



wwPDB EM Validation Summary Report ⓘ

Jul 15, 2025 – 10:49 AM JST

PDB ID : 8K5A / pdb_00008k5a
EMDB ID : EMD-36899
Title : The cryo-EM map of open TIEA-TEC complex
Authors : Zhang, K.N.; Liu, Y.; Chen, M.; Wang, Y.; Lin, W.; Li, M.; Zhang, X.; Gao, Y.; Gong, Q.; Chen, H.; Steve, M.; Li, S.; Zhang, K.; Liu, B.
Deposited on : 2023-07-21
Resolution : 3.30 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 Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

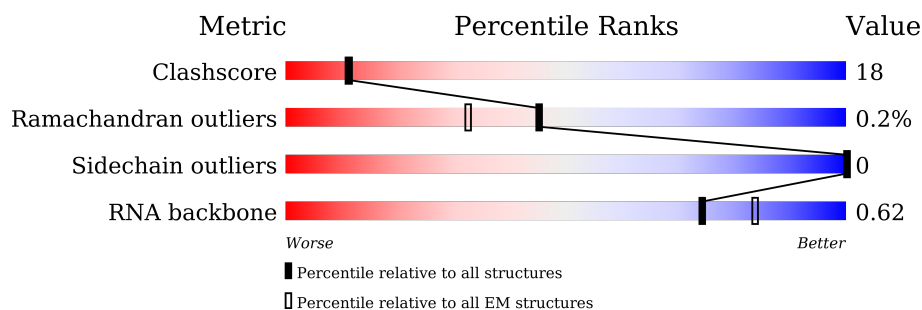
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	A	231	66% 33%
1	B	231	56% 42% .
2	C	1340	62% 38%
3	D	1363	62% 37% .
4	E	76	46% 53% .
5	G	129	55% 45%
6	H	29	69% 31%
7	I	29	34% 41% 24%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	J	10	<div><div></div><div>30%</div><div>70%</div></div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 27505 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	230	Total	C	N	O	S	0	0
			1788	1112	317	353	6		
1	B	228	Total	C	N	O	S	0	0
			1767	1100	312	349	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0
			10570	6631	1841	2055	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1352	Total	C	N	O	S	0	0
			10494	6587	1869	1988	50		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	76	Total	C	N	O	S	0	0
			606	368	115	122	1		

- Molecule 5 is a protein called 15 kDa RNA polymerase-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	129	Total	C	N	O	S	0	0
			1031	637	188	200	6		

- Molecule 6 is a DNA chain called DNA (29-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	29	Total	C	N	O	P	0	0
			583	279	99	177	28		

- Molecule 7 is a DNA chain called DNA (29-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	22	Total	C	N	O	P	0	0
			448	214	89	125	20		

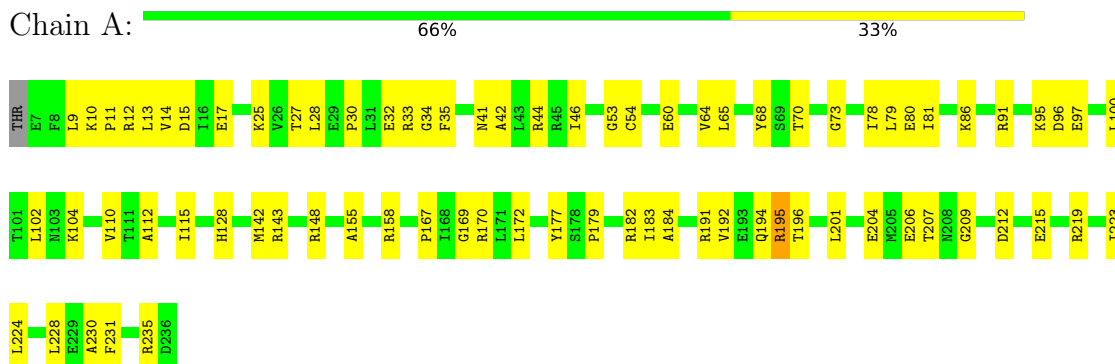
- Molecule 8 is a RNA chain called RNA (5'-R(*CP*GP*GP*AP*GP*AP*GP*GP*UP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	10	Total	C	N	O	P	0	0
			218	98	45	66	9		

