



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 27, 2017 – 10:18 AM EDT

PDB ID : 5N60
EMDB ID: : EMD-3592
Title : Cryo-EM structure of RNA polymerase I in complex with Rrn3 and Core Factor (Orientation I)
Authors : Engel, C.; Gubbey, T.; Neyer, S.; Sainsbury, S.; Oberthuer, C.; Baejen, C.; Bernecky, C.; Cramer, P.
Deposited on : unknown
Resolution : 7.70 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

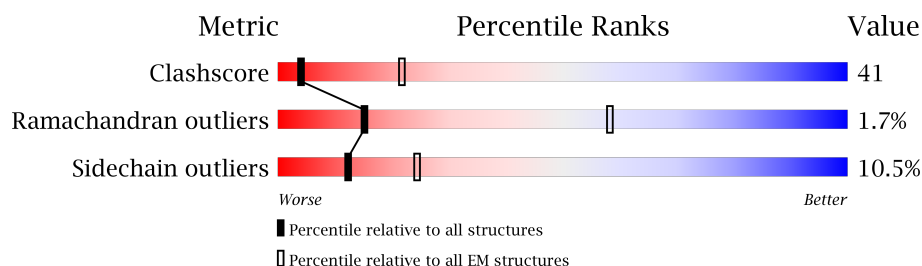
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.70 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.




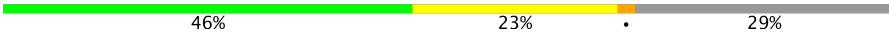


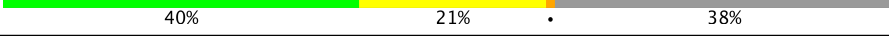
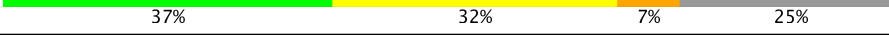
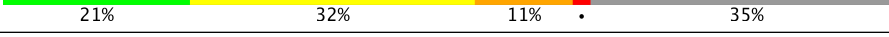
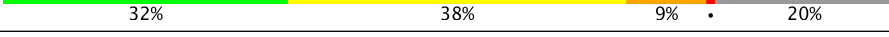

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	1664	61% 23% • 12%
2	B	1203	63% 30% • •
3	C	335	67% 22% • • 9%
4	D	137	31% 9% • • 58%
5	E	215	78% 17% • •
6	F	155	48% 14% • 35%
7	G	326	42% 16% • 41%
8	H	146	68% 21% • 10%
9	I	125	52% 26% • 21%

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Mol	Chain	Length	Quality of chain
10	J	70	
11	K	142	
12	L	70	
13	M	415	
14	N	233	
15	O	627	
16	P	894	
17	Q	514	
18	R	507	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 48004 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 I subunit RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1467	Total	C	N	O	S	0	0
			11598	7327	2017	2193	61		

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1172	Total	C	N	O	S	0	0
			9312	5891	1633	1738	50		

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	305	Total	C	N	O	S	0	0
			2423	1539	416	460	8		

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit RPA14.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	58	Total	C	N	O	0	0
			459	289	78	92		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	212	Total	C	N	O	S	0	0
			1735	1102	306	316	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	100	Total	C	N	O	S	0	0
			823	522	144	154	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	193	Total	C	N	O	S	0	0
			1526	985	262	274	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	131	Total	C	N	O	S	0	0
			1052	664	176	208	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	99	Total	C	N	O	S	0	0
			755	472	125	149	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			793	496	130	162	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	44	Total	C	N	O	S	0	0
			352	217	70	61	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	108	Total	C	N	O		0	0
			856	543	142	171			

- Molecule 14 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	145	Total	C	N	O	S	0	0
			1151	735	188	224	4		

- Molecule 15 is a protein called RNA polymerase I-specific transcription initiation factor RRN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	473	Total	C	N	O	S	0	0
			3907	2533	642	711	21		

- Molecule 16 is a protein called RNA polymerase I-specific transcription initiation factor RRN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	583	Total	C	N	O	S	0	0
			4729	3010	803	905	11		

