



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 01:52 pm BST

PDB ID : 4A3B
Title : RNA Polymerase II initial transcribing complex with a 4nt DNA-RNA hybrid
Authors : Cheung, A.C.M.; Sainsbury, S.; Cramer, P.
Deposited on : 2011-09-30
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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

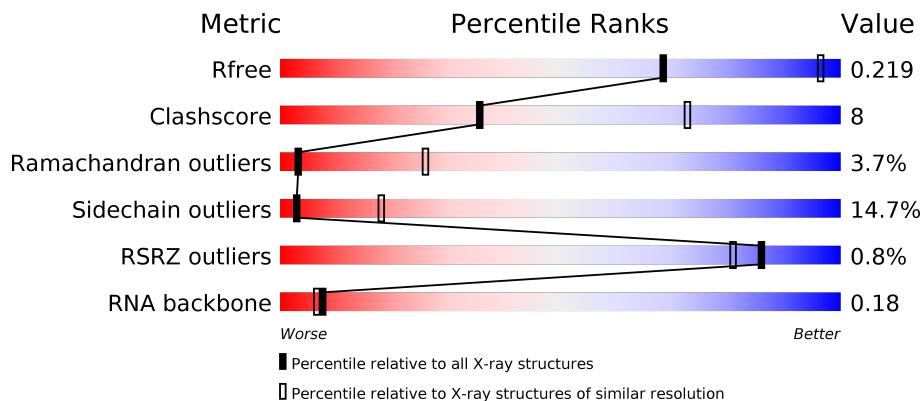
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	1732	 58% 20% 18%
2	B	1224	 61% 26% 9%
3	C	318	 57% 22% 16%
4	D	221	 54% 22% 19%

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	N	14	
14	P	4	
15	T	26	

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 31612 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
			Total	C	N	O	S			
1	A	1422	11174	7037	1954	2121	62	0	0	0

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1115	8859	5609	1554	1641	55	0	0	0

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

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

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	178	1434	887	257	288	2	0	0	0

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

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

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	84	679	434	115	127	3	0	0	0

- Molecule 7 is a protein called RPB7, DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	171	1340	861	222	249	8	0	0	0

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

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

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

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

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

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

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	115	920	590	157	171	2	0	0	1

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

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

- Molecule 13 is a DNA chain called NON TEMPLATE DNA 5'-D(*TP*AP*AP*GP*TP*A P*CP*TP*TP*GP*AP*GP*CP*TP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
13	N	4	84	40	17	23	4	0	0	0

- Molecule 14 is a RNA chain called TRANSCRIPT RNA 5'-R(*AP*GP*GP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
14	P	4	90	40	20	26	4	0	0	0

- Molecule 15 is a DNA chain called TEMPLATE DNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	Br	C	N	O	P			
15	T	12	242	1	116	36	77	12	0	0	0

