



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 20, 2016 – 01:15 PM EST

PDB ID : 5M3M
EMDB ID: : EMD-4148
Title : Free monomeric RNA polymerase I at 4.0Å resolution
Authors : Neyer, S.; Kunz, M.; Geiss, C.; Hantsche, M.; Hodirnau, V.-V.; Seybert, A.;
Engel, C.; Scheffer, M.P.; Cramer, P.; Frangakis, A.S.
Deposited on : 2016-10-15
Resolution : 4.00 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
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

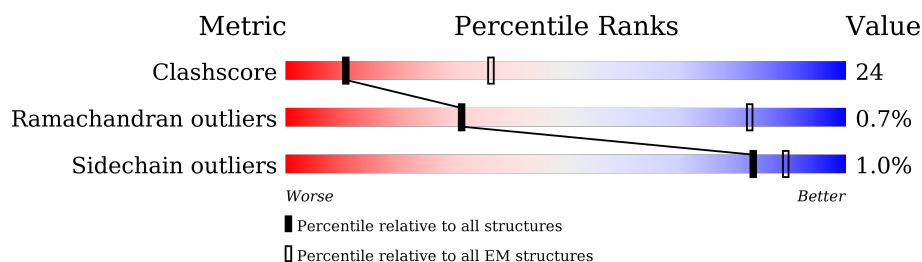
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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.



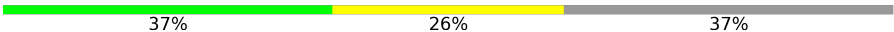

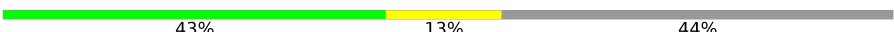

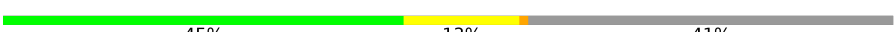
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	44% 43% 12%
2	B	1203	49% 48% .
3	C	335	41% 49% 9%
4	E	215	44% 54% .
5	F	155	32% 31% 37%
6	H	146	48% 42% 10%
7	I	125	46% 46% 7%
8	J	70	44% 54% .
9	K	142	33% 38% 29%

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Mol	Chain	Length	Quality of chain
10	L	70	
11	M	415	
12	N	233	
13	D	137	
14	G	326	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	SO4	B	1301	-	-	X	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 33233 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	1462	Total	C	N	O	S	0	0
			11558	7304	2006	2187	61		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1166	Total	C	N	O	S	0	0
			9266	5864	1617	1734	51		

- 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 polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	212	Total	C	N	O	S	0	0
			1735	1102	306	316	11		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	98	Total	C	N	O	S	0	0
			807	512	142	150	3		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	116	Total	C	N	O	S	0	0
			883	550	148	176	9		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 9 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 11 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	97	Total	C	N	O		0	0
			771	490	124	157			

- Molecule 12 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	131	Total	C	N	O	S	0	0
			1035	660	171	200	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA14.

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

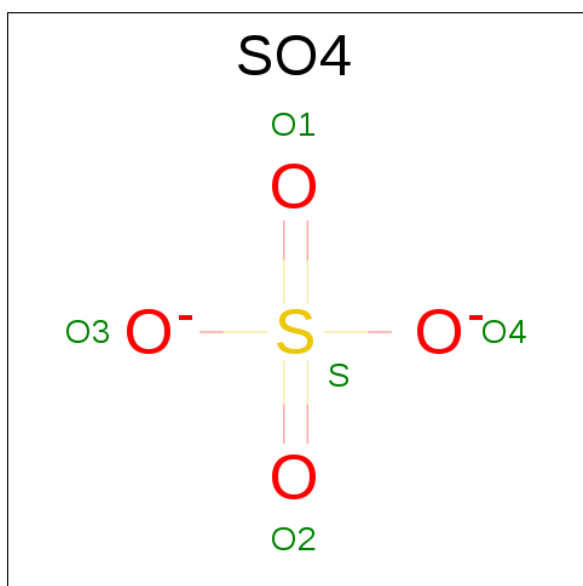
- Molecule 14 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	192	Total	C	N	O	S	0	0
			1518	979	261	273	5		

- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
15	B	1	Total	Zn	0
			1	1	
15	A	2	Total	Zn	0
			2	2	
15	L	1	Total	Zn	0
			1	1	
15	J	1	Total	Zn	0
			1	1	
15	I	2	Total	Zn	0
			2	2	

