



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:07 PM GMT

PDB ID : 1NIK
Title : Wild Type RNA Polymerase II
Authors : Bushnell, D.A.; Kornberg, R.D.
Deposited on : 2002-12-24
Resolution : 4.10 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

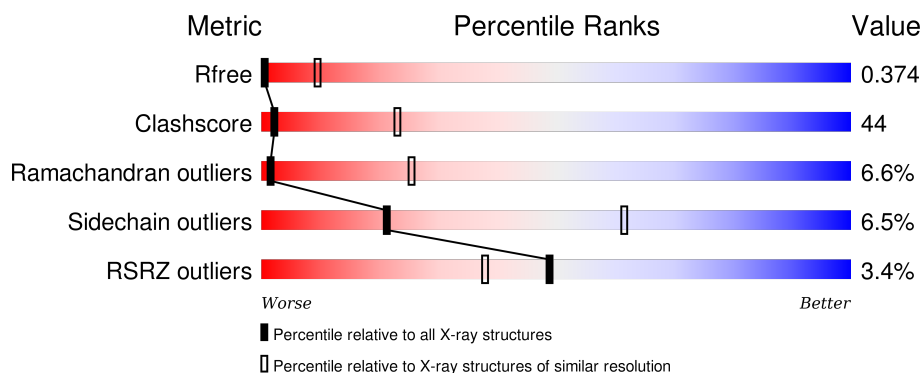
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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	1018 (4.60-3.60)
Clashscore	102246	1117 (4.60-3.60)
Ramachandran outliers	100387	1063 (4.60-3.60)
Sidechain outliers	100360	1049 (4.60-3.60)
RSRZ outliers	91569	1022 (4.60-3.60)

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	A	1733	 2% 32% 40% 7% 20%
2	B	1224	 3% 32% 51% 7% 10%
3	C	318	 2% 37% 40% 7% 16%
4	D	161	 91% 5% 5%
5	E	215	 5% 42% 55% 5% 5%

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Mol	Chain	Length	Quality of chain
6	F	155	<p>2% 18% 32% 46%</p>
7	G	170	<p>95% 5%</p>
8	H	146	<p>4% 30% 52% 9% 9%</p>
9	I	122	<p>11% 35% 51% 11% 2%</p>
10	J	70	<p>4% 31% 51% 9% 7%</p>
11	K	120	<p>1% 41% 50% 5% 3%</p>
12	L	70	<p>7% 17% 33% 13% 34%</p>

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 28295 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 RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1388	Total	C	N	O	S	0	0	7
			10864	6858	1899	2046	61			

- Molecule 2 is a protein called ORF YOR151c.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1097	Total	C	N	O	S	0	0	0
			8721	5526	1523	1618	54			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	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, chain RPB4.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	D	153	Total C 153 153	0	0	153

- Molecule 5 is a protein called DNA-directed RNA polymerase II, chain RPB5.

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

- Molecule 6 is a protein called DNA-directed RNA polymerase I, II and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	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, chain RPB7.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
7	G	170	Total	C	0	0	170
			170	170			

- Molecule 8 is a protein called DNA-directed RNA polymerase subunit RPB8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	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, chain RPB9.

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

- Molecule 10 is a protein called DNA-directed RNA polymerase II, chain RPB10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	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, chain RPB11.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II, chain RPB12.

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

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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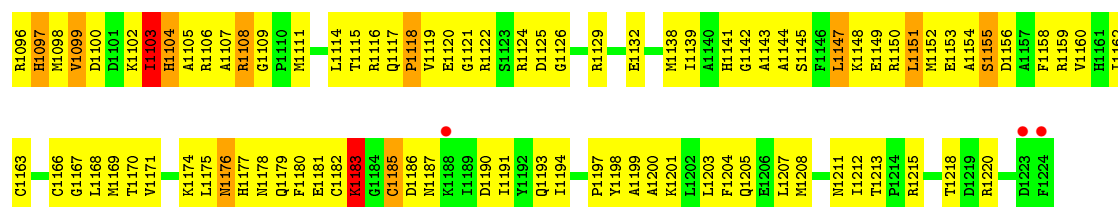
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	C	1	Total 1	Zn 1	0	0
13	J	1	Total 1	Zn 1	0	0
13	I	2	Total 2	Zn 2	0	0

