



wwPDB EM Validation Summary Report ⓘ

May 10, 2026 – 12:28 AM JST

PDB ID : 9K13 / pdb_00009k13
EMDB ID : EMD-61963
Title : A cryo-EM structure of *B. oleracea* RNA polymerase V in complex with 2U 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

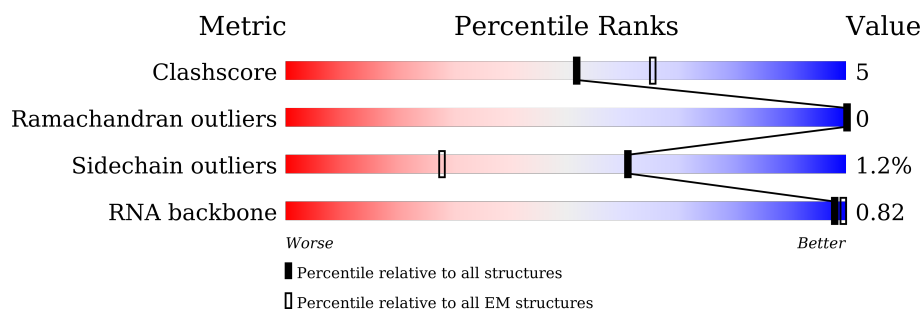
1 Overall quality at a glance

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	26% (green), 24% (yellow), 50% (grey)
2	N	34	41% (green), 15% (yellow), 44% (grey)
3	P	20	10% (green), 30% (yellow), 60% (grey)
4	A	2032	36% (green), 5% (yellow), 58% (grey)
5	C	319	83% (green), 7% (yellow), 10% (grey)
6	F	144	48% (green), 8% (yellow), 44% (grey)
7	J	71	82% (green), 7% (yellow), 11% (grey)
8	K	116	84% (green), 9% (yellow), 7% (grey)

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Mol	Chain	Length	Quality of chain
9	L	51	 76% 12% 12%
10	H	146	 72% 24% • •
11	I	114	 62% 21% • 15%
12	E	230	 61% 29% • 9%
13	B	1169	 76% 7% 17%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 23483 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	17	Total	C	N	O	P	0	0
			345	164	64	100	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	19	Total	C	N	O	P	0	0
			392	186	72	115	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	8	Total	C	N	O	P	0	0
			171	76	30	57	8		

- 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	4175	1136	1253	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	97	Total	C	N	O	S	0	0
			787	482	150	143	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



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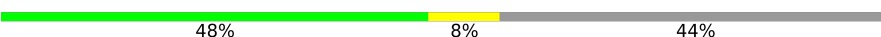
- Molecule 5: DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein

Chain C:  83% 7% 10%

MET ASP THR G3 I14 M33 V40 E44 S59 L62 R80 M84 T114 D115 Q116 F137 GLY ASP SER SER GLY ALA ASP SER SER SER GLU Q148 R158 G159 Q160 D175 H176 M200 Y237 L255 T258 K261 T285 L288 L297

S298 D299 ASP THR VAL GLU ALA ASP ASP PHE GLY LEU GLY ALA HIS MET ARG GLY

- Molecule 6: DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein

Chain F:  48% 8% 44%

MET ALA GLU ASP ASP TYR ASN GLU VAL ASP ASP LEU TYR GLU ASP GLU PRO ALA GLU PRO GLU ILE GLU GLY ILE GLU GLY ASP ASP MET LYS ASP ASN ASP ASP ILE ASN GLY PRO LEU GLU THR GLU LYS VAL THR GLU PRO VAL ARG P59 T61

M65 T95 L98 M102 R116 P119 W126 E130 L131 W137 LYS ARG GLN VAL GLY ASP

- Molecule 7: DNA-directed RNA polymerase II, IV and V subunit 10

Chain J:  82% 7% 11%

M1 I2 I3 P4 L24 Y48 M63 THR LEU GLU LYS SER ASP ALA ASN

- Molecule 8: DNA-directed RNA polymerase RBP11-like dimerisation domain-containing protein

Chain K:  84% 9% 7%

MET ASN ALA PRO ASP R6 F10 I45 F53 H76 T77 T78 S79 Q80 M84 L98 K102 E108 S113 ASN PRO TYR

- Molecule 9: DNA-directed RNA polymerase II, IV and V subunit 12

Chain L:  76% 12% 12%

MET ASP GLN SER GLU P7 I27 C32 G33 Y34 R35 I36 L37 R51

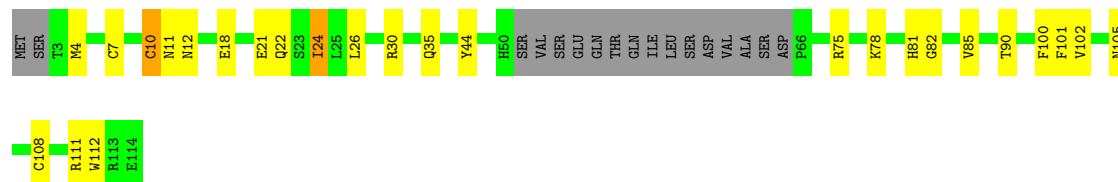
- Molecule 10: DNA-directed RNA polymerase II, IV and V subunit 8

Chain H:  72% 24% ..



