



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 02:18 PM UTC

PDB ID : 4E10 / pdb\_00004e10  
Title : Protelomerase tela Y201A covalently complexed with substrate DNA  
Authors : Shi, K.; Aihara, H.  
Deposited on : 2012-03-05  
Resolution : 2.51 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

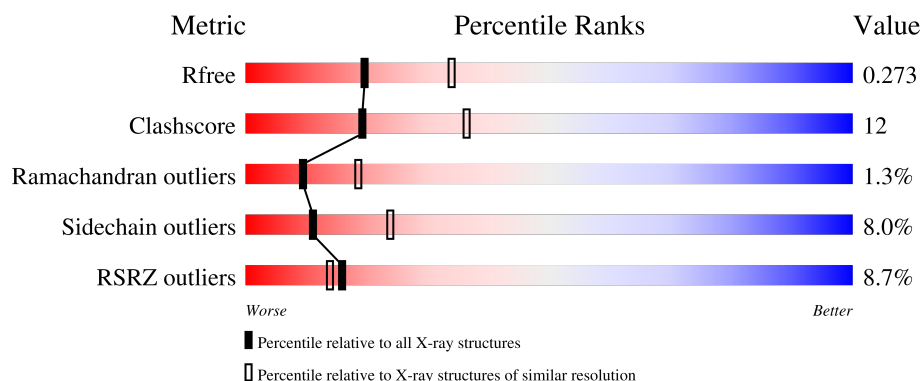
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.51 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))
$R_{free}$	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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  $\geq 3$ , 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	A	462	<div> <div>5%</div> <div>47%</div> <div>19%</div> <div>.</div> <div>31%</div> </div>
2	C	13	<div> <div>15%</div> <div>46%</div> <div>38%</div> <div>15%</div> </div>
3	D	18	<div> <div>17%</div> <div>17%</div> <div>50%</div> <div>17%</div> <div>17%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3278 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 protein called Protelomerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	318	2514	1594	436	470	1	13	0	0	0

