



## wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Mar 10, 2018 – 09:14 PM EST

PDB ID : 6FLP  
EMDB ID: : EMD-4274  
Title : CryoEM structure of E.coli RNA polymerase paused elongation complex without RNA hairpin bound to NusA  
Authors : Guo, X.; Weixlbaumer, A.  
Deposited on : 2018-01-26  
Resolution : 4.10 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB 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/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

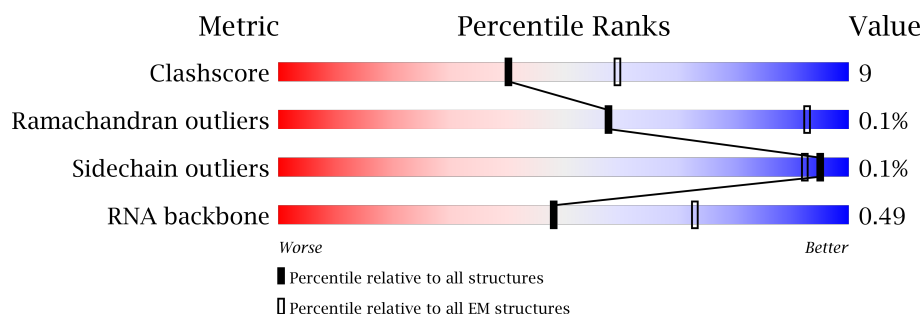
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.10 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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

Mol	Chain	Length	Quality of chain
1	A	329	54% 16% 30%
1	B	329	50% 16% 34%
2	C	1342	78% 20% •
3	D	1407	74% 21% 5%
4	E	91	89% 10% •
5	N	31	32% 68%
6	R	10	40% 40% 20%
7	T	39	49% 51%

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 26512 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 protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	229	Total	C	N	O	S	0	0
			1767	1100	313	348	6		
1	B	217	Total	C	N	O	S	0	0
			1667	1041	293	327	6		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1314	Total	C	N	O	S	0	0
			10363	6502	1806	2012	43		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1334	Total	C	N	O	S	0	0
			10357	6510	1846	1952	49		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	90	Total	C	N	O	S	0	0
			709	430	136	142	1		

- Molecule 5 is a DNA chain called DNA (30-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	31	Total	C	N	O	P	0	0
			647	304	131	181	31		

- Molecule 6 is a RNA chain called RNA (5'-R(P\*GP\*AP\*UP\*GP\*UP\*GP\*UP\*GP\*CP\*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	10	Total	C	N	O	P	0	0
			214	95	36	73	10		

- Molecule 7 is a DNA chain called DNA (39-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	39	Total	C	N	O	P	0	0
			785	375	135	236	39		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
8	D	1	Total	Mg	0
			1	1	

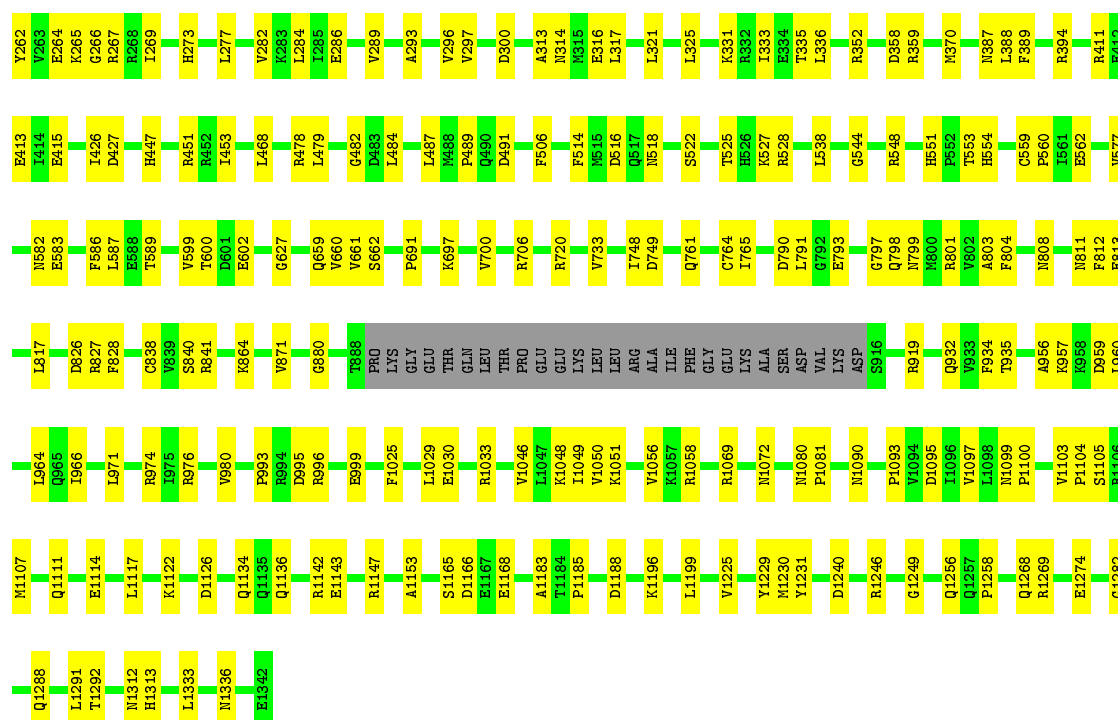
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
9	D	2	Total	Zn	0
			2	2	



