



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 25, 2026 – 02:22 AM UTC

PDB ID : 3H0G / pdb_00003h0g
Title : RNA Polymerase II from Schizosaccharomyces pombe
Authors : Spahr, H.; Calero, G.; Bushnell, D.A.; Kornberg, R.D.
Deposited on : 2009-04-09
Resolution : 3.65 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

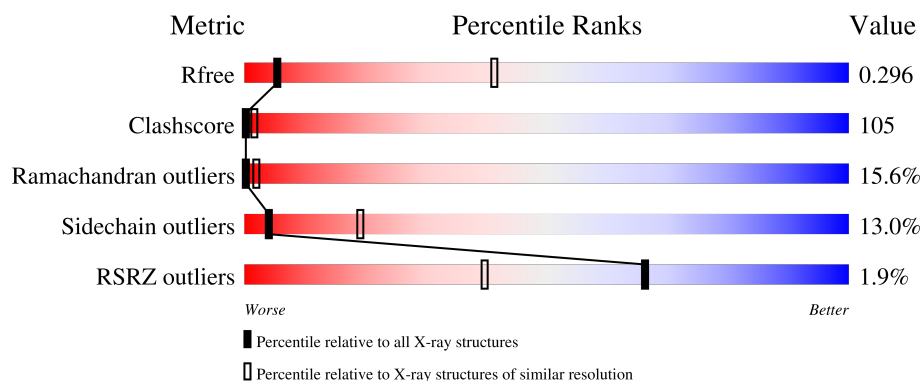
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.65 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}	180053	1062 (3.78-3.54)
Clashscore	190562	1009 (3.76-3.56)
Ramachandran outliers	187476	1054 (3.78-3.54)
Sidechain outliers	187428	1052 (3.78-3.54)
RSRZ outliers	180081	1061 (3.78-3.54)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1752	
1	M	1752	
2	B	1210	
2	N	1210	
3	C	297	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	O	297	
4	D	135	
4	P	135	
5	E	210	
5	Q	210	
6	F	142	
6	R	142	
7	G	172	
7	S	172	
8	H	125	
8	T	125	
9	I	113	
9	U	113	
10	J	71	
10	V	71	
11	K	123	
11	W	123	
12	L	63	
12	X	63	

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 62870 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	A	1496	Total	C	N	O	S	0	0	0
			11802	7415	2071	2246	70			
1	M	1476	Total	C	N	O	S	0	0	0
			11666	7334	2047	2216	69			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1150	Total	C	N	O	S	0	0	0
			9180	5772	1630	1716	62			
2	N	1150	Total	C	N	O	S	0	0	0
			9180	5772	1630	1716	62			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	263	Total	C	N	O	S	0	0	0
			2088	1315	355	406	12			
3	O	263	Total	C	N	O	S	0	0	0
			2088	1315	355	406	12			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit rpb4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	130	Total	C	N	O	S	0	0	0
			1036	649	176	205	6			
4	P	130	Total	C	N	O	S	0	0	0
			1036	649	176	205	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	207	Total	C	N	O	S	0	0	0
			1663	1050	301	306	6			
5	Q	207	Total	C	N	O	S	0	0	0
			1663	1050	301	306	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	83	Total	C	N	O	S	0	0	0
			656	416	112	125	3			
6	R	83	Total	C	N	O	S	0	0	0
			656	416	112	125	3			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit rpb7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	170	Total	C	N	O	S	0	0	0
			1330	860	217	247	6			
7	S	170	Total	C	N	O	S	0	0	0
			1330	860	217	247	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	124	Total	C	N	O	S	0	0	0
			996	631	167	195	3			
8	T	124	Total	C	N	O	S	0	0	0
			996	631	167	195	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	111	Total	C	N	O	S	0	0	0
			902	551	164	176	11			
9	U	111	Total	C	N	O	S	0	0	0
			902	551	164	176	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	64	Total	C	N	O	S	0	0	0
			518	330	87	94	7			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	V	64	Total	C	N	O	S	0	0	0
			518	330	87	94	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	119	Total	C	N	O	S	0	0	0
			955	608	159	182	6			
11	W	119	Total	C	N	O	S	0	0	0
			955	608	159	182	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	45	Total	C	N	O	S	0	0	0
			368	225	74	61	8			
12	X	45	Total	C	N	O	S	0	0	0
			368	225	74	61	8			

- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	2	Total	Zn	0	0
			2	2		
13	B	1	Total	Zn	0	0
			1	1		
13	C	1	Total	Zn	0	0
			1	1		
13	I	2	Total	Zn	0	0
			2	2		
13	J	1	Total	Zn	0	0
			1	1		
13	L	1	Total	Zn	0	0
			1	1		
13	M	2	Total	Zn	0	0
			2	2		
13	N	1	Total	Zn	0	0
			1	1		
13	O	1	Total	Zn	0	0
			1	1		
13	U	2	Total	Zn	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	V	1	Total 1	Zn 1	0	0
13	X	1	Total 1	Zn 1	0	0

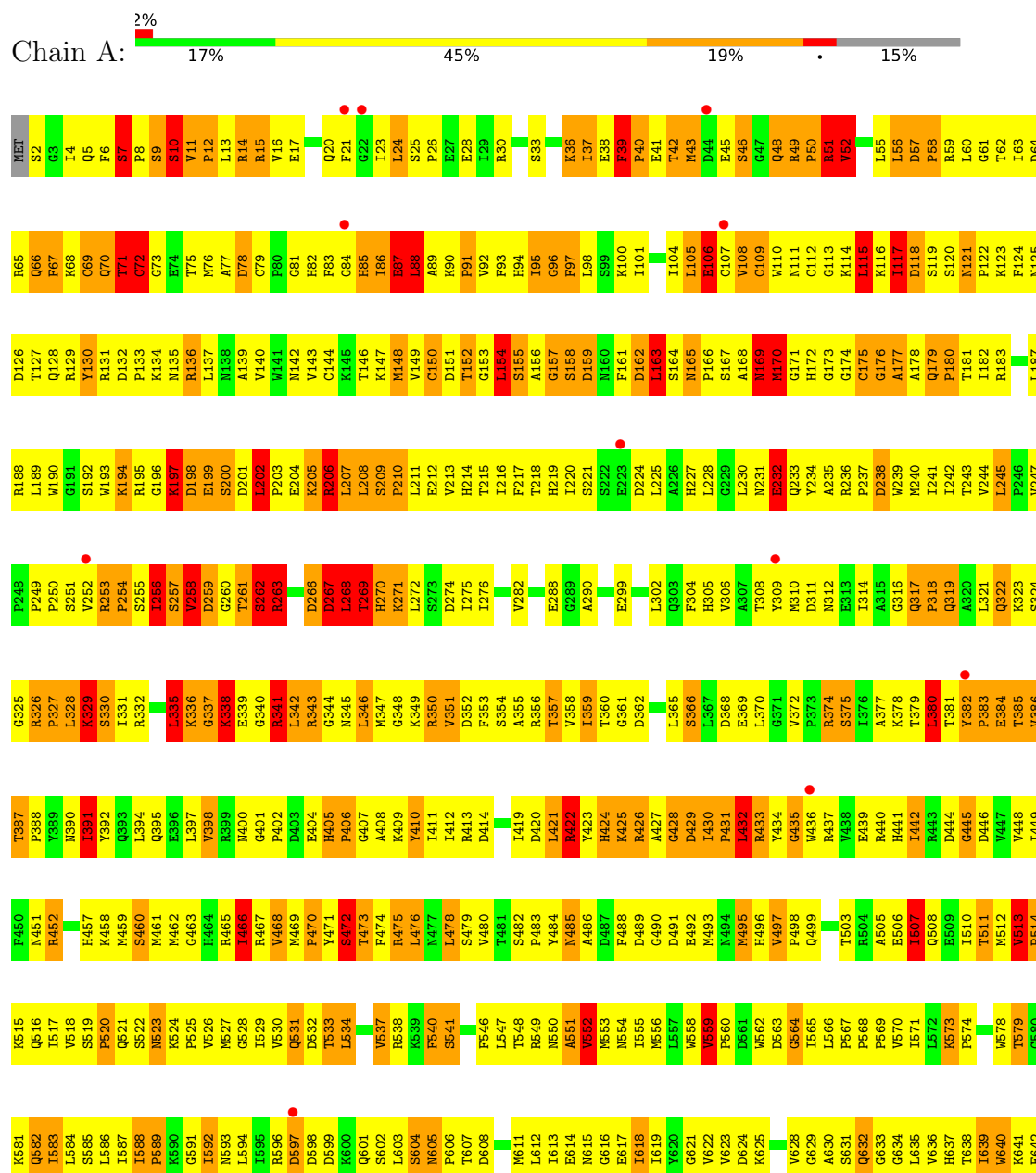
- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total 1	Mg 1	0	0
14	M	1	Total 1	Mg 1	0	0

