



wwPDB EM Validation Summary Report ⓘ

Mar 19, 2026 – 08:19 PM UTC

PDB ID : 9GDR / pdb_00009gdr
EMDB ID : EMD-51276
Title : Cryo-EM structure of Vibrio cholerae RNA polymerase Transcription Activation Complex with TcpP transcription factor and a toxT promoter DNA fragment
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Deposited on : 2024-08-06
Resolution : 2.70 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 : 0.0.1.dev132
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

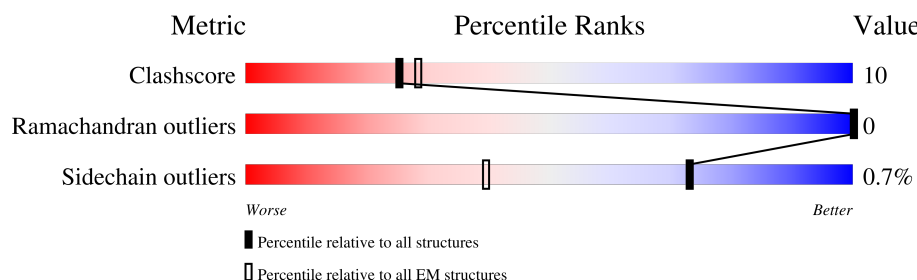
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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

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	H	115	59% 36% 5%
1	K	115	61% 34% . .
2	N	71	28% 68% .
3	T	71	37% 58% 6%
4	A	330	58% 12% 30%
4	B	330	53% 14% 33%
4	G	330	12% 9% 78%
5	C	1341	77% 22% .
6	D	1401	68% 18% 14%

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Mol	Chain	Length	Quality of chain
7	E	90	 73% 23%
8	F	621	 54% 20% 25%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 32797 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 Toxin co-regulated pilus biosynthesis protein P.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	109	Total	C	N	O	S	0	0
			898	581	152	161	4		
1	K	110	Total	C	N	O	S	0	0
			909	587	156	162	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	19	ALA	CYS	engineered mutation	UNP A0A0H3AHV1
K	19	ALA	CYS	engineered mutation	UNP A0A0H3AHV1

- Molecule 2 is a DNA chain called toxT promoter non-template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	68	Total	C	N	O	P	0	0
			1399	675	237	419	68		

- Molecule 3 is a DNA chain called toxT promoter template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	67	Total	C	N	O	P	0	0
			1374	660	264	384	66		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	71	Total	C	N	O	S	0	0
			557	353	98	104	2		
4	A	231	Total	C	N	O	S	0	0
			1776	1111	312	348	5		
4	B	222	Total	C	N	O	S	0	0
			1697	1064	295	333	5		

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	1328	Total	C	N	O	S	1	0
			10421	6547	1811	2025	38		

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	1202	Total	C	N	O	S	0	0
			9408	5912	1675	1774	47		

- Molecule 7 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	69	Total	C	N	O	S	0	0
			545	332	102	110	1		

- Molecule 8 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	468	Total	C	N	O	S	0	0
			3810	2384	690	719	17		

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

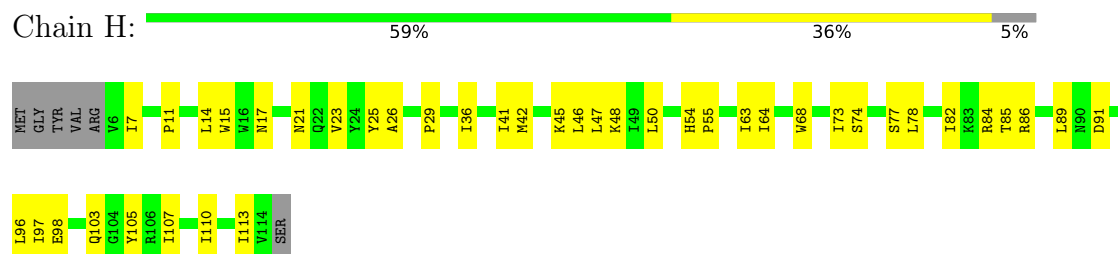
- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

