



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 15, 2020 – 11:43 pm BST

PDB ID : 4OIP  
Title : Crystal structure of Thermus thermophilus transcription initiation complex soaked with GE23077, ATP, and CMPcPP  
Authors : Zhang, Y.; Ebright, R.H.; Arnold, E.  
Deposited on : 2014-01-20  
Resolution : 3.40 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

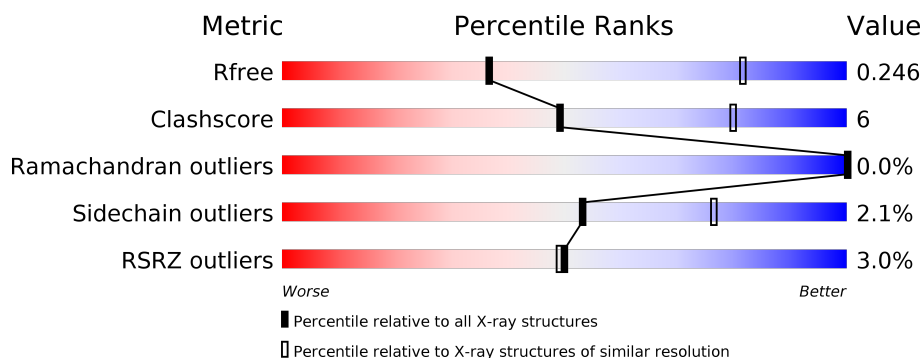
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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.




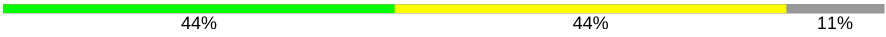

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	<div> <div>2%</div> <div>60% 13% 27%</div> </div>
1	B	315	<div> <div>2%</div> <div>57% 14% 28%</div> </div>
2	C	1119	<div> <div>2%</div> <div>83% 16% ..</div> </div>
3	D	1524	<div> <div>4%</div> <div>80% 17% .</div> </div>
4	E	99	<div> <div>2%</div> <div>84% 10% . 5%</div> </div>
5	F	443	<div> <div>2%</div> <div>67% 11% 22%</div> </div>

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Mol	Chain	Length	Quality of chain
6	G	21	 71% 5% 24%
7	H	27	 44% 44% 11%
8	I	7	 86% 14%

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 28603 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
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
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
3	D	1486	Total	C	N	O	S	0	1	0
			11746	7446	2070	2195	35			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			758	483	132	139	4			

- Molecule 5 is a protein called DNA directed RNA polymerase sigma factor A.

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

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	EXPRESSION TAG	UNP Q5SKW1
F	-18	GLY	-	EXPRESSION TAG	UNP Q5SKW1
F	-17	SER	-	EXPRESSION TAG	UNP Q5SKW1
F	-16	SER	-	EXPRESSION TAG	UNP Q5SKW1
F	-15	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-14	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-13	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-12	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-11	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-10	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-9	SER	-	EXPRESSION TAG	UNP Q5SKW1
F	-8	SER	-	EXPRESSION TAG	UNP Q5SKW1
F	-7	GLY	-	EXPRESSION TAG	UNP Q5SKW1
F	-6	LEU	-	EXPRESSION TAG	UNP Q5SKW1
F	-5	VAL	-	EXPRESSION TAG	UNP Q5SKW1
F	-4	PRO	-	EXPRESSION TAG	UNP Q5SKW1
F	-3	ARG	-	EXPRESSION TAG	UNP Q5SKW1
F	-2	GLY	-	EXPRESSION TAG	UNP Q5SKW1
F	-1	SER	-	EXPRESSION TAG	UNP Q5SKW1
F	0	HIS	-	EXPRESSION TAG	UNP Q5SKW1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	16	Total	C	N	O	P	0	0	0
			331	156	63	96	16			

- Molecule 7 is a DNA chain called 5'-D(\*TP\*AP\*TP\*AP\*AP\*TP\*GP\*GP\*GP\*AP\*GP\*CP\*TP\*GP\*TP\*CP\*AP\*CP\*GP\*GP\*AP\*TP\*GP\*CP\*AP\*GP\*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	24	Total	C	N	O	P	0	0	0
			495	236	94	142	23			

- Molecule 8 is a protein called GE23077.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	I	7	Total	C	N	O	0	0	0
			50	26	9	15			

