



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 04:20 am BST

PDB ID : 4Q4Z  
Title : Thermus thermophilus RNA polymerase de novo transcription initiation complex  
Authors : Murakami, K.S.  
Deposited on : 2014-04-15  
Resolution : 2.90 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.

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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

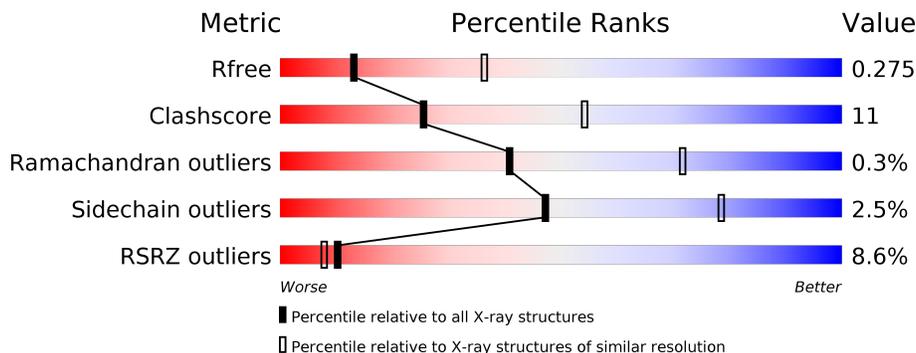
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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  $\geq 3$ , 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	315	
1	B	315	
2	C	1119	
3	D	1524	
4	E	99	
5	F	423	

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Mol	Chain	Length	Quality of chain
6	G	22	
7	H	27	

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
10	MG	D	2004	-	-	-	X

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 28755 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-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	231	Total	C	N	O	S	0	0	0
			1809	1155	315	337	2			
1	B	227	Total	C	N	O	S	0	0	0
			1789	1143	310	334	2			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	1112	Total	C	N	O	S	0	0	0
			8774	5550	1565	1635	24			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	1494	Total	C	N	O	S	0	1	0
			11808	7484	2083	2205	36			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	346	Total	C	N	O	S	0	0	0
			2807	1770	509	524	4			

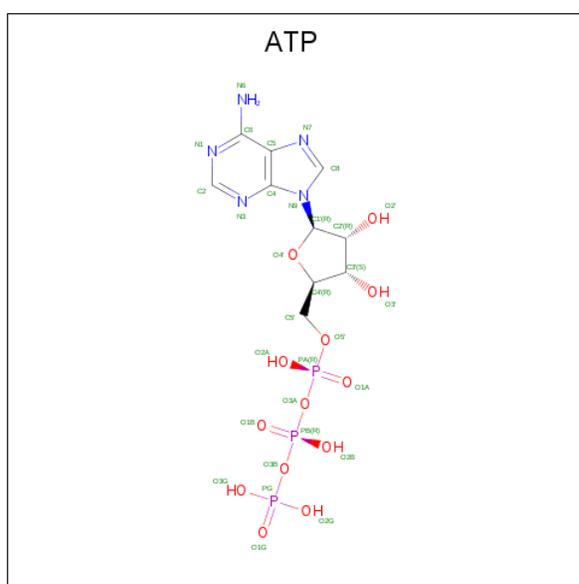
- Molecule 6 is a DNA chain called DNA (5'-D(\*CP\*CP\*TP\*GP\*CP\*AP\*TP\*CP\*CP\*GP\*TP\*GP\*AP\*GP\*TP\*GP\*CP\*AP\*GP\*CP\*CP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
6	G	18	370	175	68	109	18	0	0	0

- Molecule 7 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
7	H	25	516	246	99	147	24	0	0	0

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
8	C	1	31	10	5	13	3	0	0

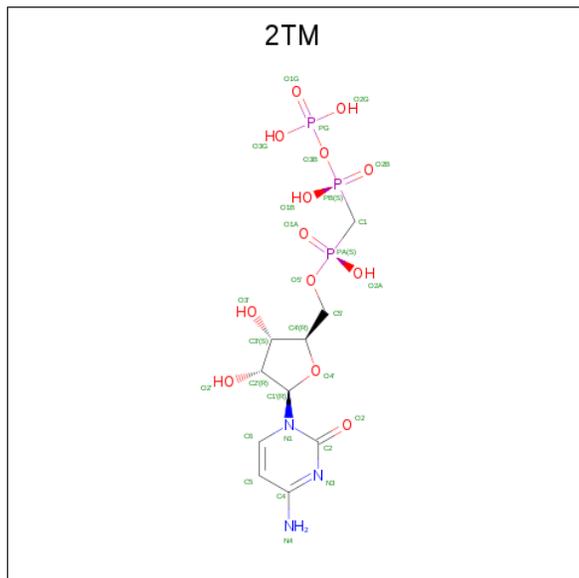
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
9	D	2	2	2	0	0

