



wwPDB EM Validation Summary Report ⓘ

Oct 27, 2024 – 03:44 PM JST

PDB ID : 7EIZ
EMDB ID : EMD-31146
Title : Coupling of N7-methyltransferase and 3'-5' exoribonuclease with SARS-CoV-2 polymerase reveals mechanisms for capping and proofreading
Authors : Yan, L.; Yang, Y.X.; Li, M.Y.; Zhang, Y.; Zheng, L.T.; Ge, J.; Huang, Y.C.; Liu, Z.Y.; Wang, T.; Gao, S.; Zhang, R.; Huang, Y.Y.; Guddat, L.W.; Gao, Y.; Rao, Z.H.; Lou, Z.Y.
Deposited on : 2021-04-01
Resolution : Not provided

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.dev113
MolProbity : 4.02b-467
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) : 2.39

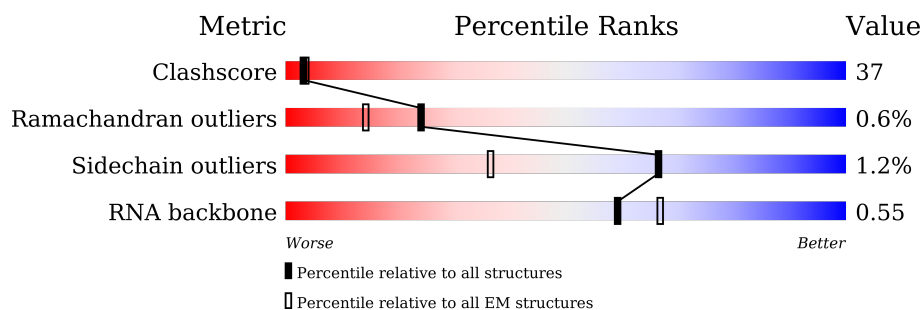
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

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	929	47% 50% .
2	B	198	46% 47% . 6%
2	D	198	41% 51% . 6%
3	C	83	40% 47% 13%
4	G	113	48% 51% .
5	H	139	39% 55% 6%
6	I	25	. 56% 40%
7	J	27	15% 52% 30% .

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Mol	Chain	Length	Quality of chain
8	K	527	 58% 41% ..
9	E	601	 26% 70% ..
9	F	601	 37% 60% ..

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 27083 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 RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	926	Total	C	N	O	S	0	0
			7458	4763	1251	1390	54		

- Molecule 2 is a protein called Non-structural protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	187	Total	C	N	O	S	0	0
			1396	872	240	273	11		
2	D	186	Total	C	N	O	S	0	0
			1414	889	242	272	11		

- Molecule 3 is a protein called Non-structural protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	72	Total	C	N	O	S	0	0
			553	349	91	107	6		

- Molecule 4 is a protein called Non-structural protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	113	Total	C	N	O	S	0	0
			868	549	150	164	5		

- Molecule 5 is a protein called Non-structural protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	131	Total	C	N	O	S	0	0
			955	593	160	186	16		

- Molecule 6 is a RNA chain called primer.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	25	Total	C	N	O	P	0	0
			545	242	105	173	25		

- Molecule 7 is a RNA chain called template.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	27	Total	C	N	O	P	0	0
			565	253	94	191	27		

- Molecule 8 is a protein called Proofreading exoribonuclease.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	523	Total	C	N	O	S	0	0
			4169	2674	710	749	36		

- Molecule 9 is a protein called Helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	587	Total	C	N	O	S	1	0
			4544	2893	765	851	35		
9	F	590	Total	C	N	O	S	0	0
			4602	2926	781	861	34		

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	A	2	Total	Zn	0
			2	2	
10	H	2	Total	Zn	0
			2	2	
10	K	3	Total	Zn	0
			3	3	
10	E	3	Total	Zn	0
			3	3	
10	F	3	Total	Zn	0
			3	3	

