



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:58 AM GMT

PDB ID : 3CQZ  
Title : Crystal structure of 10 subunit RNA polymerase II in complex with the inhibitor alpha-amanitin  
Authors : Kaplan, C.D.; Larsson, K.-M.; Kornberg, R.D.  
Deposited on : 2008-04-03  
Resolution : 2.80 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

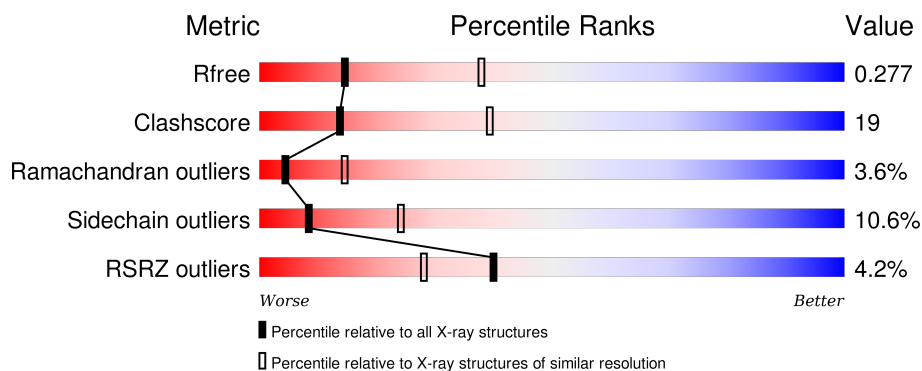
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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>3%</div> <div>50% 22% . . 22%</div> </div>
2	B	1224	<div> <div>4%</div> <div>57% 24% . . 13%</div> </div>
3	C	318	<div> <div>2%</div> <div>57% 23% . 17%</div> </div>
4	E	215	<div> <div>3%</div> <div>60% 27% 10% . .</div> </div>
5	F	155	<div> <div>%</div> <div>40% 12% . 46%</div> </div>

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Mol	Chain	Length	Quality of chain
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	M	8	

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 27340 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	1349	Total	C	N	O	S	0	0	0
			10616	6710	1838	2009	59			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1061	Total	C	N	O	S	0	0	0
			8419	5340	1465	1563	51			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	265	Total	C	N	O	S	0	0	0
			2087	1313	347	414	13			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUB-UNIT RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	213	Total	C	N	O	S	0	0	0
			1744	1107	308	318	11			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUB-UNIT RPABC2.

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

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUB-UNIT RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	116	Total	C	N	O	S	0	0	0
			932	589	154	185	4			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	121	Total	C	N	O	S	0	0	0
			989	608	181	190	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	113	Total	C	N	O	S	0	0	0
			911	585	155	170	1			

- 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	43	Total	C	N	O	S	0	0	0
			342	211	68	59	4			

- Molecule 11 is a protein called ALPHA-AMANITIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	M	8	Total	C	N	O	S	0	0	0
			64	39	10	14	1			

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	J	1	Total	Zn	0	0
			1	1		
12	B	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	I	2	Total 2	Zn 2	0	0
12	C	1	Total 1	Zn 1	0	0
12	A	2	Total 2	Zn 2	0	0
12	L	1	Total 1	Zn 1	0	0

