



wwPDB EM Validation Summary Report ⓘ

Nov 22, 2022 – 02:22 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

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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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

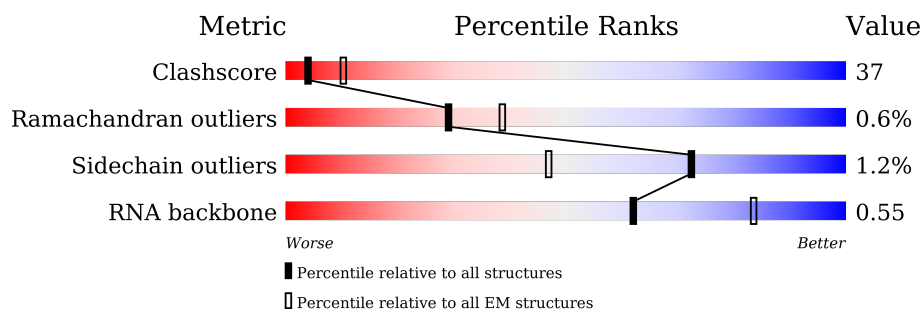
1 Overall quality at a glance

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

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	

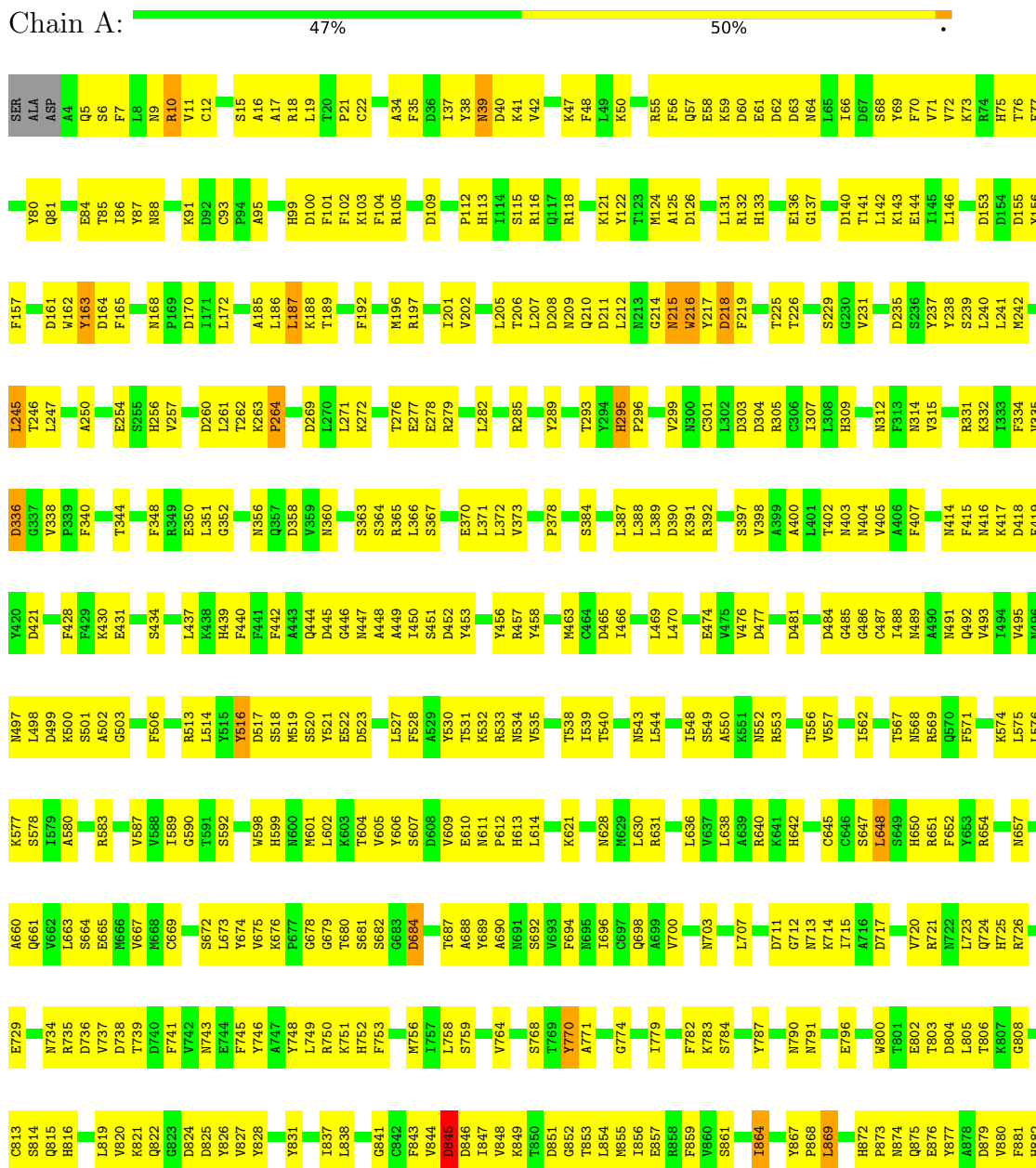
- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

