



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 06:14 am BST

PDB ID : 4M8O
Title : TERNARY COMPLEX OF DNA POLYMERASE EPSILON WITH AN IN-COMING dATP
Authors : Sauer-Eriksson, A.E.; Hogg, M.; Osterman, P.; Johansson, E.
Deposited on : 2013-08-13
Resolution : 2.20 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

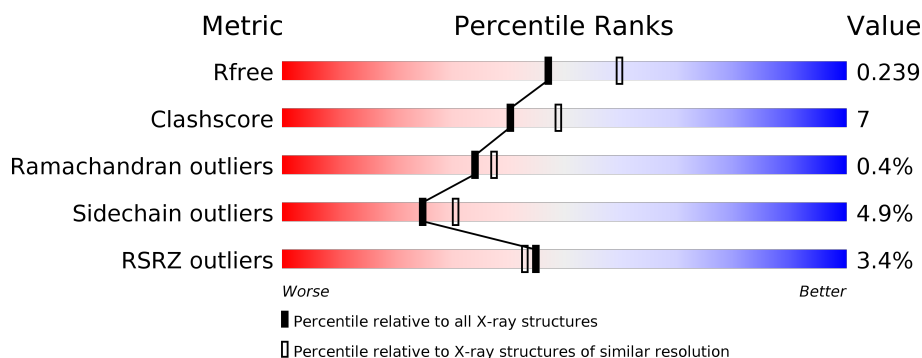
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1228	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>12%</div> <div>• 8%</div> </div> </div>
2	P	11	<div> <div>73%</div> <div>27%</div> </div>
3	T	16	<div> <div>69%</div> <div>25%</div> <div>6%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	C38	T	3	-	-	X	-
3	5IU	T	4[A]	-	-	X	-
7	TAU	A	1304	-	X	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 10235 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 DNA polymerase epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1126	Total	C	N	O	S	0	0	0
			9173	5870	1539	1719	45			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	290	ALA	ASP	ENGINEERED MUTATION	UNP P21951
A	292	ALA	GLU	ENGINEERED MUTATION	UNP P21951

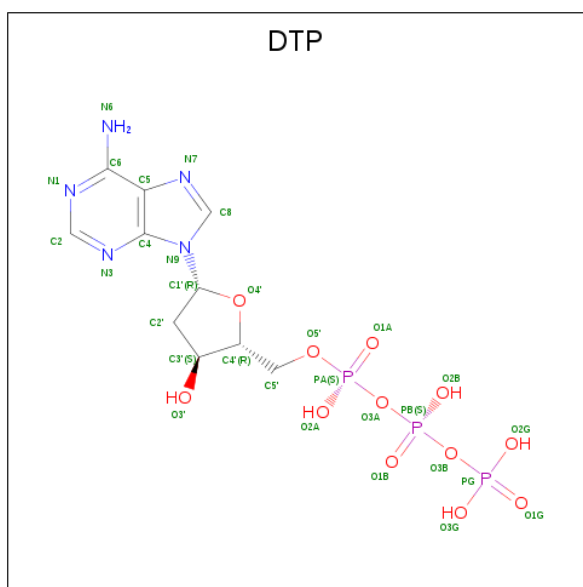
- Molecule 2 is a DNA chain called PRIMER DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	11	Total	C	I	N	O	P	0	0
			224	103	6	38	66	11		

- Molecule 3 is a DNA chain called TEMPLATE DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	15	Total	C	I	N	O	P	0	1
			331	152	8	56	99	16		

