



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 02:55 am BST

PDB ID : 3H0G
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

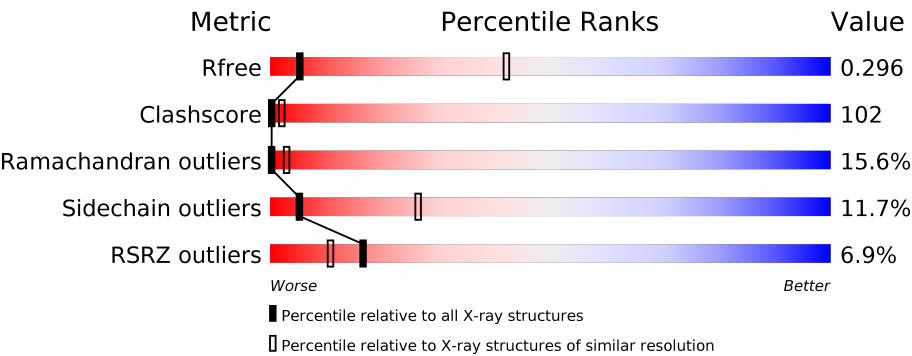
1 Overall quality at a glance i

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}	130704	1557 (3.82-3.50)
Clashscore	141614	1037 (3.80-3.52)
Ramachandran outliers	138981	1004 (3.80-3.52)
Sidechain outliers	138945	1002 (3.80-3.52)
RSRZ outliers	127900	1441 (3.82-3.50)

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 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	<div><div>5%</div><div><div>19%</div><div>45%</div><div>18%</div><div>•</div><div>15%</div></div></div>
1	M	1752	<div><div>10%</div><div><div>19%</div><div>45%</div><div>17%</div><div>•</div><div>16%</div></div></div>
2	B	1210	<div><div>2%</div><div><div>25%</div><div>54%</div><div>14%</div><div>•</div><div>5%</div></div></div>
2	N	1210	<div><div>10%</div><div><div>25%</div><div>54%</div><div>14%</div><div>•</div><div>5%</div></div></div>
3	C	297	<div><div><div>30%</div><div>48%</div><div>10%</div><div>•</div><div>11%</div></div></div>
3	O	297	<div><div><div>30%</div><div>49%</div><div>9%</div><div>•</div><div>11%</div></div></div>

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Mol	Chain	Length	Quality of chain
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	

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
14	MG	A	2458	-	-	-	X

2 Entry composition

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			

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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 (three-letter code: ZN) (formula: Zn).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	L	1	Total 1	Zn 1	0	0
13	M	2	Total 2	Zn 2	0	0

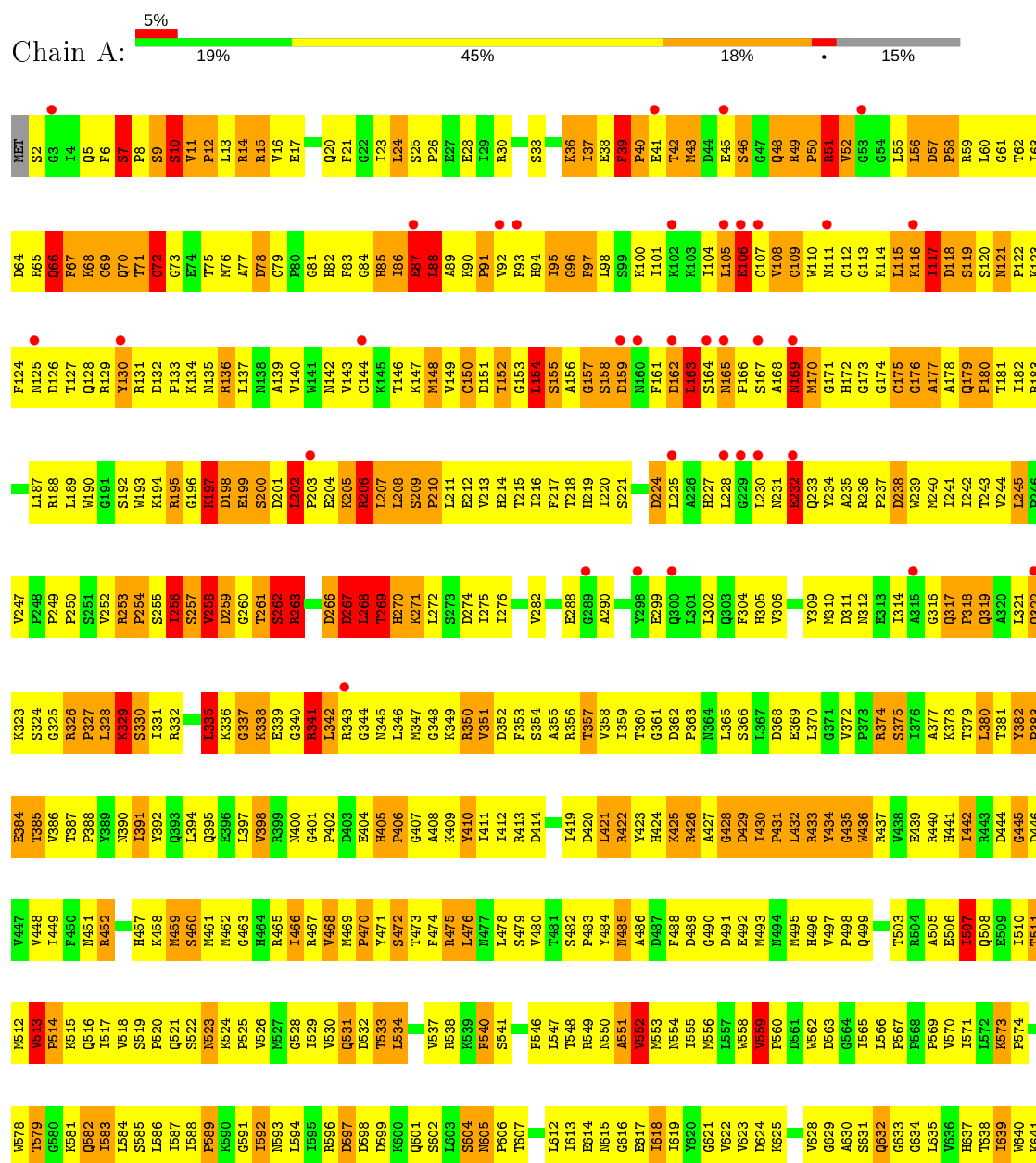
- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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 [i](#)