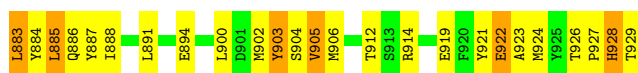
Mol	Chain	Residues	Atoms		AltConf
11	K	1	Total	Mg	0
			1	1	

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.

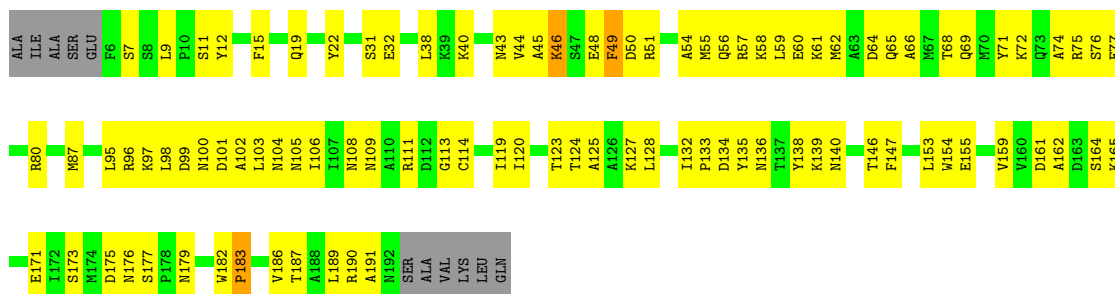
• Molecule 1: RNA-directed RNA polymerase





