



## wwPDB EM Validation Summary Report ⓘ

Feb 19, 2025 – 06:11 am GMT

PDB ID : 8RAM  
EMDB ID : EMD-19019  
Title : Structure of Sen1 bound RNA Polymerase II pre-termination complex  
Authors : Rengachari, S.; Lidsreiber, M.; Cramer, P.  
Deposited on : 2023-12-01  
Resolution : 2.80 Å(reported)  
Based on initial models : 6I59, 7NKX, ?, 2XZO

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : **FAILED**  
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) : 2.41

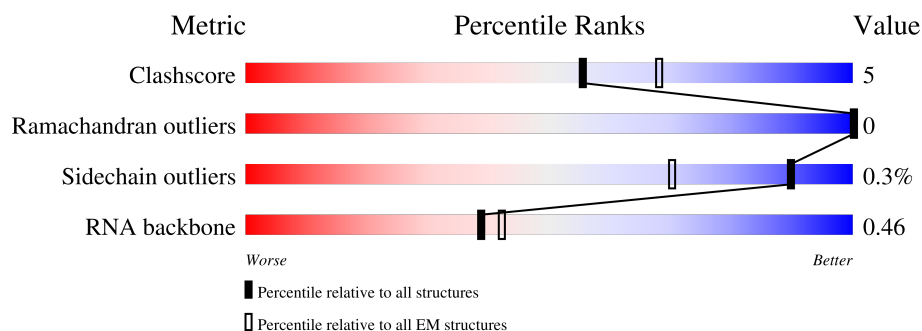
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.80 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  $\geq 3$ , 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	1733	69% (green), 12% (yellow), 19% (grey)
2	B	1224	77% (green), 14% (yellow), 9% (grey)
3	C	318	72% (green), 11% (yellow), 17% (grey)
4	D	221	64% (green), 8% (yellow), 28% (grey)
5	E	215	85% (green), 14% (yellow)
6	F	155	47% (green), 8% (yellow), 45% (grey)
7	G	171	89% (green), 11% (yellow)

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Mol	Chain	Length	Quality of chain
8	H	146	 79%12%9%
9	I	122	 88%9%.
10	J	70	 84%9%7%
11	K	120	 81%15%.
12	L	70	 54%7%39%
13	M	145	 39%6%55%
14	N	58	 45%.53%
15	O	2231	 28%.69%
16	P	35	 57%23%.17%
17	T	58	 43%22%34%
18	Y	102	 94%..
19	Z	1063	 37%.60%

## 2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 42965 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1400	Total	C	N	O	S	0	0
			11020	6948	1929	2081	62		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1113	Total	C	N	O	S	0	0
			8839	5596	1553	1635	55		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	264	Total	C	N	O	S	0	0
			2078	1308	346	411	13		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	159	Total	C	N	O	S	0	0
			1270	788	223	257	2		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1752	1111	309	321	11		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	85	Total	C	N	O	S	0	0
			688	439	116	130	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	133	Total	C	N	O	S	0	0
			1068	673	180	211	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	118	Total	C	N	O	S	0	0
			964	592	178	184	10		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	65	Total	C	N	O	S	0	0
			532	339	93	94	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	1
			920	590	157	171	2		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	43	Total	C	N	O	S	0	0
			343	211	69	59	4		

- Molecule 13 is a protein called Transcription elongation factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	65	Total	C	N	O	S	0	0
			504	311	87	101	5		

- Molecule 14 is a DNA chain called Non-template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	27	Total	C	N	O	P	0	0
			547	262	98	160	27		

- Molecule 15 is a protein called Helicase SEN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	690	Total	C	N	O	S	0	0
			5523	3491	963	1038	31		

- Molecule 16 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	29	Total	C	N	O	P	0	0
			624	278	116	201	29		

- Molecule 17 is a DNA chain called Template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	38	Total	C	N	O	P	0	0
			786	374	142	232	38		

- Molecule 18 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	100	Total	C	N	O	S	0	0
			760	474	129	147	10		

