



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:44 PM UTC

PDB ID : 3S1Q / pdb_00003s1q
Title : RNA Polymerase II Initiation Complex with a 5-nt 3'-deoxy RNA soaked with ATP
Authors : Liu, X.; Bushnell, D.A.; Silva, D.A.; Huang, X.; Kornberg, R.D.
Deposited on : 2011-05-16
Resolution : 3.30 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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

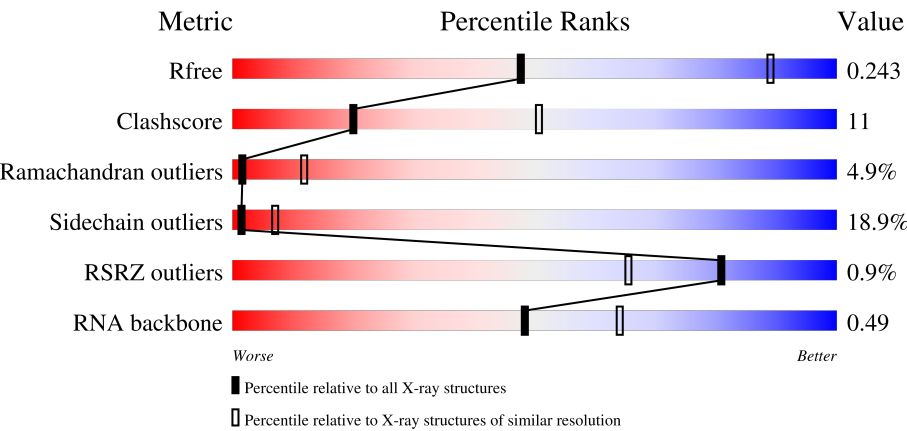
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

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	1733	% 46% 26% 8% • 19%
2	B	1224	% 52% 30% 7% • 9%
3	C	318	49% 26% 7% • 16%
4	E	215	65% 31% •

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Mol	Chain	Length	Quality of chain
5	F	155	35%17%45%
6	H	146	% 51%34%6%9%
7	I	122	2% 64%29%
8	J	70	41%33%16%7%
9	K	120	52%38%6%5%
10	L	70	4% 24%27%11%34%
11	R	5	40%60%
12	T	29	38%7%55%

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 28703 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1405	Total	C	N	O	S	0	0	0
			11043	6965	1936	2081	61			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1114	Total	C	N	O	S	0	0	0
			8861	5610	1549	1647	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	85	Total	C	N	O	S	0	0	0
			688	439	116	130	3			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 11 is a RNA chain called RNA (5'-R(*AP*GP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	5	Total	C	N	O	P	0	0	0
			109	50	25	30	4			

- Molecule 12 is a DNA chain called DNA (5'-D(*CP*TP*AP*CP*CP*GP*AP*TP*AP*AP*GP*CP*AP*GP*AP*CP*GP*AP*TP*CP*CP*TP*CP*TP*CP*GP*AP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	13	Total	C	N	O	P	0	0	0
			261	125	43	80	13			

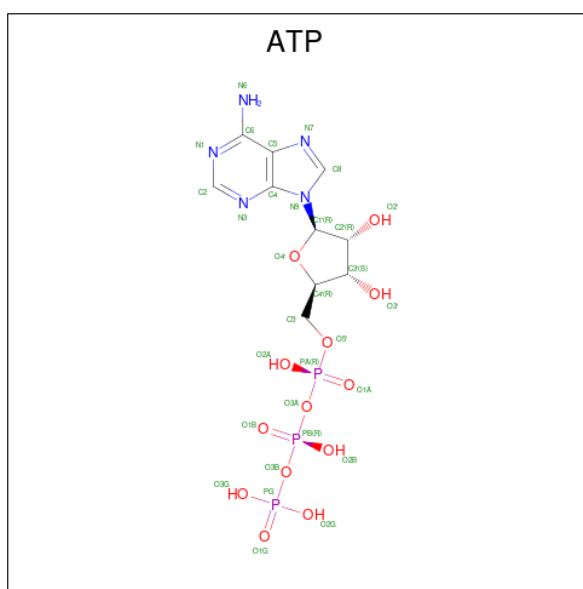
- Molecule 13 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	2	Total	Mg	0	0
			2	2		

- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	2	Total Zn 2 2	0	0
14	B	1	Total Zn 1 1	0	0
14	C	1	Total Zn 1 1	0	0
14	I	2	Total Zn 2 2	0	0
14	J	1	Total Zn 1 1	0	0
14	L	1	Total Zn 1 1	0	0

- Molecule 15 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$).