3 Residue-property plots

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

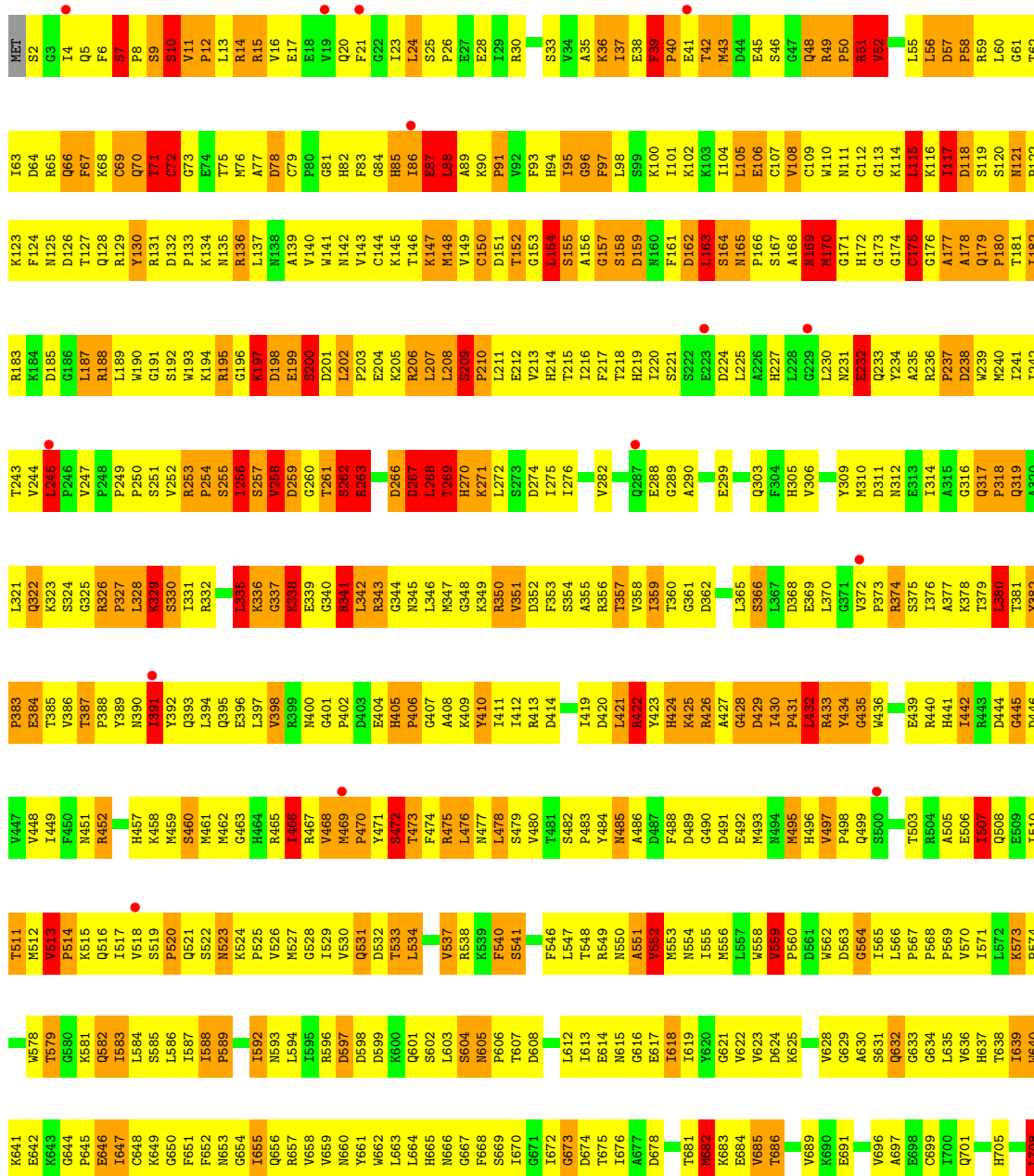
- Molecule 1: DNA-directed RNA polymerase II subunit rpb1