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

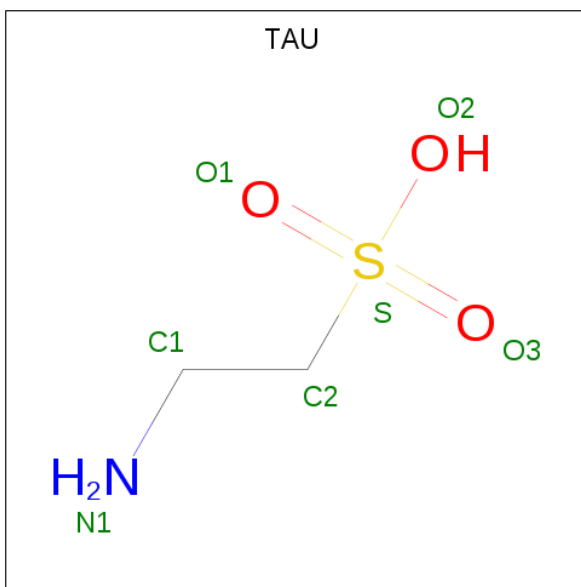
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 7 is 2-AMINOETHANESULFONIC ACID (three-letter code: TAU) (formula: C₂H₇NO₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			7	2	1	3	1		
7	A	1	Total	C	N	O	S	0	0
			7	2	1	3	1		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	P	2	Total	Cl	0	0
			2	2		

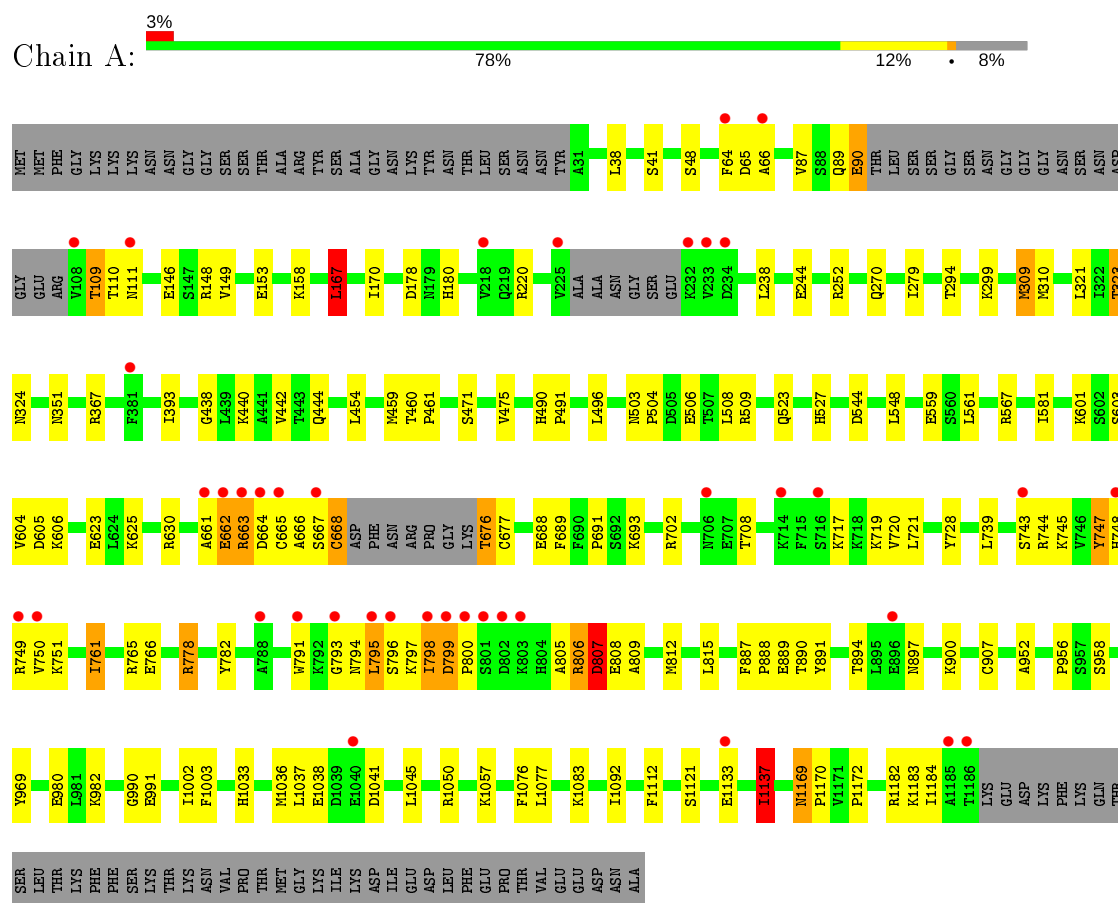
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	407	Total	O	0	0
			407	407		
9	P	22	Total	O	0	0
			22	22		
9	T	30	Total	O	0	0
			30	30		