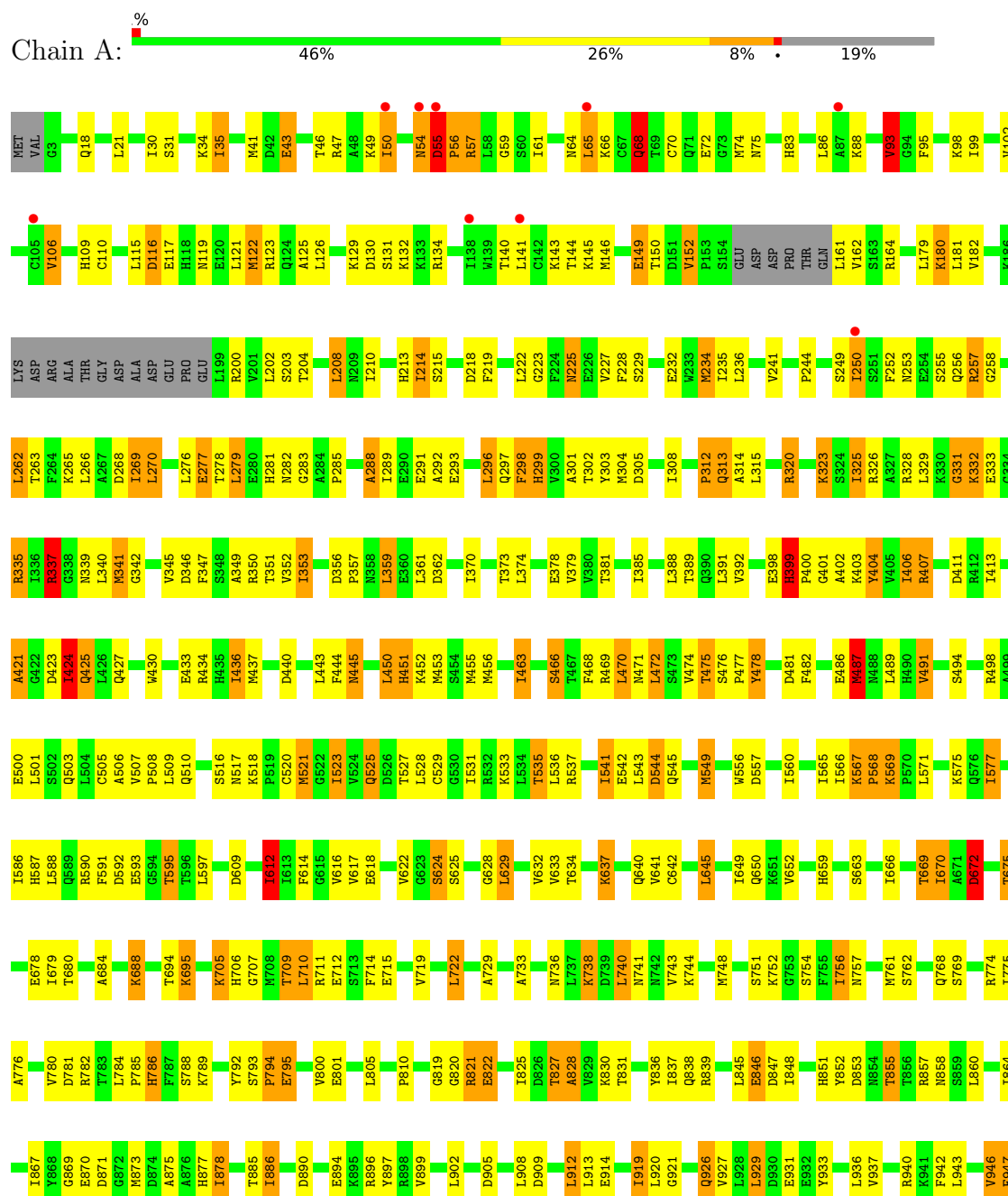


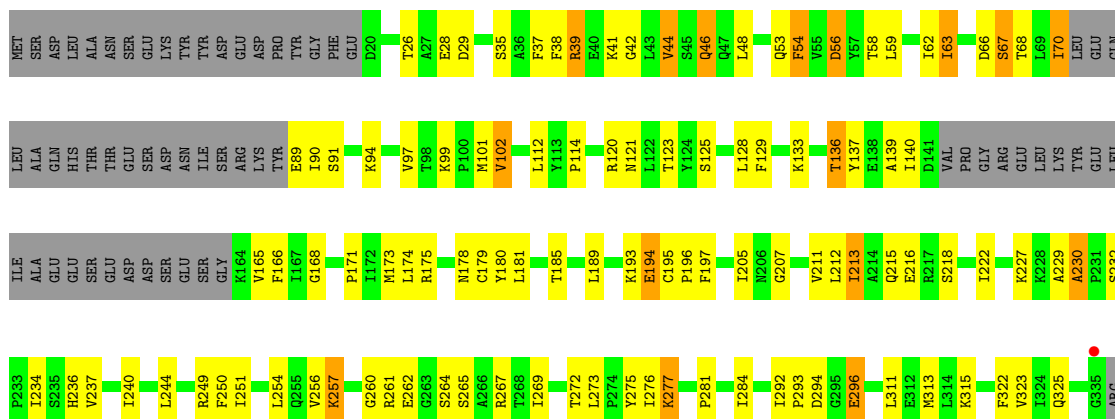
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	A	1	Total 31	C 10	N 5	O 13	P 3	0	0