- Molecule 16 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

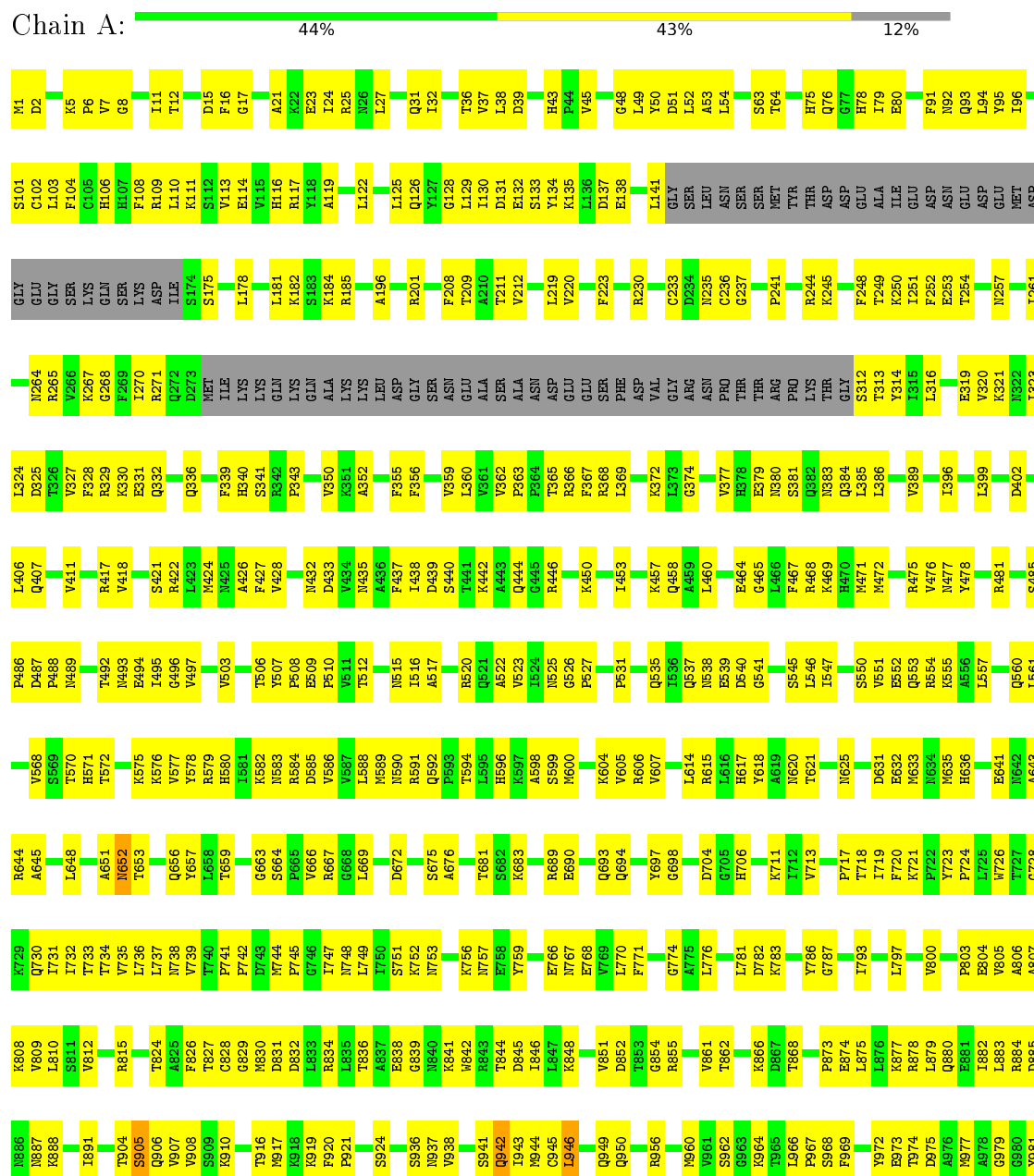


Mol	Chain	Residues	Atoms			AltConf
16	B	1	Total	O	S	0
			5	4	1	

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 errors 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

