



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:07 AM GMT

PDB ID : 3H3V
Title : Yeast RNAP II containing poly(A)-signal sequence in the active site
Authors : Dengl, S.; Cramer, P.
Deposited on : 2009-04-17
Resolution : 4.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

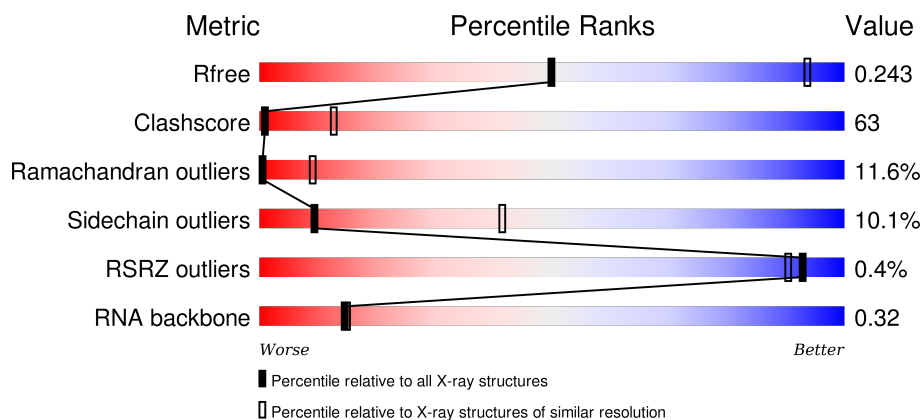
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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.




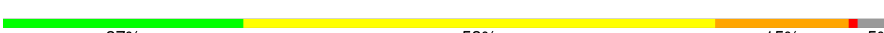



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)
RNA backbone	2183	1079 (5.04-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	1733	
2	C	1224	
3	D	318	
4	E	221	

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Mol	Chain	Length	Quality of chain
5	F	215	
6	G	155	
7	H	171	
8	I	146	
9	J	122	
10	K	70	
11	L	120	
12	M	70	
13	N	14	
14	P	16	
15	T	26	

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 31777 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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					ZeroOcc	AltConf	Trace
1	B	1416	Total	C	N	O	S	0	0	0
			11140	7021	1946	2111	62			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1108	Total	C	N	O	S	0	0	0
			8810	5580	1541	1634	55			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	177	Total	C	N	O	S	0	0	0
			1427	882	256	287	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	214	Total	C	N	O	S	0	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					ZeroOcc	AltConf	Trace
6	G	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	171	Total	C	N	O	S	0	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					ZeroOcc	AltConf	Trace
8	I	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

- Molecule 13 is a DNA chain called 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP*GP*C
P*TP*GP*CP*TP*TP*TP*AP*TP*TP*GP*CP*AP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	7	Total	C	N	O	P	11	0	0
			138	67	26	39	6			

- Molecule 14 is a RNA chain called 5'-D(*CP*AP*GP*CP*TP*AP*CP*TP*TP*GP*AP*GP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	8	Total	C	N	O	P	0	0	0
			168	77	33	51	7			

- Molecule 15 is a DNA chain called 5'-R(*UP*GP*CP*AP*UP*UP*UP*CP*GP*CP*AP*AP*UP*AP*AP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	18	Total	C	N	O	P	8	0	0
			365	177	60	111	17			

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	J	2	Total	Zn	0	0
			2	2		
16	D	1	Total	Zn	0	0
			1	1		
16	K	1	Total	Zn	0	0
			1	1		
16	B	2	Total	Zn	0	0
			2	2		
16	C	1	Total	Zn	0	0
			1	1		
16	M	1	Total	Zn	0	0
			1	1		