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
10	D	3	3	3	0	0

- Molecule 11 is 5'-O-[(S)-hydroxy{[(S)-hydroxy(phosphonoxy)phosphoryl]methyl}phosphoryl]cytidine (three-letter code: 2TM) (formula: C<sub>10</sub>H<sub>18</sub>N<sub>3</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
11	D	1	29	10	3	13	3	0	0

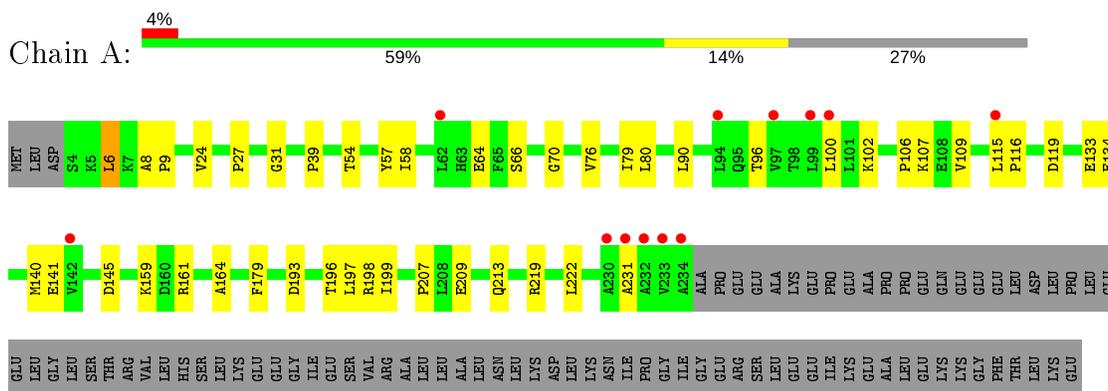
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	4	Total	O	0	0
			4	4		
12	B	1	Total	O	0	0
			1	1		
12	C	22	Total	O	0	0
			22	22		
12	D	26	Total	O	0	0
			26	26		
12	E	2	Total	O	0	0
			2	2		
12	G	1	Total	O	0	0
			1	1		

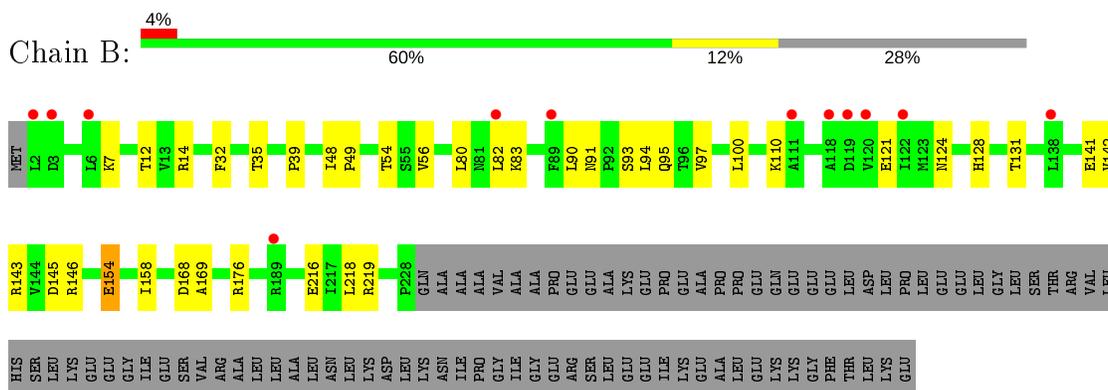
### 3 Residue-property plots [i](#)

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.

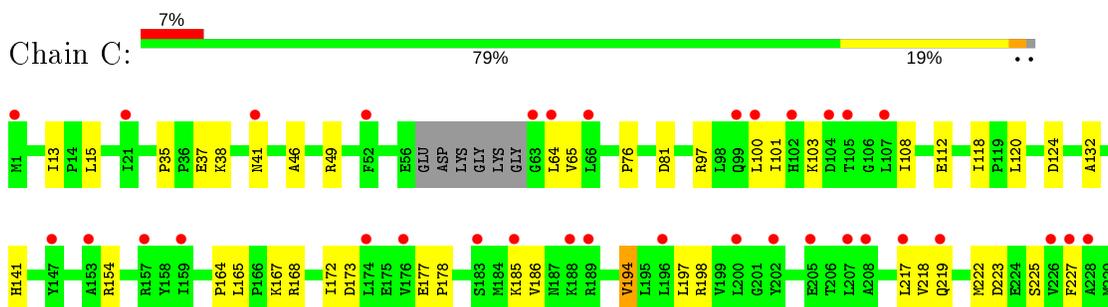
- Molecule 1: DNA-directed RNA polymerase subunit alpha

