



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:46 PM GMT

PDB ID : 3S1Q  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

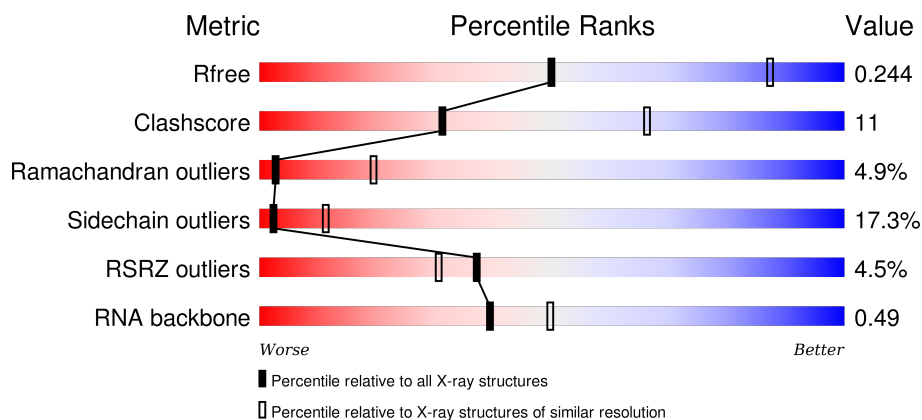
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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.




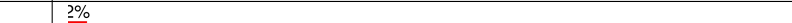

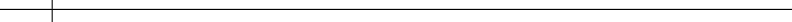



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)
RNA backbone	2183	1005 (3.82-2.78)

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. 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	<div> <div>5%</div> <div> <div></div> <div>50%</div> <div>25%</div> <div>5%</div> <div>19%</div> </div> </div>
2	B	1224	<div> <div>4%</div> <div> <div></div> <div>57%</div> <div>28%</div> <div>5%</div> <div>9%</div> </div> </div>
3	C	318	<div> <div></div> <div> <div></div> <div>52%</div> <div>25%</div> <div>6%</div> <div>16%</div> </div> </div>
4	E	215	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>28%</div> <div></div> </div> </div>

*Continued on next page...*

Mol	Chain	Length	Quality of chain
5	F	155	
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	R	5	
12	T	29	

## 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			

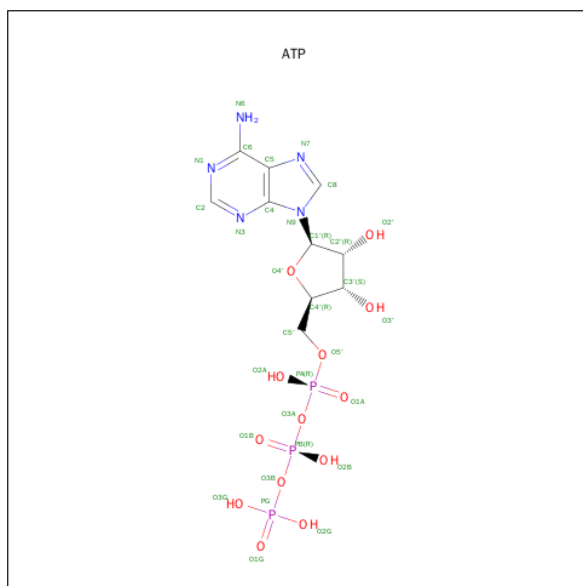
- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 15 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