There are 145 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q7CWW1
A	-18	GLY	-	expression tag	UNP Q7CWW1
A	-17	SER	-	expression tag	UNP Q7CWW1
A	-16	SER	-	expression tag	UNP Q7CWW1
A	-15	HIS	-	expression tag	UNP Q7CWW1
A	-14	HIS	-	expression tag	UNP Q7CWW1
A	-13	HIS	-	expression tag	UNP Q7CWW1
A	-12	HIS	-	expression tag	UNP Q7CWW1
A	-11	HIS	-	expression tag	UNP Q7CWW1
A	-10	HIS	-	expression tag	UNP Q7CWW1
A	-9	SER	-	expression tag	UNP Q7CWW1
A	-8	SER	-	expression tag	UNP Q7CWW1
A	-7	GLY	-	expression tag	UNP Q7CWW1
A	-6	LEU	-	expression tag	UNP Q7CWW1
A	-5	VAL	-	expression tag	UNP Q7CWW1
A	-4	PRO	-	expression tag	UNP Q7CWW1
A	-3	ARG	-	expression tag	UNP Q7CWW1
A	-2	GLY	-	expression tag	UNP Q7CWW1
A	-1	SER	-	expression tag	UNP Q7CWW1
A	0	HIS	-	expression tag	UNP Q7CWW1
A	1	MET	-	expression tag	UNP Q7CWW1
A	2	LEU	-	expression tag	UNP Q7CWW1
A	3	ALA	-	expression tag	UNP Q7CWW1
A	4	ALA	-	expression tag	UNP Q7CWW1
A	5	LYS	-	expression tag	UNP Q7CWW1
A	6	ARG	-	expression tag	UNP Q7CWW1
A	7	LYS	-	expression tag	UNP Q7CWW1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	8	THR	-	expression tag	UNP Q7CWXV1
A	9	LYS	-	expression tag	UNP Q7CWXV1
A	10	THR	-	expression tag	UNP Q7CWXV1
A	11	PRO	-	expression tag	UNP Q7CWXV1
A	12	VAL	-	expression tag	UNP Q7CWXV1
A	13	LEU	-	expression tag	UNP Q7CWXV1
A	14	VAL	-	expression tag	UNP Q7CWXV1
A	15	GLU	-	expression tag	UNP Q7CWXV1
A	16	ARG	-	expression tag	UNP Q7CWXV1
A	17	ILE	-	expression tag	UNP Q7CWXV1
A	18	ASP	-	expression tag	UNP Q7CWXV1
A	19	GLN	-	expression tag	UNP Q7CWXV1
A	20	PHE	-	expression tag	UNP Q7CWXV1
A	21	VAL	-	expression tag	UNP Q7CWXV1
A	22	GLY	-	expression tag	UNP Q7CWXV1
A	23	GLN	-	expression tag	UNP Q7CWXV1
A	24	ILE	-	expression tag	UNP Q7CWXV1
A	25	LYS	-	expression tag	UNP Q7CWXV1
A	26	GLU	-	expression tag	UNP Q7CWXV1
A	27	ALA	-	expression tag	UNP Q7CWXV1
A	28	MET	-	expression tag	UNP Q7CWXV1
A	29	LYS	-	expression tag	UNP Q7CWXV1
A	30	SER	-	expression tag	UNP Q7CWXV1
A	31	ASP	-	expression tag	UNP Q7CWXV1
A	32	ASP	-	expression tag	UNP Q7CWXV1
A	33	ALA	-	expression tag	UNP Q7CWXV1
A	34	SER	-	expression tag	UNP Q7CWXV1
A	35	ARG	-	expression tag	UNP Q7CWXV1
A	36	ASN	-	expression tag	UNP Q7CWXV1
A	37	ARG	-	expression tag	UNP Q7CWXV1
A	38	LYS	-	expression tag	UNP Q7CWXV1
A	39	ILE	-	expression tag	UNP Q7CWXV1
A	40	ARG	-	expression tag	UNP Q7CWXV1
A	41	ASP	-	expression tag	UNP Q7CWXV1
A	42	LEU	-	expression tag	UNP Q7CWXV1
A	43	TRP	-	expression tag	UNP Q7CWXV1
A	44	ASP	-	expression tag	UNP Q7CWXV1
A	45	ALA	-	expression tag	UNP Q7CWXV1
A	46	GLU	-	expression tag	UNP Q7CWXV1
A	47	VAL	-	expression tag	UNP Q7CWXV1
A	48	ARG	-	expression tag	UNP Q7CWXV1
A	49	TYR	-	expression tag	UNP Q7CWXV1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	50	HIS	-	expression tag	UNP Q7CWV1
A	51	PHE	-	expression tag	UNP Q7CWV1
A	52	ASP	-	expression tag	UNP Q7CWV1
A	53	ASN	-	expression tag	UNP Q7CWV1
A	54	GLY	-	expression tag	UNP Q7CWV1
A	55	ARG	-	expression tag	UNP Q7CWV1
A	56	THR	-	expression tag	UNP Q7CWV1
A	57	GLU	-	expression tag	UNP Q7CWV1
A	58	LYS	-	expression tag	UNP Q7CWV1
A	59	THR	-	expression tag	UNP Q7CWV1
A	60	LEU	-	expression tag	UNP Q7CWV1
A	61	GLU	-	expression tag	UNP Q7CWV1
A	62	LEU	-	expression tag	UNP Q7CWV1
A	63	TYR	-	expression tag	UNP Q7CWV1
A	64	ILE	-	expression tag	UNP Q7CWV1
A	65	MET	-	expression tag	UNP Q7CWV1
A	66	LYS	-	expression tag	UNP Q7CWV1
A	67	TYR	-	expression tag	UNP Q7CWV1
A	68	ARG	-	expression tag	UNP Q7CWV1
A	69	ASN	-	expression tag	UNP Q7CWV1
A	70	ALA	-	expression tag	UNP Q7CWV1
A	71	LEU	-	expression tag	UNP Q7CWV1
A	72	LYS	-	expression tag	UNP Q7CWV1
A	73	ALA	-	expression tag	UNP Q7CWV1
A	74	GLU	-	expression tag	UNP Q7CWV1
A	75	PHE	-	expression tag	UNP Q7CWV1
A	76	GLY	-	expression tag	UNP Q7CWV1
A	77	PRO	-	expression tag	UNP Q7CWV1
A	78	LYS	-	expression tag	UNP Q7CWV1
A	79	SER	-	expression tag	UNP Q7CWV1
A	80	THR	-	expression tag	UNP Q7CWV1
A	81	PRO	-	expression tag	UNP Q7CWV1
A	82	LEU	-	expression tag	UNP Q7CWV1
A	83	ALA	-	expression tag	UNP Q7CWV1
A	84	ILE	-	expression tag	UNP Q7CWV1
A	85	CYS	-	expression tag	UNP Q7CWV1
A	86	ASN	-	expression tag	UNP Q7CWV1
A	87	MET	-	expression tag	UNP Q7CWV1
A	88	LYS	-	expression tag	UNP Q7CWV1
A	89	LYS	-	expression tag	UNP Q7CWV1
A	90	LEU	-	expression tag	UNP Q7CWV1
A	91	ARG	-	expression tag	UNP Q7CWV1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	92	GLU	-	expression tag	UNP Q7CWV1
A	93	ARG	-	expression tag	UNP Q7CWV1
A	94	LEU	-	expression tag	UNP Q7CWV1
A	95	ASN	-	expression tag	UNP Q7CWV1
A	96	THR	-	expression tag	UNP Q7CWV1
A	97	TYR	-	expression tag	UNP Q7CWV1
A	98	ILE	-	expression tag	UNP Q7CWV1
A	99	ALA	-	expression tag	UNP Q7CWV1
A	100	ARG	-	expression tag	UNP Q7CWV1
A	101	GLY	-	expression tag	UNP Q7CWV1
A	102	ASP	-	expression tag	UNP Q7CWV1
A	201	ALA	TYR	engineered mutation	UNP Q7CWV1
A	421	LEU	-	expression tag	UNP Q7CWV1
A	422	LYS	-	expression tag	UNP Q7CWV1
A	423	ARG	-	expression tag	UNP Q7CWV1
A	424	THR	-	expression tag	UNP Q7CWV1
A	425	ASN	-	expression tag	UNP Q7CWV1
A	426	GLU	-	expression tag	UNP Q7CWV1
A	427	ARG	-	expression tag	UNP Q7CWV1
A	428	THR	-	expression tag	UNP Q7CWV1
A	429	LEU	-	expression tag	UNP Q7CWV1
A	430	GLN	-	expression tag	UNP Q7CWV1
A	431	GLN	-	expression tag	UNP Q7CWV1
A	432	MET	-	expression tag	UNP Q7CWV1
A	433	ALA	-	expression tag	UNP Q7CWV1
A	434	THR	-	expression tag	UNP Q7CWV1
A	435	ILE	-	expression tag	UNP Q7CWV1
A	436	ALA	-	expression tag	UNP Q7CWV1
A	437	PRO	-	expression tag	UNP Q7CWV1
A	438	VAL	-	expression tag	UNP Q7CWV1
A	439	SER	-	expression tag	UNP Q7CWV1
A	440	ARG	-	expression tag	UNP Q7CWV1
A	441	LYS	-	expression tag	UNP Q7CWV1
A	442	GLY	-	expression tag	UNP Q7CWV1