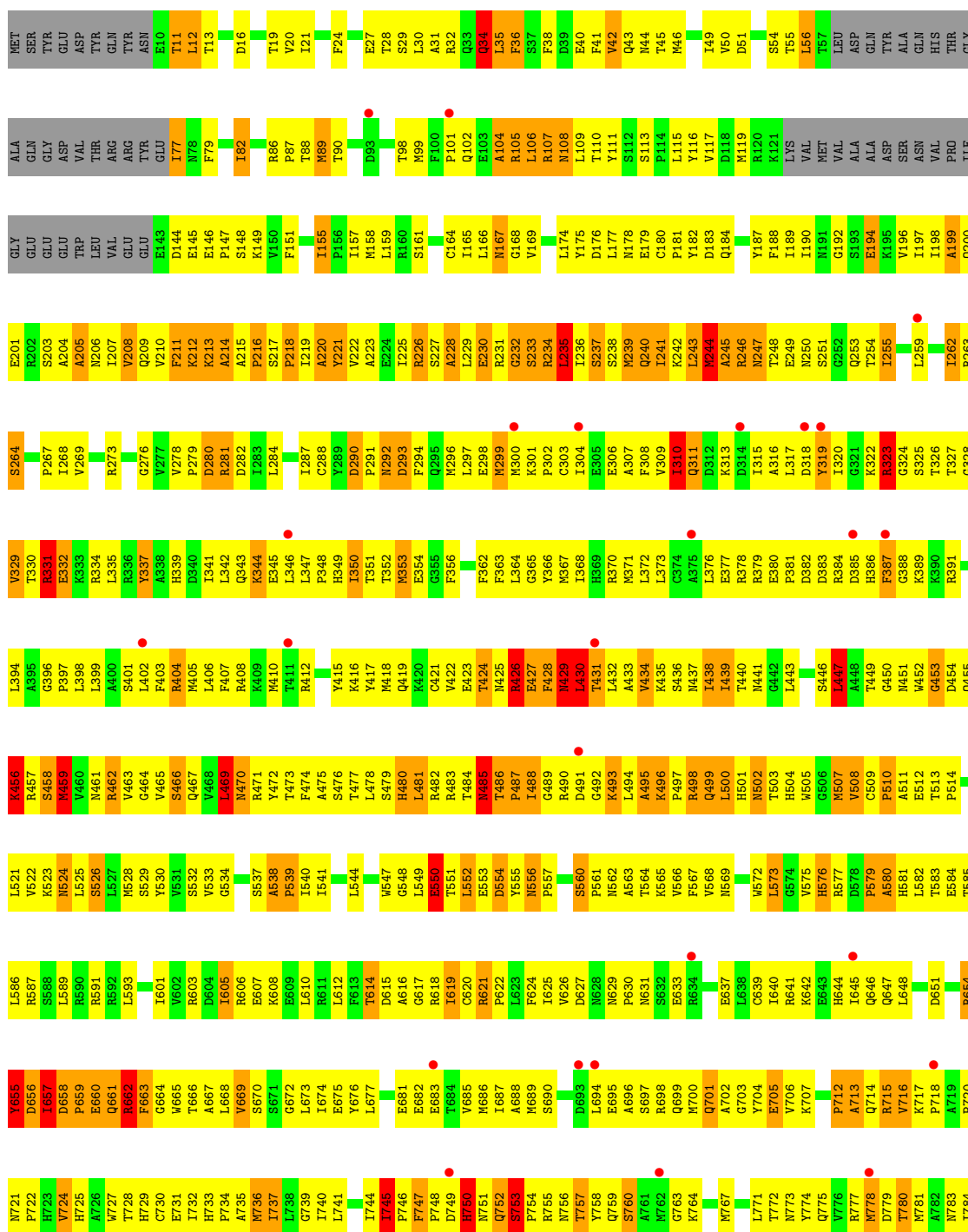
P1490	D1426	D1365	D1301	A1236	L1166	K1105	R1039	Q972	L907	Y842	L981	K643
M1491	C1427	G1366	G1302	D1237	E1167	E1106	L1040	Y973	M908	L943	M714	G644
D1493	G1428	S1367	F1304	L1239	D1168	I1107	M1041	F974	E909	Q844	T715	P645
	G1429	Y1368	F1304	L1239	D1169	I1108	K1042	H975		R845	L716	E646
	I1430	V1369	E1305	I1240	K1170	M1109	V1043	L976	L913	R846	R717	I647
	S1431	M1370	R1366	I1241	D1171	V1110	A1044	E977	S914	L847		C648
	E1432	Y1371	A1307	R1242	F1172	K1111	F1045	A978	L915	V948	F720	K649
	N1433	H1372	D1308	C1243	E1173	K1112	A1046	K979	Y916	K849	E721	G650
	I1434	H1373	E1309	R1244	E1174	N1113	W1047	M917	Y916	K849	A722	P651
	M1435	L1374	W1310	I1245	K1114	I1114	M1048	P981	K980	A850	A722	F652
	L1436	A1375	V1311	I1246	F1175	K1115	M1049	P982	E918	M851	K723	N653
	G1437	L1376	R1247	R1247	F1177	K1116	G1050	P983	N919	E852	V724	G654
	Q1438	L1377	E1313	D1248	F1178	P1117	E1051	L984	I921	V853	S725	
	L1439	G1378	F1314	D1249	I1179	S1118	V1052	L985	E922	D854	R726	I655
	A1440	D1379	D1315	D1250	P1180	L1119	E1053	P986	N923	M855	I727	Q656
	P1441	V1380	G1316	R1251	D1181	T1120		S987	D924	R857	L728	R657
	M1442	F1381	I1317	K1252	E1182	I1121	V1061	P988	S925	Y858	N729	V658
	G1443	L1382	A1253	A1253	S1183	Y1122	S1062	P989	S926	D859	Q731	V659
	V1444	S1383	L1319	E1254	V1184	M1123	P1063	I990	V927	G860	R732	Y661
	G1445	R1384	T1320	D1255	E1185	M1124	G1064		Q928	T861	D733	W662
		G1385	E1321	D1256	E1186	P1125	E1065	L993	D929	V862		L663
	I1449	H1386	A1322	D1257	M1187	W1126	M1066	L996	E933	R863	A739	L664
	Y1450	L1387	M1323	N1258	L1188	I1127	V1067			N864	E740	H665
	L1451	M1388	V1325	I1260	Y1189	A1128	G1068	L997	E934	A865	H741	N666
	Q1452	L1389	E1326	E1261	Q1191	M1130	L1070	K999	Q937	D868	S742	G667
	GLY	T1391	G1327	E1262	S1192	M1131	A1071	L1000	L938	E807	L743	F668
	M1455	R1392	V1328	D1263	P1193	D1132	A1072	T1001	V939	N808	K744	S669
		H1393	D1329	V1265	W1194	L1133	G1073	L1002	A940	Q871	D745	I670
	Y1459	G1394	A1330	F1265	L1195	M1134	I1075	F1003	F872	S809	S746	G671
	S1460	L1395	T1331	L1266	L1196	K1135	I1075	R1004	A873	R811	N747	I672
	TYR	R1396	R1332			K1136	G1076	I1005	E943	R812	W748	G673
	GLY	R1397	T1333			V1137	E1077	S1006	L944	G813	N749	D674
	L1461	A1398	Y1334			T1139	D1078	L1007	L945	E876	T675	T675
	LEU	E1399	S1335			M1140	A1079	R1008	D877	D877	Q751	I676
	GLY	T1400	G1340			Q1141	T1080	I1009	G878	G878	M752	A677
	ALA	G1401	F1338			E1142	M1081	T1010	L879	L879	G756	D678
	ALA	A1402	V1339			E1143	M1082	R1011	D880	D880		T681
	SER	L1403	E1340			M1205	T1083	P950	A881	P950	S757	T681
	PRO	M1404	L1274			K1209	L1084	P951	T882	T882	K758	M652
	TYR	C1405	L1279			A1216	T1085	Q952	L883	V884	S759	K653
	GLY	A1406	R1280			G1217	V1092	Q1022	V884	H822	S760	E684
	GLY	S1407	G1281			K1218	S1093	L1023	G953	A823	F761	V685
	VAL	F1408	V1282			L1219	S1094	L1024	D954	M824	I762	T686
	GLN	E1409	P1283			A1220	K1095	L1025	A955	A825	N763	
	GLN	E1410	M1284			V1156	Y1089	L1019	R956	Q887	I764	V689
	PRO	T1411	I1285			S1151	A1090	L1020	Q957	V888		K690
	PRO	S1475	A1349			A1152	G1091	F1021	P958	F889	M767	E691
	GLY	Q1477	T1350			T1153	V1092	Q1022	L959	E828	S768	
	TYR	E1413	R1351			E1154	S1093	L1023	P960	G829	A769	V696
	THR	L1414	V1288			I1155	K1094	L1024	V961	L893	C770	
	SER	L1415	Y1289			H1156	K1095	L1025	N962	L894	V771	Q701
	PRO	M1416	M1290			D1157	M1096	R1026	N963	S995	G772	
	PHE	D1417	M1291			D1158	V1097	S1027	Q964	A834	G773	H705
	SER	A1418	E1292			F1223	T1098	K1028	R965	Q898	Q774	N706
	SER	L1419	H1293			P1159	L1099	F1029	I966	K836	I775	R707
	ALA	A1420	K1294			D1160	G1100	A1030	I967	K902	Y776	L708
	ALA	S1421	I1295			Q1162	V1101	V1031	Q968	Y903	E777	K709
	MET	G1422				D1163	P1102	K1032	N969	R904	G778	P710
	PRO		I1299			T1230	R1103		E839	I905	K779	E711
	GLY	D1425	E1300			V1165	L1104	Y1038	L971	D906	R790	P712

[illegible]