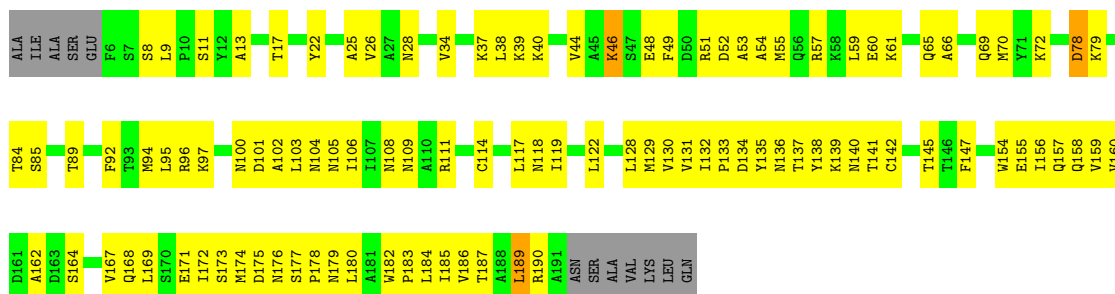
• Molecule 2: Non-structural protein 8

Chain B: 46% 47% 6%



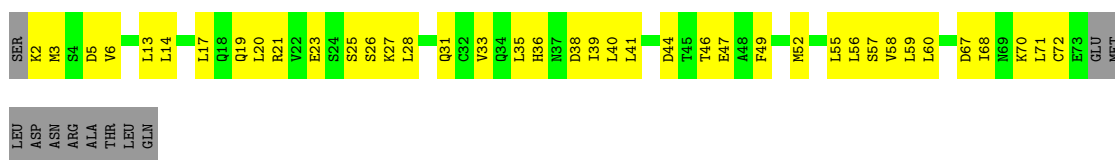
• Molecule 2: Non-structural protein 8

Chain D: 41% 51% 6%



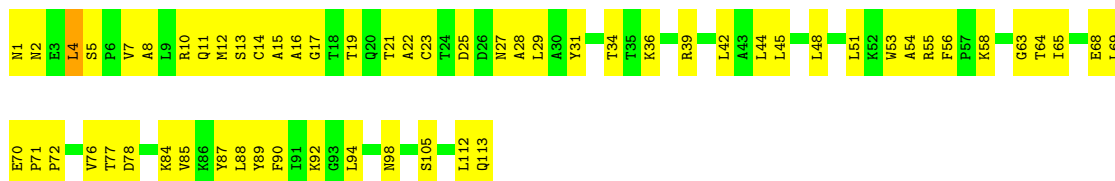
• Molecule 3: Non-structural protein 7

Chain C: 40% 47% 13%

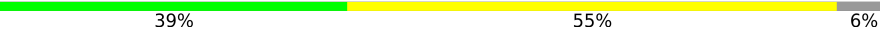


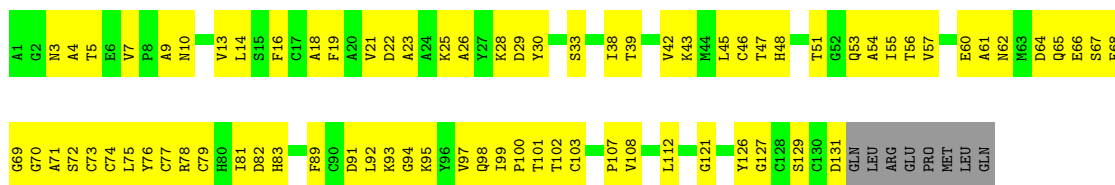
• Molecule 4: Non-structural protein 9

Chain G: 48% 51%

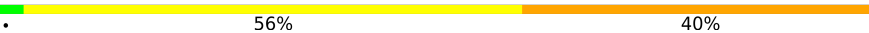


• Molecule 5: Non-structural protein 10

Chain H:  39% 55% 6%

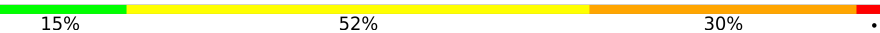


- Molecule 6: primer

Chain I:  56% 40%



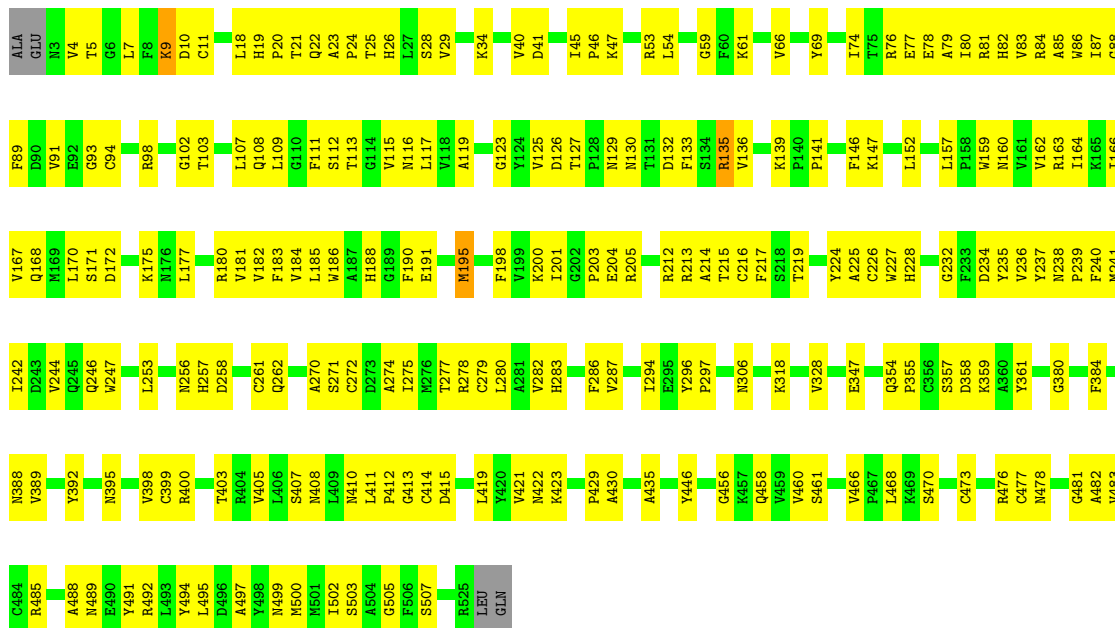
- Molecule 7: template

Chain J:  15% 52% 30%

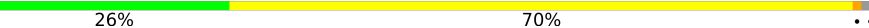


- Molecule 8: Proofreading exoribonuclease

Chain K:  58% 41%



- Molecule 9: Helicase

Chain E:  26% 70%



S69	E136	G202	V272	I334	Y396	L461	P529	ARG
Y70	L137	G203	G273	P335	V397	K462	T530	ARG
Y71	L138		M274	A336	Y398	A463	T531	ASN
C72	K139	D207	Q275	ARG	Y399	H464	T532	VAL
K73	A140	A208	K276	ALA	G400	K465	V533	ALA
S74	T141	V209	Y277	ARG	D401	D466	D534	THR
H75	T142	V210	S278	VAL	P402	K467	S535	LEU
K76	E143	V211	T279	GLU	A403	S468	S536	GLN
P77	E144	R212	L280	C342	Q404	A469	S537	
	K146	G213	Q281	F343	L405	A470	G538	
		T214	G282	D344	P406	C471	S539	
		T215	P283	K345	A407	K472	E540	
F81	Y149		P284	F346	P408	K473	Y541	
P82	G150	K218	G285	K347	R409	M474	D542	
L83	I151	L219	T286			Y475	Y543	
C84	T152	N220	G287	N349	L412	Y476	V544	
	T153	V221	K288	E353	T413		T545	
G87	V154	G222	S289	E354	K414	V479	F546	
