



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 03:28 AM UTC

PDB ID : 3CQZ / pdb_00003cqz
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:

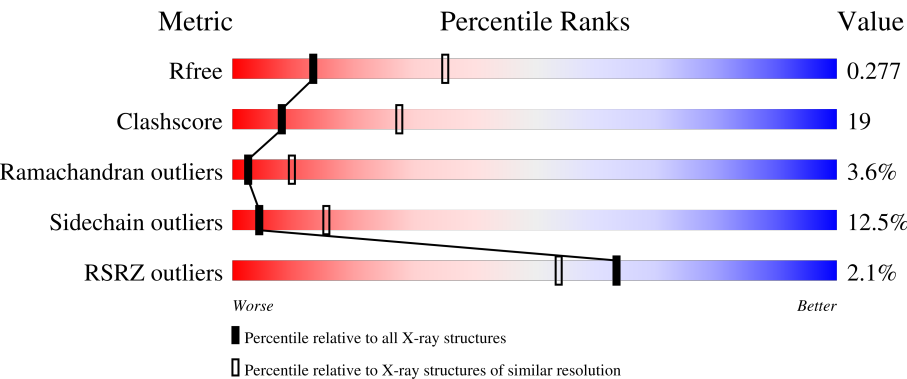
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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	2% 48%23%••22%
2	B	1224	2% 55%25%5%•13%
3	C	318	55%23%5%17%
4	E	215	2% 58%28%10%••
5	F	155	38%13%••46%

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Mol	Chain	Length	Quality of chain
6	H	146	3% 32% 29% 16% • 21%
7	I	122	% 55% 38% 7% •
8	J	70	57% 27% 9% 7%
9	K	120	% 56% 35% • • 6%
10	L	70	29% 26% 7% 39%
11	M	8	50% 38% 12%

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 (CCD ID: 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		

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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

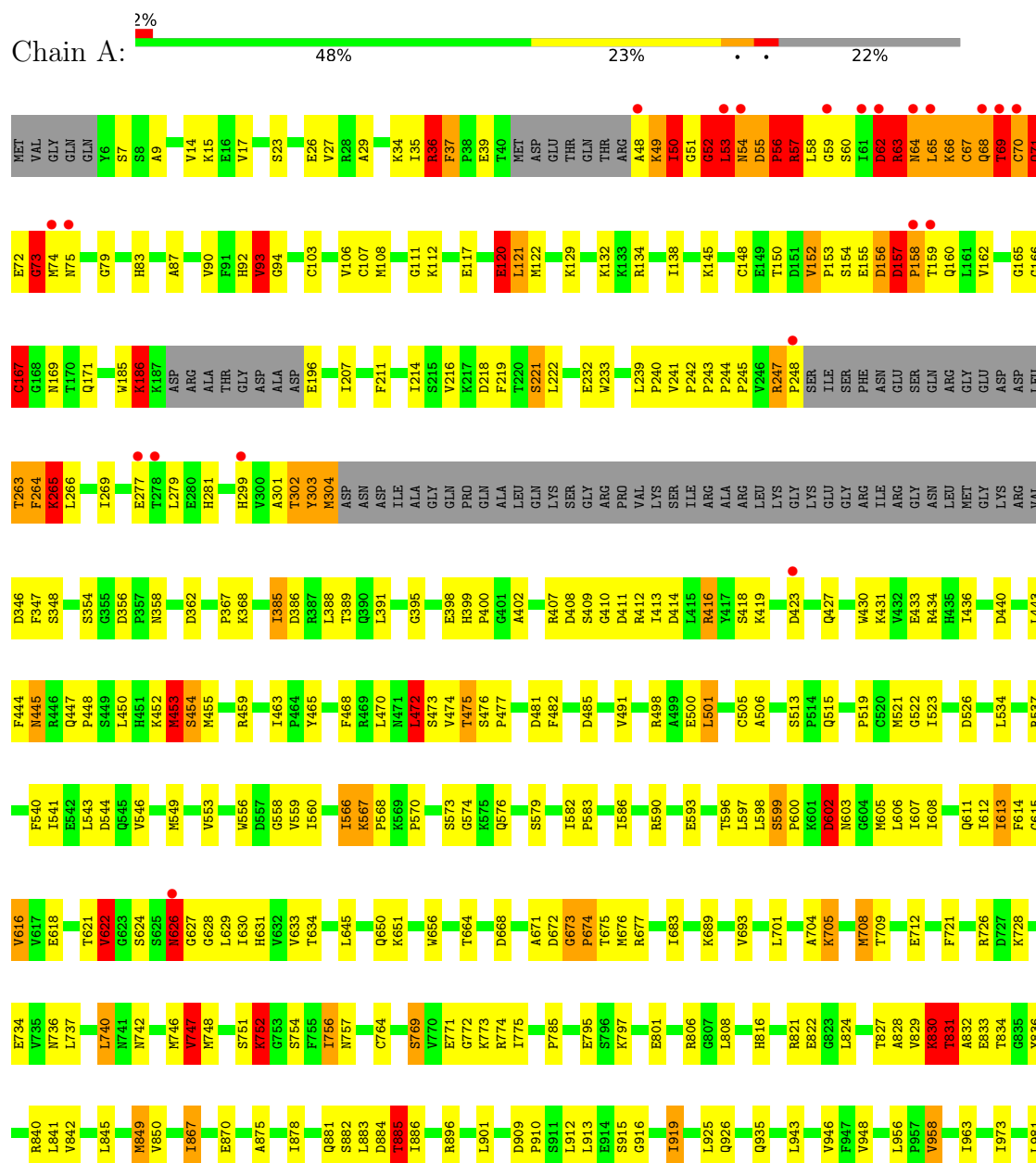
- Molecule 13 is water.

