



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 03:18 am BST

PDB ID : 1K4T
Title : HUMAN DNA TOPOISOMERASE I (70 KDA) IN COMPLEX WITH THE POISON TOPOTECAN AND COVALENT COMPLEX WITH A 22 BASE PAIR DNA DUPLEX
Authors : Staker, B.L.; Hjerrild, K.; Feese, M.D.; Behnke, C.A.; Burgin Jr., A.B.; Stewart, L.J.
Deposited on : 2001-10-08
Resolution : 2.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

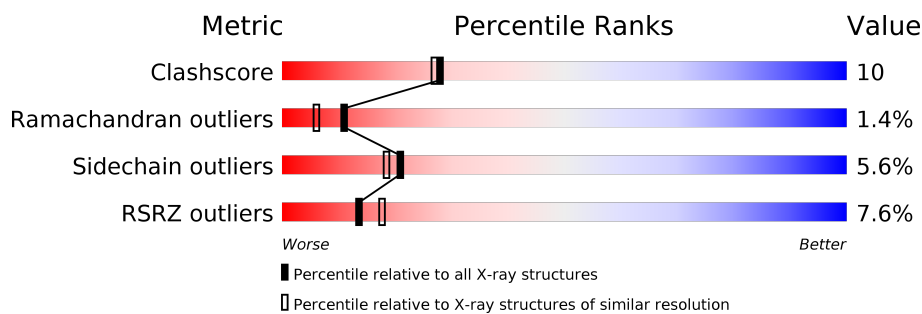
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 on 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	B	10	<div> <div>10%</div> <div>40%</div> <div>60%</div> </div>
2	C	12	<div> <div>8%</div> <div>50%</div> <div>50%</div> </div>
3	D	22	<div> <div>9%</div> <div>41%</div> <div>55%</div> <div>5%</div> </div>
4	A	592	<div> <div>7%</div> <div>77%</div> <div>17%</div> <div>5%</div> </div>

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5883 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			

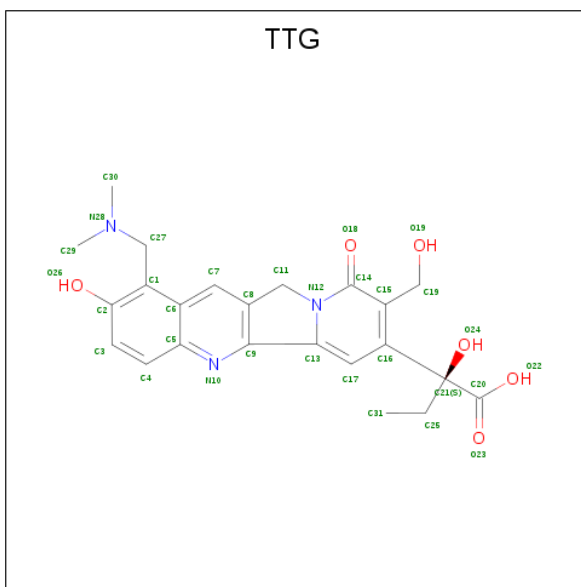
- Molecule 4 is a protein called DNA topoisomerase I.

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:

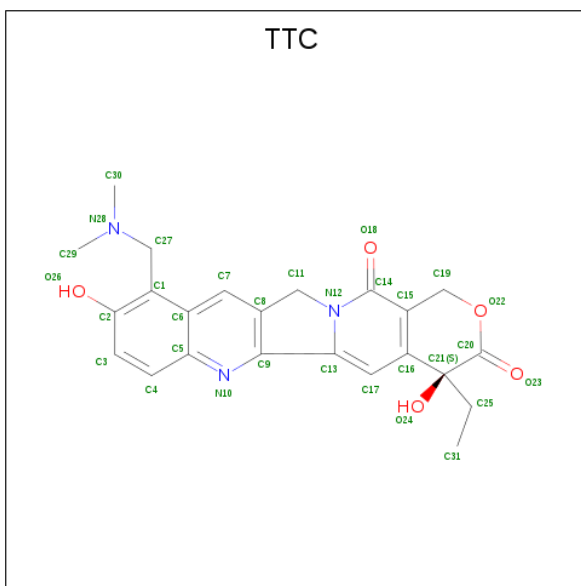
Chain	Residue	Modelled	Actual	Comment	Reference
A	723	PTR	TYR	MODIFIED RESIDUE	UNP P11387

- Molecule 5 is 2-(1-DIMETHYLAMINOMETHYL-2-HYDROXY-8-HYDROXYMETHYL-9-OXO-9,11-DIHYDRO-INDOLIZINO[1,2-B]QUINOLIN-7-YL)-2-HYDROXY-BUTYRIC ACID (three-letter code: TTG) (formula: C₂₃H₂₅N₃O₆).



