	4:A:464:ASP:HB2	2.01	0.41
4:A:599:GLN:HE22	4:A:764:GLU:HA	1.84	0.41
4:A:508:ARG:HH12	4:A:511:HIS:CE1	2.38	0.41
4:A:541:VAL:HA	4:A:542:PRO:HD3	1.76	0.41
2:C:20:DT:H2''	2:C:21:DT:OP2	2.20	0.41
4:A:644:MET:O	4:A:648:GLN:HB2	2.20	0.41
3:D:120:DT:H5'	3:D:120:DT:C6	2.46	0.40

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	562/592 (95%)	508 (90%)	41 (7%)	13 (2%)	5 23

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	213	GLU
4	A	236	GLU
4	A	467	SER
4	A	638	LYS
4	A	202	LYS
4	A	407	ASP
4	A	351	ALA
4	A	223	LYS
4	A	212	PRO
4	A	675	MET
4	A	724	LEU
4	A	740	ILE
4	A	233	PRO

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	508/535 (95%)	442 (87%)	66 (13%)	4 18

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	211	TYR
4	A	236	GLU
4	A	246	VAL
4	A	263	MET
4	A	264	LEU
4	A	271	LYS
4	A	298	SER
4	A	304	GLN
4	A	305	MET
4	A	328	LYS
4	A	329	GLU
4	A	331	ASN
4	A	335	LEU
4	A	352	ASN

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Mol	Chain	Res	Type
4	A	354	LYS
4	A	368	PRO
4	A	375	ARG
4	A	378	MET
4	A	388	LYS
4	A	396	PRO
4	A	408	ASN
4	A	411	THR
4	A	421	GLN
4	A	435	ILE
4	A	438	GLU
4	A	462	ARG
4	A	470	MET
4	A	471	LYS
4	A	479	LEU
4	A	484	LYS
4	A	487	LEU
4	A	493	LYS
4	A	517	GLU
4	A	518	LEU
4	A	525	VAL
4	A	541	VAL
4	A	549	LYS
4	A	556	GLU
4	A	557	ASN
4	A	569	ASN
4	A	573	LEU
4	A	587	LYS
4	A	591	THR
4	A	600	GLN
4	A	601	GLN
4	A	609	ASP
4	A	611	ASN
4	A	612	ILE
4	A	617	LEU
4	A	618	SER
4	A	623	ASN
4	A	647	LEU
4	A	654	LYS
4	A	663	ARG
4	A	671	ASP
4	A	674	VAL

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Mol	Chain	Res	Type
4	A	682	LYS
4	A	695	GLU
4	A	699	MET
4	A	701	LEU
4	A	703	VAL
4	A	706	THR
4	A	719	SER
4	A	746	LYS
4	A	749	ARG
4	A	761	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	266	HIS
4	A	277	ASN
4	A	352	ASN
4	A	367	HIS
4	A	385	ASN
4	A	408	ASN
4	A	419	ASN
4	A	430	ASN
4	A	460	GLN
4	A	511	HIS
4	A	550	ASN
4	A	569	ASN
4	A	578	GLN
4	A	599	GLN
4	A	611	ASN
4	A	620	ASN
4	A	623	ASN
4	A	633	GLN
4	A	648	GLN
4	A	697	GLN
4	A	704	GLN
4	A	722	ASN
4	A	745	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	TPC	C	11	3,2	17,17,21	0.44	0	23,24,31	0.69	1 (4%)
4	PTR	A	723	4,1	15,16,17	1.10	1 (6%)	17,22,24	1.06	2 (11%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	723	PTR	CE2-CD2	2.50	1.42	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	11	TPC	C5'-C4'-C3'	2.60	121.40	115.02
4	A	723	PTR	O2P-P-OH	2.43	112.49	105.32
4	A	723	PTR	O2P-P-O1P	2.01	118.67	110.83

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	11	TPC	O4'-C4'-C5'-S5'

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	11	TPC	3	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	AI3	D	901	-	27,28,28	3.75	15 (55%)	36,42,42	1.99	10 (27%)