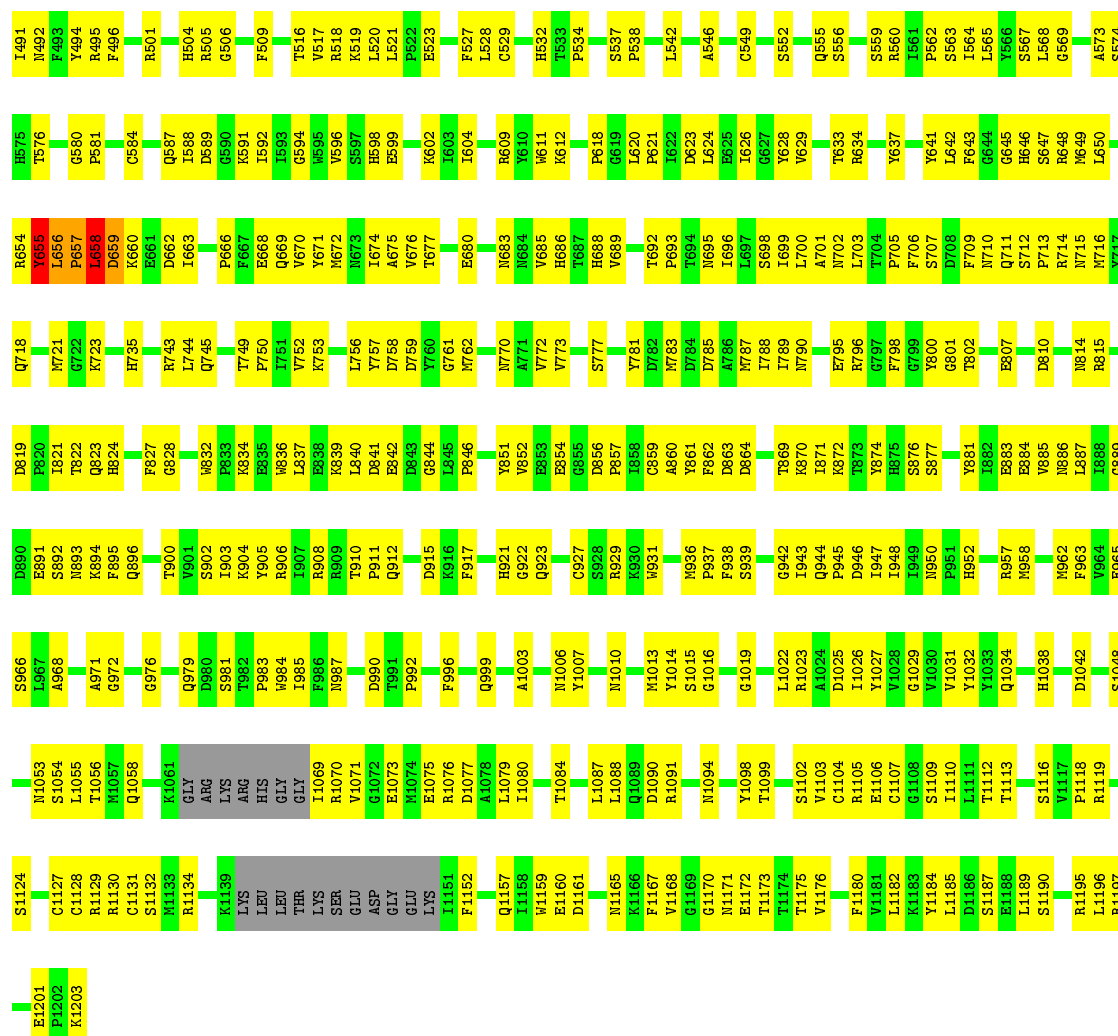


S1609	V1520	V1442	Q1314	F1166	Y1074	V982
F1610	T1521	Q1443	M1315	Q1250	Q1251	K983
M1611	V1524	R1446	I1317	A1251	L1172	G984
K1612		R1447	ASP		K1173	R985
Y1615	M1529	Q1448	S1318	F1254	Y1174	F986
E1616	M1530	A1449	M1319	C1255	K1079	
T1617	W1530	A1450	Q1320	K1256	M1175	Y987
T1618		I1450	F1321	S1257	R1176	S988
C1619	E1533	I1451	I1322	I1258	P1082	
	F1535	S1452	H1323	S1259	L1085	Y996
K1624	F1536	H1453	L1324	K1260	A1094	M1000
A1625	D1537	H1454	L1325	G1186	S1098	G1005
V1626	I1537	R1455	E1326	I1187	K1089	L1006
L1627	V1538	F1456	Q1336	L1263	K1100	I1007
D1628	D1539	I1457	ARG	A1189	T1101	T1008
M1629	T1542	T1458	K1337	E1265	S1190	D1009
		K1459	ALA	V1266	Q1191	A1010
L1634		Y1460	THR	I1287	Y1104	VAL
D1635	D1545	M1461	THR	D1288	R1105	LYS
S1636	V1546	F1462	GLY	G1194	H1108	THR
P1637	A1547	D1463	PRO	E1195		SER
S1638	A1548		ASP	T1272	P1196	ARG
A1639	V1549	W1469	ILE	E1274	E1111	ARG
R1640	L1550	C1470	GLY	T1275	P1112	THR
I1641	Y1553	E1471	VAL	T1276	M1200	ARG
V1642	G1554	F1472	ALA	GLY	T1204	SER
V1643		K1473	VAL	THR	T1205	GLY