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

- Molecule 6 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 (three-letter code: TTC) (formula: $C_{23}H_{23}N_3O_5$).

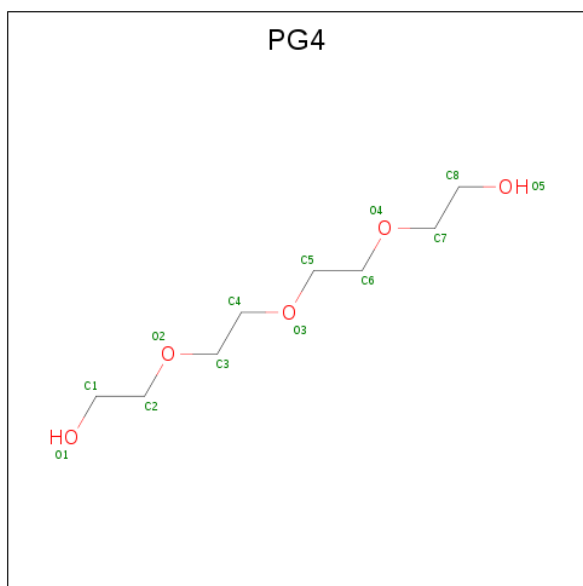


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	N	O	0	1
			31	23	3	5		

- Molecule 7 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Hg 1 1	0	0

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 13 8 5	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	18	Total O 18 18	0	0
9	C	8	Total O 8 8	0	0
9	D	26	Total O 26 26	0	0
9	A	175	Total O 175 175	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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(*AP*AP*AP*AP*AP*GP*AP*CP*TP*T)-3'



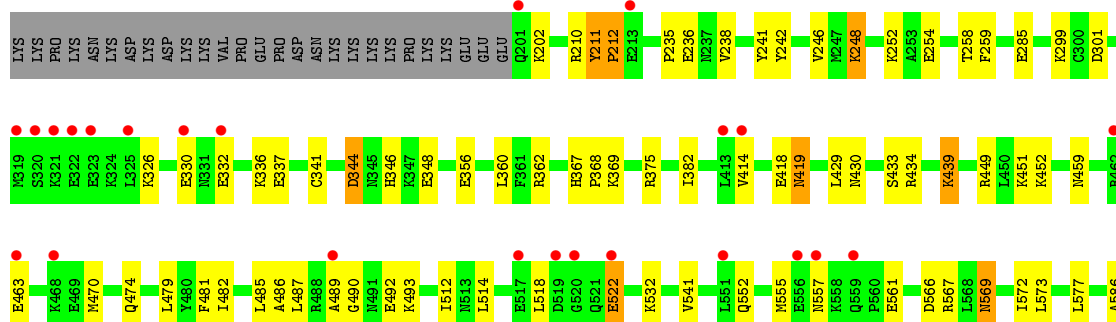
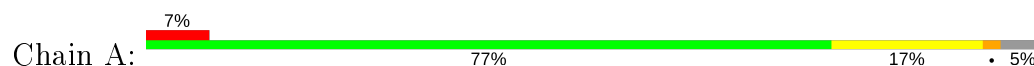
- Molecule 2: 5'-D(*(TGP)P*GP*AP*AP*AP*AP*AP*TP*TP*TP*TP*T)-3'

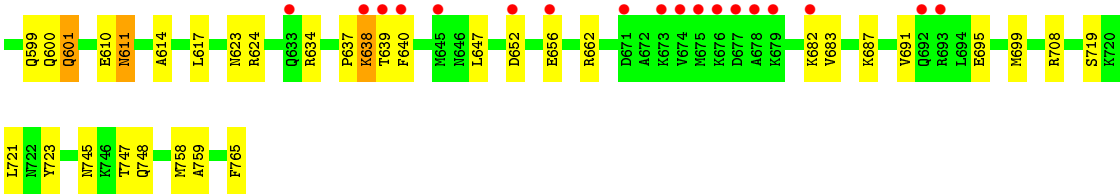


- Molecule 3: 5'-D(*AP*AP*AP*AP*AP*TP*TP*TP*TP*TP*CP*CP*AP*AP*GP*TP*CP*TP*TP*TP*TP*T)-3'



- Molecule 4: DNA topoisomerase I





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.09 Å 116.26 Å 75.22 Å 90.00° 94.16° 90.00°	Depositor
Resolution (Å)	19.89 – 2.10 19.89 – 1.99	Depositor EDS
% Data completeness (in resolution range)	80.2 (19.89-2.10) 65.8 (19.89-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 1.99 Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.229 , 0.269 0.226 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5883	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TGP, HG, PG4, TTC, TTG, 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	0.39	0/229	0.69	0/351
2	C	0.32	0/254	0.68	0/390
3	D	0.40	0/494	0.74	0/760
4	A	0.36	0/4770	0.57	0/6401
All	All	0.36	0/5747	0.60	0/7902