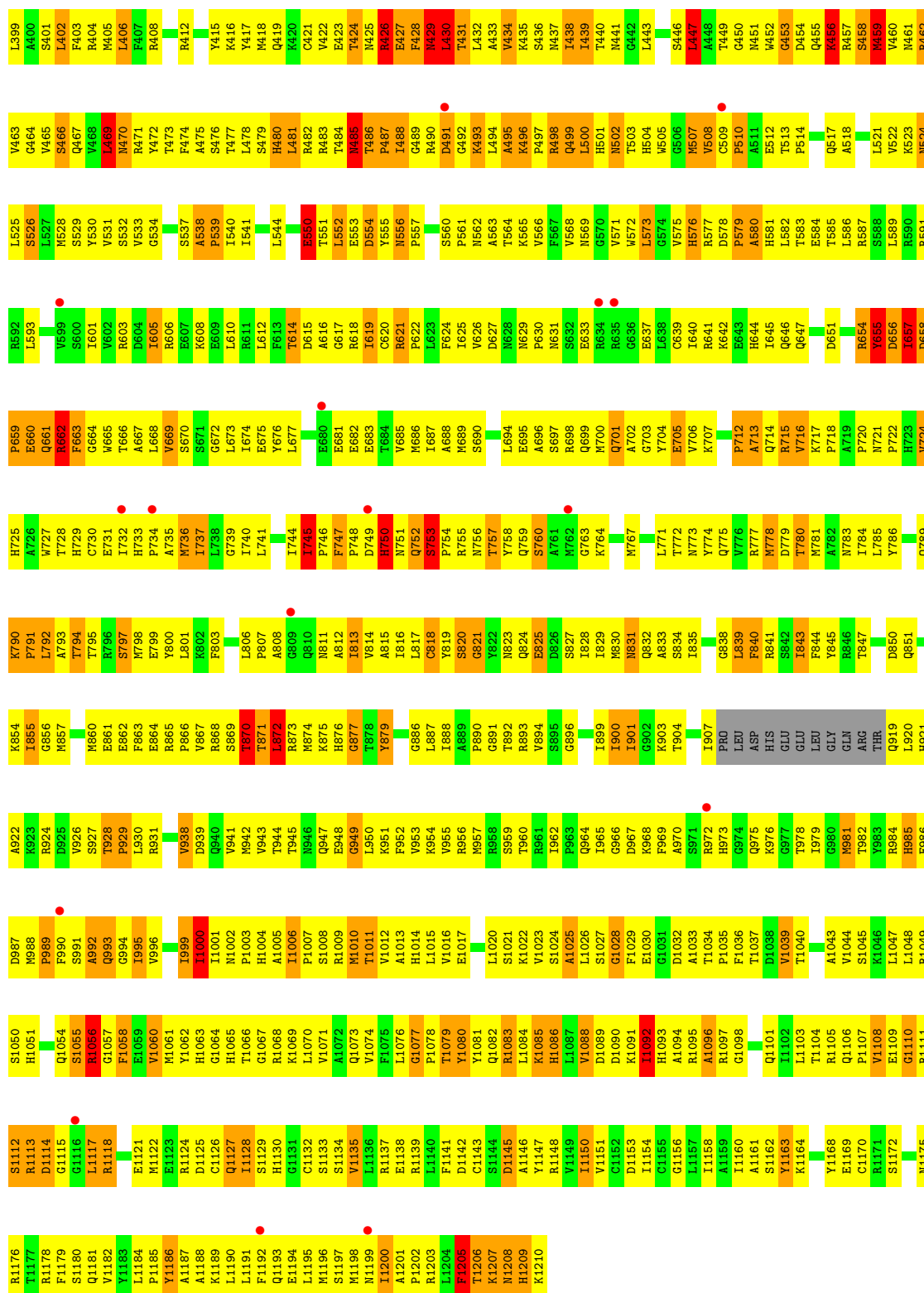
Chain M:

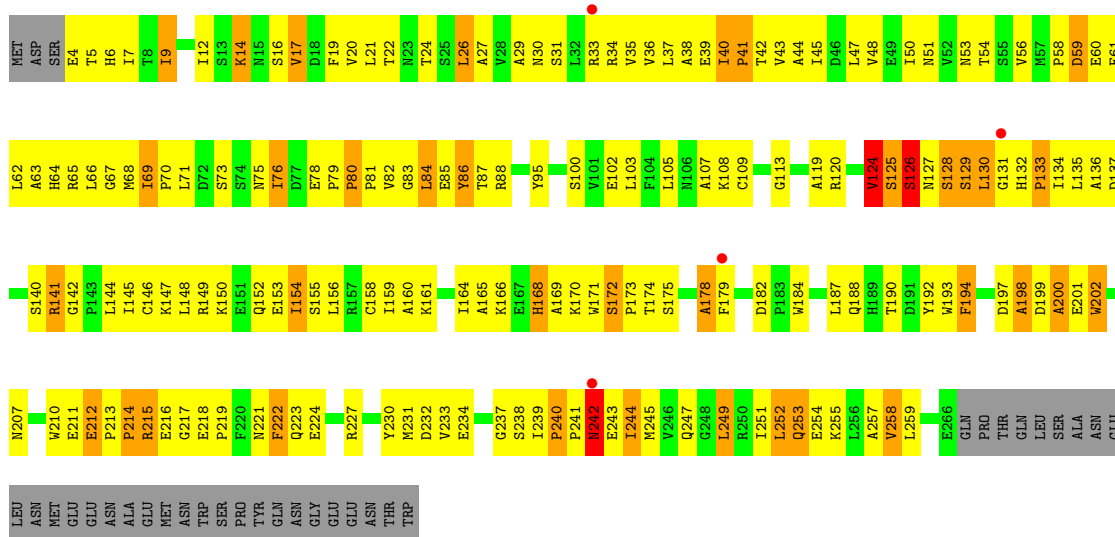


SER	PHE	ALA	K1356	M1291	Q1162	G1100	A1030	I967	K902	A838	V776	K709
PRO	SER	GLY	E1357	E1292	D1163	V1101	V1031	Q968	I903	E839	E777	P710
TYR	SER	THR	L1358	H1293	T1164	P1102	K1032	N969	R904	T840	E778	E711
SER	ALA	PRO	K1359	K1294	V1165	R1103	G	A970	I905	G841	K779	P712
ALA	SER	TYR	L1360	I1295	I1166	L1104	Y1039	L971	D906	Y842	K780	G713
THR	SER	GLY	V1361	I1299	E1167	K1105	R1038	D972	L907	T843	L781	M714
THR	PRO	ARG	I1362	E1362	E1168	E1106	L1040	I973	M908	Q844	P782	T715
SER	GLY	SER	E1363	E1426	E1169	L1107	M1041	F974	E909	R845	F783	L716
PRO	TYR	PRO	F1364	E1300	K1170	L1108	K1042	H975	G	G784	G784	R717
SER	GLY	GLY	D1365	G1302	K1171	M1109	V1043	L976	S914	V848	F785	
TYR	LEU	TYR	G1366	T1303	F1172	V1110	A1044	E977	L913			
SER	THR	SER	S1367	F1304	V1173	A1111	E1046	A978	L915			
PRO	SER	SER	Y1368	E1305	E1174	K1112	E1047	K979	Y916	A850		
THR	PRO	PRO	V1369	A1306	A1175	H1113	M1047	K980	M917	N851		
SER	SER	THR	M1370	A1307	F1176	L1114	M1048	P981	E918	E852		
PRO	TYR	TYR	Y1371	D1308	F1177	K1115	T982	T982	N919	D853		
SER	SER	SER	R1372	E1309	A1178	T1116	G1050	D983	S920	N854		
TYR	PRO	TYR	H1373	V1310	A1179	P1117	E1051	L984	I921	F793		
SER	SER	SER	L1374	V1311	E1185	S1118	Y085	L985	E922	K795		
PRO	SER	PRO	A1375	L1312	E1186	L1119	E1052	P986	N923	R857		
THR	THR	THR	L1376	E1313	E1187	P1125	E1065	S987	D924	Y858		
THR	GLY	GLY	L1377	T1314	E1188	M1120	V1061		S925	F798		
PRO	TYR	PRO	C1378	D1315	V1184	Y1122	S1062	P988	S926	G860		
SER	SER	SER	D1379	T1316	V1185	L1123	P1063	I989	G860	F799		
TYR	THR	TYR	V1380	G1316	E1186	M1124	G1064	I990	Q928	P800		
SER	SER	SER	M1381	N1318	E1187	P1125	E1065	L993	D929	V862		
PRO	PRO	PRO	T1382	L1319	L1188	M1126	M1066		E933	R863		
THR	ALA	THR	S1383	T1320	Y1189	W1127	E1067	L996	E934	N864		
SER	GLY	GLY	R1384	E1321	K1190	A1128	G1068	I997		A865		
PRO	MET	GLY	G1385	A1322	Q1191	A1129	A998		Q937	G867		
SER	PRO	SER	L1386	M1323	S1192	N1130	L1070	K999	D868	T869		
TYR	THR	GLY	L1387	T1324	P1193	M1131	A1071	L1000	L938	N808		
SER	SER	GLY	M1388	V1325	E1261	D1132	A1072	T1001	V939	S809		
PRO	PRO	ARG	A1389	E1326	E1262	L1133	I1002	I1009	A940	Y810		
THR	SER	GLY	L1390	G1327	D1263	A1134	S1074	T1003	D941	P871		
SER	TYR	GLY	T1391	V1328	L1196	K1135	I1075	R1004	R942	L811		
PRO	SER	PHE	R1392	D1329	R1197	N1136	G1076	G1005	E943	A873		
SER	PRO	GLY	H1393	A1330	E1199	V1137	E1077	S1006	L944	G875		
TYR	THR	ASP	G1394	T1331	L1269	Q1138	P1078	D1007	L945	E876		
SER	SER	TYR	T1395	R1332	E1270	T1139	A1079	R1008	C946	D877		
PRO	PRO	GLY	M1396	T1333	G1271	Q1140	T1080	I1009	K947	G878		
THR	SER	THR	R1397	Y1334	H1272	I1141	Q1081	T1010	F948	L879		
SER	TYR	ALA	A1398	S1335	M1273	E1142	M1082	R1011	I949	D880		
PRO	SER	VAL	E1399	M1336	L1274	H1143	T1083	P1012	F950	A881		
SER	PRO	ALA	T1400	S1337	E1275	T1144	L1084	V1013	P951	T820		
TYR	THR	THR	G1401	F1338	S1276	T1145	M1085		K952	L883		
SER	SER	LEU	A1402	V1339	K1209	L1146	T1086	M1016	G953	A823		
THR	PRO	ALA	L1403	E1340	L1210	V1149	H1087	A1017	D954	N824		
SER	PRO	GLY	M1404	I1341	S1278	T1150	F1088	T1018	A955	A825		
PRO	TYR	LYS	R1405	L1342	M1212	S1151	Y1089	L1019	R956	G826		
PRO	SER	GLY	C1406	G1281	G1281	A1152	A1090	L1020	W957	N827		
SER	PRO	VAL	F1407	L1345	V1215		G1091	F1021	P958	E989		
TYR	THR	GLN	F1408	G1346	A1216	T1155	V1092	Q1022	L959	E828		
SER	SER	THR	E1409	I1347	G1217	H1156	S1093	I1023	P960	G829		
PRO	PRO	PRO	E1410	E1348	K1218	Y1157	S1094	L1024	V961	L892		
THR	SER	GLN	T1411	A1349	L1219	H1157	K1095	L1025	N962	N894		
SER	TYR	LEU	V1412	T1350	A1220	D1158	N1096	R1028	V963	S895		
PRO	THR	THR	E1413	R1351	E1221	P1159	T1097	S1027	Q964	W835		
SER	PRO	GLU	T1414	G	S1222	L1160	K1098	K1028	R965	K836		
TYR	TYR	PRO	L1415	L1355	F1223	P1161	L1099	F1029	I966	T837		