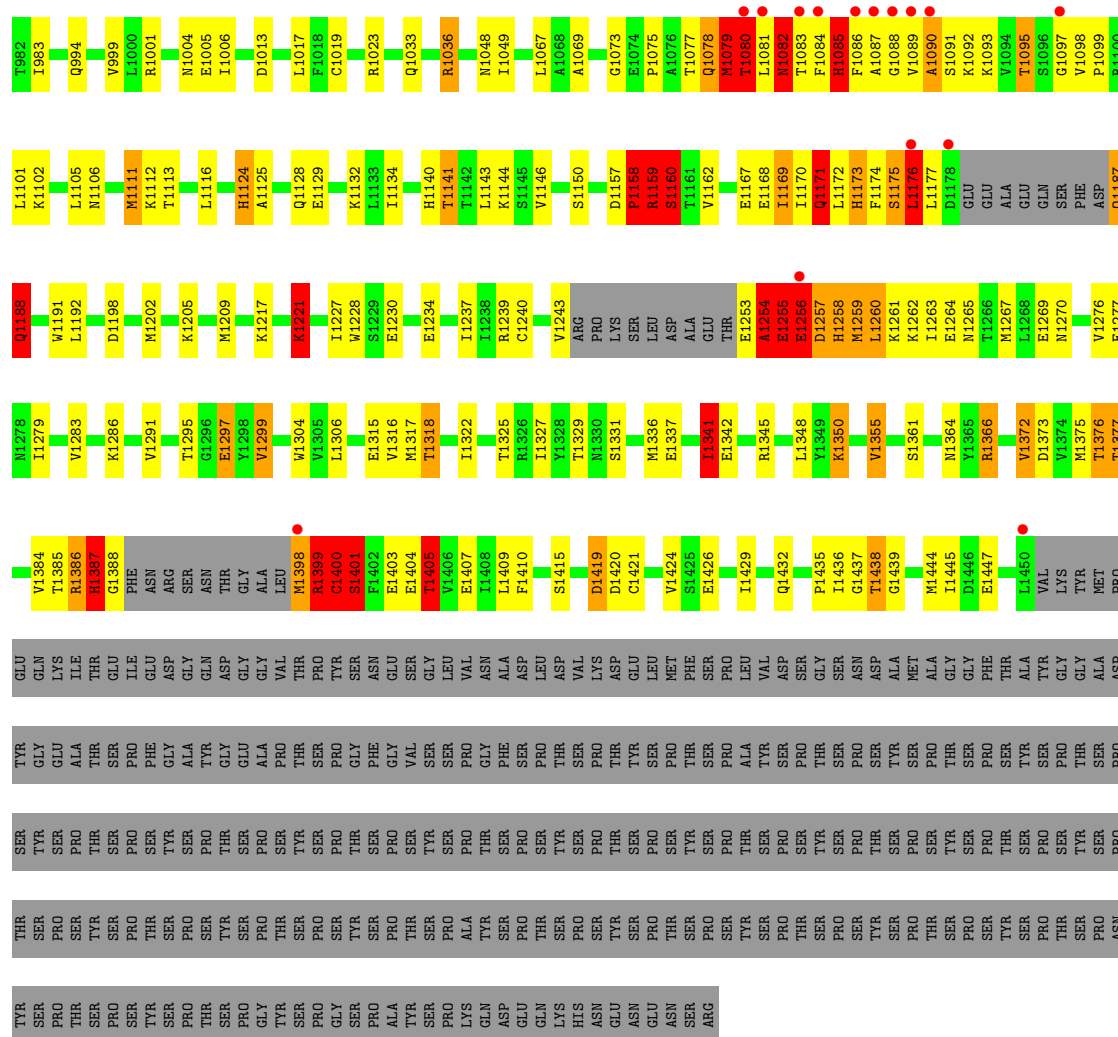
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	11	Total 11	O 11	0	0
13	B	4	Total 4	O 4	0	0
13	E	1	Total 1	O 1	0	0
13	F	1	Total 1	O 1	0	0