- Molecule 17 is a protein called RNA polymerase I-specific transcription initiation factor RRN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	410	Total	C	N	O	S	0	0
			3421	2219	579	603	20		

- Molecule 18 is a protein called RNA polymerase I-specific transcription initiation factor RRN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	303	Total	C	N	O	S	0	0
			2535	1634	456	434	11		

- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
19	J	1	Total	Zn	0
			1	1	
19	Q	1	Total	Zn	0
			1	1	
19	B	1	Total	Zn	0
			1	1	
19	I	2	Total	Zn	0
			2	2	

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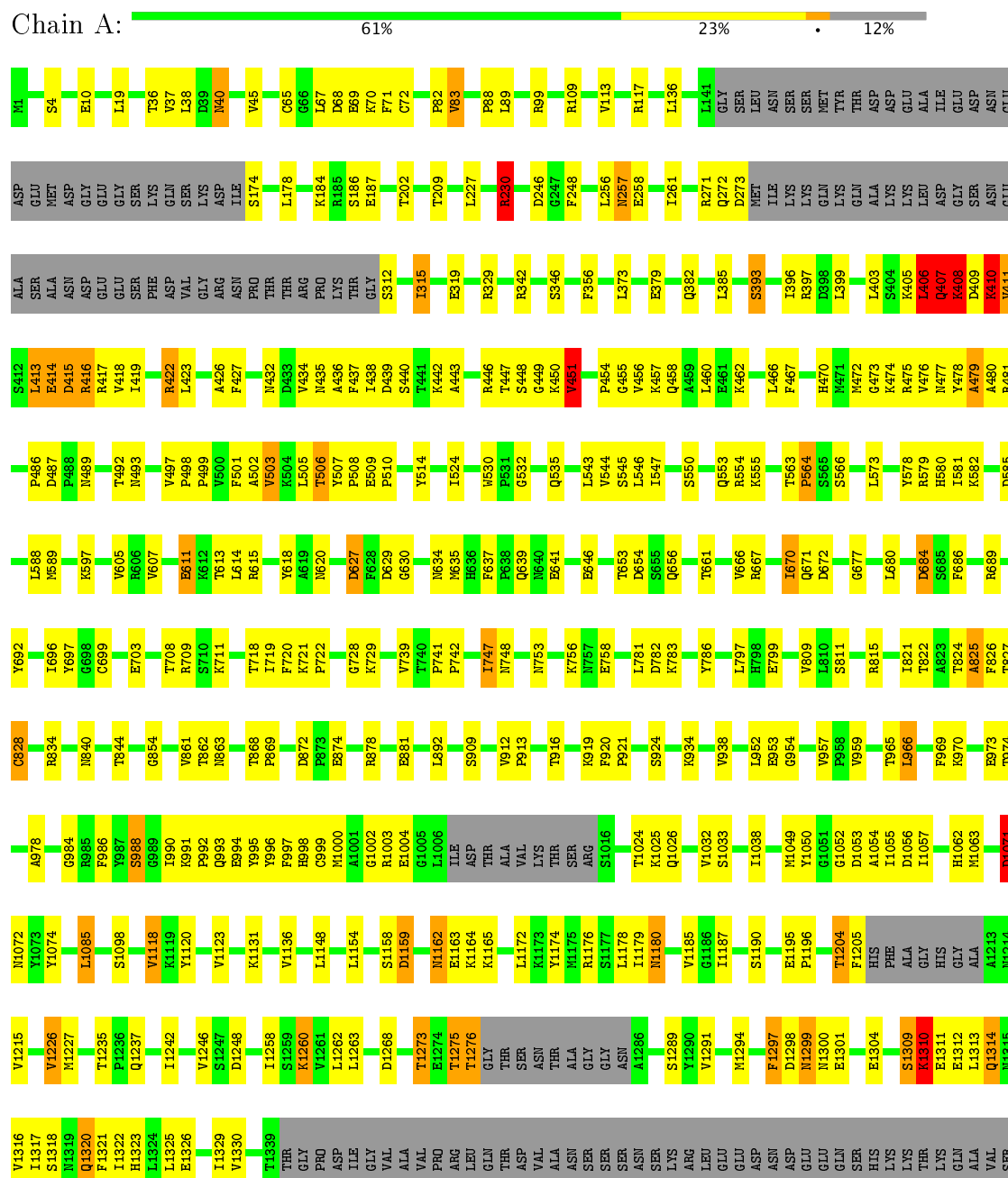
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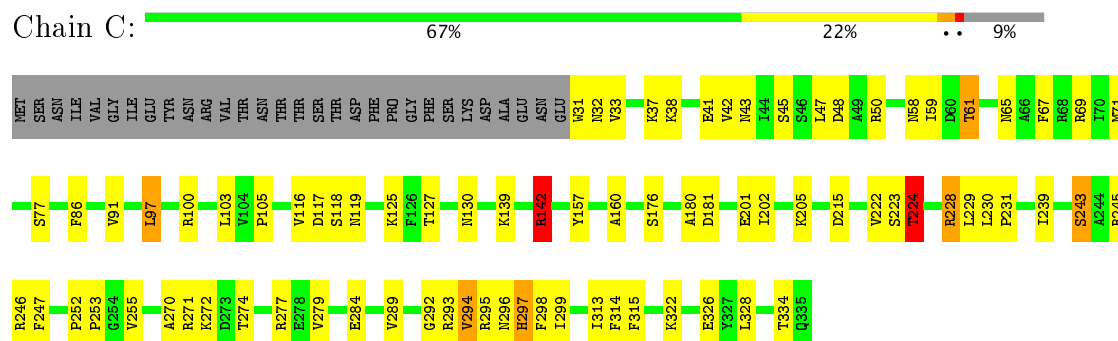
Mol	Chain	Residues	Atoms		AltConf
19	A	2	Total 2	Zn 2	0
19	L	1	Total 1	Zn 1	0