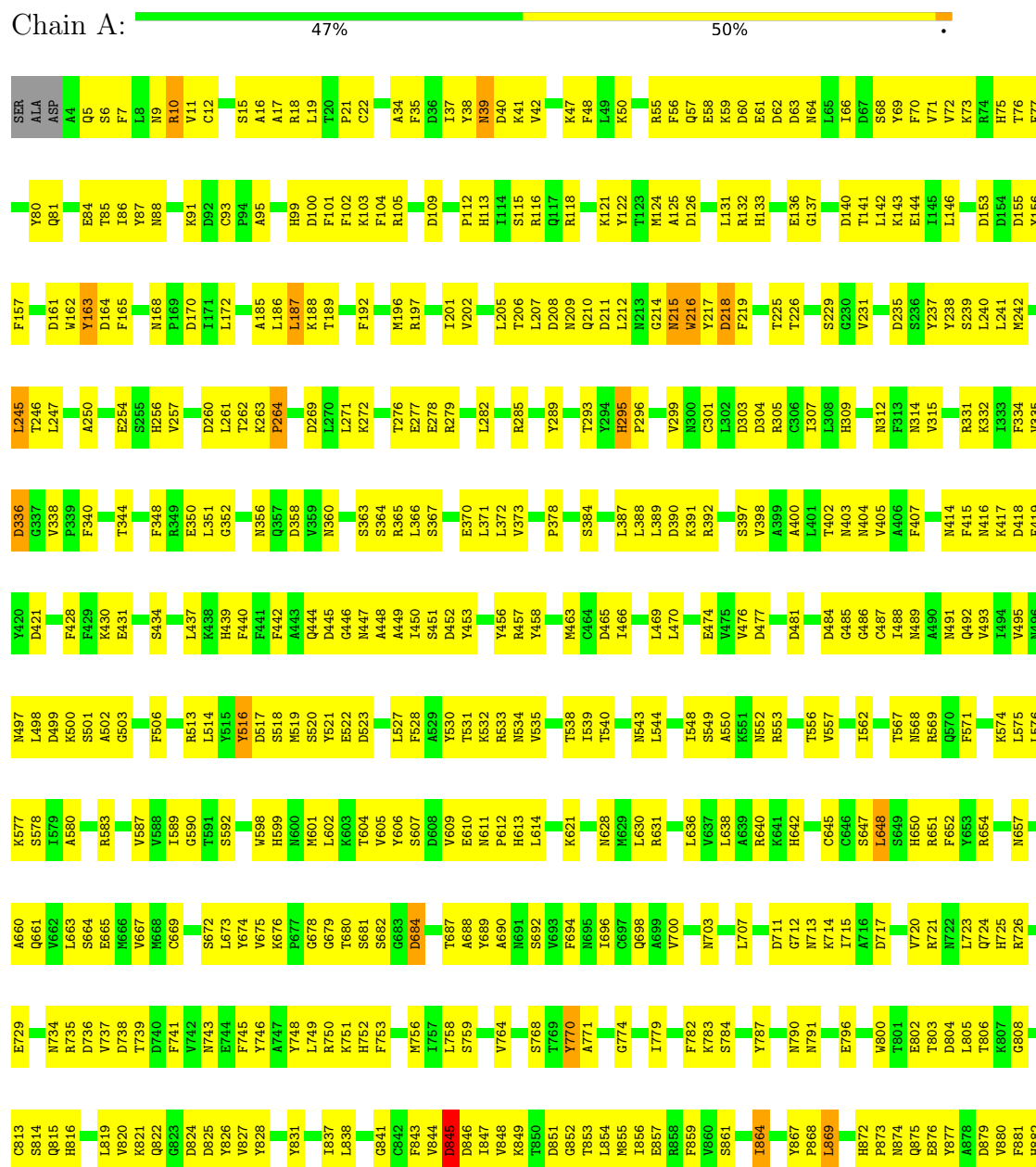
- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

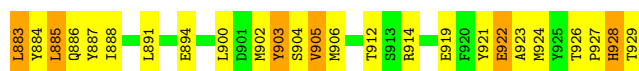
Mol	Chain	Residues	Atoms		AltConf
11	K	1	Total	Mg	0
			1	1	

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.

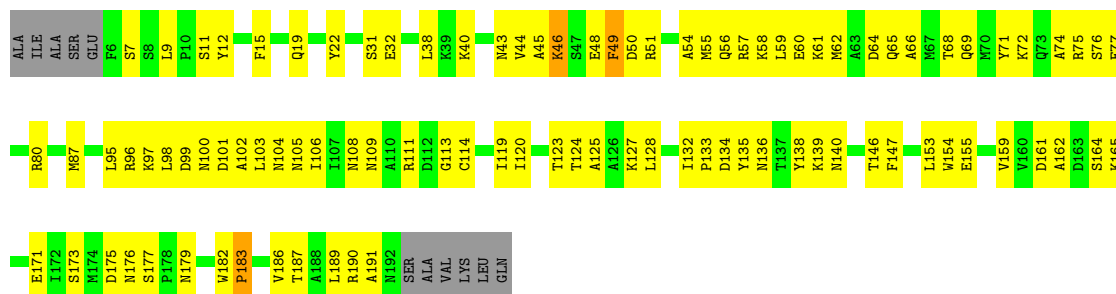
- Molecule 1: RNA-directed RNA polymerase





