



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:06 PM UTC

PDB ID : 1RRJ / pdb_00001rrj
Title : Structural Mechanisms of Camptothecin Resistance by Mutations in Human Topoisomerase I
Authors : Chrencik, J.E.; Staker, B.L.; Burgin, A.B.; Stewart, L.; Redinbo, M.R.
Deposited on : 2003-12-08
Resolution : 2.30 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

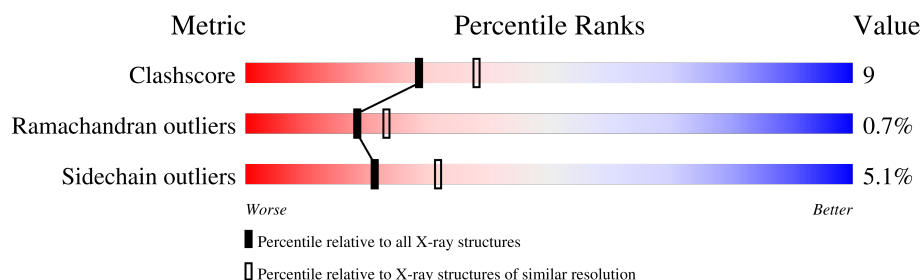
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	22	27% 73%
2	C	22	27% 64% 9%
3	A	565	86% 12% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6092 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*GP*GP*AP*AP*AP*AP*AP*TP*TP*TP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	22	Total	C	N	O	P	0	0	0
			449	219	87	123	20			

- Molecule 2 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
2	C	22	Total	C	N	O	P	0	0	0
			443	217	71	134	21			

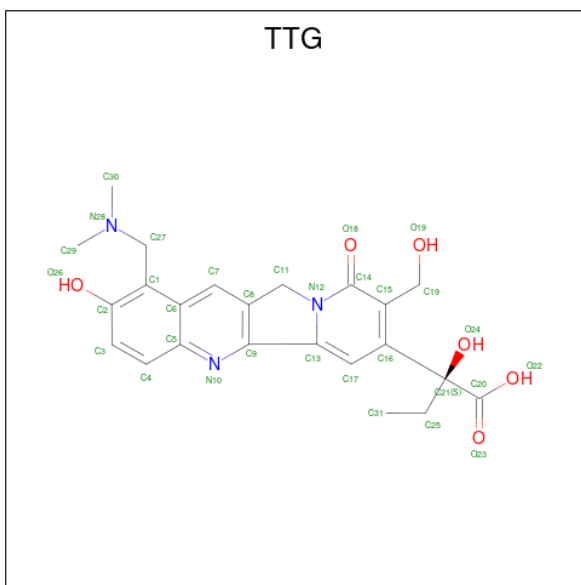
- Molecule 3 is a protein called DNA topoisomerase I.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	A	565	Total	C	N	O	P	S	0	0	0
			4701	2991	824	859	1	26			

There are 2 discrepancies between the modelled and reference sequences:

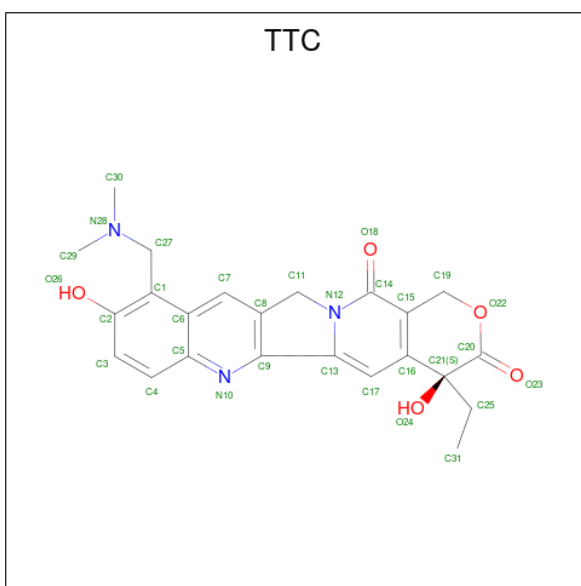
Chain	Residue	Modelled	Actual	Comment	Reference
A	722	SER	ASN	engineered mutation	UNP P11387
A	723	PTR	TYR	modified residue	UNP P11387