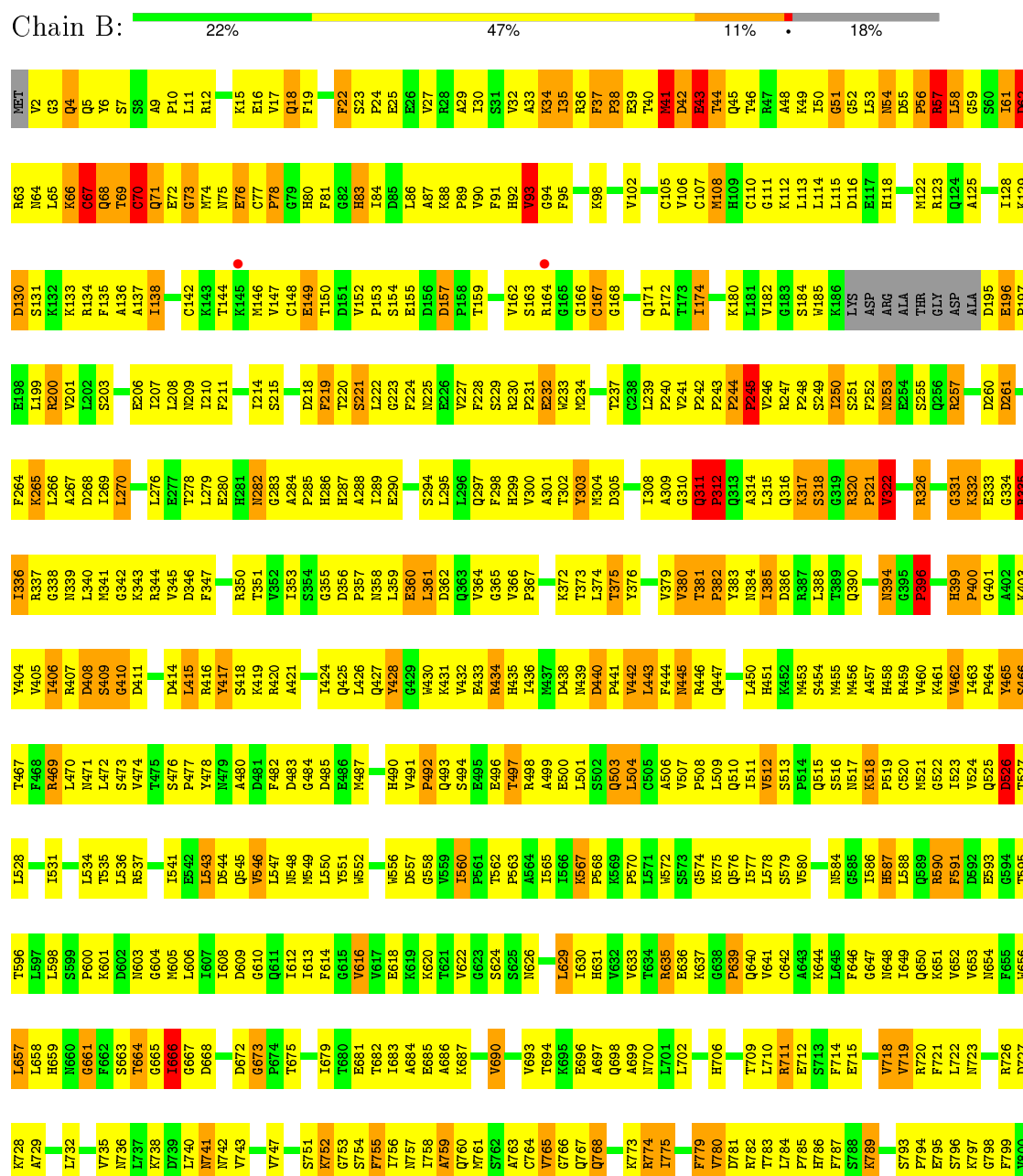
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	B	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

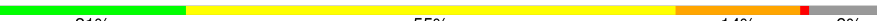
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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

