



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 15, 2025 – 07:06 pm BST

PDB ID : 9EWG / pdb_00009ewg
Title : DNA Polymerase Lambda I493K, TTP:At Ca²⁺ Ground State Ternary Complex
Authors : Nourisson, A.; Haouz, A.; Missouri, S.; Delarue, M.
Deposited on : 2024-04-03
Resolution : 2.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

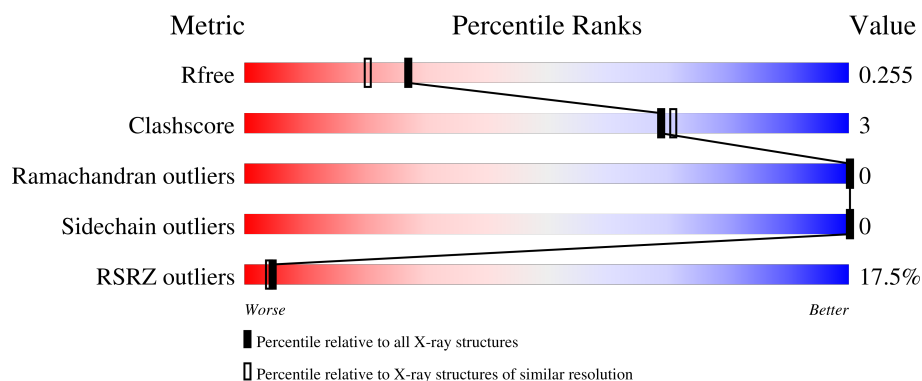
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	330	
2	D	4	
3	P	6	
4	T	11	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 5830 atoms, of which 2675 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 DNA polymerase lambda.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	316	Total	C	H	N	O	S	0	5	0
			4824	1537	2391	442	443	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLY	-	expression tag	UNP Q9UGP5
A	463	LYS	-	linker	UNP Q9UGP5
A	464	GLY	-	linker	UNP Q9UGP5
A	470	GLU	-	linker	UNP Q9UGP5
A	471	THR	-	linker	UNP Q9UGP5
A	492	LYS	ILE	engineered mutation	UNP Q9UGP5

- Molecule 2 is a DNA chain called DNA primer strand downstream.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	4	Total	C	H	N	O	P	0	0	0
			128	38	45	16	25	4			

- Molecule 3 is a DNA chain called DNA primer strand upstream.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	P	6	Total	C	H	N	O	P	0	0	0
			188	58	69	23	33	5			

- Molecule 4 is a DNA chain called DNA template strand.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	T	11	Total	C	H	N	O	P	0	0	0
			349	107	125	43	64	10			

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Na	0	0
			3	3		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

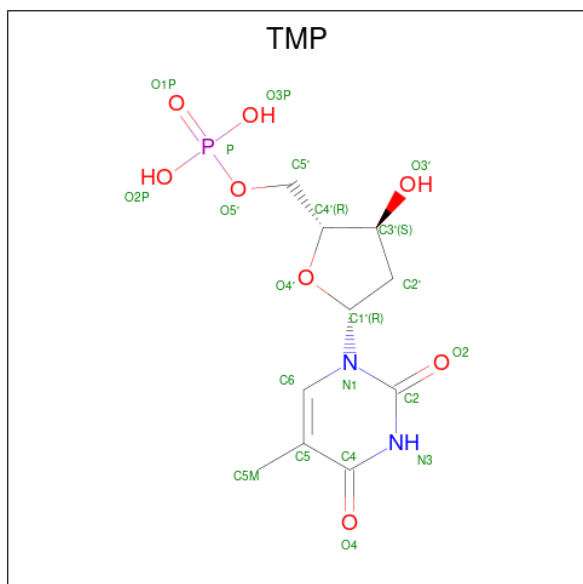
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	D	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 9 is THYMIDINE-5'-PHOSPHATE (CCD ID: TMP) (formula: $C_{10}H_{15}N_2O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
9	P	1	Total	C	H	N	O	P	0	0
			34	10	13	2	8	1		