3 Residue-property plots

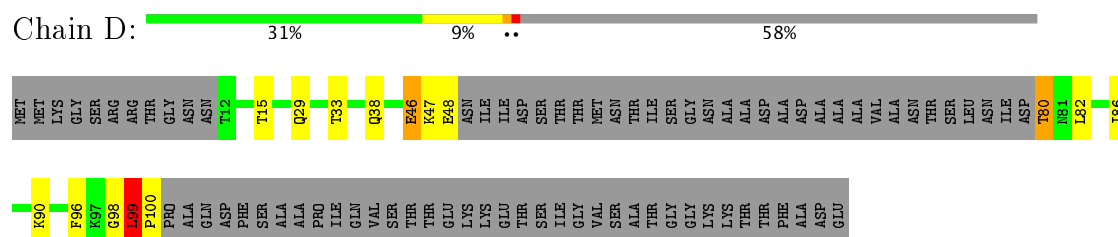
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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 I subunit RPA190

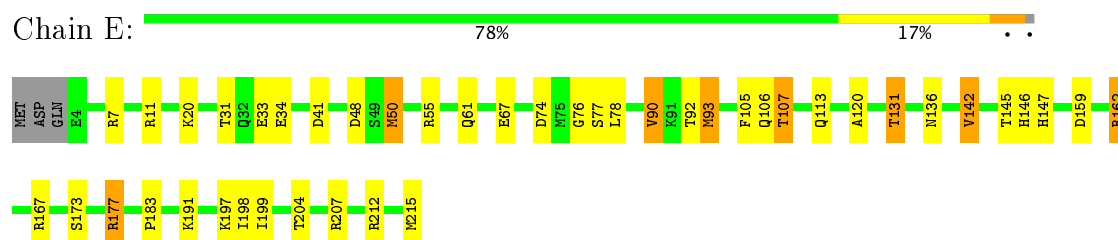




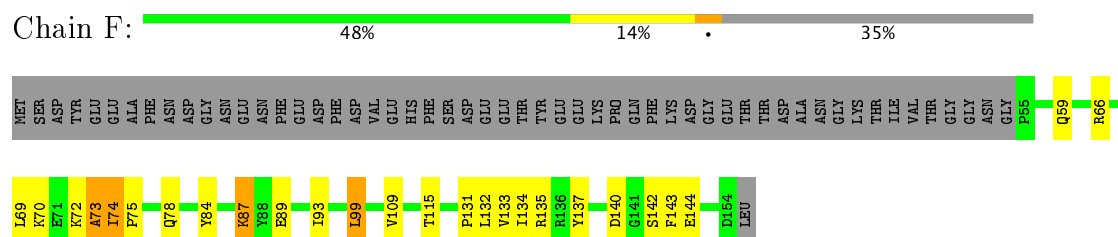
- Molecule 4: DNA-directed RNA polymerase I subunit RPA14



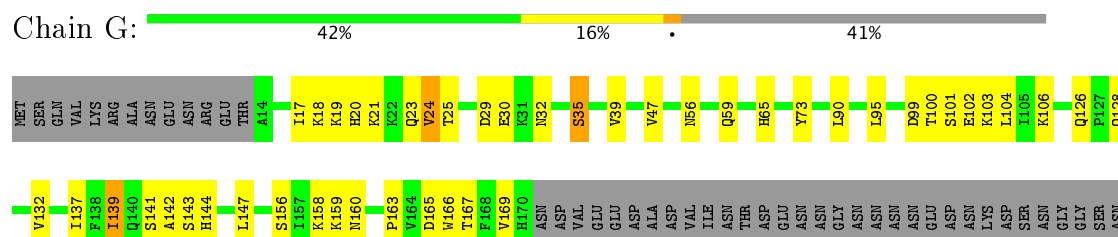
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