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	112	DC	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	203	0	112	9	0
2	C	246	0	138	12	0
3	D	443	0	255	22	0
4	A	4687	0	4720	65	0
5	C	32	0	17	4	0
6	D	31	0	19	0	0
7	A	1	0	0	0	0
8	A	13	0	18	0	0
9	A	175	0	0	4	0
9	B	18	0	0	0	0
9	C	8	0	0	3	0
9	D	26	0	0	1	0
All	All	5883	0	5279	107	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 (107) 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:C8	1.93	1.04
2:C:17:DA:H2''	2:C:18:DT:H5''	1.45	0.98
3:D:110:DT:H2''	3:D:111:DC:H5''	1.44	0.97
4:A:599:GLN:HE22	4:A:765:PHE:H	1.03	0.97
4:A:367:HIS:HD2	4:A:369:LYS:H	1.19	0.89
2:C:17:DA:H2''	2:C:18:DT:C5'	2.07	0.85
1:B:10:DT:H2''	5:C:991[B]:TTG:O19	1.77	0.84
2:C:17:DA:C2'	2:C:18:DT:H5''	2.09	0.83
3:D:110:DT:H2''	3:D:111:DC:C5'	2.09	0.82
3:D:110:DT:C2'	3:D:111:DC:H5''	2.12	0.79
4:A:419:ASN:H	4:A:419:ASN:HD22	1.33	0.76
4:A:569:ASN:ND2	4:A:572:ILE:H	1.84	0.75
1:B:10:DT:C2'	5:C:991[B]:TTG:O19	2.37	0.71
3:D:115:DG:H2'	3:D:116:DT:H72	1.73	0.70
4:A:601:GLN:HE21	4:A:601:GLN:HA	1.56	0.69
3:D:119:DT:H2''	3:D:120:DT:H5''	1.75	0.69
4:A:479:LEU:HD21	4:A:577:LEU:HD21	1.77	0.67
4:A:599:GLN:HE22	4:A:765:PHE:N	1.86	0.66
4:A:341:CYS:SG	4:A:429:LEU:HD21	2.37	0.65
4:A:419:ASN:N	4:A:419:ASN:HD22	1.95	0.64
4:A:599:GLN:NE2	4:A:765:PHE:H	1.85	0.63
4:A:241:TYR:HB2	4:A:301:ASP:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:991[B]:TTG:O22	9:C:133:HOH:O	2.15	0.63
1:B:1:DA:H2'	1:B:2:DA:H8	1.61	0.62
4:A:326:LYS:O	4:A:330:GLU:HG2	2.00	0.62
4:A:332:GLU:O	4:A:336:LYS:HG2	2.01	0.61
4:A:492:GLU:H	4:A:492:GLU:CD	2.03	0.60
4:A:652:ASP:O	4:A:656:GLU:HG2	2.01	0.60
1:B:4:DA:H2''	1:B:5:DA:H5'	1.84	0.59
3:D:115:DG:H2'	3:D:116:DT:C7	2.32	0.59
3:D:112:DC:H5'	9:A:1025:HOH:O	2.02	0.58
4:A:745:ASN:H	4:A:748:GLN:NE2	2.01	0.58
2:C:20:DT:C2'	2:C:21:DT:H72	2.34	0.58
3:D:119:DT:C2'	3:D:120:DT:H5''	2.34	0.58
1:B:4:DA:H1'	1:B:5:DA:H5''	1.86	0.57
3:D:120:DT:H2'	3:D:121:DT:H72	1.86	0.56
2:C:20:DT:H2'	2:C:21:DT:H72	1.87	0.56
3:D:105:DA:H1'	3:D:106:DT:H5''	1.87	0.56
4:A:569:ASN:C	4:A:569:ASN:HD22	2.09	0.56
4:A:611:ASN:H	4:A:611:ASN:ND2	2.04	0.55
2:C:20:DT:H2''	2:C:21:DT:C7	2.38	0.54
4:A:683:VAL:O	4:A:687:LYS:HG2	2.07	0.54
4:A:512:ILE:HD11	4:A:555:MET:SD	2.49	0.53
2:C:13:DA:OP1	4:A:634:ARG:HG3	2.08	0.53
4:A:474:GLN:OE1	4:A:566:ASP:O	2.27	0.53
4:A:481:PHE:HB3	4:A:487:LEU:HD12	1.91	0.53
4:A:569:ASN:HD21	4:A:572:ILE:HG13	1.74	0.52
4:A:624:ARG:HD2	9:A:997:HOH:O	2.09	0.52
2:C:20:DT:C2'	2:C:21:DT:C7	2.87	0.52
3:D:106:DT:H2'	3:D:107:DT:H72	1.90	0.52