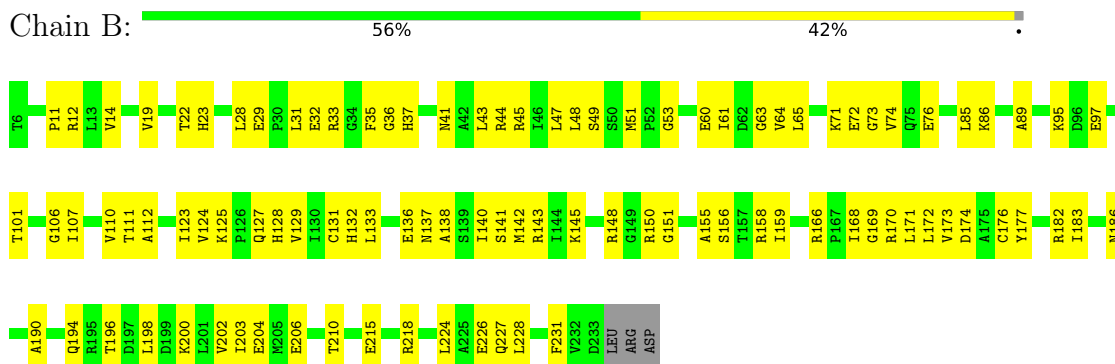
3 Residue-property plots [i](#)

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. 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. 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.

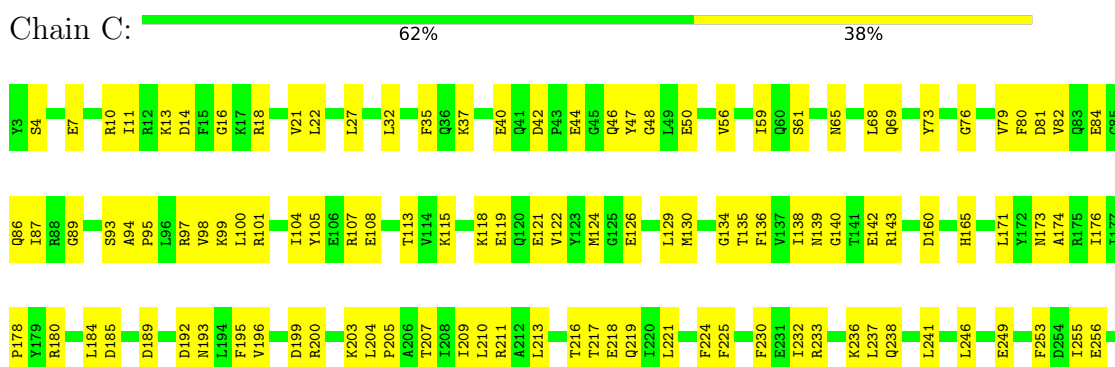
- Molecule 1: DNA-directed RNA polymerase subunit alpha