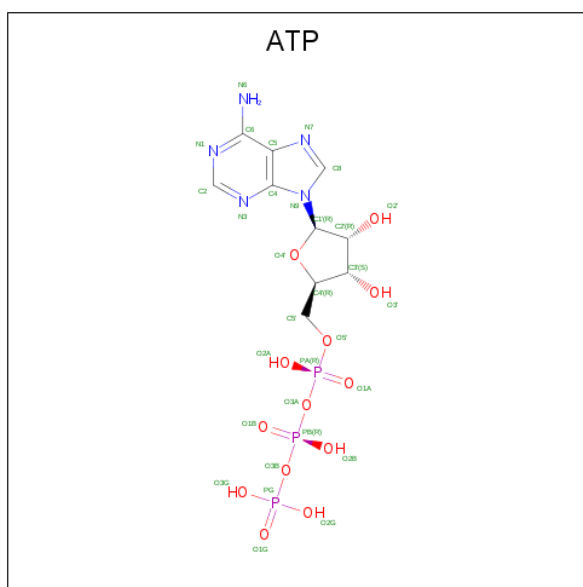
- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

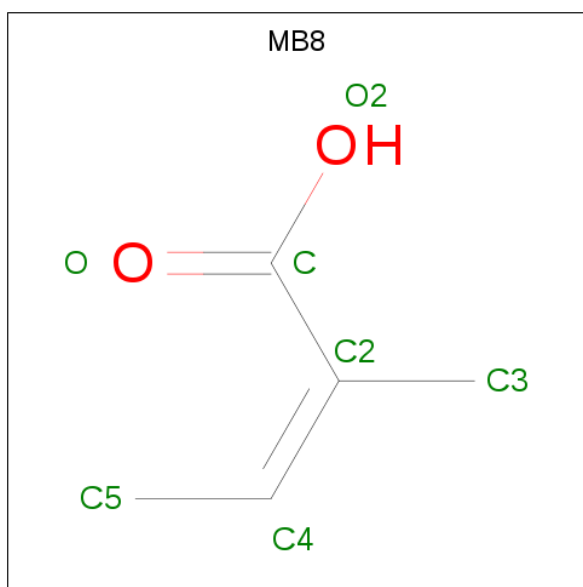
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Mg	0	0
			1	1		
9	D	4	Total	Mg	0	0
			4	4		
9	F	1	Total	Mg	0	0
			1	1		

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 11 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	I	1	Total	C	O	0	0
			2	1	1		

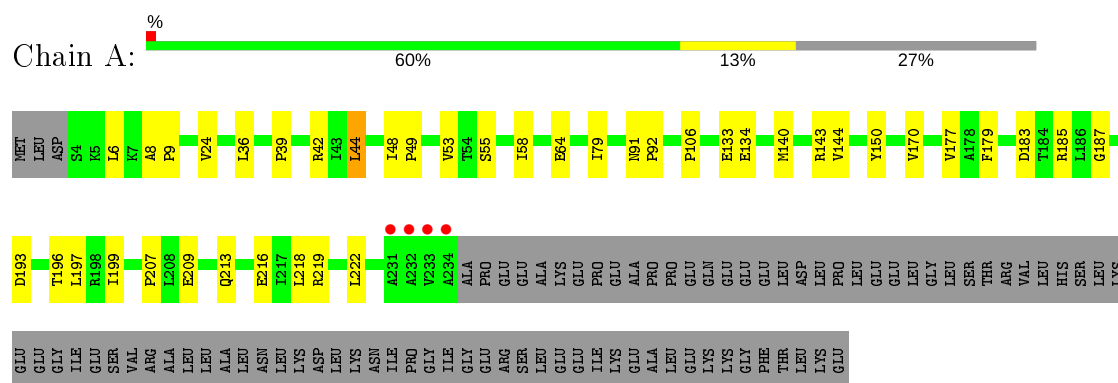
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	D	3	Total	O	0	0
			3	3		