1:B:9:DT:OP2	4:A:439:LYS:HG2	2.10	0.51
4:A:348:GLU:OE1	4:A:433:SER:HB2	2.11	0.51
4:A:449:ARG:O	4:A:452:LYS:HG2	2.11	0.50
3:D:105:DA:H2''	3:D:106:DT:H5''	1.92	0.50
2:C:11:TGP:H5'	9:C:28:HOH:O	2.11	0.50
4:A:482:ILE:O	4:A:486:ALA:HA	2.12	0.49
2:C:20:DT:H3'	9:C:202:HOH:O	2.12	0.49
3:D:106:DT:H6	3:D:106:DT:H5'	1.78	0.49
3:D:105:DA:C2'	3:D:106:DT:H5''	2.43	0.49
4:A:259:PHE:HB3	4:A:360:LEU:HG	1.95	0.48
4:A:235:PRO:HG2	4:A:238:VAL:HG23	1.95	0.48
3:D:121:DT:H2'	3:D:122:DT:H72	1.94	0.48
1:B:4:DA:H2''	1:B:5:DA:C5'	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:DA:C2'	1:B:2:DA:C8	2.83	0.47
4:A:346:HIS:HD2	9:A:1047:HOH:O	1.96	0.47
3:D:121:DT:H2''	3:D:122:DT:C6	2.49	0.47
4:A:662:ARG:HG3	4:A:662:ARG:HH11	1.80	0.47
4:A:638:LYS:C	4:A:640:PHE:H	2.18	0.47
4:A:569:ASN:ND2	4:A:572:ILE:HG13	2.30	0.47
4:A:489:ALA:HB2	4:A:586:ALA:CB	2.46	0.46
3:D:121:DT:H2'	3:D:122:DT:C7	2.45	0.46
4:A:419:ASN:H	4:A:419:ASN:ND2	2.06	0.46
4:A:610:GLU:HB3	4:A:614:ALA:HB3	1.97	0.46
3:D:105:DA:H2''	3:D:106:DT:C5'	2.46	0.46
4:A:691:VAL:O	4:A:695:GLU:HG3	2.15	0.46
4:A:367:HIS:HA	4:A:368:PRO:HD3	1.80	0.45
4:A:382:ILE:HG23	4:A:414:VAL:HG13	1.99	0.45
4:A:569:ASN:HD21	4:A:572:ILE:H	1.62	0.45
4:A:344:ASP:O	9:A:1047:HOH:O	2.20	0.45
4:A:566:ASP:O	4:A:567:ARG:HB2	2.16	0.45
5:C:991[B]:TTG:O23	4:A:532:LYS:NZ	2.43	0.45
4:A:367:HIS:CD2	4:A:369:LYS:H	2.11	0.45
4:A:451:LYS:NZ	4:A:451:LYS:HB3	2.32	0.45
3:D:119:DT:H2''	3:D:120:DT:C5'	2.44	0.45
4:A:569:ASN:HD22	4:A:572:ILE:H	1.60	0.44
4:A:248:LYS:HD3	4:A:248:LYS:O	2.17	0.44
4:A:485:LEU:HD11	4:A:541:VAL:HG11	1.99	0.44
2:C:17:DA:H2''	2:C:18:DT:H5'	1.96	0.44
4:A:241:TYR:CE2	4:A:246:VAL:HG22	2.53	0.43
4:A:254:GLU:O	4:A:258:THR:HG23	2.18	0.43
4:A:758:MET:SD	4:A:758:MET:O	2.76	0.43
4:A:522:GLU:CD	4:A:522:GLU:H	2.22	0.43
2:C:20:DT:H2''	2:C:21:DT:C6	2.55	0.42
4:A:367:HIS:CD2	4:A:368:PRO:HD2	2.55	0.42
3:D:120:DT:H6	3:D:120:DT:H5'	1.84	0.42
3:D:104:DA:H1'	9:D:1010:HOH:O	2.18	0.42
4:A:514:LEU:HD13	4:A:552:GLN:HG2	2.02	0.41
4:A:647:LEU:HD11	4:A:708:ARG:HD2	2.02	0.41
3:D:111:DC:H6	3:D:111:DC:H5'	1.84	0.41
4:A:459:ASN:O	4:A:463:GLU:HG3	2.20	0.41
4:A:611:ASN:H	4:A:611:ASN:HD22	1.68	0.41
4:A:242:TYR:CE1	4:A:299:LYS:HB3	2.56	0.41
4:A:211:TYR:HA	4:A:212:PRO:HD3	1.91	0.41
4:A:252:LYS:HG2	4:A:285:GLU:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:482:ILE:HD12	4:A:573:LEU:HD21	2.03	0.40
4:A:682:LYS:HD3	4:A:682:LYS:HA	1.84	0.40
4:A:719:SER:HA	4:A:723:PTR:HD1	2.04	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%)	542 (96%)	12 (2%)	8 (1%)	11	6