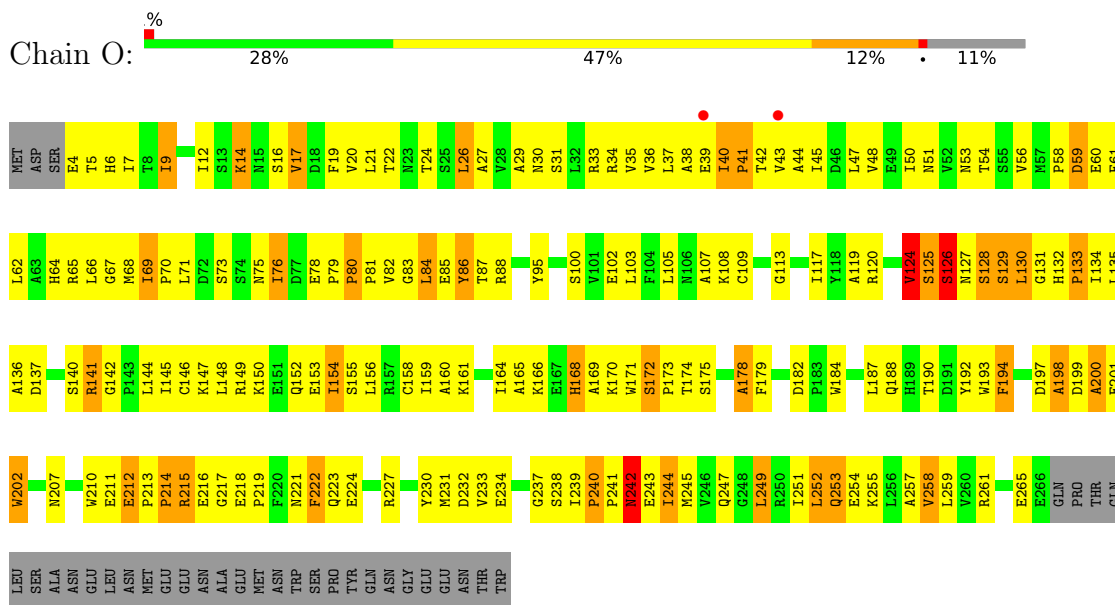




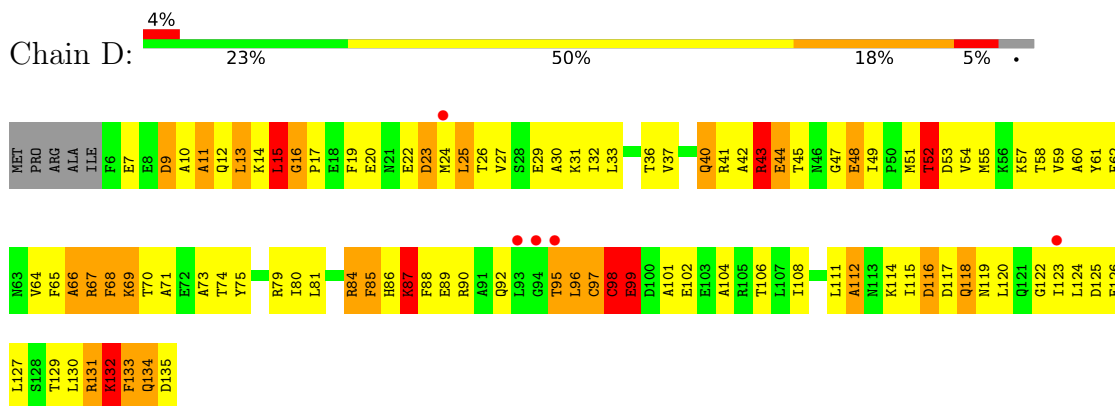




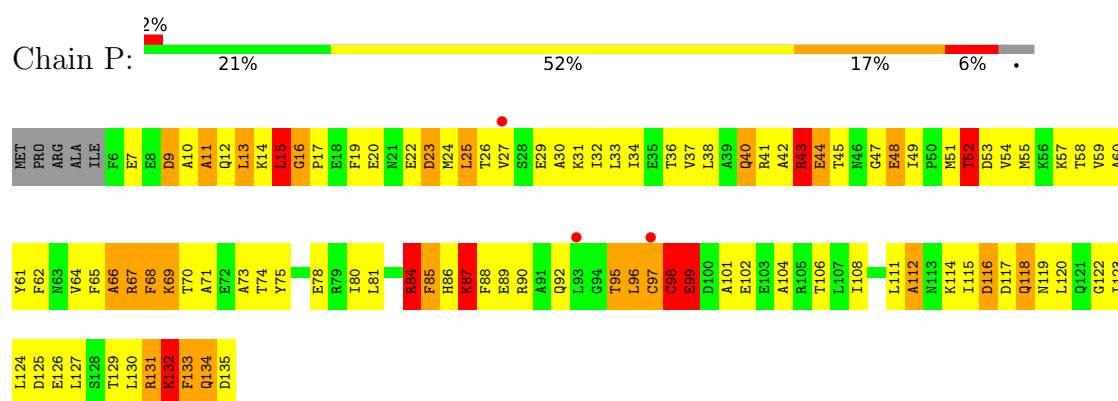
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



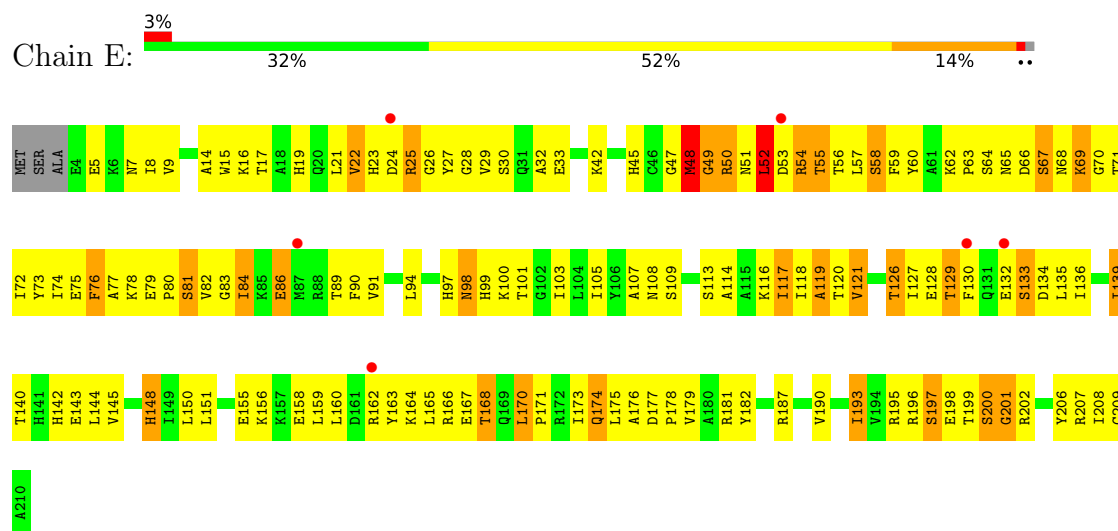
• Molecule 4: DNA-directed RNA polymerase II subunit rpb4



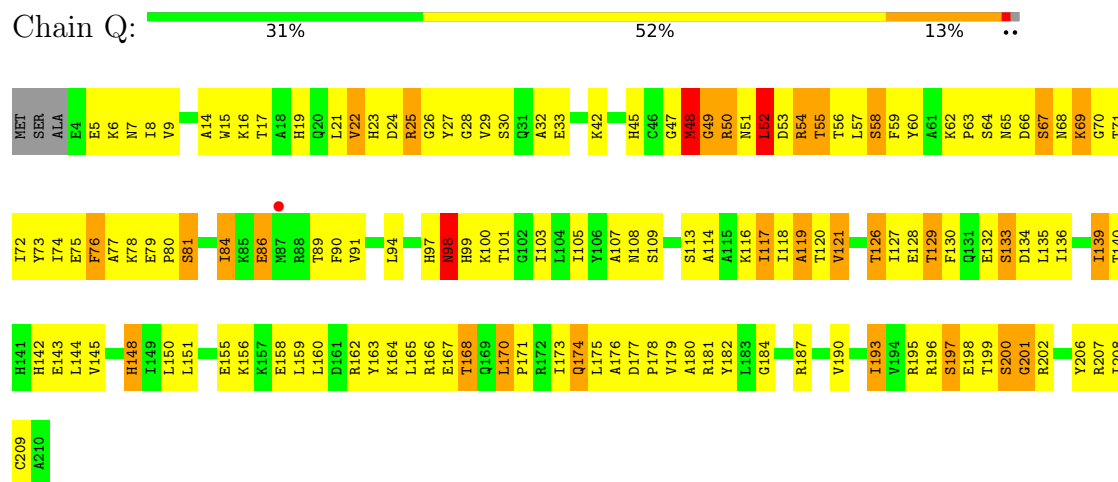
• Molecule 4: DNA-directed RNA polymerase II subunit rpb4



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



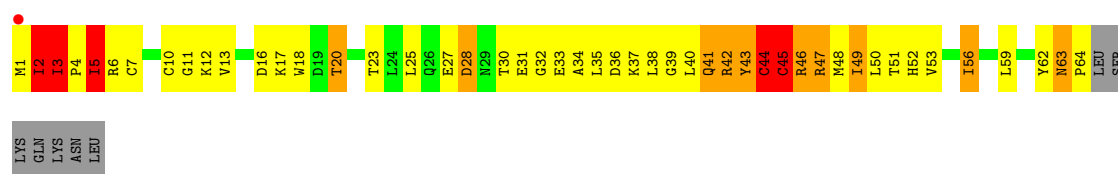
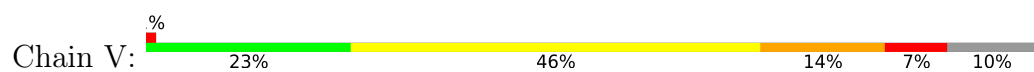
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



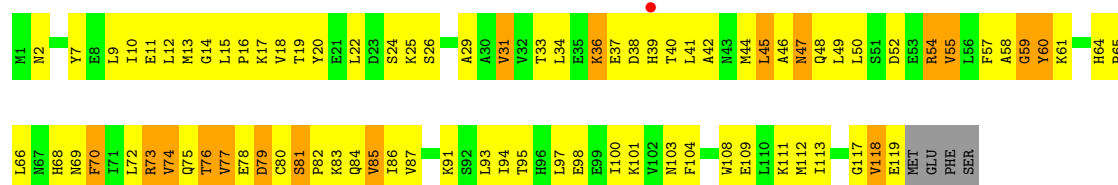
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