3 Residue-property plots [i](#)

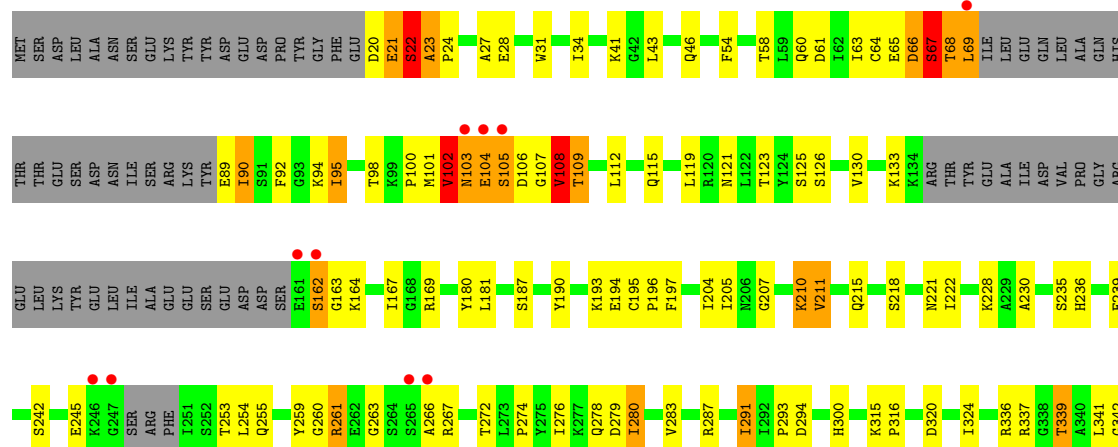
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

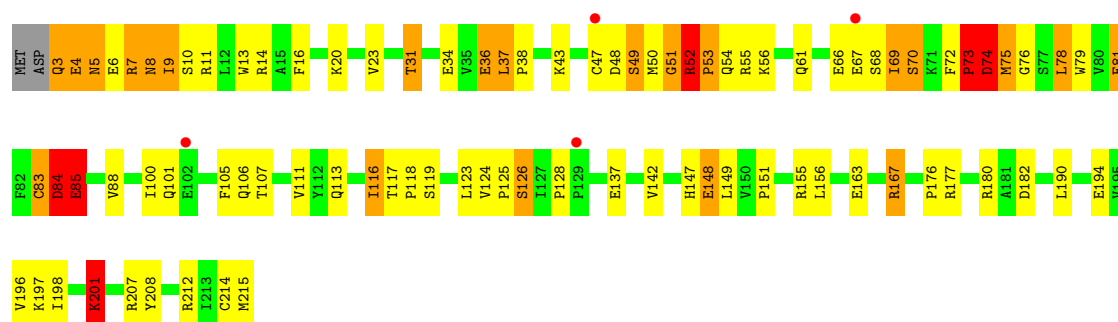
• Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1