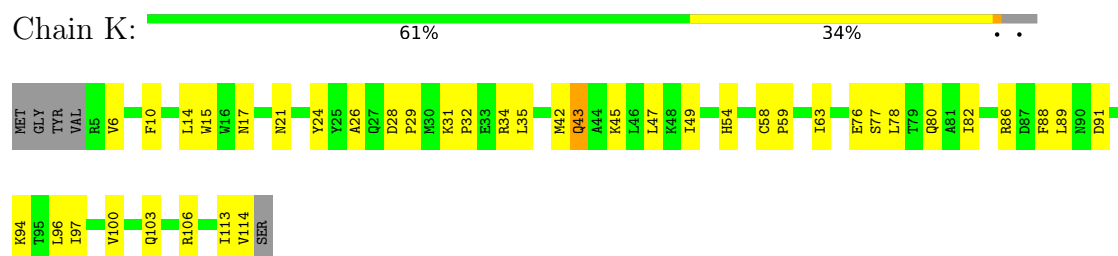
3 Residue-property plots [i](#)

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.

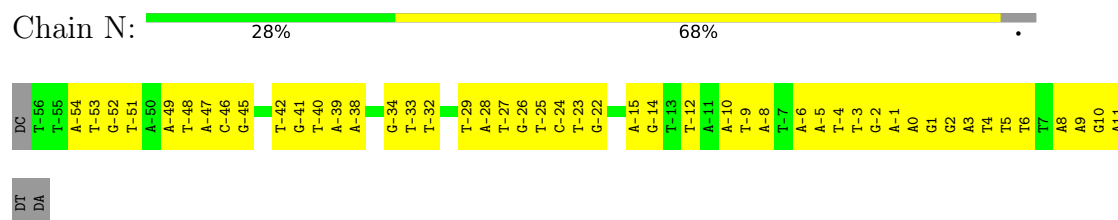
- Molecule 1: Toxin co-regulated pilus biosynthesis protein P



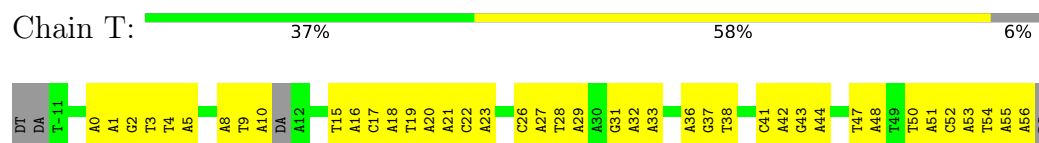
- Molecule 1: Toxin co-regulated pilus biosynthesis protein P