GLU	ASN	PRO	SER	ASP	A1416	V1352	R1281	R1215	A1149	ASN	G1019	Y933	Q855	P794
THR	THR	THR	PRO	LEU	E417	I1356	V1282	I1216	S1150	THR	G1020	Y936	F866	E795
LYS	SER	TYR	THR	ASP	L1418	I1355	M1283	I1217	E1151	PHE	L1021	L936	I867	
ASN	PRO	PRO	PRO	VAL	D1419	I1356	M1284	Q1218	I1152	HIS	L1022	L940	Y868	S803
GLU	PRO	PRO	LYS	LYS	C1421	D1359	S1293	T1219	Y1153	PHE	S1024	R940	Q869	Y804
ASN	TYR	THR	ASP	ASP		G1360	P1294	F1220	Y1154	ALA	R1025	L943	E870	L808
PRO	PRO	TYR	LEU	LEU	V1424	S1361	P1294	K1221	D1155	GLY	R1025		D871	
ASN	PRO	SER	LEU	LEU	S1425	Y1362	T1295	M1222	P1158	VAL	L1026		Q872	T809
ASN	TYR	THR	PHE	PHE		V1363	G1296	L1223	R1159	ALA	A1027	Y948	M873	P810
SER	TYR	THR	THR	THR	V1428	Y1364	E1297	L1224	S1160	SER	R1028	D949	D874	
PRO	PRO	PRO	PRO	PRO	L1429	Y1365	E1298	F1225	T1161	K1092	T1029		A875	F813
THR	THR	THR	ALA	LEU	L1430	R1366	V1299	V1226	T1162	R1093	R1030	A952		F814
SER	SER	SER	VAL	VAL	G1431	K1367	K1300	I1227	V1162	V1094	R1031	A954		F815
PRO	PRO	PRO	ASP	ASP	Q1432	M1368		M1228	I1163	T1095	L1032	P955		H816
THR	THR	THR	SER	SER		A1369	V1305	N1232	D1166	S1096		P957		A817
SER	TYR	THR	GLY	GLY	P1435	V1372	L1306		E1167	G1097	Y1035	P957		Q880
PRO	TYR	THR	SER	SER	I1436	T1308	E1307	L1236	E1168	V1098	L1036	P957		Q880
PRO	PRO	PRO	ASN	ASN	G1437	V1374	T1309	I1237	E1169	P1099	L1037	P957		Q881
TYR	THR	THR	THR	ASP	T1438	M1375	G1310	I1238	I1170	R1100	T1038	P959		G820
PRO	PRO	PRO	ALA	ALA	G1439	T1376	G1311	R1239	Q1171	L1101	K1039	P960		T885
PRO	PRO	PRO	MET	MET	F1440	T1377	N1312	C1240	L1172	K1102	A1041	R961		E822
THR	THR	THR	ALA	ALA	F1441	Q1378	L1313	R1241	H1173	E1103	F1042	R962		E823
SER	TYR	THR	GLY	GLY	D1442	G1379	S1314	V1242	F1174	I1104	D1043	R963		L824
PRO	PRO	PRO	PHE	PHE	V1443	E1380	E1315	M1243	S1175	L1105	H1044	R964		L825
TYR	THR	THR	ALA	ALA	M1444	L1381	M1316	ARG	L1176		Y1045	Q965		D826
SER	TYR	THR	ALA	ALA	I1445	T1382	M1317	PRO	LEU	A1108		Q968		T827
PRO	PRO	PRO	TYR	TYR	D1446	S1383	T1318	LYS	ASP	L1046		Q968		A828
PRO	PRO	PRO	TYR	TYR	K1452	V1384	V1319	SER	GLU	L1047		Q968		A829
PRO	PRO	PRO	GLY	GLY	THR	M1385	P1320	LEU	GLU	N1048		R896		R830
PRO	PRO	PRO	GLY	GLY	THR	R1386	G1321	ASP	ALA	R897		R896		T831
ASN	ASN	ASN	ALA	ALA	THR	H1387	I1322	ALA	GLU	R898		R898		T834
PRO	PRO	PRO	ASP	ASP	PRO	G1388	D1323	GLU	GLN	R899		R899		G835
THR	THR	THR	TYR	TYR	PRO	F1389	P1324	THR	SER	S979		D980		T837
PRO	PRO	PRO	GLN	GLN	PRO	N1390	T1325	GLU	GLU	L1054		L901		T836
PRO	PRO	PRO	LYS	LYS	THR	R1391	R1326	A1254	ASP	R1055		N903		T837
THR	THR	THR	ILE	ILE	THR	S1392	I1327	E1255	Q1187	S1056				T840
PRO	PRO	PRO	THR	THR	THR	M1393	Y1328	E1256	Q1188	Y1057				L841
PRO	PRO	PRO	ILE	ILE	GLU	T1394	T1329	D1257	S1189	V1058				Y842
PRO	PRO	PRO	ILE	ILE	PRO	G1395	M1330	H1258	P1190	D985				R843
TYR	TYR	TYR	GLY	PHE	GLU	A1396	S1331	M1259	W1191	H1059				A844
SER	SER	SER	GLY	GLY	ASP	L1397	F1332	L1260	L1192	P1060				L845
PRO	PRO	PRO	ALA	ALA	TYR	M1398	I1333	K1261	L1193	E1062				E846
PRO	PRO	PRO	TYR	TYR	GLY	R1399	D1334	K1262	R1194	L913				D847
PRO	PRO	PRO	GLY	GLY	ASP	C1400	I1335	I1263	A1195	M1063				E914
PRO	PRO	PRO	GLY	GLY	GLY	S1401	M1336	E1264	E1196	V1064				L848
GLY	GLY	GLY	ALA	ALA	GLY	F1402			Y1197	G1065				S915
TYR	TYR	TYR	VAL	VAL	VAL	E1403	L1339	M1267		V1066				E918
PRO	PRO	PRO	THR	THR	PRO	E1404	G1340	L1268	L1134	L1067				Y850
PRO	PRO	PRO	PRO	PRO	PRO	T1405	I1341	E1269	R1135	A1068				H851
PRO	PRO	PRO	PRO	PRO	PRO	V1406	E1342	M1270	R1135	A1069				L920
TYR	TYR	TYR	THR	THR	THR	E1407	A1343	I1271		G1002				D853
PRO	PRO	PRO	PHE	PHE	ASN	I1408	G1344	T1272	T1138	K1003				H854
PRO	PRO	PRO	GLY	GLY	GLU	L1409	R1345	L1273	H1140	M1004				T855
THR	THR	THR	VAL	VAL	VAL	A1346	A1347	M1209	T1142	Q1008				R857
GLY	GLY	GLY	SER	SER	SER	F1411	A1347	G1210	L1143	A1014				Y927
PRO	PRO	PRO	SER	SER	LEU	A1412	L1348	Q1211	V1146	V1015				L928
LYS	LYS	LYS	PRO	PRO	VAL	G1413	Y1349	T1212	T1147	T1016				L929
GLN	GLN	GLN	ASN	ASN	ASN	A1414	K1350	G1213	T1147	T1016				D930
ASP	ASP	ASP	SER	PHE	ALA	S1415	E1351	E1214	I1148	F1018				Y863