G1644		SER	PRO	SER	HIS	Q1020
K1645	R1559	E1475	ARG	ASN	Q1116	L1023
L1646	T1562	L1476	LEU	THR	Y1120	T1024
L1647	R1647	A1477	GLN	ALA	L1124	K1025
N1648	N1568	D1478	THR	GLY		H1031
V1649	V1569	T1479	ASP	GLY	Y1127	Y1034
G1650	F1570	K1481	VAL	ASN	N1128	
T1651	S1571	K1482	ASP	A1286	P1129	R1039
G1652	R1572	L1483	SER	A1287	Y1215	D1040
F1654	Y1573	L1484	ASP	S1289	T1216	A1041
V1655	A1574	M1485	GLU	SER		D1042
V1656	S1578	V1486	ASN	I1292	S1135	G1043
L1657	F1579	E1490	VAL	H1293	E1138	
ALA	R1580		ASP			M1049
LYS	H1581	S1496	MET	F1296	Q1141	Y1050
VAL	L1582	T1497	ASN	F1297	D1142	G1051
PRO		I1498	GLN	D1298		G1052
ASN	A1586	R1499	ILE	M1299	L1148	D1053
ALA	D1587	Q1500	ASN	ASP		A1054
ALA	M1588	I1501	ASN	E1301	K1153	I1055
		P1502	LYS	Y1302	L1154	D1056
	R1591	H1503	ILE	S1303	F1155	I1057
	A1597	I1504	GLN	GLU	K1156	T1058
			GLU	ASP	S1157	K1059
		P1510	ALA	D1307	E1060	
		E1511	ASN	HIS	S1158	S1061
			ASN	LYS	D1159	H1062
			LYS	S1309		
			THR	K1310	N1162	
		R1516	ASN	D1245	E1163	F1066
		R1517	MET	E1311	K1164	
		V1518	ASN	GLN	V1246	L1070
		L1519	ALA	ALA	S1247	
			K1441			