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

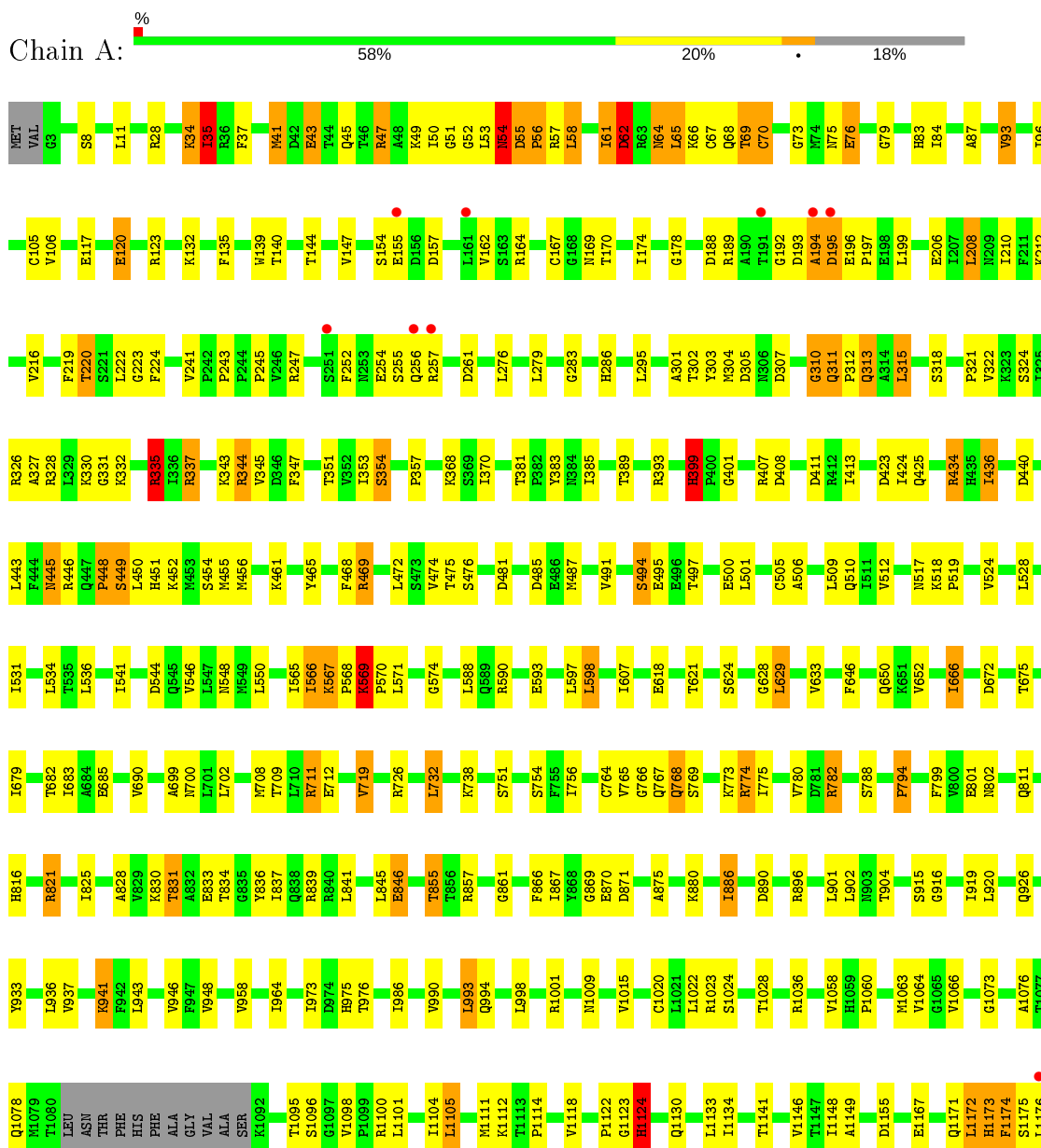
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

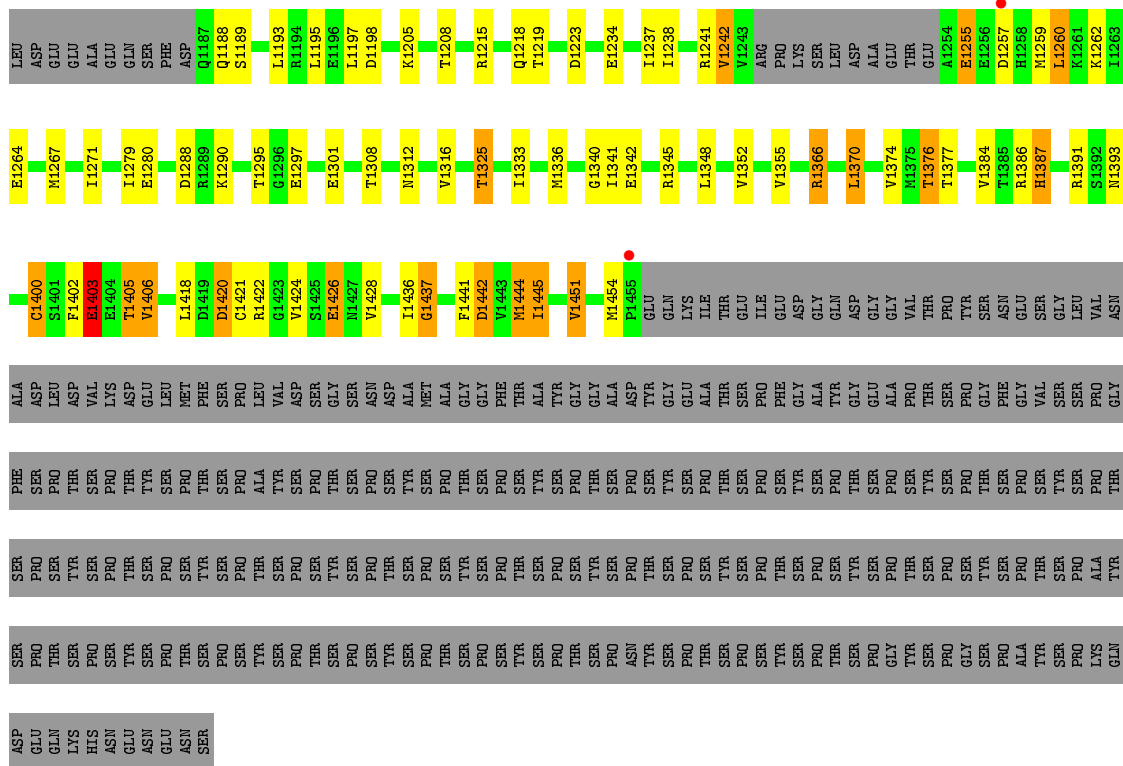
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Mg	0	0
			1	1		