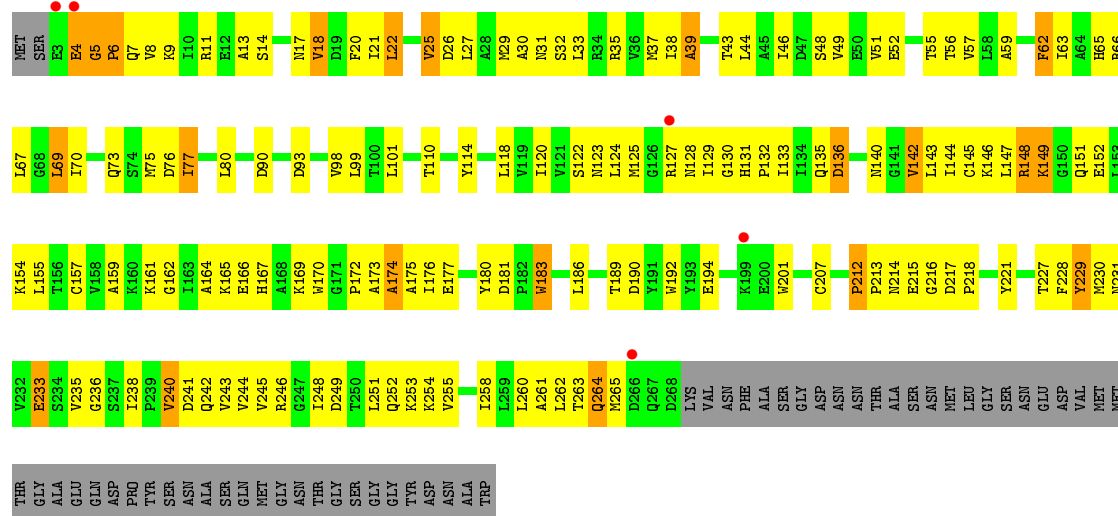
• Molecule 2: ORF YOR151c



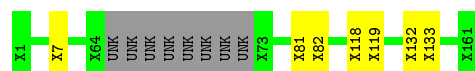
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V1023	G960	G997	G832	H761	A630	I554	L483	D407	ARG	T268	M199	K133	I70	SER
A1024	L961	L898	Y833	I762	B631	I555	L484	L408	ARG	T269	G201	K134	LEU	ASP
L1030	K962	I899	N834	I763	B632	T556	N483	L409	GLY	R270	G201	ARG	LEU	LEU
K1033	F963	P901	Q835	S764	V633	F557	R485	G410	THR	A271	F203	THR	GLN	ALA
V1034	K964	P901	E836	P765	B634	L558	Y486	G411	ALA	P274	Y202	THR	GLN	ASN
S1035	K965	R904	D837	Q770	B635	S559	T487	F417	LEU	P275	I204	GLU	LEU	SER
G1038	R966	V905	S838	Q770	B636	Q562	Y488	K418	GLY	I276	I205	ALA	LEU	GLU
G1039	R967	S906	M839	M773	B637	Q563	S489	T419	ILE	I277	N206	ALA	GLN	LYS
M1040	T970	G907	M841	M773	B638	Q563	S489	T420	LYS	I278	G207	ASP	HIS	TYR
D1043	I973	E908	N842	M778	B639	L566	R486	F421	GLY	I279	S208	VAL	THR	TYR
A1044	P974	D909	Q843	M778	B640	E567	N489	K423	GLU	I280	E209	PRO	THR	ASP
A1045	Q975	V910	S844	M779	B641	E567	T500	K424	GLY	I281	V211	ARG	SER	ASP
G1046	R976	I911	S845	V781	B642	V570	P501	T425	GLU	I282	L212	GLU	ASP	PRO
S1045	G977	I912	S846	L782	B643	H572	I502	K426	LEU	I283	G214	LEU	ASN	TYR
P1046	D978	G913	D847	T783	B644	P571	F502	T427	ASP	I284	L213	GLY	ILE	GLY
D1049	K979	K914	R848	N784	G647	Q573	ARG	D428	GLY	I285	Q215	TYR	SER	PHE
I1050	F980	T915	G849	N784	H648	Q574	ASP	F429	GLY	I286	E216	GLU	ARG	GLU
V1051	L981	T916	L850	V787	B649	P575	GLY	R430	GLY	I287	R217	LEU	LYS	D20
T1052	S982	I918	F851	R788	B650	D576	LYS	F431	LYS	I288	N221	ALA	TYR	D21
V1053	R983	S919	F855	M789	B651	A577	LEU	N432	LEU	I289	V225	GLU	GLU	S22
E1054	H984	ASP	R857	D790	B652	T578	ASP	A509	ASP	I290	F226	GLU	GLU	A23
G1054	K985	PRO	R857	M791	B653	R579	GLY	T435	GLU	I291	Y226	GLU	GLU	P24
I1055	Q866	GLU	S858	A793	B654	V580	ASP	V436	GLU	I292	F226	SER	GLU	I25
S1056	K987	GLU	T859	I794	B655	P581	GLY	V437	GLU	I293	K227	GLU	GLU	I26
K1057	G991	GLU	B659	N795	B656	V582	LYS	A447	GLU	I294	Y227	ASP	ASP	A27
L1059	R991	GLY	L860	L796	B657	V582	LYS	A448	GLU	I295	G228	ASP	ASP	E28
R1060	I992	GLN	K864	T798	B658	P582	ASP	A449	GLU	I296	A239	SER	SER	D29
E1061	T993	ARG	K865	V799	B659	G584	ASP	A450	GLU	I297	A230	GLU	GLU	T98
I1062	I994	THR	R866	Q800	B660	V585	ASP	A451	GLU	I298	P231	GLU	GLU	S30