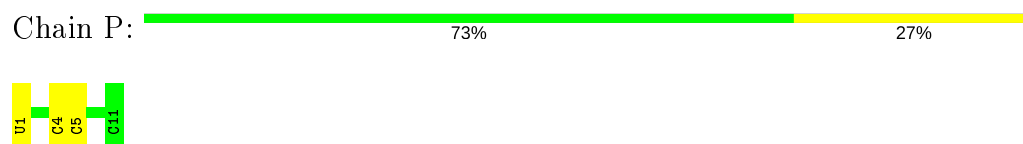
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA polymerase epsilon catalytic subunit A



- Molecule 2: PRIMER DNA



- Molecule 3: TEMPLATE DNA



C38	U2	C3	U4	T5	A16
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	148.50Å 68.92Å 149.85Å 90.00° 109.50° 90.00°	Depositor
Resolution (Å)	47.05 – 2.20 47.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.05-2.20) 99.9 (47.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.180 , 0.237 0.187 , 0.239	Depositor DCC
R_{free} test set	3667 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10235	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: TAU, ZN, CL, DOC, MG, 5IU, C38, DTP

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	0.84	4/9381 (0.0%)	0.87	8/12676 (0.1%)
2	P	0.55	0/95	0.92	0/140
3	T	1.06	1/190 (0.5%)	1.15	1/285 (0.4%)
All	All	0.85	5/9666 (0.1%)	0.88	9/13101 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	506	GLU	CD-OE1	5.74	1.31	1.25
3	T	5	DT	P-OP2	-5.31	1.40	1.49
1	A	506	GLU	CG-CD	5.26	1.59	1.51
1	A	1170	PRO	N-CD	5.22	1.55	1.47
1	A	1172	PRO	N-CD	5.03	1.54	1.47

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	747	TYR	N-CA-C	6.78	129.30	111.00
3	T	5	DT	O5'-P-OP2	-5.89	100.39	105.70
1	A	778	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	309	MET	CA-CB-CG	5.60	122.81	113.30
1	A	109	THR	CB-CA-C	-5.46	96.87	111.60

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	9173	0	9089	117	0
2	P	224	0	113	3	0
3	T	331	0	165	17	0
4	A	30	0	12	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	A	14	0	14	1	0
8	P	2	0	0	0	0
9	A	407	0	0	4	0
9	P	22	0	0	1	0
9	T	30	0	0	5	0
All	All	10235	0	9393	137	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.

The worst 5 of 137 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)
3:T:4[B]:5IU:O2	9:T:120:HOH:O	1.63	1.16
1:A:178:ASP:OD1	1:A:664:ASP:HB3	1.50	1.07
1:A:110:THR:HG22	1:A:111:ASN:H	1.25	1.01
1:A:64:PHE:CB	1:A:270:GLN:HG2	1.90	1.00
1:A:603:SER:OG	1:A:606:LYS:HE2	1.61	1.00

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	1118/1228 (91%)	1066 (95%)	47 (4%)	5 (0%)	34 37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	798	ILE
1	A	807	ASP
1	A	799	ASP
1	A	1169	ASN
1	A	1137	ILE

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
1	A	1017/1102 (92%)	967 (95%)	50 (5%)	25 31

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	717	LYS
1	A	745	LYS
1	A	1121	SER
1	A	719	LYS
1	A	721	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	434	GLN
1	A	523	GLN
1	A	713	ASN
1	A	360	GLN

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Mol	Chain	Res	Type
1	A	527	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

