



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 23, 2023 – 12:54 PM EDT

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

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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

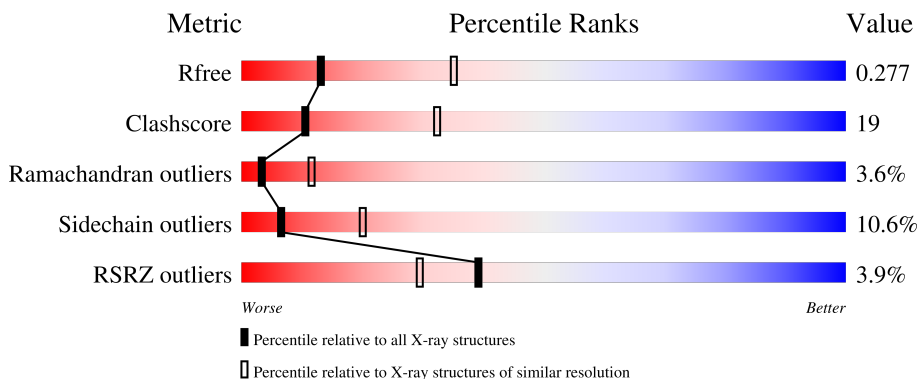
1 Overall quality at a glance

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 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	 3% 50% 22% 22%
2	B	1224	 4% 57% 24% 13%
3	C	318	 2% 57% 23% 17%
4	E	215	 3% 60% 27% 10% 2%
5	F	155	 % 40% 12% 46%

Continued on next page...

Continued from previous page...

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

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
			Total	C	N	O	S			
1	A	1349	10616	6710	1838	2009	59	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	1061	8419	5340	1465	1563	51	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	265	2087	1313	347	414	13	0	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	I	121	989	608	181	190	10	0	0	0

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC5.

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

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	K	113	911	585	155	170	1	0	0	0

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	L	43	342	211	68	59	4	0	0	0

- Molecule 11 is a protein called ALPHA-AMANITIN.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	2	Total	Zn	0	0
			2	2		
12	B	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

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

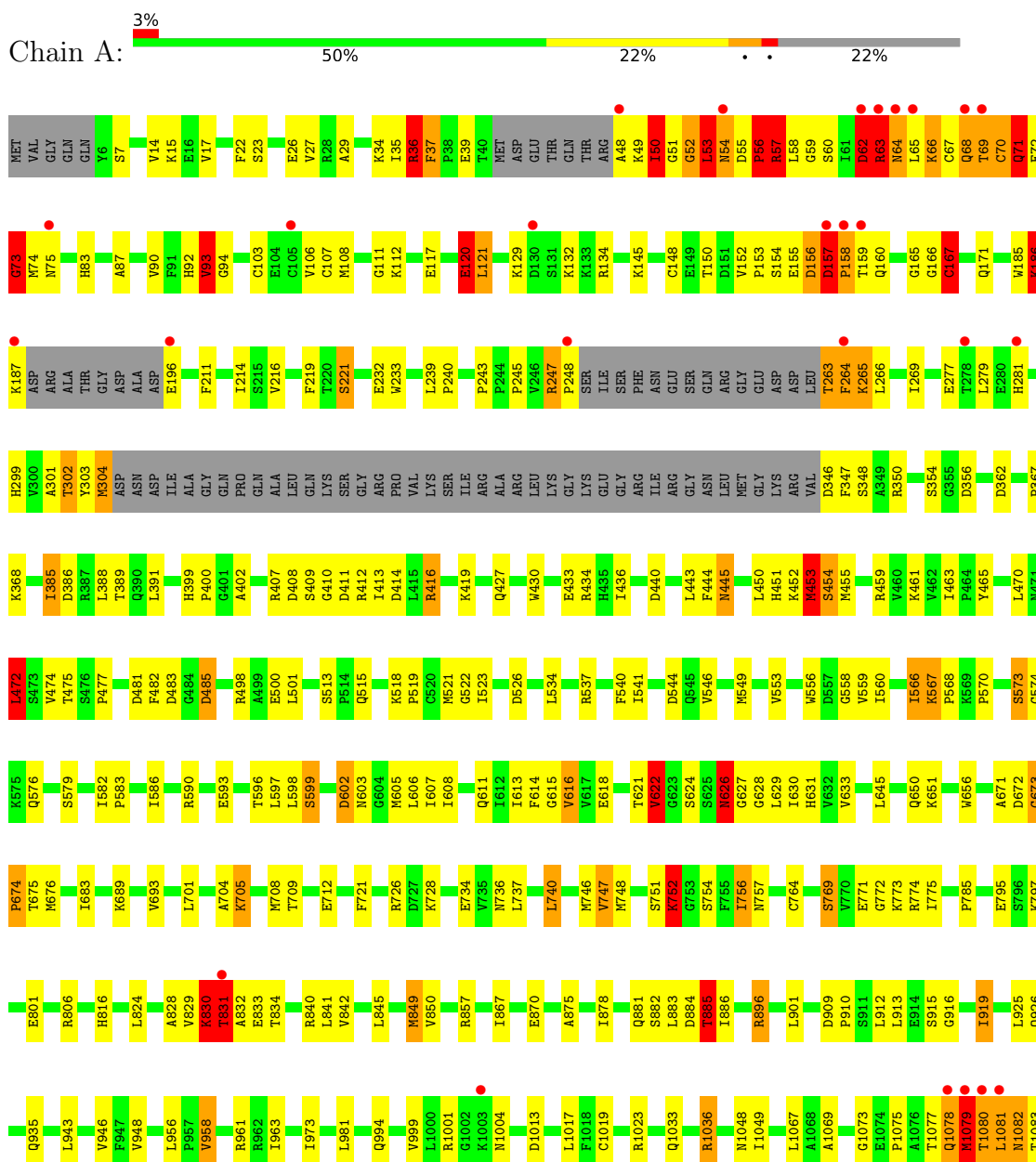
- Molecule 13 is water.