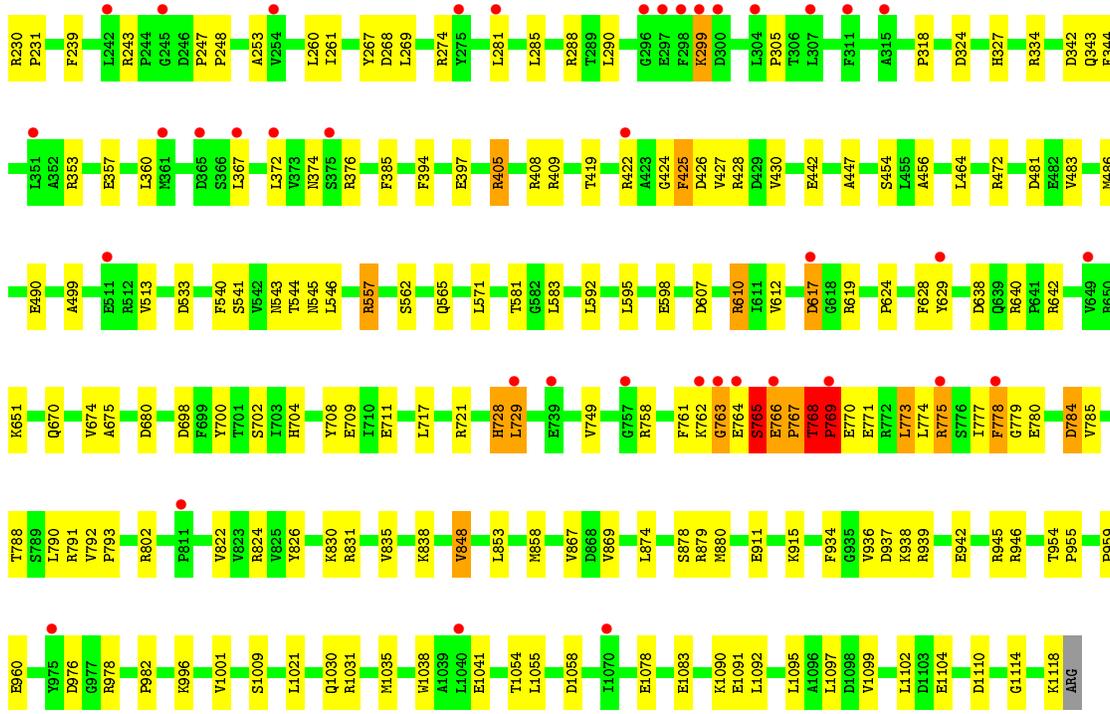


- Molecule 1: DNA-directed RNA polymerase subunit alpha

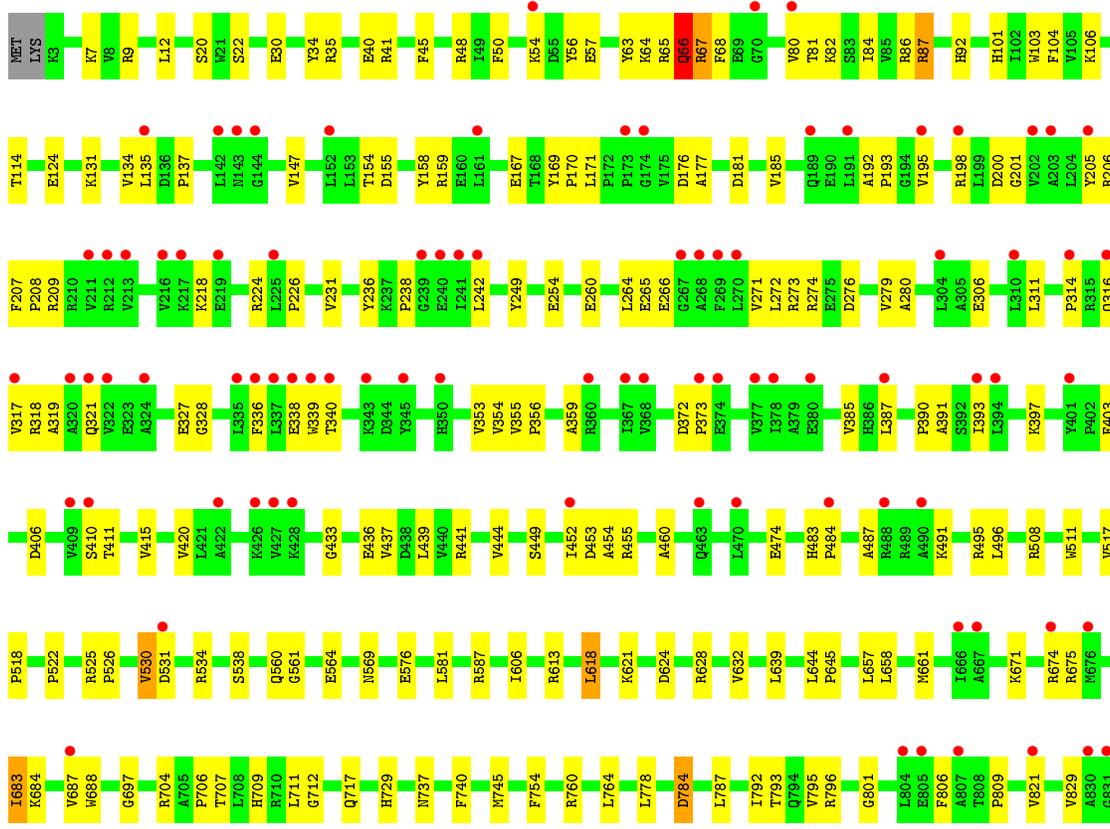
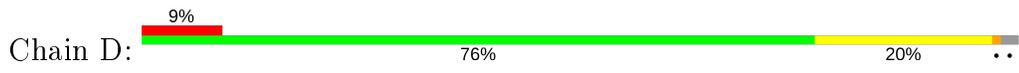