15 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$
3	5IU	T	2	3	14,21,22	0.79	0	16,30,33	2.68	4 (25%)
3	C38	T	11	3,2	14,21,22	1.19	1 (7%)	18,30,33	1.87	3 (16%)
2	C38	P	4	3,2	14,21,22	0.93	1 (7%)	18,30,33	2.21	5 (27%)
2	5IU	P	9	3,2	14,21,22	1.42	1 (7%)	16,30,33	2.87	6 (37%)
3	5IU	T	15	3,2	14,21,22	0.96	1 (7%)	16,30,33	2.12	3 (18%)
2	C38	P	5	3,2	14,21,22	1.07	1 (7%)	18,30,33	1.41	4 (22%)
2	DOC	P	11	3,2	14,19,20	1.16	1 (7%)	13,26,29	1.97	3 (23%)
3	5IU	T	4[B]	3	14,21,22	1.04	1 (7%)	16,30,33	3.08	4 (25%)
2	5IU	P	10	3,2	14,21,22	1.10	1 (7%)	16,30,33	2.88	4 (25%)
2	C38	P	7	3,2	14,21,22	0.98	1 (7%)	18,30,33	2.15	7 (38%)
3	5IU	T	14	3,2	14,21,22	1.19	3 (21%)	16,30,33	2.67	3 (18%)
3	C38	T	9	3,2	14,21,22	1.03	1 (7%)	18,30,33	1.67	4 (22%)
3	5IU	T	4[A]	3	14,21,22	1.48	1 (7%)	16,30,33	3.94	7 (43%)
2	5IU	P	1	3,2	14,21,22	0.92	1 (7%)	16,30,33	2.09	3 (18%)
3	C38	T	3	3	14,21,22	0.67	0	18,30,33	2.95	7 (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
3	5IU	T	2	3	-	1/4/21/22	0/2/2/2
3	C38	T	11	3,2	-	1/4/21/22	0/2/2/2
2	C38	P	4	3,2	-	3/4/21/22	0/2/2/2
2	5IU	P	9	3,2	-	1/4/21/22	0/2/2/2
3	5IU	T	15	3,2	-	1/4/21/22	0/2/2/2
2	C38	P	5	3,2	-	1/4/21/22	0/2/2/2
2	DOC	P	11	3,2	-	2/4/18/19	0/2/2/2
3	5IU	T	4[B]	3	-	0/4/21/22	0/2/2/2
2	5IU	P	10	3,2	-	1/4/21/22	0/2/2/2
2	C38	P	7	3,2	-	1/4/21/22	0/2/2/2
3	5IU	T	14	3,2	-	0/4/21/22	0/2/2/2
3	C38	T	9	3,2	-	0/4/21/22	0/2/2/2
3	5IU	T	4[A]	3	-	1/4/21/22	0/2/2/2
2	5IU	P	1	3,2	-	3/4/21/22	0/2/2/2
3	C38	T	3	3	-	0/4/21/22	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	4[A]	5IU	C6-C5	4.28	1.43	1.38
2	P	9	5IU	C2-N3	-4.09	1.30	1.38
3	T	4[B]	5IU	C6-C5	2.60	1.41	1.38
2	P	7	C38	C6-C5	2.59	1.41	1.38
2	P	11	DOC	C4-N3	-2.48	1.31	1.35

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	4[A]	5IU	C6-C5-I5	12.34	128.54	118.52
2	P	10	5IU	C4-N3-C2	9.86	123.47	115.14
3	T	4[B]	5IU	C6-C5-I5	9.34	126.11	118.52
2	P	9	5IU	C4-N3-C2	9.09	122.81	115.14
3	T	14	5IU	C4-N3-C2	8.43	122.26	115.14

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	T	11	C38	O4'-C1'-N1-C6
2	P	4	C38	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
3	T	15	5IU	O4'-C1'-N1-C6
2	P	5	C38	O4'-C1'-N1-C6
2	P	11	DOC	C3'-C4'-C5'-O5'