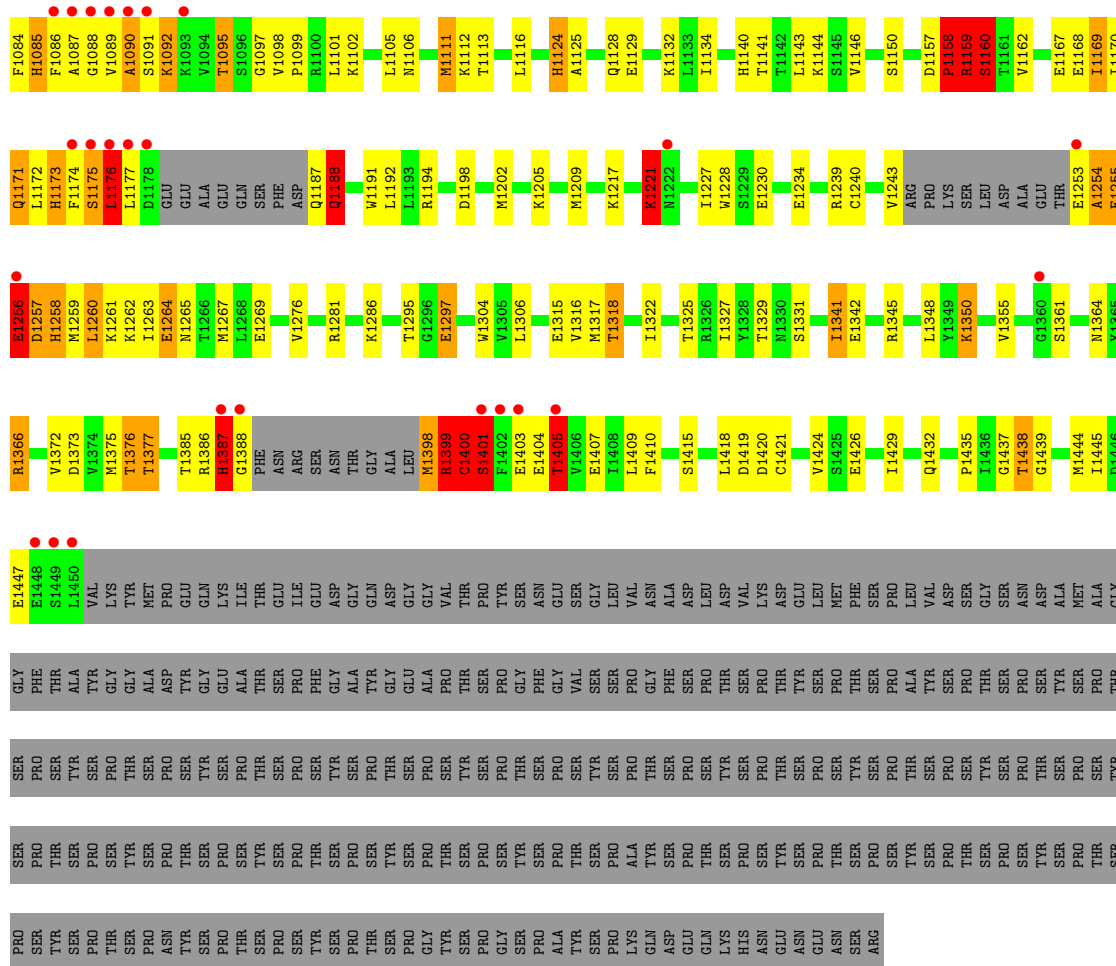
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	11	Total 11	O 11	0	0
13	B	4	Total 4	O 4	0	0
13	E	1	Total 1	O 1	0	0
13	F	1	Total 1	O 1	0	0