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	638	LYS
4	A	490	GLY
4	A	344	ASP
4	A	637	PRO
4	A	202	LYS
4	A	759	ALA
4	A	639	THR
4	A	212	PRO

5.3.2 Protein sidechains [i](#)

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%)	476 (94%)	28 (6%)	21	18

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	210	ARG
4	A	211	TYR
4	A	236	GLU
4	A	248	LYS
4	A	337	GLU
4	A	356	GLU
4	A	362	ARG
4	A	375	ARG
4	A	418	GLU
4	A	419	ASN
4	A	430	ASN
4	A	434	ARG
4	A	439	LYS
4	A	470	MET
4	A	493	LYS
4	A	518	LEU
4	A	522	GLU
4	A	557	ASN
4	A	561	GLU
4	A	569	ASN
4	A	600	GLN
4	A	601	GLN
4	A	611	ASN
4	A	617	LEU
4	A	623	ASN
4	A	699	MET
4	A	721	LEU
4	A	747	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	277	ASN
4	A	331	ASN
4	A	346	HIS
4	A	367	HIS
4	A	419	ASN

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Mol	Chain	Res	Type
4	A	421	GLN
4	A	430	ASN
4	A	459	ASN
4	A	460	GLN
4	A	474	GLN
4	A	513	ASN
4	A	515	HIS
4	A	569	ASN
4	A	599	GLN
4	A	601	GLN
4	A	620	ASN
4	A	631	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	18,21,25	1.16	2 (11%)	19,31,38	2.65	5 (26%)
4	PTR	A	723	1,4	15,16,17	0.87	0	19,22,24	0.86	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TGP	C	11	3,2	-	1/2/18/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PTR	A	723	1,4	-	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)
2	C	11	TGP	C6-N1	3.89	1.39	1.33
2	C	11	TGP	C8-N7	-2.04	1.31	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	11	TGP	C5-C6-N1	-8.56	111.72	123.43
2	C	11	TGP	C6-N1-C2	5.76	125.09	115.93
2	C	11	TGP	C2-N3-C4	-3.00	111.92	115.36
2	C	11	TGP	N3-C2-N1	-2.60	123.75	127.22
2	C	11	TGP	C6-C5-C4	-2.12	118.77	120.80

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	723	PTR	CE2-CZ-OH-P
2	C	11	TGP	O4'-C4'-C5'-S5'

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	11	TGP	1	0
4	A	723	PTR	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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	TTG	C	991[B]	-	30,35,35	2.91	7 (23%)	32,54,54	2.58	7 (21%)
8	PG4	A	901	-	12,12,12	0.45	0	11,11,11	0.28	0
6	TTC	D	990[A]	-	34,35,35	2.62	11 (32%)	35,55,55	1.88	9 (25%)

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	TTG	C	991[B]	-	-	1/15/29/29	0/4/4/4
8	PG4	A	901	-	-	8/10/10/10	-
6	TTC	D	990[A]	-	-	2/7/32/32	0/5/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	990[A]	TTC	O24-C21	-9.67	1.32	1.42
5	C	991[B]	TTG	C9-N10	8.27	1.45	1.32
5	C	991[B]	TTG	C14-C15	7.81	1.58	1.41
5	C	991[B]	TTG	C27-C1	7.70	1.56	1.51
6	D	990[A]	TTC	O23-C20	4.89	1.32	1.20
5	C	991[B]	TTG	C13-N12	4.46	1.45	1.36
6	D	990[A]	TTC	C13-C9	-3.84	1.40	1.47
6	D	990[A]	TTC	C27-C1	3.61	1.53	1.51
6	D	990[A]	TTC	C9-C8	3.58	1.47	1.41
6	D	990[A]	TTC	O22-C20	3.54	1.38	1.34
6	D	990[A]	TTC	O18-C14	3.36	1.32	1.24
5	C	991[B]	TTG	C5-N10	-3.29	1.32	1.37
6	D	990[A]	TTC	C4-C5	-3.07	1.36	1.41
6	D	990[A]	TTC	C15-C16	2.92	1.43	1.38
5	C	991[B]	TTG	C2-C1	2.69	1.41	1.38
6	D	990[A]	TTC	C13-N12	-2.38	1.31	1.36
6	D	990[A]	TTC	C4-C3	2.14	1.41	1.36
5	C	991[B]	TTG	C6-C5	2.07	1.45	1.42