G1063	R995	ALA	Y866	K801	B661	V586	ASN	A452	GLU	I299	S232	SER	GLY	I31
Q1064	R996	THR	S869	L802	B662	G588	ASN	A453	GLU	I300	P233	GLY	GLY	I31
Y1065	E997	HIS	L870	L803	B663	V589	MET	A454	GLU	I301	I234	SER	GLY	I31
S1066	D998	S933	T871	G804	B664	H590	LYS	A455	GLU	I302	G235	GLY	GLY	I31
R1067	M999	K834	E872	T805	B665	P593	LYS	A456	GLU	I303	H236	GLU	GLU	I31
G1068	P1000	R935	T873	T806	B666	R601	LYS	A457	GLU	I304	V237	GLU	GLU	I31
F1069	F1001	D936	F874	R807	B667	T602	LYS	A458	GLU	I305	A238	GLU	GLU	I31
E1070	T1002	A937	E875	A808	B668	L603	LYS	A459	GLU	I306	E239	GLU	GLU	I31
V1071	A1003	S938	K876	M809	B669	R604	LYS	A460	GLU	I307	R240	GLU	GLU	I31
M1072	E1004	GLY	P877	E810	B670	G605	LYS	A461	GLU	I308	A242	GLU	GLU	I31
Y1073	G1005	L941	Q878	L811	B671	L609	LYS	A462	GLU	I309	L244	GLU	GLU	I31
T1077	V1007	T944	R879	L812	B672	T609	LYS	A463	GLU	I310	G247	GLU	GLU	I31
K1078	P1008	E945	N881	F814	B673	E612	LYS	A464	GLU	I311	S248	GLU	GLU	I31
K1079	D1009	N946	T882	R815	B674	V613	LYS	A465	GLU	I312	R249	GLU	GLU	I31
K1080	L1010	G947	L883	R815	B675	S614	LYS	A466	GLU	I313	F250	GLU	GLU	I31
L1081	I1011	I948	R884	P818	B676	S615	LYS	A467	GLU	I314	T253	GLU	GLU	I31
Q1084	M1012	V949	M885	Q821	B677	L616	LYS	A468	GLU	I315	G256	GLU	GLU	I31
I1085	P1014	Q951	K886	N822	B678	R617	LYS	A469	GLU	I316	V256	GLU	GLU	I31
F1086	H1015	V952	H887	A823	B679	D618	LYS	A470	GLU	I317	K257	GLU	GLU	I31
F1087	L1016	L953	G888	A823	B680	I619	LYS	A471	GLU	I318	L258	GLU	GLU	I31
I1017	G1016	T899	T899	V825	B681	V619	LYS	A472	GLU	I319	Y259	GLU	GLU	I31
P1018	P1018	V954	Y890	V825	B682	L624	LYS	A473	GLU	I320	G260	GLU	GLU	I31
S1019	S1019	T955	D891	A826	B683	K625	LYS	A474	GLU	I321	R261	GLU	GLU	I31
R1094	R1094	T956	R892	I827	B684	L626	LYS	A475	GLU	I322	G263	GLU	GLU	I31
L1095	M1021	Q958	L893	Y830	B685	T627	LYS	A476	GLU	I323	G263	GLU	GLU	I31
										I324				
										I325				
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										I374				
										I375				
										I376				
										I377				
										I378				
										I379				
										I380				
										I381				
										I382				
										I383				
										I384				
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										I395				
										I396				
										I397				
										I398				
										I399				
										I400				
										I401				
										I402				