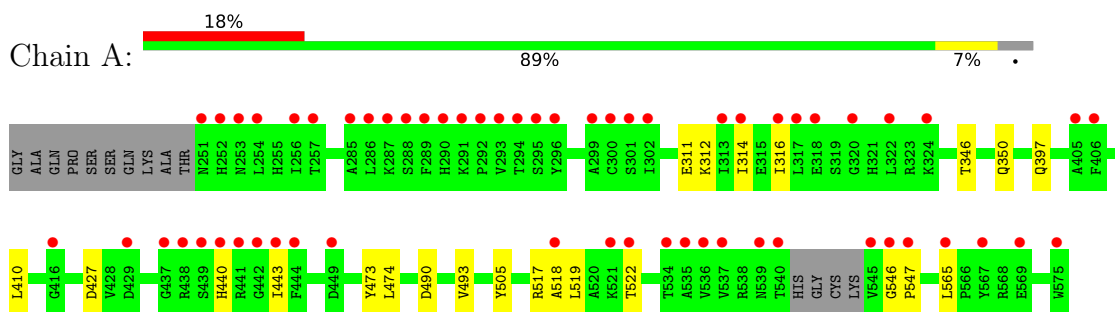
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	183	Total 183	O 183	0	0
10	D	2	Total 2	O 2	0	0
10	P	26	Total 26	O 26	0	0
10	T	37	Total 37	O 37	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: DNA polymerase lambda



- Molecule 2: DNA primer strand downstream

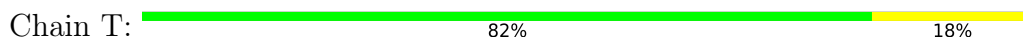


There are no outlier residues recorded for this chain.

- Molecule 3: DNA primer strand upstream



- Molecule 4: DNA template strand



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.04Å 62.50Å 141.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.70 – 2.00 70.70 – 2.00	Depositor EDS
% Data completeness (in resolution range)	73.2 (70.70-2.00) 73.2 (70.70-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.205 , 0.252 0.208 , 0.255	Depositor DCC
R_{free} test set	32382 reflections (7.86%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 60.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5830	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.06% 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: NA, TMP, EDO, CA, GOL

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	0.21	0/2498	0.37	0/3378
2	D	0.22	0/92	0.47	0/138
3	P	0.35	0/133	0.60	0/203
4	T	0.36	0/251	0.62	0/386
All	All	0.23	0/2974	0.41	0/4105

There are no bond length outliers.

There are no bond angle outliers.

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	2433	2391	2370	17	0
2	D	83	45	45	0	0
3	P	119	69	69	1	0
4	T	224	125	125	1	0
5	A	3	0	0	0	0
6	A	16	24	24	0	0
7	A	1	0	0	0	0
7	D	1	0	0	0	0
8	A	6	8	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	P	21	13	13	1	0
10	A	183	0	0	1	0
10	D	2	0	0	0	0
10	P	26	0	0	0	0
10	T	37	0	0	0	0
All	All	3155	2675	2654	19	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 3.