- Molecule 4 is 2-(1-DIMETHYLAMINOMETHYL-2-HYDROXY-8-HYDROXYMETHYL-9-OXO-9,11-DIHYDRO-INDOLIZINO[1,2-B]QUINOLIN-7-YL)-2-HYDROXY-BUTYRIC ACID (CCD ID: TTG) (formula: C₂₃H₂₅N₃O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			32	23	3	6		

- Molecule 5 is (S)-10-[(DIMETHYLAMINO)METHYL]-4-ETHYL-4,9-DIHYDROXY-1H-PYRANO[3',4':6,7]INOLIZINO[1,2-B]-QUINOLINE-3,14(4H,12H)-DIONE (CCD ID: TTC) (formula: $C_{23}H_{23}N_3O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			31	23	3	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	44	Total 44	O 44	0	0
6	C	37	Total 37	O 37	0	0
6	A	355	Total 355	O 355	0	0

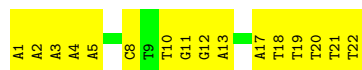
3 Residue-property plots

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.

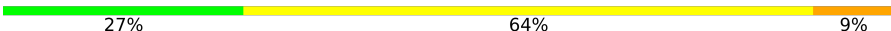
Note EDS was not executed.

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

Chain B: 



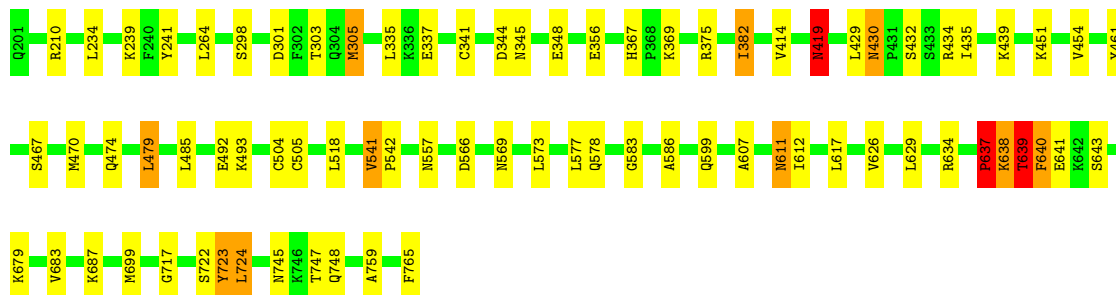
- Molecule 2: 5'-D(*AP*AP*AP*AP*AP*TP*TP*TP*TP*TP*CP*CP*AP*AP*GP*TP*CP*TP*TP*TP*TP*T)-3'

Chain C: 



- Molecule 3: 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	57.33Å 115.35Å 75.17Å 90.00° 94.33° 90.00°	Depositor
Resolution (Å)	43.69 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (43.69-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.246 , 0.278	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6092	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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: TTG, TTC, 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	0.28	0/505	0.67	0/776
2	C	0.30	0/494	0.80	2/760 (0.3%)
3	A	1.05	5/4785 (0.1%)	1.19	21/6419 (0.3%)
All	All	0.96	5/5784 (0.1%)	1.12	23/7955 (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
3	A	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	640	PHE	N-CA	53.57	2.17	1.46
3	A	724	LEU	N-CA	12.70	1.70	1.46
3	A	612	ILE	CA-CB	8.26	1.58	1.54
3	A	541	VAL	CA-CB	5.85	1.58	1.54
3	A	305	MET	SD-CE	-5.73	1.65	1.79