3 Residue-property plots

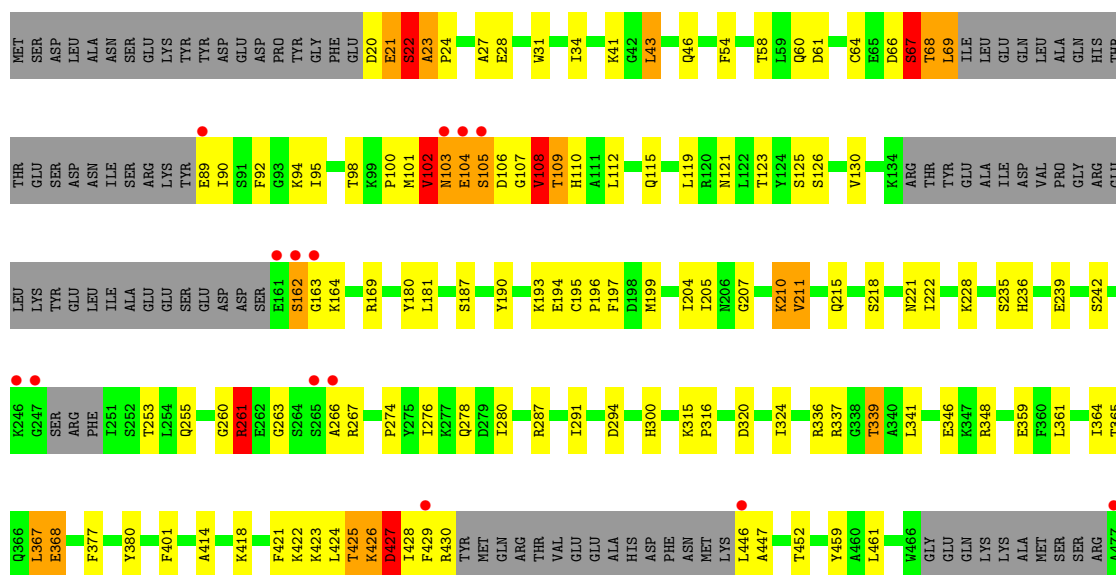
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