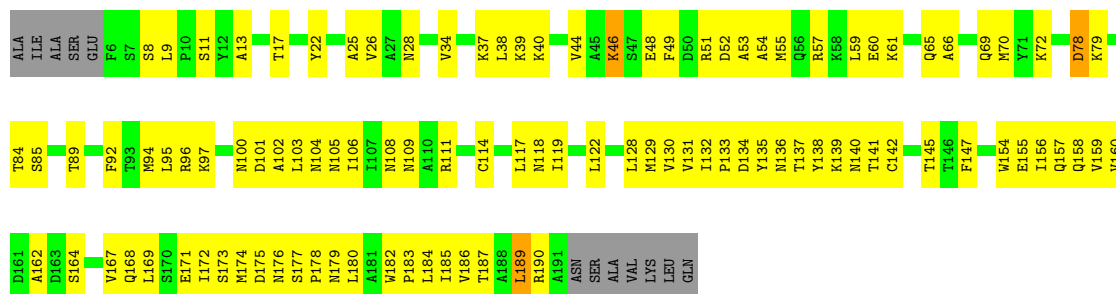
• Molecule 2: Non-structural protein 8

Chain B: 46% 47% 6%



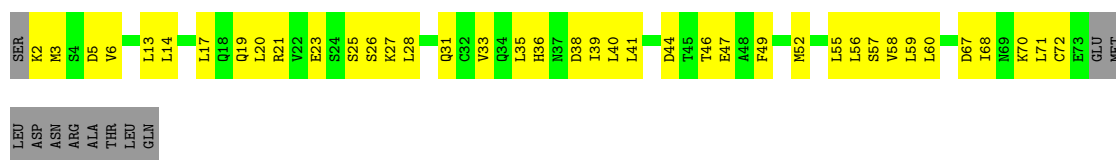
• Molecule 2: Non-structural protein 8

Chain D: 41% 51% 6%



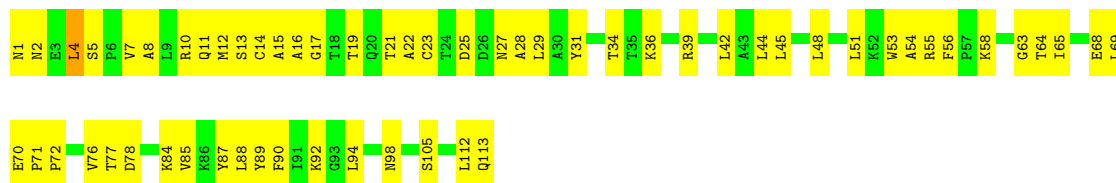
• Molecule 3: Non-structural protein 7

Chain C: 40% 47% 13%



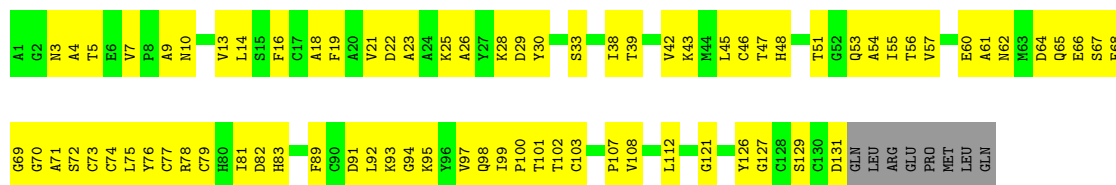
• Molecule 4: Non-structural protein 9

Chain G: 48% 51%

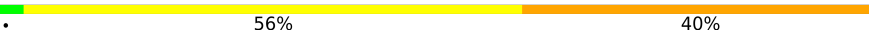


• Molecule 5: Non-structural protein 10

Chain H:  39% 55% 6%

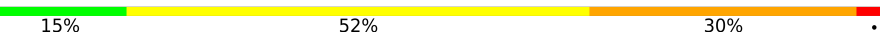


