



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:42 AM UTC

PDB ID : 4DWP / pdb\_00004dwp  
Title : SeMet protelomerase tela covalently complexed with substrate DNA  
Authors : Shi, K.; Aihara, H.  
Deposited on : 2012-02-26  
Resolution : 2.35 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](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>.

---

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

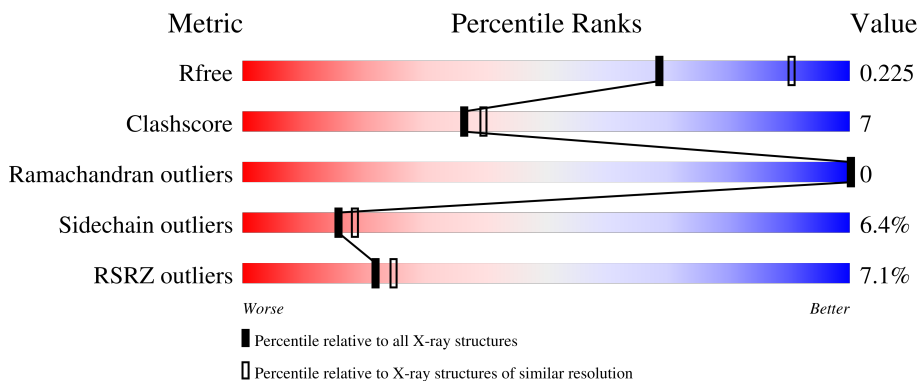
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	
2	C	15	
3	D	19	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3542 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	Se			
1	A	319	2544	1618	438	474	1	2	11	0	1	0

There are 143 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	expression tag	UNP Q7CWV1
A	-18	GLY	-	expression tag	UNP Q7CWV1
A	-17	SER	-	expression tag	UNP Q7CWV1
A	-16	SER	-	expression tag	UNP Q7CWV1
A	-15	HIS	-	expression tag	UNP Q7CWV1
A	-14	HIS	-	expression tag	UNP Q7CWV1
A	-13	HIS	-	expression tag	UNP Q7CWV1
A	-12	HIS	-	expression tag	UNP Q7CWV1
A	-11	HIS	-	expression tag	UNP Q7CWV1
A	-10	HIS	-	expression tag	UNP Q7CWV1
A	-9	SER	-	expression tag	UNP Q7CWV1
A	-8	SER	-	expression tag	UNP Q7CWV1
A	-7	GLY	-	expression tag	UNP Q7CWV1
A	-6	LEU	-	expression tag	UNP Q7CWV1
A	-5	VAL	-	expression tag	UNP Q7CWV1
A	-4	PRO	-	expression tag	UNP Q7CWV1
A	-3	ARG	-	expression tag	UNP Q7CWV1
A	-2	GLY	-	expression tag	UNP Q7CWV1
A	-1	SER	-	expression tag	UNP Q7CWV1
A	0	HIS	-	expression tag	UNP Q7CWV1
A	1	MSE	-	expression tag	UNP Q7CWV1
A	2	LEU	-	expression tag	UNP Q7CWV1
A	3	ALA	-	expression tag	UNP Q7CWV1
A	4	ALA	-	expression tag	UNP Q7CWV1
A	5	LYS	-	expression tag	UNP Q7CWV1
A	6	ARG	-	expression tag	UNP Q7CWV1
A	7	LYS	-	expression tag	UNP Q7CWV1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	THR	-	expression tag	UNP Q7CWV1
A	9	LYS	-	expression tag	UNP Q7CWV1
A	10	THR	-	expression tag	UNP Q7CWV1
A	11	PRO	-	expression tag	UNP Q7CWV1
A	12	VAL	-	expression tag	UNP Q7CWV1
A	13	LEU	-	expression tag	UNP Q7CWV1
A	14	VAL	-	expression tag	UNP Q7CWV1
A	15	GLU	-	expression tag	UNP Q7CWV1
A	16	ARG	-	expression tag	UNP Q7CWV1
A	17	ILE	-	expression tag	UNP Q7CWV1
A	18	ASP	-	expression tag	UNP Q7CWV1
A	19	GLN	-	expression tag	UNP Q7CWV1
A	20	PHE	-	expression tag	UNP Q7CWV1
A	21	VAL	-	expression tag	UNP Q7CWV1
A	22	GLY	-	expression tag	UNP Q7CWV1
A	23	GLN	-	expression tag	UNP Q7CWV1
A	24	ILE	-	expression tag	UNP Q7CWV1
A	25	LYS	-	expression tag	UNP Q7CWV1
A	26	GLU	-	expression tag	UNP Q7CWV1
A	27	ALA	-	expression tag	UNP Q7CWV1
A	28	MSE	-	expression tag	UNP Q7CWV1
A	29	LYS	-	expression tag	UNP Q7CWV1
A	30	SER	-	expression tag	UNP Q7CWV1
A	31	ASP	-	expression tag	UNP Q7CWV1
A	32	ASP	-	expression tag	UNP Q7CWV1
A	33	ALA	-	expression tag	UNP Q7CWV1
A	34	SER	-	expression tag	UNP Q7CWV1
A	35	ARG	-	expression tag	UNP Q7CWV1
A	36	ASN	-	expression tag	UNP Q7CWV1
A	37	ARG	-	expression tag	UNP Q7CWV1
A	38	LYS	-	expression tag	UNP Q7CWV1
A	39	ILE	-	expression tag	UNP Q7CWV1
A	40	ARG	-	expression tag	UNP Q7CWV1
A	41	ASP	-	expression tag	UNP Q7CWV1
A	42	LEU	-	expression tag	UNP Q7CWV1
A	43	TRP	-	expression tag	UNP Q7CWV1
A	44	ASP	-	expression tag	UNP Q7CWV1
A	45	ALA	-	expression tag	UNP Q7CWV1
A	46	GLU	-	expression tag	UNP Q7CWV1
A	47	VAL	-	expression tag	UNP Q7CWV1
A	48	ARG	-	expression tag	UNP Q7CWV1
A	49	TYR	-	expression tag	UNP Q7CWV1