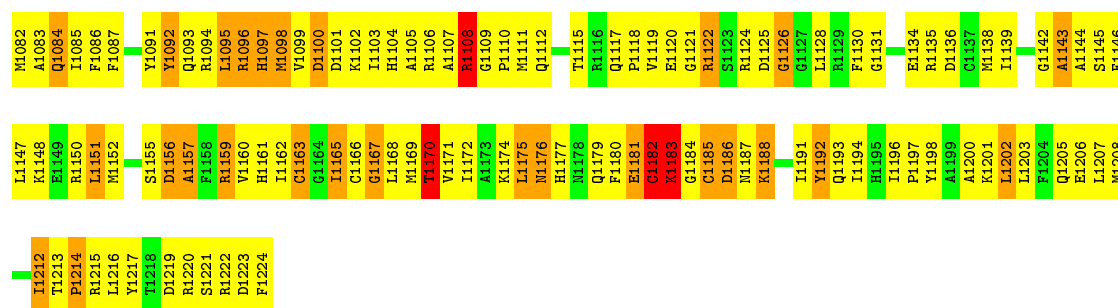


PRO	SER	SER	GLY	D1446	T1385	E1256	S1189	A1126	M1063	K1003	V937	I867	E801
SER	PRO	THR	PHE	E1447	R1386	M1259	L1192	D1127	V1064	M1004	R940	Y868	I802
THR	THR	ALA	THR	E1448	F1389	L1260	L1193	Q1128	G1065	I1006	R940	G869	S803
ALA	ALA	ALA	THR	V1451	M1390	K1261	R1194	Q1130	V1066	I1006	K941	E870	T804
THR	THR	THR	GLY		D1323	K1262	K1131	K1132	L1067	Q1008	F942	D871	L805
GLY	GLY	GLY	GLY		D1324	L1263	L1197	K1133	A1068	Q1008	L943	G872	R806
ALA	ALA	ALA	ALA		T1325	E1263	D1198	L1134		M1009	R944	M873	G807
ASP	ASP	ASP	ASP		R1326	E1265		L1134		A1010	E945	D874	L808
GLY	GLY	GLY	GLY		I1327	M1266	A1201		I1072	Q1011	V946	A875	T809
LYS	LYS	LYS	LYS		F1328	M1267	M1202		G1073	R1012	F947	A876	
ILE	ILE	ILE	THR		L1329	L1268		A1137	E1074	D1013	R877	H877	E812
THR	THR	THR	THR		M1330	E1269	K1205	I1138	A1076	A1015	V948	I878	F813
THR	THR	THR	THR		S1331	M1270	D1206	E1139	Q1076	V1016			F814
SER	SER	SER	SER		F1332	T1271	D1207	H1140	M1079	T1017	E851	Q881	F815
PRO	PRO	PRO	PRO		I1333	T1272	L1207	T1141	T1080	F1018	A852	S882	H816
THR	THR	THR	THR		G1401	T1273	M1209	T1142	L1081	A817	N953	L883	A817
GLY	GLY	GLY	GLY		F1402	R1273	K1274	K1143	ASN	C1019	P955	D884	M818
ASP	ASP	ASP	ALA		E1403	G1275	Q1211	S1145	THR	C1020	L956	T885	G819
GLY	GLY	GLY	THR		E1404	V1276	V1212	V1146	PHE	L1021	P957	I886	G820
GLN	GLN	GLN	THR		T1405	E1277	V1213	T1147	HIS	L1022	V958	G857	R821
ASP	ASP	ASP	GLY		E1407	M1278	E1214	I1148	PHE	S1024	N959	D890	I825
GLY	GLY	GLY	GLY		T1408	I1279	R1215	A1149	ALA	R1025	I960	D826	D826
VAL	VAL	VAL	PRO		L1409	E1280	Q1218	S1150	GLY	L1026	R962	R896	T827
THR	THR	THR	THR		E1411	V1282	T1219	I1152	ALA	A1027	I963	Y897	A828
PRO	PRO	PRO	SER		E1412	F1284	K1221	Y1153	SER	T1028	I964	R898	T829
GLY	GLY	GLY	THR		A1413	M1284	M1222	D1155	K1093	V1031	Q965	R899	R830
ASN	ASN	ASN	PHE		E1414	A1346	D1223	P1156	L1094	L1032	D900	L901	T831
GLU	GLU	GLU	GLY		S1415	A1347	D1224	D1157	T1095	E1033	Q968	L902	T834
SER	SER	SER	VAL		E1416	L1348	D1288	F1158	S1086	E1034	F971	T903	N903