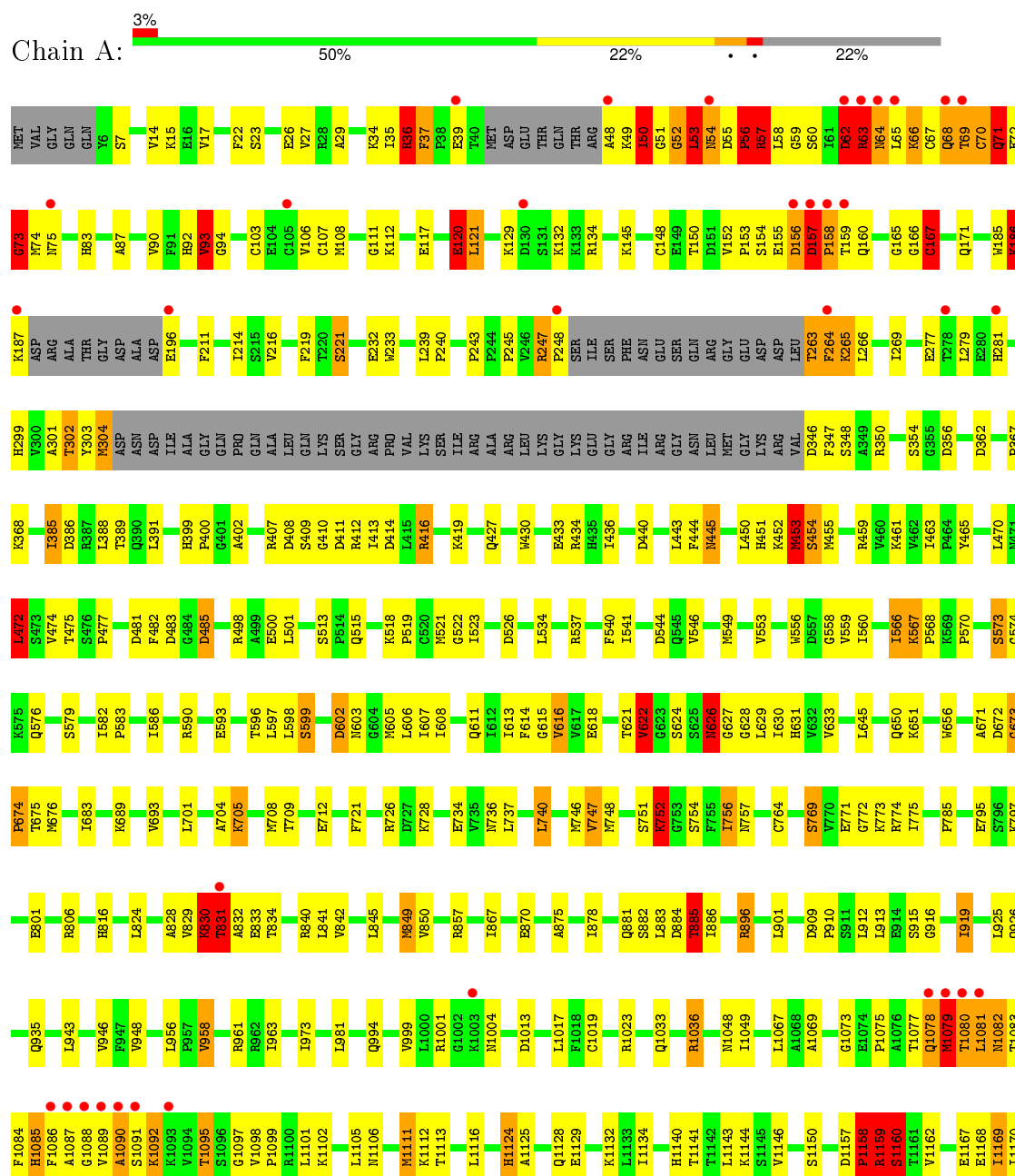
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	11	Total 11	O 11	0	0
13	B	4	Total 4	O 4	0	0
13	E	1	Total 1	O 1	0	0
13	F	1	Total 1	O 1	0	0