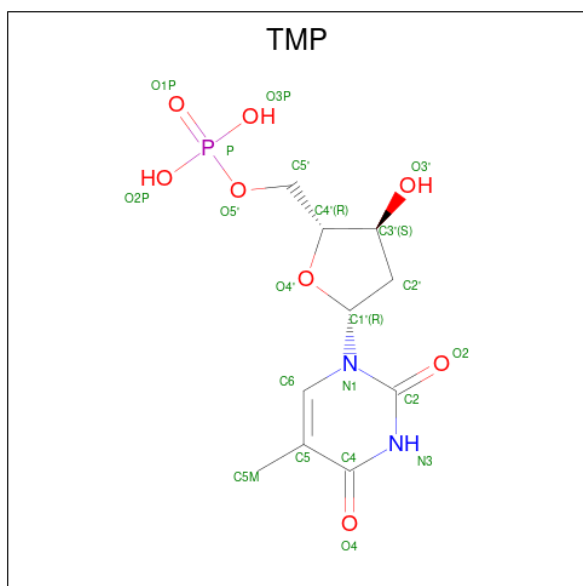
- Molecule 2 is a DNA chain called DNA (5'-D(\*CP\*AP\*TP\*AP\*AP\*(BRU)P\*AP\*AP\*CP\*AP\*AP\*(BRU)P\*AP\*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	13	Total	Br	C	N	O	P	0	0	0
			263	3	125	52	71	12			