SER	SER	SER	GLY		E1417	Y1349	E1289	P1158	Q1096	E1034	H972	T904	G835
PRO	PRO	PRO	LEU		L1418	K1390	V1226	A1159	R1036	T1037	D974	H906	R839
ALA	ALA	ALA	VAL		D1419	E1351	I1227	S1160	L1037	T1038	H975	T907	R840
GLN	GLN	GLN	GLY		R1420	F1352	M1228	T1161	L1101	K1039	T976	L908	
ASP	ASP	ASP	PHE		C1421	Y1353	S1229	V1163	L1102	Q1039	K977	L912	K843
ASP	ASP	ASP	PRO		R1422	M1354	E1230	I1163	E1103	Q1040	P978	L913	A844
LEU	LEU	LEU	THR		G1423	V1355	D1231	P1164	L1104	F1042	S979	L914	L845
ASP	ASP	ASP	THR		E1424	T1296	M1232	E1166	L1106	D1043	D980	E915	E846
VAL	VAL	VAL	VAL		S1425	E1297		D1167	N1107	W1044	L981	S915	D847
LYS	LYS	LYS	THR		E1426	Y1298	L1236	E1167	V1107	W1045	T982	G916	T848
ASP	ASP	ASP	THR		M1427	V1299	I1237	I1170	A1108	V1046	I983	I919	M849
GLU	GLU	GLU	THR		V1428	K1300	I1238		K1109	L1046	K984	L920	V850
LEU	LEU	LEU	SER		I1429	F1301	R1239	H1173	M1110	S1047	D985	L921	H851
MET	MET	MET	PRO		L1430	P1302	C1240	F1174	M1111	M1048	G921	L922	H852
PHE	PHE	PHE	THR		Q1431	E1303	R1241	S1175	K1112	I1049	V987	D922	D853
SER	SER	SER	SER		Q1432	M1368	V1242	L1176	T1113	E1050	L988	L923	T854
PRO	PRO	PRO	PRO		M1433	L1370	V1243	LEU	P1114	A1051	K924	K924	T855
ALA	ALA	ALA	ALA		A1434	L1371	ARG	ASP	S1115	Q1052	D982	L925	T856
LEU	LEU	LEU	THR		F1435	F1307	PRO	GLU	L1116	F1053	L993	Q926	H857
VAL	VAL	VAL	THR		I1436	T1308	LYS	GLU	T1117	L1054	Q994	V927	H858
ASP	ASP	ASP	PRO		D1437	D1309	SER	GLU	T1118	R1055	V1118	L928	S859
SER	SER	SER	THR		T1438	M1375	LEU	ALA	Y1119	S1056	N996	L929	L860
GLY	GLY	GLY	SER		G1439	T1376	ASP	GLU	GLN	V1057	L997	L932	G861
PRO	PRO	PRO	PRO		T1377	M1312	ALA	GLN	E1121	V1058	L998	E932	H862
ASN	ASN	ASN	THR		A1440	Q1378	GLY	THR	H1059	P1060	V999	Y933	V863
ASP	ASP	ASP	THR		F1441	T1379	THR	PHE	G1123	R1000	R934	L934	H864
ALA	ALA	ALA	TYR		D1442	G1379	GLU	ASP	H1124	Q1001	R935	L936	Q865
MET	MET	MET	PRO		V1443	E1380	GLU	Q1187	A1125	E1062	G1002		F866
M1444	M1444	M1444	ALA			V1316							
ALA	ALA	ALA	THR		I1445	M1317							