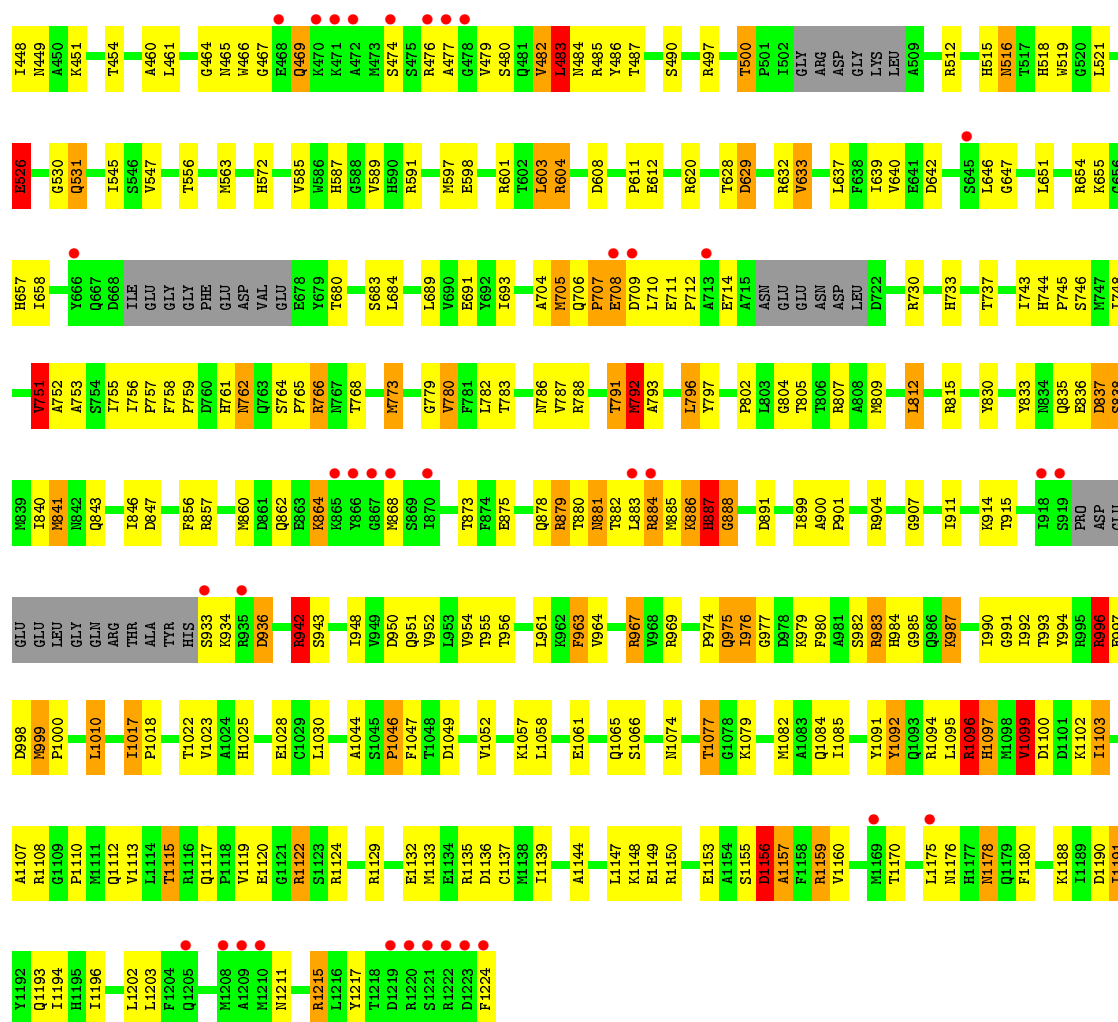
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		