- Molecule 19 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	429	Total	C	N	O	S	0	0
			3397	2150	605	633	9		

- Molecule 20 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
20	A	2	Total	Zn	0
			2	2	
20	B	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
20	C	1	Total 1	Zn 1	0
20	I	2	Total 2	Zn 2	0
20	J	1	Total 1	Zn 1	0
20	L	1	Total 1	Zn 1	0
20	M	1	Total 1	Zn 1	0

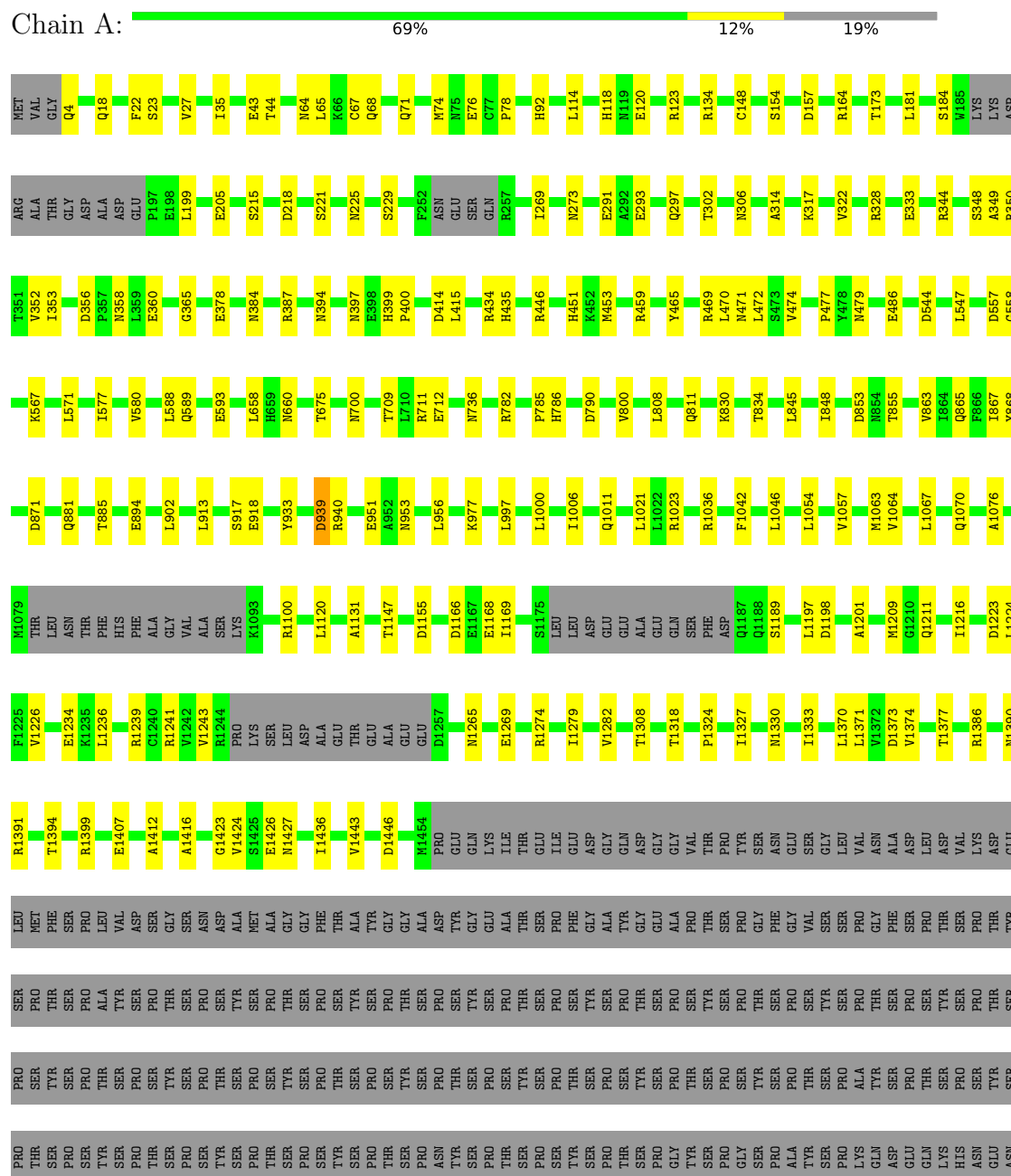
- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total 1	Mg 1	0