### 3 Residue-property plots

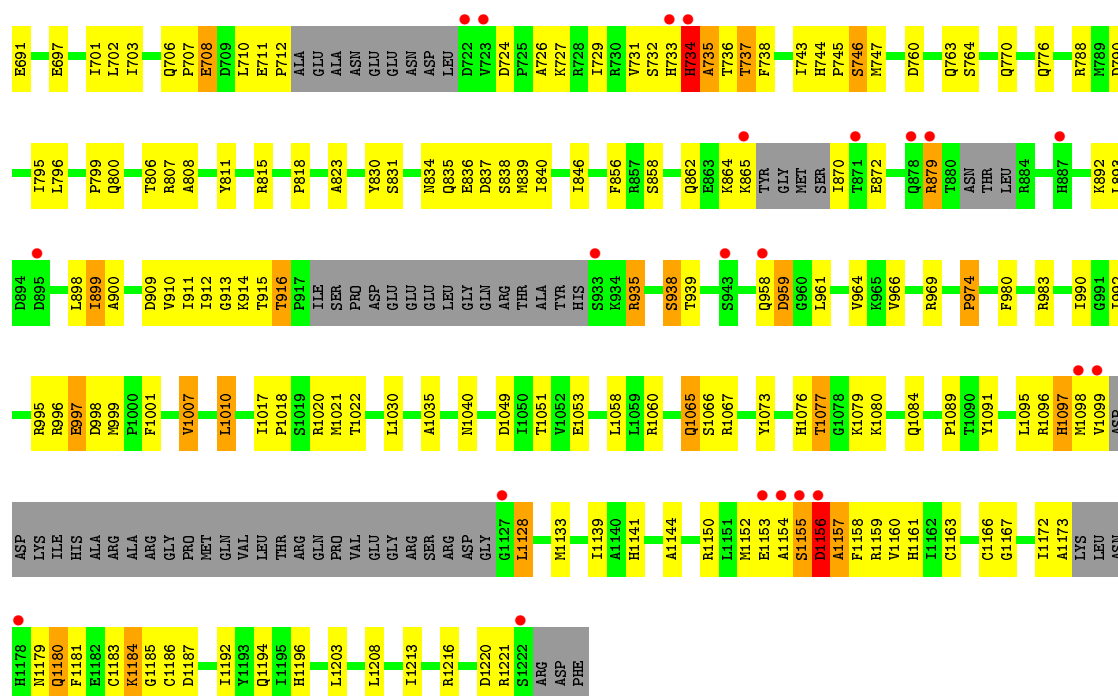
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

