



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 03:10 am BST

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

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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



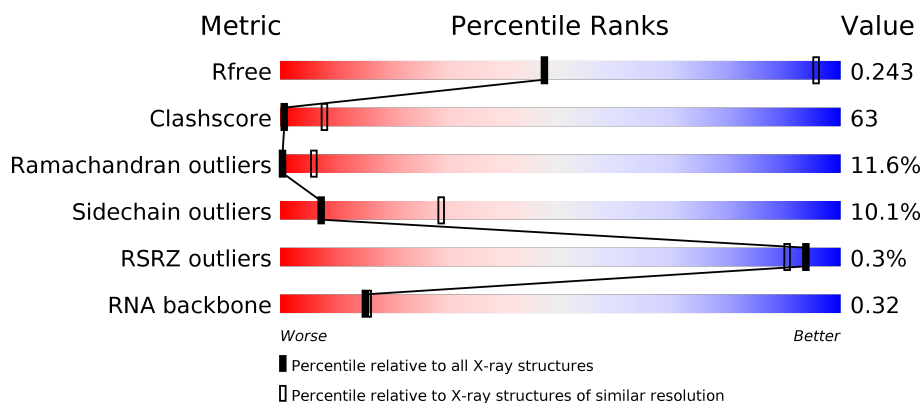
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)
RNA backbone	3102	1048 (5.00-3.00)


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  $\geq 3$ , 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	B	1733	
2	C	1224	
3	D	318	
4	E	221	

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



## 2 Entry composition [i](#)

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

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	1416	Total	C	N	O	S	0	0	0
			11140	7021	1946	2111	62			

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

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

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

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

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

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

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

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

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

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



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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

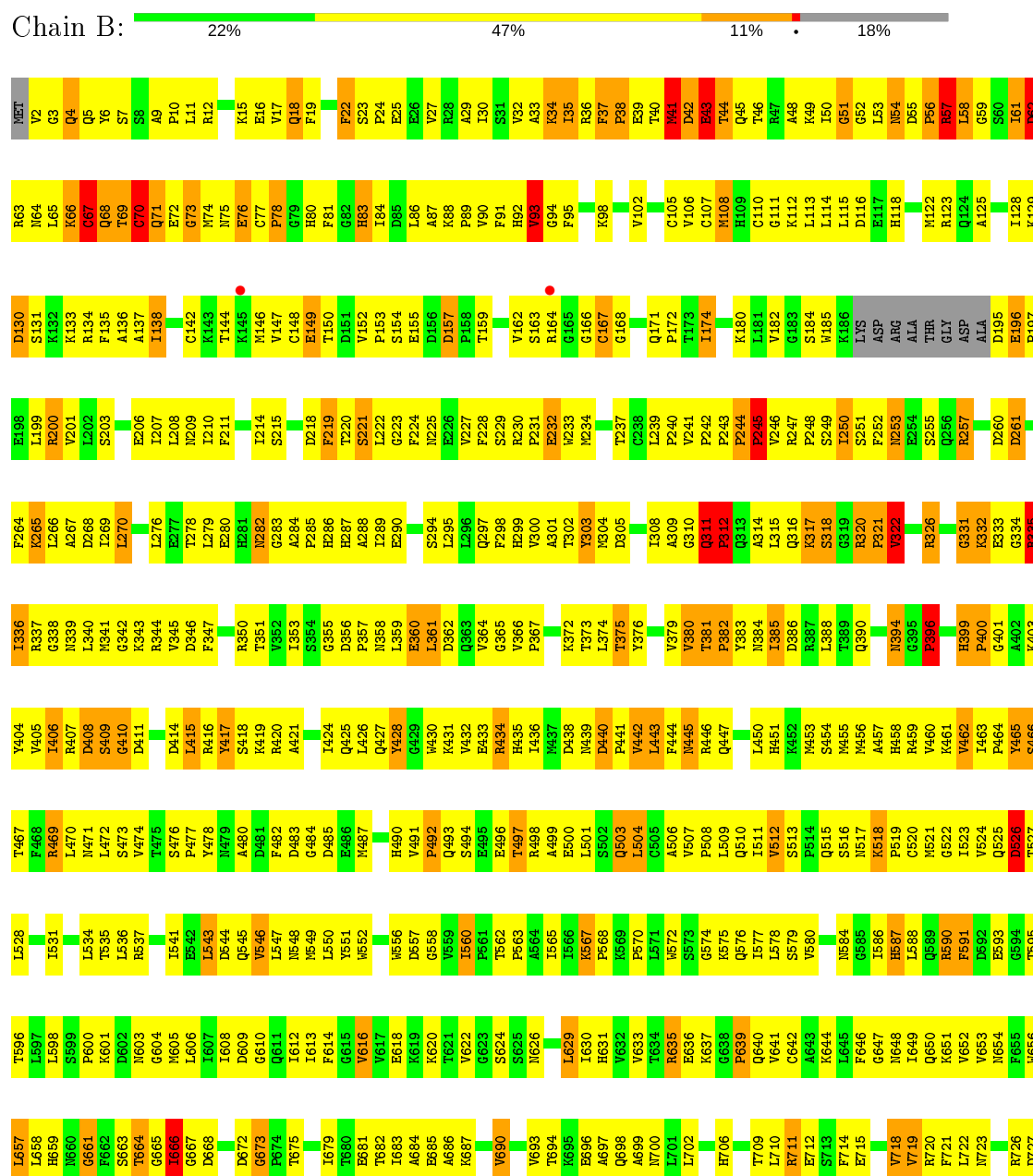
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	B	1	Total	Mg	0	0
			1	1		



### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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





PRO	SER	SER	PRO	SER	GLY	D1446	T1385	T1318	E1256	S1189	A1126	M1063	K1003	V937	I867	E801	K728
SER	PRO	THR	THR	THR	PHE	E1447	R1386	V1319	M1259	L1192	D1127	V1064	M1004	R940	Y868	N802	A729
SER	THR	ALA	ALA	ALA	THR	S1448	F1389	G1321	L1260	L1193	Q1128	G1065	I1006	R941	G869	S803	
PRO	PRO	PRO	PRO	PRO	TYR	V1450	R1390	I1322	K1261	R1194	Q1130	E1086	I1006	K941	E870	Y804	L732
THR	SER	GLY	GLY	GLY	GLY	V1451	R1391	D1323	K1262		A1131	A1068	Q1008	L943	G872	R806	V735
PRO	THR	GLY	GLY	GLY	GLY		S1392	P1324	T1263	L1197	K1132		Q1009	R944	M873	G807	M736
ASN	SER	ASP	ASP	ASP	ASP		R1393	T1325	E1264	D1196	L1133		A1010	E945	D874	L808	L737
GLN	PRO	GLN	GLN	GLN	GLN		P1455	R1326	M1265	A1201	I1134		Q1011	V946	K738	T809	K739
GLY	PRO	GLY	GLY	GLY	GLY		P1456	R1327	T1266			G1073	R1012	F947	D739	L740	L740
THR	THR	THR	THR	THR	THR			T1329	M1267	A1202	A1137	E1074	D1013	R947	E812	E812	E812
THR	THR	THR	THR	THR	THR			M1330	E1268		T1138	A1076	A1014	V948	F813	F814	N741
THR	THR	THR	THR	THR	THR			S1331	E1269	K1205	H1139	T1077	V1015		F814	F815	N742
PRO	PRO	PRO	PRO	PRO	PRO			F1332	M1270	D1206	H1140	Q1078	T1016		F815	F816	V743
PRO	PRO	PRO	PRO	PRO	PRO			I1333	T1271	L1207	T1141	M1079	L1017		A817	A817	V747
THR	THR	THR	THR	THR	THR			D1334	T1272	T1208	T1142	T1080	F1018		M818	M818	
GLY	GLY	GLY	GLY	GLY	GLY			I1335	R1273	M1209	L1143	L1081	C1019		G819	G819	S751
GLY	GLY	GLY	GLY	GLY	GLY			M1336	R1274	G1210	K1144	ASN	C1020		G820	G820	K752
THR	THR	THR	THR	THR	THR			E1337	G1275	V1211	T1145	THR	L1021		R831	R831	G753
GLY	GLY	GLY	GLY	GLY	GLY			T1338	V1276	V1212	V1146	PHE	L1022		S754	S754	
GLY	GLY	GLY	GLY	GLY	GLY			L1339	T1277	G1213	T1147	HIS	R1023		F755	F755	
GLY	GLY	GLY	GLY	GLY	GLY			G1340	M1278	E1214	T1148	PHE	S1024		D826	D826	I756
THR	THR	THR	THR	THR	THR			I1341	E1280	R1215	A1149	ALA	R1025		T827	T827	N757
THR	THR	THR	THR	THR	THR			A1342	E1281		S1150	GLY	L1026		A828	A828	I758
PRO	PRO	PRO	PRO	PRO	PRO			A1343	V1282	T1219	T1152	ALA	T1028		R829	R829	A759
GLY	GLY	GLY	GLY	GLY	GLY			G1344	V1283	F1220	V1153	SER	R1029		K830	K830	Q760
PRO	PRO	PRO	PRO	PRO	PRO			R1345	M1284	K1221	V1154	K1093	R1030		M761	M761	Q761
ALA	ALA	ALA	ALA	ALA	ALA			A1346		N1222	D1155	T1094	V1031		S762	S762	
GLY	GLY	GLY	GLY	GLY	GLY			A1347	Y1287	D1223	P1156	T1095	L1032		T834	T834	A763
GLY	GLY	GLY	GLY	GLY	GLY			L1348	R1288	L1224	D1157	S1096	Q1033		G835	G835	C764
GLY	GLY	GLY	GLY	GLY	GLY			Y1349	R1289	F1225	P1158	G1097	E1034		Y836	Y836	V765
GLY	GLY	GLY	GLY	GLY	GLY			K1350	E1290	V1226	R1159		Y1035		G766	G766	
GLY	GLY	GLY	GLY	GLY	GLY			E1351	V1291	I1227	S1160	K1036	R1037		R839	R839	Q767
GLY	GLY	GLY	GLY	GLY	GLY			D1352	P1292	W1228	T1161	L1037	T907		K840	K840	Q768
GLY	GLY	GLY	GLY	GLY	GLY			C1421	S1293	S1229	V1162	T1038	T976		K843	K843	
GLY	GLY	GLY	GLY	GLY	GLY			M1354	P1294	E1230	T1163	K1039	K977		A844	A844	K773
GLY	GLY	GLY	GLY	GLY	GLY			V1355	T1295	D1231	P1164	E1103	Q1040		L845	L845	R774
GLY	GLY	GLY	GLY	GLY	GLY				G1296	N1232	E1165	L1104	A1041		E846	E846	I775
GLY	GLY	GLY	GLY	GLY	GLY			D1359	E1297		E1167	L1105	F1042		D847	D847	F779
GLY	GLY	GLY	GLY	GLY	GLY				Y1298	L1236		M1106	D1043		I848	I848	V780
GLY	GLY	GLY	GLY	GLY	GLY			M1364	V1299	I1237		T1107	W1044		M849	M849	D781
GLY	GLY	GLY	GLY	GLY	GLY			Y1365	K1300	R1238		K1109	L1045		V850	V850	R782
GLY	GLY	GLY	GLY	GLY	GLY			R1366	E1301	R1239		M1110	S1047		H851	H851	T783
GLY	GLY	GLY	GLY	GLY	GLY			H1367	P1302	C1240		M1111	N1048		Y852	Y852	L784
GLY	GLY	GLY	GLY	GLY	GLY			M1368	W1304	R1241	F1174	K1112	D922		D853	D853	P785
GLY	GLY	GLY	GLY	GLY	GLY			A1369	E1303	V1242	S1175	T1113	E1050		N854	N854	H786
GLY	GLY	GLY	GLY	GLY	GLY			L1370	L1305	V1243	L1176	P1114	A1051		T855	T855	F787
GLY	GLY	GLY	GLY	GLY	GLY			L1371	L1306	ARG	LEU	P1114	A1051		T856	T856	S788
GLY	GLY	GLY	GLY	GLY	GLY			V1372	E1307	PRO	ASP	S1115	Q1052		R857	R857	K789
GLY	GLY	GLY	GLY	GLY	GLY			D1373	T1308	LYS	GLU	L1116	F1053		L858	L858	
GLY	GLY	GLY	GLY	GLY	GLY			V1374	D1309	SER	GLU	T1117	L1054		S793	S793	
GLY	GLY	GLY	GLY	GLY	GLY			M1375	E1310	LEU	ALA	T1118	R1055		S859	S859	P794
GLY	GLY	GLY	GLY	GLY	GLY			T1376	V1311	ASP	GLU	Y1119	S1056		G861	G861	E795
GLY	GLY	GLY	GLY	GLY	GLY			T1377	M1312	ALA	GLN	L1120	V1057		V862	V862	S796
GLY	GLY	GLY	GLY	GLY	GLY			T1378	M1313	GLU	SER	E1121	V1058		V863	V863	K797
GLY	GLY	GLY	GLY	GLY	GLY			G1379	S1314	THR	PHE	P1122	H1059		L864	L864	G798
GLY	GLY	GLY	GLY	GLY	GLY			G1380	E1315	GLY	ASP	G1123	P1060		Q865	Q865	F799
GLY	GLY	GLY	GLY	GLY	GLY			L1381	M1316	ALA	Q1187	G1123	G1061		V866	V866	
GLY	GLY	GLY	GLY	GLY	GLY				M1317	E1255	Q1188	A1125	E1062				