### 3 Residue-property plots

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 II subunit RPB1

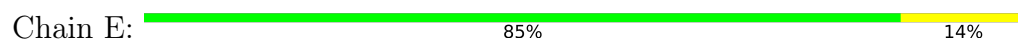




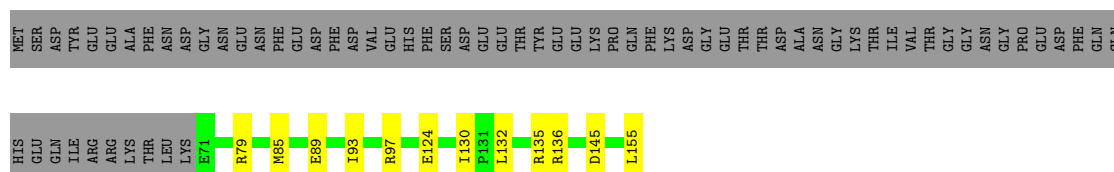




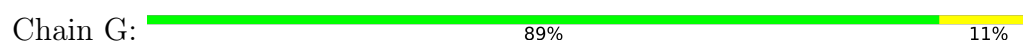
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



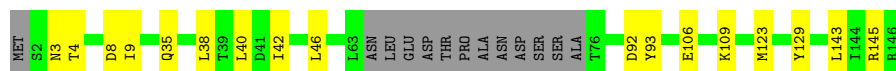
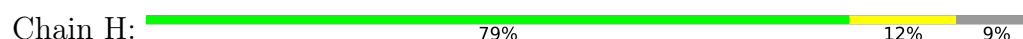
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



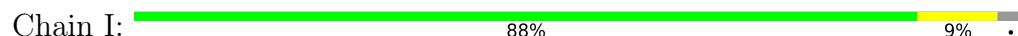
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



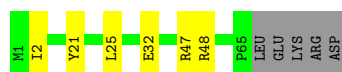
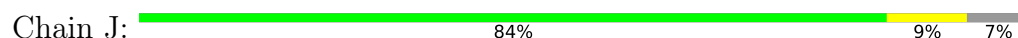
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 11: DNA-directed RNA polymerase II subunit RPB11

M1	L11	E36	K37	E38	D39	H40	T41	L42	R47	F58	H65	A69	R70	E79	C91	L98	G99	A100	N104	L111	A115	ALA	ASP	ASP	ALA	PHE
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- |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | SER | ARG | GLU | GLY | PHE | GLN | ILE | PRO | THR | ASN | LEU | ASP | ALA | ALA | ALA | ALA | GLY | THR | SER | GLN | GLN | ALA | ARG | THR | ALA | ALA | THR | LEU | K28 | L40 | L56 | V65 | Q66 | R70 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

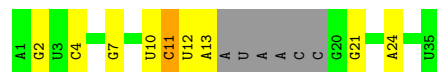
- |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| THR | GLN | ASN | ASP | GLY | GLU | ILE | ASP | SER | ASP | GLU | GLU | VAL | ASP | SER | GLY | GLU | GLU | GLU | ARG | ILE | GLY | GLN | VAL | LYS | T37 | L38 | D39 | R42 | S43 | T46 | L47 | Q65 | G85 | SER | ASP | THR | THR | ASP | GLY | ASP | GLU | GLY | GLY | SER | ASP | GLU | GLU | GLN | ASP | ALA | LYS |
| MET | GLY | LYS | ARG | LYS | LYS | SER | THR | ARG | LYS | PRO | THR | LYS | ARG | LEU | VAL | GLN | LYS | LEU | ASP | T21 | V34 | T37 | L38 | D39 | R42 | S43 | T46 | L47 | Q65 | G85 | SER | ASP | THR | THR | ASP | GLY | ASP | GLU | GLY | GLY | SER | ASP | GLU | GLU | GLN | ASP | ALA | LYS |     |     |     |