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

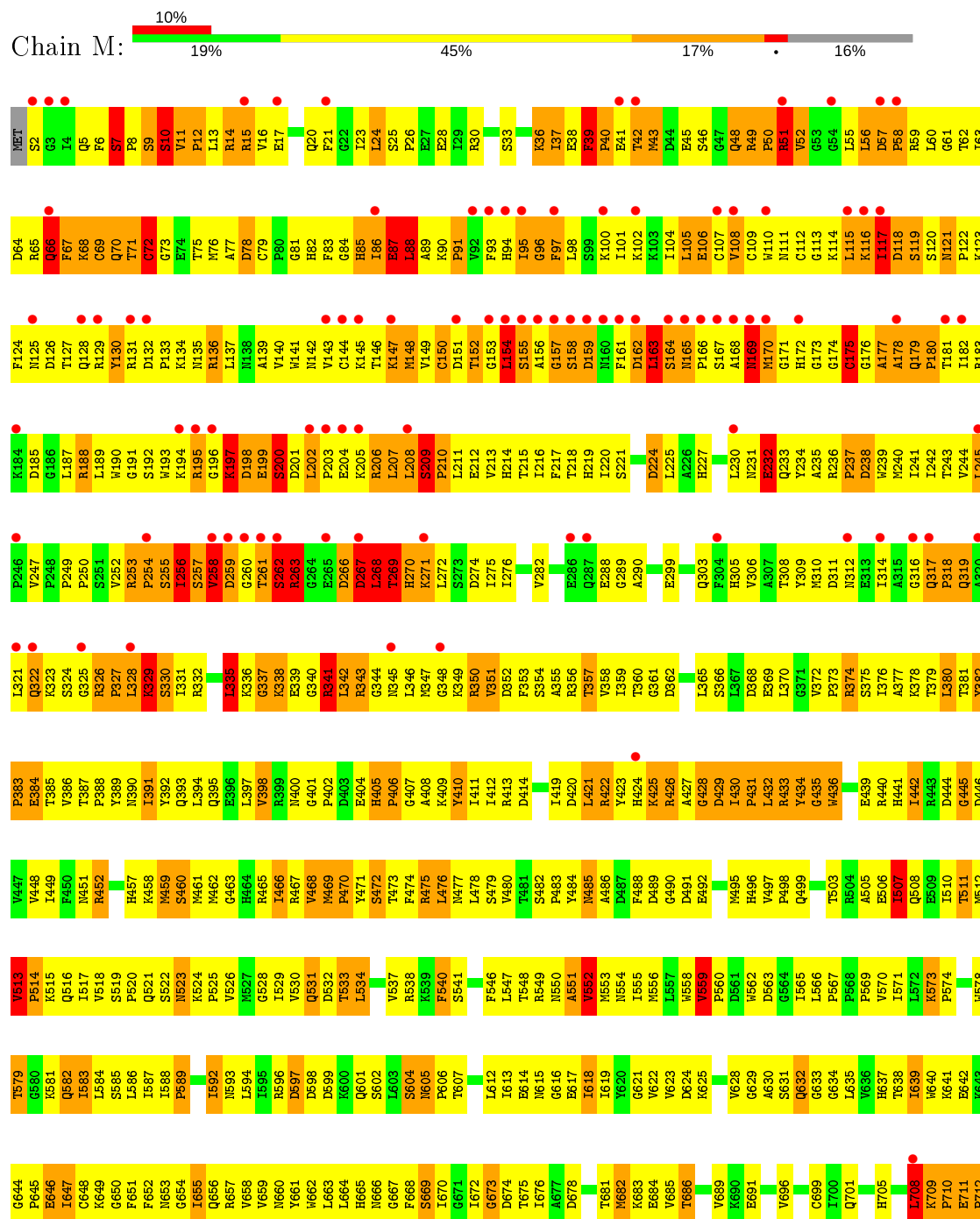
- Molecule 1: DNA-directed RNA polymerase II subunit rpb1



SER	M1435	H1373	E1309	R1244	A1175	K1115	M1049	T982	R919	R846	P782	P712	E642
SER	L1436	L1374	W1310	I1245	F1176	T1116	G1050	D983	S920	L847	F783	G713	K643
PRO	Q1437	A1375	V1311	I1246	A1177	S1118	O1051	I984	I921	V848	G784	M714	G644
GLY	Q1438	L1376	L1312	R1247	A1178	S1118	E1052	L985	E922	R849	F785	T715	P645
THR	L1439	L1377	E1313	D1248	L1179	L1120	E1053	P986	N923	A850	K786	R716	E646
SER	A1440	G1378	T1314	D1249	P1180	T1121	V1061	S987	D924	K851	Y787	L717	I647
PRO	P1441	D1379	D1315	D1250	D1181	I1121	V1062	D988	S925	E852	R788	F720	C648
LEU	P1442	T1382	G1316	R1251	E1182	Y1122	S1063	I989	S926	D853	R789	F721	G650
SER	M1443	T1382	I1317	K1252	E1183	L1123	P1063	I990	Y927	H854	L790	E721	G650
ALA	T1444	S1383	N1318	A1253	E1184	M1124	E1064	E989	Q928	V856	A722	K723	F651
THR	L1445	L1384	L1319	E1254	E1185	P1125	E1065	V939	H792	R857	H792	K724	N653
GLY	I1449	G1385	T1320	D1255	E1186	W1126	M1066	I1002	D929	Y858	S725	F725	G654
PRO	L1450	H1386	E1321	D1256	N1187	I1127	V1067	I986	E933	D859	R726	R726	I655
SER	D1452	L1387	A1322	D1257	L1188	A1128	G1068	I997	E934	E860	K795	I727	K656
GLY	M1455	A1388	M1323	M1258	Y1189	A1129	T1069	A998	Q937	T861	P800	I728	K657
PRO	M1456	T1390	V1326	M1259	L1190	M1130	L1070	K999	L938	V862	E801	N729	V658
GLY	N1458	L1391	E1326	E1261	Q1191	D1132	A1071	M1131	L938	R863	S802	Q730	V659
THR	L1459	R1392	G1327	E1262	P1193	L1133	Q1073	T1001	V939	R864	R803	A731	N660
PRO	L1460	H1393	V1328	D1263	W1194	A1134	S1074	F1003	D941	A865	R804	R732	Y661
ASP	S1460	G1394	D1329	D1264	L1195	K1135	I1075	R1004	E943	D868	R806	F745	L663
THR	L1461	I1395	A1330	F1265	L1196	M1136	G1076	G1005	L944	I869	E807	D746	L664
PRO	G1462	L1396	T1331	L1266	R1197	V1137	E1077	S1006	L945	I870	N808	S746	G671
GLY	T1463	R1397	R1332	L1267	L1198	Q1138	A1078	D1007	L945	I871	S809	N747	N665
LEU	A1464	A1398	L1333	I1269	L1199	T1139	P1079	R1008	C946	R872	H741	N747	N666
SER	V1465	E1399	Y1384	I1270	L1200	Q1140	T1080	I1009	K947	F872	S742	N748	G667
PRO	P1466	T1400	S1335	M1273	D1201	F1141	Q1081	T1010	F948	A873	L811	V749	D674
THR	L1467	G1401	L1342	L1274	R1202	E1142	M1082	T1011	R949	I874	R812	M752	T675
SER	L1468	A1402	V1338	E1275	A1203	H1143	T1083	L1018	F950	G875	L813	D746	I670
PRO	A1469	L1403	F1339	S1276	K1204	L1144	L1084	L1019	P951	E876	D745	S746	G671
THR	G1470	M1404	E1340	I1277	M1205	T1145	N1085	L1020	K952	D877	T815	N747	D672
SER	S1471	R1405	I1341	S1278	L1206	L1146	T1086	F1021	P953	C878	P816	N748	G673
GLY	L1472	C1406	L1342	L1279	K1209	S1147	F1087	A1017	D954	L879	Q817	V749	D674
VAL	M1473	S1407	L1345	L1280	L1210	T1148	H1088	L1018	A955	D880	F819	M752	I676
THR	F1474	F1408	L1346	G1281	S1211	V1149	H1089	L1019	R956	A881	F820	S757	D678
SER	T1475	E1409	G1346	V1282	M1212	T1150	A1090	L1020	P957	L883	F821	K758	K758
PRO	E1410	P1283	I1347	P1283	S1151	G1091	G1091	F1021	P958	L884	R822	G759	G759
GLY	Q1477	N1284	E1348	N1284	A1152	Y1092	Y1092	Q1022	L959	E885	A823	G759	G759
THR	L1478	I1285	A1349	I1285	T1153	S1093	S1093	I1023	P960	E886	M824	S760	M882
SER	P1479	T1286	T1350	T1286	E1154	S1094	S1094	L1024	Y961	Q887	A825	F761	K683
PRO	E1480	L1414	R1351	L1287	H1155	L1155	K1095	L1025	N962	V888	G826	I762	E884
THR	G1481	V1288	L1415	L1288	I1219	H1156	N1096	R1026	N963	F889	R827	N763	V685
SER	A1482	Y1289	L1355	L1289	A1220	Y1157	Y1097	S1027	Q964	E828	E827	I764	T686
PRO	E1483	M1416	L1356	M1290	E1221	D1158	T1098	K1028	N965	S895	G829	M767	V689
SER	T1484	D1417	E1357	M1291	S1222	P1159	L1099	F1029	Y966	L830	L830	A769	K690
ALA	A1419	L1419	L1358	E1292	F1223	D1160	G1100	A1030	Q968	Q898	T833	C770	E691
SER	Y1486	A1420	R1359	H1293	P1161	Y1101	Q968	V1031	Q969	K902	A834	G771	V696
ALA	E1487	K1294	M1360	K1294	Q1162	P1102	P1102	K1032	N969	Y903	V835	G772	G772
THR	R1488	G1422	V1361	I1295	L1227	D1163	R1103	X1038	A970	R904	K836	Q773	Q701
GLY	S1489	D1425	I1362	I1295	F1228	D1164	L1104	R1039	Q972	Y906	T837	Q774	Q774
PRO	F1490	D1426	E1363	I1299	I1230	V1165	K1105	L1040	Q973	D906	A838	I775	H705
THR	M1491	D1426	F1364	E1300	A1236	E1167	E1107	L1041	N975	L907	E839	I776	N706
LEU	V1492	G1427	D1365	D1301	D1237	E1168	L1108	K1042	H976	N908	T840	E777	E707
SER	D1493	K1428	G1366	G1302	K1238	D1169	T1109	V1043	E977	E909	G841	G778	L708
PRO	G1429	T1303	S1367	F1304	L1239	K1170	V1110	A1044	Q977	Y942	K843	R779	K709
THR	L1430	F1304	E1368	E1305	I1240	D1171	A1111	F1045	Q978	Y946	T843	G778	P710
SER	S1491	S1431	V1369	E1306	I1241	F1172	K1112	E1046	R979	M917	Q844	R779	K709
PRO	V1497	G1432	M1370	R1306	L1242	Y1173	M1113	W1047	K980	E948	R845	I781	E711
GLY	SER	GLY	SER	GLY	C1243	E1174	I1114	I1048	P981				
SER	PRO	PRO	PRO	PRO									