3 Residue-property plots [i](#)

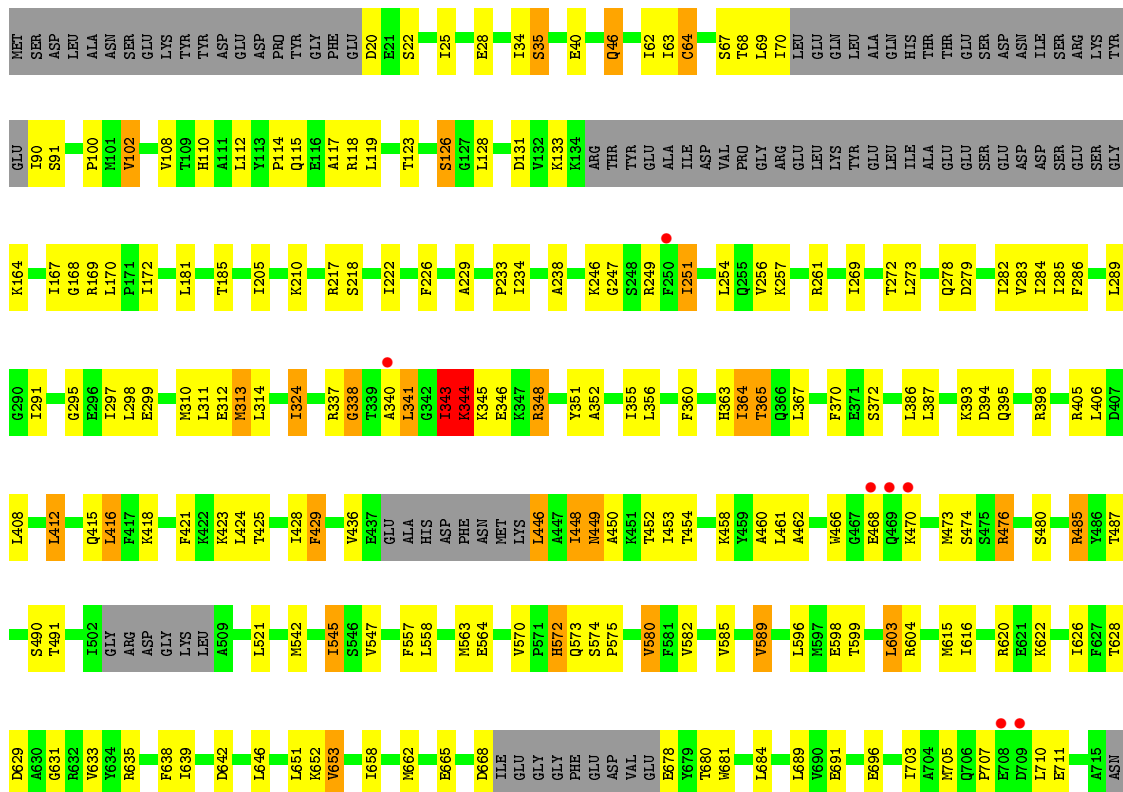
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