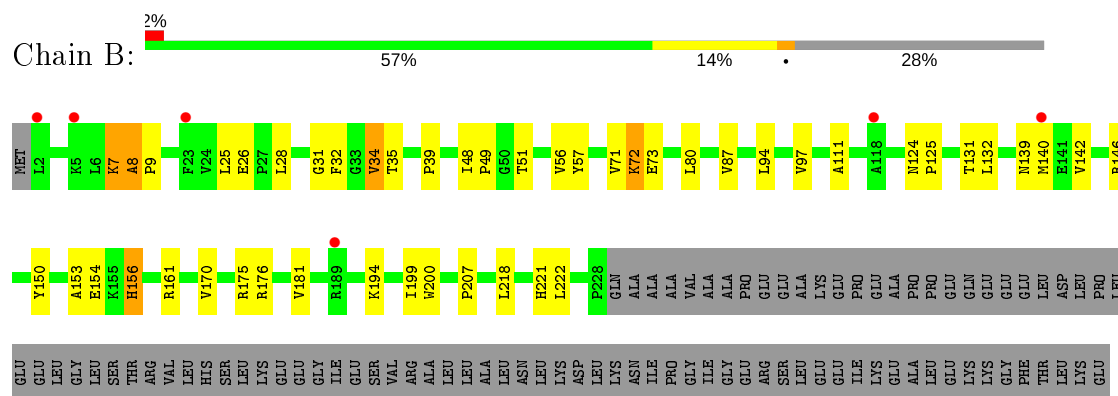
### 3 Residue-property plots [i](#)

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.

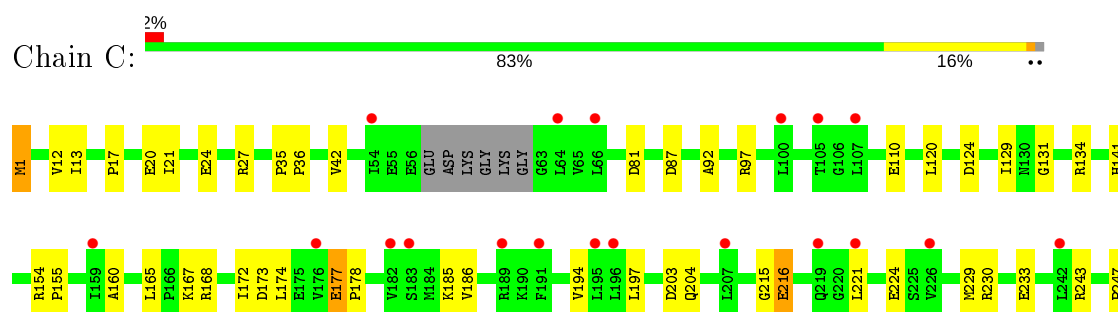
- Molecule 1: DNA-directed RNA polymerase subunit alpha



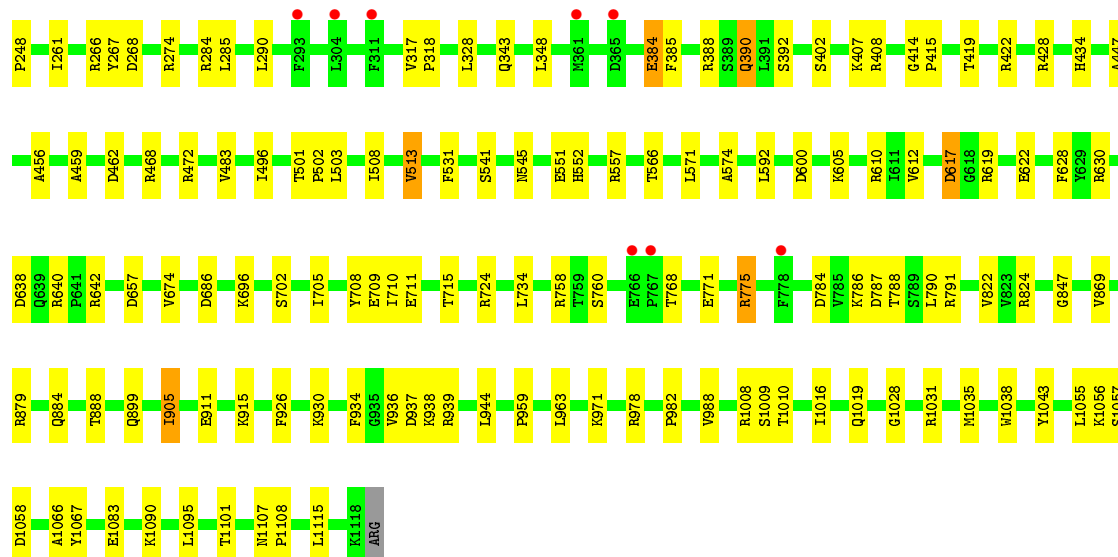
- Molecule 1: DNA-directed RNA polymerase subunit alpha