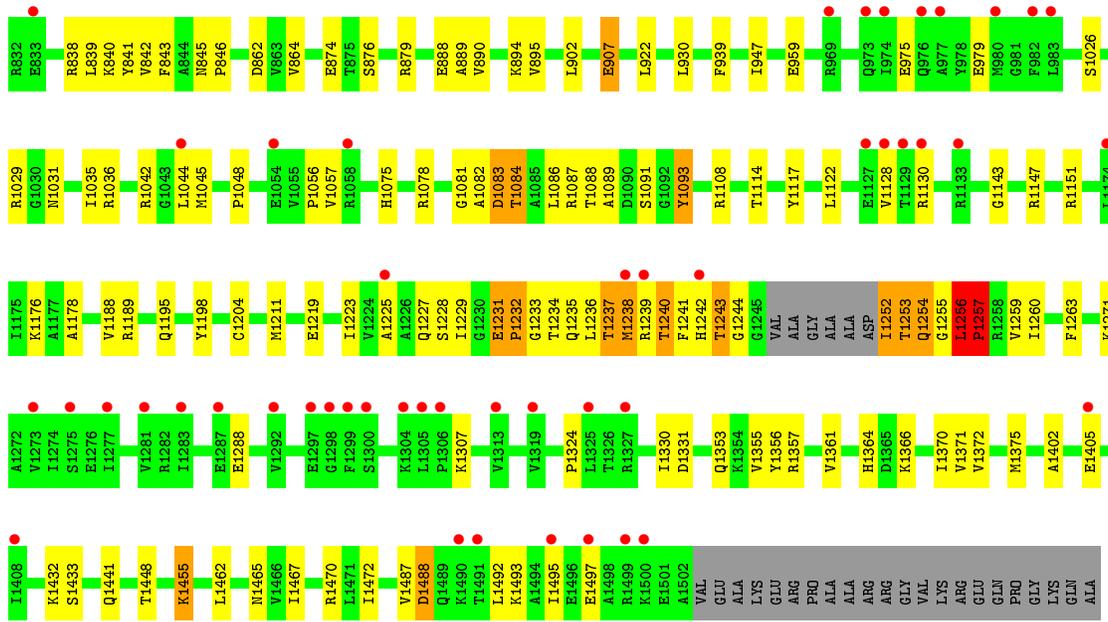
- Molecule 2: DNA-directed RNA polymerase subunit beta



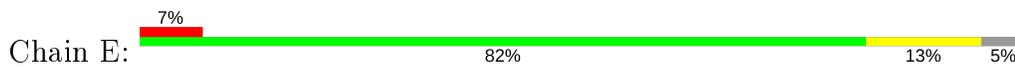


● Molecule 3: DNA-directed RNA polymerase subunit beta'





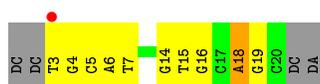
• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 5: RNA polymerase sigma factor SigA



• Molecule 6: DNA (5'-D(\*CP\*CP\*TP\*GP\*CP\*AP\*TP\*CP\*CP\*GP\*TP\*GP\*AP\*GP\*TP\*GP\*CP\*AP\*GP\*CP\*CP\*A)-3')



● Molecule 7: DNA (25-MER)



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	184.49Å 102.16Å 294.72Å 90.00° 98.96° 90.00°	Depositor
Resolution (Å)	29.78 – 2.90 43.54 – 2.85	Depositor EDS
% Data completeness (in resolution range)	89.5 (29.78-2.90) 84.3 (43.54-2.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 2.86Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.256 , 0.275 0.258 , 0.275	Depositor DCC
$R_{free}$ test set	1753 reflections (1.57%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.3	Xtrriage
Anisotropy	0.753	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 18.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	28755	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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: 2TM, MG, ZN, ATP