- Molecule 3 is a DNA chain called DNA (5'-D(\*CP\*AP\*TP\*GP\*AP\*TP\*AP\*(BRU)P\*(BRU)P\*GP\*(BRU)P\*(BRU)P\*AP\*(BRU)P\*(BRU)P\*AP\*(BRU)P\*G)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D	15	Total	Br	C	N	O	P	0	0	0
			307	7	143	51	92	14			

- Molecule 4 is THYMIDINE-5'-PHOSPHATE (CCD ID: TMP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>2</sub>O<sub>8</sub>P).



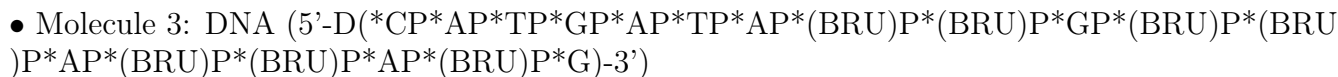
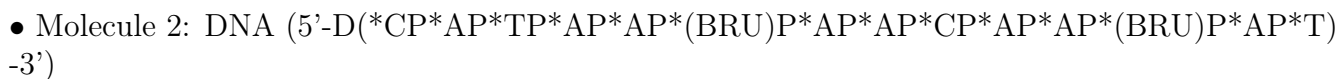
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			17	10	2	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	144	Total	O	0	0
			144	144		
5	C	15	Total	O	0	0
			15	15		
5	D	18	Total	O	0	0
			18	18		



- Molecule 1: Protelomerase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.34Å 119.66Å 56.63Å 90.00° 111.30° 90.00°	Depositor
Resolution (Å)	35.05 – 2.51 35.05 – 2.51	Depositor EDS
% Data completeness (in resolution range)	73.5 (35.05-2.51) 73.5 (35.05-2.51)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.06 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.183 , 0.270 0.190 , 0.273	Depositor DCC
$R_{free}$ test set	956 reflections (4.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.5	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 86.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3278	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PTR, TMP, BRU

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	A	0.91	1/2551 (0.0%)	1.13	9/3445 (0.3%)
2	C	0.56	0/227	1.31	2/340 (0.6%)
3	D	0.62	0/185	1.33	4/275 (1.5%)
All	All	0.87	1/2963 (0.0%)	1.16	15/4060 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	212	ILE	CA-CB	-8.47	1.44	1.54

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	LYS	CA-C-N	6.76	128.29	119.84
1	A	127	LYS	C-N-CA	6.76	128.29	119.84
1	A	370	ALA	N-CA-C	-6.33	104.30	111.14
1	A	192	LYS	N-CA-C	-6.26	105.68	113.38
2	C	13	DA	C2'-C3'-O3'	-5.81	102.78	111.50

There are no chirality outliers.

There are no planarity outliers.

### 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	A	2514	0	2498	60	0
2	C	263	0	139	7	0
3	D	307	0	154	6	0
4	A	17	0	13	3	0
5	A	144	0	0	8	0
5	C	15	0	0	1	0
5	D	18	0	0	1	0
All	All	3278	0	2804	69	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 12.