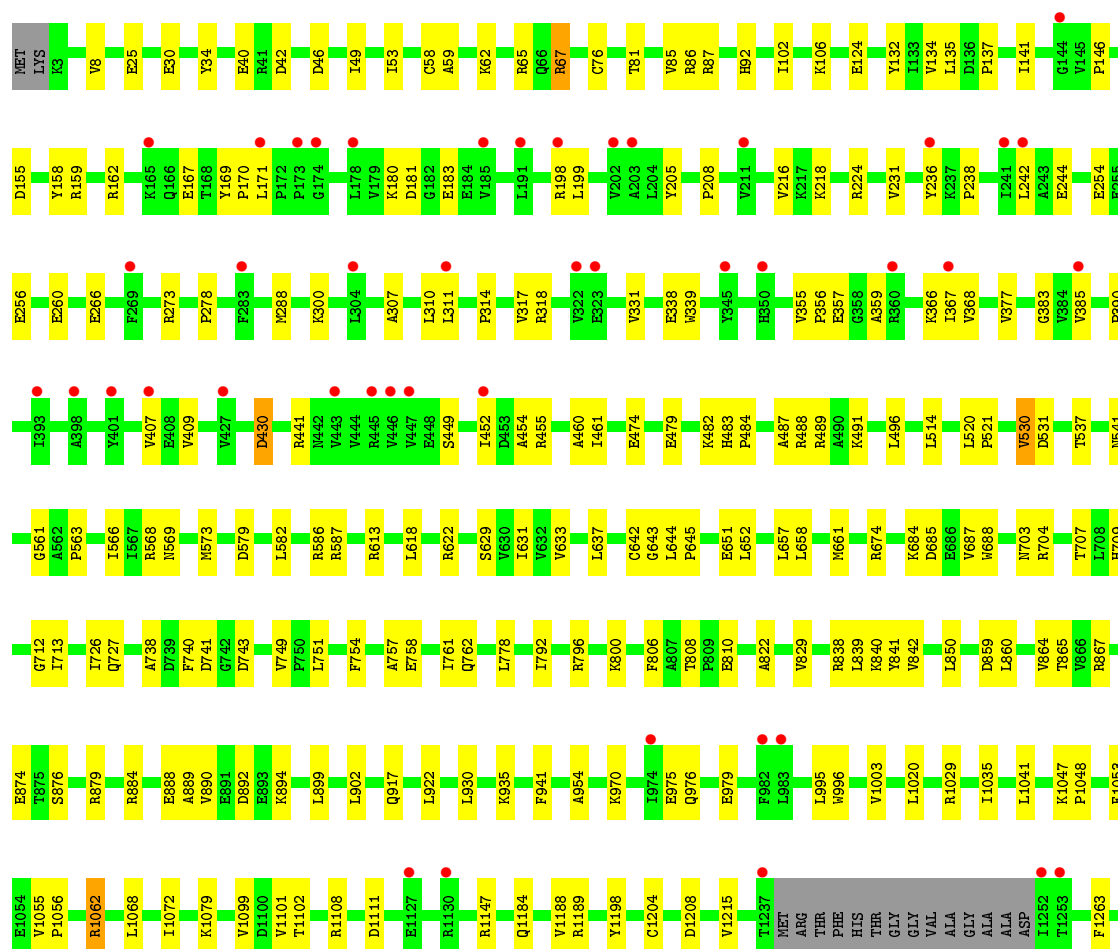
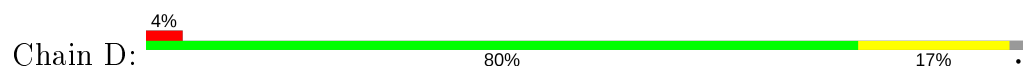
- Molecule 2: DNA-directed RNA polymerase subunit beta

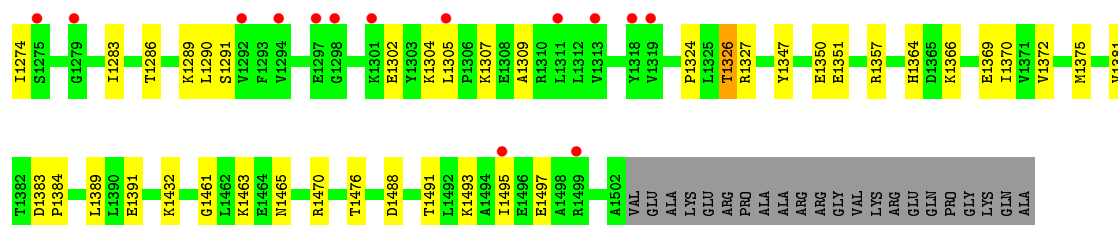




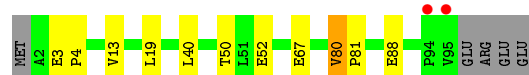
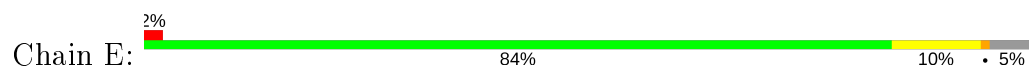