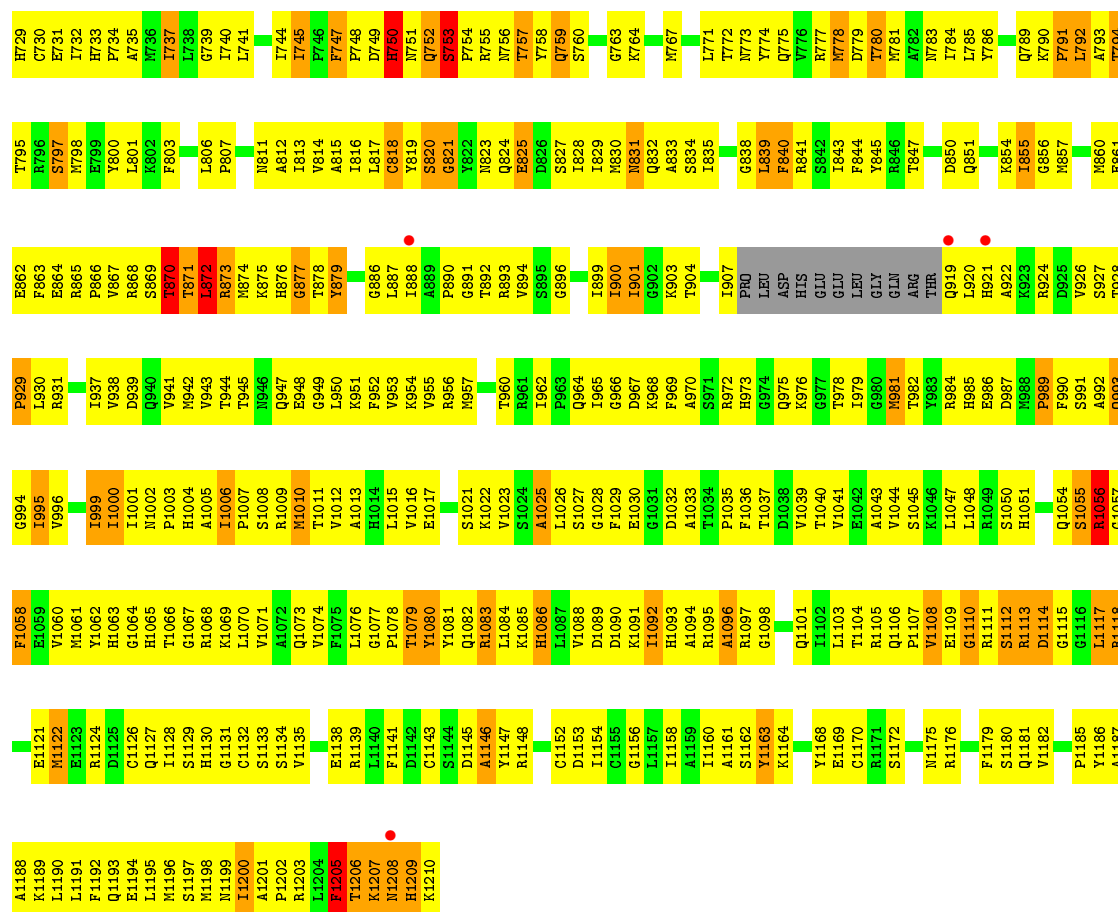
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- Molecule 1: DNA-directed RNA polymerase II subunit rpb1