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

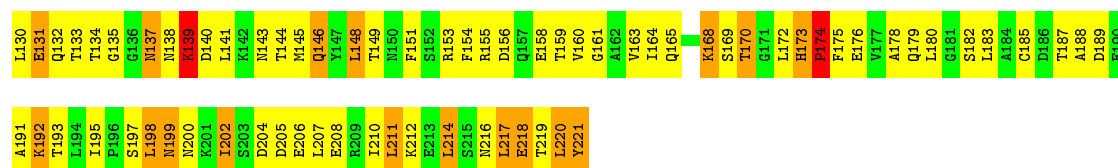
Chain C: 

MET	SER	ASP	LEU	ALA	ASN	SER	GLU	LYS	LEU	GLN	TYR	THR	ASP	GLU	ASP	ASP	PRO	THR	GLY	PHE	GLU	D20	D29	S30	S31	S91	A32	V33	S34	S35	S36	S37	S38	S39	S40	S41	S42	S43	S44	S45	S46	S47	S48	S49	S50	S51	S52	S53	S54	S55	S56	S57	S58	S59	S60	S61	S62	S63	S64	S65	S66	S67	S68	S69	S70	S71	S72	S73	S74	S75	S76	S77	S78	S79	S80	S81	S82	S83	S84	S85	S86	S87	S88	S89	S90	S91	S92	S93	S94	S95	S96	S97	S98	S99	S100	S101	S102	S103	S104	S105	S106	S107	S108	S109	S110	S111	S112	S113	S114	S115	S116	S117	S118	S119	S120	S121	S122	S123	S124	S125	S126	S127	S128	S129	S130	S131	S132	S133	S134	S135	S136	S137	S138	S139	S140	S141	S142	S143	S144	S145	S146	S147	S148	S149	S150	S151	S152	S153	S154	S155	S156	S157	S158	S159	S160	S161	S162	S163	S164	S165	S166	S167	S168	S169	S170	S171	S172	S173	S174	S175	S176	S177	S178	S179	S180	S181	S182	S183	S184	S185	S186	S187	S188	S189	S190	S191	S192	S193	S194	S195	S196	S197	S198	S199	S200	S201	S202	S203	S204	S205	S206	S207	S208	S209	S210	S211	S212	S213	S214	S215	S216	S217	S218	S219	S220	S221	S222	S223	S224	S225	S226	S227	S228	S229	S230	S231	S232	S233	S234	S235	S236	S237	S238	S239	S240	S241	S242	S243	S244	S245	S246	S247	S248	S249	S250	S251	S252	S253	S254	S255	S256	S257	S258	S259	S260	S261	S262	S263	S264	S265	S266	S267	S268	S269	S270	S271	S272	S273	S274	S275	S276	S277	S278	S279	S280	S281	S282	S283	S284	S285	S286	S287	S288	S289	S290	S291	S292	S293	S294	S295	S296	S297	S298	S299	S300	S301	S302	S303	S304	S305	S306	S307	S308	S309	S310	S311	S312	S313	S314	S315	S316	S317	S318	S319	S320	S321	S322	S323	S324	S325	S326	S327	S328	S329	S330	S331	S332	S333	S334	S335	S336	S337	S338	S339	S340	S341	S342	S343	S344	S345	S346	S347	S348	S349	S350	S351	S352	S353	S354	S355	S356	S357	S358	S359	S360	S361	S362	S363	S364	S365	S366	S367	S368	S369	S370	S371	S372	S373	S374	S375	S376	S377	S378	S379	S380	S381	S382	S383	S384	S385	S386	S387	S388	S389	S390	S391	S392	S393	S394	S395	S396	S397	S398	S399	S400	S401	S402	S403	S404	S405	S406	S407	S408	S409	S410	S411	S412	S413	S414	S415	S416	S417	S418	S419	S420	S421	S422	S423	S424	S425	S426	S427	S428	S429	S430	S431	S432	S433	S434	S435	S436	S437	S438	S439	S440	S441	S442	S443	S444	S445	S446	S447	S448	S449	S450	S451	S452	S453	S454	S455	S456	S457	S458	S459	S460	S461	S462	S463	S464	S465	S466	S467	S468	S469	S470	S471	S472	S473	S474	S475	S476	S477	S478	S479	S480	S481	S482	S483	S484	S485	S486	S487	S488	S489	S490	S491	S492	S493	S494	S495	S496	S497	S498	S499	S500	S501	S502	S503	S504	S505	S506	S507	S508	S509	S510	S511	S512	S513	S514	S515	S516	S517	S518	S519	S520	S521	S522	S523	S524	S525	S526	S527	S528	S529	