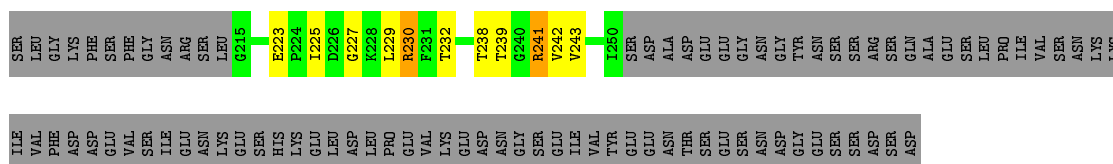


- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

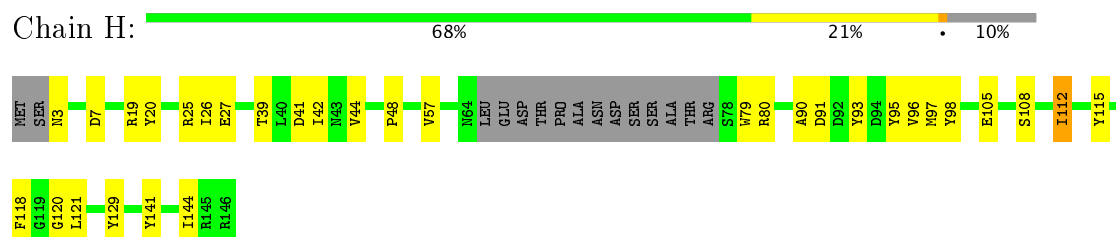


- Molecule 7: DNA-directed RNA polymerase I subunit RPA43

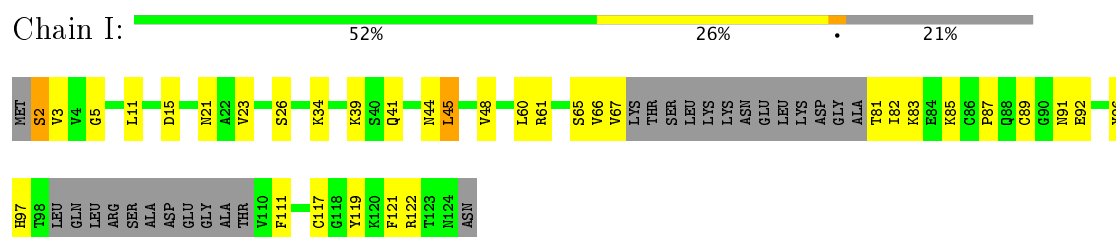




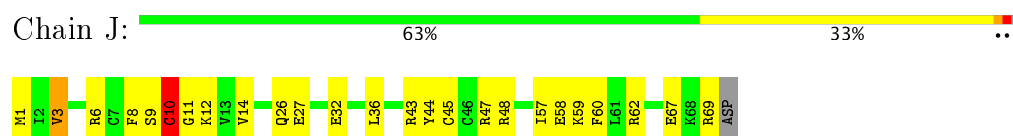
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



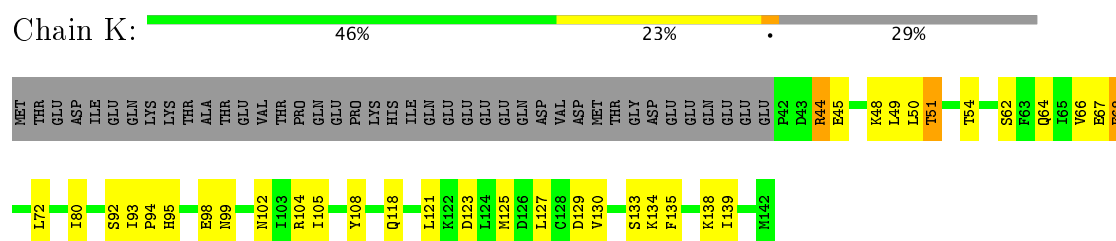
- Molecule 9: DNA-directed RNA polymerase I subunit RPA12



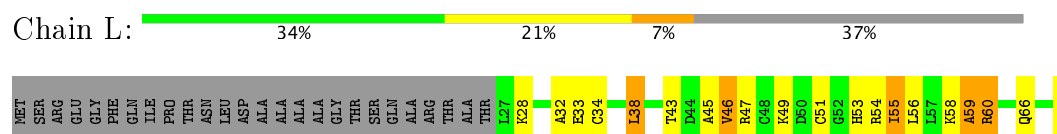
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