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	0.24	0/1841	0.46	0/2504
1	B	0.22	0/1821	0.44	0/2476
2	C	0.31	1/8941 (0.0%)	0.50	6/12092 (0.0%)
3	D	0.35	1/12019 (0.0%)	0.50	4/16248 (0.0%)
4	E	0.24	0/775	0.41	0/1045
5	F	0.23	0/2852	0.40	0/3837
6	G	0.72	2/414 (0.5%)	1.16	3/637 (0.5%)
7	H	0.57	0/580	1.13	3/895 (0.3%)
All	All	0.33	4/29243 (0.0%)	0.52	16/39734 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1093	TYR	CE2-CZ	-6.38	1.30	1.38
6	G	18	DA	O3'-P	-5.67	1.54	1.61
6	G	3	DT	O3'-P	-5.63	1.54	1.61
2	C	769	PRO	N-CD	5.43	1.55	1.47

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	761	PHE	O-C-N	-10.43	106.01	122.70
6	G	18	DA	O4'-C1'-N9	9.34	114.54	108.00
3	D	1257	PRO	CA-N-CD	-8.41	99.72	111.50
3	D	1232	PRO	CA-N-CD	-7.58	100.88	111.50
2	C	761	PHE	C-N-CA	7.11	139.47	121.70

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	1809	0	1863	38	0
1	B	1789	0	1841	24	0
2	C	8774	0	8877	226	3
3	D	11808	0	12041	258	4
4	E	761	0	778	9	1
5	F	2807	0	2882	101	2
6	G	370	0	202	19	0
7	H	516	0	283	31	1
8	C	31	0	11	2	0
9	D	2	0	0	0	0
10	D	3	0	0	0	0
11	D	29	0	14	2	0
12	A	4	0	0	9	0
12	B	1	0	0	0	0
12	C	22	0	0	29	0
12	D	26	0	0	26	0
12	E	2	0	0	1	0
12	G	1	0	0	0	0
All	All	28755	0	28792	605	6

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 11.

The worst 5 of 605 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)
2:C:773:LEU:CD2	5:F:373:LYS:HG3	1.14	1.60
5:F:358:LEU:HD13	5:F:370:LYS:NZ	1.33	1.41
2:C:773:LEU:CD2	5:F:373:LYS:CG	2.03	1.36
2:C:778:PHE:HE2	5:F:419:ARG:NH2	1.25	1.35
2:C:764:GLU:O	2:C:766:GLU:N	1.62	1.32

The worst 5 of 6 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:306:GLU:OE1	7:H:1:DT:O5'[4_745]	1.70	0.50
2:C:318:PRO:CB	4:E:87:LYS:CG[1_545]	1.77	0.43
3:D:34:TYR:OH	3:D:327:GLU:OE1[4_755]	1.89	0.31
3:D:328:GLY:O	5:F:303:ARG:NH2[4_745]	2.11	0.09
2:C:37:GLU:OE1	3:D:1151:ARG:NH1[3_545]	2.12	0.08

### 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	229/315 (73%)	226 (99%)	3 (1%)	0	100	100
1	B	225/315 (71%)	222 (99%)	3 (1%)	0	100	100
2	C	1108/1119 (99%)	1076 (97%)	26 (2%)	6 (0%)	29	61
3	D	1491/1524 (98%)	1454 (98%)	33 (2%)	4 (0%)	41	71
4	E	92/99 (93%)	89 (97%)	3 (3%)	0	100	100
5	F	344/423 (81%)	336 (98%)	7 (2%)	1 (0%)	41	71
All	All	3489/3795 (92%)	3403 (98%)	75 (2%)	11 (0%)	41	71

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	425	PHE
2	C	765	SER
2	C	769	PRO
3	D	1240	THR
2	C	779	GLY

#### 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	200/273 (73%)	196 (98%)	4 (2%)	55	82
1	B	200/273 (73%)	196 (98%)	4 (2%)	55	82
2	C	936/941 (100%)	907 (97%)	29 (3%)	40	74
3	D	1260/1279 (98%)	1229 (98%)	31 (2%)	47	78
4	E	83/88 (94%)	83 (100%)	0	100	100
5	F	301/371 (81%)	296 (98%)	5 (2%)	60	86
All	All	2980/3225 (92%)	2907 (98%)	73 (2%)	47	79