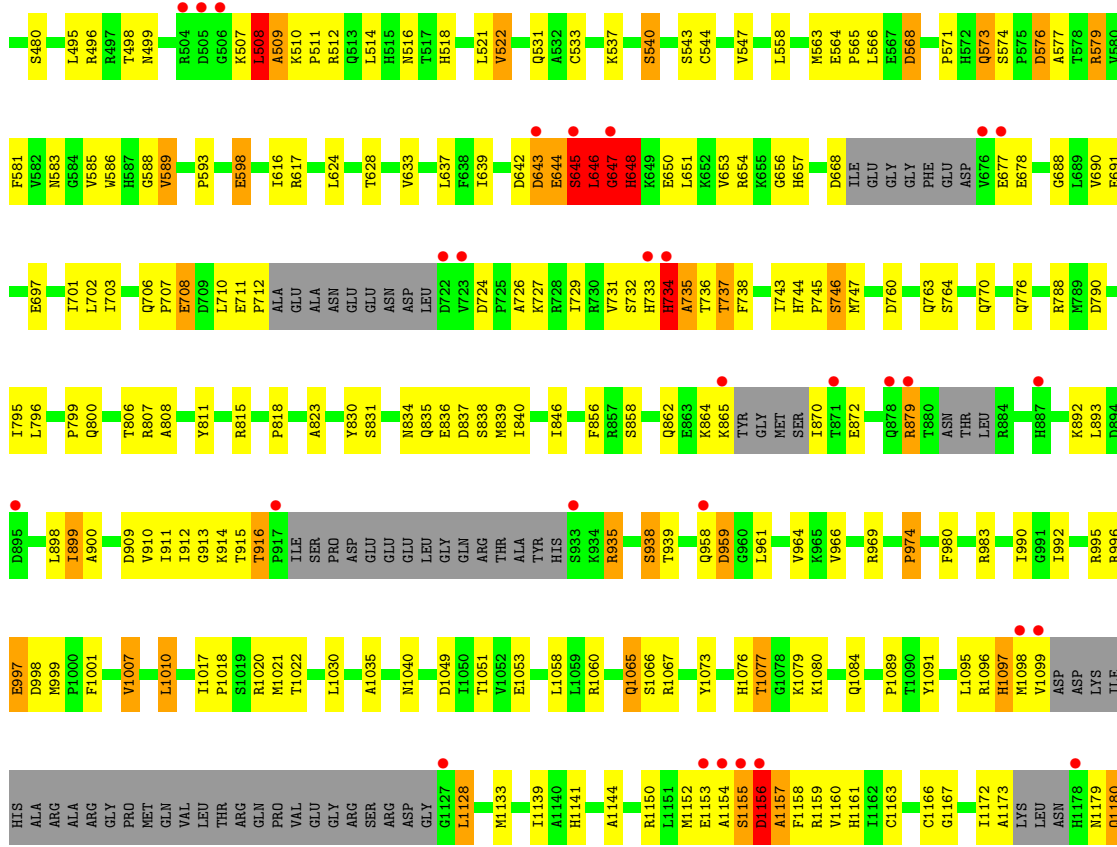
- Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1