● Molecule 2: DNA-directed RNA polymerase II subunit RPB2

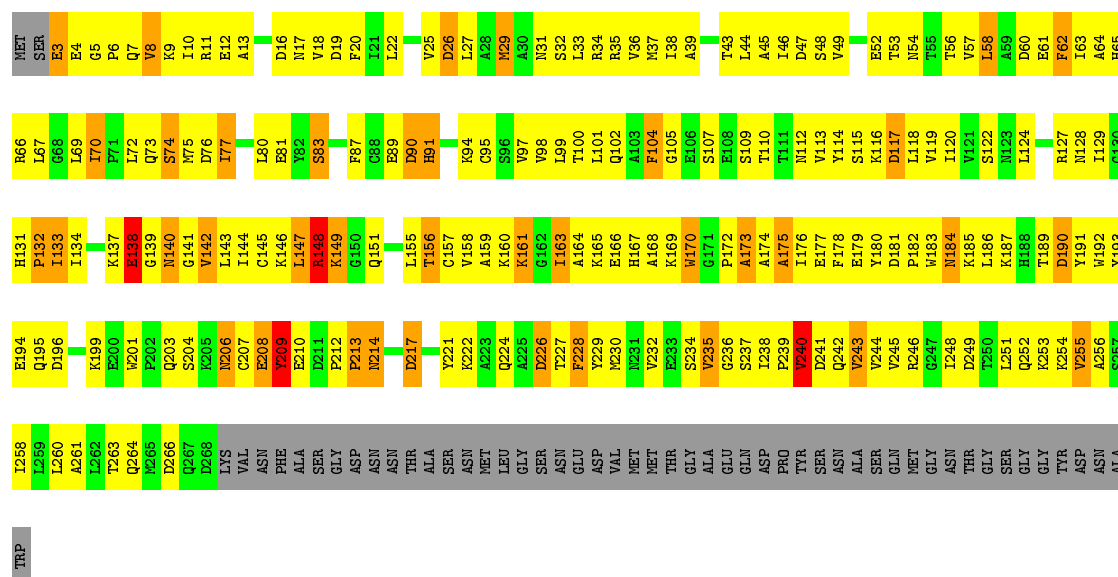
Chain C:  21% 55% 14% 9%





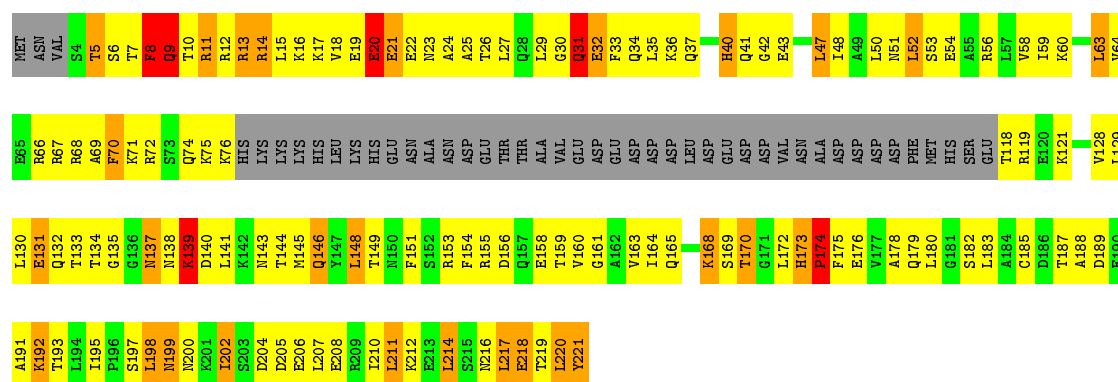
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain D: 21% 49% 12% 16%



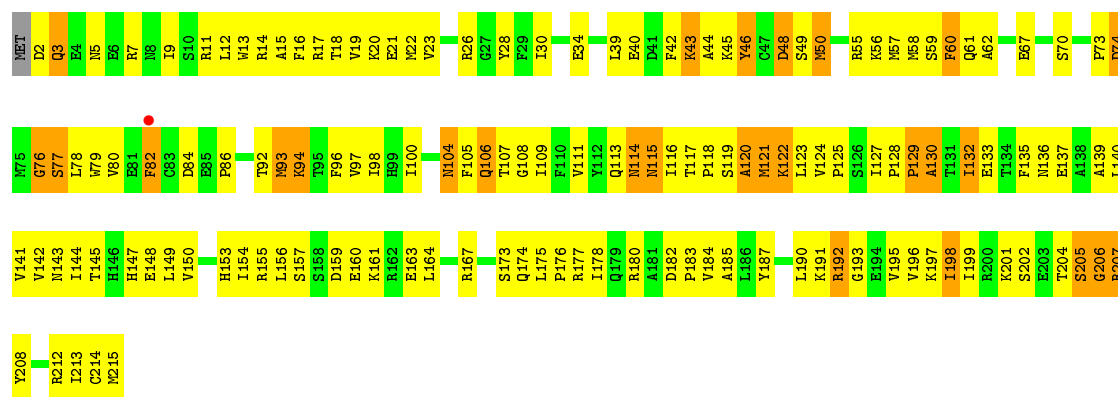
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain E: 19% 45% 13% 20%