S530	S531	S532	S533	S534	S535	S536	S537	S538	S539	S540	S541	S542	S543	S544	S545	S546	S547	S548	S549	S550	S551	S552	S553	S554	S555	S556	S557	S558	S559	S560	S561	S562	S563	S564	S565	S566	S567	S568	S569	S570	S571	S572	S573	S574	S575	S576	S577	S578	S579	S580	S581	S582	S583	S584	S585	S586	S587	S588	S589	S590	S591	S592	S593	S594	S595	S596	S597	S598	S599	S600	S601	S602	S603	S604	S605	S606	S607	S608	S609	S610	S611	S612	S613	S614	S615	S616	S617	S618	S619	S620	S621	S622	S623	S624	S625	S626	S627	S628	S629	S630	S631	S632	S633	S634	S635	S636	S637	S638	S639	S640	S641	S642	S643	S644	S645	S646	S647	S648	S649	S650	S651	S652	S653	S654	S655	S656	S657	S658	S659	S660	S661	S662	S663	S664	S665	S666	S667	S668	S669	S670	S671	S672	S673	S674	S675	S676	S677	S678	S679	S680	S681	S682	S683	S684	S685	S686	S687	S688	S689	S690	S691	S692	S693	S694	S695	S696	S697	S698	S699	S700	S701	S702	S703	S704	S705	S706	S707	S708	S709	S710	S711	S712	S713	S714	S715	S716	S717	S718	S719	S720	S721	S722	S723	S724	S725	S726	S727	S728	S729	S730	S731	S732	S733	S734	S735	S736	S737	S738	S739	S740	S741	S742	S743	S744	S745	S746	S747	S748	S749	S750	S751	S752	S753	S754	S755	S756	S757	S758	S759	S760	S761	S762	S763	S764	S765	S766	S767	S768	S769	S770	S771	S772	S773	S774	S775	S776	S777	S778	S779	S780	S781	S782	S783	S784	S785	S786	S787	S788	S789	S790	S791	S792	S793	S794	S795	S796	S797	S798	S799	S800	S801	S802	S803	S804	S805	S806	S807	S808	S809	S810	S811	S812	S813	S814	S815	S816	S817	S818	S819	S820	S821	S822	S823	S824	S825	S826	S827	S828	S829	S830	S831	S832	S833	S834	S835	S836	S837	S838	S839	S840	S841	S842	S843	S844	S845	S846	S847	S848	S849	S850	S851	S852	S853	S854	S855	S856	S857	S858	S859	S860	S861	S862	S863	S864	S865	S866	S867	S868	S869	S870	S871	S872	S873	S874	S875	S876	S877	S878	S879	S880	S881	S882	S883	S884	S885	S886	S887	S888	S889	S890	S891	S892	S893	S894	S895	S896	S897	S898	S899	S900	S901	S902	S903	S904	S905	S906	S907	S908	S909	S910	S911	S912	S913	S914	S915	S916	S917	S918	S919	S920	S921	S922	S923	S924	S925	S926	S927	S928	S929	S930	S931	S932	S933	S934	S935	S936	S937	S938	S939	S940	S941	S942	S943	S944	S945	S946	S947	S948	S949	S950	S951	S952	S953	S954	S955	S956	S957	S958	S959	S960	S961	S962	S963	S964	S965	S966	S967	S968	S969	S970	S971	S972	S973	S974	S975	S976	S977	S978	S979	S980	S981	S982	S983	S984	S985	S986	S987	S988	S989	S990	S991	S992	S993	S994	S995	S996	S997	S998	S999	S1000	S1001	S1002	S1003	S1004	S1005	S1006	S1007	S1008	S1009	S1010	S1011	S1012	S1013	S1014	S1015	S1016	S1017	S1018	S1019	S1020	S1021	S1022	S1023	S1024	S1025	S1026	S1027	S1028	S1029	S1030	S1031	S1032	S1033	S1034	S1035	S1036	S1037	S1038	S1039	S1040	S1041	S1042	S1043	S1044	S1045	S1046	S1047	S1048	