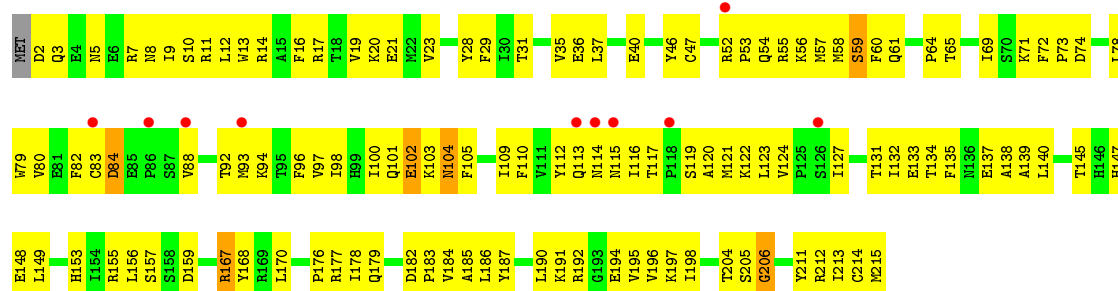
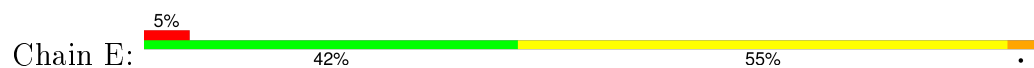
• Molecule 3: DNA-directed RNA polymerase II, chain RPB3