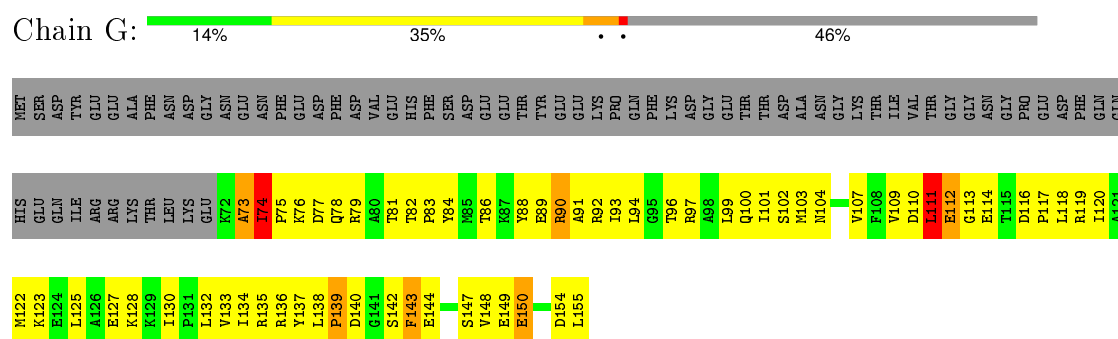


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

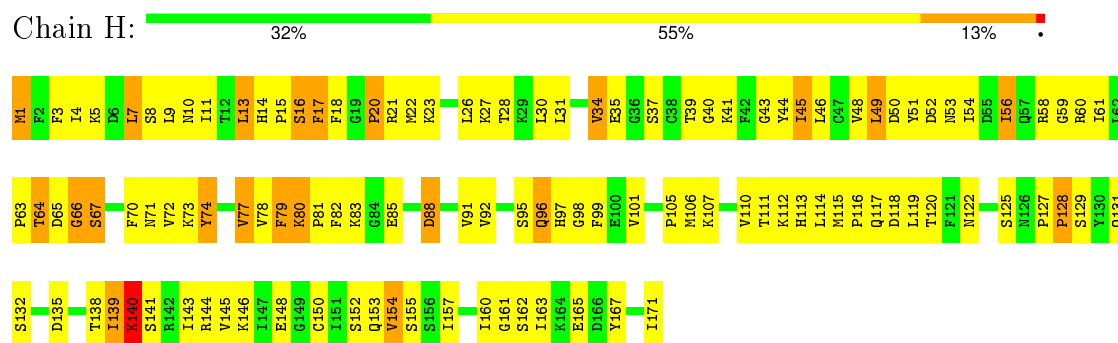
Chain F: 33% 53% 13%



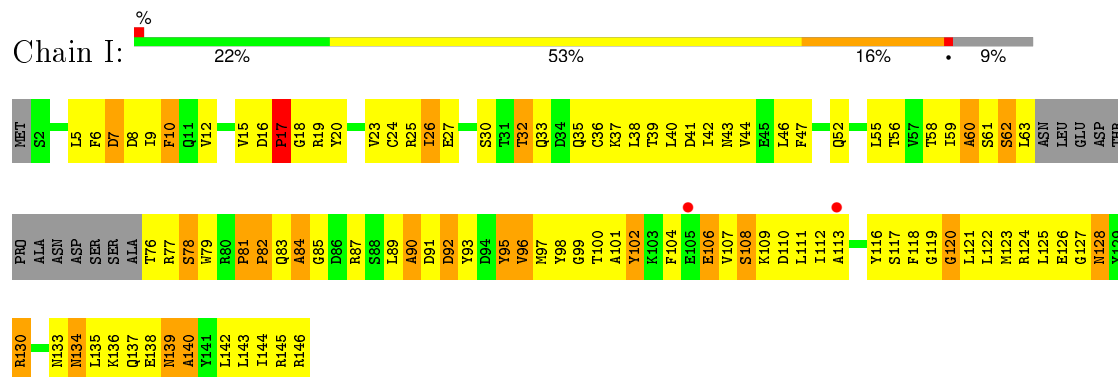
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



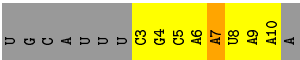
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



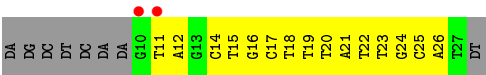
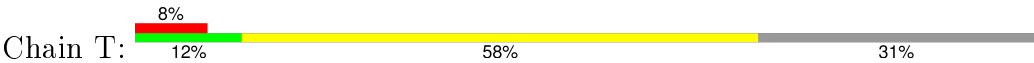
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Chain P: 