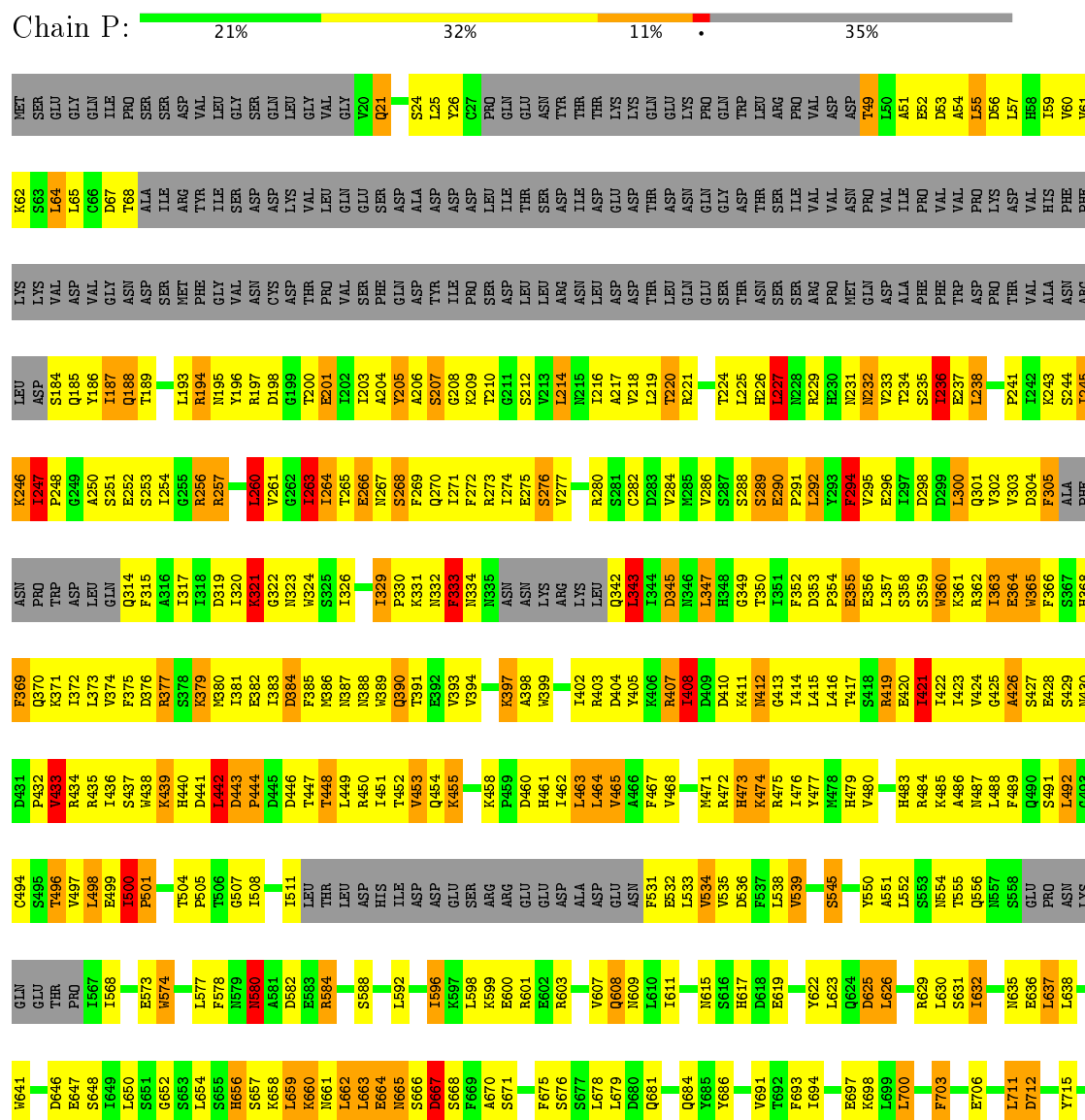
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2



- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



- Molecule 13: DNA-directed RNA polymerase I subunit RPA49



GLU	SER	I318	I253
ARG	ARG	N319	Q254
ASP	GLN	N320	V255
VAL	PHE	Q321	E256
ALA	VAL	K322	I257
ASN	ASN	S323	L258
VAL	ASP	N324	D259
TYR	ASN	PRO	N260
ASP	LYS	SER	N263
SER	ASN	SER	S264
ILE	ASN	SER	S265
ASP	ASP	ASN	S266
ASN	LEU	ILE	S267
SER	ILE	ILE	L268
SER	GLY	ASP	D269
VAL	SER	LYS	F270
GLU	ASP	PRO	L271
ASN	ARG	PHE	Q272
SER	ASP	ASP	N273
PHE	ILE	THR	
GLY	LYS	GLU	
ASP	I401	ASN	I277
VAL	N402	ASP	Y278
VAL		LEU	S279
TYR		LEU	
GLU	I405	GLN	S282
THR	K406	GLU	ARG
ASN			PHE
ALA	H409	L345	VAL
GLU	Y410	I346	GLN
PHE	V411	D347	ASN
LEU	R412	K348	ILE
ASP	T413	I349	ASN
THR	F414	S350	ASN
GLN		E351	TYR
LEU	I417	W352	R291
MET	C418	V353	S292
ASP	L419	L354	
LEU	D420	T355	P295
SER	K421	P356	F296
PHO	G422	P357	F297
GLU		F358	Q298
ASP	A425	M359	T299
ASN	V426	E360	G300
GLY	P427	D361	S301
LEU	S428	A362	R302
ASP		E363	T303
GLU	K436	V364	H304
MET		W365	T305
HIS	E439	F366	A306
TYR	S440	I367	K307
SER	ARG	Y368	F308
ASP	LEU	A369	A309
GLU	TYR		I310
ASP	GLY	H372	T311
SER	GLU	L373	Y312
SER	ALA	L374	I313
SER	GLN		W314
GLU	ASP	D377	S315
	ILE	THR	S316
	GLN	LEU	L317