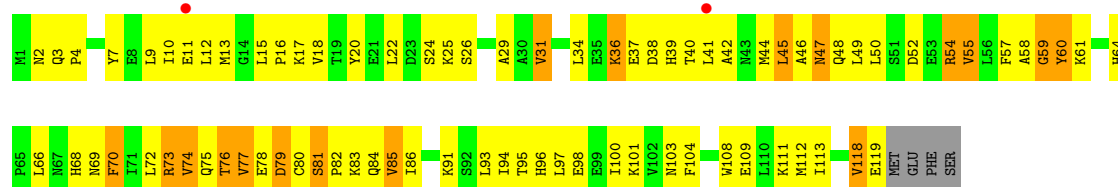




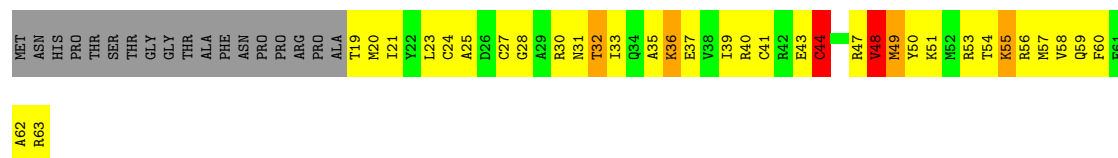
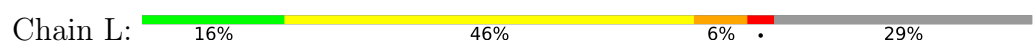
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



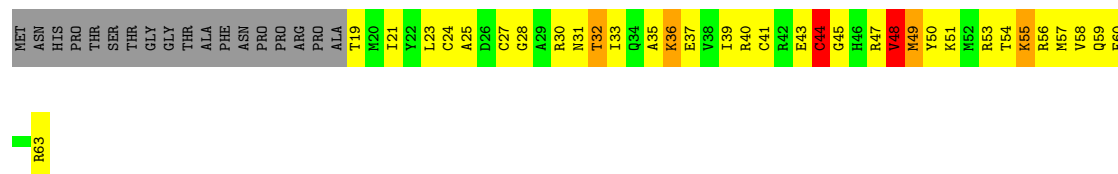
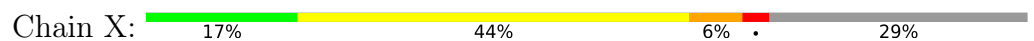
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	163.03Å 202.68Å 391.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.70 – 3.65 48.70 – 3.65	Depositor EDS
% Data completeness (in resolution range)	92.8 (48.70-3.65) 96.1 (48.70-3.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.67Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.297 , 0.321 0.292 , 0.296	Depositor DCC
R_{free} test set	6932 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	125.6	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 177.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	62870	wwPDB-VP
Average B, all atoms (Å ²)	203.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, 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	A	0.54	4/12026 (0.0%)	0.87	36/16260 (0.2%)
1	M	0.55	6/11887 (0.1%)	0.86	30/16069 (0.2%)
2	B	0.58	3/9360 (0.0%)	0.91	36/12643 (0.3%)
2	N	0.57	2/9360 (0.0%)	0.90	35/12643 (0.3%)
3	C	0.59	0/2135	0.95	10/2904 (0.3%)
3	O	0.59	0/2135	0.95	10/2904 (0.3%)
4	D	0.29	0/1049	0.64	1/1412 (0.1%)
4	P	0.29	0/1049	0.64	1/1412 (0.1%)
5	E	0.50	0/1695	0.91	7/2287 (0.3%)
5	Q	0.50	0/1695	0.90	7/2287 (0.3%)
6	F	0.68	0/666	1.12	10/901 (1.1%)
6	R	0.67	0/666	1.12	10/901 (1.1%)
7	G	0.33	0/1361	0.78	3/1847 (0.2%)
7	S	0.33	0/1361	0.79	3/1847 (0.2%)
8	H	0.53	0/1010	0.88	1/1363 (0.1%)
8	T	0.53	0/1010	0.88	2/1363 (0.1%)
9	I	0.26	0/921	0.52	0/1246
9	U	0.29	0/921	0.52	0/1246
10	J	0.78	0/526	1.13	4/709 (0.6%)
10	V	0.78	0/526	1.13	4/709 (0.6%)
11	K	0.59	0/972	0.91	0/1317
11	W	0.59	0/972	0.90	0/1317
12	L	0.46	0/371	0.84	0/491
12	X	0.46	0/371	0.84	0/491
All	All	0.54	15/64045 (0.0%)	0.88	210/86569 (0.2%)

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	35	ALA	C-N	8.17	1.44	1.34
1	M	1445	GLY	C-N	8.15	1.44	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	346	LEU	C-N	-7.41	1.23	1.33
2	B	1150	ILE	C-N	6.72	1.43	1.33
2	B	480	HIS	C-N	6.42	1.42	1.33

The worst 5 of 210 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	997	ILE	N-CA-C	-10.34	102.62	112.96
1	A	997	ILE	N-CA-C	-10.29	102.67	112.96
10	V	45	CYS	N-CA-C	-10.00	101.41	114.31
10	J	45	CYS	N-CA-C	-9.99	101.42	114.31
5	E	201	GLY	N-CA-C	9.85	121.50	111.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11802	0	11784	3392	0
1	M	11666	0	11647	3341	0
2	B	9180	0	9163	1716	0
2	N	9180	0	9164	1721	0
3	C	2088	0	2045	286	0
3	O	2088	0	2045	289	0
4	D	1036	0	1025	358	0
4	P	1036	0	1025	324	0
5	E	1663	0	1684	208	0
5	Q	1663	0	1684	213	0
6	F	656	0	679	83	0
6	R	656	0	679	89	0
7	G	1330	0	1329	426	0
7	S	1330	0	1329	428	0
8	H	996	0	1006	168	0
8	T	996	0	1006	178	0
9	I	902	0	840	281	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	U	902	0	839	272	0
10	J	518	0	529	95	0
10	V	518	0	529	96	0
11	K	955	0	968	127	0
11	W	955	0	968	121	0
12	L	368	0	380	39	0
12	X	368	0	380	38	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	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
13	M	2	0	0	0	0
13	N	1	0	0	0	0
13	O	1	0	0	0	0
13	U	2	0	0	0	0
13	V	1	0	0	0	0
13	X	1	0	0	0	0
14	A	1	0	0	0	0
14	M	1	0	0	0	0
All	All	62870	0	62727	13231	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 105.

The worst 5 of 13231 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1161:PRO:HG2	1:M:1190:LYS:CG	1.29	1.62
1:A:1161:PRO:HG2	1:A:1190:LYS:CG	1.29	1.58
1:M:1161:PRO:CG	1:M:1190:LYS:HG2	1.33	1.57
1:M:1091:GLY:HA3	1:M:1092:VAL:CG1	1.35	1.56
1:M:267:ASP:CB	1:M:268:LEU:HB2	1.35	1.54

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 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	1494/1752 (85%)	939 (63%)	280 (19%)	275 (18%)	0	1
1	M	1472/1752 (84%)	932 (63%)	281 (19%)	259 (18%)	0	1
2	B	1142/1210 (94%)	735 (64%)	245 (22%)	162 (14%)	0	2
2	N	1142/1210 (94%)	738 (65%)	243 (21%)	161 (14%)	0	2
3	C	261/297 (88%)	178 (68%)	56 (22%)	27 (10%)	0	4
3	O	261/297 (88%)	178 (68%)	56 (22%)	27 (10%)	0	4
4	D	128/135 (95%)	86 (67%)	20 (16%)	22 (17%)	0	1
4	P	128/135 (95%)	86 (67%)	20 (16%)	22 (17%)	0	1
5	E	205/210 (98%)	137 (67%)	43 (21%)	25 (12%)	0	3
5	Q	205/210 (98%)	137 (67%)	43 (21%)	25 (12%)	0	3
6	F	81/142 (57%)	58 (72%)	15 (18%)	8 (10%)	0	5
6	R	81/142 (57%)	57 (70%)	16 (20%)	8 (10%)	0	5
7	G	168/172 (98%)	128 (76%)	24 (14%)	16 (10%)	0	5
7	S	168/172 (98%)	128 (76%)	24 (14%)	16 (10%)	0	5
8	H	122/125 (98%)	73 (60%)	27 (22%)	22 (18%)	0	1
8	T	122/125 (98%)	73 (60%)	27 (22%)	22 (18%)	0	1
9	I	109/113 (96%)	46 (42%)	27 (25%)	36 (33%)	0	0
9	U	109/113 (96%)	45 (41%)	25 (23%)	39 (36%)	0	0
10	J	62/71 (87%)	41 (66%)	15 (24%)	6 (10%)	0	5
10	V	62/71 (87%)	41 (66%)	15 (24%)	6 (10%)	0	5
11	K	117/123 (95%)	80 (68%)	24 (20%)	13 (11%)	0	3
11	W	117/123 (95%)	80 (68%)	24 (20%)	13 (11%)	0	3
12	L	43/63 (68%)	23 (54%)	12 (28%)	8 (19%)	0	1
12	X	43/63 (68%)	23 (54%)	12 (28%)	8 (19%)	0	1
All	All	7842/8826 (89%)	5042 (64%)	1574 (20%)	1226 (16%)	0	2