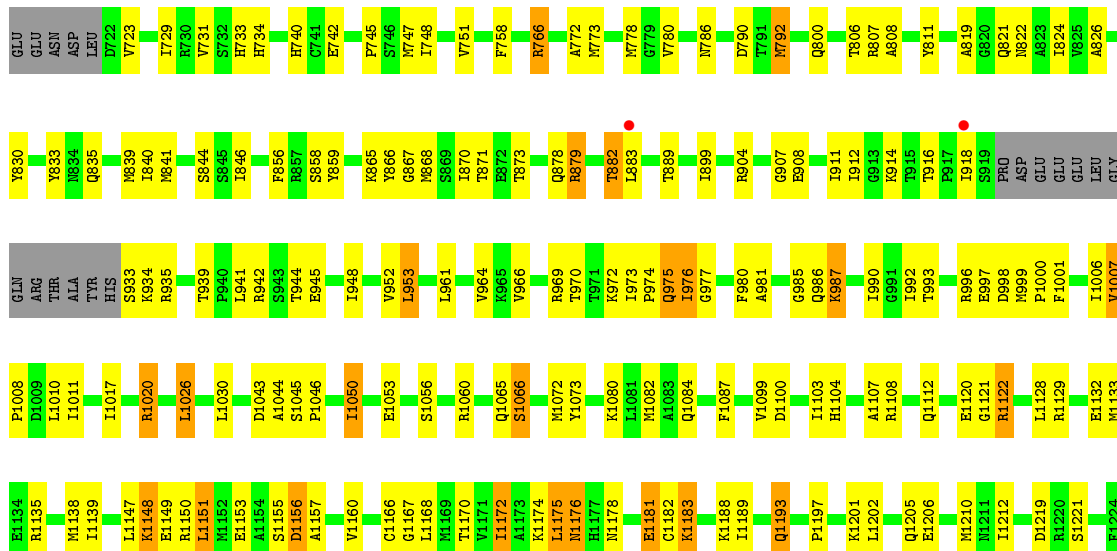
- Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1