The worst 5 of 69 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:A:266:SER:HB2	1:A:280:LEU:HB2	1.62	0.79
2:C:4:DA:H2'	2:C:5:DA:C8	2.17	0.79
1:A:384:LYS:HG2	1:A:406:MET:HE2	1.68	0.76
1:A:354:TRP:CD1	1:A:355:PRO:HD2	2.27	0.70
3:D:18:DG:N7	5:D:111:HOH:O	2.25	0.69

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
1	A	315/462 (68%)	283 (90%)	28 (9%)	4 (1%)	<b>9</b> <b>18</b>

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	ALA

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Mol	Chain	Res	Type
1	A	330	SER
1	A	310	VAL
1	A	333	ASP

### 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	
1	A	262/388 (68%)	241 (92%)	21 (8%)	11	24

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	293	THR
1	A	330	SER
1	A	408	TYR
1	A	356	LYS
1	A	325	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	166	GLN
1	A	227	GLN
1	A	385	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

11 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	BRU	C	3	3,2	18,21,22	1.97	8 (44%)	25,30,33	3.28	14 (56%)
3	BRU	D	22	3,2	18,21,22	2.06	8 (44%)	25,30,33	2.85	11 (44%)
3	BRU	D	25	3,2	18,21,22	1.96	7 (38%)	25,30,33	2.22	10 (40%)
3	BRU	D	23	3,2	18,21,22	2.15	8 (44%)	25,30,33	2.14	9 (36%)
3	BRU	D	26	3,2	18,21,22	2.03	8 (44%)	25,30,33	2.40	6 (24%)
1	PTR	A	405	1	11,15,17	2.20	1 (9%)	10,19,24	0.25	0
2	BRU	C	12	3,2	18,21,22	2.00	8 (44%)	25,30,33	2.45	11 (44%)
3	BRU	D	31	3,2	18,21,22	2.02	10 (55%)	25,30,33	2.26	7 (28%)
3	BRU	D	28	3,2	18,21,22	2.00	9 (50%)	25,30,33	2.21	8 (32%)
3	BRU	D	29	3,2	18,21,22	2.27	10 (55%)	25,30,33	2.43	8 (32%)
2	BRU	C	6	3,2	18,21,22	2.02	8 (44%)	25,30,33	2.21	6 (24%)

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	BRU	C	3	3,2	-	6/7/21/22	0/2/2/2
3	BRU	D	22	3,2	-	2/7/21/22	0/2/2/2
3	BRU	D	25	3,2	-	2/7/21/22	0/2/2/2
3	BRU	D	23	3,2	-	0/7/21/22	0/2/2/2
3	BRU	D	26	3,2	-	0/7/21/22	0/2/2/2
1	PTR	A	405	1	-	0/7/10/13	0/1/1/1
2	BRU	C	12	3,2	-	0/7/21/22	0/2/2/2
3	BRU	D	31	3,2	-	0/7/21/22	0/2/2/2
3	BRU	D	28	3,2	-	2/7/21/22	0/2/2/2
3	BRU	D	29	3,2	-	2/7/21/22	0/2/2/2
2	BRU	C	6	3,2	-	0/7/21/22	0/2/2/2

The worst 5 of 85 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	405	PTR	OH-CZ	-7.07	1.29	1.40
3	D	23	BRU	C4-C5	-4.63	1.35	1.45
2	C	3	BRU	C2'-C3'	-3.89	1.43	1.52
2	C	6	BRU	C4-C5	-3.64	1.37	1.45
3	D	23	BRU	C2'-C3'	-3.48	1.44	1.52

The worst 5 of 90 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	BRU	BR-C5-C4	8.65	127.98	118.02
3	D	22	BRU	BR-C5-C4	7.53	126.69	118.02
3	D	29	BRU	C5-C4-N3	6.30	120.59	113.34
3	D	26	BRU	C5-C4-N3	5.92	120.15	113.34
2	C	3	BRU	C5-C4-N3	5.80	120.02	113.34

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	22	BRU	O4'-C4'-C5'-O5'
2	C	3	BRU	C3'-C4'-C5'-O5'
2	C	3	BRU	O4'-C4'-C5'-O5'
2	C	3	BRU	C2'-C1'-N1-C6
3	D	22	BRU	C3'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	23	BRU	1	0
1	A	405	PTR	4	0
3	D	29	BRU	2	0
2	C	6	BRU	1	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	$\# Z  > 2$
4	TMP	A	501	-	18,18,22	0.68	0	26,26,33	2.20	10 (38%)

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	TMP	A	501	-	-	4/6/18/22	0/2/2/2

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	A	501	TMP	C1'-N1-C6	-4.52	113.15	120.74
4	A	501	TMP	C1'-N1-C2	4.46	126.37	117.66
4	A	501	TMP	C5-C4-N3	-3.46	112.31	115.32
4	A	501	TMP	C5M-C5-C6	-3.46	118.17	122.85
4	A	501	TMP	C5M-C5-C4	3.28	122.28	118.78

There are no chirality outliers.