S1049	S1050	S1051	S1052	S1053	S1054	S1055	S1056	S1057	S1058	S1059	S1060	S1061	S1062	S1063	S1064	S1065	S1066	S1067	S1068	S1069	S1070	S1071	S1072	S1073	S1074	S1075	S1076	S1077	S1078	S1079	S1080	S1081	S1082	S1083	S1084	S1085	S1086	S1087	S1088	S1089	S1090	S1091	S1092	S1093	S1094	S1095	S1096	S1097	S1098	S1099	S1100	S1101	S1102	S1103	S1104	S1105	S1106	S1107	S1108	S1109	S1110	S1111	S1112	S1113	S1114	S1115	S1116	S1117	S1118	S1119	S1120	S1121	S1122	S1123	S1124	S1125	S1126	S1127	S1128	S1129	S1130	S1131	S1132	S1133	S1134	S1135	S1136	S1137	S1138	S1139	S1140	S1141	S1142	S1143	S1144	S1145	S1146	S1147	S1148	S1149	S1150	S1151	S1152	S1153	S1154	S1155	S1156	S1157	S1158	S1159	S1160	S1161	S1162	S1163	S1164	S1165	S1166	S1167	S1168	S1169	S1170	S1171	S1172	S1173	S1174	S1175	S1176	S1177	S1178	S1179	S1180	S1181	S1182	S1183	S1184	S1185	S1186	S1187	S1188	S1189	S1190	S1191	S1192	S1193	S1194	S1195	S1196	S1197	S1198	S1199	S1200	S1201	S1202	S1203	S1204	S1205	S1206	S1207	S1208	S1209	S1210	S1211	S1212	S1213	S1214	S1215	S1216	S1217	S1218	S1219	S1220	S1221	S1222	S1223	S1224	S1225	S1226	S1227	S1228	S1229	S1230	S1231	S1232	S1233	S1234	S1235	S1236	S1237	S1238	S1239	S1240	S1241	S1242	S1243	S1244	S1245	S1246	S1247	S1248	S1249	S1250	S1251	S1252	S1253	S1254	S1255	S1256	S1257	S1258	S1259	S1260	S1261	S1262	S1263	S1264	S1265	S1266	S1267	S1268	S1269	S1270	S1271	S1272	S1273	S1274	S1275	S1276	S1277	S1278	S1279	S1280	S1281	S1282	S1283	S1284	S1285	S1286	S1287	S1288	S1289	S1290	S1291	S1292	S1293	S1294	S1295	S1296	S1297	S1298	S1299	S1300	S1301	S1302	S1303	S1304	S1305	S1306	S1307	S1308	S1309	S1310	S1311	S1312	S1313	S1314	S1315	S1316	S1317	S1318	S1319	S1320	S1321	S1322	S1323	S1324	S1325	S1326	S1327	S1328	S1329	S1330	S1331	S1332	S1333	S1334	S1335	S1336	S1337	S1338	S1339	S1340	S1341	S1342	S1343	S1344	S1345	S1346	S1347	S1348	S1349	S1350	S1351	S1352	S1353	S1354	S1355	S1356	S1357	S1358	S1359	S1360	S1361	S1362	S1363	S1364	S1365	S1366	S1367	S1368	S1369	S1370	S1371	S1372	S1373	S1374	S1375	S1376	S1377	S1378	S1379	S1380	S1381	S1382	S1383	S1384	S1385	S1386	S1387	S1388	S1389	S1390	S1391	S1392	S1393	S1394	S1395	S1396	S1397	S1398	S1399	S1400	S1401	S1402	S1403	S1404	S1405	S1406	S1407	S1408	S1409	S1410	S1411	S1412	S1413	S1414	S1415	S1416	S1417	S1418	S1419	S1420	S1421	S1422	S1423	S1424	S1425	S1426	S1427	S1428	S1429	S1430	S1431	S1432	S1433	S1434	S1435	S1436	S1437	S1438	S1439	S1440	S1441	S1442	S1443	S1444	S1445	S1446	S1447	S1448	S1449	S1450	S1451	S1452	S1453	S1454	S1455	S1456	S1457	S1458	S1459	S1460	S1461	S1462	S1463	S1464	S1465	S1466	S1467	S1468	S1469	S1470	S147
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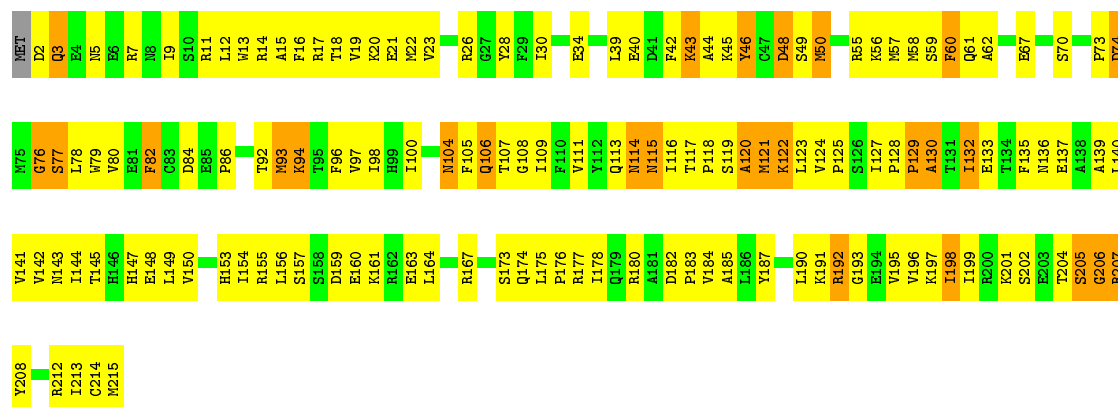