All (19) 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:474:LEU:HD22	1:A:490:ASP:CG	2.23	0.64
1:A:518:ALA:O	1:A:522:THR:HG23	1.98	0.63
1:A:519:LEU:HD21	1:A:565:LEU:HD21	1.87	0.56
4:T:9:DC:H2''	4:T:10:DT:H5'	1.89	0.54
1:A:312:LYS:O	1:A:316:ILE:HG13	2.08	0.53
1:A:474:LEU:HD22	1:A:490:ASP:OD1	2.12	0.50
1:A:346:THR:O	1:A:350:GLN:HG3	2.13	0.49
1:A:440:HIS:HB2	1:A:493[A]:VAL:CG1	2.44	0.48
1:A:427:ASP:OD2	1:A:427:ASP:C	2.55	0.48
1:A:519:LEU:CD2	1:A:565:LEU:HD21	2.43	0.48
1:A:505:TYR:CD1	1:A:517:ARG:NH2	2.82	0.47
1:A:311:GLU:O	1:A:314:ILE:HG22	2.14	0.47
1:A:473:TYR:O	1:A:474:LEU:HD23	2.18	0.44
1:A:410:LEU:HD11	1:A:443:ILE:HD13	1.98	0.43
1:A:311:GLU:HA	1:A:314:ILE:HG22	2.00	0.43
3:P:1:DC:H2'	3:P:2:DA:C8	2.53	0.43
1:A:546:GLY:N	1:A:547:PRO:CD	2.82	0.42
1:A:397:GLN:NE2	10:A:710:HOH:O	2.51	0.42
1:A:427:ASP:OD1	9:P:101:TMP:O3P	2.39	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	317/330 (96%)	309 (98%)	8 (2%)	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	251/275 (91%)	251 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	270	GLN
1	A	355	GLN
1	A	400	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	$\# Z > 2$
6	EDO	A	608	-	3,3,3	0.28	0	2,2,2	0.26	0
6	EDO	A	605	-	3,3,3	0.24	0	2,2,2	0.45	0
6	EDO	A	604	-	3,3,3	0.28	0	2,2,2	0.21	0
9	TMP	P	101	5	22,22,22	0.19	0	33,33,33	0.51	0
6	EDO	A	606	-	3,3,3	0.27	0	2,2,2	0.29	0
8	GOL	A	609	-	5,5,5	0.34	0	5,5,5	0.36	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
6	EDO	A	608	-	-	0/1/1/1	-
6	EDO	A	605	-	-	1/1/1/1	-
6	EDO	A	604	-	-	1/1/1/1	-
9	TMP	P	101	5	-	0/10/22/22	0/2/2/2
6	EDO	A	606	-	-	0/1/1/1	-
8	GOL	A	609	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