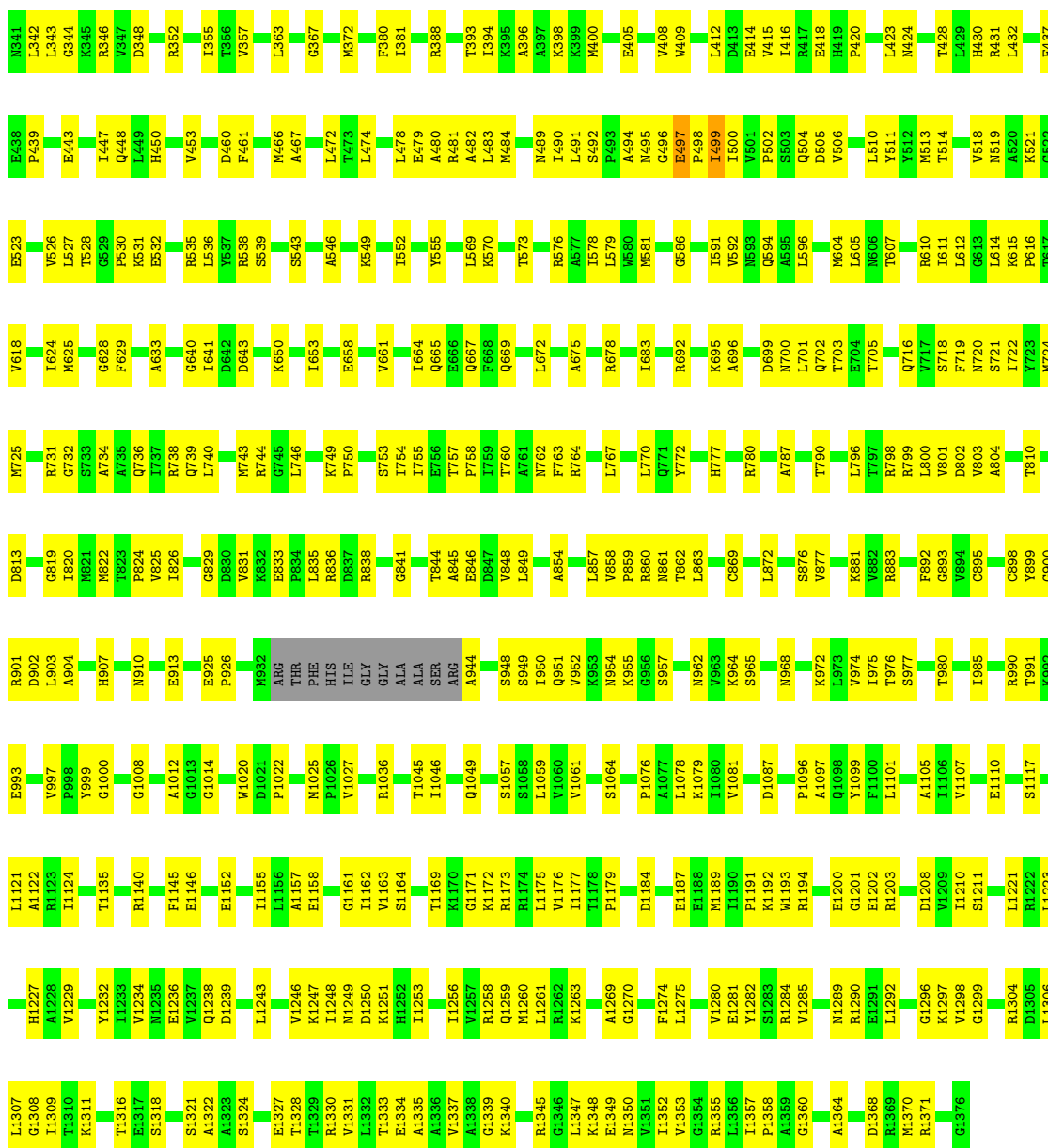
- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 2: DNA-directed RNA polymerase subunit beta

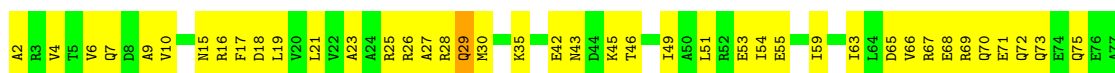






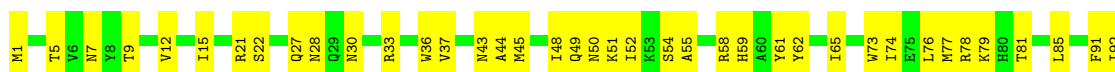
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 46% 53%