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	8317	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	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (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

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 > 2$	RMSZ	# $ Z > 2$
1	A	0.49	0/11809	0.72	20/15943 (0.1%)
10	J	0.57	1/578 (0.2%)	0.59	0/775
11	K	0.46	0/804	0.78	3/1083 (0.3%)
12	L	0.42	0/354	0.60	0/468
13	M	0.40	0/872	0.55	0/1170
14	N	0.40	0/1172	0.54	0/1580
15	O	0.35	0/3996	0.54	0/5401
16	P	0.41	0/4822	0.68	4/6525 (0.1%)
17	Q	0.39	0/3502	0.64	2/4727 (0.0%)
18	R	0.36	0/2591	0.65	6/3483 (0.2%)
2	B	0.50	2/9518 (0.0%)	0.78	26/12863 (0.2%)
3	C	0.42	0/2475	0.67	3/3354 (0.1%)
4	D	0.40	0/465	0.59	0/630
5	E	0.40	0/1771	0.66	3/2383 (0.1%)
6	F	0.45	0/838	0.58	0/1129
7	G	0.37	0/1563	0.66	3/2124 (0.1%)
8	H	0.42	0/1070	0.61	0/1449
9	I	0.44	0/765	0.58	0/1030
All	All	0.44	3/48965 (0.0%)	0.68	70/66117 (0.1%)

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	15
12	L	0	2
13	M	0	3
14	N	0	1
15	O	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	P	0	26
17	Q	0	8
18	R	0	8
2	B	0	4
3	C	0	1
6	F	0	1
All	All	0	73

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	10	CYS	CB-SG	7.64	1.95	1.82
2	B	281	CYS	CB-SG	-6.94	1.70	1.82
2	B	859	CYS	CB-SG	-6.10	1.71	1.82

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	7	GLY	C-N-CD	-15.26	87.03	120.60
2	B	1023	ARG	NE-CZ-NH2	-13.71	113.44	120.30
2	B	452	ARG	NE-CZ-NH2	-13.22	113.69	120.30
1	A	397	ARG	NE-CZ-NH1	13.09	126.85	120.30
2	B	448	ARG	NE-CZ-NH2	-13.08	113.76	120.30

There are no chirality outliers.

5 of 73 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	405	LYS	Peptide
1	A	406	LEU	Peptide
1	A	407	GLN	Peptide
1	A	410	LYS	Peptide
1	A	411	VAL	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	11598	0	11666	1134	0
2	B	9312	0	9200	973	0
3	C	2423	0	2412	140	0
4	D	459	0	462	7	0
5	E	1735	0	1764	30	0
6	F	823	0	839	91	0
7	G	1526	0	1534	148	0
8	H	1052	0	1021	54	0
9	I	755	0	728	103	0
10	J	569	0	584	53	0
11	K	793	0	790	55	0
12	L	352	0	371	59	0
13	M	856	0	852	58	0
14	N	1151	0	1168	168	0
15	O	3907	0	3902	406	0
16	P	4729	0	4675	620	0
17	Q	3421	0	3463	519	0
18	R	2535	0	2600	729	0
19	A	2	0	0	1	0
19	B	1	0	0	0	0
19	I	2	0	0	0	0
19	J	1	0	0	0	0
19	L	1	0	0	0	0
19	Q	1	0	0	0	0
All	All	48004	0	48031	3895	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 41.