- |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |     |     |    |    |    |    |    |    |    |    |    |    |    |     |     |     |    |    |    |    |    |
|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|-----|-----|----|----|----|----|----|----|----|----|----|----|----|-----|-----|-----|----|----|----|----|----|
| DC | DG | DG | DT | DC | DT | DG | DC | DA | DT | DG | DT | DA | DA | DA | C16 | T24 | DA | DT | DT | DC | DG | DA | DG | DT | DT | DA | DG | C37 | T45 | C54 | DT | DT | DG | DC | DC |
|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|-----|-----|----|----|----|----|----|----|----|----|----|----|----|-----|-----|-----|----|----|----|----|----|

- [illegible]



- Molecule 16: RNA



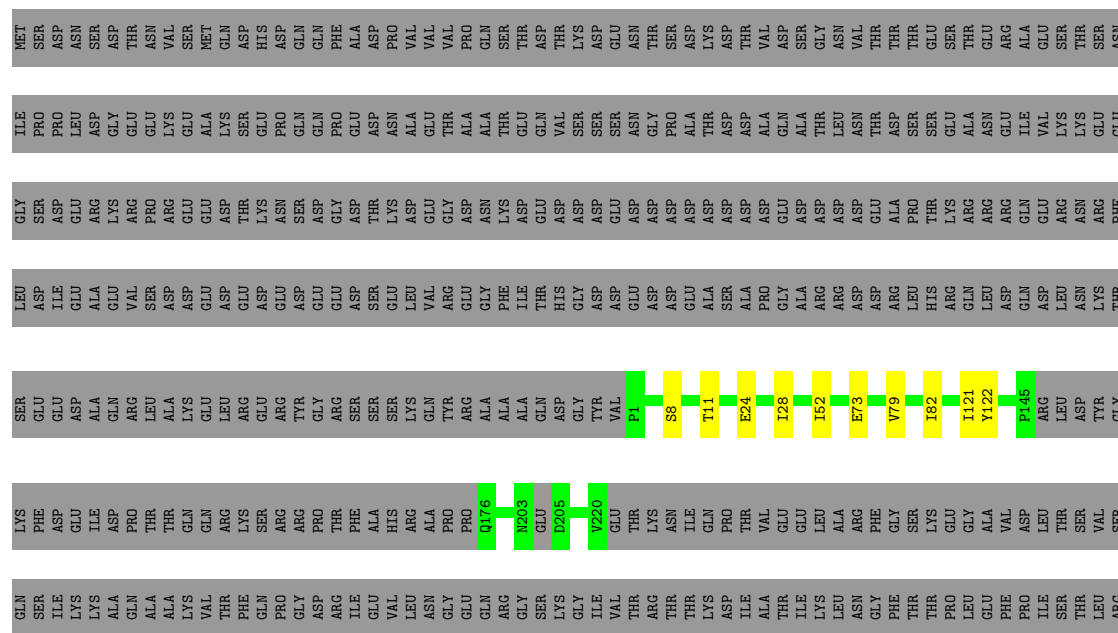
- Molecule 17: Template strand



- Molecule 18: Transcription elongation factor SPT4



- Molecule 19: Transcription elongation factor SPT5



HIS	GLY	GLY	ASN	ASN	SER	LYS
	GLY	THR	GLY	ALA	MET	ILE
	GLY	ASP	GLY	THR	GLY	F584
	ARG	SER	SER	GLY	PRO	D600
	ALA	ALA	ALA	ILE	PRO	A601
	TRP	ALA	TRP	SER	SER	S616
	TVR	GLY	GLY	ALA	LYS	S620
	GLY	GLY	ALA	GLY	THR	S620
	GLY	ALA	ALA	PHE	THR	T625
	ALA	GLY	ALA	GLN	GLN	T626
	SER	THR	GLY	THR	PRO	N629
	TRP	ALA	ALA	SER	ILE	N629
	GLY	GLY	SER	SER	GLN	D635
	GLY	ALA	ALA	GLY	SER	THR
	ASN	TRP	TRP	LEU	ARG	THR
	ASN	GLY	GLY	SER	GLY	THR
	ASN	GLY	GLY	GLY	GLY	ALA
	LYS	GLN	GLN	GLY	R797	THR
	SER	THR	THR	MET	GLY	SER
	THR	ALA	GLY	THR	L801	SER
	ALA	GLY	GLY	PRO	G802	GLU
	ARG	ASP	ALA	GLY	V805	T643
	GLY	THR	SER	TRP	THR	D699
	GLY	THR	THR	SER	SER	Y830
	ALA	TRP	PHE	SER	E830	N703
	SER	GLY	GLY	ASP	H832	Y711
	ALA	GLY	GLY	GLY	T839	Y732