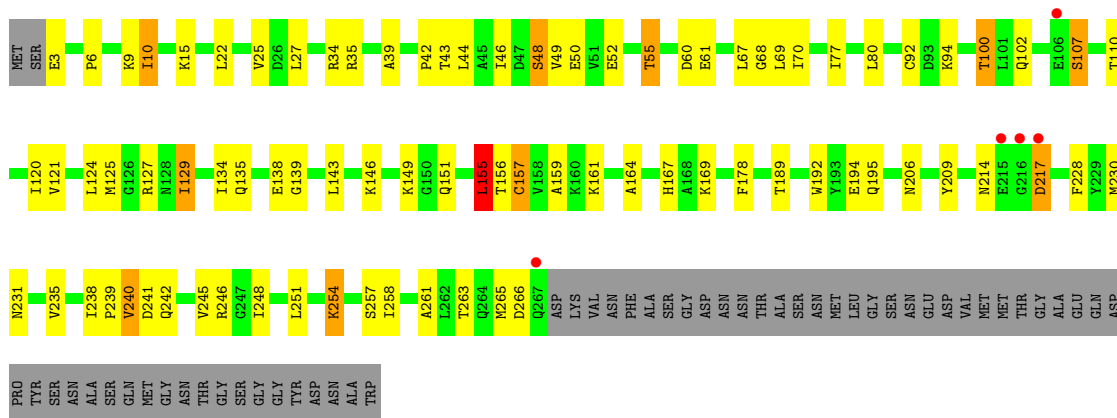


● Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2



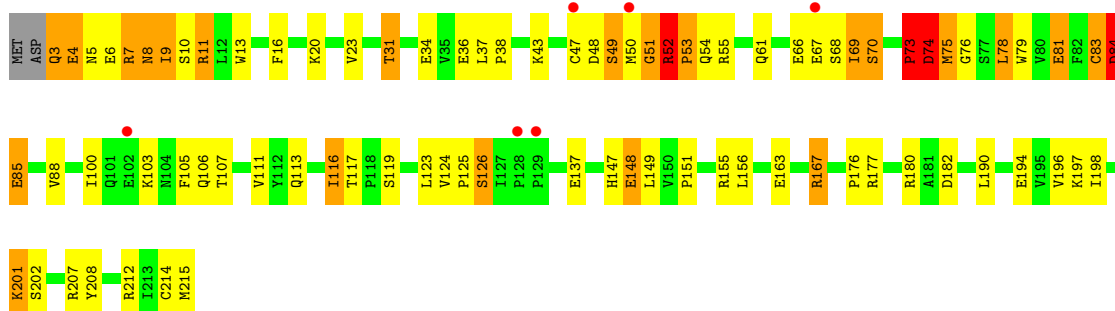


● Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

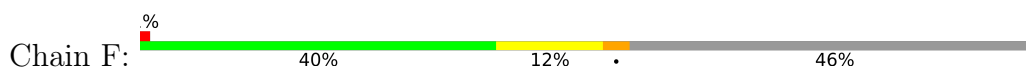


● Molecule 4: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1

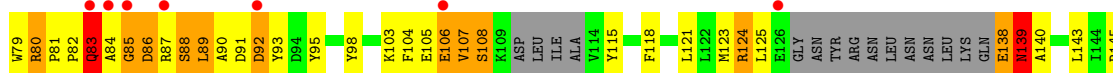




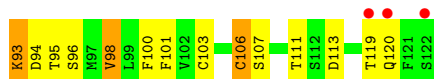
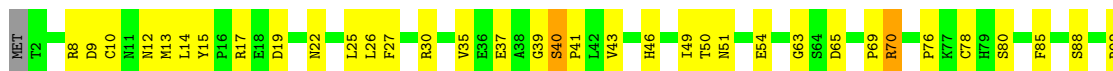
- Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2



- 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

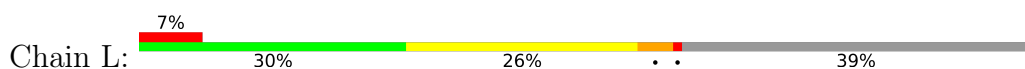




- Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11



- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.79Å)	Xtrriage
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 (2.80%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtrriage
Anisotropy	0.352	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27340	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage'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.*

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: TRX, ILX, CSX, ZN, HYP

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

Continued on next page...

Continued from previous page...

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 9
2	B	1035/1224 (85%)	920 (89%)	79 (8%)	36 (4%)	3 12
3	C	263/318 (83%)	243 (92%)	19 (7%)	1 (0%)	34 66
4	E	211/215 (98%)	189 (90%)	12 (6%)	10 (5%)	2 7
5	F	82/155 (53%)	78 (95%)	4 (5%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	H	108/146 (74%)	76 (70%)	17 (16%)	15 (14%)	0	0
7	I	119/122 (98%)	106 (89%)	11 (9%)	2 (2%)	9	29
8	J	63/70 (90%)	62 (98%)	1 (2%)	0	100	100
9	K	111/120 (92%)	99 (89%)	10 (9%)	2 (2%)	8	28
10	L	39/70 (56%)	29 (74%)	9 (23%)	1 (3%)	5	18
11	M	4/8 (50%)	3 (75%)	1 (25%)	0	100	100
All	All	3368/4181 (81%)	2973 (88%)	273 (8%)	122 (4%)	3	11

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 [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	1182/1520 (78%)	1049 (89%)	133 (11%)	6	18
2	B	919/1061 (87%)	841 (92%)	78 (8%)	10	31
3	C	233/274 (85%)	207 (89%)	26 (11%)	6	18
4	E	195/197 (99%)	170 (87%)	25 (13%)	4	13
5	F	74/137 (54%)	67 (90%)	7 (10%)	8	25
6	H	102/128 (80%)	81 (79%)	21 (21%)	1	3
7	I	115/116 (99%)	105 (91%)	10 (9%)	10	30
8	J	60/65 (92%)	53 (88%)	7 (12%)	5	16
9	K	98/102 (96%)	91 (93%)	7 (7%)	14	39
10	L	38/57 (67%)	32 (84%)	6 (16%)	2	8

Continued on next page...

Continued from previous page...