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	778	PHE
3	D	134	VAL
3	D	1488	ASP
3	D	66	GLN
3	D	354	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	560	GLN
3	D	737	ASN
3	D	1441	GLN
3	D	669	ASN
3	D	717	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	ATP	C	1201	10	26,33,33	0.92	1 (3%)	31,52,52	1.19	4 (12%)
11	2TM	D	2006	-	24,30,30	2.52	9 (37%)	30,47,47	1.83	7 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ATP	C	1201	10	-	8/18/38/38	0/3/3/3
11	2TM	D	2006	-	-	5/17/38/38	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	2006	2TM	C6-N1	-4.88	1.29	1.35
11	D	2006	2TM	PB-O3B	4.39	1.63	1.58
11	D	2006	2TM	PB-O1B	-4.10	1.46	1.56
11	D	2006	2TM	C2'-C1'	-3.88	1.47	1.53
11	D	2006	2TM	C5-C4	-3.61	1.32	1.41

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	2006	2TM	C2-N3-C4	4.03	120.43	116.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	2006	2TM	O3G-PG-O1G	3.81	125.58	110.68
11	D	2006	2TM	O1B-PB-O2B	3.63	122.18	110.07
11	D	2006	2TM	N4-C4-N3	3.20	121.55	116.49
11	D	2006	2TM	C6-N1-C2	-3.20	116.11	121.20

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

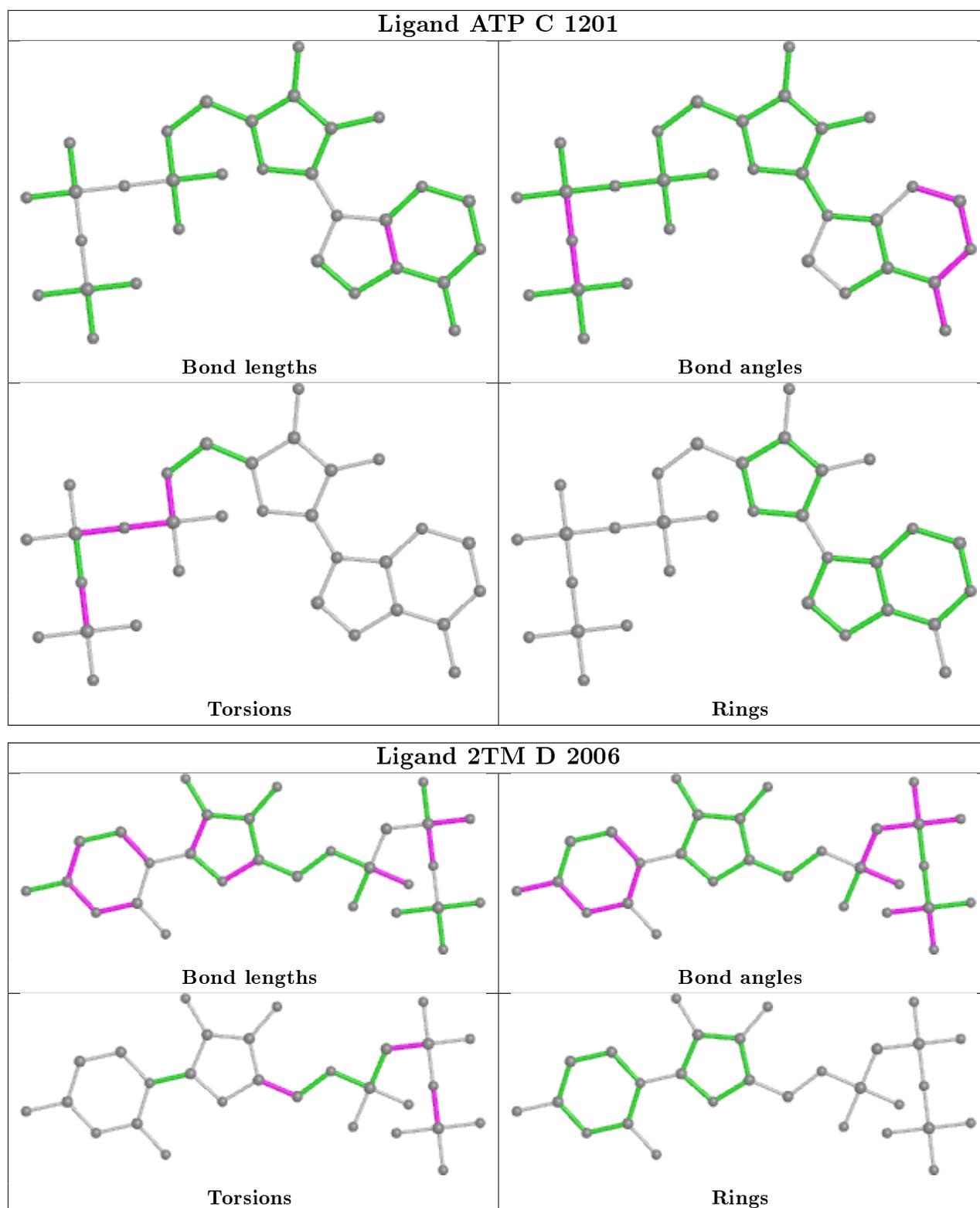
Mol	Chain	Res	Type	Atoms
8	C	1201	ATP	PB-O3B-PG-O3G
8	C	1201	ATP	C5'-O5'-PA-O3A
11	D	2006	2TM	O4'-C4'-C5'-O5'
11	D	2006	2TM	PB-O3B-PG-O2G
11	D	2006	2TM	PA-C1-PB-O2B