	TRP	ALA	ALA	GLY	R840	Y746
	GLY	ASN	ALA	THR	LYS	Y746
	GLN	TRP	TRP	PRO	ALA	Y752
	ASP	GLY	GLY	ALA	ALA	V752
	ASP	GLY	ASN	VAL	Y847	V755
	GLY	GLY	LYS	ASN	Y848	ALA
	ASN	ASN	SER	SER	N849	V755
	ARG	SER	SER	HIS	GLY	ALA
	SER	TRP	TRP	GLY	GLY	SER
	ALA	ALA	GLY	GLY	E854	LYS
	TRP	TRP	GLY	SER	E860	ASP
	ASN	ASN	ALA	GLY	GLY	ASN
	GLN	SER	THR	GLY	R864	LEU
	GLY	TRP	TRP	GLY	GLY	SER
	ASN	ALA	VAL	GLY	P869	ASN
	LYS	SER	SER	VAL	Q870	LYS
	SER	GLY	GLY	SER	A871	THR
	SER	GLY	GLY	ARG	THR	ASP
	ASN	GLY	TRP	TRP	MET	MET
	TVR	GLY	GLU	GLY	GLY	LEU
	GLY	GLY	SER	GLY	PRO	SER
	ASN	GLY	ASN	ALA	SER	LYS
	SER	GLY	GLY	SER	TYR	MET
	THR	THR	ALA	THR	VAL	ASN
	TRP	TRP	MET	TRP	SER	PRO
	GLY	GLY	GLY	GLY	ALA	GLU
	GLY	THR	THR	GLY	PRO	ILE
	GLY	TRP	GLN	GLY	ARG	THR

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	95644	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 ( $e^-/\text{\AA}^2$ )	40.02	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k 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	A	0.23	0/11217	0.39	0/15166
2	B	0.24	0/9011	0.40	0/12149
3	C	0.23	0/2116	0.40	0/2868
4	D	0.24	0/1279	0.38	0/1716
5	E	0.24	0/1788	0.38	0/2406
6	F	0.23	0/700	0.38	0/945
7	G	0.25	0/1368	0.41	0/1844
8	H	0.24	0/1086	0.43	0/1470
9	I	0.24	0/982	0.42	0/1321
10	J	0.24	0/541	0.38	0/727
11	K	0.24	0/938	0.38	0/1267
12	L	0.22	0/345	0.41	0/457
13	M	0.24	0/512	0.39	0/689
14	N	0.51	0/611	0.89	0/936
15	O	0.24	0/5625	0.37	0/7580
16	P	0.11	0/697	0.65	0/1083
17	T	0.52	0/881	0.94	0/1360
18	Y	0.23	0/776	0.39	0/1050
19	Z	0.23	0/3443	0.40	0/4632
All	All	0.25	0/43916	0.43	0/59666

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.