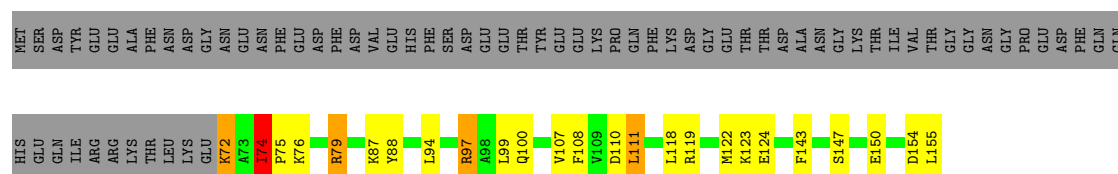
● Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2





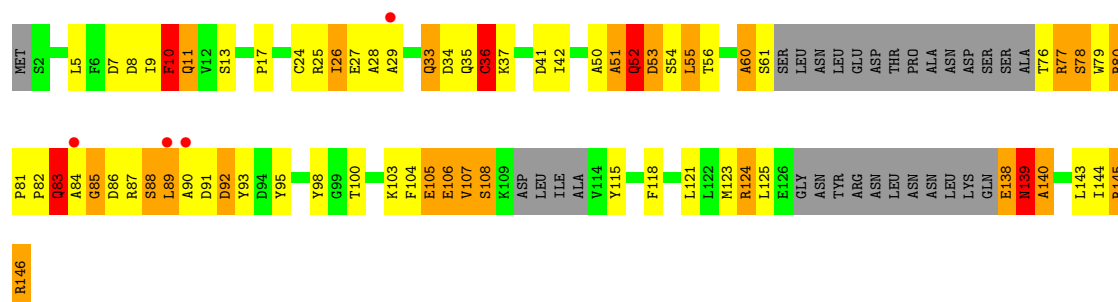
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2

Chain F: 38% 13% 46%



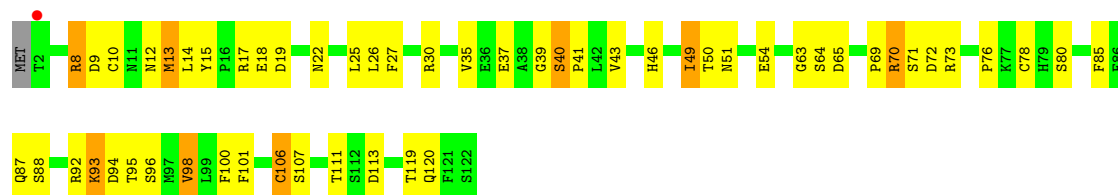
• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC3

Chain H: 3% 32% 29% 16% 21%



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

Chain I: 55% 38% 7%

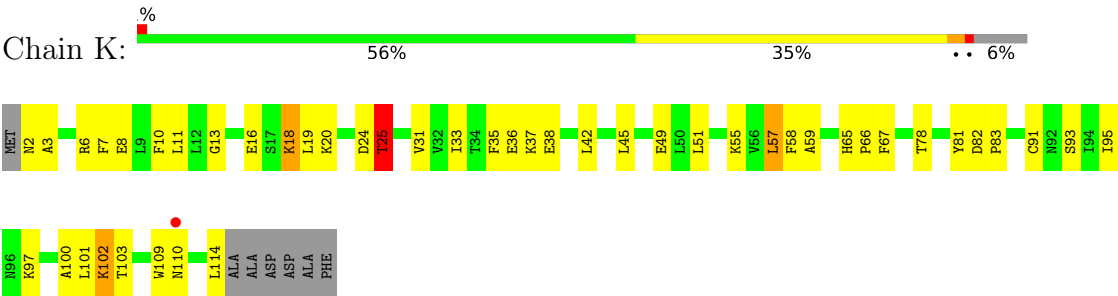


• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC5

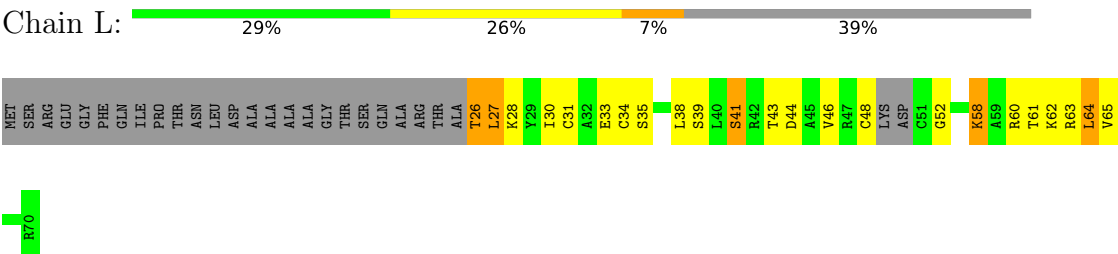
Chain J: 57% 27% 9% 7%



● 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) 92.7 (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)	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 (2.80%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 25.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27340	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HYP, ILX, CSX, TRX, ZN