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	640	PHE	N-CA-C	-26.91	77.24	113.30
3	A	639	THR	CA-C-N	-13.39	101.73	122.49
3	A	639	THR	C-N-CA	-13.39	101.73	122.49
3	A	724	LEU	N-CA-CB	11.40	129.89	110.50
3	A	541	VAL	N-CA-C	8.62	117.86	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	382	ILE	N-CA-C	7.60	119.53	108.58
3	A	419	ASN	N-CA-C	7.49	121.68	112.54
3	A	717	GLY	N-CA-C	7.35	121.53	112.64
3	A	504	CYS	N-CA-C	6.84	118.42	110.97
3	A	724	LEU	N-CA-C	-6.28	93.41	111.00
3	A	454	VAL	N-CA-C	6.05	116.83	110.72
3	A	639	THR	N-CA-CB	-6.02	100.32	110.49
3	A	303	THR	N-CA-C	5.90	118.47	111.33
3	A	586	ALA	N-CA-C	5.67	117.46	111.28
2	C	112	DC	C5'-C4'-C3'	-5.61	106.49	114.90
3	A	239	LYS	N-CA-C	5.37	118.86	110.32
3	A	607	ALA	CA-C-N	5.37	124.83	119.24
3	A	607	ALA	C-N-CA	5.37	124.83	119.24
3	A	643	SER	N-CA-C	-5.22	106.89	113.20
3	A	298	SER	N-CA-C	5.09	118.59	112.38
3	A	639	THR	N-CA-C	5.07	121.59	110.80
2	C	115	DG	C5'-C4'-C3'	-5.05	107.33	114.90
3	A	467	SER	N-CA-C	5.02	117.18	110.35