*Continued on next page...*

*Continued from previous page...*

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	MSE	-	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	MSE	-	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

*Continued on next page...*

Continued from previous page...

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	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	MSE	-	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

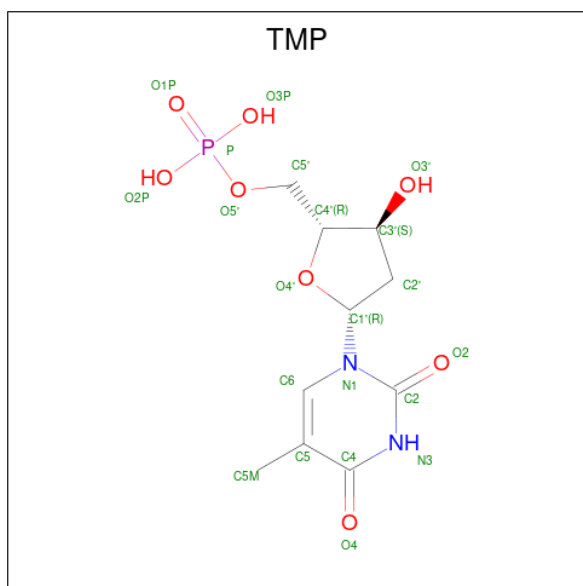
- Molecule 2 is a DNA chain called DNA (5'-D(\*TP\*TP\*AP\*CP\*AP\*AP\*TP\*AP\*AP\*CP\*AP\*AP\*TP\*AP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	14	283	138	54	78	13	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	D	17	351	170	58	106	17	0	0	0