• Molecule 4: DNA-directed RNA polymerase II, chain RPB4

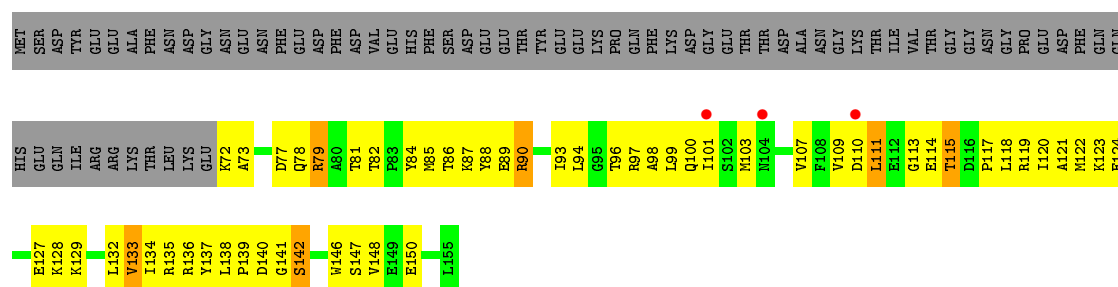


• Molecule 5: DNA-directed RNA polymerase II, chain RPB5



• Molecule 6: DNA-directed RNA polymerase I, II and III 23 kDa polypeptide





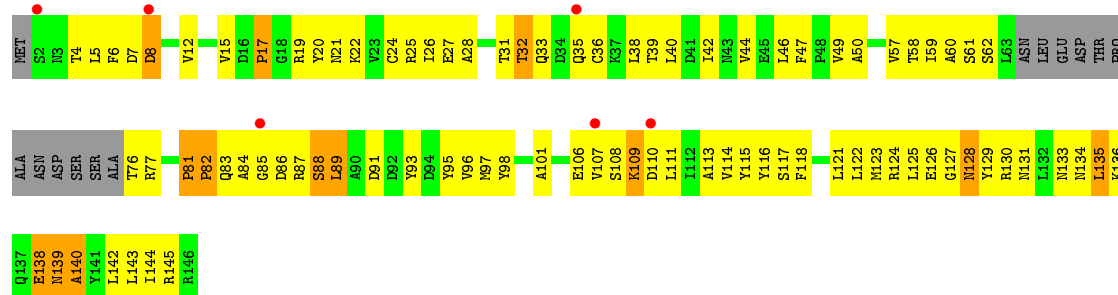
- Molecule 7: DNA-directed RNA polymerase II, chain RPB7

Chain G: 95% 5%



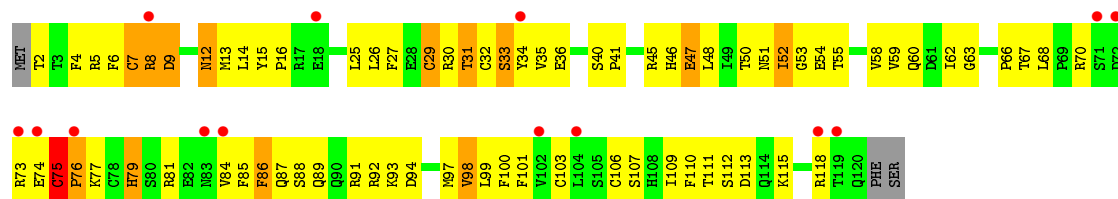
- Molecule 8: DNA-directed RNA polymerase subunit RPB8

Chain H: 4% 30% 52% 9% 9%



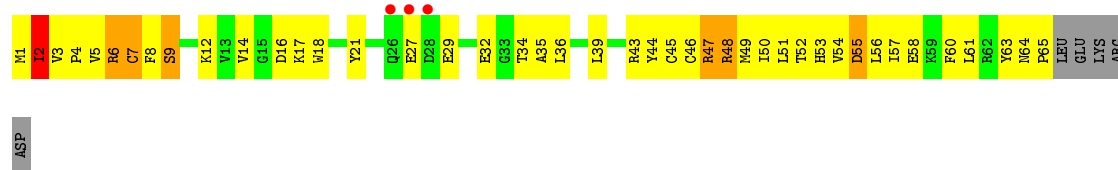
- Molecule 9: DNA-directed RNA polymerase II, chain RPB9

