



wwPDB EM Validation Summary Report ⓘ

May 10, 2026 – 12:24 AM JST

PDB ID : 9K17 / pdb_00009k17
EMDB ID : EMD-61967
Title : A cryo-EM structure of *B. oleracea* RNA polymerase V in complex with 6U scaffold at 3.04 Angstrom
Authors : Xie, G.; Du, X.; Du, J.
Deposited on : 2024-10-16
Resolution : 3.04 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : **FAILED**
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

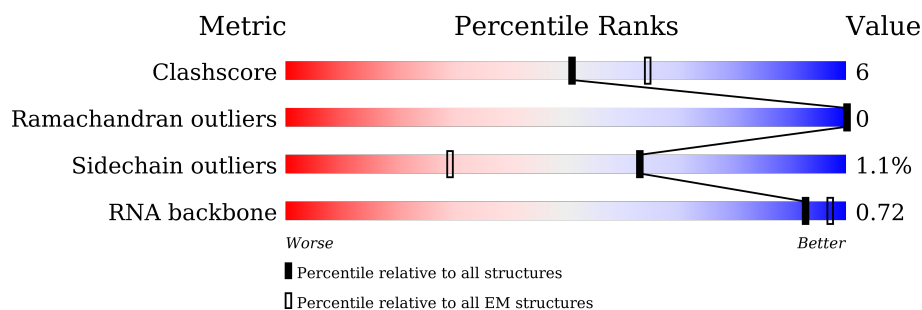
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.04 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RNA backbone	8273	3508

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	T	34	
2	N	34	
3	P	20	
4	A	2032	
5	C	319	
6	F	144	
7	J	71	
8	K	116	

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Mol	Chain	Length	Quality of chain
9	L	51	 82%6%12%
10	H	146	 68%27%. .
11	I	114	 68%15%.16%
12	E	230	 69%22%9%
13	B	1169	 75%8%17%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 23142 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 DNA chain called DNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	T	9	Total	C	N	O	P	0	0
			185	88	38	50	9		

- Molecule 2 is a DNA chain called DNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	16	Total	C	N	O	P	0	0
			329	156	60	97	16		

- Molecule 3 is a RNA chain called RNA (5'-R(*UP*AP*UP*AP*UP*GP*CP*AP*GP*AP*AP*AP*GP*CP*UP*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	3	Total	C	N	O	P	0	0
			60	27	6	24	3		

- Molecule 4 is a protein called DNA-directed RNA polymerase V largest subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	844	Total	C	N	O	S	0	0
			6608	4176	1136	1252	44		

- Molecule 5 is a protein called DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	287	Total	C	N	O	S	0	0
			2256	1418	380	445	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	THR	SER	conflict	UNP A0A0D3D418

- Molecule 6 is a protein called DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	80	Total	C	N	O	S	0	0
			660	420	114	122	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	51	GLU	ASP	conflict	UNP A0A0D3BZZ8

- Molecule 7 is a protein called DNA-directed RNA polymerase II, IV and V subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	63	Total	C	N	O	S	0	0
			507	324	85	91	7		

- Molecule 8 is a protein called DNA-directed RNA polymerase RBP11-like dimerisation domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	108	Total	C	N	O	S	0	0
			890	565	156	167	2		

- Molecule 9 is a protein called DNA-directed RNA polymerase II, IV and V subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	45	Total	C	N	O	S	0	0
			365	224	70	67	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	18	GLU	LYS	conflict	UNP A0A0D2ZPP3
L	32	CYS	ARG	conflict	UNP A0A0D2ZPP3

- Molecule 10 is a protein called DNA-directed RNA polymerase II, IV and V subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	141	Total	C	N	O	S	0	0
			1129	729	183	208	9		

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	96	Total	C	N	O	S	0	0
			780	477	149	142	12		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	20	ARG	LYS	conflict	UNP A0A0D3A7P5
I	40	ASP	ASN	conflict	UNP A0A0D3A7P5

- Molecule 12 is a protein called RNA polymerase subunit H/Rpb5 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	209	Total	C	N	O	S	0	0
			1706	1085	303	316	2		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	101	GLY	SER	conflict	UNP A0A0D3DTU3
E	182	GLN	HIS	conflict	UNP A0A0D3DTU3
E	210	ILE	VAL	conflict	UNP A0A0D3DTU3