- Molecule 2: toxT promoter non-template DNA strand

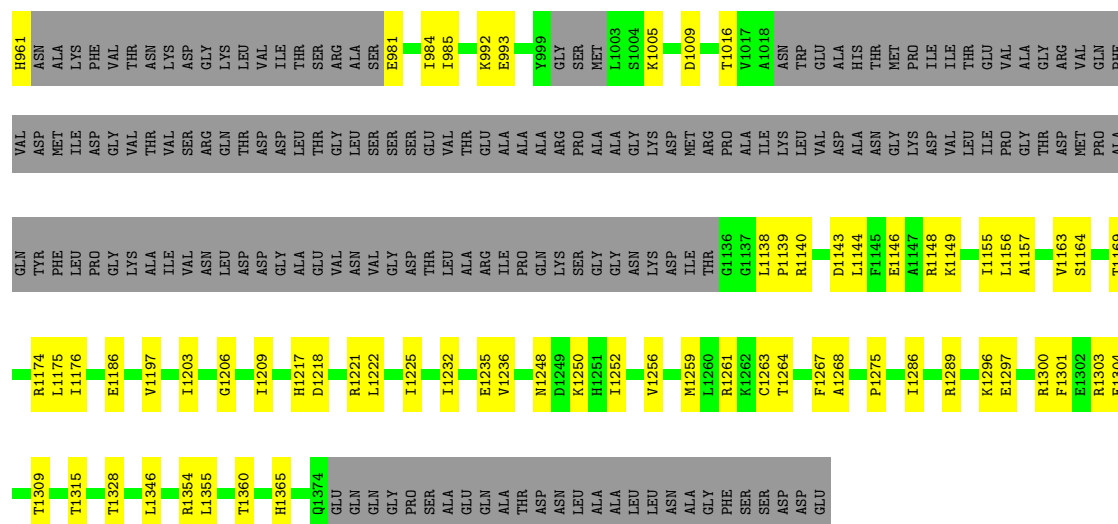


- Molecule 3: toxT promoter template DNA strand

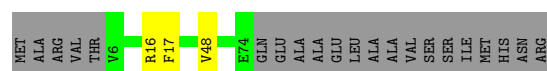


- Molecule 4: DNA-directed RNA polymerase subunit alpha

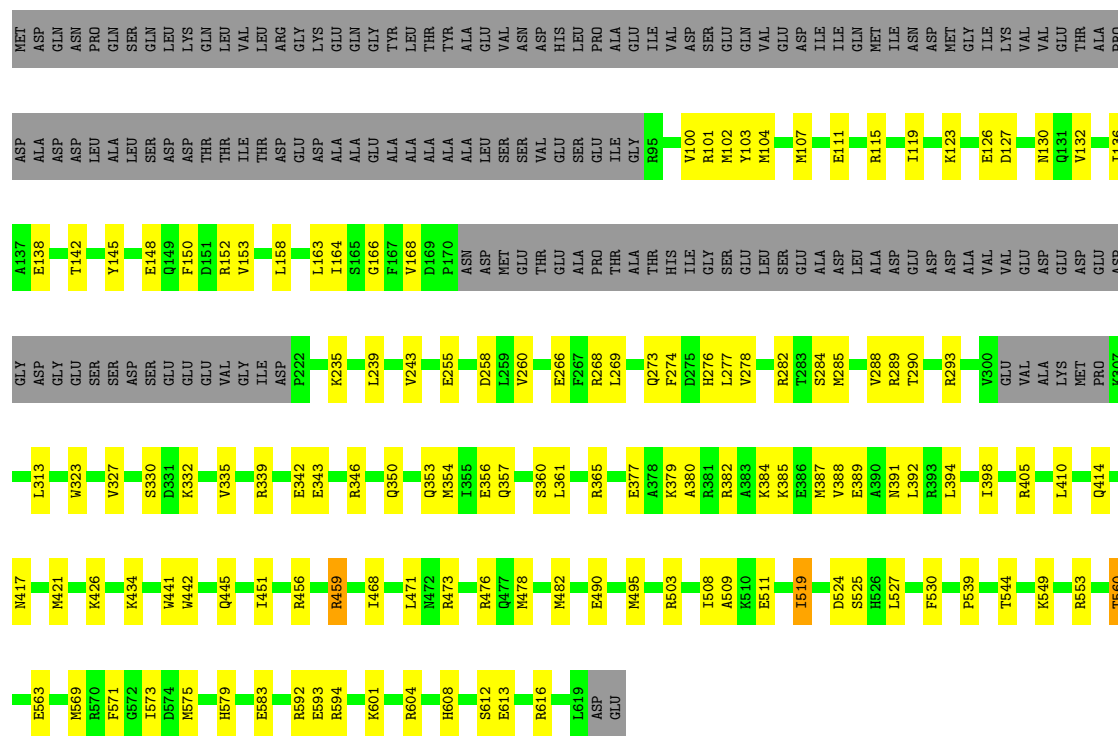




- Molecule 7: DNA-directed RNA polymerase subunit omega



- Molecule 8: RNA polymerase sigma factor RpoD



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	159379	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.26	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (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: 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	H	0.18	0/922	0.41	0/1255
1	K	0.15	0/933	0.39	0/1269
2	N	0.23	0/1566	0.45	0/2418
3	T	0.23	0/1546	0.40	0/2380
4	A	0.14	0/1798	0.29	0/2437
4	B	0.15	0/1717	0.29	0/2327
4	G	0.20	0/563	0.49	0/761
5	C	0.17	0/10585	0.36	1/14288 (0.0%)
6	D	0.16	0/9552	0.33	0/12881
7	E	0.08	0/547	0.19	0/734
8	F	0.17	0/3861	0.42	0/5184
All	All	0.17	0/33590	0.36	1/45934 (0.0%)

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
5	C	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	213	LEU	N-CA-C	-5.06	107.06	113.18

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	C	211	ARG	Sidechain

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	H	898	0	901	31	0
1	K	909	0	914	29	0
2	N	1399	0	780	44	0
3	T	1374	0	757	30	0
4	A	1776	0	1802	25	0
4	B	1697	0	1728	31	0
4	G	557	0	591	24	0
5	C	10421	0	10444	224	0
6	D	9408	0	9587	180	0
7	E	545	0	551	3	0
8	F	3810	0	3891	114	0
9	D	2	0	0	0	0
10	D	1	0	0	0	0
All	All	32797	0	31946	672	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 10.

The worst 5 of 672 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)
8:F:478:MET:HE1	8:F:490:GLU:HB3	1.54	0.89
8:F:100:VAL:HG22	8:F:410:LEU:HD11	1.55	0.86