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	1201	ATP	2	0
11	D	2006	2TM	2	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

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	231/315 (73%)	0.44	12 (5%) 27 23	36, 68, 92, 101	0
1	B	227/315 (72%)	0.43	12 (5%) 26 22	41, 69, 100, 122	0
2	C	1112/1119 (99%)	0.48	73 (6%) 18 14	25, 58, 115, 135	0
3	D	1494/1524 (98%)	0.59	135 (9%) 9 7	19, 58, 122, 214	0
4	E	94/99 (94%)	0.53	7 (7%) 14 11	34, 73, 111, 114	0
5	F	346/423 (81%)	0.93	61 (17%) 1 1	43, 79, 152, 176	0
6	G	18/22 (81%)	0.19	1 (5%) 24 20	55, 81, 139, 140	0
7	H	25/27 (92%)	0.39	3 (12%) 4 3	70, 100, 149, 169	0
All	All	3547/3844 (92%)	0.57	304 (8%) 10 8	19, 64, 124, 214	0

The worst 5 of 304 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	173	PRO	8.7
2	C	311	PHE	7.6
2	C	300	ASP	7.5
3	D	211	VAL	7.1
3	D	427	VAL	7.0

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

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

### 6.3 Carbohydrates [i](#)

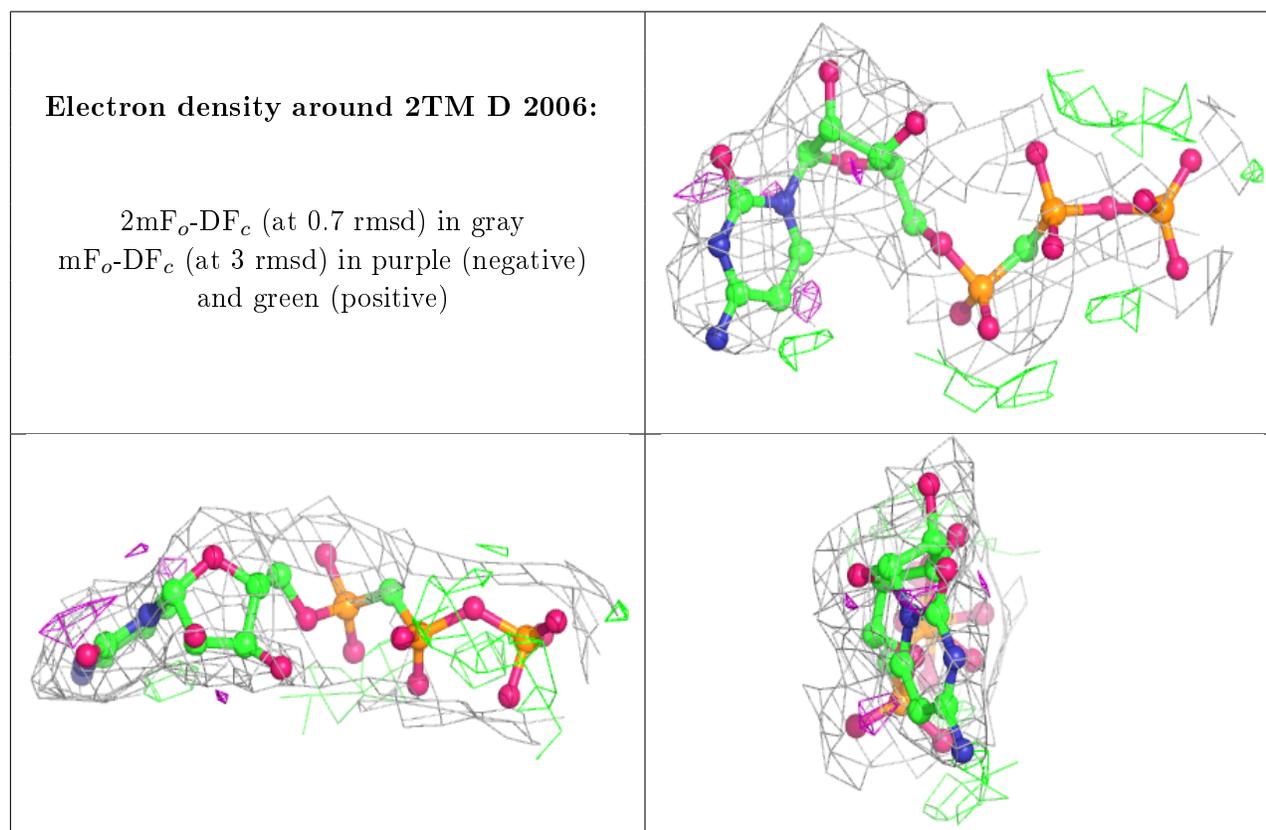
There are no carbohydrates in this entry.