- Molecule 13 is a protein called DNA-directed RNA polymerase IV and V subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	B	967	Total	C	N	O	S	0	0
			7660	4827	1357	1432	44		

- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
14	A	1	Total	Mg	0
			1	1	

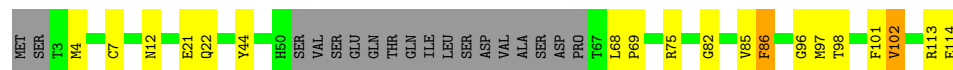
- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total 1	Zn 1	0
15	C	1	Total 1	Zn 1	0
15	J	1	Total 1	Zn 1	0
15	L	1	Total 1	Zn 1	0
15	I	2	Total 2	Zn 2	0

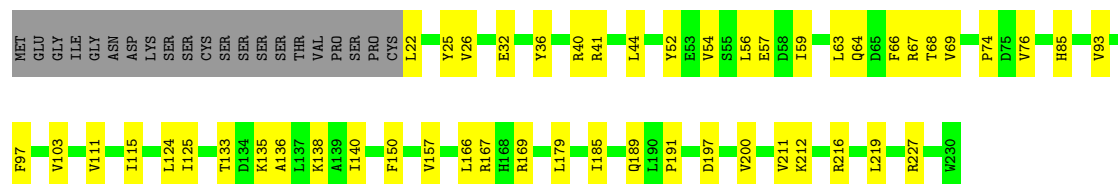




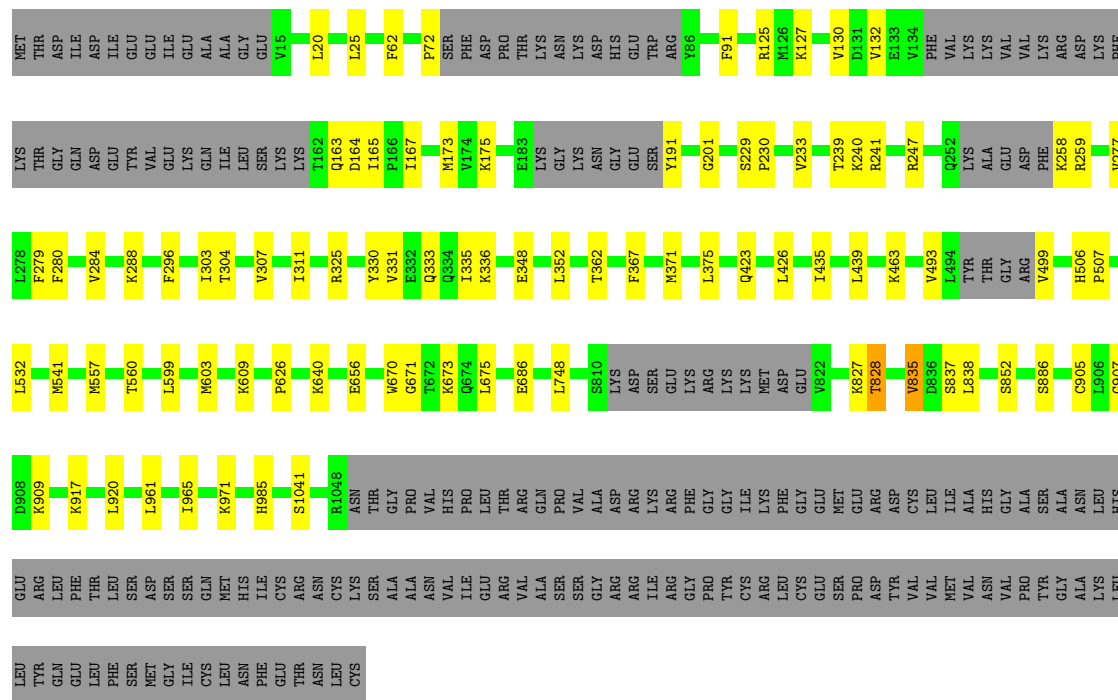
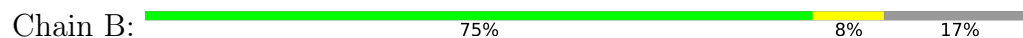
• Molecule 11: DNA-directed RNA polymerase subunit