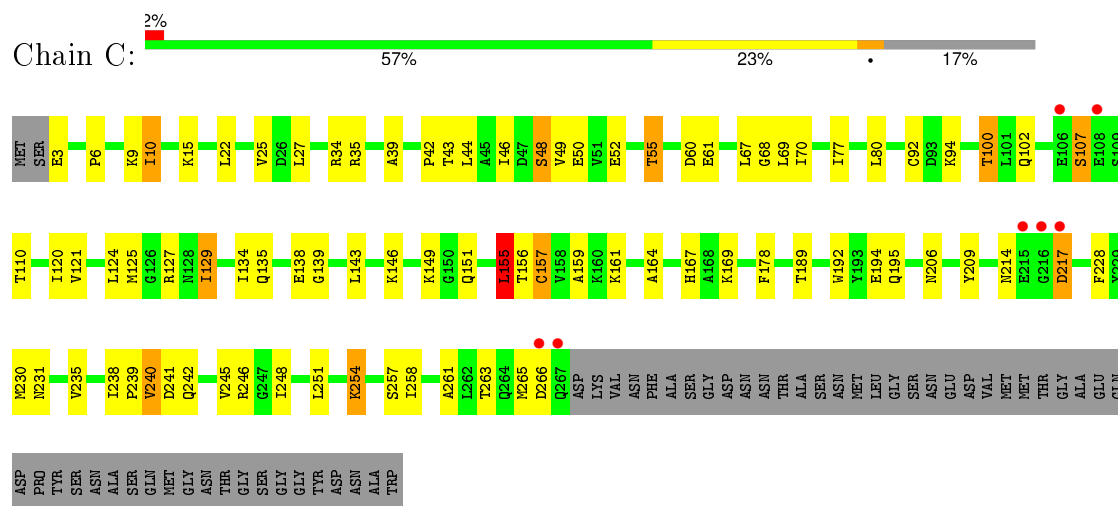




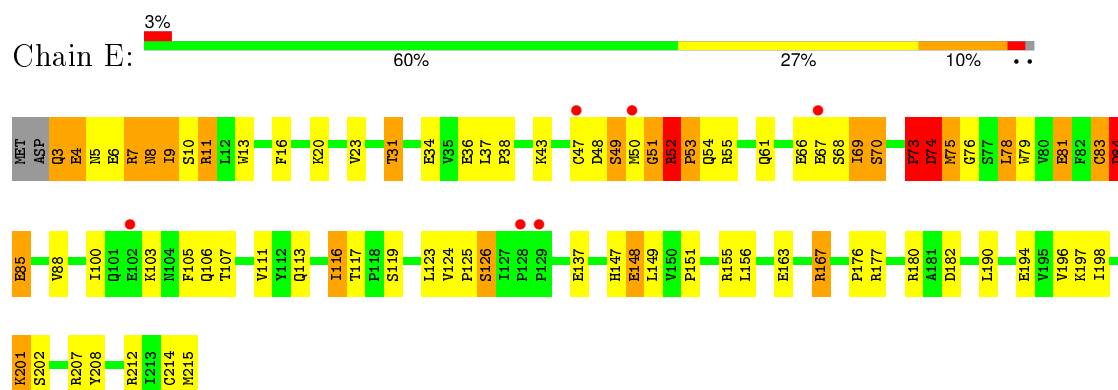




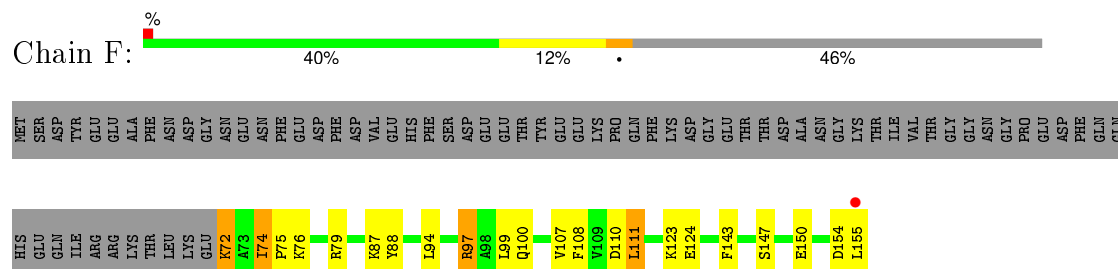
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3



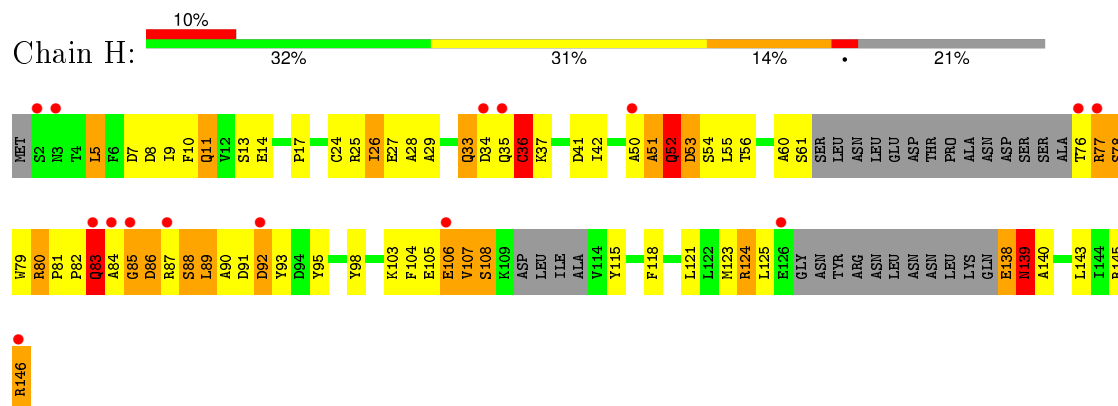
• Molecule 4: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1



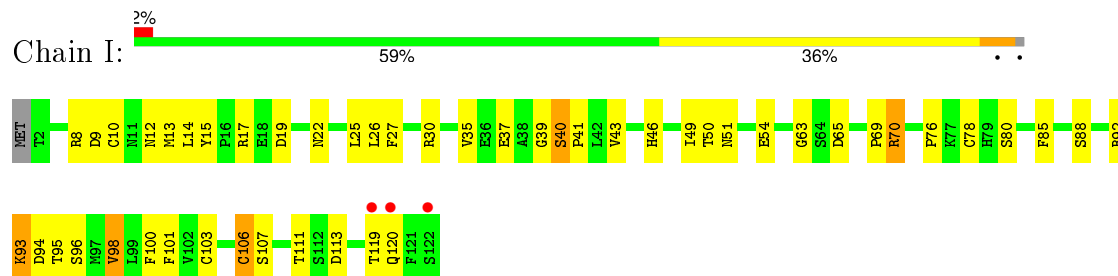
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2