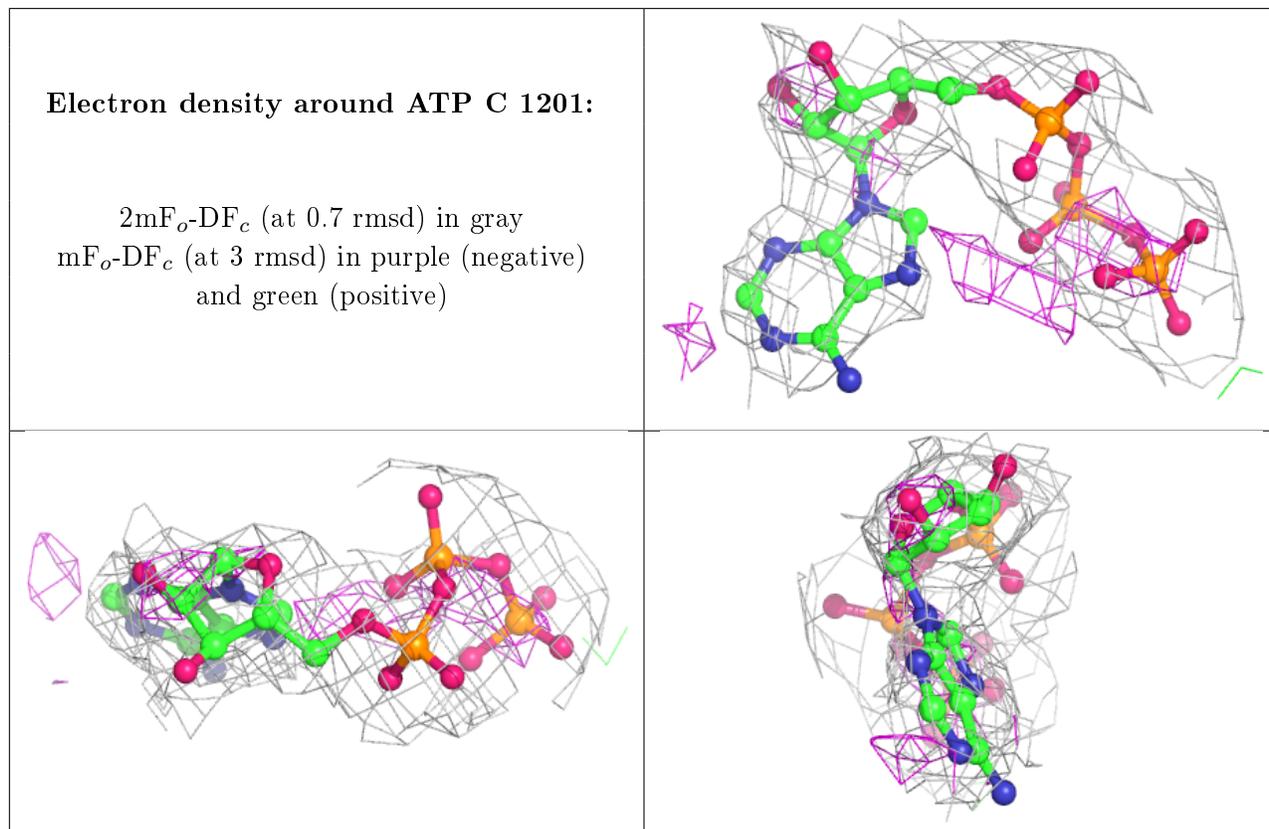
## 6.4 Ligands [\(i\)](#)

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, 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
10	MG	D	2004	1/1	0.41	0.66	54,54,54,54	0
11	2TM	D	2006	29/29	0.85	0.19	38,51,69,94	0
8	ATP	C	1201	31/31	0.88	0.19	38,47,75,83	0
10	MG	D	2003	1/1	0.95	0.26	38,38,38,38	0
10	MG	D	2005	1/1	0.96	0.31	45,45,45,45	0
9	ZN	D	2002	1/1	0.97	0.02	59,59,59,59	0
9	ZN	D	2001	1/1	0.97	0.17	38,38,38,38	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.