- 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
			Total	C	N	O		
4	D	1	17	10	2	5	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	266	Total	O	0	0
			266	266		
5	C	37	Total	O	0	0
			37	37		
5	D	44	Total	O	0	0
			44	44		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.85Å 119.77Å 65.98Å 90.00° 108.63° 90.00°	Depositor
Resolution (Å)	40.84 – 2.35 40.84 – 2.35	Depositor EDS
% Data completeness (in resolution range)	81.3 (40.84-2.35) 81.3 (40.84-2.35)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.75 (at 2.34Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.189 , 0.227 0.183 , 0.225	Depositor DCC
$R_{free}$ test set	1452 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.3	Xtrriage
Anisotropy	0.054	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 65.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3542	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.55	1/2573 (0.0%)	0.86	0/3460
2	C	0.36	0/318	1.05	1/488 (0.2%)
3	D	0.37	0/392	1.05	1/604 (0.2%)
All	All	0.51	1/3283 (0.0%)	0.91	2/4552 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	ALA	C-O	-5.12	1.18	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	DC	C4'-C3'-O3'	6.20	119.30	110.00
3	D	18	DG	C4'-C3'-O3'	5.85	118.78	110.00

There are no chirality outliers.

There are no planarity outliers.

### 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	A	2544	0	2529	34	0
2	C	283	0	159	5	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	351	0	197	9	0
4	D	17	0	13	0	0
5	A	266	0	0	4	0
5	C	37	0	0	0	0
5	D	44	0	0	1	0
All	All	3542	0	2898	44	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 7.

All (44) 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:293:THR:HG22	1:A:295:PHE:H	1.38	0.88
1:A:329:MSE:HE2	1:A:334:PHE:HA	1.58	0.83
3:D:31:DT:H2''	3:D:32:DA:H5''	1.67	0.76
1:A:232:CYS:HB2	1:A:251:MSE:HE3	1.76	0.68
3:D:19:DA:N1	5:D:232:HOH:O	2.26	0.68
1:A:154:TRP:HB2	1:A:190:MSE:HE1	1.76	0.66
1:A:266:SER:HB3	1:A:280:LEU:HB2	1.81	0.62
1:A:154:TRP:HB2	1:A:190:MSE:CE	2.32	0.59
1:A:238:SER:O	1:A:316:ARG:NH2	2.30	0.56
1:A:276:LYS:HE3	1:A:306:ARG:HD2	1.86	0.56
1:A:249[B]:ILE:HD13	1:A:259:VAL:HG21	1.89	0.55
1:A:288:LYS:O	1:A:293:THR:HG21	2.08	0.52
1:A:384:LYS:HG2	1:A:406:MSE:HE2	1.93	0.50
1:A:161:MSE:HE2	1:A:176:TYR:CE1	2.47	0.49
1:A:316:ARG:NH1	5:A:731:HOH:O	2.46	0.48
1:A:235:CYS:HB3	1:A:243:MSE:O	2.14	0.48
1:A:343:ARG:NH1	5:A:624:HOH:O	2.42	0.48
1:A:414:ARG:NH2	5:A:755:HOH:O	2.38	0.47
1:A:133:ARG:NH2	1:A:157:GLU:OE2	2.42	0.47
1:A:167:THR:CG2	2:C:10:DA:H2'	2.45	0.46
1:A:167:THR:HG22	2:C:10:DA:H2'	1.97	0.46
3:D:22:DT:H2''	3:D:23:DT:H5''	1.97	0.46
1:A:317:LEU:O	1:A:320:SER:OG	2.32	0.46
3:D:22:DT:H2'	3:D:23:DT:C6	2.51	0.45
5:A:572:HOH:O	3:D:29:DT:H5'	2.18	0.44
1:A:292:GLY:HA2	1:A:396:ASN:ND2	2.32	0.44
2:C:3:DC:H2''	2:C:4:DA:O5'	2.17	0.44
1:A:287:THR:OG1	1:A:293:THR:HG23	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ARG:HD3	1:A:254:ARG:HA	1.68	0.43
1:A:167:THR:HG21	2:C:11:DA:H8	1.84	0.43
1:A:260:PHE:O	1:A:326:TRP:HB3	2.18	0.43
1:A:223:GLU:OE1	1:A:414:ARG:NH1	2.39	0.42
1:A:288:LYS:NZ	3:D:21:DA:OP1	2.46	0.42
1:A:240:ASP:HA	1:A:241:PRO:HD3	1.86	0.42
1:A:263:ALA:O	1:A:314:TYR:OH	2.24	0.42
1:A:418:LEU:HD12	1:A:418:LEU:HA	1.71	0.42
2:C:3:DC:H2'	2:C:4:DA:C8	2.55	0.42
1:A:222:PHE:CE1	1:A:355:PRO:HD3	2.55	0.41
1:A:215:LYS:HB3	1:A:215:LYS:HE2	1.81	0.41
3:D:18:DG:H2''	3:D:19:DA:C8	2.56	0.41
3:D:18:DG:H2''	3:D:19:DA:H5''	2.02	0.41
3:D:31:DT:H2''	3:D:32:DA:C8	2.56	0.41
1:A:354:TRP:CD1	1:A:355:PRO:HD2	2.56	0.41
1:A:253:GLY:O	1:A:366:ARG:NH1	2.51	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
1	A	317/462 (69%)	303 (96%)	14 (4%)	0	100 100