- Molecule 6: primer

Chain I:  56% 40%



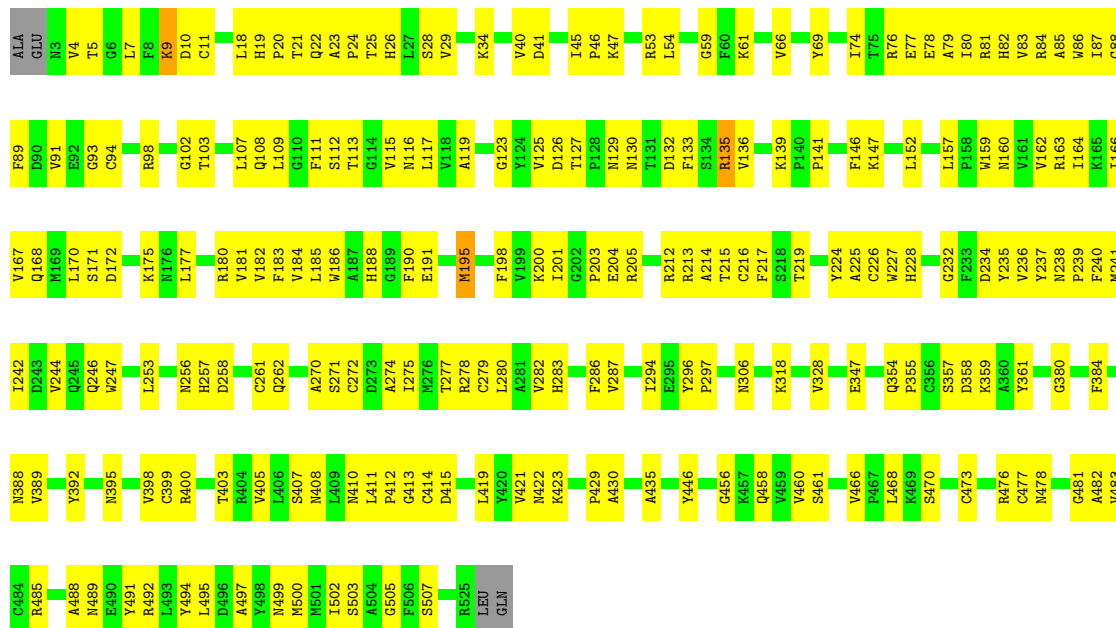
- Molecule 7: template

Chain J:  15% 52% 30%



- Molecule 8: Proofreading exoribonuclease

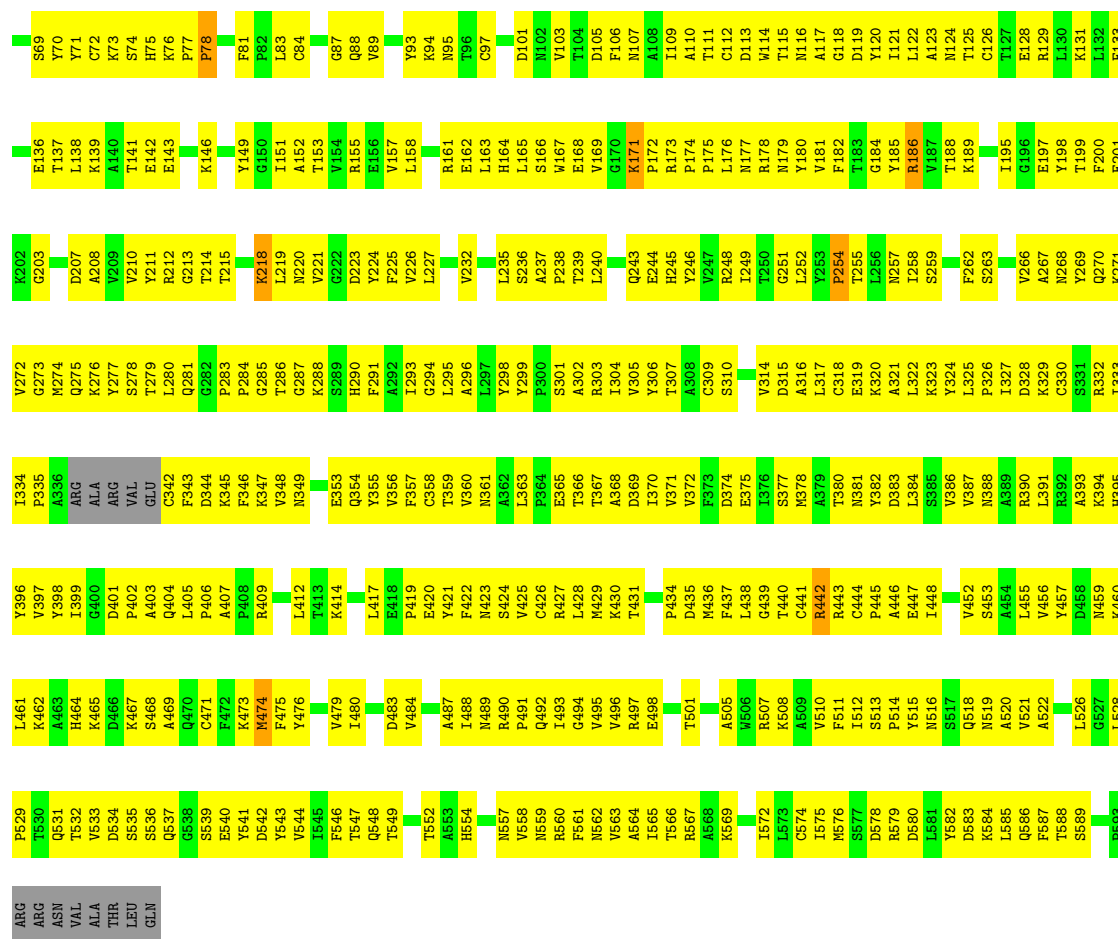
Chain K:  58% 41%



- Molecule 9: Helicase

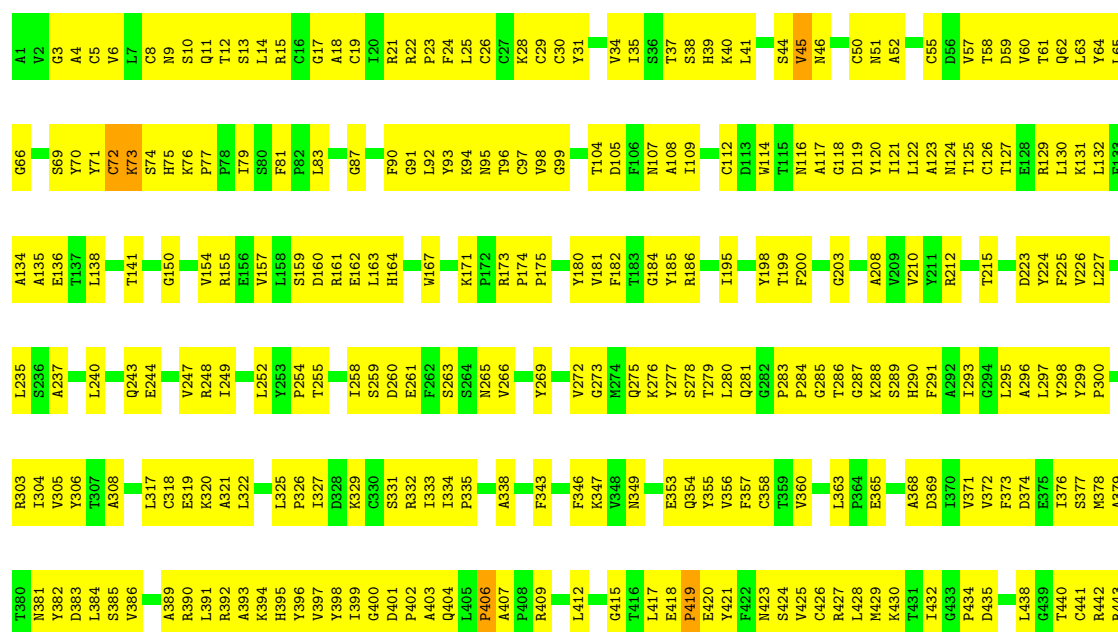
Chain E:  26% 70%





• Molecule 9: Helicase

Chain F: 37% 60% ..





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80256	Depositor
Resolution determination method	Not provided	
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (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 >5	RMSZ	# Z >5
1	A	0.98	1/7647 (0.0%)	0.73	10/10379 (0.1%)
2	B	0.63	0/1414	0.63	0/1922
2	D	0.58	0/1433	0.64	1/1944 (0.1%)
3	C	0.79	0/556	0.76	1/749 (0.1%)
4	G	0.30	0/884	0.55	1/1200 (0.1%)
5	H	0.31	0/976	0.54	0/1327
6	I	1.49	5/611 (0.8%)	1.29	1/953 (0.1%)
7	J	1.46	2/628 (0.3%)	1.23	3/974 (0.3%)
8	K	0.29	0/4288	0.49	0/5831
9	E	0.45	0/4647	0.58	0/6329
9	F	0.42	0/4706	0.56	0/6402
All	All	0.70	8/27790 (0.0%)	0.66	17/38010 (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
1	A	0	2
2	B	0	1
8	K	0	1
9	E	0	1
9	F	0	2
All	All	0	7