## 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	11020	0	11104	144	0
2	B	8839	0	8896	112	0
3	C	2078	0	2041	25	0
4	D	1270	0	1287	11	0
5	E	1752	0	1776	20	0
6	F	688	0	707	7	0
7	G	1340	0	1357	12	0
8	H	1068	0	1040	14	0
9	I	964	0	922	9	0
10	J	532	0	542	5	0
11	K	920	0	929	15	0
12	L	343	0	363	4	0
13	M	504	0	480	5	0
14	N	547	0	306	1	0
15	O	5523	0	5555	34	0
16	P	624	0	315	1	0
17	T	786	0	431	11	0
18	Y	760	0	741	3	0
19	Z	3397	0	3506	28	0
20	A	2	0	0	0	0
20	B	1	0	0	0	0
20	C	1	0	0	0	0
20	I	2	0	0	0	0
20	J	1	0	0	0	0
20	L	1	0	0	0	0
20	M	1	0	0	0	0
21	A	1	0	0	0	0
All	All	42965	0	42298	410	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 5.

The worst 5 of 410 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:956:LEU:HD13	1:A:1021:LEU:HD22	1.46	0.97
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.53	0.90
1:A:853:ASP:OD1	1:A:855:THR:OG1	1.95	0.83
19:Z:8:SER:HG	19:Z:11:THR:HG1	1.27	0.81
2:B:971:THR:OG1	3:C:61:GLU:OE1	2.00	0.80

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	1388/1733 (80%)	1350 (97%)	38 (3%)	0	100	100
2	B	1099/1224 (90%)	1070 (97%)	29 (3%)	0	100	100
3	C	262/318 (82%)	255 (97%)	7 (3%)	0	100	100
4	D	155/221 (70%)	152 (98%)	3 (2%)	0	100	100
5	E	212/215 (99%)	210 (99%)	2 (1%)	0	100	100
6	F	83/155 (54%)	81 (98%)	2 (2%)	0	100	100
7	G	169/171 (99%)	169 (100%)	0	0	100	100
8	H	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
9	I	116/122 (95%)	113 (97%)	3 (3%)	0	100	100
10	J	63/70 (90%)	63 (100%)	0	0	100	100
11	K	113/120 (94%)	113 (100%)	0	0	100	100
12	L	41/70 (59%)	40 (98%)	1 (2%)	0	100	100
13	M	63/145 (43%)	63 (100%)	0	0	100	100
15	O	684/2231 (31%)	676 (99%)	8 (1%)	0	100	100
18	Y	98/102 (96%)	98 (100%)	0	0	100	100
19	Z	417/1063 (39%)	412 (99%)	5 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5092/8106 (63%)	4990 (98%)	102 (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	A	1225/1520 (81%)	1222 (100%)	3 (0%)	92	97
2	B	964/1061 (91%)	959 (100%)	5 (0%)	86	95
3	C	232/274 (85%)	230 (99%)	2 (1%)	75	92
4	D	141/200 (70%)	140 (99%)	1 (1%)	81	94
5	E	196/197 (100%)	196 (100%)	0	100	100
6	F	75/137 (55%)	75 (100%)	0	100	100
7	G	152/152 (100%)	152 (100%)	0	100	100
8	H	117/128 (91%)	117 (100%)	0	100	100
9	I	112/116 (97%)	112 (100%)	0	100	100
10	J	60/65 (92%)	60 (100%)	0	100	100
11	K	99/102 (97%)	99 (100%)	0	100	100
12	L	38/57 (67%)	38 (100%)	0	100	100
13	M	60/131 (46%)	60 (100%)	0	100	100
15	O	615/2010 (31%)	614 (100%)	1 (0%)	92	97
18	Y	85/87 (98%)	85 (100%)	0	100	100
19	Z	376/876 (43%)	376 (100%)	0	100	100
All	All	4547/7113 (64%)	4535 (100%)	12 (0%)	90	97

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	961	LEU

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Mol	Chain	Res	Type
3	C	4	GLU
15	O	1277	ARG
3	C	249	ASP
2	B	61	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	47	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	27/35 (77%)	8 (29%)	0

5 of 8 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	2	G
16	P	4	C
16	P	7	G
16	P	10	U
16	P	11	C

There are no RNA pucker outliers to report.

## 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 10 ligands modelled in this entry, 10 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.