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%)	6	20

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

Mol	Chain	Res	Type
3	C	240	VAL
6	H	138	GLU
4	E	7	ARG
4	E	201	LYS
8	J	1	MET

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

Mol	Chain	Res	Type
4	E	3	GLN
9	K	2	ASN
4	E	32	GLN
6	H	33	GLN
2	B	115	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	CSX	M	6	11	3,6,7	2.76	2 (66%)	1,6,8	1.00	0

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	3.83	4 (28%)	15,22,24	3.27	7 (46%)
11	HYP	M	8	11	6,8,9	0.73	0	5,10,12	1.12	0
11	ILX	M	1	11	8,9,10	0.90	0	9,11,13	1.66	2 (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
11	CSX	M	6	11	-	0/1/5/7	-
11	TRX	M	2	11	-	0/4/6/8	0/2/2/2
11	HYP	M	8	11	-	0/0/11/13	0/1/1/1
11	ILX	M	1	11	-	5/11/12/14	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	2	TRX	CZ2-CH2	10.69	1.56	1.37
11	M	2	TRX	CZ2-CE2	8.38	1.54	1.41
11	M	6	CSX	O-C	4.09	1.36	1.19
11	M	6	CSX	CB-CA	2.42	1.59	1.53
11	M	2	TRX	CB-CG	2.09	1.57	1.51

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	2	TRX	CH2-CZ2-CE2	-9.64	109.12	119.29
11	M	2	TRX	CG-CB-CA	4.40	121.33	114.53
11	M	2	TRX	CZ2-CE2-CD2	3.26	125.35	121.16
11	M	2	TRX	CB-CA-C	3.23	117.52	111.47
11	M	1	ILX	O-C-CA	-2.86	117.30	124.78

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	M	1	ILX	CG2-CB-CG1-CD1
11	M	1	ILX	OD1-CD1-CG1-OG1
11	M	1	ILX	C-CA-CB-CG2
11	M	1	ILX	OD1-CD1-CG1-CB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	M	1	ILX	O-C-CA-CB

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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	1349/1733 (77%)	-0.20	51 (3%) 40 30	2, 30, 63, 104	0
2	B	1061/1224 (86%)	-0.24	44 (4%) 37 27	6, 29, 63, 77	0
3	C	265/318 (83%)	-0.28	5 (1%) 66 59	16, 26, 43, 59	0
4	E	213/215 (99%)	-0.15	6 (2%) 53 43	13, 35, 60, 70	0
5	F	84/155 (54%)	-0.36	1 (1%) 79 73	10, 23, 41, 49	0
6	H	116/146 (79%)	0.52	14 (12%) 4 2	35, 48, 71, 72	0
7	I	121/122 (99%)	-0.21	3 (2%) 57 47	6, 24, 52, 65	0
8	J	65/70 (92%)	-0.47	0 100 100	17, 26, 45, 46	0
9	K	113/120 (94%)	-0.25	5 (4%) 34 24	17, 32, 54, 57	0
10	L	43/70 (61%)	0.44	5 (11%) 4 2	34, 57, 72, 76	0
11	M	4/8 (50%)	0.45	0 100 100	44, 45, 48, 48	0
All	All	3434/4181 (82%)	-0.20	134 (3%) 39 29	2, 30, 62, 104	0

The worst 5 of 134 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	247	GLY	8.6
1	A	1089	VAL	6.8
1	A	1087	ALA	6.0
1	A	62	ASP	5.8
2	B	265	SER	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. 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(\AA^2)	Q<0.9
11	ILX	M	1	10/11	0.94	0.21	37,40,44,44	0
11	TRX	M	2	15/16	0.94	0.20	44,50,51,51	0
11	CSX	M	6	7/8	0.95	0.25	48,50,52,54	0
11	HYP	M	8	8/9	0.95	0.19	42,47,48,48	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(\AA^2)	Q<0.9
12	ZN	A	3008	1/1	0.94	0.04	77,77,77,77	0
12	ZN	L	3005	1/1	0.96	0.04	73,73,73,73	0
12	ZN	C	3002	1/1	0.97	0.03	39,39,39,39	0
12	ZN	I	3004	1/1	0.98	0.05	46,46,46,46	0
12	ZN	I	3003	1/1	0.98	0.04	33,33,33,33	0
12	ZN	A	3006	1/1	0.99	0.02	46,46,46,46	0
12	ZN	J	3001	1/1	0.99	0.03	34,34,34,34	0
12	ZN	B	3007	1/1	0.99	0.02	60,60,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.