• Molecule 12: RNA polymerase subunit H/Rpb5 C-terminal domain-containing protein



• Molecule 13: DNA-directed RNA polymerase IV and V subunit 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70717	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.5625	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

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

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	T	0.13	0/207	0.25	0/314
2	N	0.19	0/367	0.37	0/562
3	P	0.04	0/65	0.09	0/98
4	A	0.14	0/6722	0.41	0/9076
5	C	0.12	0/2286	0.36	0/3087
6	F	0.15	0/673	0.43	0/905
7	J	0.12	0/515	0.32	0/696
8	K	0.13	0/908	0.29	0/1224
9	L	0.12	0/369	0.32	0/493
10	H	0.16	0/1155	0.48	0/1557
11	I	0.13	0/796	0.38	0/1070
12	E	0.14	0/1732	0.44	0/2332
13	B	0.12	0/7809	0.36	0/10524
All	All	0.13	0/23604	0.38	0/31938

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	T	185	0	102	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	329	0	182	4	0
3	P	60	0	31	0	0
4	A	6608	0	6661	90	0
5	C	2256	0	2269	18	0
6	F	660	0	669	17	0
7	J	507	0	512	3	0
8	K	890	0	883	7	0
9	L	365	0	364	2	0
10	H	1129	0	1128	31	0
11	I	780	0	728	16	0
12	E	1706	0	1759	30	0
13	B	7660	0	7600	60	0
14	A	1	0	0	0	0
15	A	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
All	All	23142	0	22888	255	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 6.

The worst 5 of 255 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)
4:A:592:LYS:HG3	4:A:596:GLU:HG3	1.60	0.81
11:I:113:ARG:HG2	11:I:114:GLU:HG2	1.64	0.78
5:C:104:VAL:HG21	5:C:132:VAL:HG21	1.73	0.71
13:B:258:LYS:HG3	13:B:259:ARG:HG2	1.73	0.71
12:E:76:VAL:HB	12:E:97:PHE:HB2	1.73	0.70

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	
4	A	836/2032 (41%)	806 (96%)	30 (4%)	0	100	100
5	C	283/319 (89%)	276 (98%)	7 (2%)	0	100	100
6	F	78/144 (54%)	72 (92%)	6 (8%)	0	100	100
7	J	61/71 (86%)	60 (98%)	1 (2%)	0	100	100
8	K	106/116 (91%)	102 (96%)	4 (4%)	0	100	100
9	L	43/51 (84%)	41 (95%)	2 (5%)	0	100	100
10	H	139/146 (95%)	126 (91%)	13 (9%)	0	100	100
11	I	92/114 (81%)	88 (96%)	4 (4%)	0	100	100
12	E	207/230 (90%)	200 (97%)	7 (3%)	0	100	100
13	B	953/1169 (82%)	926 (97%)	27 (3%)	0	100	100
All	All	2798/4392 (64%)	2697 (96%)	101 (4%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	
4	A	749/1709 (44%)	747 (100%)	2 (0%)	86	88
5	C	253/276 (92%)	252 (100%)	1 (0%)	84	87
6	F	72/128 (56%)	68 (94%)	4 (6%)	19	49
7	J	56/63 (89%)	55 (98%)	1 (2%)	51	74
8	K	98/105 (93%)	96 (98%)	2 (2%)	48	73
9	L	40/46 (87%)	40 (100%)	0	100	100
10	H	123/127 (97%)	121 (98%)	2 (2%)	55	76
11	I	84/101 (83%)	82 (98%)	2 (2%)	43	70
12	E	190/209 (91%)	184 (97%)	6 (3%)	34	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
13	B	846/1026 (82%)	838 (99%)	8 (1%)	70 82
All	All	2511/3790 (66%)	2483 (99%)	28 (1%)	63 80

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	E	26	VAL
13	B	985	HIS
12	E	179	LEU
13	B	835	VAL
12	E	133	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
13	B	951	GLN
13	B	1016	ASN
10	H	42	HIS
10	H	67	ASN
10	H	106	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	P	2/20 (10%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 7 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.