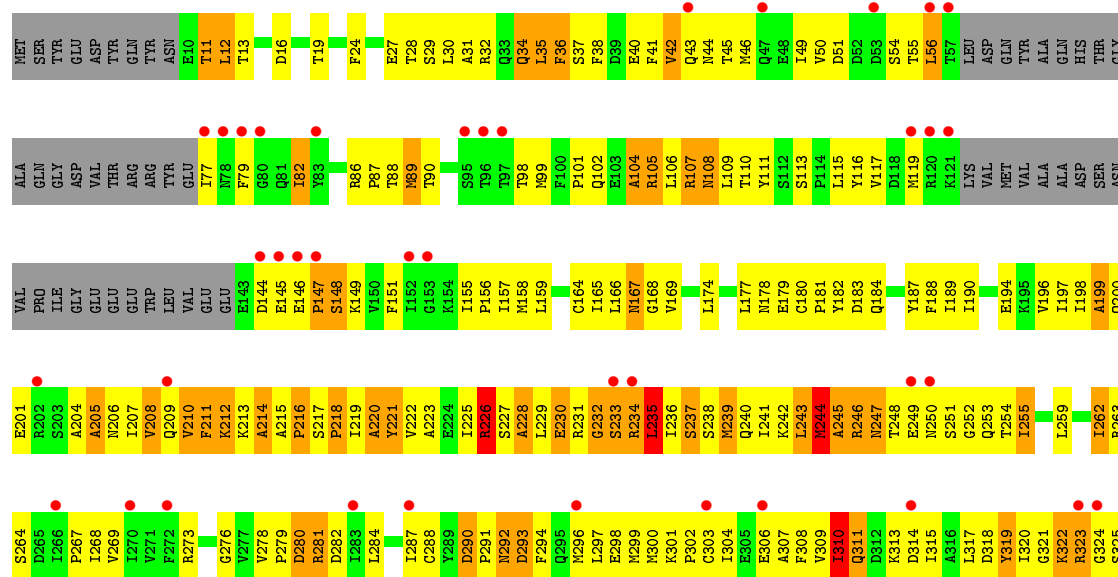


WORLDWIDE
PDB
PROTEIN DATA BANK





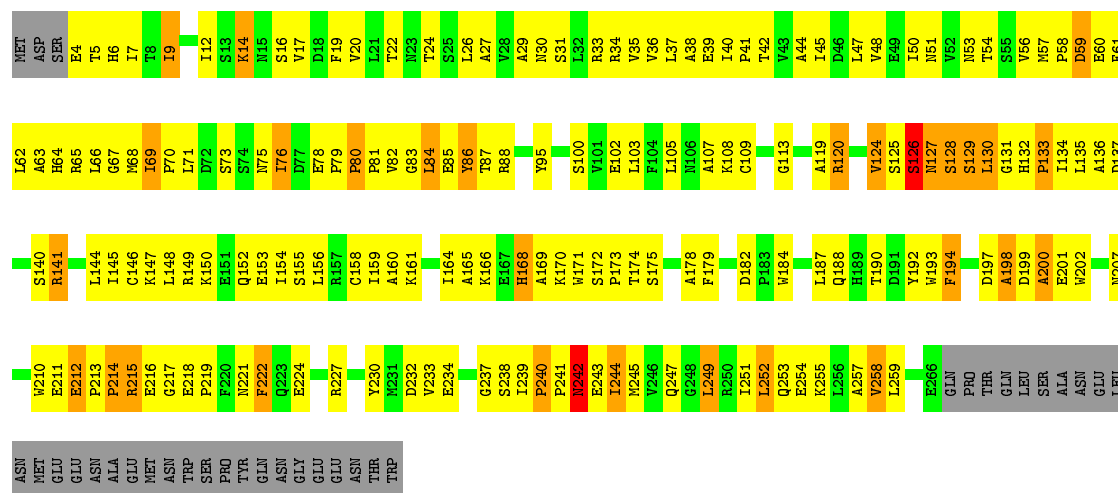
● Molecule 2: DNA-directed RNA polymerase II subunit RPB2





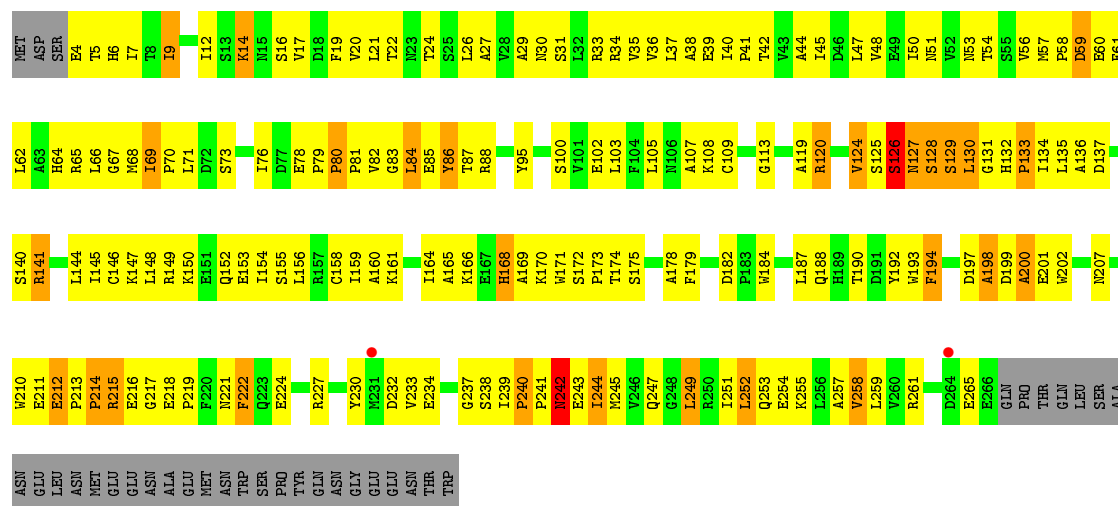
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 



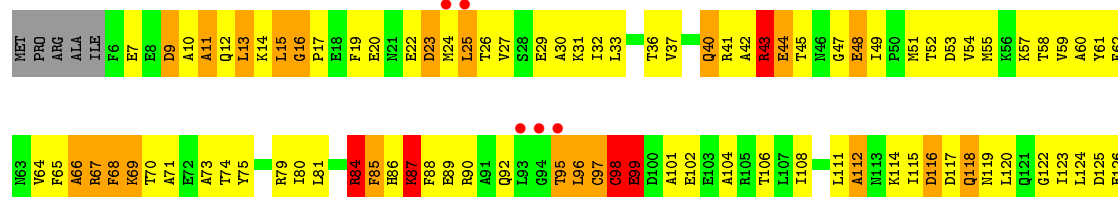
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain O: 



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

Chain D: 



L127
S128
T129
L130
R131
K132
F133
Q134
D135

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

Chain P: 6% 21% 53% 18%

MET PRO ARG ALA ILE F6 E7 E8 D9 A10 A11 Q12 Q13 K14 L15 G16 F17 F18 F19 E20 E21 E22 E23 M24 L25 L26 V27 S28 E29 A30 A31 I32 L33 L34 E35 E36 T36 V37 L38 A39 Q40 R41 A42 A43 R44 E44 T45 R46 G47 G48 E49 I49 F50 M51 T52 D53 V54 M55 M56 K57 T58 V59 A60