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	AI3	D	901	-	-	0/4/18/18	0/4/5/5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	901	AI3	C1-C6	10.04	1.55	1.38
5	D	901	AI3	C2-C3	6.97	1.51	1.41
5	D	901	AI3	C4-C5	6.49	1.49	1.38
5	D	901	AI3	C24-C23	-5.46	1.32	1.39
5	D	901	AI3	C32-C23	4.67	1.46	1.39
5	D	901	AI3	C4-C3	-4.64	1.32	1.40
5	D	901	AI3	C29-C24	4.60	1.47	1.39
5	D	901	AI3	O45-C6	4.31	1.44	1.37
5	D	901	AI3	O38-C39	3.80	1.50	1.43
5	D	901	AI3	C32-C31	-3.59	1.32	1.38
5	D	901	AI3	C22-C23	3.19	1.56	1.50
5	D	901	AI3	O40-C39	2.67	1.48	1.43
5	D	901	AI3	O40-C30	2.55	1.42	1.38
5	D	901	AI3	C6-C5	-2.47	1.35	1.40
5	D	901	AI3	O38-C31	-2.05	1.34	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	901	AI3	C23-C22-C16	-5.67	96.89	102.90
5	D	901	AI3	C3-C2-C16	-4.93	115.01	119.73
5	D	901	AI3	C51-O49-C5	-4.15	111.42	117.51
5	D	901	AI3	C29-C24-C15	-2.65	128.87	133.42
5	D	901	AI3	C23-C24-C15	2.49	109.13	106.96
5	D	901	AI3	O38-C31-C32	-2.38	124.70	127.86
5	D	901	AI3	C22-C23-C24	2.37	113.12	110.25
5	D	901	AI3	C2-C3-C13	2.15	119.89	118.04
5	D	901	AI3	C31-C32-C23	-2.12	117.91	121.10
5	D	901	AI3	C39-O40-C30	-2.04	102.58	105.32

There are no chirality outliers.

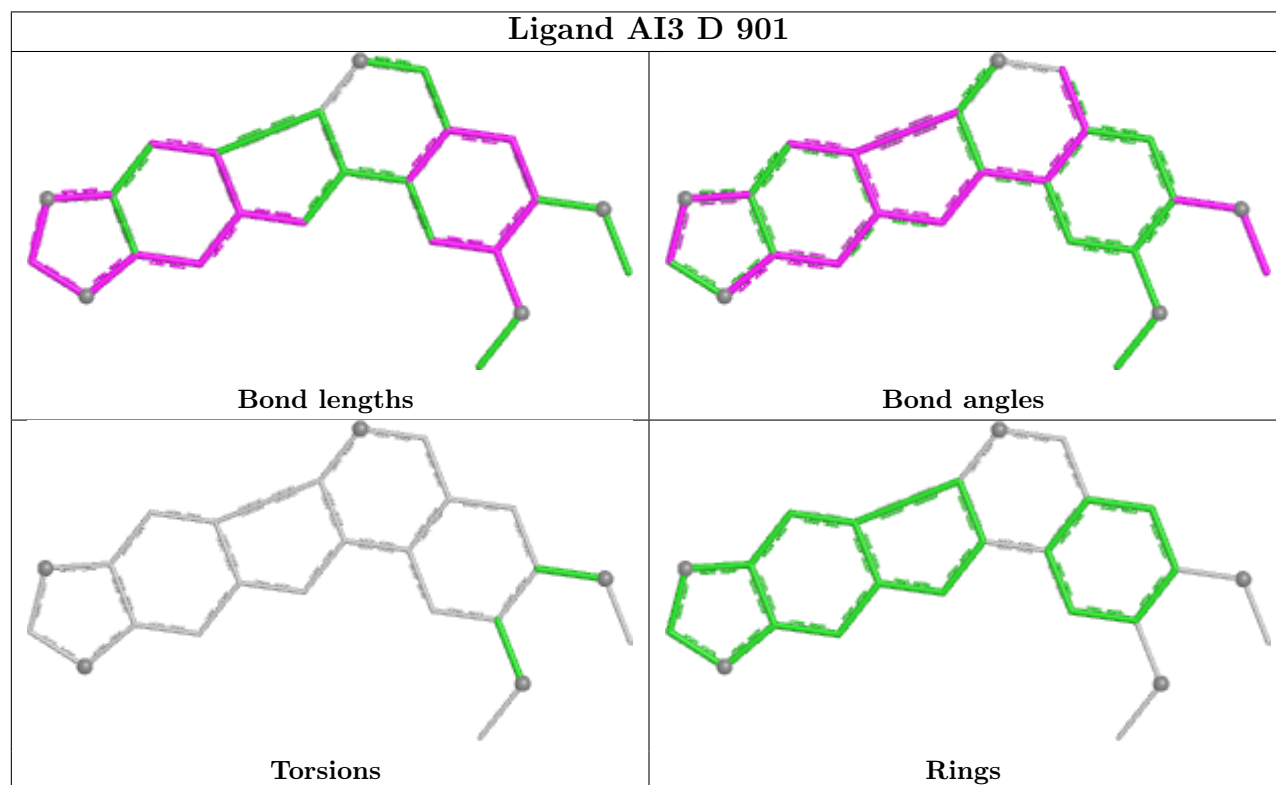
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [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 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.