Chain I: 11% 35% 51% 11%

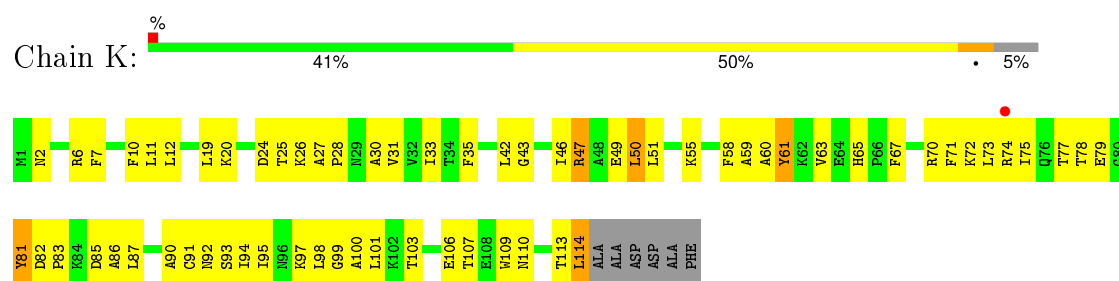


- Molecule 10: DNA-directed RNA polymerase II, chain RPB10

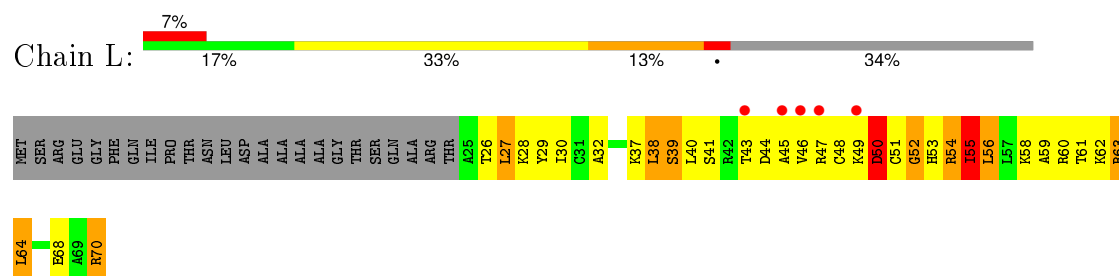
Chain J: 4% 31% 51% 9% 7%



- Molecule 11: DNA-directed RNA polymerase II, chain RPB11



- Molecule 12: DNA-directed RNA polymerase II, chain RPB12



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	224.10Å 394.46Å 284.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 4.10 39.97 – 4.11	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-4.10) 86.4 (39.97-4.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 4.13Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.334 , 0.360 0.351 , 0.374	Depositor DCC
R_{free} test set	3272 reflections (4.02%)	DCC
Wilson B-factor (Å ²)	114.0	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 168.4	EDS
Estimated twinning fraction	0.044 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.047 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 96816 reflections	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	28295	wwPDB-VP
Average B, all atoms (Å ²)	194.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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

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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/11048	0.71	6/14936 (0.0%)
2	B	0.46	0/8891	0.71	1/11990 (0.0%)
3	C	0.48	0/2133	0.76	2/2891 (0.1%)
5	E	0.37	0/1788	0.65	0/2406
6	F	0.40	0/691	0.64	0/933
8	H	0.40	0/1086	0.73	0/1470
9	I	0.48	0/989	0.76	1/1331 (0.1%)
10	J	0.53	0/541	0.78	0/727
11	K	0.46	0/937	0.68	0/1265
12	L	0.49	0/366	0.78	0/485
All	All	0.44	0/28470	0.71	10/38434 (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
2	B	0	1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1392	SER	N-CA-C	6.34	128.13	111.00
3	C	39	ALA	N-CA-C	6.06	127.35	111.00
1	A	398	GLU	N-CA-C	-5.77	95.43	111.00
3	C	183	TRP	N-CA-C	-5.61	95.86	111.00
2	B	647	GLY	N-CA-C	5.22	126.15	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	811	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	A	10864	0	10959	1032	1
2	B	8721	0	8746	900	0
3	C	2095	0	2052	162	1
4	D	153	0	0	4	0
5	E	1752	0	1776	129	0
6	F	679	0	701	66	0
7	G	170	0	0	5	0
8	H	1068	0	1040	134	0
9	I	971	0	933	101	0
10	J	532	0	544	77	0
11	K	919	0	929	84	0
12	L	364	0	390	50	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	1	0
13	J	1	0	0	1	0
All	All	28295	0	28070	2499	1

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 44.