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	991[B]	TTG	C13-C9-N10	8.11	130.00	118.19
5	C	991[B]	TTG	C17-C13-C9	5.28	136.19	124.70
5	C	991[B]	TTG	C27-C1-C2	-5.10	115.49	119.86
5	C	991[B]	TTG	C15-C14-N12	-5.06	114.73	120.23
5	C	991[B]	TTG	C8-C9-N10	-4.70	120.70	125.87
6	D	990[A]	TTC	C13-C9-N10	4.50	124.74	118.19
6	D	990[A]	TTC	C27-C1-C2	-4.26	116.21	119.86
5	C	991[B]	TTG	C27-C1-C6	3.89	125.66	120.96
6	D	990[A]	TTC	C17-C13-N12	3.65	122.12	119.63
5	C	991[B]	TTG	C13-C17-C16	3.59	125.27	120.38
6	D	990[A]	TTC	C17-C16-C15	-3.47	111.81	118.67
6	D	990[A]	TTC	C27-C1-C6	3.07	124.67	120.96
6	D	990[A]	TTC	C4-C5-C6	3.01	122.58	119.13
6	D	990[A]	TTC	C4-C5-N10	-2.81	114.42	118.69
6	D	990[A]	TTC	C11-C8-C7	2.68	135.94	127.26
6	D	990[A]	TTC	C13-C17-C16	2.34	123.56	120.38

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	990[A]	TTC	C1-C27-N28-C30
6	D	990[A]	TTC	C1-C27-N28-C29
8	A	901	PG4	O2-C3-C4-O3
8	A	901	PG4	O3-C5-C6-O4
8	A	901	PG4	O1-C1-C2-O2
8	A	901	PG4	C6-C5-O3-C4
8	A	901	PG4	C1-C2-O2-C3
8	A	901	PG4	C3-C4-O3-C5
8	A	901	PG4	C5-C6-O4-C7
5	C	991[B]	TTG	C17-C16-C21-C25
8	A	901	PG4	O4-C7-C8-O5

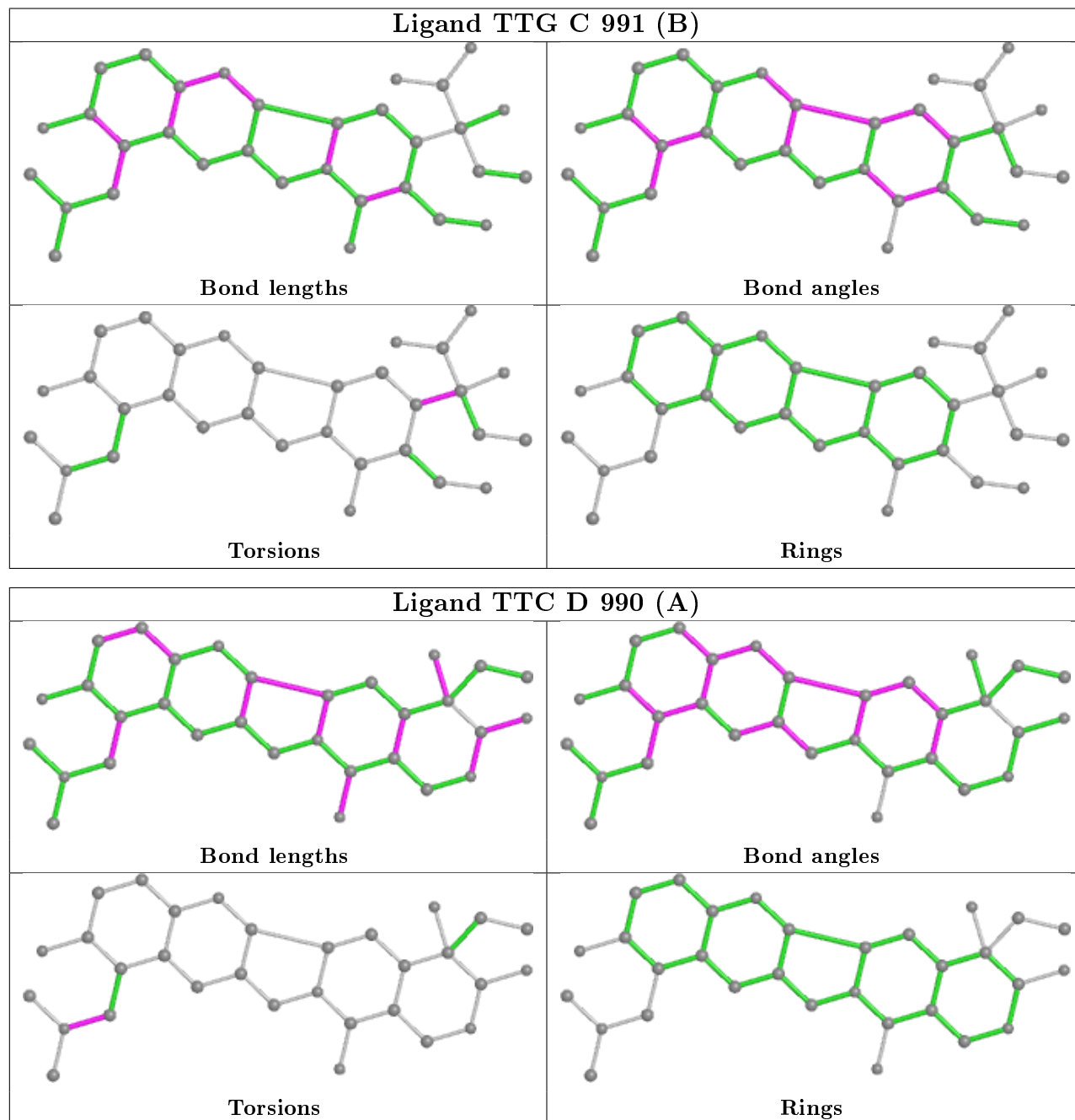
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	991[B]	TTG	4	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