● Molecule 15: 5'-R(*UP*GP*CP*AP*UP*UP*UP*CP*GP*CP*AP*AP*UP*AP*AP*A)-3',



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	222.47Å 391.62Å 284.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 4.00 48.99 – 4.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-4.00) 100.0 (48.99-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 4.00Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.205 , 0.241 0.215 , 0.243	Depositor DCC
R_{free} test set	8343 reflections (7.99%)	DCC
Wilson B-factor (Å ²)	131.8	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 82.8	EDS
Estimated twinning fraction	0.024 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.024 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 202368 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	31777	wwPDB-VP
Average B, all atoms (Å ²)	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	B	0.43	0/11339	0.71	4/15334 (0.0%)
2	C	0.43	0/8981	0.69	1/12108 (0.0%)
3	D	0.43	0/2133	0.71	0/2891
4	E	0.43	0/1437	0.69	0/1925
5	F	0.42	0/1788	0.67	0/2406
6	G	0.48	0/691	0.77	0/933
7	H	0.47	0/1368	0.73	0/1844
8	I	0.41	0/1086	0.69	0/1470
9	J	0.40	0/989	0.66	0/1331
10	K	0.44	0/541	0.75	0/727
11	L	0.45	0/937	0.69	0/1265
12	M	0.48	0/366	0.72	0/485
13	N	0.70	0/154	0.88	0/235
14	P	0.55	0/188	0.94	0/291
15	T	0.42	0/407	0.95	0/627
All	All	0.44	0/32405	0.71	5/43872 (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
10	K	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	311	GLN	N-CA-C	5.60	126.11	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	56	PRO	N-CA-C	-5.54	97.71	112.10
1	B	425	GLN	N-CA-C	-5.38	96.48	111.00
2	C	1163	CYS	N-CA-C	-5.21	96.94	111.00
1	B	440	ASP	N-CA-C	-5.02	97.44	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	K	44	TYR	Sidechain

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	B	11140	0	11215	1481	0
2	C	8810	0	8847	1266	0
3	D	2095	0	2051	295	0
4	E	1427	0	1451	175	0
5	F	1752	0	1776	183	0
6	G	679	0	701	98	0
7	H	1340	0	1357	185	0
8	I	1068	0	1040	166	0
9	J	971	0	929	123	0
10	K	532	0	542	122	0
11	L	919	0	929	135	0
12	M	364	0	388	57	0
13	N	138	0	80	8	0
14	P	168	0	88	15	0
15	T	365	0	208	48	0
16	B	2	0	0	0	0
16	C	1	0	0	0	0
16	D	1	0	0	0	0
16	J	2	0	0	0	0
16	K	1	0	0	0	0
16	M	1	0	0	0	0
17	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	31777	0	31602	3977	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 63.

The worst 5 of 3977 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)
15:T:21:DA:C2'	15:T:22:DT:H5'	1.58	1.32
15:T:21:DA:H2''	15:T:22:DT:C5'	1.65	1.25
15:T:20:DT:C2'	15:T:21:DA:H5'	1.73	1.18
11:L:47:ARG:HH11	11:L:47:ARG:HB3	1.11	1.15
15:T:20:DT:H2'	15:T:21:DA:H5'	1.13	1.12

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 X-ray entries followed by that with respect to entries of similar resolution.

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	B	1406/1733 (81%)	965 (69%)	284 (20%)	157 (11%)	0	10
2	C	1090/1224 (89%)	719 (66%)	243 (22%)	128 (12%)	0	9
3	D	264/318 (83%)	163 (62%)	70 (26%)	31 (12%)	0	9
4	E	173/221 (78%)	107 (62%)	43 (25%)	23 (13%)	0	6
5	F	212/215 (99%)	154 (73%)	36 (17%)	22 (10%)	1	12
6	G	82/155 (53%)	62 (76%)	13 (16%)	7 (8%)	1	17
7	H	169/171 (99%)	129 (76%)	26 (15%)	14 (8%)	1	18
8	I	129/146 (88%)	79 (61%)	30 (23%)	20 (16%)	0	5
9	J	117/122 (96%)	80 (68%)	24 (20%)	13 (11%)	0	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	K	63/70 (90%)	38 (60%)	12 (19%)	13 (21%)	0	2
11	L	112/120 (93%)	81 (72%)	24 (21%)	7 (6%)	2	27
12	M	44/70 (63%)	22 (50%)	8 (18%)	14 (32%)	0	0
All	All	3861/4565 (85%)	2599 (67%)	813 (21%)	449 (12%)	0	9

5 of 449 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	4	GLN
1	B	41	MET
1	B	48	ALA
1	B	54	ASN
1	B	57	ARG

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 X-ray entries followed by that with respect to entries of similar resolution.