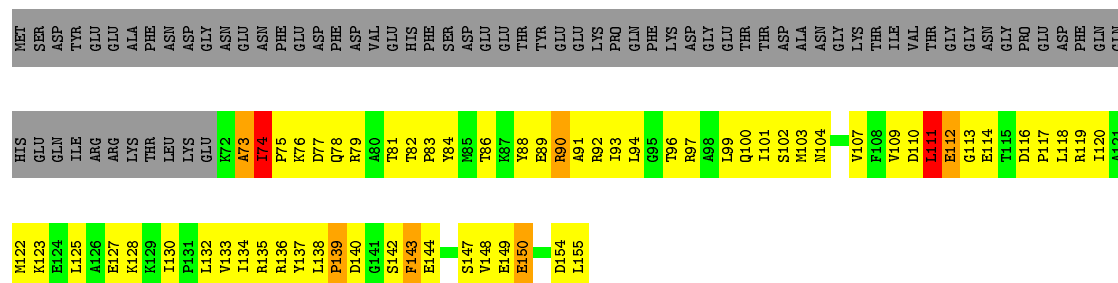
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain F: 33% 53% 13%



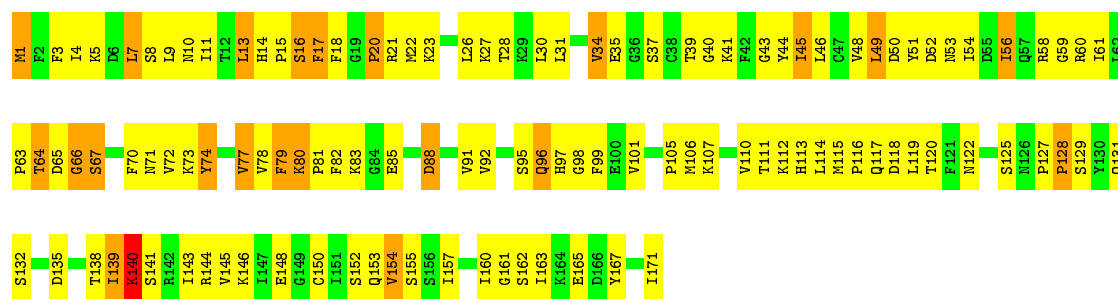
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain G: 14% 35% 46%