Q88	R155	D223	H290	Q354	L417	I480	T547	
V89	E156	F224	F291	Y355	E418		Q548	
	V157	F225	I293	V356	P419	D483	T549	
Y93	L158	L227	G294	C358	E420	V484		
K94			L295	T359	Y421	A487	T552	
N95			A296	V360	F422	I488	A553	
T96	R161	V232	L297	N361	M423	N489	H554	
C97	L163		Y298	A362	S424	R490	N557	
	L164	L235	Y299	L363	V425	P491	V558	
D101	L165	S236	Y299	P364	C426	Q492	N559	
N102	S166	A237	F300	E365	R427	I493	R560	
V103	W167	P238	S301	T366	L428	G494	F561	
T104	E168	T239	A302	T367	M429	V495	N562	
D105	V169	L240	R303	A368	K430	V496	V563	
F106	G170		I304	D369	T431	R497	T565	
A107	K171	Q243	Y306	I370		E498	T566	
I109	R172	H245	T307	V371	P434	T501	R567	
A110	P174	Y246	A308	V372	M435	A505	A568	
T111	P175	V247	C309	F373	M436	W506	K569	
C112	L176	R248	S310	D374	F437			
D113	N177	I249		E375	L438	A505	I572	
W114	R178	T250	V314	I376	G439	R507	L573	
T115	N179	G251	D315	S377	T440	K508	C574	
N116	V180	L252	A316	M378	C441	A509	I575	
A117	V181	Y253	L317	A379	R442	V510	M576	
G118	F182	P254	C318	T380	R443	F511	S577	
D119	T183	T255	E319	N381	C444	I512		
Y120	G184	L256	K320	Y382	P445	S513	D578	
I121	Y185	N257	A321	D383	A446	P514	R579	
L122	R186	I258	L322	L384	E447	Y515	D580	
A123	W187	S259	K323	S385	I448	N516	I581	
N124	T188		Y324	V386		S517	Y582	
T125	K189	F262	L325	V387	V452	Q518	D583	
C126	T127	S263	P326	N388	S453	N519	K584	
E128	G196	V266	I327	A389	A454	A520	L585	
R129	E197	N268	D328	R390	V456	V521	Q586	
L130	Y198	K329	K329	L391	Y457	A522	F587	
K131	T199	Y269	C330	R392			T588	
L132	F200	N268	S331	A393	D458	L526	S589	
F133	F200	K271	I333	K394	G527	G527	P593	

• Molecule 9: Helicase

Chain F: 37% 60% ..