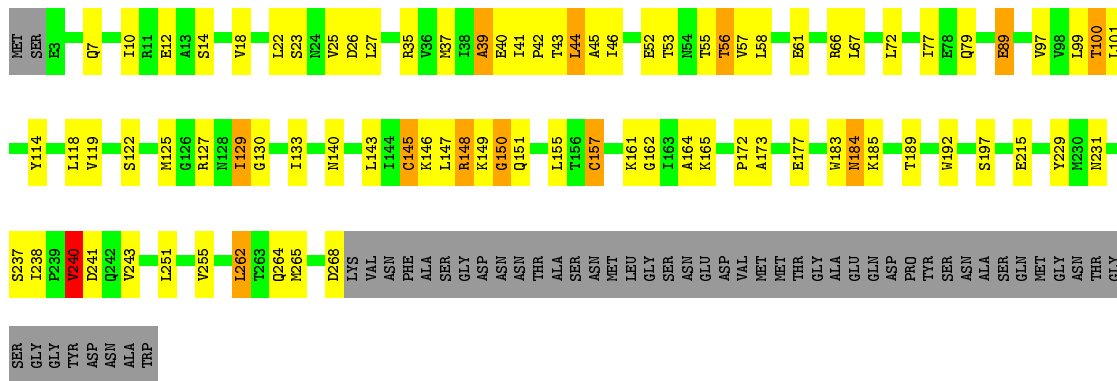


● Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2

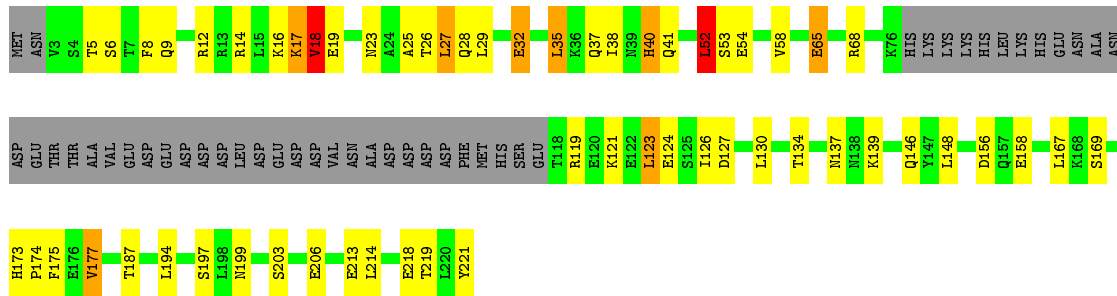




• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

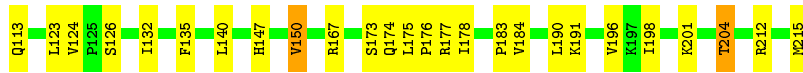
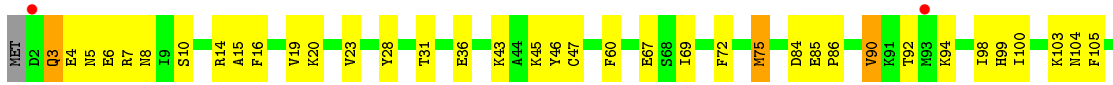


• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4

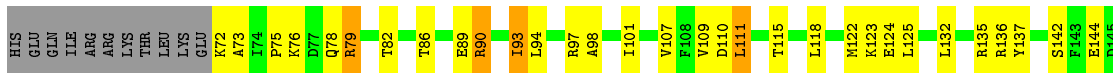
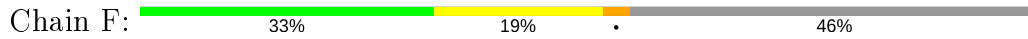


• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1

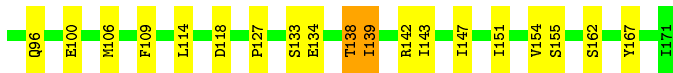
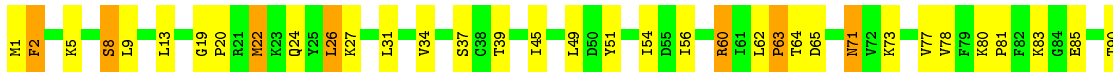




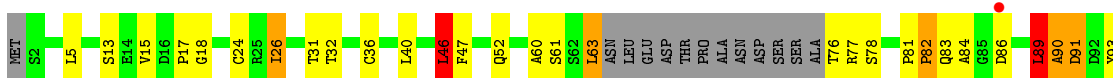
- Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2



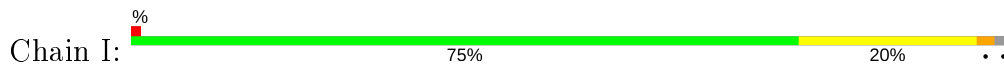
- Molecule 7: RPB7, DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7



- Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3



- Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9



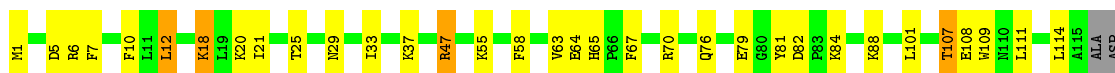
- Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

Chain J: 




- Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

Chain K: 



ASP
ALA
PHE

- Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

Chain L: 



- Molecule 13: NON TEMPLATE DNA 5'-D(*TP*AP*AP*GP*TP*AP*CP*TP*TP*GP*AP*GP*CP*TP)-3'

Chain N: 


DT, A2, A3, G4, T5, DA, DC, DT, DG, DA, DC, DT

- Molecule 14: TRANSCRIPT RNA 5'-R(*AP*GP*GP*A)-3'

Chain P: 

A7, G8, G9, A10

- Molecule 15: TEMPLATE DNA

Chain T: 