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	B	10/10 (100%)	0.26	1 (10%) 7 9	17, 24, 60, 68	0
2	C	11/12 (91%)	0.56	1 (9%) 9 12	32, 46, 70, 76	0
3	D	22/22 (100%)	0.36	2 (9%) 9 12	15, 42, 61, 70	0
4	A	564/592 (95%)	0.49	42 (7%) 14 18	12, 36, 75, 103	0
All	All	607/636 (95%)	0.48	46 (7%) 13 18	12, 36, 75, 103	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	675	MET	7.2
4	A	638	LYS	6.0
4	A	639	THR	4.7
4	A	321	LYS	4.0
4	A	677	ASP	3.9
4	A	693	ARG	3.6
4	A	674	VAL	3.5
4	A	414	VAL	3.5
4	A	678	ALA	3.4
4	A	682	LYS	3.4
4	A	673	LYS	3.3
4	A	213	GLU	3.2
4	A	557	ASN	3.1
4	A	519	ASP	3.0
4	A	676	LYS	2.9
4	A	640	PHE	2.9
4	A	645	MET	2.9
4	A	325	LEU	2.9
4	A	322	GLU	2.8
4	A	413	LEU	2.7
4	A	633	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
4	A	320	SER	2.6
4	A	319	MET	2.6
4	A	656	GLU	2.5
4	A	692	GLN	2.5
4	A	652	ASP	2.5
4	A	323	GLU	2.5
4	A	679	LYS	2.5
4	A	517	GLU	2.4
4	A	201	GLN	2.4
4	A	468	LYS	2.4
4	A	520	GLY	2.3
2	C	22	DT	2.3
4	A	559	GLN	2.3
3	D	101	DA	2.3
4	A	330	GLU	2.3
4	A	522	GLU	2.3
4	A	462	ARG	2.2
1	B	1	DA	2.2
4	A	463	GLU	2.1
4	A	556	GLU	2.1
4	A	671	ASP	2.1
4	A	551	LEU	2.1
3	D	103	DA	2.0
4	A	332	GLU	2.0
4	A	489	ALA	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	TGP	C	11	19/23	0.97	0.10	16,24,48,58	0
4	PTR	A	723	16/17	0.98	0.14	21,24,28,36	0

