



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 01:54 PM GMT

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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

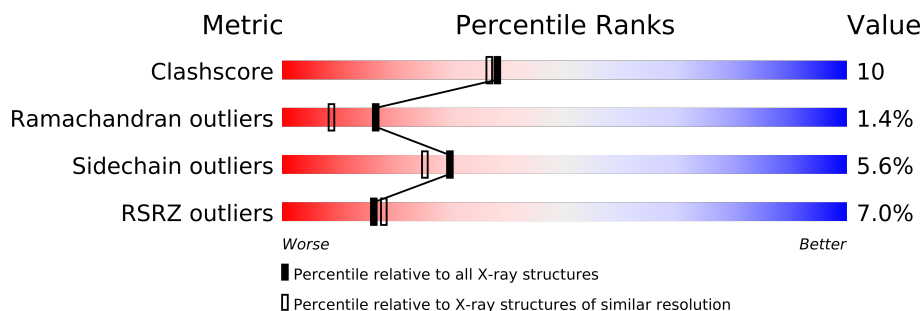
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	B	10	
2	C	12	
3	D	22	
4	A	592	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
8	PG4	A	901	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5883 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

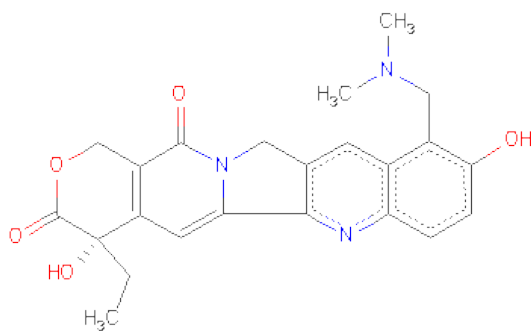
- Molecule 4 is a protein called DNA topoisomerase I.

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 (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: C₂₃H₂₃N₃O₅).

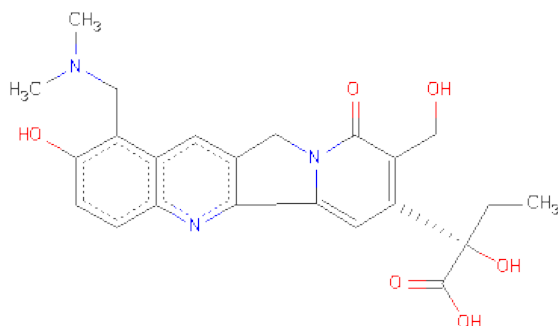


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	N	O	0	1
			31	23	3	5		

- Molecule 6 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

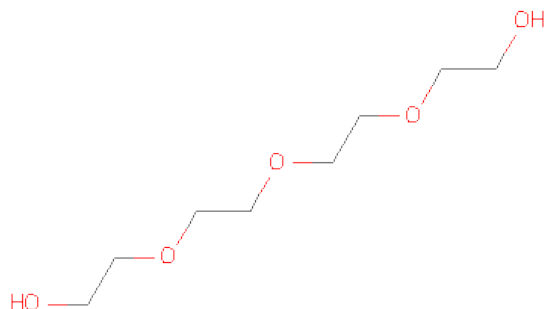
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Hg	0	0
			1	1		

- Molecule 7 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
7	C	1	Total	C	N	O	0	1
			32	23	3	6		

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



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

- Molecule 9 is water.

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

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 errors 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.

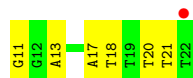
- Molecule 1: 5'-D(*AP*AP*AP*AP*AP*GP*AP*CP*TP*T)-3'

Chain B: 



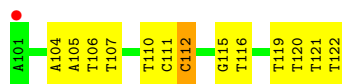
- Molecule 2: 5'-D(*(TGP)P*GP*AP*AP*AP*AP*AP*TP*TP*TP*TP*T)-3'

Chain C: 