Y61 F62 R63 F64 F65 A66 A67 R68 R69 A70 A71 E72 E73 A74 T74 T75 R76 R77 R78 R79 R80 L81 R84 R85 R86 R87 R88 R89 R90 R91 Q92 T95 T96 C97 C98 C99 D100 A101 E102 E103 A104 R105 T106 R107 I108 L111 A112 A113 H114 I115 D116 D117 Q118 M119 L120 Q121 G122 T123 L124

D125 E126 S127 T129 L130 R131 K132 F133 Q134 D135

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

Chain E: 2% 34% 51% 12%

MET SER ALA E4 E5 K6 N7 I8 V9 A14 A15 K16 T17 A18 H19 H20 Q21 L21 Y22 H23 H24 R25 G26 G27 Y28 G29 V29 S30 Q31 A32 E33 K42 A43 A44 M44 H45 C46 G47 R48 G49 R50 N51 L52 D53 B54 T55 T56 L57 S58 F59 Y60 A61 R62 P63 S64 M65 D66 S67 M68 K69 G70

T71 I72 Y73 I74 E75 F76 A77 K78 R79 P80 S81 V82 G83 I84 K85 R86 T89 F90 V91 L94 H97 N98 H99 K100 T101 G102 L103 I104 I105 I106 A107 M108 N109 S113 A114 A115 N117 I118 D119 B120 T121 Q124 F125 T126 I127 A128 T129 F130 S131 Q132 S133 D134 L135 I136

I139 T140 H141 E142 E143 L144 V145 H148 A149 L150 L151 E155 K156 E158 L159 L160 D161 R162 L165 R166 E167 T168 Q169 L170 P171 Q174 L175 D177 P178 R181 Y182 R187 V190 I193 V194 R195 S197 E198 T199 S200 G201 M202 Y206 R207 I208 K209 A210

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

Chain Q: 2% 33% 52% 12%

MET SER ALA E4 E5 K6 N7 I8 V9 A14 A15 K16 T17 A18 H19 H20 Q21 L21 Y22 H23 H24 R25 G26 G27 Y28 G29 V29 S30 Q31 A32 E33 K42 A43 A44 M44 H45 C46 G47 R48 G49 R50 N51 L52 D53 B54 T55 T56 L57 S58 F59 Y60 A61 R62 P63 S64 M65 D66 S67 M68 K69 G70

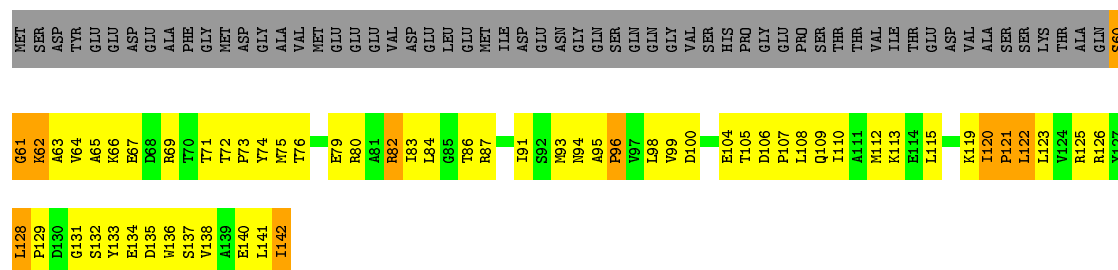
T71 I72 Y73 I74 E75 F76 A77 K78 R79 P80 S81 V82 G83 I84 K85 R86 T89 F90 V91 L94 H97 N98 H99 K100 T101 G102 L103 I104 I105 I106 A107 M108 N109 S113 A114 A115 N117 I118 D119 B120 T121 Q124 F125 T126 I127 A128 T129 F130 S131 Q132 S133 D134 L135 I136

I139 T140 H141 E142 E143 L144 V145 H148 A149 L150 L151 E155 K156 E158 L159 L160 D161 R162 L165 R166 E167 T168 Q169 L170 P171 Q174 L175 D177 P178 R181 Y182 R187 V190 I193 V194 R195 S197 E198 T199 S200 G201 M202 Y206 R207 I208