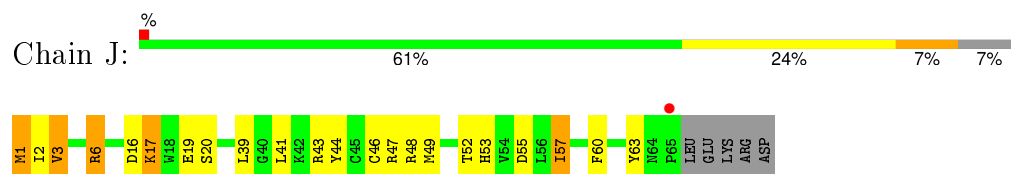
• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC3



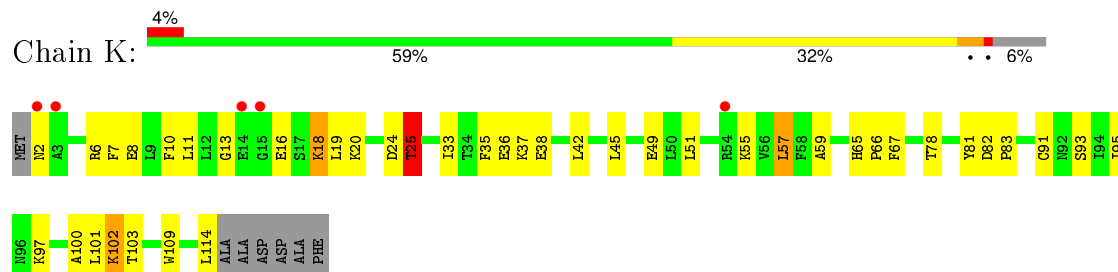
• Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9



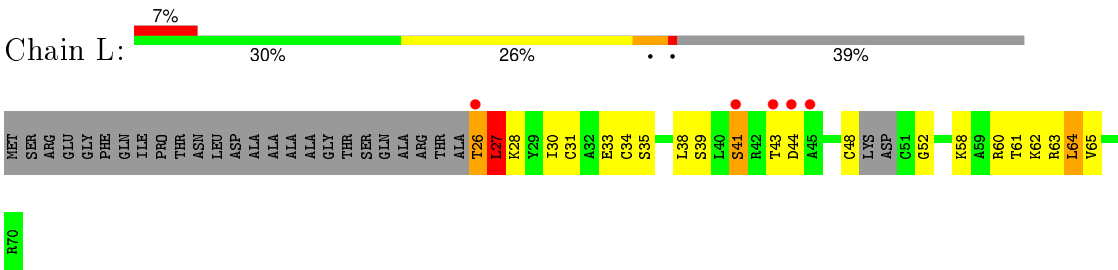
• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC5



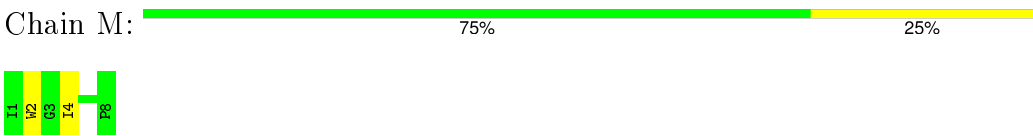
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11



● Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4



● Molecule 11: ALPHA-AMANITIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.51Å 222.48Å 374.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.4 (20.00-2.80) 93.4 (20.00-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.200 , 0.273 0.209 , 0.277	Depositor DCC
$R_{free}$ test set	3507 reflections (3.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.5	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 53.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 125151 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	27340	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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: HYP, TRX, ZN, CSX, ILX

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	0.74	0/10809	0.91	20/14624 (0.1%)
2	B	0.73	0/8579	0.86	10/11565 (0.1%)
3	C	0.62	0/2125	0.74	1/2880 (0.0%)
4	E	0.71	0/1780	0.82	2/2395 (0.1%)
5	F	0.72	0/691	0.80	0/933
6	H	0.60	0/947	0.90	1/1279 (0.1%)
7	I	0.80	1/1008 (0.1%)	0.81	0/1355
8	J	0.68	0/541	0.90	0/727
9	K	0.63	0/929	0.74	0/1255
10	L	0.61	0/343	0.87	1/453 (0.2%)
11	M	1.99	1/22 (4.5%)	1.58	0/26
All	All	0.72	2/27774 (0.0%)	0.86	35/37492 (0.1%)

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
1	A	0	16
2	B	0	12
4	E	0	2
8	J	0	1
All	All	0	31

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	4	ILE	C-O	7.28	1.37	1.23
7	I	103	CYS	CB-SG	5.83	1.92	1.82

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	472	LEU	CA-CB-CG	-8.37	96.05	115.30
3	C	155	LEU	CA-CB-CG	7.16	131.76	115.30
2	B	508	LEU	CA-CB-CG	6.93	131.24	115.30
4	E	74	ASP	N-CA-C	-6.77	92.72	111.00
2	B	1128	LEU	CA-CB-CG	6.55	130.36	115.30

There are no chirality outliers.