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	639	THR	Peptide
3	A	722	SER	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	B	449	0	251	31	0
2	C	443	0	255	19	0
3	A	4701	0	4749	46	0
4	B	32	0	21	3	0
5	B	31	0	19	0	0
6	A	355	0	0	4	0
6	B	44	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	37	0	0	2	0
All	All	6092	0	5295	95	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 (95) 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:A:724:LEU:CA	3:A:724:LEU:N	1.70	1.50
3:A:640:PHE:N	3:A:641:GLU:H	1.23	1.33
3:A:640:PHE:N	3:A:641:GLU:N	1.89	1.18
3:A:640:PHE:N	3:A:640:PHE:CA	2.17	1.08
1:B:1:DA:H2'	1:B:2:DA:C8	1.99	0.97
2:C:110:DT:H2''	2:C:111:DC:H5''	1.50	0.91
3:A:419:ASN:HD22	3:A:419:ASN:H	1.14	0.90
2:C:115:DG:H2'	2:C:116:DT:H72	1.57	0.87
3:A:723:PTR:O	3:A:724:LEU:CA	2.22	0.86
3:A:611:ASN:HD22	3:A:611:ASN:H	1.18	0.85
1:B:17:DA:H2''	1:B:18:DT:H5''	1.57	0.85
3:A:724:LEU:N	3:A:724:LEU:C	2.34	0.85
1:B:10:DT:H2''	4:B:991:TTG:O19	1.77	0.84
3:A:640:PHE:N	3:A:640:PHE:C	2.36	0.83
3:A:638:LYS:O	3:A:639:THR:OG1	2.03	0.77
2:C:110:DT:C2'	2:C:111:DC:H5''	2.16	0.75
2:C:110:DT:H2''	2:C:111:DC:C5'	2.17	0.74
2:C:115:DG:H2'	2:C:116:DT:C7	2.17	0.73
1:B:17:DA:C2'	1:B:18:DT:H5''	2.17	0.73
3:A:640:PHE:H	3:A:641:GLU:H	1.34	0.73
3:A:599:GLN:HE22	3:A:765:PHE:H	1.35	0.72
3:A:578:GLN:HE22	3:A:583:GLY:H	1.36	0.72
3:A:637:PRO:O	3:A:640:PHE:N	2.22	0.72
3:A:639:THR:C	3:A:641:GLU:H	1.98	0.71
3:A:419:ASN:HD22	3:A:419:ASN:N	1.89	0.70
1:B:17:DA:H2''	1:B:18:DT:C5'	2.21	0.69
2:C:106:DT:H2'	2:C:107:DT:H72	1.75	0.69
1:B:1:DA:H2'	1:B:2:DA:H8	1.56	0.67
1:B:19:DT:H5''	6:B:2068:HOH:O	1.94	0.67
1:B:18:DT:H4'	6:B:2030:HOH:O	1.94	0.66
3:A:419:ASN:H	3:A:419:ASN:ND2	1.92	0.66
3:A:341:CYS:SG	3:A:429:LEU:HD21	2.36	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:611:ASN:H	3:A:611:ASN:ND2	1.93	0.64
3:A:234:LEU:HD11	3:A:305:MET:HE3	1.79	0.64
2:C:119:DT:H2''	2:C:120:DT:H5''	1.80	0.63
2:C:120:DT:H2'	2:C:121:DT:H72	1.80	0.63
2:C:112:DC:H5'	6:A:2221:HOH:O	1.97	0.63
6:B:2112:HOH:O	2:C:105:DA:H2	1.83	0.62
2:C:105:DA:H1'	2:C:106:DT:H5''	1.81	0.61
3:A:626:VAL:HG11	3:A:724:LEU:HD21	1.83	0.60
3:A:578:GLN:NE2	3:A:583:GLY:H	1.98	0.59
1:B:11:DG:C2'	1:B:12:DG:C8	2.85	0.59
3:A:639:THR:C	3:A:640:PHE:CA	2.77	0.58
3:A:474:GLN:OE1	3:A:566:ASP:O	2.23	0.57
1:B:4:DA:H1'	1:B:5:DA:H5''	1.87	0.56
1:B:21:DT:H2'	1:B:22:DT:H71	1.87	0.56
1:B:20:DT:H3'	6:B:2209:HOH:O	2.04	0.56
3:A:492:GLU:H	3:A:492:GLU:CD	2.14	0.56
1:B:10:DT:C2'	4:B:991:TTG:O19	2.51	0.55
1:B:11:DG:H2''	1:B:12:DG:C8	2.42	0.55
2:C:109:DT:H2'	2:C:110:DT:H72	1.88	0.54
1:B:11:DG:H2'	1:B:12:DG:C8	2.42	0.54
3:A:611:ASN:HD22	3:A:611:ASN:N	1.98	0.53
1:B:13:DA:OP1	3:A:634:ARG:HG3	2.09	0.52
3:A:485:LEU:HD11	3:A:541:VAL:HG11	1.90	0.52
1:B:17:DA:H5''	6:A:2291:HOH:O	2.10	0.52
2:C:104:DA:H1'	6:C:2002:HOH:O	2.08	0.51
3:A:367:HIS:HD2	3:A:369:LYS:H	1.59	0.51
3:A:479:LEU:HD21	3:A:577:LEU:HD21	1.93	0.51
1:B:3:DA:C2	1:B:4:DA:C4	2.99	0.51
1:B:2:DA:N6	6:B:2118:HOH:O	2.42	0.50
1:B:8:DC:H3'	6:B:2000:HOH:O	2.11	0.50
3:A:723:PTR:O	3:A:724:LEU:HA	2.09	0.50
2:C:106:DT:H6	2:C:106:DT:H5'	1.77	0.49
1:B:4:DA:H2''	1:B:5:DA:H5'	1.94	0.49
1:B:11:DG:O5'	6:B:2319:HOH:O	1.79	0.49
2:C:119:DT:C2'	2:C:120:DT:H5''	2.41	0.49
2:C:121:DT:H2'	2:C:122:DT:H72	1.94	0.49
1:B:11:DG:H2'	1:B:12:DG:N7	2.28	0.48
3:A:638:LYS:C	3:A:639:THR:HG1	2.07	0.48
3:A:345:ASN:ND2	6:A:2316:HOH:O	2.34	0.47
1:B:17:DA:H1'	6:B:2195:HOH:O	2.15	0.47
3:A:745:ASN:H	3:A:748:GLN:NE2	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:DA:H1'	1:B:3:DA:C8	2.50	0.46
1:B:20:DT:C2'	1:B:21:DT:H72	2.45	0.46
3:A:382:ILE:HG23	3:A:414:VAL:HG13	1.96	0.46
3:A:639:THR:C	3:A:641:GLU:N	2.63	0.46
1:B:12:DG:H5'	4:B:991:TTG:H311	1.98	0.46
3:A:241:TYR:HB2	3:A:301:ASP:HB3	1.98	0.45
2:C:101:DA:H2''	2:C:102:DA:C8	2.51	0.45
3:A:724:LEU:HA	3:A:724:LEU:HD23	1.78	0.45
3:A:599:GLN:NE2	3:A:765:PHE:H	2.10	0.44
3:A:430:ASN:ND2	3:A:432:SER:H	2.16	0.43
3:A:541:VAL:HA	3:A:542:PRO:HD3	1.88	0.43
1:B:19:DT:C6	1:B:20:DT:H72	2.53	0.43
1:B:20:DT:H2'	1:B:21:DT:H72	2.01	0.43
3:A:683:VAL:O	3:A:687:LYS:HG2	2.19	0.42
1:B:18:DT:C6	1:B:19:DT:H72	2.55	0.42
3:A:505:CYS:SG	3:A:573:LEU:HD22	2.60	0.42
1:B:1:DA:C6	1:B:2:DA:C6	3.07	0.41
3:A:723:PTR:CD1	3:A:723:PTR:N	2.83	0.41
3:A:434:ARG:NH1	6:A:2103:HOH:O	2.44	0.41
2:C:109:DT:P	6:C:2050:HOH:O	2.78	0.41
2:C:106:DT:H2'	2:C:107:DT:C7	2.47	0.41
3:A:724:LEU:C	3:A:724:LEU:H	2.22	0.41