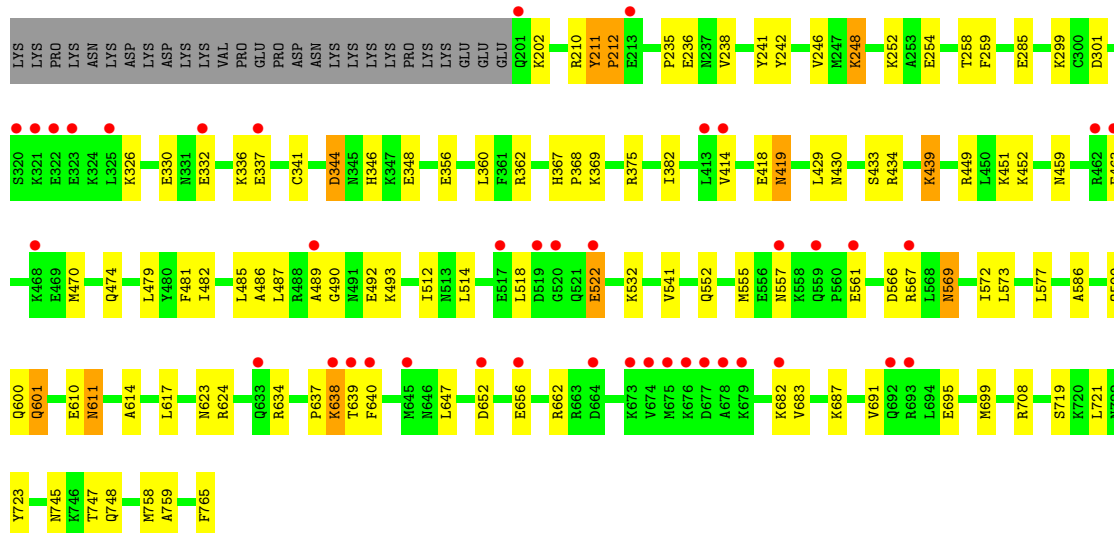
- Molecule 3: 5'-D(*AP*AP*AP*AP*AP*TP*TP*TP*TP*TP*CP*CP*AP*AP*GP*TP*CP*TP*TP*TP*TP*T)-3'

Chain D: 



- Molecule 4: DNA topoisomerase I

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.09Å 116.26Å 75.22Å 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	2.65 (at 1.99Å)	Xtriage
Refinement program	CNX 2000.1	Depositor
R, R_{free}	0.229 , 0.269 0.228 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 29.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 45708 reflections (0.002%)	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 5.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the

Clashes column.

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	D	31	0	19	0	0
6	A	1	0	0	0	0
7	C	32	0	17	4	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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (107) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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''	7: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'	7: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
7:C:991[B]:TTG:O22	9:C:133:HOH:O	2.15	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:241:TYR:HB2	4:A:301:ASP:HB3	1.81	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
3:D:115:DG:H2'	3:D:116:DT:C7	2.32	0.59
1:B:4:DA:H2''	1:B:5:DA:H5'	1.84	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
3:D:119:DT:C2'	3:D:120:DT:H5''	2.34	0.58
2:C:20:DT:C2'	2:C:21:DT:H72	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
2:C:13:DA:OP1	4:A:634:ARG:HG3	2.08	0.53
4:A:512:ILE:HD11	4:A:555:MET:SD	2.49	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
3:D:105:DA:H2''	3:D:106:DT:H5''	1.92	0.50
4:A:449:ARG:O	4:A:452:LYS:HG2	2.11	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
1:B:1:DA:C2'	1:B:2:DA:C8	2.83	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:121:DT:H2''	3:D:122:DT:C6	2.49	0.47
4:A:346:HIS:HD2	9:A:1047:HOH:O	1.96	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
3:D:121:DT:H2'	3:D:122:DT:C7	2.45	0.46
4:A:489:ALA:HB2	4:A:586:ALA:CB	2.46	0.46
4:A:419:ASN:ND2	4:A:419:ASN:H	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:569:ASN:HD21	4:A:572:ILE:H	1.62	0.45
4:A:382:ILE:HG23	4:A:414:VAL:HG13	1.99	0.45
7:C:991[B]:TTG:O23	4:A:532:LYS:NZ	2.43	0.45
4:A:566:ASP:O	4:A:567:ARG:HB2	2.16	0.45
4:A:344:ASP:O	9:A:1047:HOH:O	2.20	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:485:LEU:HD11	4:A:541:VAL:HG11	1.99	0.44
4:A:248:LYS:HD3	4:A:248:LYS:O	2.17	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:H5'	3:D:111:DC:H6	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
4:A:482:ILE:HD12	4:A:573:LEU:HD21	2.03	0.40
4:A:719:SER:HA	4:A:723:PTR:HD1	2.04	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:682:LYS:HD3	4:A:682:LYS:HA	1.84	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%)	542 (96%)	12 (2%)	8 (1%)	16 9