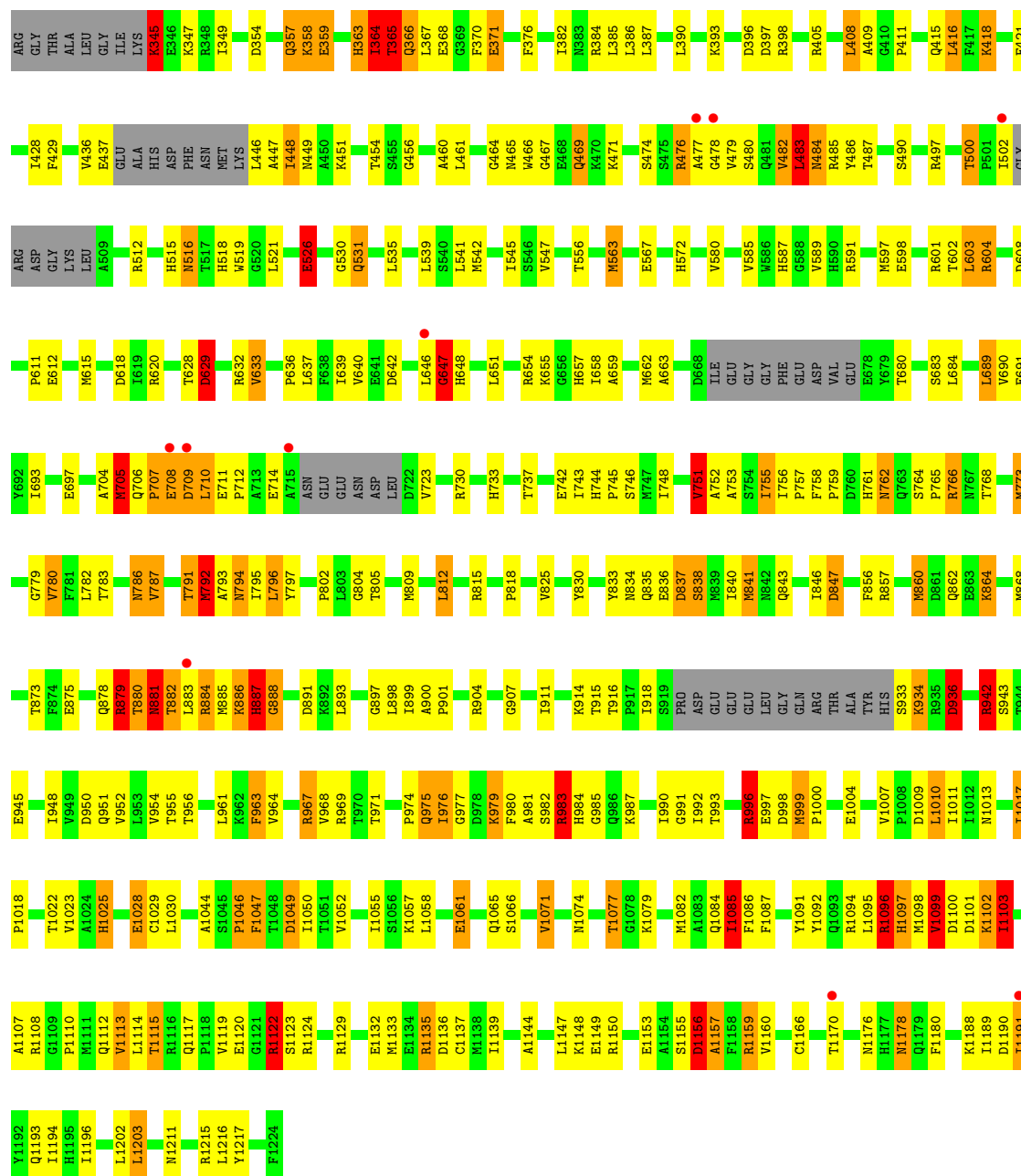
3 Residue-property plots

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.

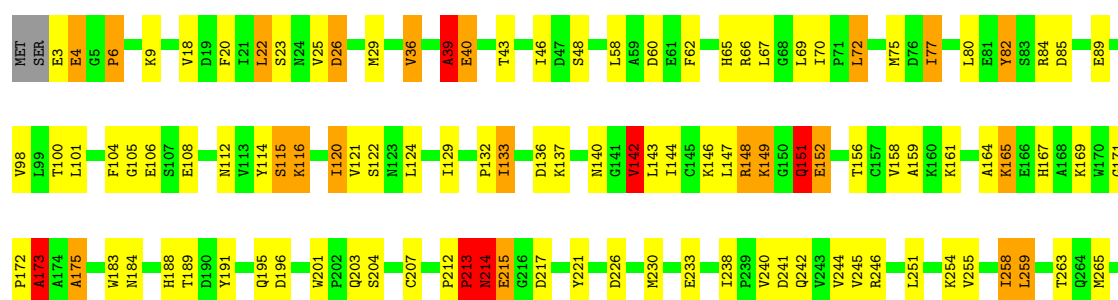
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