• Molecule 3: DNA-directed RNA polymerase subunit beta'

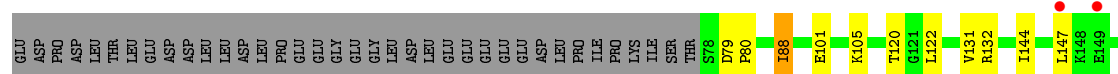
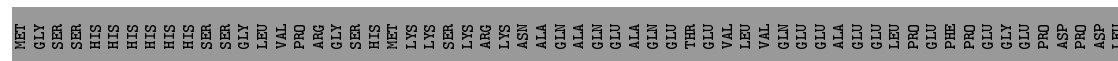




- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 5: DNA directed RNA polymerase sigma factor A



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



- Molecule 7: 5'-D(\*TP\*AP\*TP\*AP\*AP\*TP\*GP\*GP\*GP\*AP\*GP\*CP\*TP\*GP\*TP\*CP\*AP\*C P\*GP\*GP\*AP\*TP\*GP\*CP\*AP\*GP\*G)-3'



- Molecule 8: GE23077

Chain I:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.92Å 104.39Å 294.21Å 90.00° 98.97° 90.00°	Depositor
Resolution (Å)	49.12 – 3.40 49.12 – 3.40	Depositor EDS
% Data completeness (in resolution range)	81.5 (49.12-3.40) 81.5 (49.12-3.40)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.208 , 0.246 0.211 , 0.246	Depositor DCC
$R_{free}$ test set	1643 reflections (2.66%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	95.8	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 26.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.018 for $1/2^*h-3/2^*k,-1/2^*h-1/2^*k,-1/2^*h+1/2^*k-l$ 0.014 for $1/2^*h+3/2^*k,1/2^*h-1/2^*k,-1/2^*h-1/2^*k-l$	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	28603	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FGL, ZN, 2TL, DVA, MG, 2RA, DSN, MB8, ATP, 0QZ, R2T

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	0.22	0/1841	0.44	0/2504
1	B	0.22	0/1821	0.45	0/2476
2	C	0.22	0/8941	0.42	0/12092
3	D	0.22	0/11955	0.42	0/16163
4	E	0.23	0/772	0.39	0/1040
5	F	0.21	0/2852	0.38	0/3837
6	G	0.44	0/371	0.93	0/571
7	H	0.46	0/556	1.02	0/858
All	All	0.23	0/29109	0.45	0/39541

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
8	I	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	I	5	2TL	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1809	0	1863	29	0
1	B	1789	0	1841	32	0
2	C	8774	0	8877	110	0
3	D	11746	0	11984	154	0
4	E	758	0	770	6	0
5	F	2807	0	2882	31	0
6	G	331	0	180	2	0
7	H	495	0	272	12	0
8	I	50	0	37	0	0
9	B	1	0	0	0	0
9	D	4	0	0	0	0
9	F	1	0	0	0	0
10	D	2	0	0	0	0
11	D	31	0	12	1	0
12	I	2	0	0	0	0
13	D	3	0	0	0	0
All	All	28603	0	28718	337	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 6.

The worst 5 of 337 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:42:ARG:NH2	1:B:31:GLY:O	2.18	0.77
2:C:165:LEU:HB2	2:C:168:ARG:HG3	1.68	0.74
1:A:44:LEU:HA	1:A:48:ILE:HG12	1.70	0.73
3:D:273:ARG:HB3	3:D:278:PRO:HA	1.71	0.72
3:D:65:ARG:NH1	5:F:378:GLY:O	2.23	0.72

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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%)	227 (99%)	2 (1%)	0	100	100
1	B	225/315 (71%)	221 (98%)	3 (1%)	1 (0%)	34	67
2	C	1108/1119 (99%)	1088 (98%)	20 (2%)	0	100	100
3	D	1483/1524 (97%)	1463 (99%)	20 (1%)	0	100	100
4	E	92/99 (93%)	91 (99%)	1 (1%)	0	100	100
5	F	344/443 (78%)	339 (98%)	5 (2%)	0	100	100
All	All	3481/3815 (91%)	3429 (98%)	51 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	8	ALA