There are no Ramachandran outliers to report.

### 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	266/372 (72%)	249 (94%)	17 (6%)	16 18

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	LYS
1	A	158	ILE
1	A	167	THR
1	A	197	ASP
1	A	206	ARG
1	A	223	GLU
1	A	237	LYS
1	A	264	GLU
1	A	274	VAL
1	A	325	LEU
1	A	329	MSE
1	A	339	ARG
1	A	344	ASP
1	A	363	TYR
1	A	382	VAL
1	A	418	LEU
1	A	421	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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
1	PTR	A	405	1,2	11,15,17	2.05	1 (9%)	10,19,24	0.74	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
1	PTR	A	405	1,2	-	2/7/10/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	405	PTR	OH-CZ	-6.57	1.30	1.40

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	405	PTR	CE1-CZ-OH-P
1	A	405	PTR	CE2-CZ-OH-P

There are no ring outliers.

No monomer is involved in short contacts.

## 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	D	101	-	18,18,22	0.35	0	26,26,33	1.27	4 (15%)

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	D	101	-	-	2/6/18/22	0/2/2/2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	D	101	TMP	C5M-C5-C4	2.64	121.60	118.78
4	D	101	TMP	O4-C4-C5	-2.58	121.97	124.92
4	D	101	TMP	C1'-N1-C6	-2.35	116.80	120.74
4	D	101	TMP	C1'-N1-C2	2.24	122.04	117.66

There are no chirality outliers.

All (2) torsion outliers are listed below:

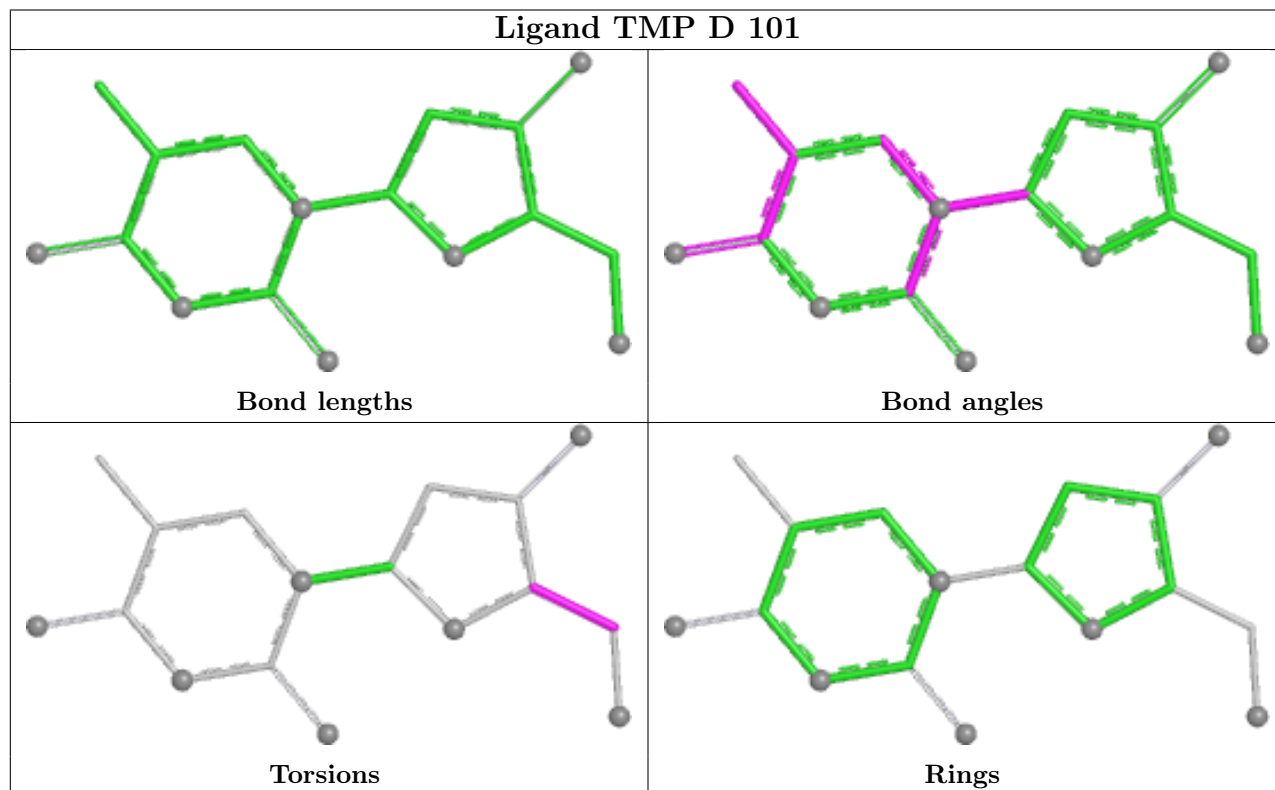
Mol	Chain	Res	Type	Atoms
4	D	101	TMP	C3'-C4'-C5'-O5'
4	D	101	TMP	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight  $> 250$  and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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	307/462 (66%)	0.26	18 (5%) 28 32	10, 35, 70, 96	1 (0%)
2	C	14/15 (93%)	0.32	4 (28%) 1 1	13, 35, 123, 123	0
3	D	17/19 (89%)	0.17	2 (11%) 9 10	14, 40, 103, 120	0
All	All	338/496 (68%)	0.25	24 (7%) 22 25	10, 35, 74, 123	1 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	421	LEU	6.6
1	A	121	PHE	5.3
3	D	33	DA	3.9
2	C	0	DT	3.1
1	A	306	ARG	2.8
1	A	347	PHE	2.8
2	C	2	DA	2.8
1	A	145	ASP	2.7
1	A	123	THR	2.7
3	D	32	DA	2.6
1	A	148	GLN	2.6
1	A	272	LYS	2.4
1	A	419	ALA	2.4
1	A	420	ARG	2.4
1	A	270	TYR	2.4
1	A	314	TYR	2.3
2	C	1	DT	2.3
2	C	3	DC	2.3
1	A	166	GLN	2.3
1	A	124	ALA	2.3
1	A	106	THR	2.2
1	A	118	ARG	2.2
1	A	416	ASN	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	162	ASN	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, 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
1	PTR	A	405	15/17	0.98	0.06	10,14,20,21	0