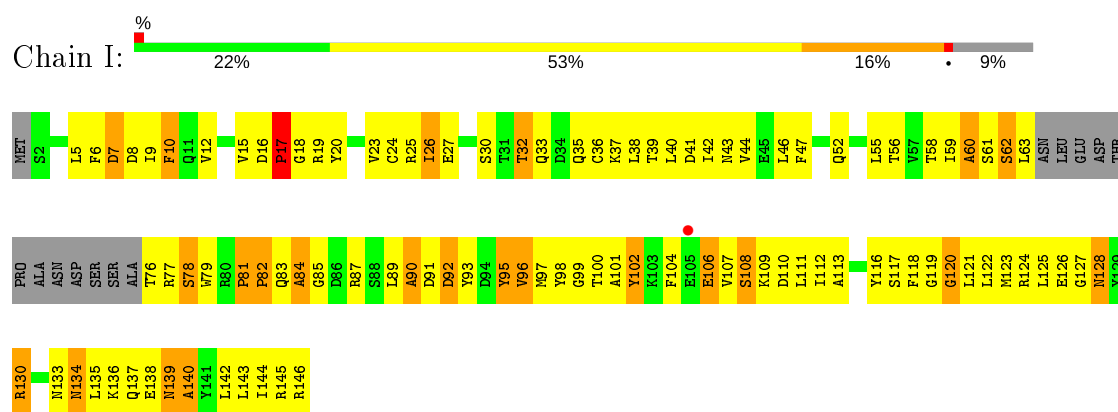
• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain H: 32% 55% 13%

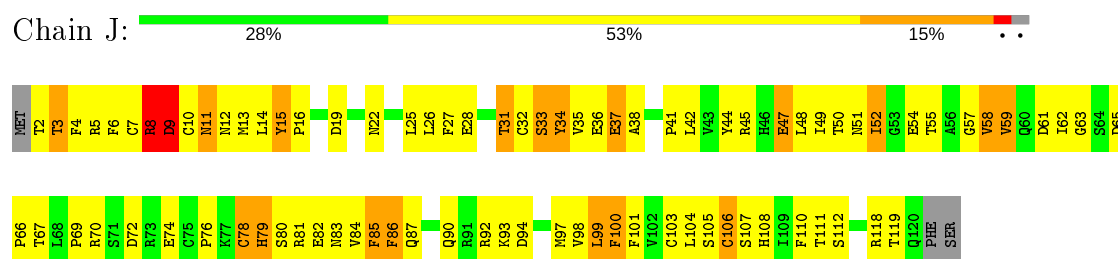


• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

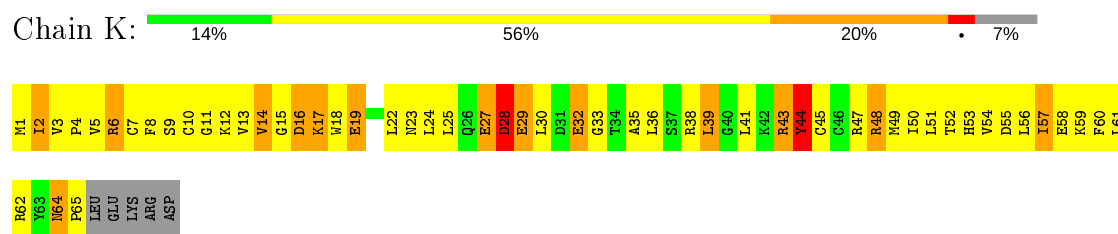




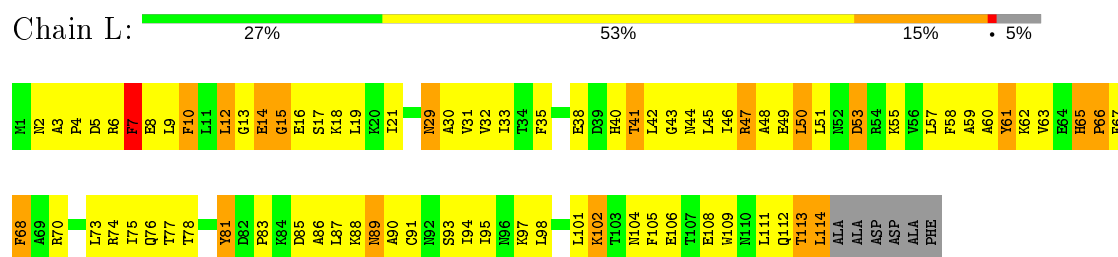
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



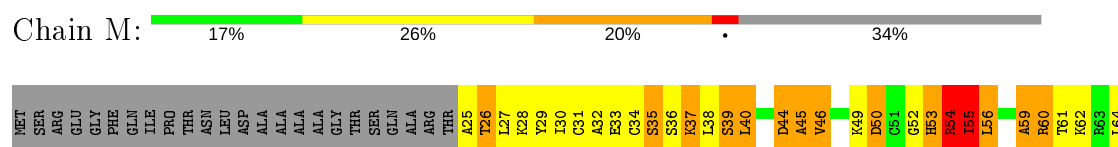
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



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



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



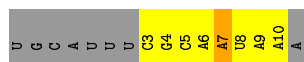




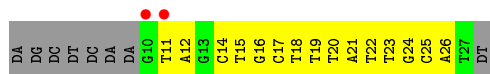
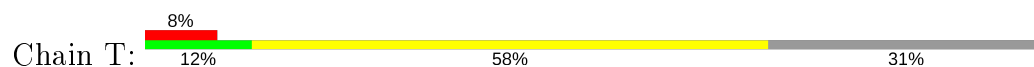
- Molecule 13: 5'-D(\*AP\*GP\*CP\*TP\*CP\*AP\*AP\*GP\*TP\*AP\*GP\*CP\*TP\*GP\*CP\*TP\*TP\*TP\*AP\*TP\*TP\*GP\*CP\*AP\*TP\*T)-3'



- Molecule 14: 5'-D(\*CP\*AP\*GP\*CP\*TP\*AP\*CP\*TP\*TP\*GP\*AP\*GP\*CP\*T)-3'



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	222.47Å 391.62Å 284.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 4.00 48.99 – 4.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-4.00) 100.0 (48.99-4.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.57 (at 4.00Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.205 , 0.241 0.215 , 0.243	Depositor DCC
$R_{free}$ test set	16372 reflections (8.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	131.8	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 82.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.024 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.024 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	31777	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	138.0	wwPDB-VP

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

<sup>1</sup>Intensities estimated from amplitudes.