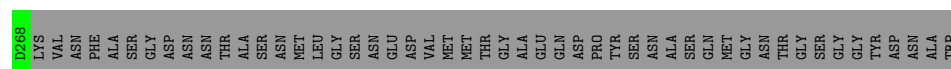






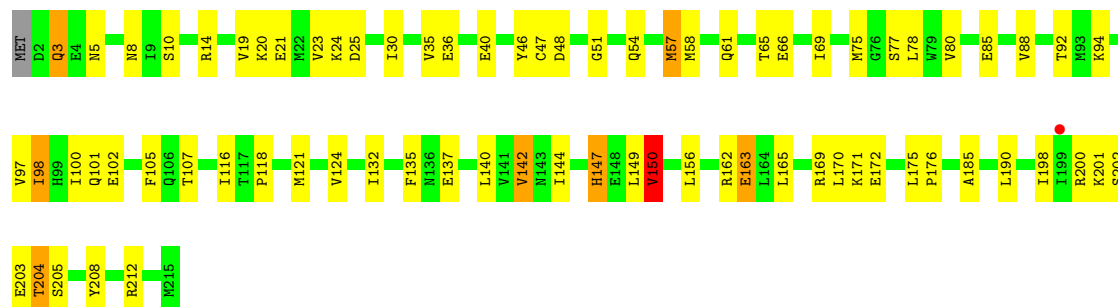
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3





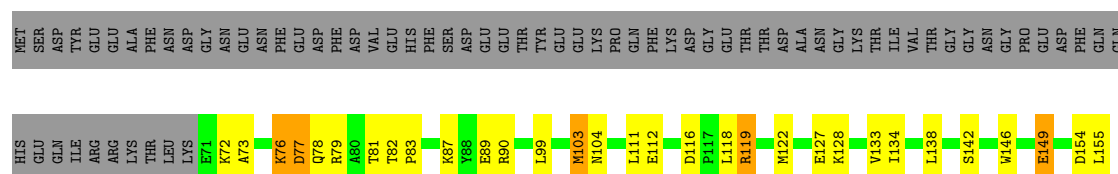
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 65% 31% .