- Molecule 11: DNA-directed RNA polymerase subunit

Chain I: 62% 21% 15%



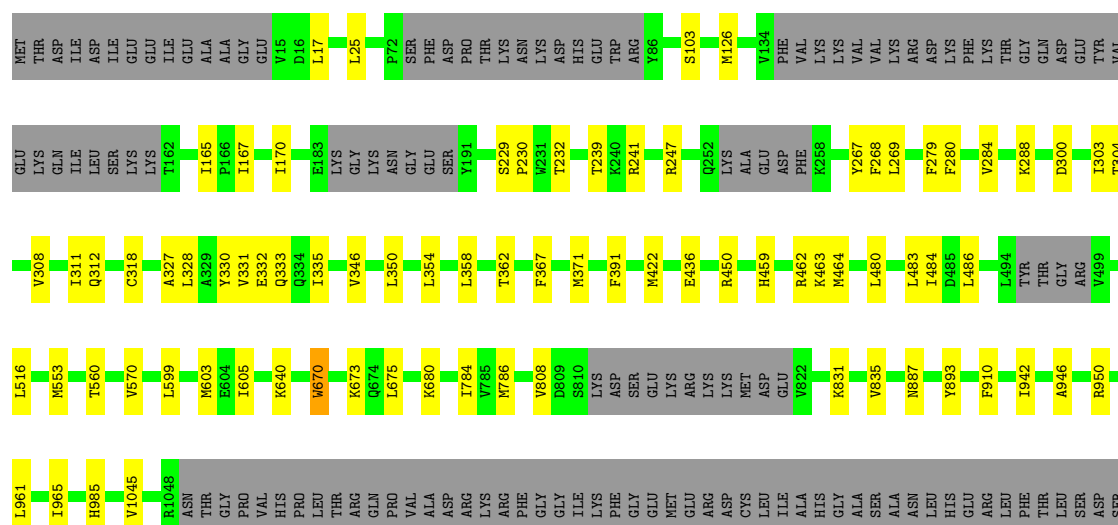
- Molecule 12: RNA polymerase subunit H/Rpb5 C-terminal domain-containing protein

Chain E: 61% 29% 9%



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

Chain B: 76% 7% 17%



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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46670	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	0.19	0/385	0.36	0/588
2	N	0.20	0/438	0.37	0/672
3	P	0.07	0/190	0.17	0/294
4	A	0.16	0/6720	0.42	0/9070
5	C	0.13	0/2286	0.37	0/3087
6	F	0.15	0/673	0.40	0/905
7	J	0.14	0/515	0.36	0/696
8	K	0.15	0/908	0.31	0/1224
9	L	0.15	0/369	0.37	0/493
10	H	0.15	0/1155	0.46	0/1557
11	I	0.14	0/804	0.42	1/1081 (0.1%)
12	E	0.14	0/1732	0.43	0/2332
13	B	0.14	0/7809	0.35	0/10524
All	All	0.15	0/23984	0.39	1/32523 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
11	I	24	ILE	N-CA-C	-5.43	108.56	113.71

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	345	0	192	8	0
2	N	392	0	216	3	0
3	P	171	0	87	5	0
4	A	6608	0	6661	85	0
5	C	2256	0	2269	18	0
6	F	660	0	669	9	0
7	J	507	0	512	4	0
8	K	890	0	883	9	0
9	L	365	0	364	4	0
10	H	1129	0	1128	23	0
11	I	787	0	736	20	0
12	E	1706	0	1759	48	0
13	B	7660	0	7600	47	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	23483	0	23076	252	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 5.

The worst 5 of 252 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:940:HIS:CE1	4:A:989:CYS:SG	2.63	0.92
4:A:885:ARG:HE	12:E:22:LEU:HB2	1.40	0.86
4:A:804:SER:HA	12:E:189:GLN:HB3	1.62	0.82
12:E:135:LYS:HA	12:E:138:LYS:HE3	1.71	0.73
1:T:17:DA:H61	3:P:20:U:H3	1.37	0.72

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	834/2032 (41%)	796 (95%)	38 (5%)	0	100	100
5	C	283/319 (89%)	277 (98%)	6 (2%)	0	100	100
6	F	78/144 (54%)	71 (91%)	7 (9%)	0	100	100
7	J	61/71 (86%)	58 (95%)	3 (5%)	0	100	100
8	K	106/116 (91%)	105 (99%)	1 (1%)	0	100	100
9	L	43/51 (84%)	40 (93%)	3 (7%)	0	100	100
10	H	139/146 (95%)	124 (89%)	15 (11%)	0	100	100
11	I	93/114 (82%)	87 (94%)	6 (6%)	0	100	100
12	E	207/230 (90%)	197 (95%)	10 (5%)	0	100	100
13	B	953/1169 (82%)	918 (96%)	35 (4%)	0	100	100
All	All	2797/4392 (64%)	2673 (96%)	124 (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%)	738 (98%)	11 (2%)	57	77
5	C	253/276 (92%)	252 (100%)	1 (0%)	84	87
6	F	72/128 (56%)	72 (100%)	0	100	100
7	J	56/63 (89%)	56 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	K	98/105 (93%)	98 (100%)	0	100	100
9	L	40/46 (87%)	40 (100%)	0	100	100
10	H	123/127 (97%)	121 (98%)	2 (2%)	55	76
11	I	85/101 (84%)	84 (99%)	1 (1%)	63	79
12	E	190/209 (91%)	183 (96%)	7 (4%)	30	61
13	B	846/1026 (82%)	837 (99%)	9 (1%)	65	80
All	All	2512/3790 (66%)	2481 (99%)	31 (1%)	61	79

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	I	10	CYS
13	B	670	TRP
12	E	115	ILE
13	B	985	HIS
13	B	391	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
13	B	251	ASN
13	B	333	GLN
13	B	1039	HIS
13	B	714	GLN
13	B	951	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	P	7/20 (35%)	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.