A11	G66	A134	L235	R303	T380
V2		A135	S236	I304	N381
G3	S69	E136	A237	V305	S382
A4	Y70	T137		Y306	D383
C5	Y71	L138	L240	T307	L384
V6	C72		Q243	A308	S385
L7	K73	T141	E244		V386
C8	S74	G150	V247	L317	A389
N9	H75	V154	R248	C318	R390
S10	K76	R155	I249	E319	L391
Q11	P77	R455	L252	K320	R392
T12	P78	E157	Y253	A321	A393
S13	I79	S60	F262	L322	K394
L14	S80	F81	T255		H395
R15	P82	L158	L258	L325	R396
C16	L83	D160	S259	P326	Y397
G17		R161	E261	I327	V398
A18	G87	E162	F262	D328	I399
C19		L163	S263	C330	G400
I20	F90	H164	N265	S331	D401
R21	G91		V266	R332	P402
R22	C91	W167	Y269	I333	A403
P23	L92	K171		I334	Q404
F24	Y93	P172		P335	L405
L25	K94	R173			P406
C26	N95	P174		A338	A407
C27	C97	P175		F343	R409
K28	V98				L412
C29	G99	Y180	V272	F346	G415
C30		I181	G273	K347	T416
C31	T104	F182	M274	V348	L417
V34	D105	T183	Q275	N349	E418
I35	F106	G184	K276		P419
S36	N107	Y185	Y277	E353	E420
T37	A108	R186	S278	Q354	Y421
S38	I109		T279	V355	F422
H39			L280	V356	N423
K40			Q281	F357	S424
L41	C112	I195			V425
S44	D113	Y198	G282	C358	C426
V45	T115	T199	P283	T359	R427
M46	N116	F200	P284	V360	L428
	A117	G203	G285		M429
	G118		T286	L363	K430
C50	D119	A208	G287	P364	I432
N51	Y120	V209	K288	E365	G433
A52	I121	L121	H290	D369	P434
	L122	Y211	F291	I370	D435
C55	A123	R212	A292	V371	L438
D56	N124	T215	G294	V372	G439
V57	T125	C126	L294	F373	T440
T58	T127	F225	A296	D374	R442
D59	D223	Y224	L297	F375	R443
V60	R129	F225	Y298	I376	
Q62	L130	V226	P300	S377	
L63	K131	L132		M378	
Y64	L132				
L65	F133				



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 [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	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%)	17	17
2	B	185/198 (93%)	163 (88%)	21 (11%)	1 (0%)	29	29
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%)	47	47
9	E	584/601 (97%)	429 (74%)	149 (26%)	6 (1%)	15	15
9	F	588/601 (98%)	460 (78%)	124 (21%)	4 (1%)	22	22
All	All	3296/3389 (97%)	2565 (78%)	711 (22%)	20 (1%)	29	25

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%)	55	55
2	B	144/167 (86%)	141 (98%)	3 (2%)	53	53
2	D	149/167 (89%)	147 (99%)	2 (1%)	69	69
3	C	67/77 (87%)	66 (98%)	1 (2%)	65	65
4	G	94/94 (100%)	94 (100%)	0	100	100
5	H	105/113 (93%)	104 (99%)	1 (1%)	76	76
8	K	458/462 (99%)	454 (99%)	4 (1%)	78	78
9	E	503/523 (96%)	499 (99%)	4 (1%)	81	81
9	F	513/523 (98%)	510 (99%)	3 (1%)	86	86
All	All	2850/2946 (97%)	2816 (99%)	34 (1%)	72	71

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 monosaccharides 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 surface views

This section was not generated.

6.5 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.