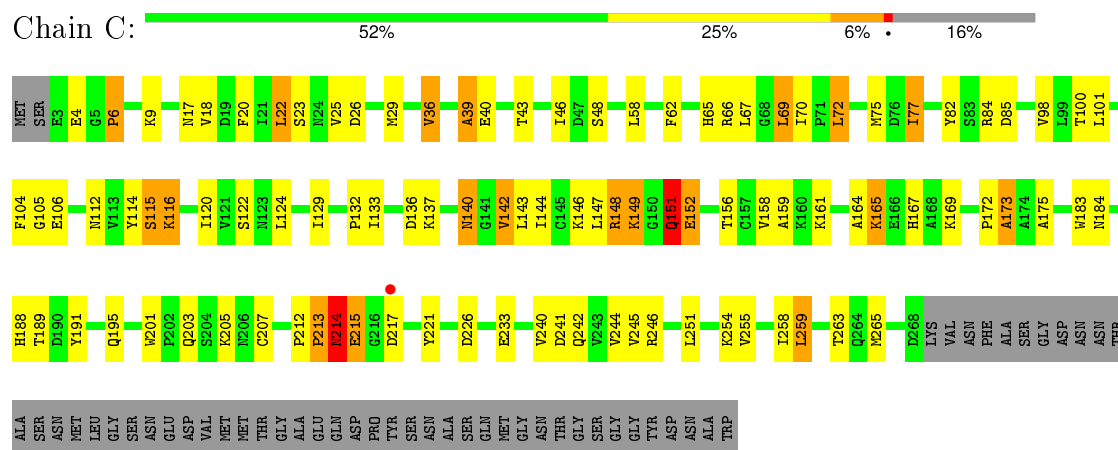


K345	G247	SER	THR	MET
E346	S248	GLU	GLU	SER
K347	R249	SER	ASP	ASP
	F250	GLY	ASN	LEU
D354		K164	ASN	ALA
	L254	V165	ILE	ASN
Q357	Q255	F166	SER	SER
K358	V256	I167	ARG	GLU
E359	R257	G168	LYS	LYS
			TYR	TYR
H363	G260	P171	E89	
I364	R261	I172	I90	ASP
I365	R262	M173	S91	GLU
Q366		L174		ASP
L367	S265	R175	K94	PRQ
E368	A266			TYR
G369	R267	G179	M101	GLY
F370	T268	I180	V102	PHE
E371	I269	L181		
			L112	D20
F376	T272	T185	V113	
	L273		P114	T26
I382	P274	L189		A27
K383	V275		R120	E28
R384	I276	K193	M121	D29
L385	R277	E194	L122	
L386	Q278	C195	T123	S35
		P196	V124	
D396	P281	F197	S125	F38
D397		D198		R39
R398	I284	M199	L128	E40
			F129	K41
R405	T292	I205	K133	G42
L408	P293	L206	L133	L43
A409	D294	G207	K134	V44
G410	D295	S208	R135	S45
C410	E296		T136	Q46
P411		V211	V137	Q47
L416	L311	L212	E138	L48
F417	E312	I213	A139	
K418	K313	A214	I140	Q53
	L314	Q215	D141	F54
I428	K315	E216	VAL	
F429	F322	R217	PRO	T58
		S218	GLY	I63
Q433	Q325	E227	ARG	
			GLU	D66
V436	F333	A230	LEU	S67
E437	L334	P231	LYS	
GLU	G335	S232	TYR	T68
ALA	ARG	P233	GLU	L69
HIS	ARG	T234	LEU	I70
ASP	GLY	S235	ILE	LEU
PHE	THR	R236	ALA	GLU
ASN	ALA	V237	GLN	LEU
MET	LEU		GLU	ALA
	GLY	L244	SER	GLY
L446	GLY	E245	GLU	HIS
L447	TYR	E246	ASP	THR