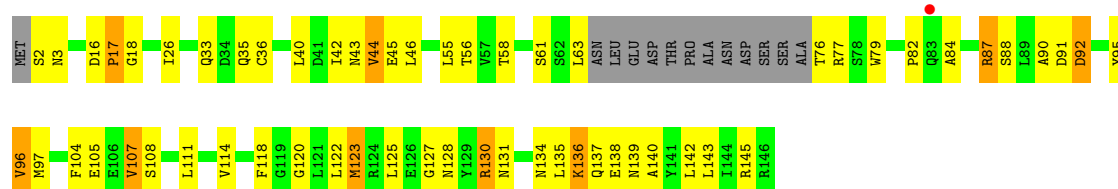
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 35% 17% . 45%



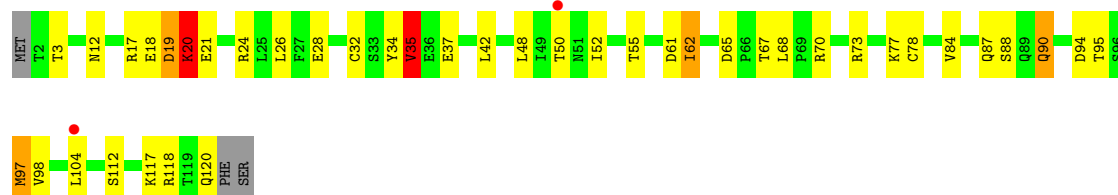
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 51% 34% 6% 9%

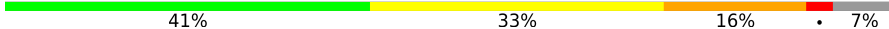


- Molecule 7: DNA-directed RNA polymerase II subunit RPB9

Chain I: 2% 64% 29% . . .



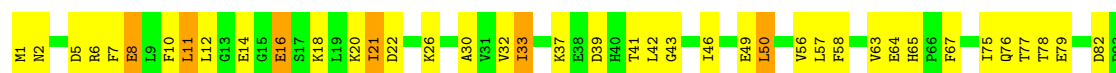
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 



- Molecule 9: DNA-directed RNA polymerase II subunit RPB11

Chain K: 



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L: 



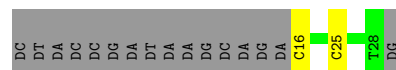
- Molecule 11: RNA (5'-R(*AP*GP*AP*GP*G)-3')

Chain R: 



- Molecule 12: DNA (5'-D(*CP*TP*AP*CP*CP*GP*AP*TP*AP*AP*GP*CP*AP*GP*AP*CP*GP*AP*TP*CP*CP*TP*CP*TP*CP*GP*AP*TP*G)-3')

Chain T: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	161.94Å 220.53Å 193.72Å 90.00° 98.48° 90.00°	Depositor
Resolution (Å)	29.67 – 3.30 29.67 – 3.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.67-3.30) 99.1 (29.67-3.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 3.31Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.8.0, BUSTER 2.8.0	Depositor
R, R_{free}	0.176 , 0.229 0.192 , 0.243	Depositor DCC
R_{free} test set	4995 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	97.3	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 113.7	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	0.96	EDS
Total number of atoms	28703	wwPDB-VP
Average B, all atoms (Å ²)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ZN, MG

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	0.88	3/11241 (0.0%)	1.56	142/15199 (0.9%)
2	B	0.92	4/9033 (0.0%)	1.53	115/12181 (0.9%)
3	C	0.84	2/2133 (0.1%)	1.48	26/2891 (0.9%)
4	E	0.81	0/1788	1.46	20/2406 (0.8%)
5	F	0.84	0/700	1.41	3/945 (0.3%)
6	H	0.83	0/1086	1.33	7/1470 (0.5%)
7	I	0.85	0/989	1.42	7/1331 (0.5%)
8	J	1.01	2/541 (0.4%)	1.71	10/727 (1.4%)
9	K	0.80	0/937	1.46	7/1265 (0.6%)
10	L	0.97	0/365	1.78	9/485 (1.9%)
11	R	0.50	0/123	1.07	0/191
12	T	0.48	0/290	1.38	3/444 (0.7%)
All	All	0.88	11/29226 (0.0%)	1.52	349/39535 (0.9%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	1	MET	SD-CE	6.91	1.96	1.79
8	J	6	ARG	CA-C	6.80	1.61	1.52
2	B	563	MET	SD-CE	-6.31	1.63	1.79
1	A	487	MET	SD-CE	-6.27	1.63	1.79
2	B	705	MET	SD-CE	-5.97	1.64	1.79

The worst 5 of 349 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	GLU	N-CA-C	-9.89	103.35	114.62
3	C	172	PRO	CA-C-N	9.02	138.77	121.54
3	C	172	PRO	C-N-CA	9.02	138.77	121.54
2	B	881	ASN	CA-C-N	8.96	133.02	120.29
2	B	881	ASN	C-N-CA	8.96	133.02	120.29

There are no chirality outliers.