All (4) torsion outliers are listed below:

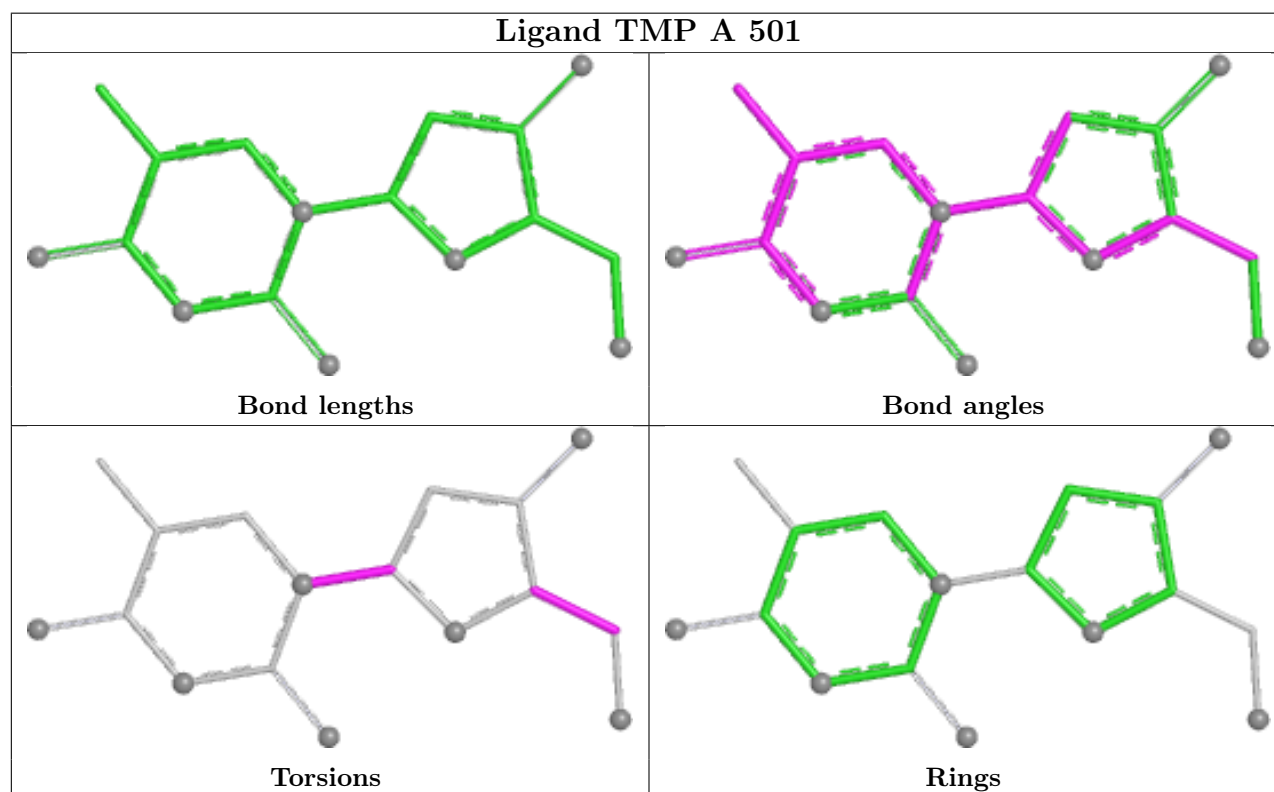
Mol	Chain	Res	Type	Atoms
4	A	501	TMP	O4'-C4'-C5'-O5'
4	A	501	TMP	C2'-C1'-N1-C2
4	A	501	TMP	C2'-C1'-N1-C6
4	A	501	TMP	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	TMP	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	317/462 (68%)	0.67	24 (7%) 20 17	29, 63, 97, 125	0
2	C	10/13 (76%)	0.64	2 (20%) 3 2	52, 69, 123, 129	0
3	D	8/18 (44%)	1.22	3 (37%) 1 1	48, 82, 113, 141	0
All	All	335/493 (67%)	0.69	29 (8%) 16 14	29, 64, 102, 141	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	421	LEU	4.5
1	A	121	PHE	3.9
1	A	105	LYS	3.8
1	A	276	LYS	3.6
3	D	18	DG	3.4