### 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	200/273 (73%)	198 (99%)	2 (1%)	76	88
1	B	200/273 (73%)	194 (97%)	6 (3%)	41	68
2	C	936/941 (100%)	913 (98%)	23 (2%)	47	72
3	D	1254/1279 (98%)	1231 (98%)	23 (2%)	59	79
4	E	82/88 (93%)	80 (98%)	2 (2%)	49	74
5	F	301/388 (78%)	296 (98%)	5 (2%)	60	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2973/3242 (92%)	2912 (98%)	61 (2%)	53 76

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	775	ARG
3	D	81	THR
5	F	88	ILE
2	C	905	ILE
2	C	1057	SER

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

Mol	Chain	Res	Type
2	C	834	GLN
3	D	696	HIS
3	D	724	GLN
3	D	762	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 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	$\# Z  > 2$
8	R2T	I	4	8	8,10,11	1.87	2 (25%)	6,13,15	1.04	0
8	2TL	I	5	8	5,6,7	1.02	0	6,7,9	0.86	0
8	FGL	I	7	8	2,6,7	0.60	0	0,7,9	0.00	-
8	2RA	I	1	8,12	3,5,6	0.62	0	1,5,7	0.29	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	0QZ	I	6	8	4,5,6	1.56	1 (25%)	2,5,7	0.63	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
8	R2T	I	4	8	-	2/13/14/16	-
8	2TL	I	5	8	-	1/5/6/8	-
8	FGL	I	7	8	-	0/0/6/8	-
8	2RA	I	1	8,12	-	0/2/4/6	-
8	0QZ	I	6	8	-	1/3/4/6	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	4	R2T	CD-NE2	4.19	1.43	1.32
8	I	6	0QZ	OB-CA	-2.95	1.38	1.43
8	I	4	R2T	OB1-CB	-2.24	1.37	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	5	2TL	O-C-CA-CB
8	I	6	0QZ	N-C1-CA-C
8	I	4	R2T	OE1-CD-CG-OG1
8	I	4	R2T	NE2-CD-CG-OG1

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 10 ligands modelled in this entry, 8 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	$\# Z  > 2$
12	MB8	I	101	8	0,1,6	0.00	-	-		
11	ATP	D	2007	9	26,33,33	0.93	1 (3%)	31,52,52	1.59	5 (16%)

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
11	ATP	D	2007	9	-	6/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	2007	ATP	C5-C4	2.50	1.47	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	2007	ATP	PA-O3A-PB	-3.58	120.53	132.83
11	D	2007	ATP	PB-O3B-PG	-3.39	121.19	132.83
11	D	2007	ATP	C3'-C2'-C1'	3.32	105.97	100.98
11	D	2007	ATP	N3-C2-N1	-3.23	123.63	128.68
11	D	2007	ATP	C4-C5-N7	-2.69	106.59	109.40