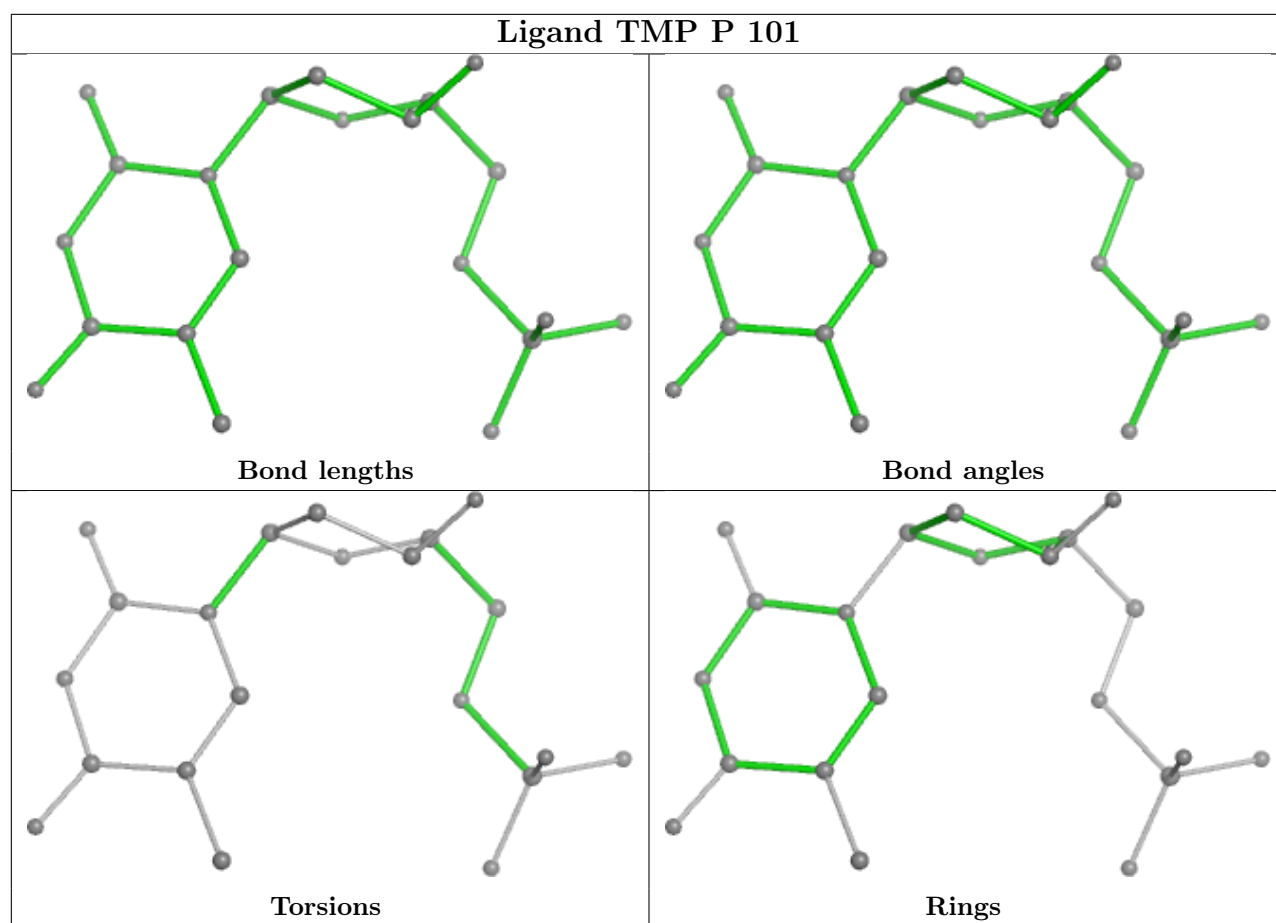
Mol	Chain	Res	Type	Atoms
6	A	605	EDO	O1-C1-C2-O2
6	A	604	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	P	101	TMP	1	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	A	316/330 (95%)	0.85	59 (18%)	4 3	19, 52, 116, 171	3 (0%)
2	D	4/4 (100%)	-0.28	0	100 100	51, 56, 59, 61	0
3	P	6/6 (100%)	-0.75	0	100 100	26, 29, 36, 54	0
4	T	11/11 (100%)	0.04	0	100 100	36, 47, 55, 65	0
All	All	337/351 (96%)	0.79	59 (17%)	5 4	19, 52, 115, 171	3 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	535	ALA	9.5
1	A	536	VAL	6.2
1	A	537	VAL	6.2
1	A	442	GLY	6.1
1	A	540	THR	5.9
1	A	443	ILE	5.6
1	A	289	PHE	5.1
1	A	299	ALA	4.9
1	A	293	VAL	4.8
1	A	440	HIS	4.7
1	A	545	VAL	4.7
1	A	286	LEU	4.4
1	A	534	THR	4.0
1	A	546	GLY	4.0
1	A	294	THR	3.9
1	A	539	ASN	3.8
1	A	441	ARG	3.7
1	A	575	TRP	3.7
1	A	290	HIS	3.6
1	A	439	SER	3.6
1	A	522	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	314	ILE	3.4
1	A	317	LEU	3.4
1	A	292	PRO	3.4
1	A	547	PRO	3.2
1	A	285	ALA	3.2
1	A	444	PHE	3.1
1	A	316	ILE	3.0
1	A	300	CYS	2.9
1	A	438	ARG	2.9
1	A	567	TYR	2.9
1	A	254	LEU	2.8
1	A	322	LEU	2.6
1	A	318	GLU	2.6
1	A	288	SER	2.6
1	A	296	TYR	2.6
1	A	406	PHE	2.6
1	A	313	ILE	2.6
1	A	251	ASN	2.6
1	A	301	SER	2.6
1	A	295	SER	2.5
1	A	256	ILE	2.4
1	A	518	ALA	2.4
1	A	416	GLY	2.4
1	A	291	LYS	2.4
1	A	253	ASN	2.3
1	A	324	LYS	2.3
1	A	257	THR	2.3
1	A	302	ILE	2.3
1	A	437	GLY	2.2
1	A	569	GLU	2.2
1	A	429	ASP	2.2
1	A	320	GLY	2.2
1	A	287	LYS	2.1
1	A	565	LEU	2.1
1	A	252	HIS	2.1
1	A	405	ALA	2.0
1	A	521	LYS	2.0
1	A	449	ASP	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