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
3	A	562/565 (100%)	541 (96%)	17 (3%)	4 (1%)	18 23

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	344	ASP
3	A	638	LYS
3	A	759	ALA
3	A	637	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	
3	A	508/508 (100%)	482 (95%)	26 (5%)	21	32

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	210	ARG
3	A	264	LEU
3	A	335	LEU
3	A	337	GLU
3	A	348	GLU
3	A	356	GLU
3	A	375	ARG
3	A	419	ASN
3	A	430	ASN
3	A	435	ILE
3	A	439	LYS
3	A	451	LYS
3	A	461	TYR
3	A	470	MET
3	A	479	LEU
3	A	493	LYS
3	A	518	LEU
3	A	557	ASN
3	A	569	ASN
3	A	611	ASN
3	A	617	LEU
3	A	629	LEU
3	A	637	PRO

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Mol	Chain	Res	Type
3	A	679	LYS
3	A	699	MET
3	A	747	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	277	ASN
3	A	331	ASN
3	A	366	ASN
3	A	367	HIS
3	A	419	ASN
3	A	421	GLN
3	A	430	ASN
3	A	442	GLN
3	A	459	ASN
3	A	474	GLN
3	A	515	HIS
3	A	569	ASN
3	A	578	GLN
3	A	593	ASN
3	A	599	GLN
3	A	600	GLN
3	A	611	ASN
3	A	620	ASN
3	A	631	ASN
3	A	633	GLN
3	A	657	GLN
3	A	697	GLN
3	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 ⓘ

1 non-standard protein/DNA/RNA residue 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
3	PTR	A	723	3,1	15,16,17	1.29	2 (13%)	17,22,24	0.91	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
3	PTR	A	723	3,1	-	1/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	723	PTR	CE1-CD1	2.46	1.42	1.38
3	A	723	PTR	CE2-CD2	2.17	1.42	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	723	PTR	O2P-P-O1P	2.08	118.93	110.83

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	723	PTR	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	723	PTR	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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	$\# Z > 2$
5	TTC	B	990	-	31,35,35	2.42	13 (41%)	35,55,55	2.64	10 (28%)
4	TTG	B	991	-	33,35,35	3.76	14 (42%)	39,54,54	2.60	12 (30%)

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	TTC	B	990	-	-	2/7/32/32	0/5/5/5
4	TTG	B	991	-	-	6/15/29/29	0/4/4/4