The worst 5 of 3895 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)
17:Q:20:TRP:CZ3	17:Q:22:ILE:CG2	1.76	1.69
17:Q:381:MET:SD	18:R:212:HIS:HB3	1.26	1.68
3:C:272:LYS:HA	14:N:175:TYR:CE1	1.16	1.63
1:A:995:TYR:CD2	2:B:708:ASP:HA	1.29	1.62
1:A:545:SER:HB2	17:Q:34:VAL:CG2	1.13	1.61

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	A	1449/1664 (87%)	1375 (95%)	60 (4%)	14 (1%)	18	61
2	B	1164/1203 (97%)	1095 (94%)	51 (4%)	18 (2%)	12	53
3	C	303/335 (90%)	287 (95%)	13 (4%)	3 (1%)	18	61
4	D	54/137 (39%)	50 (93%)	2 (4%)	2 (4%)	4	33
5	E	210/215 (98%)	197 (94%)	11 (5%)	2 (1%)	18	61
6	F	98/155 (63%)	95 (97%)	2 (2%)	1 (1%)	18	61
7	G	187/326 (57%)	173 (92%)	12 (6%)	2 (1%)	17	60
8	H	127/146 (87%)	121 (95%)	6 (5%)	0	100	100
9	I	91/125 (73%)	80 (88%)	8 (9%)	3 (3%)	4	35
10	J	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
11	K	99/142 (70%)	92 (93%)	7 (7%)	0	100	100
12	L	42/70 (60%)	36 (86%)	4 (10%)	2 (5%)	2	28
13	M	106/415 (26%)	96 (91%)	8 (8%)	2 (2%)	9	47
14	N	139/233 (60%)	123 (88%)	13 (9%)	3 (2%)	8	44
15	O	467/627 (74%)	426 (91%)	35 (8%)	6 (1%)	14	56
16	P	569/894 (64%)	473 (83%)	76 (13%)	20 (4%)	4	34
17	Q	398/514 (77%)	347 (87%)	41 (10%)	10 (2%)	6	41
18	R	289/507 (57%)	240 (83%)	39 (14%)	10 (4%)	4	34
All	All	5859/7778 (75%)	5369 (92%)	392 (7%)	98 (2%)	15	50

5 of 98 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	408	LYS
1	A	479	ALA
1	A	1651	THR
2	B	111	ASP

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Mol	Chain	Res	Type
2	B	895	PHE

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	1297/1465 (88%)	1215 (94%)	82 (6%)	21	53
2	B	1025/1053 (97%)	960 (94%)	65 (6%)	21	53
3	C	269/296 (91%)	253 (94%)	16 (6%)	23	55
4	D	55/116 (47%)	49 (89%)	6 (11%)	7	30
5	E	194/197 (98%)	180 (93%)	14 (7%)	17	49
6	F	90/137 (66%)	86 (96%)	4 (4%)	33	63
7	G	171/291 (59%)	159 (93%)	12 (7%)	18	50
8	H	115/128 (90%)	111 (96%)	4 (4%)	41	69
9	I	89/110 (81%)	84 (94%)	5 (6%)	25	57
10	J	64/65 (98%)	57 (89%)	7 (11%)	7	30
11	K	91/130 (70%)	84 (92%)	7 (8%)	15	47
12	L	39/57 (68%)	36 (92%)	3 (8%)	15	47
13	M	98/371 (26%)	85 (87%)	13 (13%)	4	24
14	N	135/220 (61%)	129 (96%)	6 (4%)	33	63
15	O	439/576 (76%)	387 (88%)	52 (12%)	6	27
16	P	539/828 (65%)	395 (73%)	144 (27%)	0	4
17	Q	383/476 (80%)	318 (83%)	65 (17%)	2	15
18	R	286/474 (60%)	227 (79%)	59 (21%)	1	8
All	All	5379/6990 (77%)	4815 (90%)	564 (10%)	12	32

5 of 564 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	O	180	LEU

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Mol	Chain	Res	Type
16	P	246	LYS
18	R	155	GLN
15	O	205	ARG
15	O	489	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
15	O	70	GLN
15	O	228	GLN
18	R	184	ASN
15	O	105	ASN
15	O	117	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
7	G	1
18	R	1
9	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	24:VAL	C	25:THR	N	4.53
1	R	206:ARG	C	207:ASN	N	3.86
1	I	45:LEU	C	46:LYS	N	3.17
1	A	438:ILE	C	439:ASP	N	2.97
1	A	991:LYS	C	992:PRO	N	2.86