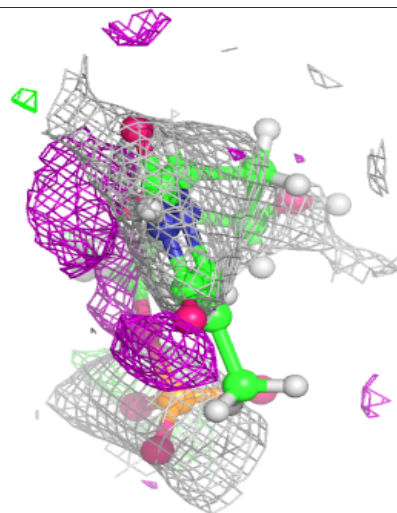
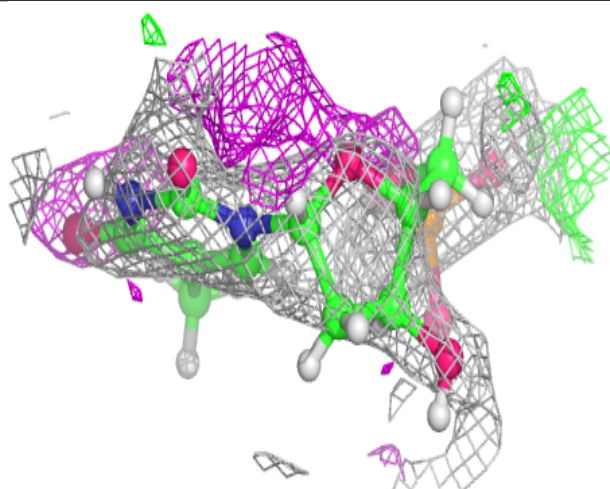
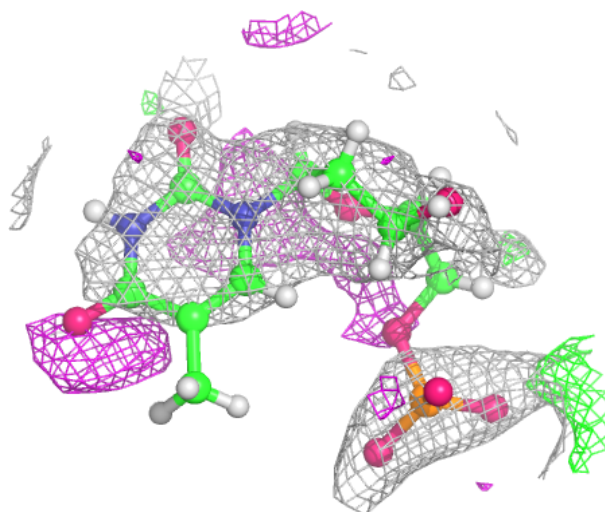
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	EDO	A	608	4/4	0.63	0.22	94,113,138,138	0
6	EDO	A	606	4/4	0.68	0.26	79,95,113,123	0
8	GOL	A	609	6/6	0.70	0.15	74,95,129,133	0
9	TMP	P	101	21/21	0.72	0.24	64,93,133,141	0
7	CA	D	101	1/1	0.77	0.29	97,97,97,97	0
7	CA	A	607	1/1	0.80	0.18	77,77,77,77	0
6	EDO	A	605	4/4	0.84	0.17	65,78,86,86	0
6	EDO	A	604	4/4	0.86	0.18	43,64,72,78	0
5	NA	A	601	1/1	0.86	0.18	79,79,79,79	0
5	NA	A	603	1/1	0.94	0.05	21,21,21,21	0
5	NA	A	602	1/1	0.96	0.11	74,74,74,74	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 P 101:

$2mF_o-DF_c$ (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.