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	991	TTG	C21-C16	15.63	1.65	1.51
4	B	991	TTG	C14-C15	6.33	1.59	1.44
4	B	991	TTG	C11-N12	6.02	1.53	1.47
4	B	991	TTG	C9-C13	-5.04	1.40	1.46
5	B	990	TTC	C2-C1	4.94	1.43	1.38
5	B	990	TTC	C27-C1	4.67	1.56	1.51
4	B	991	TTG	C15-C16	4.64	1.43	1.36
5	B	990	TTC	C11-N12	4.58	1.51	1.47
5	B	990	TTC	C9-C13	-4.18	1.41	1.46
5	B	990	TTC	C14-C15	4.04	1.54	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	991	TTG	C2-C1	4.00	1.42	1.38
5	B	990	TTC	O22-C20	-3.77	1.29	1.34
4	B	991	TTG	C27-C1	3.52	1.54	1.51
4	B	991	TTG	C4-C3	3.34	1.43	1.36
4	B	991	TTG	C4-C5	-3.33	1.36	1.41
5	B	990	TTC	C5-N10	3.19	1.42	1.37
4	B	991	TTG	C5-N10	3.14	1.42	1.37
5	B	990	TTC	O22-C19	2.90	1.50	1.45
5	B	990	TTC	C4-C3	2.42	1.41	1.36
4	B	991	TTG	C14-N12	-2.40	1.36	1.40
5	B	990	TTC	C13-N12	-2.28	1.35	1.40
4	B	991	TTG	C19-C15	2.25	1.55	1.51
4	B	991	TTG	C13-N12	-2.17	1.35	1.40
5	B	990	TTC	C9-N10	2.16	1.35	1.32
5	B	990	TTC	C17-C13	2.06	1.41	1.37
4	B	991	TTG	C29-N28	2.03	1.52	1.46
5	B	990	TTC	C7-C6	2.01	1.46	1.42

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	990	TTC	C8-C9-N10	-8.09	121.03	125.61
5	B	990	TTC	C13-C9-N10	6.94	129.67	125.32
4	B	991	TTG	C17-C16-C15	-6.92	112.86	120.25
4	B	991	TTG	C8-C9-N10	-6.91	121.70	125.61
4	B	991	TTG	C13-C9-N10	6.75	129.55	125.32
5	B	990	TTC	C17-C16-C15	-5.64	114.22	120.25
4	B	991	TTG	C9-C13-N12	4.64	109.69	107.06
4	B	991	TTG	C27-C1-C2	-4.48	116.10	119.85
5	B	990	TTC	C13-N12-C14	-4.43	120.44	124.57
5	B	990	TTC	C9-C13-N12	4.07	109.37	107.06
4	B	991	TTG	C3-C2-C1	-3.63	119.13	121.39
4	B	991	TTG	C13-C17-C16	3.52	125.62	119.09
5	B	990	TTC	C11-C8-C9	-3.42	107.02	109.56
4	B	991	TTG	C13-N12-C14	-3.20	121.58	124.57
4	B	991	TTG	C1-C27-N28	3.07	117.80	112.52
5	B	990	TTC	C27-C1-C2	-2.93	117.40	119.85
4	B	991	TTG	C27-C1-C6	2.90	124.47	120.96
5	B	990	TTC	C13-C17-C16	2.44	123.62	119.09
5	B	990	TTC	C27-C1-C6	2.41	123.88	120.96
4	B	991	TTG	C11-C8-C9	-2.17	107.95	109.56
5	B	990	TTC	C4-C5-C6	2.13	121.43	119.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	991	TTG	O22-C20-O23	-2.04	117.33	123.86

There are no chirality outliers.