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	0.91	1/10809 (0.0%)	1.22	80/14624 (0.5%)
2	B	0.90	0/8579	1.16	33/11565 (0.3%)
3	C	0.77	0/2125	1.04	3/2880 (0.1%)
4	E	0.83	1/1780 (0.1%)	1.16	13/2395 (0.5%)
5	F	0.86	0/691	1.17	2/933 (0.2%)
6	H	0.75	0/947	1.25	10/1279 (0.8%)
7	I	0.89	0/1008	1.05	2/1355 (0.1%)
8	J	0.79	0/541	1.17	1/727 (0.1%)
9	K	0.76	0/929	1.01	3/1255 (0.2%)
10	L	0.76	0/343	1.02	0/453
11	M	3.43	2/22 (9.1%)	2.06	0/26
All	All	0.88	4/27774 (0.0%)	1.17	147/37492 (0.4%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	4	ILE	C-O	13.26	1.37	1.24
11	M	4	ILE	CA-C	5.94	1.59	1.52
4	E	128	PRO	CA-C	5.74	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	476	SER	N-CA	-5.00	1.42	1.46

The worst 5 of 147 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	ASP	CA-C-N	16.60	140.59	119.84
1	A	157	ASP	C-N-CA	16.60	140.59	119.84
1	A	1257	ASP	N-CA-C	11.91	127.69	108.63
6	H	105	GLU	N-CA-C	11.31	123.15	108.34
4	E	5	ASN	N-CA-C	-9.58	101.52	113.02

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

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	475	0
2	B	8419	0	8450	308	0
3	C	2087	0	2047	67	0
4	E	1744	0	1772	88	0
5	F	679	0	701	21	0
6	H	932	0	899	75	0
7	I	989	0	942	35	0
8	J	532	0	542	17	0
9	K	911	0	917	38	0
10	L	342	0	363	17	0
11	M	64	0	51	1	0
12	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	1058	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 1058 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%)	2 8
2	B	1035/1224 (85%)	920 (89%)	79 (8%)	36 (4%)	3 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	263/318 (83%)	243 (92%)	19 (7%)	1 (0%)	30	60
4	E	211/215 (98%)	189 (90%)	12 (6%)	10 (5%)	2	6
5	F	82/155 (53%)	78 (95%)	4 (5%)	0	100	100
6	H	108/146 (74%)	76 (70%)	17 (16%)	15 (14%)	0	0
7	I	119/122 (98%)	106 (89%)	11 (9%)	2 (2%)	7	25
8	J	63/70 (90%)	62 (98%)	1 (2%)	0	100	100
9	K	111/120 (92%)	99 (89%)	10 (9%)	2 (2%)	6	23
10	L	39/70 (56%)	29 (74%)	9 (23%)	1 (3%)	4	15
11	M	4/8 (50%)	3 (75%)	1 (25%)	0	100	100
All	All	3368/4181 (81%)	2973 (88%)	273 (8%)	122 (4%)	2	10

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%)	1033 (87%)	149 (13%)	4	15
2	B	919/1061 (87%)	823 (90%)	96 (10%)	7	22
3	C	233/274 (85%)	200 (86%)	33 (14%)	3	12
4	E	195/197 (99%)	169 (87%)	26 (13%)	4	14
5	F	74/137 (54%)	66 (89%)	8 (11%)	6	21
6	H	102/128 (80%)	79 (78%)	23 (22%)	1	3
7	I	115/116 (99%)	100 (87%)	15 (13%)	4	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	J	60/65 (92%)	50 (83%)	10 (17%)	2	8
9	K	98/102 (96%)	90 (92%)	8 (8%)	10	33
10	L	38/57 (67%)	30 (79%)	8 (21%)	1	4
11	M	2/2 (100%)	2 (100%)	0	100	100
All	All	3018/3659 (82%)	2642 (88%)	376 (12%)	4	15