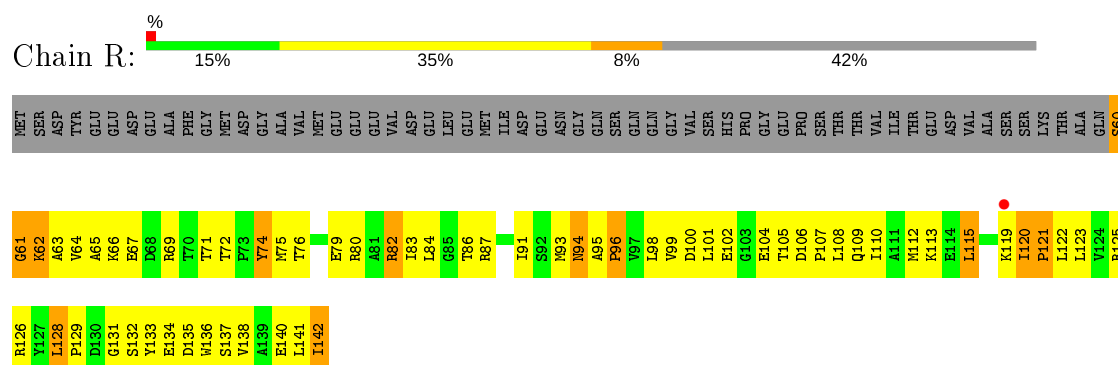
C209 A210

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

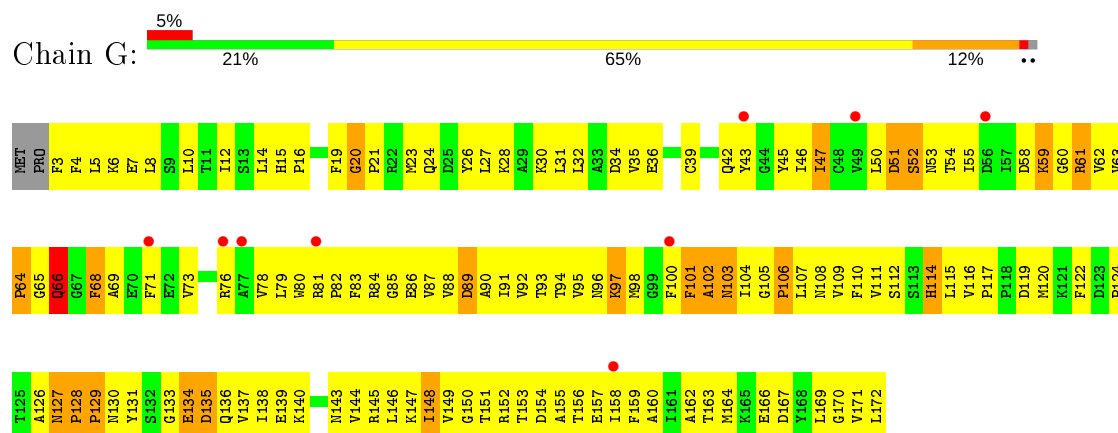
Chain F: 16% 35% 7% 42%



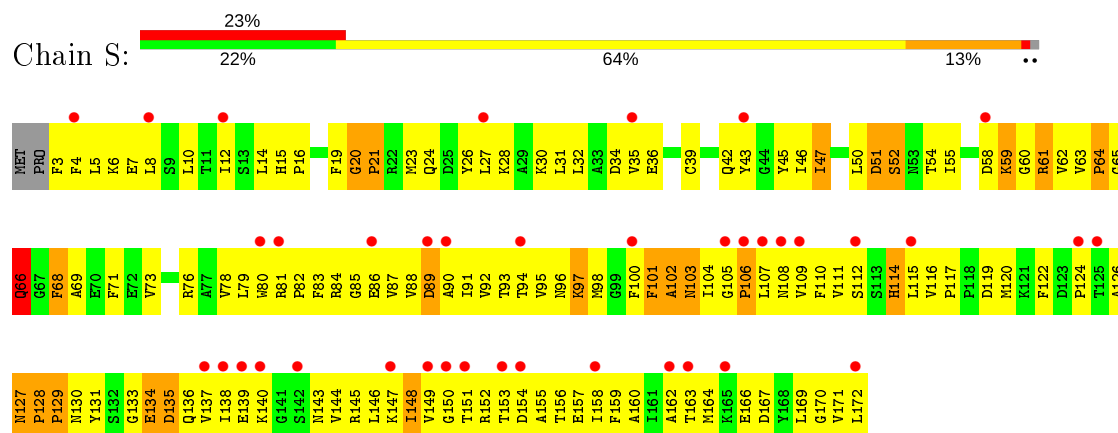
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



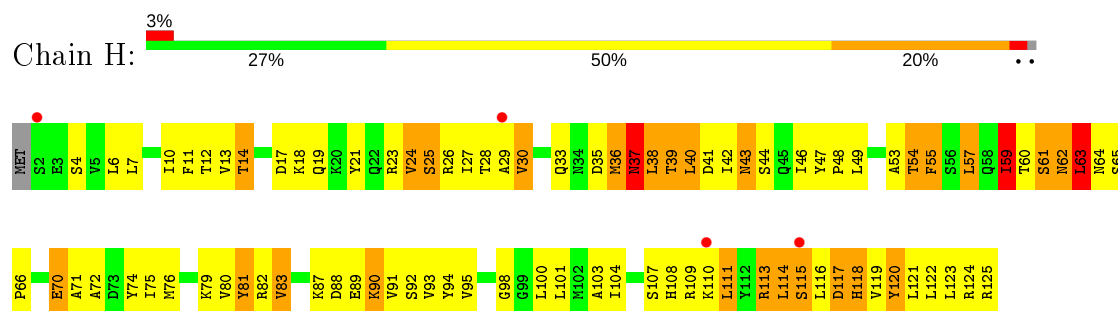
- Molecule 7: DNA-directed RNA polymerase II subunit rpb7



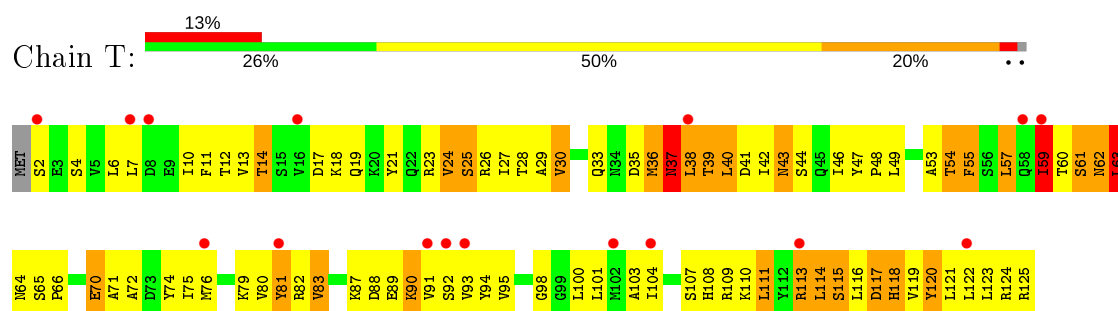
- Molecule 7: DNA-directed RNA polymerase II subunit rpb7



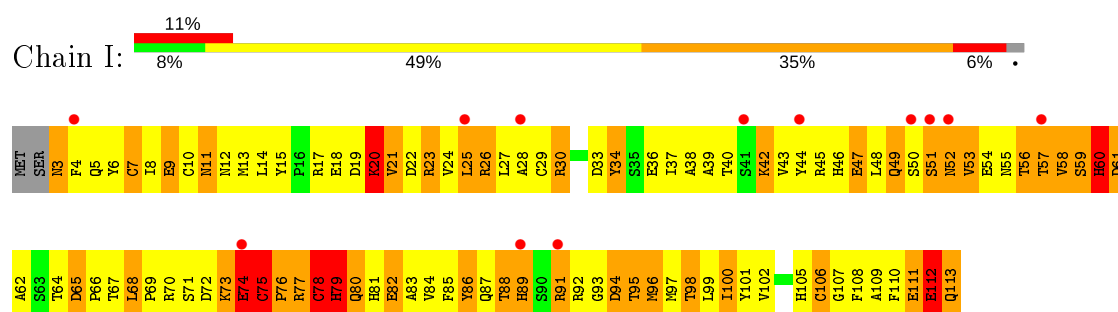
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



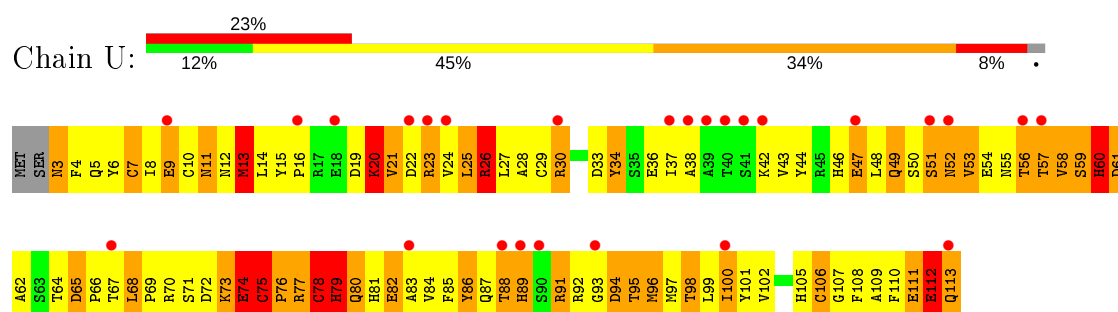
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



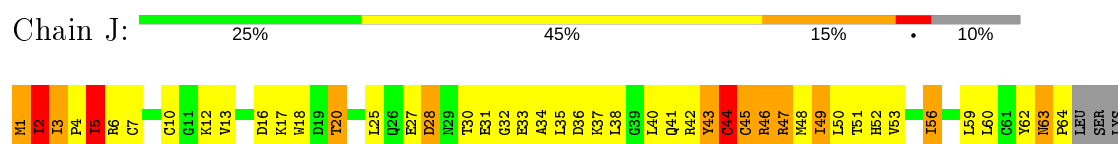
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