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	BRU	C	3	20/21	0.91	0.18	128,133,149,151	0
3	BRU	D	29	20/21	0.92	0.14	102,108,127,138	0
3	BRU	D	31	20/21	0.93	0.15	113,120,135,170	0
3	BRU	D	28	20/21	0.96	0.11	88,95,116,120	0
2	BRU	C	12	20/21	0.97	0.10	44,56,79,97	0
3	BRU	D	22	20/21	0.97	0.09	46,53,67,82	0
3	BRU	D	26	20/21	0.97	0.10	66,72,82,105	0
2	BRU	C	6	20/21	0.98	0.09	74,85,92,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BRU	D	25	20/21	0.98	0.10	57,63,79,92	0
1	PTR	A	405	15/17	0.98	0.07	33,41,49,50	0
3	BRU	D	23	20/21	0.99	0.07	45,50,70,74	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

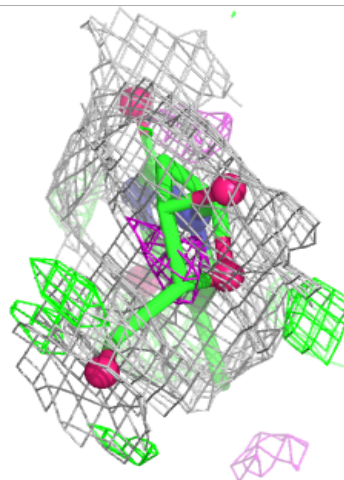
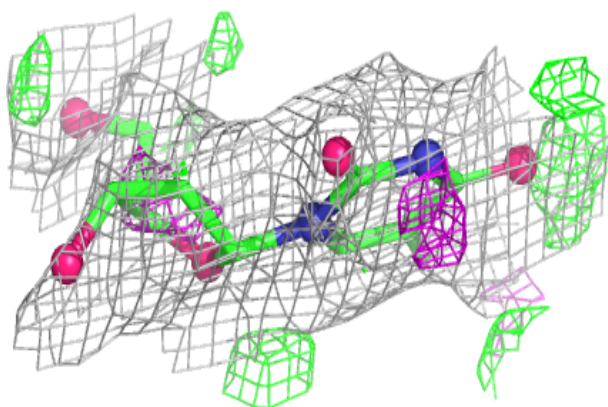
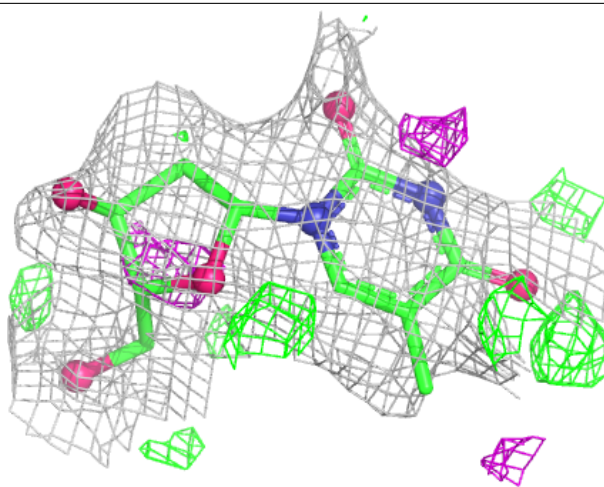
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	TMP	A	501	17/21	0.84	0.22	72,80,121,121	0

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 TMP A 501:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.