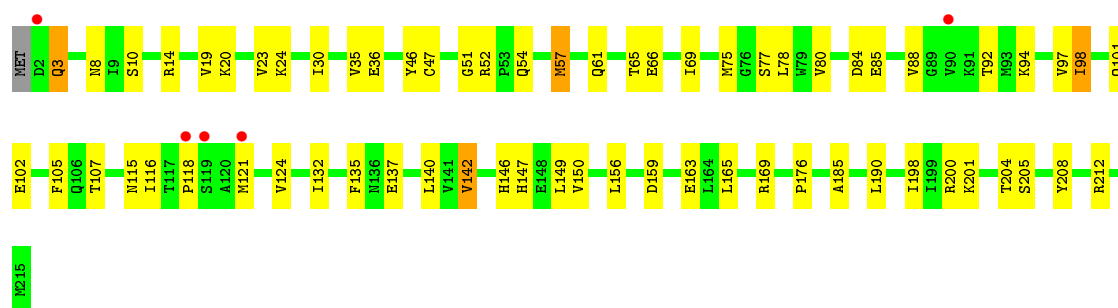


- Molecule 3: DNA-directed RNA polymerase II subunit RPB3



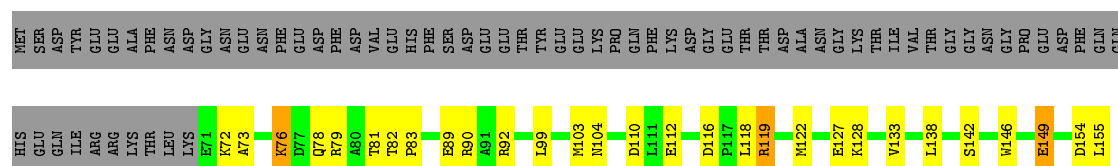
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1





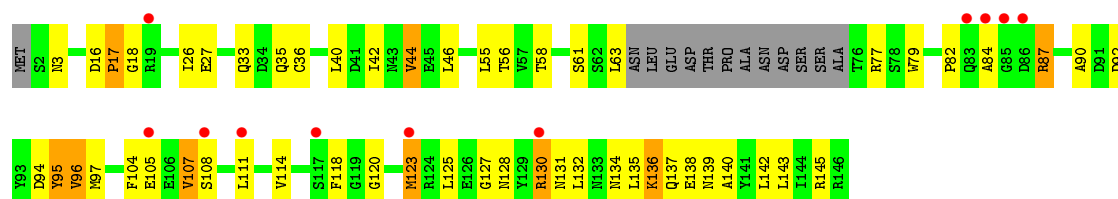
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 36% 17% 45%



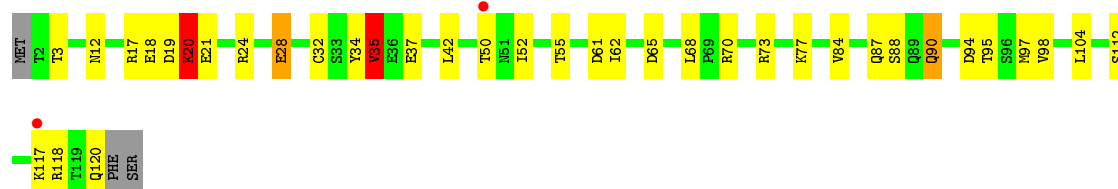
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 8% 54% 31% 6% 9%



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

Chain I: 2% 67% 27%



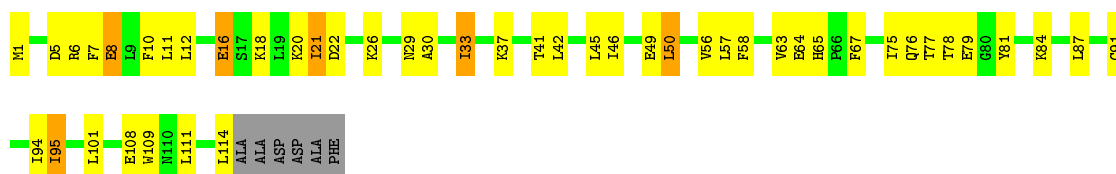
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 43% 41% 9% 7%

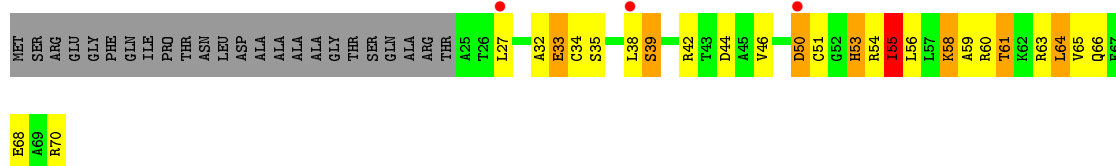
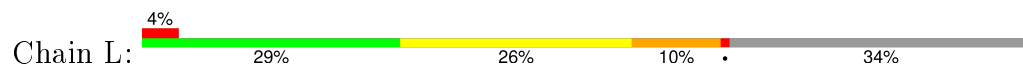