There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	T	2	5IU	2	0
2	P	4	C38	1	0
2	P	5	C38	2	0
3	T	4[B]	5IU	6	0
3	T	4[A]	5IU	8	0
2	P	1	5IU	1	0
3	T	3	C38	7	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 4 are 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	$\# Z > 2$
7	TAU	A	1305	-	6,6,6	2.72	2 (33%)	6,8,8	2.32	3 (50%)
4	DTP	A	1301	5	26,32,32	1.31	5 (19%)	30,50,50	1.62	6 (20%)
7	TAU	A	1304	-	6,6,6	3.08	2 (33%)	6,8,8	2.71	3 (50%)

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
7	TAU	A	1305	-	-	1/4/4/4	-
4	DTP	A	1301	5	-	4/18/34/34	0/3/3/3
7	TAU	A	1304	-	-	3/4/4/4	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1304	TAU	C2-S	-5.93	1.69	1.77
7	A	1305	TAU	C2-S	-5.36	1.69	1.77
7	A	1304	TAU	O2-S	4.55	1.63	1.47
7	A	1305	TAU	O2-S	3.81	1.61	1.47
4	A	1301	DTP	PB-O2B	-2.55	1.43	1.55

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1304	TAU	O3-S-C2	5.31	113.31	106.92
4	A	1301	DTP	C2'-C1'-N9	-4.64	103.56	114.27
7	A	1305	TAU	O1-S-C2	3.69	111.36	106.92
4	A	1301	DTP	C5-C6-N6	-3.66	114.79	120.35
4	A	1301	DTP	N3-C2-N1	-2.95	124.08	128.68

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1304	TAU	C1-C2-S-O1
4	A	1301	DTP	PB-O3B-PG-O3G
7	A	1304	TAU	C1-C2-S-O2
4	A	1301	DTP	PB-O3B-PG-O2G
4	A	1301	DTP	PA-O3A-PB-O1B