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	157	ASP	Peptide
1	A	158	PRO	Peptide
1	A	36	ARG	Peptide
1	A	62	ASP	Peptide
1	A	73	GLY	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10616	0	10675	454	0
2	B	8419	0	8450	294	0
3	C	2087	0	2047	62	0
4	E	1744	0	1772	87	0
5	F	679	0	701	18	0
6	H	932	0	899	75	0
7	I	989	0	942	34	0
8	J	532	0	542	18	0
9	K	911	0	917	35	0
10	L	342	0	363	16	0
11	M	64	0	51	1	0
12	A	2	0	0	0	0
12	B	1	0	0	0	0
12	C	1	0	0	0	0
12	I	2	0	0	0	0
12	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	1	0	0	0	0
13	A	11	0	0	2	0
13	B	4	0	0	1	0
13	E	1	0	0	0	0
13	F	1	0	0	0	0
All	All	27340	0	27359	1013	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 19.

The worst 5 of 1013 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:1399:ARG:HB3	1:A:1400:CYS:CB	1.60	1.30
4:E:53:PRO:HB2	4:E:54:GLN:CA	1.65	1.25
1:A:1399:ARG:CB	1:A:1400:CYS:HB3	1.68	1.24
4:E:53:PRO:CB	4:E:54:GLN:HA	1.64	1.22
1:A:1398:MET:HA	1:A:1399:ARG:HB2	1.24	1.17

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	1333/1733 (77%)	1168 (88%)	110 (8%)	55 (4%)	3	11
2	B	1035/1224 (85%)	920 (89%)	79 (8%)	36 (4%)	4	15
3	C	263/318 (83%)	243 (92%)	19 (7%)	1 (0%)	39	74
4	E	211/215 (98%)	189 (90%)	12 (6%)	10 (5%)	3	9
5	F	82/155 (53%)	78 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	H	108/146 (74%)	76 (70%)	17 (16%)	15 (14%)	0	1
7	I	119/122 (98%)	106 (89%)	11 (9%)	2 (2%)	11	36
8	J	63/70 (90%)	62 (98%)	1 (2%)	0	100	100
9	K	111/120 (92%)	99 (89%)	10 (9%)	2 (2%)	11	34
10	L	39/70 (56%)	29 (74%)	9 (23%)	1 (3%)	7	22
11	M	4/8 (50%)	3 (75%)	1 (25%)	0	100	100
All	All	3368/4181 (81%)	2973 (88%)	273 (8%)	122 (4%)	4	14

5 of 122 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	ILE
1	A	56	PRO
1	A	63	ARG
1	A	70	CYS
1	A	157	ASP

### 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	1182/1520 (78%)	1049 (89%)	133 (11%)	7	22
2	B	919/1061 (87%)	841 (92%)	78 (8%)	13	36
3	C	233/274 (85%)	207 (89%)	26 (11%)	7	22
4	E	195/197 (99%)	170 (87%)	25 (13%)	5	16
5	F	74/137 (54%)	67 (90%)	7 (10%)	11	30
6	H	102/128 (80%)	81 (79%)	21 (21%)	1	4
7	I	115/116 (99%)	105 (91%)	10 (9%)	13	35
8	J	60/65 (92%)	53 (88%)	7 (12%)	7	20
9	K	98/102 (96%)	91 (93%)	7 (7%)	18	46
10	L	38/57 (67%)	32 (84%)	6 (16%)	3	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	M	2/2 (100%)	2 (100%)	0	100	100
All	All	3018/3659 (82%)	2698 (89%)	320 (11%)	8	24