4:G:313:LEU:HD12	4:G:314:SER:H	1.42	0.81
4:G:265:VAL:O	4:G:269:ASN:HB2	1.82	0.80
6:D:335:GLN:HE22	8:F:524:ASP:HA	1.49	0.78

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	H	107/115 (93%)	102 (95%)	5 (5%)	0	100	100
1	K	108/115 (94%)	104 (96%)	4 (4%)	0	100	100
4	A	227/330 (69%)	224 (99%)	3 (1%)	0	100	100
4	B	218/330 (66%)	217 (100%)	1 (0%)	0	100	100
4	G	69/330 (21%)	66 (96%)	3 (4%)	0	100	100
5	C	1323/1341 (99%)	1300 (98%)	23 (2%)	0	100	100
6	D	1192/1401 (85%)	1165 (98%)	27 (2%)	0	100	100
7	E	67/90 (74%)	67 (100%)	0	0	100	100
8	F	462/621 (74%)	449 (97%)	13 (3%)	0	100	100
All	All	3773/4673 (81%)	3694 (98%)	79 (2%)	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	
1	H	101/106 (95%)	98 (97%)	3 (3%)	36	66
1	K	102/106 (96%)	101 (99%)	1 (1%)	68	86
4	A	195/283 (69%)	195 (100%)	0	100	100
4	B	186/283 (66%)	186 (100%)	0	100	100
4	G	63/283 (22%)	60 (95%)	3 (5%)	23	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	C	1129/1144 (99%)	1122 (99%)	7 (1%)	78	91
6	D	1012/1168 (87%)	1007 (100%)	5 (0%)	81	92
7	E	58/74 (78%)	58 (100%)	0	100	100
8	F	417/544 (77%)	413 (99%)	4 (1%)	68	86
All	All	3263/3991 (82%)	3240 (99%)	23 (1%)	73	90

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	D	565	THR
6	D	759	ILE
6	D	743	MET
6	D	913	GLU
4	G	305	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
6	D	910	ASN
8	F	251	HIS
6	D	911	GLN
4	B	104	ASN
8	F	477	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-51276. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections ⓘ

This section was not generated.

6.2 Central slices ⓘ

This section was not generated.

6.3 Largest variance slices ⓘ

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

This section was not generated.

6.5 Orthogonal surface views ⓘ

This section was not generated.

6.6 Mask visualisation ⓘ

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.