• Molecule 2: DNA-directed RNA polymerase I subunit RPA135

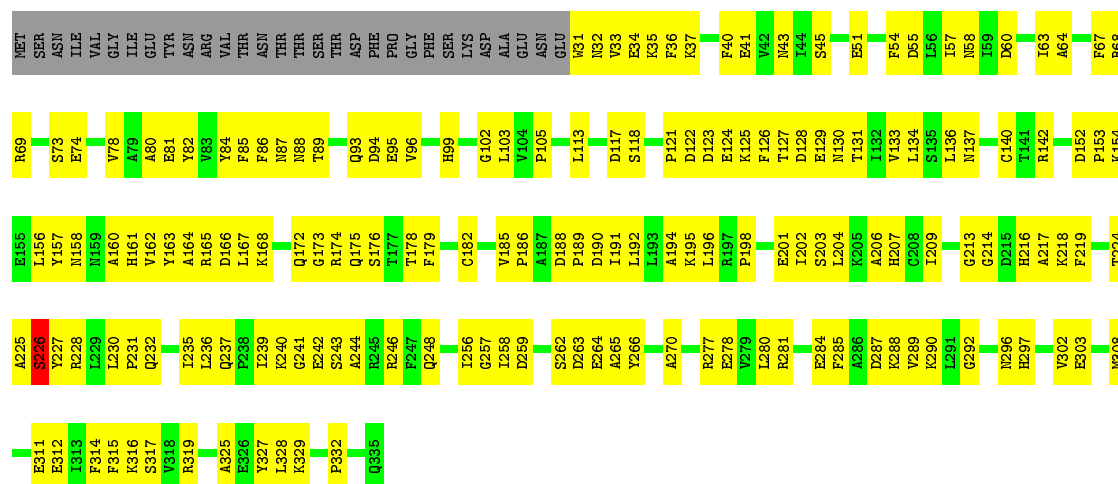
Chain B:  49% 48%

MET	SER	LYS	VAL	ILE	PRO	PRO	GLY	GLN	ALA	ARG	THR	ALA	D15	R17	L18	L19	E20	E21	E22	S23	R24	R25	I26	N27	P28	P29	K30	D31	K32	F35	V42	I46	N50	A51	E54	D57	G58	G59	L60	L61	N62	L63	V65	I68	G69	E70	K71	V72	I73
F74	D75	G76	H80	SER	GLU	ASP	GLU	ILE	SER	ASN	S88	G92	R93	K94	L95	S96	I97	S98	V102	S103	I104	I105	K106	P107	N110	I118	V121	I122	Q128	S132	Y133	R134	G135	K136	L137	L138	L139	W143	S144	V145	M146	E149	E150	N151	L152	R156	G160		
L161	P162	V163	M164	S167	M168	R169	C170	H171	L172	M173	K174	M175	S176	P177	Y178	E179	L180	V181	H183	K184	E185	E186	E189	I190	F194	I195	V196	K201	L202	V208	Q209	R210	R211	N212	M215	I218	F222	R225	S228	Y229	S230	H231	I234	S238	V239	R240			
S245	T247	Y249	Y252	L253	D254	D255	G256	Q257	R261	F262	S263	R264	R265	K266	E268	V274	W275	L276	L277	L280	D285	R286	F289	D290	F301	R305	L306	E307	L308	L309	R311	K314	K315	L320	Q321	R322	R323	T324	Q325	V326	L327								
Q328	R329	G331	R335	A340	S341	P342	D343	Q344	S345	D346	V349	E352	V353	R356	V358	L359	V360	H361	L362	Q368	D369	K370	F371	R372	L375	F376	M377	I378	R379	L381	R380	R382	A386	G387	E388	N393	A396	T397	Q398	H399	Q400	E401	L404	F407					
N411	T417	L421	T424	Q427	V428	D431	R434	G435	N436	K441	D442	K443	Y445	N446	S447	R448	V449	L450	R452	N455	N456	L457	K460	N461	Q462	N463	F464	L465	S466	T467	Q468	L470	N471	Q473	S474	Q480	N481	Y484	T485	V486	V487	A488	E489	K490					



- Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C: 41% 49% 9%



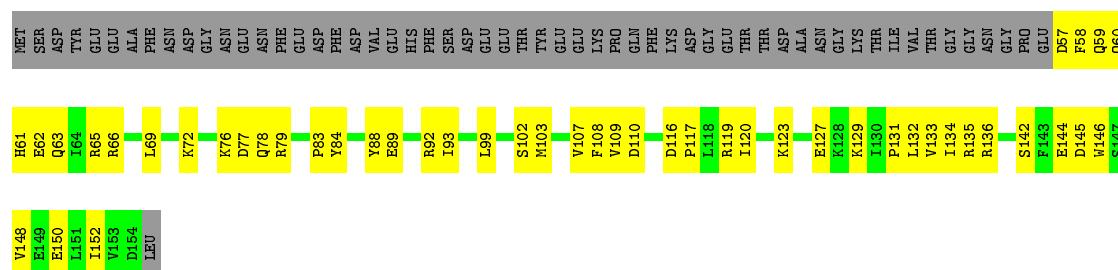
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 



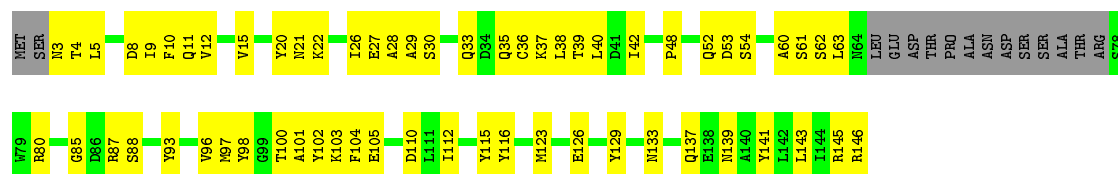
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 