6.3 Carbohydrates [i](#)

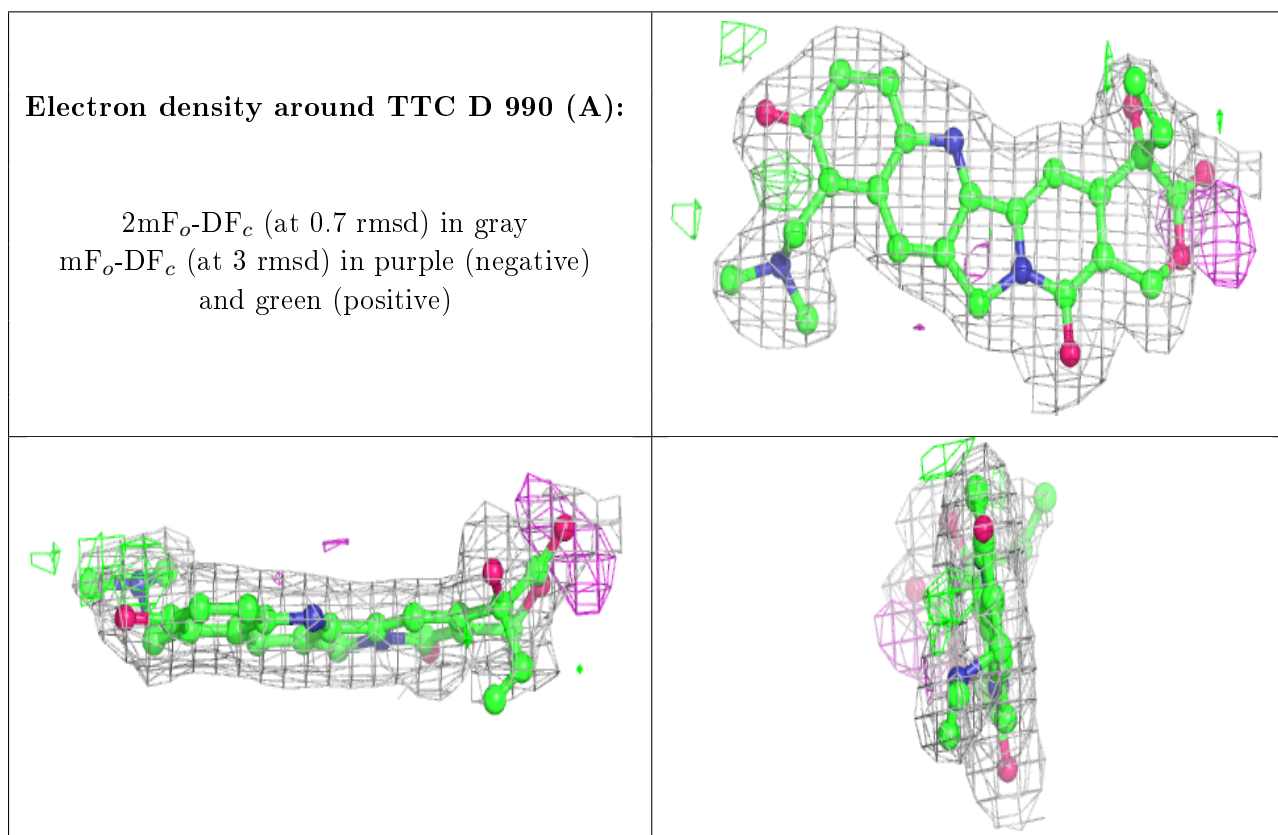
There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

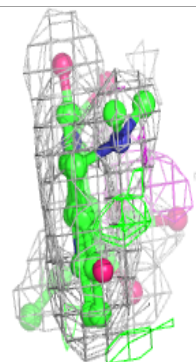
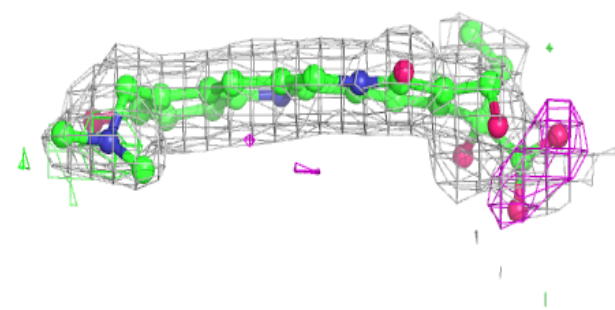
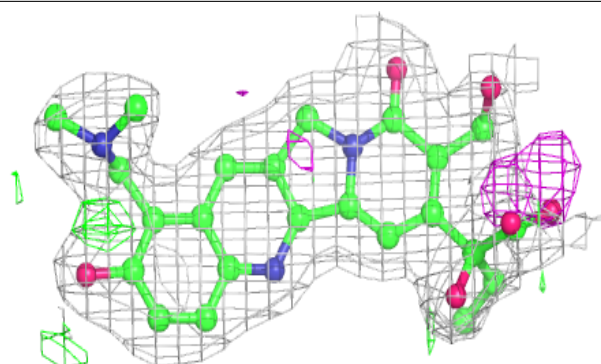
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	PG4	A	901	13/13	0.65	0.27	48,56,63,63	0
7	HG	A	900	1/1	0.89	0.07	75,75,75,75	1
6	TTC	D	990[A]	31/31	0.96	0.11	13,22,33,37	31
5	TTG	C	991[B]	32/32	0.96	0.12	13,23,33,37	32

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around TTG C 991 (B):

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.