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



GLN
LYS
ASN
LEU

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

Chain V: 27% 42% 17% • 10%

M1 I2 I3 P4 I5 I6 C7 C10 G11 G12 K13 V13 D16 K17 W18 D19 T20 L25 Q26 E27 D28 N29 T30 E31 G32 E33 A34 L35 D36 K37 L38 G39 L40 L41 Q41 R42 Y43 C44 R46 R47 M48 I49 L50 T51 H52 V53 I56 L59 Y62 M63 P64 L60 SER LYS GLN

LYS
ASN
LEU

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

Chain K: 30% 57% 10% •

M1 N2 L9 I10 E11 L12 M13 G14 T16 L15 P16 V17 K18 T19 Y20 E21 L22 D23 K25 S26 A29 A30 I31 V32 T33 G32 E33 A34 L35 D36 K37 L38 G39 L40 L41 Q41 R42 Y43 C44 R46 R47 M48 I49 L50 T51 H52 V53 I56 L59 Y62 M63 P64 L60 SER LYS GLN

H68 M69 F70 I71 L72 R73 V74 Q75 T76 W77 E78 C80 S81 P82 K83 Q84 W85 I86 V87 K91 S92 A93 I94 T95 H96 E98 E99 I100 K101 V102 N103 F104 M108 E109 L110 K111 M112 I113 G117 V118 E119 MET GLU PHE SER

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

Chain W: 2% 33% 54% 10% •

M1 N2 P4 L9 I10 E11 L12 M13 G14 L15 P16 K17 V18 T19 Y20 E21 L22 D23 K25 S26 A29 A30 I31 V32 T33 G32 E33 A34 L35 D36 K37 L38 G39 L40 L41 Q41 R42 Y43 C44 R46 R47 M48 I49 L50 T51 H52 V53 I56 L59 Y62 M63 P64 L60 SER LYS GLN

M67 H68 M69 F70 I71 L72 R73 V74 Q75 T76 W77 E78 C80 S81 P82 K83 Q84 W85 I86 V87 K91 S92 A93 I94 T95 H96 E98 E99 I100 K101 V102 N103 F104 M108 E109 L110 K111 M112 I113 G117 V118 E119 MET GLU PHE SER

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

Chain L: 2% 19% 41% 8% • 29%

MET ASN HIS PRO THR SER THR GLY THR THR ALA PHE ASN ASN PRO ARG ARG ALA T19 M20 L21 Y22 L23 L24 A25 D26 C27 G28 A29 R30 N31 T32 A35 K36 E37 V38 I39 R40 C41 R42 E43 C44 R47 V48 M49 Y50 K51 M52 R53 R54 K55 R56 M57 Q58 F59 F60 A62

R63

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

Chain X: 17% 19% 41% 8% • 29%

MET ASN HIS PRO THR SER THR GLY THR THR ALA PHE ASN ASN PRO ARG ARG ALA T19 M20 L21 Y22 L23 L24 A25 D26 C27 G28 A29 R30 N31 T32 A35 K36 E37 V38 I39 R40 C41 R42 E43 C44 R47 V48 M49 Y50 K51 M52 R53 R54 K55 R56 M57 Q58 F59 F60 A62



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 48.69 – 3.65	Depositor EDS
% Data completeness (in resolution range)	92.8 (48.70-3.65) 96.2 (48.69-3.65)	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)	0.26 , 139.6	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	0.88	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 [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	A	0.41	0/12026	0.57	1/16260 (0.0%)
1	M	0.42	0/11887	0.56	1/16069 (0.0%)
2	B	0.44	0/9360	0.60	5/12643 (0.0%)
2	N	0.43	0/9360	0.59	5/12643 (0.0%)
3	C	0.44	0/2135	0.60	0/2904
3	O	0.44	0/2135	0.59	0/2904
4	D	0.24	0/1049	0.38	0/1412
4	P	0.24	0/1049	0.38	0/1412
5	E	0.38	0/1695	0.60	0/2287
5	Q	0.39	0/1695	0.60	0/2287
6	F	0.50	0/666	0.67	0/901
6	R	0.50	0/666	0.67	0/901
7	G	0.26	0/1361	0.57	3/1847 (0.2%)
7	S	0.26	0/1361	0.57	3/1847 (0.2%)
8	H	0.42	0/1010	0.65	0/1363
8	T	0.42	0/1010	0.65	0/1363
9	I	0.22	0/921	0.37	0/1246
9	U	0.24	0/921	0.37	0/1246
10	J	0.57	0/526	0.77	0/709
10	V	0.57	0/526	0.76	0/709
11	K	0.47	0/972	0.61	0/1317
11	W	0.47	0/972	0.61	0/1317
12	L	0.36	0/371	0.57	0/491
12	X	0.37	0/371	0.57	0/491
All	All	0.41	0/64045	0.58	18/86569 (0.0%)

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	992	ALA	N-CA-C	-5.71	95.59	111.00
2	N	992	ALA	N-CA-C	-5.69	95.65	111.00
7	G	167	ASP	CB-CG-OD2	5.38	123.14	118.30
7	S	167	ASP	CB-CG-OD2	5.35	123.12	118.30
2	N	711	ASP	CB-CG-OD2	5.30	123.07	118.30

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	3283	0
1	M	11666	0	11647	3212	0
2	B	9180	0	9163	1630	0
2	N	9180	0	9164	1653	0
3	C	2088	0	2045	267	0
3	O	2088	0	2045	269	0
4	D	1036	0	1025	349	0
4	P	1036	0	1025	318	0
5	E	1663	0	1684	205	0
5	Q	1663	0	1684	209	0
6	F	656	0	679	75	0
6	R	656	0	679	82	0
7	G	1330	0	1329	424	0
7	S	1330	0	1329	425	0
8	H	996	0	1006	168	0
8	T	996	0	1006	178	0
9	I	902	0	840	282	0
9	U	902	0	839	268	0
10	J	518	0	529	90	0
10	V	518	0	529	90	0
11	K	955	0	968	120	0
11	W	955	0	968	113	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	368	0	380	38	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	12749	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 102.