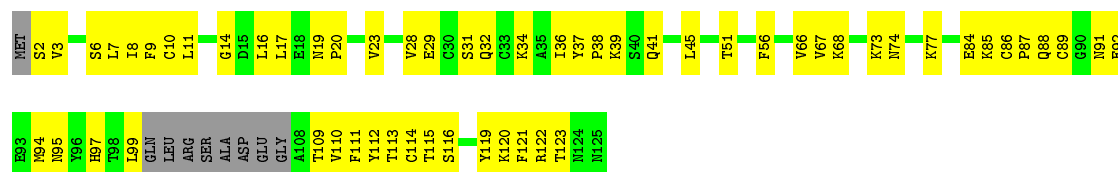
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 



- Molecule 7: DNA-directed RNA polymerase I subunit RPA12

Chain I: 

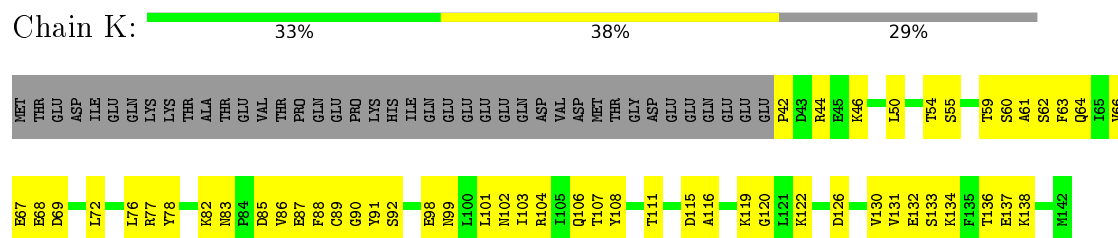


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

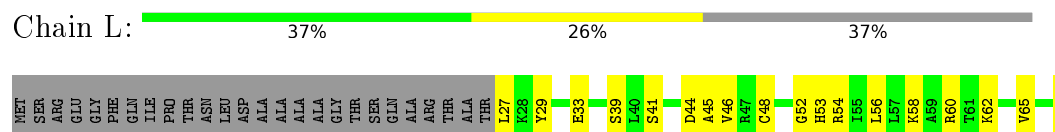
Chain J: 



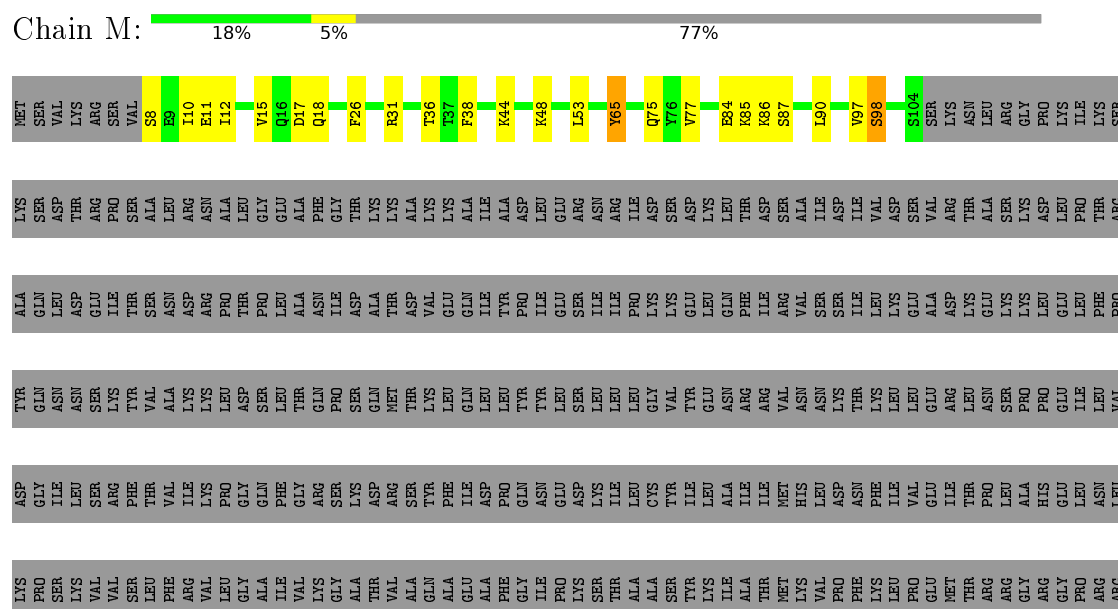
- Molecule 9: DNA-directed RNA polymerases I and III subunit RPAC2