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 ⓘ

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%)	30 25

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
4	A	421	GLN
4	A	430	ASN
4	A	459	ASN
4	A	460	GLN
4	A	474	GLN
4	A	513	ASN

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Mol	Chain	Res	Type
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 chains 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	$\# Z > 2$
4	PTR	A	723	1,4	16,16,17	4.43	2 (12%)	20,22,24	1.37	2 (10%)
2	TGP	C	11	3,2	21,21,25	0.74	0	27,31,38	5.60	3 (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
4	PTR	A	723	1,4	-	0/9/11/13	0/1/1/1
2	TGP	C	11	3,2	-	0/4/18/22	0/1/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	723	PTR	O-C	17.21	1.23	1.11
4	A	723	PTR	CA-C	2.55	1.53	1.48

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	11	TGP	C6-C5-N7	-28.55	130.30	134.14
4	A	723	PTR	C-CA-N	4.80	118.62	113.83
2	C	11	TGP	C6-N1-C2	3.19	125.09	119.51
4	A	723	PTR	O2P-P-O1P	2.34	118.08	110.44
2	C	11	TGP	C2-N3-C4	-2.25	111.92	115.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
8	PG4	A	901	-	12,12,12	0.45	0	11,11,11	0.28	0
7	TTG	C	991[B]	-	35,35,35	2.95	9 (25%)	52,54,54	3.05	14 (26%)
5	TTC	D	990[A]	-	35,35,35	2.48	11 (31%)	53,55,55	1.99	17 (32%)

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
8	PG4	A	901	-	-	0/10/10/10	0/0/0/0
7	TTG	C	991[B]	-	-	0/21/29/29	0/0/4/4
5	TTC	D	990[A]	-	-	0/7/32/32	0/0/5/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	990[A]	TTC	O24-C21	-9.17	1.32	1.42
7	C	991[B]	TTG	C9-N10	9.06	1.45	1.32
7	C	991[B]	TTG	C27-C1	7.92	1.56	1.51
7	C	991[B]	TTG	C14-C15	6.91	1.58	1.42
7	C	991[B]	TTG	C21-C16	5.30	1.59	1.53
5	D	990[A]	TTC	O23-C20	4.62	1.32	1.20
5	D	990[A]	TTC	O18-C14	4.28	1.32	1.24
7	C	991[B]	TTG	C13-N12	4.20	1.45	1.36
7	C	991[B]	TTG	C2-C1	3.97	1.41	1.38
5	D	990[A]	TTC	C27-C1	3.63	1.53	1.51
7	C	991[B]	TTG	C21-C20	3.56	1.61	1.52
5	D	990[A]	TTC	O22-C20	3.40	1.38	1.34
5	D	990[A]	TTC	C13-C9	-3.21	1.40	1.47
7	C	991[B]	TTG	C5-N10	-3.03	1.32	1.37
5	D	990[A]	TTC	C4-C5	-2.89	1.36	1.41
5	D	990[A]	TTC	C15-C16	2.63	1.43	1.38
5	D	990[A]	TTC	C2-C1	2.44	1.40	1.38
5	D	990[A]	TTC	C4-C3	2.16	1.41	1.36
7	C	991[B]	TTG	C6-C5	2.06	1.45	1.42
5	D	990[A]	TTC	C13-N12	-2.04	1.31	1.36