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	D	2007	ATP	C5'-O5'-PA-O1A

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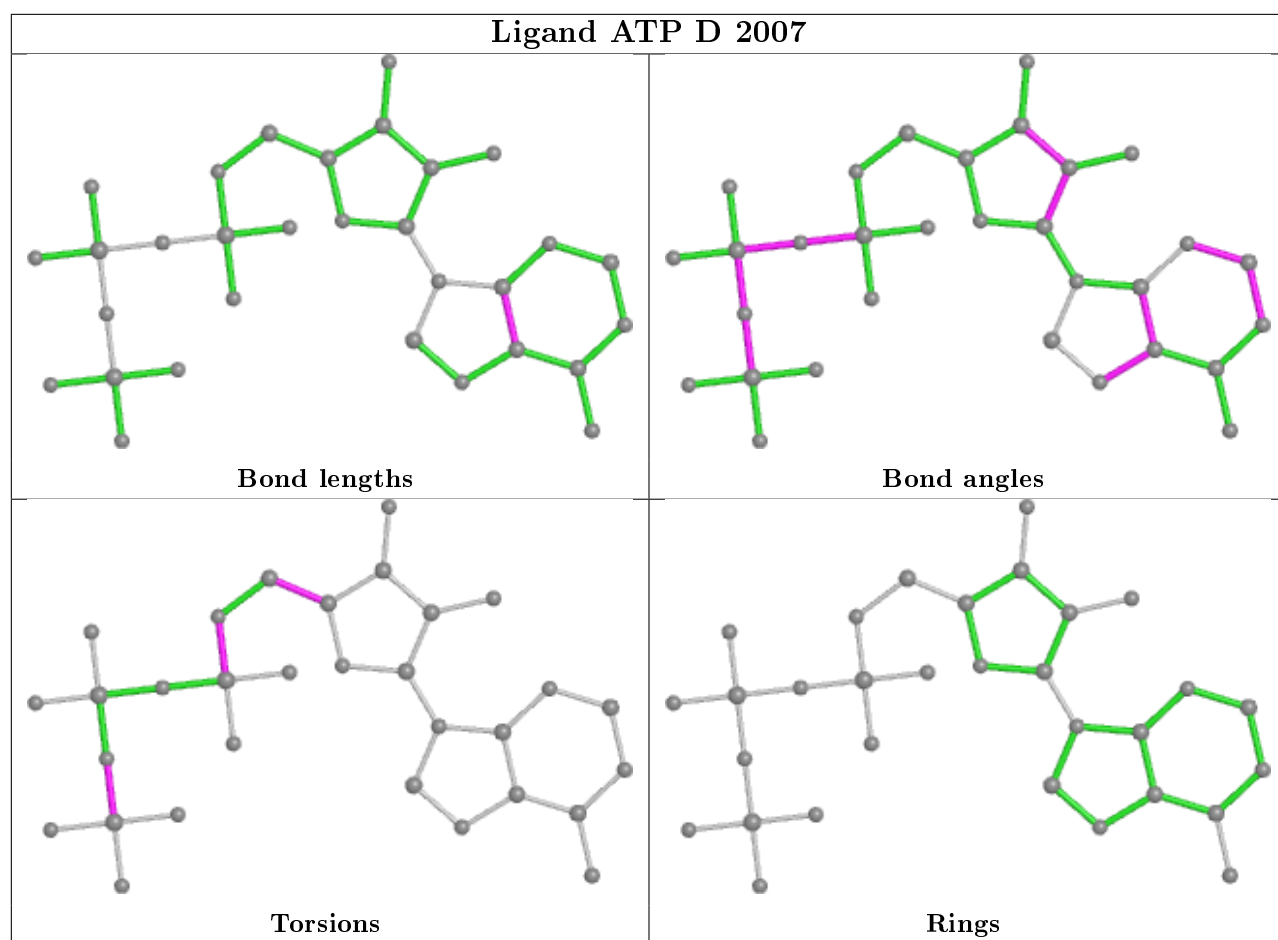
Mol	Chain	Res	Type	Atoms
11	D	2007	ATP	C5'-O5'-PA-O2A
11	D	2007	ATP	C3'-C4'-C5'-O5'
11	D	2007	ATP	O4'-C4'-C5'-O5'
11	D	2007	ATP	PB-O3B-PG-O1G

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	2007	ATP	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, 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%)	-0.08	4 (1%) 70 68	38, 57, 83, 133	0
1	B	227/315 (72%)	-0.03	6 (2%) 56 54	39, 69, 97, 117	0
2	C	1112/1119 (99%)	0.08	27 (2%) 59 57	19, 52, 116, 143	0
3	D	1486/1524 (97%)	0.16	58 (3%) 39 38	21, 56, 116, 157	0
4	E	94/99 (94%)	-0.20	2 (2%) 63 62	32, 60, 98, 101	0
5	F	346/443 (78%)	0.04	8 (2%) 60 59	31, 73, 124, 144	0
6	G	16/21 (76%)	-0.26	0 100 100	65, 94, 203, 205	0
7	H	24/27 (88%)	-0.29	0 100 100	65, 123, 198, 228	0
8	I	0/7	-	-	-	-
All	All	3536/3870 (91%)	0.08	105 (2%) 50 49	19, 59, 117, 228	0

The worst 5 of 105 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1237	THR	8.8
5	F	422	LEU	5.5
2	C	64	LEU	5.5
5	F	414	ARG	5.1
2	C	221	LEU	5.0

### 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, 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	FGL	I	7	7/8	0.90	0.23	33,36,38,39	0
8	R2T	I	4	11/12	0.92	0.21	34,36,45,46	0
8	2RA	I	1	6/7	0.94	0.15	33,35,41,50	0
8	DSN	I	2	6/7	0.95	0.20	34,37,50,56	0
8	0QZ	I	6	6/7	0.97	0.22	33,33,37,38	0
8	2TL	I	5	7/8	0.97	0.22	37,41,43,44	0
8	DVA	I	3	7/8	0.98	0.18	33,36,41,47	0