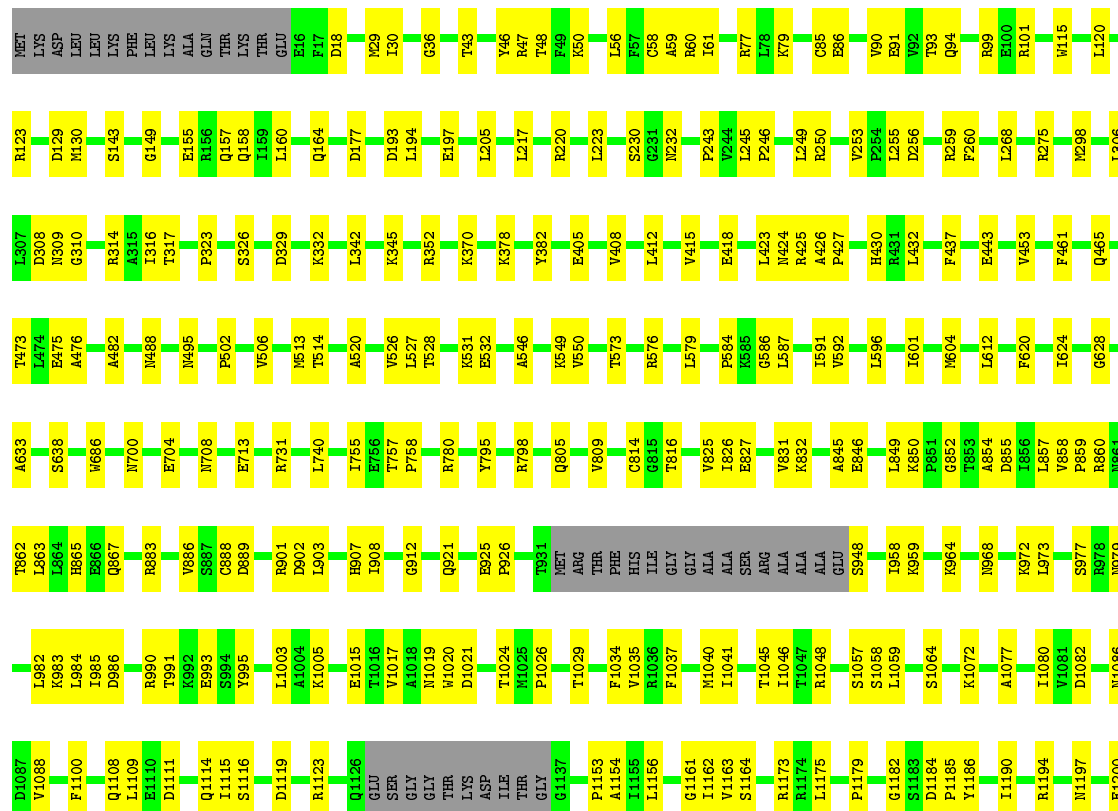
- Molecule 1: DNA-directed RNA polymerase subunit alpha