There are no planarity outliers.

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	11043	0	11133	293	0
2	B	8861	0	8884	228	0
3	C	2095	0	2051	58	0
4	E	1752	0	1776	39	0
5	F	688	0	707	10	0
6	H	1068	0	1040	21	0
7	I	971	0	927	13	0
8	J	532	0	542	22	0
9	K	919	0	929	28	0
10	L	363	0	386	14	0
11	R	109	0	55	2	0
12	T	261	0	148	0	0
13	A	2	0	0	0	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	31	0	12	5	0
All	All	28703	0	28590	651	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 11.

The worst 5 of 651 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)
15:A:1736:ATP:H5'1	15:A:1736:ATP:H8	1.25	1.01
1:A:1123:GLY:HA3	1:A:1124:HIS:HB2	1.45	0.99
1:A:855:THR:HG21	1:A:857:ARG:HE	1.37	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:830:LYS:HG3	1:A:1098:VAL:HG11	1.55	0.87
1:A:525:GLN:HB2	2:B:835:GLN:HE21	1.43	0.84

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	1395/1733 (80%)	1177 (84%)	149 (11%)	69 (5%)	1	12
2	B	1096/1224 (90%)	927 (85%)	110 (10%)	59 (5%)	1	10
3	C	264/318 (83%)	235 (89%)	19 (7%)	10 (4%)	2	16
4	E	212/215 (99%)	199 (94%)	11 (5%)	2 (1%)	14	43
5	F	83/155 (54%)	73 (88%)	7 (8%)	3 (4%)	2	17
6	H	129/146 (88%)	93 (72%)	24 (19%)	12 (9%)	0	3
7	I	117/122 (96%)	103 (88%)	10 (8%)	4 (3%)	3	18
8	J	63/70 (90%)	55 (87%)	6 (10%)	2 (3%)	3	19
9	K	112/120 (93%)	101 (90%)	8 (7%)	3 (3%)	4	22
10	L	44/70 (63%)	28 (64%)	7 (16%)	9 (20%)	0	0
All	All	3515/4173 (84%)	2991 (85%)	351 (10%)	173 (5%)	1	12

5 of 173 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	215	SER
1	A	250	ILE
1	A	312	PRO
1	A	556	TRP

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	1225/1520 (81%)	980 (80%)	245 (20%)	1	6
2	B	967/1061 (91%)	790 (82%)	177 (18%)	2	7
3	C	234/274 (85%)	192 (82%)	42 (18%)	2	8
4	E	196/197 (100%)	173 (88%)	23 (12%)	5	20
5	F	75/137 (55%)	59 (79%)	16 (21%)	1	5
6	H	117/128 (91%)	98 (84%)	19 (16%)	2	11
7	I	113/116 (97%)	91 (80%)	22 (20%)	1	6
8	J	60/65 (92%)	44 (73%)	16 (27%)	0	2
9	K	99/102 (97%)	82 (83%)	17 (17%)	2	10
10	L	40/57 (70%)	26 (65%)	14 (35%)	0	1
All	All	3126/3657 (86%)	2535 (81%)	591 (19%)	1	7

5 of 591 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	265	MET
9	K	95	ILE
4	E	107	THR
3	C	263	THR
6	H	136	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	657	HIS
2	B	1097	HIS
2	B	744	HIS
2	B	862	GLN
3	C	17	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	3/5 (60%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 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	$\# Z > 2$
15	ATP	A	1736	13	32,33,33	1.47	7 (21%)	48,52,52	1.37	8 (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
15	ATP	A	1736	13	-	6/22/38/38	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1736	ATP	PA-O3A	3.65	1.63	1.59
15	A	1736	ATP	PB-O3A	3.64	1.63	1.59
15	A	1736	ATP	C2-N1	2.43	1.38	1.33
15	A	1736	ATP	PB-O1B	2.38	1.59	1.50
15	A	1736	ATP	C2-N3	2.13	1.37	1.33