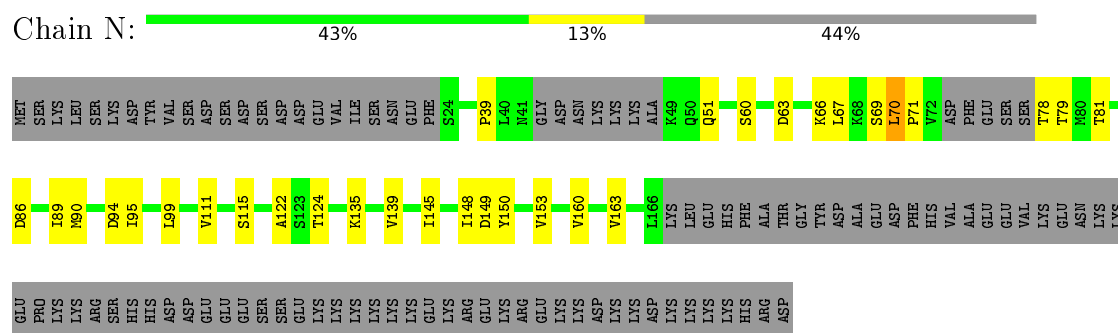
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



- Molecule 11: DNA-directed RNA polymerase I subunit RPA49

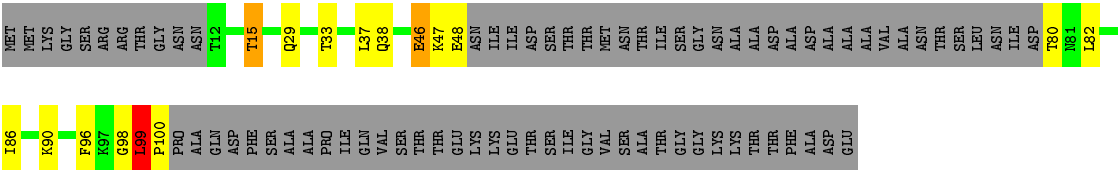


- Molecule 12: DNA-directed RNA polymerase I subunit RPA34

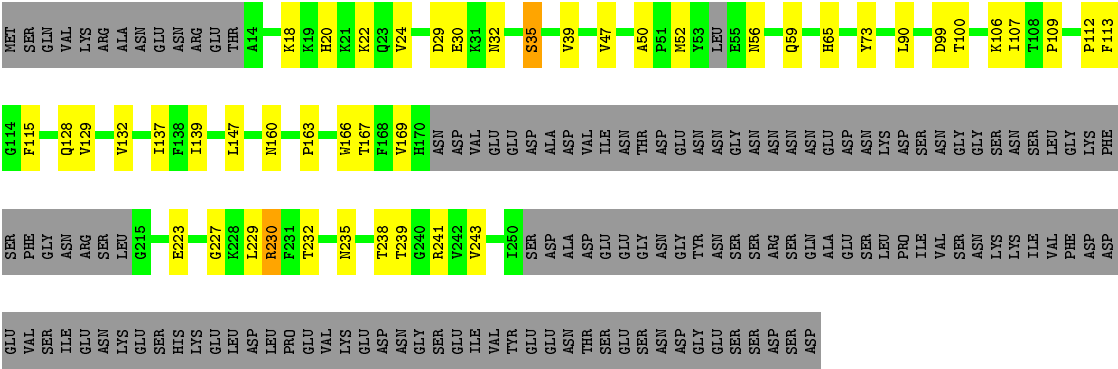


- Molecule 13: DNA-directed RNA polymerase I subunit RPA14





● Molecule 14: DNA-directed RNA polymerase I subunit RPA43



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	94000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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, SO4