- Molecule 9: DNA-directed RNA polymerase II subunit RPB11

Chain K: 56% 34% 5% 5%



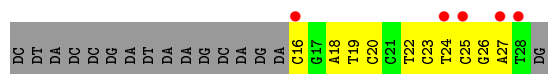
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



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



- 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')



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 99.3 (29.67-3.30)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 3.31Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, $R_{free}$	0.176 , 0.229 0.192 , 0.244	Depositor DCC
$R_{free}$ test set	4989 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	97.3	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 110.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 99956 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	28703	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, MG, 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	0.51	0/11241	0.83	6/15199 (0.0%)
2	B	0.54	0/9033	0.83	3/12181 (0.0%)
3	C	0.49	0/2133	0.84	1/2891 (0.0%)
4	E	0.46	0/1788	0.72	0/2406
5	F	0.49	0/700	0.74	0/945
6	H	0.49	0/1086	0.82	0/1470
7	I	0.50	0/989	0.81	0/1331
8	J	0.59	0/541	0.93	0/727
9	K	0.46	0/937	0.74	0/1265
10	L	0.58	0/365	1.05	0/485
11	R	0.93	0/123	1.42	0/191
12	T	1.14	0/290	2.13	17/444 (3.8%)
All	All	0.53	0/29226	0.85	27/39535 (0.1%)

There are no bond length outliers.

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	16	DC	P-O3'-C3'	10.52	132.32	119.70
12	T	25	DC	O4'-C1'-N1	9.54	114.68	108.00
12	T	23	DC	O4'-C1'-N1	8.20	113.74	108.00
12	T	22	DT	C4'-C3'-C2'	-8.13	95.78	103.10
12	T	24	DT	O4'-C1'-N1	8.12	113.69	108.00

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	280	0
2	B	8861	0	8884	215	0
3	C	2095	0	2051	56	0
4	E	1752	0	1776	36	0
5	F	688	0	707	9	0
6	H	1068	0	1040	20	0
7	I	971	0	927	11	0
8	J	532	0	542	23	0
9	K	919	0	929	27	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	619	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 619 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:H8	15:A:1736:ATP:H5'1	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
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 ⓘ

### 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	1395/1733 (80%)	1177 (84%)	149 (11%)	69 (5%)	3	19
2	B	1096/1224 (90%)	927 (85%)	110 (10%)	59 (5%)	2	17
3	C	264/318 (83%)	235 (89%)	19 (7%)	10 (4%)	4	26
4	E	212/215 (99%)	199 (94%)	11 (5%)	2 (1%)	21	60
5	F	83/155 (54%)	73 (88%)	7 (8%)	3 (4%)	4	28
6	H	129/146 (88%)	93 (72%)	24 (19%)	12 (9%)	1	6
7	I	117/122 (96%)	103 (88%)	10 (8%)	4 (3%)	5	29
8	J	63/70 (90%)	55 (87%)	6 (10%)	2 (3%)	5	31
9	K	112/120 (93%)	101 (90%)	8 (7%)	3 (3%)	6	35
10	L	44/70 (63%)	28 (64%)	7 (16%)	9 (20%)	0	1
All	All	3515/4173 (84%)	2991 (85%)	351 (10%)	173 (5%)	3	19

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%)	1008 (82%)	217 (18%)	2	10
2	B	967/1061 (91%)	811 (84%)	156 (16%)	3	14
3	C	234/274 (85%)	191 (82%)	43 (18%)	2	9
4	E	196/197 (100%)	173 (88%)	23 (12%)	7	28
5	F	75/137 (55%)	60 (80%)	15 (20%)	1	6
6	H	117/128 (91%)	96 (82%)	21 (18%)	2	10
7	I	113/116 (97%)	91 (80%)	22 (20%)	2	7
8	J	60/65 (92%)	46 (77%)	14 (23%)	1	4
9	K	99/102 (97%)	83 (84%)	16 (16%)	3	14
10	L	40/57 (70%)	26 (65%)	14 (35%)	0	1
All	All	3126/3657 (86%)	2585 (83%)	541 (17%)	2	11