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	32	A	N9-C4	-7.70	1.33	1.37
6	I	29	A	N3-C4	-5.83	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	29	A	N9-C4	-5.71	1.34	1.37
6	I	31	C	N1-C6	-5.60	1.33	1.37
7	J	26	A	N9-C4	-5.43	1.34	1.37

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	885	LEU	CA-CB-CG	-7.54	97.97	115.30
7	J	34	C	N1-C2-O2	-6.39	115.06	118.90
1	A	187	LEU	CA-CB-CG	-6.31	100.79	115.30
4	G	4	LEU	CA-CB-CG	5.79	128.62	115.30
1	A	503	GLY	C-N-CA	-5.69	107.48	121.70

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	246	THR	Peptide
1	A	848	VAL	Peptide
2	B	182	TRP	Peptide
9	E	406	PRO	Peptide
8	K	195	MET	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	7458	0	7191	430	0
2	B	1396	0	1365	95	0
2	D	1414	0	1416	103	0
3	C	553	0	585	38	0
4	G	868	0	880	59	0
5	H	955	0	911	72	0
6	I	545	0	272	67	0
7	J	565	0	291	64	0
8	K	4169	0	4050	196	0
9	E	4544	0	4480	524	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	F	4602	0	4577	390	0
10	A	2	0	0	0	0
10	E	3	0	0	0	0
10	F	3	0	0	0	0
10	H	2	0	0	0	0
10	K	3	0	0	0	0
11	K	1	0	0	0	0
All	All	27083	0	26018	1952	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 37.

The worst 5 of 1952 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)
9:F:55:CYS:SG	9:F:75:HIS:HE1	1.60	1.24
9:E:214:THR:HG1	9:E:342:CYS:N	1.45	1.14
9:E:471:CYS:HA	9:E:572:ILE:O	1.49	1.11
9:E:561:PHE:O	9:E:565:ILE:HB	1.55	1.07
9:F:8:CYS:SG	9:F:26:CYS:HB3	1.97	1.04

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	924/929 (100%)	690 (75%)	226 (24%)	8 (1%)	14	14
2	B	185/198 (93%)	163 (88%)	21 (11%)	1 (0%)	25	25
2	D	184/198 (93%)	152 (83%)	32 (17%)	0	100	100
3	C	70/83 (84%)	48 (69%)	22 (31%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	G	111/113 (98%)	94 (85%)	17 (15%)	0	100	100
5	H	129/139 (93%)	105 (81%)	24 (19%)	0	100	100
8	K	521/527 (99%)	424 (81%)	96 (18%)	1 (0%)	44	44
9	E	584/601 (97%)	429 (74%)	149 (26%)	6 (1%)	13	13
9	F	588/601 (98%)	460 (78%)	124 (21%)	4 (1%)	19	19
All	All	3296/3389 (97%)	2565 (78%)	711 (22%)	20 (1%)	24	22

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	PRO
1	A	296	PRO
1	A	905	VAL
1	A	928	HIS
2	B	183	PRO

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	817/820 (100%)	801 (98%)	16 (2%)	50	50
2	B	144/167 (86%)	141 (98%)	3 (2%)	48	48
2	D	149/167 (89%)	147 (99%)	2 (1%)	65	65
3	C	67/77 (87%)	66 (98%)	1 (2%)	60	60
4	G	94/94 (100%)	94 (100%)	0	100	100
5	H	105/113 (93%)	104 (99%)	1 (1%)	73	73
8	K	458/462 (99%)	454 (99%)	4 (1%)	75	75
9	E	503/523 (96%)	499 (99%)	4 (1%)	79	79
9	F	513/523 (98%)	510 (99%)	3 (1%)	84	84
All	All	2850/2946 (97%)	2816 (99%)	34 (1%)	66	67

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	E	218	LYS
9	E	474[A]	MET
9	F	73	LYS
1	A	770	TYR
1	A	684	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
9	F	354	GLN
9	F	489	ASN
3	C	19	GLN
2	B	108	ASN
9	F	518	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	I	24/25 (96%)	6 (25%)	1 (4%)
7	J	26/27 (96%)	8 (30%)	0
All	All	50/52 (96%)	14 (28%)	1 (2%)

5 of 14 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	I	10	C
6	I	11	G
6	I	15	G
6	I	16	U
6	I	23	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	I	22	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 14 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.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31146. 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.