DA, DG, DC, DT, DA, DA, DG, DT, A13, C14, T15, T16, T17, T18, T19, C20, C21, G24, DT, DC, DA, DT

4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	222.09Å 392.97Å 281.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.89 – 3.50 48.89 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.89-3.50) 98.9 (48.89-3.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 3.48Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.166 , 0.197 0.190 , 0.219	Depositor DCC
R_{free} test set	3021 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	112.6	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 100.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.025 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.023 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	31612	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.54	0/11374	0.84	12/15383 (0.1%)
2	B	0.52	0/9029	0.80	1/12171 (0.0%)
3	C	0.49	0/2133	0.79	1/2891 (0.0%)
4	D	0.52	0/1444	0.84	2/1935 (0.1%)
5	E	0.48	0/1788	0.74	0/2406
6	F	0.61	0/691	0.82	0/933
7	G	0.50	0/1368	0.78	0/1844
8	H	0.52	0/1086	0.80	0/1470
9	I	0.46	0/989	0.77	0/1331
10	J	0.54	0/541	0.83	0/727
11	K	0.50	0/938	0.72	0/1267
12	L	0.56	0/365	1.06	1/485 (0.2%)
13	N	1.22	0/94	0.97	0/143
14	P	1.08	0/101	0.78	0/156
15	T	1.42	2/245 (0.8%)	1.14	0/373
All	All	0.54	2/32186 (0.0%)	0.82	17/43515 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	15	DT	C1'-N1	5.44	1.56	1.49
15	T	21	DC	C1'-N1	5.12	1.55	1.49

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	LYS	C-N-CA	7.41	140.22	121.70
1	A	399	HIS	N-CA-CB	6.52	122.34	110.60
1	A	56	PRO	C-N-CA	5.87	136.38	121.70
1	A	194	ALA	C-N-CA	5.67	135.87	121.70
2	B	338	GLY	C-N-CA	5.54	135.56	121.70

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	11174	0	11233	186	0
2	B	8859	0	8901	171	0
3	C	2095	0	2051	45	0
4	D	1434	0	1460	22	0
5	E	1752	0	1776	27	0
6	F	679	0	701	23	0
7	G	1340	0	1357	29	0
8	H	1068	0	1040	19	0
9	I	971	0	927	13	0
10	J	532	0	542	14	0
11	K	920	0	929	14	0
12	L	363	0	386	9	0
13	N	84	0	46	3	0
14	P	90	0	45	1	0
15	T	242	0	136	3	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	A	1	0	0	0	0
All	All	31612	0	31530	509	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 8.

The worst 5 of 509 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:867:ILE:CD1	1:A:867:ILE:CG1	1.75	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LEU:HD23	1:A:54:ASN:H	1.27	0.98
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.46	0.97
6:F:90:ARG:HG3	6:F:90:ARG:HH11	1.31	0.94
1:A:855:THR:HG21	1:A:857:ARG:HE	1.32	0.94

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	1414/1732 (82%)	1211 (86%)	145 (10%)	58 (4%)	3	23
2	B	1095/1224 (90%)	951 (87%)	114 (10%)	30 (3%)	5	33
3	C	264/318 (83%)	231 (88%)	26 (10%)	7 (3%)	5	33
4	D	174/221 (79%)	147 (84%)	19 (11%)	8 (5%)	2	21
5	E	212/215 (99%)	194 (92%)	11 (5%)	7 (3%)	4	28
6	F	82/155 (53%)	75 (92%)	6 (7%)	1 (1%)	13	50
7	G	169/171 (99%)	158 (94%)	7 (4%)	4 (2%)	6	35
8	H	129/146 (88%)	100 (78%)	15 (12%)	14 (11%)	0	6
9	I	117/122 (96%)	99 (85%)	16 (14%)	2 (2%)	9	42
10	J	63/70 (90%)	54 (86%)	5 (8%)	4 (6%)	1	14
11	K	113/120 (94%)	104 (92%)	8 (7%)	1 (1%)	17	56
12	L	44/70 (63%)	30 (68%)	6 (14%)	8 (18%)	0	2
All	All	3876/4564 (85%)	3354 (86%)	378 (10%)	144 (4%)	3	26

5 of 144 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	ARG

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Mol	Chain	Res	Type
1	A	57	ARG
1	A	58	LEU
1	A	69	THR
1	A	193	ASP