5 of 541 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	273	LEU
2	B	743	ILE
8	J	9	SER
2	B	322	PHE
2	B	469	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1364	ASN
2	B	518	HIS
7	I	60	GLN
2	B	46	GLN
2	B	366	GLN

### 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 [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 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	24,33,33	1.20	3 (12%)	31,52,52	1.54	7 (22%)

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	-	0/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1736	ATP	PB-O1B	2.16	1.59	1.51
15	A	1736	ATP	C2-N1	2.28	1.38	1.33
15	A	1736	ATP	C2-N3	3.13	1.37	1.32

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1736	ATP	N3-C2-N1	-3.22	126.42	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1736	ATP	C1'-N9-C4	-2.60	123.01	126.94
15	A	1736	ATP	PA-O3A-PB	2.31	139.23	132.73
15	A	1736	ATP	O3'-C3'-C4'	2.38	118.19	111.05
15	A	1736	ATP	C4-C5-N7	2.61	111.88	109.48

There are no chirality outliers.

There are no torsion outliers.

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

## 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	1405/1733 (81%)	0.09	86 (6%) 25 20	78, 133, 223, 254	0
2	B	1114/1224 (91%)	-0.03	49 (4%) 38 31	71, 115, 183, 241	0
3	C	266/318 (83%)	-0.21	1 (0%) 93 92	87, 113, 153, 215	0
4	E	214/215 (99%)	-0.04	5 (2%) 64 57	102, 159, 206, 216	0
5	F	85/155 (54%)	-0.13	0 100 100	109, 139, 178, 196	0
6	H	133/146 (91%)	0.38	11 (8%) 14 11	131, 172, 202, 222	0
7	I	119/122 (97%)	-0.14	2 (1%) 73 67	93, 138, 185, 200	0
8	J	65/70 (92%)	-0.16	0 100 100	81, 104, 136, 151	0
9	K	114/120 (95%)	-0.21	0 100 100	87, 123, 150, 175	0
10	L	46/70 (65%)	0.27	3 (6%) 22 18	99, 155, 188, 214	0
11	R	5/5 (100%)	0.30	0 100 100	148, 153, 180, 183	0
12	T	13/29 (44%)	1.44	5 (38%) 0 1	150, 170, 237, 245	0
All	All	3579/4207 (85%)	0.01	162 (4%) 37 30	71, 128, 208, 254	0

The worst 5 of 162 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	69	THR	8.9
2	B	1222	ARG	7.1
2	B	1224	PHE	6.9
1	A	1176	LEU	6.5
1	A	66	LYS	6.3

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

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

### 6.3 Carbohydrates [i](#)

There are no 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
15	ATP	A	1736	31/31	0.88	0.23	-0.07	162,165,195,197	0
14	ZN	J	101	1/1	0.98	0.20	-0.59	102,102,102,102	0
14	ZN	I	203	1/1	0.98	0.08	-0.88	134,134,134,134	0
14	ZN	A	1735	1/1	0.95	0.15	-1.02	198,198,198,198	0
14	ZN	C	319	1/1	0.99	0.09	-1.18	113,113,113,113	0
14	ZN	I	204	1/1	0.99	0.07	-1.30	112,112,112,112	0
14	ZN	L	105	1/1	0.97	0.03	-1.53	142,142,142,142	0
13	MG	A	2002	1/1	0.92	0.14	-1.67	131,131,131,131	0
14	ZN	B	1307	1/1	0.82	0.10	-1.72	221,221,221,221	0
14	ZN	A	1734	1/1	0.24	0.15	-1.78	300,300,300,300	0
13	MG	A	2001	1/1	0.90	0.04	-4.05	102,102,102,102	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.