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1736	ATP	O3'-C3'-C2'	3.31	122.43	111.82
15	A	1736	ATP	O4'-C1'-N9	3.19	114.22	108.09
15	A	1736	ATP	O3A-PA-O1A	2.87	119.35	110.70
15	A	1736	ATP	O3'-C3'-C4'	2.47	118.19	111.08
15	A	1736	ATP	O3G-PG-O3B	2.43	112.78	104.64

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

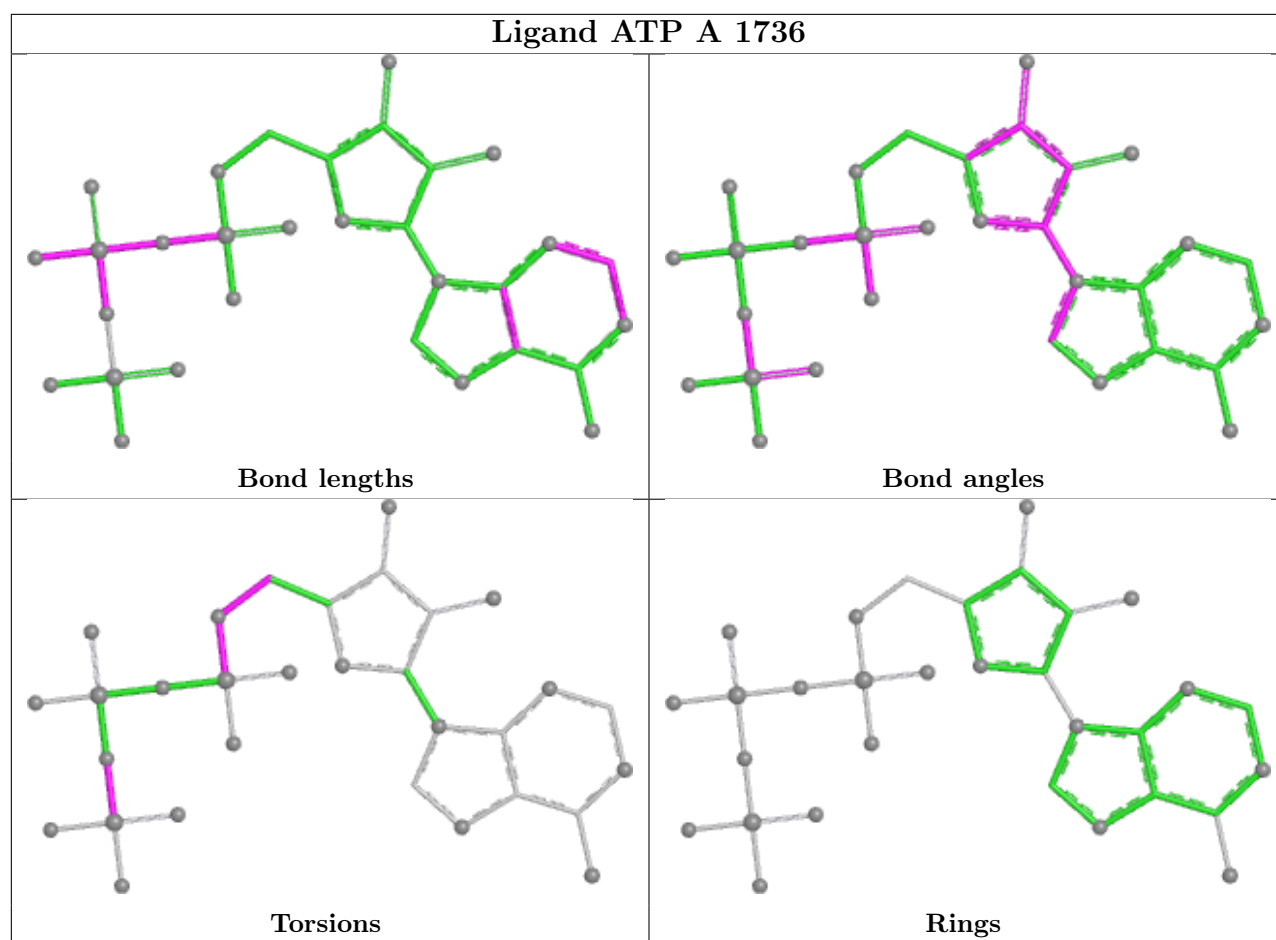
Mol	Chain	Res	Type	Atoms
15	A	1736	ATP	PB-O3B-PG-O3G
15	A	1736	ATP	C5'-O5'-PA-O3A
15	A	1736	ATP	PB-O3B-PG-O2G
15	A	1736	ATP	C4'-C5'-O5'-PA
15	A	1736	ATP	C5'-O5'-PA-O1A