The worst 5 of 2499 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)
4:D:132:UNK:CA	4:D:133:UNK:CA	2.01	1.36
12:L:60:ARG:HG3	12:L:61:THR:H	1.05	1.17
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.18	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:111:THR:HG22	9:I:113:ASP:H	1.05	1.14
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	1.65	1.11

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:LYS:NZ	3:C:90:ASP:N[4_555]	1.74	0.46

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	A	1365/1733 (79%)	1022 (75%)	251 (18%)	92 (7%)	1	25
2	B	1077/1224 (88%)	839 (78%)	169 (16%)	69 (6%)	2	26
3	C	264/318 (83%)	208 (79%)	40 (15%)	16 (6%)	2	27
5	E	212/215 (99%)	170 (80%)	33 (16%)	9 (4%)	3	36
6	F	82/155 (53%)	64 (78%)	15 (18%)	3 (4%)	4	40
8	H	129/146 (88%)	93 (72%)	21 (16%)	15 (12%)	0	9
9	I	117/122 (96%)	93 (80%)	15 (13%)	9 (8%)	1	20
10	J	63/70 (90%)	47 (75%)	12 (19%)	4 (6%)	2	27
11	K	112/120 (93%)	96 (86%)	15 (13%)	1 (1%)	21	67
12	L	44/70 (63%)	22 (50%)	13 (30%)	9 (20%)	0	2
All	All	3465/4173 (83%)	2654 (77%)	584 (17%)	227 (7%)	1	25

5 of 227 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	A	48	ALA
1	A	55	ASP
1	A	56	PRO
1	A	74	MET

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	A	1206/1520 (79%)	1128 (94%)	78 (6%)	21	61
2	B	952/1061 (90%)	886 (93%)	66 (7%)	19	59
3	C	234/274 (85%)	222 (95%)	12 (5%)	29	68
5	E	196/197 (100%)	189 (96%)	7 (4%)	42	76
6	F	74/137 (54%)	68 (92%)	6 (8%)	15	53
8	H	117/128 (91%)	112 (96%)	5 (4%)	35	72
9	I	113/116 (97%)	104 (92%)	9 (8%)	15	53
10	J	60/65 (92%)	56 (93%)	4 (7%)	20	60
11	K	99/102 (97%)	90 (91%)	9 (9%)	12	47
12	L	40/57 (70%)	35 (88%)	5 (12%)	6	32
All	All	3091/3657 (84%)	2890 (94%)	201 (6%)	21	61

5 of 201 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	261	ARG
2	B	644	GLU
10	J	47	ARG
2	B	309	GLN
2	B	466	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	325	GLN
2	B	538	ASN
9	I	12	ASN
2	B	363	HIS
2	B	513	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 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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	A	1388/1733 (80%)	-0.05	42 (3%) 54 41	20, 181, 283, 321	0
2	B	1097/1224 (89%)	0.01	31 (2%) 56 45	74, 189, 297, 321	0
3	C	266/318 (83%)	0.00	5 (1%) 70 60	87, 180, 262, 321	0
4	D	0/161	-	-	-	-
5	E	214/215 (99%)	0.21	10 (4%) 35 27	88, 223, 305, 321	0
6	F	84/155 (54%)	0.08	3 (3%) 46 36	90, 163, 254, 321	0
7	G	0/170	-	-	-	-
8	H	133/146 (91%)	0.41	6 (4%) 37 28	139, 242, 318, 321	0
9	I	119/122 (97%)	0.74	14 (11%) 6 6	139, 241, 318, 321	0
10	J	65/70 (92%)	-0.12	3 (4%) 36 27	68, 173, 284, 313	0
11	K	114/120 (95%)	-0.04	1 (0%) 85 79	98, 170, 245, 304	0
12	L	46/70 (65%)	0.24	5 (10%) 7 6	134, 233, 304, 321	0
All	All	3526/4504 (78%)	0.04	120 (3%) 49 38	20, 189, 294, 321	0

The worst 5 of 120 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	114	LEU	5.5
2	B	715	ALA	5.2
1	A	199	LEU	4.8
3	C	4	GLU	4.5
2	B	869	SER	4.5

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
13	ZN	I	203	1/1	0.90	0.18	-0.86	172,172,172,172	0
13	ZN	A	1735	1/1	0.90	0.12	-1.14	172,172,172,172	0
13	ZN	C	319	1/1	0.94	0.07	-1.15	172,172,172,172	0
13	ZN	I	204	1/1	0.93	0.23	-1.45	172,172,172,172	0
13	ZN	J	101	1/1	0.94	0.12	-1.90	172,172,172,172	0
13	ZN	A	1734	1/1	0.94	0.16	-2.14	172,172,172,172	0
13	ZN	B	1307	1/1	0.99	0.06	-	172,172,172,172	0

6.5 Other polymers [i](#)

There are no such residues in this entry.