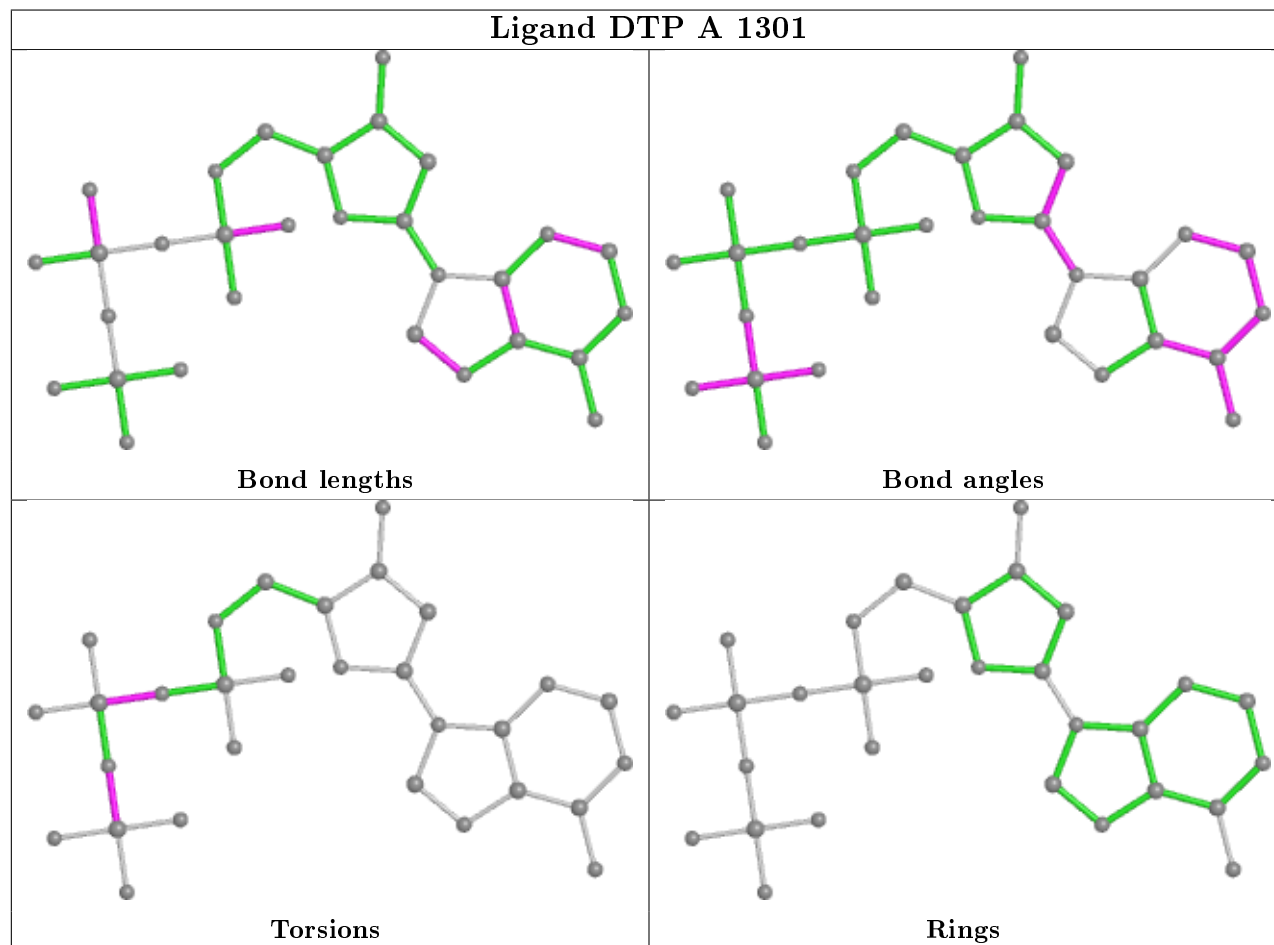
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1305	TAU	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	1126/1228 (91%)	-0.06	39 (3%) 44 42	15, 33, 73, 146	0
2	P	4/11 (36%)	-0.49	0 100 100	20, 31, 46, 48	0
3	T	8/16 (50%)	-0.50	0 100 100	16, 19, 34, 41	0
All	All	1138/1255 (90%)	-0.07	39 (3%) 45 43	15, 33, 73, 146	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	663	ARG	11.9
1	A	664	ASP	10.3
1	A	798	ILE	7.4
1	A	800	PRO	6.6
1	A	1186	THR	5.9

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. 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
3	5IU	T	2	20/21	0.60	0.36	98,115,123,126	1
3	C38	T	3	20/21	0.81	0.14	37,68,94,110	1
2	5IU	P	1	20/21	0.91	0.19	43,56,140,144	1
3	5IU	T	4[B]	20/21	0.92	0.17	26,37,56,73	20
3	5IU	T	4[A]	20/21	0.92	0.17	26,37,58,87	20
2	C38	P	4	20/21	0.94	0.10	29,47,65,72	1
2	C38	P	5	20/21	0.95	0.10	25,44,56,66	1
3	5IU	T	15	20/21	0.96	0.10	32,39,43,52	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	C38	P	7	20/21	0.98	0.12	19,24,29,35	1
3	5IU	T	14	20/21	0.98	0.11	30,35,38,39	1
3	C38	T	9	20/21	0.98	0.11	16,21,25,28	1
2	DOC	P	11	18/19	0.98	0.16	17,19,24,24	0
3	C38	T	11	20/21	0.98	0.12	22,26,30,32	1
2	5IU	P	10	20/21	0.98	0.16	13,18,20,25	1
2	5IU	P	9	20/21	0.99	0.15	16,18,23,23	1