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	1736	ATP	5	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 [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, 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	1405/1733 (81%)	-0.12	13 (0%) 81 65	78, 133, 223, 254	0
2	B	1114/1224 (91%)	-0.13	11 (0%) 79 63	71, 115, 183, 241	0
3	C	266/318 (83%)	-0.29	0 100 100	87, 113, 153, 215	0
4	E	214/215 (99%)	-0.23	1 (0%) 87 76	102, 159, 206, 216	0
5	F	85/155 (54%)	-0.30	0 100 100	109, 139, 178, 196	0
6	H	133/146 (91%)	0.04	1 (0%) 82 68	131, 172, 202, 222	0
7	I	119/122 (97%)	-0.10	2 (1%) 69 50	93, 138, 185, 200	0
8	J	65/70 (92%)	-0.34	0 100 100	81, 104, 136, 151	0
9	K	114/120 (95%)	-0.32	0 100 100	87, 123, 150, 175	0
10	L	46/70 (65%)	0.30	3 (6%) 25 17	99, 155, 188, 214	0
11	R	5/5 (100%)	0.02	0 100 100	148, 153, 180, 183	0
12	T	13/29 (44%)	0.16	0 100 100	150, 170, 237, 245	0
All	All	3579/4207 (85%)	-0.14	31 (0%) 81 65	71, 128, 208, 254	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1086	PHE	4.7
2	B	715	ALA	3.5
2	B	708	GLU	3.2
4	E	199	ILE	3.2
2	B	478	GLY	3.1

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

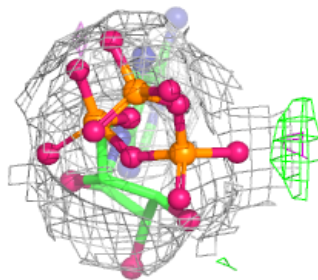
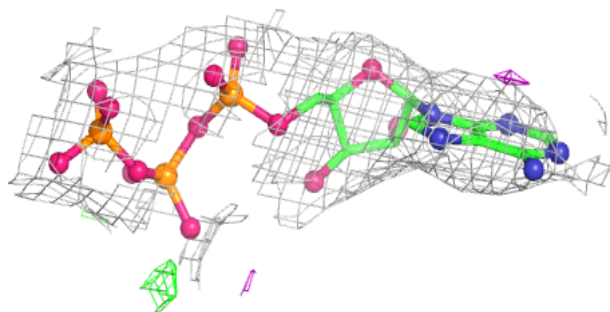
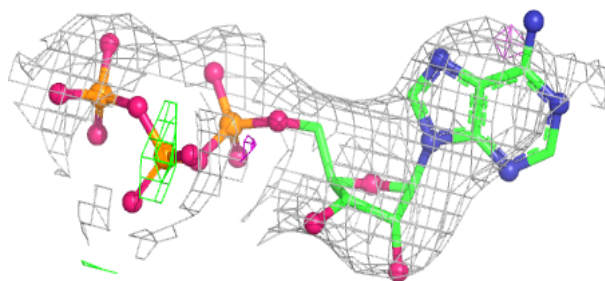
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	ZN	A	1734	1/1	0.84	0.09	300,300,300,300	0
15	ATP	A	1736	31/31	0.89	0.10	162,165,195,197	0
14	ZN	B	1307	1/1	0.93	0.06	221,221,221,221	0
13	MG	A	2002	1/1	0.95	0.05	131,131,131,131	0
14	ZN	A	1735	1/1	0.96	0.04	198,198,198,198	0
14	ZN	C	319	1/1	0.99	0.02	113,113,113,113	0
14	ZN	I	203	1/1	0.99	0.02	134,134,134,134	0
14	ZN	I	204	1/1	0.99	0.02	112,112,112,112	0
14	ZN	J	101	1/1	0.99	0.04	102,102,102,102	0
14	ZN	L	105	1/1	0.99	0.02	142,142,142,142	0
13	MG	A	2001	1/1	0.99	0.06	102,102,102,102	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 ATP A 1736:

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.