5 of 376 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	964	VAL
4	E	52	ARG
2	B	1065	GLN
3	C	129	ILE
4	E	142	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	131	HIS
5	F	100	GLN
3	C	167	HIS
4	E	3	GLN
7	I	12	ASN

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	TRX	M	2	11	15,16,17	4.35	7 (46%)	17,22,24	2.24	5 (29%)
11	CSX	M	6	11	3,6,7	2.84	2 (66%)	1,6,8	0.85	0
11	HYP	M	8	11	7,8,9	0.70	0	5,10,12	1.15	0
11	ILX	M	1	11	8,9,10	0.95	0	8,11,13	1.65	2 (25%)

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	TRX	M	2	11	-	3/5/6/8	0/2/2/2
11	CSX	M	6	11	-	0/2/5/7	-
11	HYP	M	8	11	-	0/0/11/13	0/1/1/1
11	ILX	M	1	11	-	4/11/12/14	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	2	TRX	CZ2-CH2	11.87	1.56	1.39
11	M	2	TRX	CZ2-CE2	9.74	1.54	1.39
11	M	6	CSX	O-C	4.28	1.36	1.20
11	M	2	TRX	CB-CG	3.66	1.57	1.50
11	M	2	TRX	CD1-CG	3.03	1.41	1.36

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	2	TRX	CE2-CZ2-CH2	-5.56	109.12	117.87
11	M	2	TRX	CZ2-CE2-NE1	-4.20	125.14	131.62
11	M	2	TRX	CZ2-CE2-CD2	3.55	125.35	122.52
11	M	1	ILX	O-C-CA	-2.91	117.30	124.77
11	M	1	ILX	CG2-CB-CG1	2.68	115.36	111.09

There are no chirality outliers.

5 of 7 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

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Mol	Chain	Res	Type	Atoms
11	M	2	TRX	CA-CB-CG-CD2
11	M	1	ILX	C-CA-CB-CG2
11	M	2	TRX	CA-CB-CG-CD1

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 oligosaccharides 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 ⓘ

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, 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%)	-0.06	36 (2%) 56 46	2, 30, 63, 104	0
2	B	1061/1224 (86%)	-0.15	25 (2%) 59 49	6, 29, 63, 77	0
3	C	265/318 (83%)	-0.10	0 100 100	16, 26, 43, 59	0
4	E	213/215 (99%)	-0.04	4 (1%) 66 57	13, 35, 60, 70	0
5	F	84/155 (54%)	-0.38	0 100 100	10, 23, 41, 49	0
6	H	116/146 (79%)	0.62	4 (3%) 48 39	35, 48, 71, 72	0
7	I	121/122 (99%)	-0.28	1 (0%) 82 75	6, 24, 52, 65	0
8	J	65/70 (92%)	-0.29	0 100 100	17, 26, 45, 46	0
9	K	113/120 (94%)	0.01	1 (0%) 81 74	17, 32, 54, 57	0
10	L	43/70 (61%)	0.44	0 100 100	34, 57, 72, 76	0
11	M	4/8 (50%)	0.36	0 100 100	44, 45, 48, 48	0
All	All	3434/4181 (82%)	-0.08	71 (2%) 63 54	2, 30, 62, 104	0

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1090	ALA	5.2
1	A	54	ASN	5.0
1	A	69	THR	4.7
1	A	62	ASP	4.7
1	A	1083	THR	4.4

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	ILX	M	1	10/11	0.91	0.10	37,40,44,44	0
11	CSX	M	6	7/8	0.91	0.09	48,50,52,54	0
11	TRX	M	2	15/16	0.93	0.10	44,50,51,51	0
11	HYP	M	8	8/9	0.95	0.08	42,47,48,48	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
12	ZN	L	3005	1/1	0.95	0.05	73,73,73,73	0
12	ZN	A	3008	1/1	0.96	0.06	77,77,77,77	0
12	ZN	C	3002	1/1	0.97	0.04	39,39,39,39	0
12	ZN	I	3004	1/1	0.98	0.03	46,46,46,46	0
12	ZN	A	3006	1/1	0.98	0.02	46,46,46,46	0
12	ZN	B	3007	1/1	0.99	0.03	60,60,60,60	0
12	ZN	J	3001	1/1	0.99	0.02	34,34,34,34	0
12	ZN	I	3003	1/1	0.99	0.02	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.