6.3 Carbohydrates [i](#)

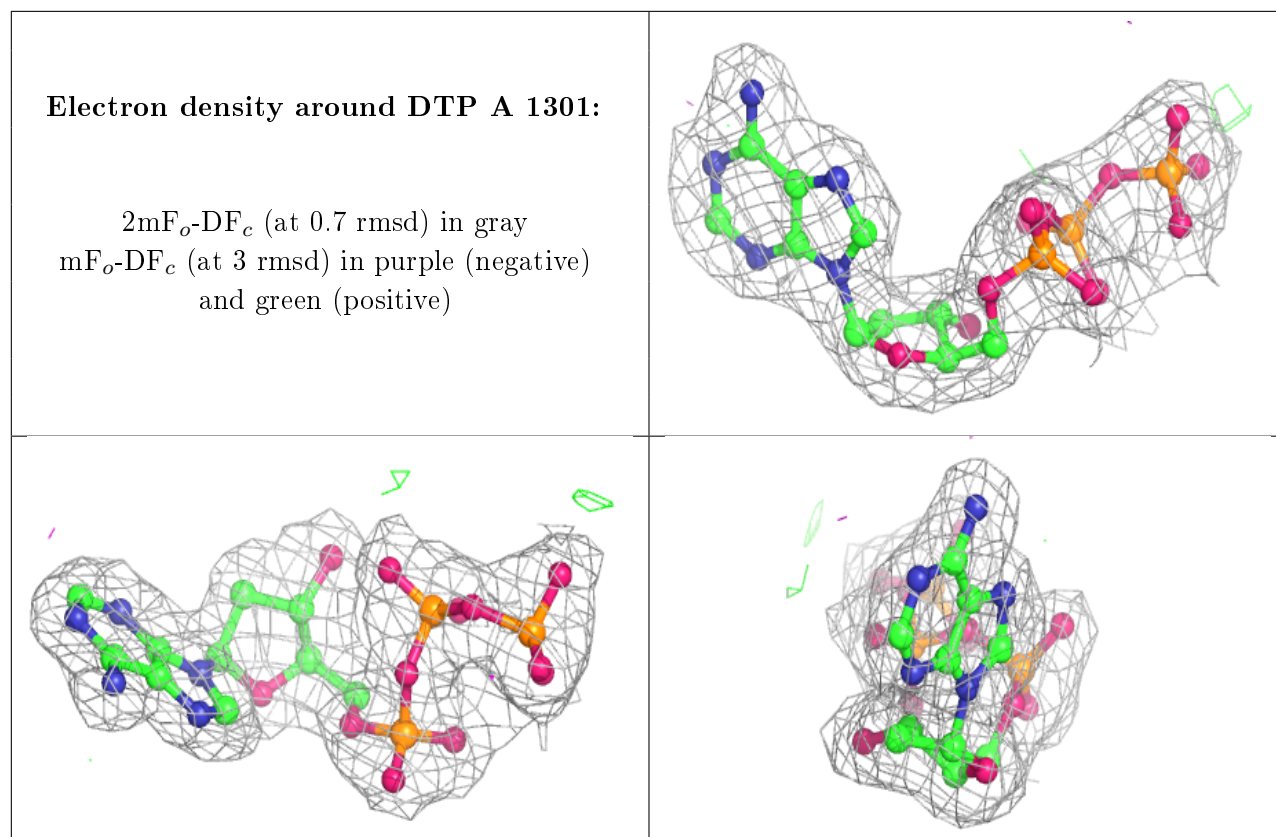
There are no carbohydrates in this entry.

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(\AA^2)	Q<0.9
7	TAU	A	1304	7/7	0.84	0.28	66,79,82,88	0
7	TAU	A	1305	7/7	0.87	0.30	50,59,67,68	7
5	MG	A	1302	1/1	0.96	0.10	21,21,21,21	0
6	ZN	A	1303	1/1	0.99	0.07	41,41,41,41	0
4	DTP	A	1301	30/30	0.99	0.13	13,14,23,24	0
8	CL	P	102	1/1	0.99	0.28	24,24,24,24	1
8	CL	P	101	1/1	1.00	0.25	9,9,9,9	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.