• Molecule 5: 15 kDa RNA polymerase-binding protein

Chain G: 55% 45%

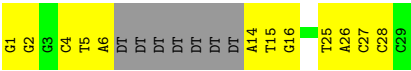




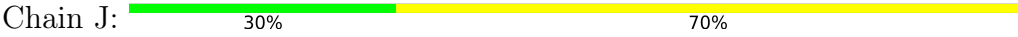
● Molecule 6: DNA (29-MER)



● Molecule 7: DNA (29-MER)



● Molecule 8: RNA (5'-R(*CP*GP*GP*AP*GP*AP*GP*GP*UP*A)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	225078	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.20	0/1810	0.45	0/2451
1	B	0.20	0/1789	0.50	0/2425
2	C	0.20	0/10739	0.43	2/14489 (0.0%)
3	D	0.19	0/10652	0.47	3/14382 (0.0%)
4	E	0.26	0/608	0.87	2/817 (0.2%)
5	G	0.17	0/1046	0.54	1/1411 (0.1%)
6	H	0.15	0/650	0.31	0/1000
7	I	0.16	0/503	0.31	0/773
8	J	0.08	0/245	0.19	0/382
All	All	0.20	0/28042	0.46	8/38130 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	29	GLN	CA-C-N	-6.72	110.30	121.92
4	E	29	GLN	C-N-CA	-6.72	110.30	121.92
5	G	12	VAL	N-CA-C	-6.58	106.59	112.90
2	C	1162	SER	N-CA-C	-6.24	106.63	114.56
3	D	499	ILE	N-CA-C	-5.69	107.44	112.90

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	A	1788	0	1810	70	0
1	B	1767	0	1789	96	0
2	C	10570	0	10582	393	0
3	D	10494	0	10712	409	0
4	E	606	0	612	46	0
5	G	1031	0	1026	47	0
6	H	583	0	329	9	0
7	I	448	0	249	10	0
8	J	218	0	111	6	0
All	All	27505	0	27220	963	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 18.

The worst 5 of 963 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:155:ALA:HA	1:A:158:ARG:HH12	1.24	0.99
1:A:231:PHE:HE1	1:B:28:LEU:HD13	1.37	0.89
1:A:104:LYS:HD3	1:A:110:VAL:HG22	1.56	0.88
2:C:1119:MET:HE3	2:C:1204:LEU:HD13	1.59	0.84
1:A:158:ARG:HH21	1:A:172:LEU:HB3	1.43	0.83

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 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	228/231 (99%)	211 (92%)	16 (7%)	1 (0%)	30	61
1	B	226/231 (98%)	219 (97%)	7 (3%)	0	100	100
2	C	1338/1340 (100%)	1280 (96%)	57 (4%)	1 (0%)	48	76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	1348/1363 (99%)	1290 (96%)	53 (4%)	5 (0%)	30	61
4	E	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
5	G	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	46
All	All	3341/3370 (99%)	3191 (96%)	142 (4%)	8 (0%)	45	71

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	79	LYS
3	D	1097	ALA
3	D	594	GLN
2	C	1158	LYS
3	D	1152	GLU

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	198/199 (100%)	198 (100%)	0	100	100
1	B	196/199 (98%)	196 (100%)	0	100	100
2	C	1155/1155 (100%)	1155 (100%)	0	100	100
3	D	1129/1136 (99%)	1129 (100%)	0	100	100
4	E	65/65 (100%)	65 (100%)	0	100	100
5	G	112/112 (100%)	112 (100%)	0	100	100
All	All	2855/2866 (100%)	2855 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	1038	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	G	29	GLN
3	D	477	GLN
5	G	71	ASN
3	D	1367	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	J	9/10 (90%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	J	12	G

There are no RNA pucker outliers to report.

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

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](#)

There are no ligands in this entry.

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.