5 of 320 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	110	HIS
2	B	648	HIS
7	I	98	VAL
2	B	199	MET
2	B	425	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	572	HIS
2	B	957	ASN
7	I	12	ASN
2	B	583	ASN
2	B	667	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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
11	ILX	M	1	11	7,9,10	0.88	0	7,11,13	2.16	3 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	TRX	M	2	11	14,16,17	3.74	3 (21%)	10,22,24	5.18	4 (40%)
11	CSX	M	6	11	3,6,7	2.43	2 (66%)	3,6,8	1.89	1 (33%)
11	HYP	M	8	11	7,8,9	0.82	0	5,10,12	1.17	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
11	ILX	M	1	11	-	0/10/12/14	0/0/0/0
11	TRX	M	2	11	-	0/3/6/8	0/2/2/2
11	CSX	M	6	11	-	0/1/5/7	0/0/0/0
11	HYP	M	8	11	-	0/0/11/13	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	2	TRX	CE3-CZ3	2.03	1.40	1.36
11	M	6	CSX	CB-CA	2.16	1.59	1.53
11	M	6	CSX	O-C	3.56	1.36	1.19
11	M	2	TRX	CZ2-CE2	8.66	1.54	1.41
11	M	2	TRX	CZ2-CH2	10.04	1.56	1.37

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	2	TRX	CH2-CZ2-CE2	-15.43	109.12	119.19
11	M	1	ILX	O-C-CA	-3.08	117.30	125.44
11	M	6	CSX	O-C-CA	-2.99	117.71	125.49
11	M	2	TRX	CB-CG-CD1	-2.47	124.92	127.97
11	M	2	TRX	CZ2-CE2-NE1	-2.03	125.14	130.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	M	2	TRX	1	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1349/1733 (77%)	-0.20	54 (4%)	42	30	2, 30, 63, 104	0
2	B	1061/1224 (86%)	-0.24	46 (4%)	39	27	6, 29, 63, 77	0
3	C	265/318 (83%)	-0.27	7 (2%)	59	47	16, 26, 43, 59	0
4	E	213/215 (99%)	-0.14	6 (2%)	56	44	13, 35, 60, 70	0
5	F	84/155 (54%)	-0.36	1 (1%)	81	73	10, 23, 41, 49	0
6	H	116/146 (79%)	0.53	15 (12%)	5	2	35, 48, 71, 72	0
7	I	121/122 (99%)	-0.20	3 (2%)	61	48	6, 24, 52, 65	0
8	J	65/70 (92%)	-0.46	1 (1%)	76	68	17, 26, 45, 46	0
9	K	113/120 (94%)	-0.25	5 (4%)	38	26	17, 32, 54, 57	0
10	L	43/70 (61%)	0.45	5 (11%)	6	3	34, 57, 72, 76	0
11	M	4/8 (50%)	0.49	0	100	100	44, 45, 48, 48	0
All	All	3434/4181 (82%)	-0.19	143 (4%)	40	28	2, 30, 62, 104	0

The worst 5 of 143 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	247	GLY	8.7
1	A	1089	VAL	6.9
1	A	62	ASP	6.2
2	B	265	SER	5.7
1	A	1087	ALA	5.7

### 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. 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
11	TRX	M	2	15/16	0.94	0.20	-	44,50,51,51	0
11	HYP	M	8	8/9	0.95	0.18	-	42,47,48,48	0
11	ILX	M	1	10/11	0.94	0.21	-	37,40,44,44	0
11	CSX	M	6	7/8	0.95	0.26	-	48,50,52,54	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. 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
12	ZN	I	3003	1/1	0.98	0.04	-1.56	33,33,33,33	0
12	ZN	I	3004	1/1	0.98	0.05	-1.68	46,46,46,46	0
12	ZN	C	3002	1/1	0.97	0.04	-2.13	39,39,39,39	0
12	ZN	A	3008	1/1	0.94	0.04	-2.20	77,77,77,77	0
12	ZN	L	3005	1/1	0.96	0.04	-2.48	73,73,73,73	0
12	ZN	A	3006	1/1	0.99	0.02	-3.04	46,46,46,46	0
12	ZN	J	3001	1/1	0.99	0.03	-3.12	34,34,34,34	0
12	ZN	B	3007	1/1	0.99	0.02	-3.24	60,60,60,60	0

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

There are no such residues in this entry.