All (8) torsion outliers are listed below:

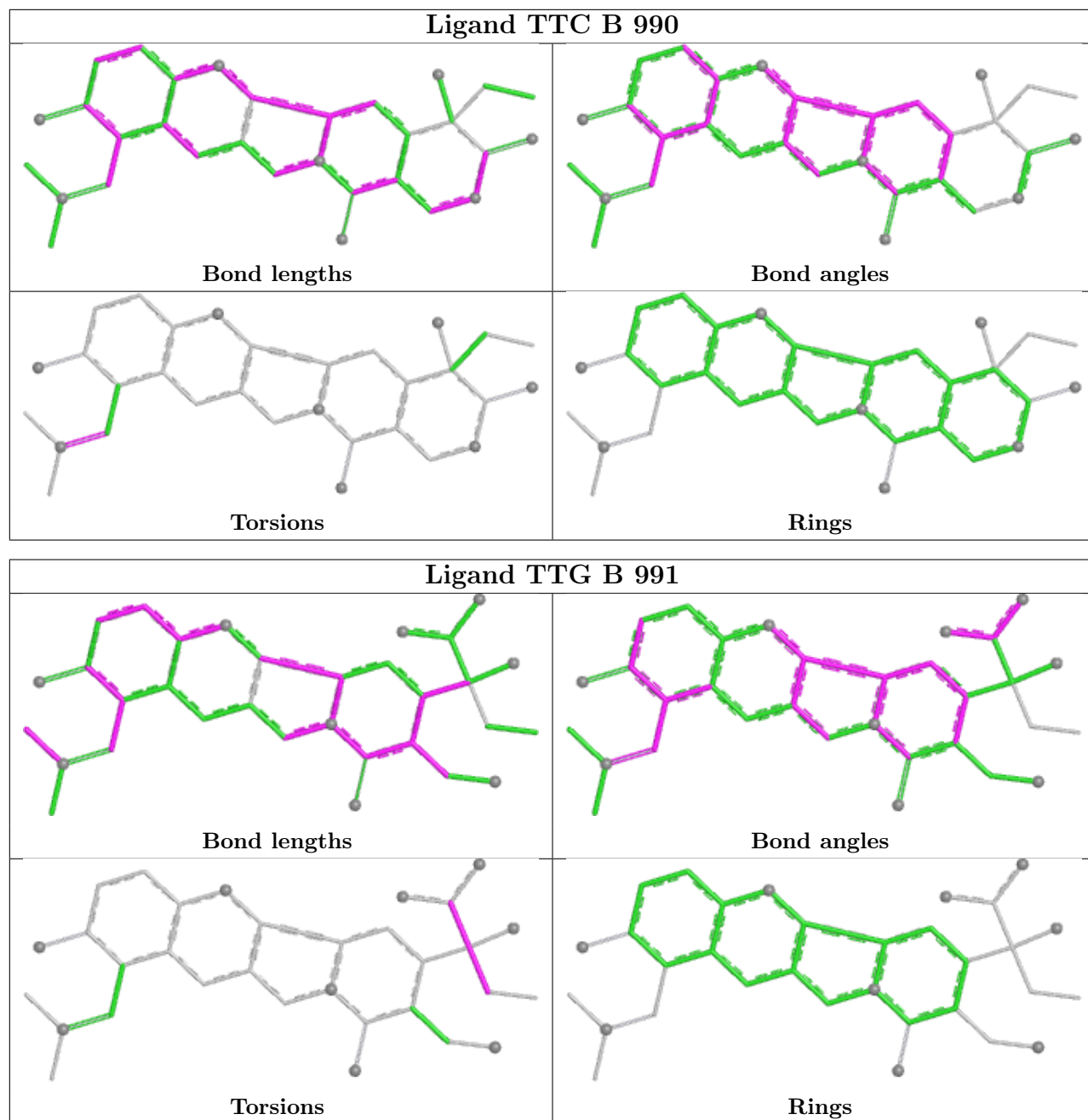
Mol	Chain	Res	Type	Atoms
4	B	991	TTG	O23-C20-C21-C25
4	B	991	TTG	O22-C20-C21-C25
4	B	991	TTG	O22-C20-C21-O24
5	B	990	TTC	C1-C27-N28-C30
5	B	990	TTC	C1-C27-N28-C29
4	B	991	TTG	O24-C21-C25-C31
4	B	991	TTG	C20-C21-C25-C31
4	B	991	TTG	O23-C20-C21-O24

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	991	TTG	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 [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.