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	B	1239/1520 (82%)	1113 (90%)	126 (10%)	9	41
2	C	962/1061 (91%)	867 (90%)	95 (10%)	10	43
3	D	234/274 (85%)	209 (89%)	25 (11%)	8	39
4	E	159/200 (80%)	136 (86%)	23 (14%)	4	27
5	F	196/197 (100%)	182 (93%)	14 (7%)	18	58
6	G	74/137 (54%)	69 (93%)	5 (7%)	20	59
7	H	152/152 (100%)	136 (90%)	16 (10%)	8	40
8	I	117/128 (91%)	107 (92%)	10 (8%)	13	51
9	J	113/116 (97%)	103 (91%)	10 (9%)	12	48
10	K	60/65 (92%)	54 (90%)	6 (10%)	9	42
11	L	99/102 (97%)	84 (85%)	15 (15%)	3	25
12	M	40/57 (70%)	36 (90%)	4 (10%)	9	42
All	All	3445/4009 (86%)	3096 (90%)	349 (10%)	9	41

5 of 349 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	502	ILE
2	C	999	MET
9	J	99	LEU
2	C	544	CYS
2	C	790	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 106 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	366	GLN
2	C	821	GLN
9	J	12	ASN
2	C	465	ASN
2	C	538	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	7/16 (43%)	1 (14%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	7	A

There are no RNA pucker outliers to report.

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

Of 9 ligands modelled in this entry, 9 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

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	1416/1733 (81%)	-0.34	4 (0%) 94 92	76, 129, 175, 200	0
2	C	1108/1224 (90%)	-0.28	3 (0%) 94 92	79, 140, 185, 200	0
3	D	266/318 (83%)	-0.38	0 100 100	93, 126, 168, 188	0
4	E	177/221 (80%)	-0.31	0 100 100	106, 142, 182, 190	0
5	F	214/215 (99%)	-0.30	1 (0%) 91 88	99, 161, 187, 200	0
6	G	84/155 (54%)	-0.50	0 100 100	73, 107, 138, 147	0
7	H	171/171 (100%)	-0.31	0 100 100	98, 127, 164, 174	0
8	I	133/146 (91%)	0.07	2 (1%) 76 66	134, 165, 186, 196	0
9	J	119/122 (97%)	-0.28	0 100 100	122, 165, 189, 200	0
10	K	65/70 (92%)	-0.57	0 100 100	92, 121, 158, 169	0
11	L	114/120 (95%)	-0.37	0 100 100	94, 128, 156, 170	0
12	M	46/70 (65%)	0.02	0 100 100	120, 172, 195, 198	0
13	N	7/14 (50%)	1.41	2 (28%) 1 1	199, 200, 200, 200	1 (14%)
14	P	8/16 (50%)	0.14	0 100 100	198, 199, 200, 200	0
15	T	18/26 (69%)	0.84	2 (11%) 7 6	178, 199, 200, 200	1 (5%)
All	All	3946/4621 (85%)	-0.30	14 (0%) 93 90	73, 136, 184, 200	2 (0%)

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1176	LEU	4.0
13	N	7	DC	3.1
2	C	471	LYS	2.9
15	T	11	DT	2.7
13	N	6	DA	2.5

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
16	ZN	J	123	1/1	0.99	0.16	0.27	136,136,136,136	0
16	ZN	K	71	1/1	0.99	0.25	0.14	113,113,113,113	0
16	ZN	D	319	1/1	0.99	0.13	-0.66	98,98,98,98	0
16	ZN	B	1735	1/1	0.99	0.12	-1.49	110,110,110,110	0
16	ZN	M	71	1/1	0.98	0.05	-1.61	174,174,174,174	0
16	ZN	B	1734	1/1	0.99	0.04	-2.66	149,149,149,149	0
16	ZN	J	124	1/1	0.92	0.03	-2.80	200,200,200,200	0
17	MG	B	1736	1/1	0.86	0.10	-	153,153,153,153	0
16	ZN	C	1225	1/1	0.99	0.23	-	104,104,104,104	0

6.5 Other polymers [i](#)

There are no such residues in this entry.