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
10	K	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

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

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

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	K	44	TYR	Sidechain

## 5.2 Too-close contacts

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 63.

The worst 5 of 3977 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:21:DA:C2'	15:T:22:DT:H5'	1.58	1.32
15:T:21:DA:H2''	15:T:22:DT:C5'	1.65	1.25
15:T:20:DT:C2'	15:T:21:DA:H5'	1.73	1.18
11:L:47:ARG:HH11	11:L:47:ARG:HB3	1.11	1.15
15:T:20:DT:H2'	15:T:21:DA:H5'	1.13	1.12

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	K	63/70 (90%)	38 (60%)	12 (19%)	13 (21%)	0	2
11	L	112/120 (93%)	81 (72%)	24 (21%)	7 (6%)	1	18
12	M	44/70 (63%)	22 (50%)	8 (18%)	14 (32%)	0	0
All	All	3861/4565 (85%)	2599 (67%)	813 (21%)	449 (12%)	0	6

5 of 449 Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	1239/1520 (82%)	1113 (90%)	126 (10%)	7	28
2	C	962/1061 (91%)	867 (90%)	95 (10%)	8	29
3	D	234/274 (85%)	209 (89%)	25 (11%)	6	27
4	E	159/200 (80%)	136 (86%)	23 (14%)	3	18
5	F	196/197 (100%)	182 (93%)	14 (7%)	14	42
6	G	74/137 (54%)	69 (93%)	5 (7%)	16	44
7	H	152/152 (100%)	136 (90%)	16 (10%)	7	27
8	I	117/128 (91%)	107 (92%)	10 (8%)	10	37
9	J	113/116 (97%)	103 (91%)	10 (9%)	10	35
10	K	60/65 (92%)	54 (90%)	6 (10%)	7	29
11	L	99/102 (97%)	84 (85%)	15 (15%)	3	16
12	M	40/57 (70%)	36 (90%)	4 (10%)	7	29
All	All	3445/4009 (86%)	3096 (90%)	349 (10%)	7	29



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

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

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

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

### 5.3.3 RNA ⓘ

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

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	7	A

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 5.6 Ligand geometry

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	B	1416/1733 (81%)	-0.37	4 (0%) 94 90	76, 129, 175, 200	0
2	C	1108/1224 (90%)	-0.32	2 (0%) 95 93	79, 140, 185, 200	0
3	D	266/318 (83%)	-0.41	0 100 100	93, 126, 168, 188	0
4	E	177/221 (80%)	-0.34	0 100 100	106, 142, 182, 190	0
5	F	214/215 (99%)	-0.33	0 100 100	99, 161, 187, 200	0
6	G	84/155 (54%)	-0.52	0 100 100	73, 107, 138, 147	0
7	H	171/171 (100%)	-0.34	0 100 100	98, 127, 164, 174	0
8	I	133/146 (91%)	0.02	1 (0%) 86 79	134, 165, 186, 196	0
9	J	119/122 (97%)	-0.31	0 100 100	122, 165, 189, 200	0
10	K	65/70 (92%)	-0.59	0 100 100	92, 121, 158, 169	0
11	L	114/120 (95%)	-0.39	0 100 100	94, 128, 156, 170	0
12	M	46/70 (65%)	-0.03	0 100 100	120, 172, 195, 198	0
13	N	7/14 (50%)	1.23	3 (42%) 0 0	199, 200, 200, 200	1 (14%)
14	P	8/16 (50%)	0.06	0 100 100	198, 199, 200, 200	0
15	T	18/26 (69%)	0.65	2 (11%) 5 5	178, 199, 200, 200	1 (5%)
All	All	3946/4621 (85%)	-0.33	12 (0%) 94 90	73, 136, 184, 200	2 (0%)

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1176	LEU	3.9
13	N	7	DC	2.9
15	T	11	DT	2.8
2	C	471	LYS	2.8
1	B	1455	PRO	2.3



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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
17	MG	B	1736	1/1	0.86	0.10	153,153,153,153	0
16	ZN	J	124	1/1	0.92	0.03	200,200,200,200	0
16	ZN	M	71	1/1	0.98	0.05	174,174,174,174	0
16	ZN	D	319	1/1	0.99	0.13	98,98,98,98	0
16	ZN	B	1735	1/1	0.99	0.12	110,110,110,110	0
16	ZN	K	71	1/1	0.99	0.25	113,113,113,113	0
16	ZN	J	123	1/1	0.99	0.16	136,136,136,136	0
16	ZN	B	1734	1/1	0.99	0.04	149,149,149,149	0
16	ZN	C	1225	1/1	0.99	0.23	104,104,104,104	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.