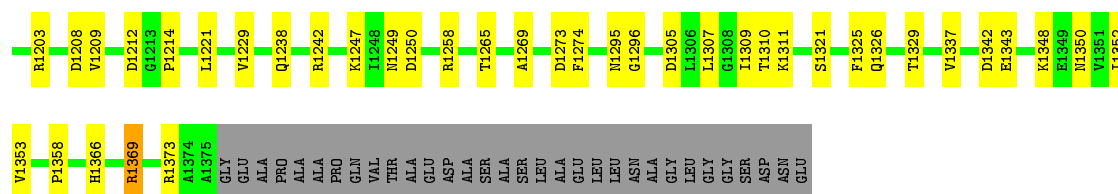




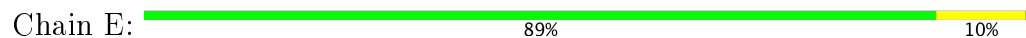
- Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D:  74% 21% 5%

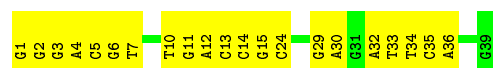




- Molecule 4: DNA-directed RNA polymerase subunit omega



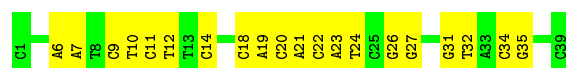
- Molecule 5: DNA (30-MER)



- Molecule 6: RNA (5'-R(P\*GP\*AP\*UP\*GP\*UP\*GP\*UP\*GP\*CP\*U)-3')



- Molecule 7: DNA (39-MER)



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	65966	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	53	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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  >2	RMSZ	# Z  >2
1	A	0.24	0/1789	0.46	0/2425
1	B	0.24	0/1686	0.47	0/2285
2	C	0.24	0/10528	0.44	0/14205
3	D	0.24	0/10514	0.43	0/14199
4	E	0.22	0/711	0.39	0/956
5	N	0.52	0/728	0.93	0/1121
6	R	0.21	0/238	0.85	0/369
7	T	0.52	0/876	0.94	0/1346
All	All	0.27	0/27070	0.49	0/36906

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
2	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	57	PHE	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	1767	0	1782	35	0
1	B	1667	0	1689	36	0
2	C	10363	0	10368	172	0
3	D	10357	0	10573	187	0
4	E	709	0	719	6	0
5	N	647	0	347	23	0
6	R	214	0	107	6	0
7	T	785	0	440	24	0
8	D	1	0	0	0	0
9	D	2	0	0	0	0
All	All	26512	0	26025	454	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 9.

The worst 5 of 454 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)
5:N:29:DG:N2	7:T:11:DC:O2	2.06	0.87
2:C:200:ARG:NH2	5:N:24:DC:OP2	2.11	0.84
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.63	0.79
1:B:64:VAL:HG13	1:B:69:SER:HB2	1.68	0.75
2:C:1274:GLU:HG2	3:D:424:ASN:HD21	1.54	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	
1	A	227/329 (69%)	204 (90%)	23 (10%)	0	100	100
1	B	213/329 (65%)	192 (90%)	21 (10%)	0	100	100
2	C	1310/1342 (98%)	1221 (93%)	87 (7%)	2 (0%)	51	84
3	D	1328/1407 (94%)	1264 (95%)	64 (5%)	0	100	100
4	E	88/91 (97%)	84 (96%)	4 (4%)	0	100	100
All	All	3166/3498 (90%)	2965 (94%)	199 (6%)	2 (0%)	58	88

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	58	PRO
2	C	57	PHE

### 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	
1	A	194/286 (68%)	193 (100%)	1 (0%)	91	96
1	B	183/286 (64%)	183 (100%)	0	100	100
2	C	1132/1157 (98%)	1132 (100%)	0	100	100
3	D	1114/1168 (95%)	1113 (100%)	1 (0%)	94	97
4	E	74/75 (99%)	74 (100%)	0	100	100
All	All	2697/2972 (91%)	2695 (100%)	2 (0%)	95	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	ARG
3	D	1369	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such

sidechains are listed below:

Mol	Chain	Res	Type
2	C	688	GLN
2	C	1146	GLN
3	D	805	GLN
2	C	1080	ASN
2	C	1136	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	R	10/10 (100%)	3 (30%)	1 (10%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	R	21	A
6	R	25	G
6	R	29	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	R	20	G

## 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	N	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	15:DG	O3'	24:DC	P	28.77