The worst 5 of 12749 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 [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	1494/1752 (85%)	939 (63%)	280 (19%)	275 (18%)	0	1
1	M	1472/1752 (84%)	932 (63%)	281 (19%)	259 (18%)	0	2
2	B	1142/1210 (94%)	735 (64%)	245 (22%)	162 (14%)	0	3
2	N	1142/1210 (94%)	738 (65%)	243 (21%)	161 (14%)	0	3
3	C	261/297 (88%)	178 (68%)	56 (22%)	27 (10%)	0	7
3	O	261/297 (88%)	178 (68%)	56 (22%)	27 (10%)	0	7
4	D	128/135 (95%)	86 (67%)	20 (16%)	22 (17%)	0	2
4	P	128/135 (95%)	86 (67%)	20 (16%)	22 (17%)	0	2
5	E	205/210 (98%)	137 (67%)	43 (21%)	25 (12%)	0	5
5	Q	205/210 (98%)	137 (67%)	43 (21%)	25 (12%)	0	5
6	F	81/142 (57%)	58 (72%)	15 (18%)	8 (10%)	0	8
6	R	81/142 (57%)	57 (70%)	16 (20%)	8 (10%)	0	8
7	G	168/172 (98%)	128 (76%)	24 (14%)	16 (10%)	0	8
7	S	168/172 (98%)	128 (76%)	24 (14%)	16 (10%)	0	8
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	8
10	V	62/71 (87%)	41 (66%)	15 (24%)	6 (10%)	0	8
11	K	117/123 (95%)	80 (68%)	24 (20%)	13 (11%)	0	5
11	W	117/123 (95%)	80 (68%)	24 (20%)	13 (11%)	0	5
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	3

5 of 1226 Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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%)	1113 (86%)	188 (14%)	3	18
1	M	1286/1536 (84%)	1097 (85%)	189 (15%)	3	18
2	B	1012/1064 (95%)	914 (90%)	98 (10%)	8	33
2	N	1012/1064 (95%)	914 (90%)	98 (10%)	8	33
3	C	236/267 (88%)	220 (93%)	16 (7%)	16	47
3	O	236/267 (88%)	220 (93%)	16 (7%)	16	47
4	D	111/115 (96%)	94 (85%)	17 (15%)	2	17
4	P	111/115 (96%)	94 (85%)	17 (15%)	2	17
5	E	182/184 (99%)	169 (93%)	13 (7%)	14	45
5	Q	182/184 (99%)	169 (93%)	13 (7%)	14	45
6	F	71/121 (59%)	64 (90%)	7 (10%)	8	32
6	R	71/121 (59%)	64 (90%)	7 (10%)	8	32
7	G	146/148 (99%)	139 (95%)	7 (5%)	25	56
7	S	146/148 (99%)	139 (95%)	7 (5%)	25	56
8	H	113/114 (99%)	99 (88%)	14 (12%)	4	23
8	T	113/114 (99%)	99 (88%)	14 (12%)	4	23
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
10	V	59/66 (89%)	46 (78%)	13 (22%)	1	6
11	K	109/113 (96%)	104 (95%)	5 (5%)	27	57
11	W	109/113 (96%)	103 (94%)	6 (6%)	21	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	39/53 (74%)	34 (87%)	5 (13%)	4	22
12	X	39/53 (74%)	34 (87%)	5 (13%)	4	22
All	All	6949/7772 (89%)	6135 (88%)	814 (12%)	5	26

5 of 814 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	I	47	GLU
1	M	262	SER
7	S	114	HIS
9	I	94	ASP
1	M	48	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 225 such sidechains are listed below:

Mol	Chain	Res	Type
8	H	33	GLN
1	M	395	GLN
6	R	94	ASN
9	I	55	ASN
1	M	48	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 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 [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	1496/1752 (85%)	0.16	84 (5%) 24 16	51, 150, 385, 628	0
1	M	1476/1752 (84%)	0.53	174 (11%) 4 3	83, 199, 449, 672	0
2	B	1150/1210 (95%)	0.05	27 (2%) 60 46	69, 143, 314, 580	0
2	N	1150/1210 (95%)	0.55	118 (10%) 6 4	85, 222, 419, 618	0
3	C	263/297 (88%)	-0.18	0 100 100	80, 126, 252, 477	0
3	O	263/297 (88%)	0.08	2 (0%) 86 77	125, 190, 350, 511	0
4	D	130/135 (96%)	0.32	5 (3%) 40 28	128, 240, 360, 596	0
4	P	130/135 (96%)	0.55	8 (6%) 20 13	152, 287, 414, 545	0
5	E	207/210 (98%)	-0.15	5 (2%) 59 45	70, 164, 293, 516	0
5	Q	207/210 (98%)	-0.05	4 (1%) 66 53	119, 181, 373, 501	0
6	F	83/142 (58%)	-0.49	0 100 100	70, 97, 170, 232	0
6	R	83/142 (58%)	-0.35	1 (1%) 79 68	111, 126, 200, 335	0
7	G	170/172 (98%)	0.35	9 (5%) 26 18	92, 199, 323, 514	0
7	S	170/172 (98%)	1.07	39 (22%) 0 0	122, 240, 388, 494	0
8	H	124/125 (99%)	0.14	4 (3%) 47 34	82, 138, 298, 408	0
8	T	124/125 (99%)	0.60	16 (12%) 3 3	115, 197, 344, 429	0
9	I	111/113 (98%)	0.50	12 (10%) 5 4	98, 239, 367, 549	0
9	U	111/113 (98%)	1.63	26 (23%) 0 0	151, 330, 482, 585	0
10	J	64/71 (90%)	-0.20	0 100 100	85, 108, 220, 304	0
10	V	64/71 (90%)	0.04	0 100 100	137, 203, 326, 373	0
11	K	119/123 (96%)	-0.34	0 100 100	60, 126, 221, 319	0
11	W	119/123 (96%)	0.15	3 (2%) 57 43	76, 168, 295, 470	0
12	L	45/63 (71%)	-0.02	1 (2%) 62 48	93, 177, 299, 481	0
12	X	45/63 (71%)	1.00	11 (24%) 0 0	153, 277, 425, 580	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	7904/8826 (89%)	0.29	549 (6%) 16 11	51, 181, 397, 672	0

The worst 5 of 549 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	U	41	SER	21.8
9	U	40	THR	16.2
9	U	39	ALA	14.8
11	W	119	GLU	14.5
1	A	107	CYS	12.1

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 carbohydrates 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	0.27	0.39	197,197,197,197	0
14	MG	A	2458	1/1	0.54	1.81	109,109,109,109	0
13	ZN	M	2456	1/1	0.63	0.26	432,432,432,432	0
13	ZN	A	2456	1/1	0.68	0.06	245,245,245,245	0
13	ZN	O	1269	1/1	0.70	0.11	189,189,189,189	0
13	ZN	U	1122	1/1	0.80	0.06	240,240,240,240	0
13	ZN	N	2225	1/1	0.80	0.22	180,180,180,180	0
13	ZN	I	1121	1/1	0.83	0.06	160,160,160,160	0
13	ZN	I	1122	1/1	0.83	0.10	126,126,126,126	0
13	ZN	X	1071	1/1	0.83	0.05	195,195,195,195	0
13	ZN	M	2457	1/1	0.83	0.14	172,172,172,172	0
13	ZN	L	1071	1/1	0.87	0.09	123,123,123,123	0
13	ZN	U	1121	1/1	0.90	0.06	284,284,284,284	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
13	ZN	C	1269	1/1	0.91	0.07	122,122,122,122	0
13	ZN	A	2457	1/1	0.94	0.20	122,122,122,122	0
13	ZN	B	2225	1/1	0.94	0.17	149,149,149,149	0
13	ZN	V	1066	1/1	0.96	0.20	155,155,155,155	0
13	ZN	J	1066	1/1	0.97	0.22	87,87,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.