5 of 1226 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	12	PRO
1	A	37	ILE
1	A	42	THR
1	A	50	PRO

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	1301/1536 (85%)	1094 (84%)	207 (16%)	2	14
1	M	1286/1536 (84%)	1076 (84%)	210 (16%)	2	13
2	B	1012/1064 (95%)	900 (89%)	112 (11%)	6	24
2	N	1012/1064 (95%)	898 (89%)	114 (11%)	5	24
3	C	236/267 (88%)	217 (92%)	19 (8%)	11	34
3	O	236/267 (88%)	216 (92%)	20 (8%)	10	32
4	D	111/115 (96%)	93 (84%)	18 (16%)	2	13
4	P	111/115 (96%)	92 (83%)	19 (17%)	2	12
5	E	182/184 (99%)	170 (93%)	12 (7%)	15	40
5	Q	182/184 (99%)	169 (93%)	13 (7%)	13	38
6	F	71/121 (59%)	65 (92%)	6 (8%)	10	32
6	R	71/121 (59%)	65 (92%)	6 (8%)	10	32
7	G	146/148 (99%)	136 (93%)	10 (7%)	14	40
7	S	146/148 (99%)	136 (93%)	10 (7%)	14	40
8	H	113/114 (99%)	99 (88%)	14 (12%)	4	20
8	T	113/114 (99%)	99 (88%)	14 (12%)	4	20
9	I	103/105 (98%)	80 (78%)	23 (22%)	1	6
9	U	103/105 (98%)	80 (78%)	23 (22%)	1	6
10	J	59/66 (89%)	46 (78%)	13 (22%)	1	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	V	59/66 (89%)	46 (78%)	13 (22%)	1	6
11	K	109/113 (96%)	100 (92%)	9 (8%)	10	33
11	W	109/113 (96%)	99 (91%)	10 (9%)	8	30
12	L	39/53 (74%)	34 (87%)	5 (13%)	4	20
12	X	39/53 (74%)	34 (87%)	5 (13%)	4	20
All	All	6949/7772 (89%)	6044 (87%)	905 (13%)	4	19

5 of 905 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	72	CYS
10	V	45	CYS
1	M	773	GLN
10	V	2	ILE
4	P	43	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 221 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	121	ASN
1	M	919	ASN
11	W	68	HIS
5	Q	98	ASN
1	M	179	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 18 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	A	1496/1752 (85%)	0.13	30 (2%) 65 39	51, 150, 385, 628	0
1	M	1476/1752 (84%)	0.12	28 (1%) 66 40	83, 199, 449, 672	0
2	B	1150/1210 (95%)	0.23	34 (2%) 52 31	69, 142, 314, 580	0
2	N	1150/1210 (95%)	0.15	27 (2%) 61 36	85, 222, 419, 618	0
3	C	263/297 (88%)	-0.05	4 (1%) 72 44	80, 126, 252, 477	0
3	O	263/297 (88%)	0.00	2 (0%) 82 59	125, 190, 350, 511	0
4	D	130/135 (96%)	0.10	5 (3%) 44 27	128, 240, 360, 596	0
4	P	130/135 (96%)	0.10	3 (2%) 61 36	152, 287, 414, 545	0
5	E	207/210 (98%)	0.04	6 (2%) 53 31	70, 164, 293, 516	0
5	Q	207/210 (98%)	0.08	1 (0%) 87 67	119, 181, 373, 501	0
6	F	83/142 (58%)	-0.40	0 100 100	70, 97, 170, 232	0
6	R	83/142 (58%)	-0.13	0 100 100	111, 126, 200, 335	0
7	G	170/172 (98%)	0.30	6 (3%) 47 28	92, 199, 323, 514	0
7	S	170/172 (98%)	0.25	1 (0%) 85 64	122, 240, 388, 494	0
8	H	124/125 (99%)	0.02	1 (0%) 82 59	82, 138, 298, 408	0
8	T	124/125 (99%)	0.03	0 100 100	115, 197, 344, 429	0
9	I	111/113 (98%)	0.05	0 100 100	98, 239, 367, 549	0
9	U	111/113 (98%)	0.07	0 100 100	151, 330, 482, 585	0
10	J	64/71 (90%)	-0.01	0 100 100	85, 108, 220, 304	0
10	V	64/71 (90%)	0.03	1 (1%) 70 43	137, 203, 326, 373	0
11	K	119/123 (96%)	-0.02	1 (0%) 82 59	60, 126, 221, 319	0
11	W	119/123 (96%)	-0.11	2 (1%) 69 41	76, 168, 295, 470	0
12	L	45/63 (71%)	0.08	0 100 100	93, 177, 299, 481	0
12	X	45/63 (71%)	0.03	0 100 100	153, 277, 425, 580	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	7904/8826 (89%)	0.11	152 (1%) 66 40	51, 181, 397, 672	0

The worst 5 of 152 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	972	ARG	6.2
1	A	107	CYS	5.4
1	M	874	TYR	4.5
2	N	314	ASP	4.4
2	B	346	LEU	4.4

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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. 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	B-factors(Å ²)	Q<0.9
14	MG	M	2458	1/1	0.51	0.20	197,197,197,197	0
14	MG	A	2458	1/1	0.65	0.11	109,109,109,109	0
13	ZN	M	2456	1/1	0.68	0.10	432,432,432,432	0
13	ZN	O	1269	1/1	0.92	0.06	189,189,189,189	0
13	ZN	U	1122	1/1	0.92	0.06	240,240,240,240	0
13	ZN	N	2225	1/1	0.93	0.07	180,180,180,180	0
13	ZN	A	2456	1/1	0.94	0.05	245,245,245,245	0
13	ZN	U	1121	1/1	0.95	0.05	284,284,284,284	0
13	ZN	B	2225	1/1	0.95	0.06	149,149,149,149	0
13	ZN	I	1121	1/1	0.95	0.05	160,160,160,160	0
13	ZN	I	1122	1/1	0.95	0.09	126,126,126,126	0
13	ZN	X	1071	1/1	0.97	0.07	195,195,195,195	0
13	ZN	A	2457	1/1	0.97	0.10	122,122,122,122	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	ZN	M	2457	1/1	0.97	0.06	172,172,172,172	0
13	ZN	C	1269	1/1	0.98	0.04	122,122,122,122	0
13	ZN	L	1071	1/1	0.98	0.05	123,123,123,123	0
13	ZN	V	1066	1/1	0.98	0.03	155,155,155,155	0
13	ZN	J	1066	1/1	1.00	0.06	87,87,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.