### 6.3 Carbohydrates [i](#)

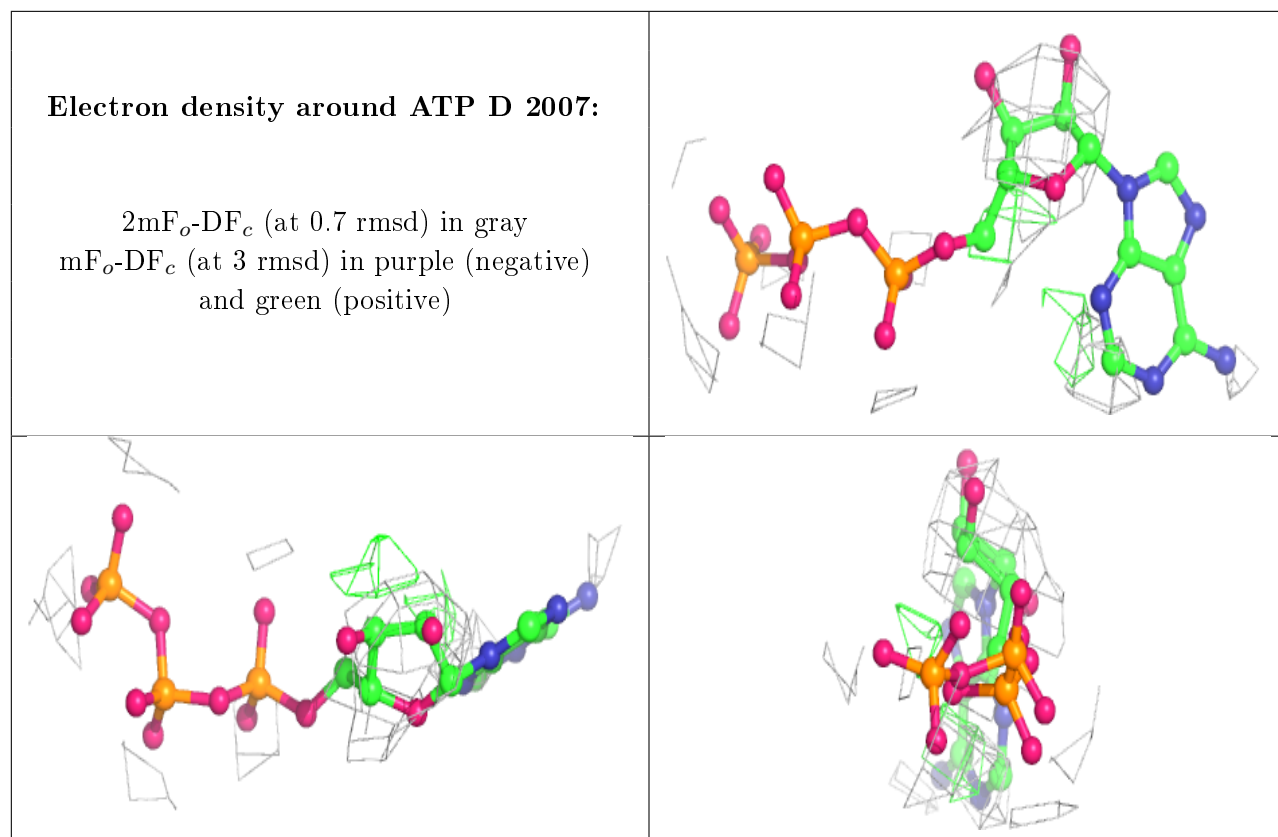
There are no carbohydrates in this entry.

### 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( $\text{\AA}^2$ )	Q<0.9
9	MG	F	2001	1/1	0.56	0.18	68,68,68,68	0
9	MG	D	2006	1/1	0.73	0.17	50,50,50,50	0
9	MG	B	2001	1/1	0.78	0.35	93,93,93,93	0
11	ATP	D	2007	31/31	0.91	0.35	53,108,121,122	10
9	MG	D	2004	1/1	0.92	0.41	69,69,69,69	0
12	MB8	I	101	2/7	0.92	0.16	34,34,34,34	0
9	MG	D	2005	1/1	0.96	0.42	33,33,33,33	0
9	MG	D	2003	1/1	0.98	0.20	26,26,26,26	0
10	ZN	D	2002	1/1	0.98	0.10	79,79,79,79	0
10	ZN	D	2001	1/1	1.00	0.19	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.