## 6.3 Carbohydrates [i](#)

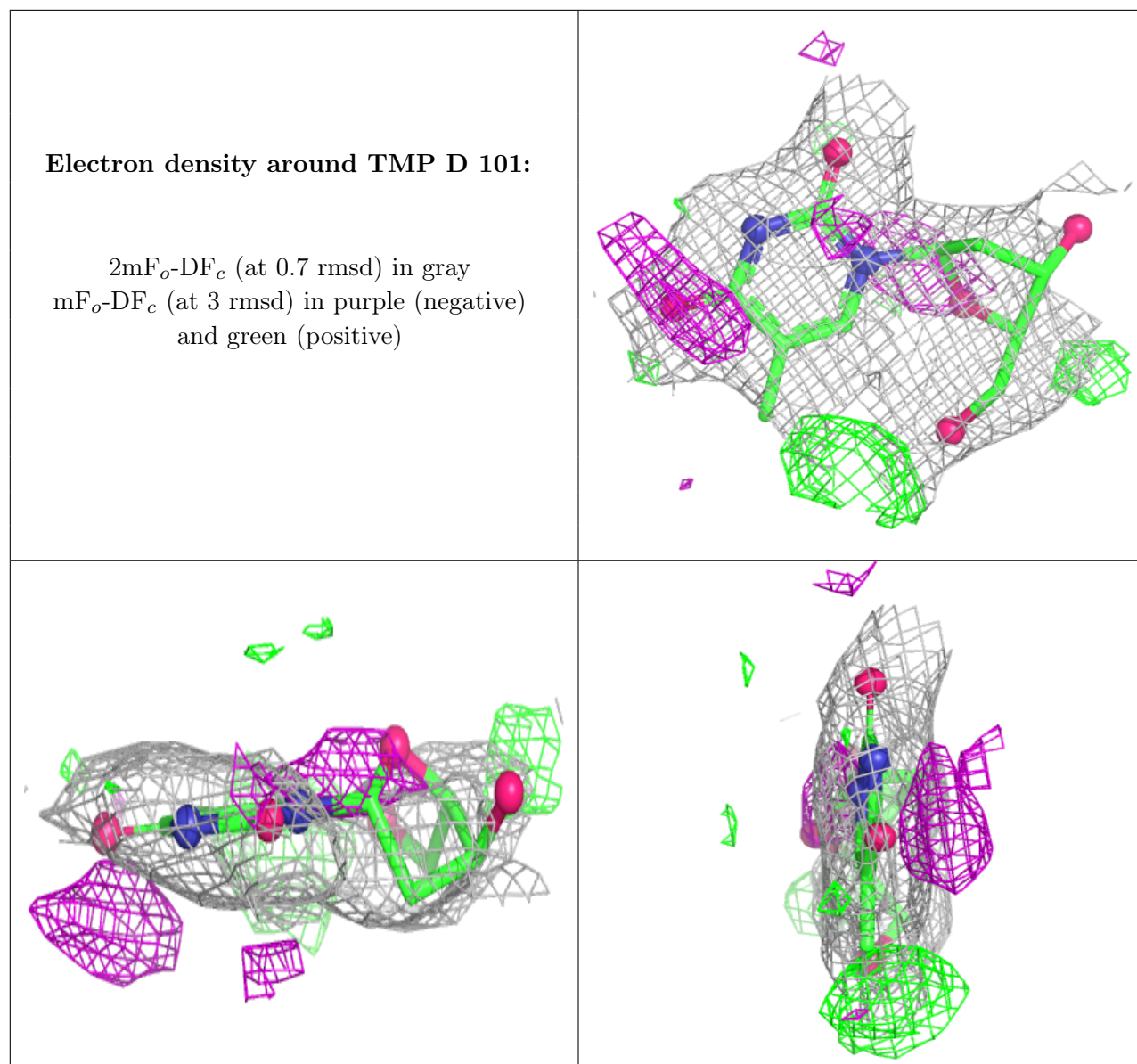
There are no oligosaccharides in this entry.

## 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(Å <sup>2</sup> )	Q<0.9
4	TMP	D	101	17/21	0.80	0.23	60,71,98,99	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.