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	991[B]	TTG	C9-C13-N12	-10.98	104.92	114.16
7	C	991[B]	TTG	C13-C9-N10	10.45	130.00	117.86
7	C	991[B]	TTG	C17-C13-C9	9.00	136.19	124.37
5	D	990[A]	TTC	C13-C9-N10	5.92	124.74	117.86
5	D	990[A]	TTC	C9-C13-N12	-5.13	109.84	114.16
7	C	991[B]	TTG	C31-C25-C21	4.65	120.23	114.16
7	C	991[B]	TTG	C16-C21-C20	4.60	118.49	109.43
7	C	991[B]	TTG	C8-C9-N10	-4.25	120.70	125.92
5	D	990[A]	TTC	C11-C8-C7	4.18	135.94	129.24
5	D	990[A]	TTC	C11-C8-C9	-3.61	106.23	109.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	991[B]	TTG	C27-C1-C2	-3.59	115.49	119.87
7	C	991[B]	TTG	C15-C14-N12	-3.48	114.73	119.74
7	C	991[B]	TTG	C19-C15-C16	3.47	123.87	120.09
7	C	991[B]	TTG	C13-C17-C16	3.38	125.27	120.15
5	D	990[A]	TTC	C14-C15-C16	3.31	123.82	118.01
7	C	991[B]	TTG	C27-C1-C6	3.12	125.66	120.96
7	C	991[B]	TTG	O24-C21-C20	-3.05	102.73	108.69
5	D	990[A]	TTC	C27-C1-C2	-2.99	116.21	119.87
5	D	990[A]	TTC	C4-C5-C6	2.96	122.58	119.08
5	D	990[A]	TTC	C17-C16-C15	-2.95	111.81	118.57
5	D	990[A]	TTC	C17-C13-N12	2.94	122.12	119.67
5	D	990[A]	TTC	C17-C13-C9	2.79	128.03	124.37
5	D	990[A]	TTC	C4-C5-N10	-2.68	114.42	118.71
5	D	990[A]	TTC	C27-C1-C6	2.46	124.67	120.96
5	D	990[A]	TTC	C9-N10-C5	-2.46	113.87	117.70
5	D	990[A]	TTC	C19-C15-C16	-2.41	116.82	120.42
7	C	991[B]	TTG	O22-C20-C21	2.35	120.41	113.36
7	C	991[B]	TTG	C19-C15-C14	-2.34	114.65	121.74
5	D	990[A]	TTC	C16-C21-C20	-2.27	107.80	113.04
5	D	990[A]	TTC	C13-C17-C16	2.25	123.56	120.15
5	D	990[A]	TTC	C17-C16-C21	2.18	127.27	120.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

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%)	0.12	0 100 100	17, 24, 60, 68	0
2	C	11/12 (91%)	0.40	1 (9%) 9 10	32, 46, 70, 76	0
3	D	22/22 (100%)	0.22	1 (4%) 32 35	15, 42, 61, 70	0
4	A	565/592 (95%)	0.43	41 (7%) 15 16	12, 36, 75, 103	0
All	All	608/636 (95%)	0.41	43 (7%) 16 17	12, 36, 75, 103	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	675	MET	6.6
4	A	638	LYS	5.5
4	A	639	THR	4.2
4	A	678	ALA	3.5
4	A	674	VAL	3.5
4	A	321	LYS	3.4
4	A	693	ARG	3.2
4	A	682	LYS	3.1
4	A	673	LYS	3.1
4	A	213	GLU	3.1
4	A	676	LYS	3.0
4	A	414	VAL	3.0
4	A	645	MET	2.8
4	A	519	ASP	2.8
4	A	677	ASP	2.8
4	A	679	LYS	2.7
4	A	322	GLU	2.7
4	A	557	ASN	2.6
4	A	323	GLU	2.6
4	A	633	GLN	2.5
4	A	325	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
4	A	201	GLN	2.5
4	A	517	GLU	2.4
4	A	559	GLN	2.3
4	A	656	GLU	2.3
4	A	664	ASP	2.3
4	A	468	LYS	2.3
4	A	522	GLU	2.2
4	A	462	ARG	2.2
4	A	692	GLN	2.2
4	A	561	GLU	2.2
3	D	101	DA	2.2
4	A	640	PHE	2.1
4	A	320	SER	2.1
4	A	337	GLU	2.1
4	A	332	GLU	2.1
2	C	22	DT	2.1
4	A	520	GLY	2.1
4	A	413	LEU	2.0
4	A	567	ARG	2.0
4	A	463	GLU	2.0
4	A	652	ASP	2.0
4	A	489	ALA	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	PTR	A	723	16/17	0.13	0.02	21,24,28,36	0
2	TGP	C	11	19/23	0.09	-0.44	16,24,48,58	0

6.3 Carbohydrates ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
8	PG4	A	901	13/13	0.27	4.44	48,56,63,63	0
7	TTG	C	991[B]	32/32	0.12	-0.23	13,23,33,37	32
5	TTC	D	990[A]	31/31	0.11	-0.56	13,22,33,37	31
6	HG	A	900	1/1	0.07	-1.25	75,75,75,75	1

6.5 Other polymers ⓘ

There are no such residues in this entry.