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	1240/1519 (82%)	1055 (85%)	185 (15%)	3	17
2	B	966/1061 (91%)	818 (85%)	148 (15%)	2	17
3	C	234/274 (85%)	199 (85%)	35 (15%)	3	17
4	D	160/200 (80%)	133 (83%)	27 (17%)	2	12
5	E	196/197 (100%)	172 (88%)	24 (12%)	5	23
6	F	74/137 (54%)	66 (89%)	8 (11%)	6	30
7	G	152/152 (100%)	130 (86%)	22 (14%)	3	18
8	H	117/128 (91%)	103 (88%)	14 (12%)	5	24
9	I	113/116 (97%)	105 (93%)	8 (7%)	14	46
10	J	60/65 (92%)	48 (80%)	12 (20%)	1	7
11	K	99/102 (97%)	85 (86%)	14 (14%)	3	19
12	L	40/57 (70%)	30 (75%)	10 (25%)	0	4
All	All	3451/4008 (86%)	2944 (85%)	507 (15%)	3	18

5 of 507 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	448	ILE
2	B	908	GLU
9	I	83	ASN
2	B	474	SER
2	B	646	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	449	ASN
2	B	986	GLN
9	I	60	GLN
2	B	590	HIS
2	B	957	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	3/4 (75%)	1 (33%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	9	G

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is 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
15	BRU	T	22	15,14	15,21,22	1.59	2 (13%)	17,30,33	2.26	3 (17%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BRU	T	22	15,14	-	0/4/21/22	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	22	BRU	C4-C5	4.95	1.44	1.38
15	T	22	BRU	C4-N3	3.33	1.38	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	22	BRU	C4-N3-C2	6.41	120.56	115.14
15	T	22	BRU	C2'-C1'-N1	-5.55	101.46	114.27
15	T	22	BRU	C5-C4-N3	-3.18	119.83	123.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	934:LYS	C	935:ARG	N	5.39
1	B	351:TYR	C	352:ALA	N	3.29

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	1422/1732 (82%)	-0.21	11 (0%) 86 81	64, 115, 172, 239	0
2	B	1115/1224 (91%)	-0.15	9 (0%) 86 81	71, 127, 187, 209	0
3	C	266/318 (83%)	-0.28	0 100 100	86, 115, 158, 185	0
4	D	178/221 (80%)	-0.21	0 100 100	96, 131, 179, 198	0
5	E	214/215 (99%)	-0.18	2 (0%) 84 79	89, 146, 193, 206	0
6	F	84/155 (54%)	-0.43	0 100 100	73, 97, 124, 137	0
7	G	171/171 (100%)	-0.21	0 100 100	85, 113, 154, 172	0
8	H	133/146 (91%)	0.29	4 (3%) 50 44	125, 157, 194, 214	0
9	I	119/122 (97%)	-0.08	1 (0%) 86 81	120, 151, 192, 199	0
10	J	65/70 (92%)	-0.31	0 100 100	95, 115, 151, 161	0
11	K	115/120 (95%)	-0.32	0 100 100	85, 114, 155, 174	0
12	L	46/70 (65%)	0.44	3 (6%) 18 17	103, 182, 199, 210	0
13	N	4/14 (28%)	0.27	0 100 100	230, 230, 234, 239	0
14	P	4/4 (100%)	0.20	0 100 100	211, 220, 228, 240	0
15	T	11/26 (42%)	0.79	2 (18%) 1 1	188, 216, 258, 264	0
All	All	3947/4608 (85%)	-0.18	32 (0%) 86 81	64, 122, 185, 264	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	L	27	LEU	5.1
12	L	26	THR	4.6
1	A	194	ALA	4.0
1	A	1455	PRO	3.8
2	B	883	LEU	3.4

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	BRU	T	22	20/21	0.84	0.21	221,231,240,243	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
17	MG	A	2458	1/1	0.75	0.33	281,281,281,281	0
16	ZN	L	1071	1/1	0.93	0.06	201,201,201,201	0
16	ZN	I	1122	1/1	0.98	0.03	201,201,201,201	0
16	ZN	A	2456	1/1	0.98	0.06	155,155,155,155	0
16	ZN	B	2225	1/1	0.99	0.20	91,91,91,91	0
16	ZN	A	2457	1/1	1.00	0.14	81,81,81,81	0
16	ZN	J	1066	1/1	1.00	0.25	101,101,101,101	0
16	ZN	I	1121	1/1	1.00	0.12	136,136,136,136	0
16	ZN	C	1269	1/1	1.00	0.12	96,96,96,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.