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	0.40	0/11770	0.51	0/15895
10	L	0.40	0/354	0.53	0/468
11	M	0.40	0/786	0.55	0/1057
12	N	0.39	0/1052	0.55	0/1418
13	D	0.40	0/465	0.58	0/630
14	G	0.37	0/1555	0.66	3/2113 (0.1%)
2	B	0.45	0/9471	0.53	0/12805
3	C	0.45	0/2475	0.51	0/3354
4	E	0.40	0/1771	0.50	0/2383
5	F	0.37	0/821	0.48	0/1106
6	H	0.46	0/1070	0.54	0/1449
7	I	0.38	0/895	0.49	0/1205
8	J	0.50	0/578	0.53	0/775
9	K	0.45	0/804	0.55	0/1083
All	All	0.42	0/33867	0.53	3/45741 (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	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	241	ARG	NE-CZ-NH1	11.80	126.20	120.30
14	G	241	ARG	NE-CZ-NH2	-11.62	114.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	241	ARG	CD-NE-CZ	6.08	132.12	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1649	VAL	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	11558	0	11642	651	0
2	B	9266	0	9151	558	0
3	C	2423	0	2412	156	0
4	E	1735	0	1764	98	0
5	F	807	0	827	45	0
6	H	1052	0	1021	47	0
7	I	883	0	879	60	0
8	J	569	0	585	36	0
9	K	793	0	790	56	0
10	L	352	0	374	20	0
11	M	771	0	755	11	0
12	N	1035	0	1069	29	0
13	D	459	0	462	8	0
14	G	1518	0	1528	31	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
16	B	5	0	0	8	0
All	All	33233	0	33259	1613	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 24.

The worst 5 of 1613 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)
2:B:656:LEU:O	12:N:153:VAL:HG11	1.62	0.97
3:C:225:ALA:O	3:C:226:SER:HB2	1.63	0.95
1:A:1501:ILE:HG22	1:A:1502:PRO:HD2	1.49	0.94
2:B:894:LYS:HG2	10:L:54:ARG:HH21	1.33	0.94
5:F:66:ARG:HA	5:F:69:LEU:HD12	1.50	0.93

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	1448/1664 (87%)	1364 (94%)	75 (5%)	9 (1%)	30	73
2	B	1158/1203 (96%)	1110 (96%)	41 (4%)	7 (1%)	30	73
3	C	303/335 (90%)	283 (93%)	19 (6%)	1 (0%)	46	82
4	E	210/215 (98%)	202 (96%)	8 (4%)	0	100	100
5	F	96/155 (62%)	94 (98%)	2 (2%)	0	100	100
6	H	127/146 (87%)	124 (98%)	3 (2%)	0	100	100
7	I	112/125 (90%)	108 (96%)	4 (4%)	0	100	100
8	J	67/70 (96%)	61 (91%)	6 (9%)	0	100	100
9	K	99/142 (70%)	95 (96%)	4 (4%)	0	100	100
10	L	42/70 (60%)	38 (90%)	4 (10%)	0	100	100
11	M	95/415 (23%)	86 (90%)	7 (7%)	2 (2%)	9	53
12	N	125/233 (54%)	108 (86%)	13 (10%)	4 (3%)	5	44
13	D	54/137 (39%)	50 (93%)	2 (4%)	2 (4%)	4	40
14	G	186/326 (57%)	171 (92%)	13 (7%)	2 (1%)	17	64
All	All	4122/5236 (79%)	3894 (94%)	201 (5%)	27 (1%)	31	71

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	946	LEU
2	B	657	PRO
2	B	658	LEU
2	B	659	ASP
3	C	226	SER

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	1292/1465 (88%)	1288 (100%)	4 (0%)	94	97
2	B	1022/1053 (97%)	1020 (100%)	2 (0%)	95	97
3	C	269/296 (91%)	268 (100%)	1 (0%)	93	97
4	E	194/197 (98%)	194 (100%)	0	100	100
5	F	88/137 (64%)	88 (100%)	0	100	100
6	H	115/128 (90%)	115 (100%)	0	100	100
7	I	103/110 (94%)	103 (100%)	0	100	100
8	J	64/65 (98%)	64 (100%)	0	100	100
9	K	91/130 (70%)	91 (100%)	0	100	100
10	L	39/57 (68%)	39 (100%)	0	100	100
11	M	88/371 (24%)	79 (90%)	9 (10%)	9	41
12	N	124/220 (56%)	120 (97%)	4 (3%)	46	78
13	D	55/116 (47%)	49 (89%)	6 (11%)	8	38
14	G	170/291 (58%)	158 (93%)	12 (7%)	18	58
All	All	3714/4636 (80%)	3676 (99%)	38 (1%)	83	92

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	N	124	THR
13	D	29	GLN

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Mol	Chain	Res	Type
14	G	230	ARG
12	N	145	ILE
13	D	38	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	248	ASN
2	B	547	HIS
6	H	35	GLN
2	B	254	ASN
2	B	427	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	SO4	B	1301	-	4,4,4	0.46	0	6,6,6	0.29	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	SO4	B	1301	-	-	0/0/0/0	0/0/0/0

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.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	1301	SO4	8	0

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.