



wwPDB X-ray Structure Validation Summary Report ⓘ

May 18, 2020 – 04:57 am BST

PDB ID : 1R9T
Title : RNA POLYMERASE II STRAND SEPARATED ELONGATION COM-
PLEX, MISMATCHED NUCLEOTIDE
Authors : Westover, K.D.; Bushnell, D.A.; Kornberg, R.D.
Deposited on : 2003-10-30
Resolution : 3.50 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
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

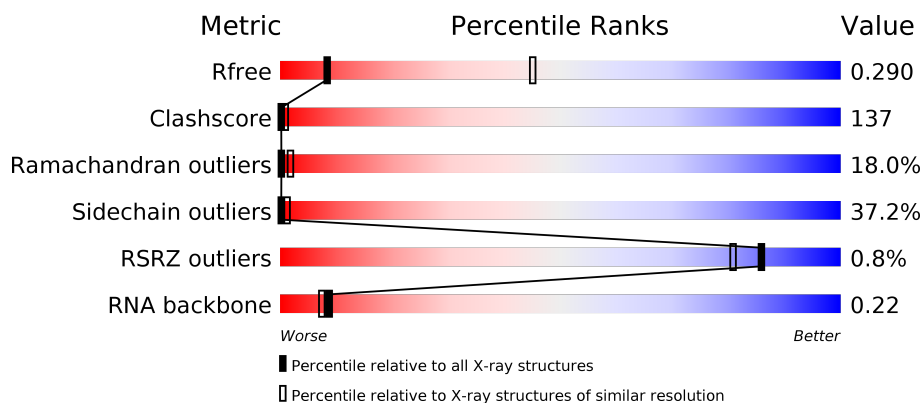
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

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 ≥ 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	R	10	<div> <div>50%</div> <div>50%</div> </div>
2	T	28	<div> <div>18%</div> <div>50%</div> <div>43%</div> <div>7%</div> </div>
3	N	14	<div> <div>36%</div> <div>71%</div> <div>29%</div> </div>
4	A	1733	<div> <div>%</div> <div>11%</div> <div>35%</div> <div>32%</div> <div>20%</div> </div>

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Mol	Chain	Length	Quality of chain
5	B	1224	
6	C	318	
7	E	215	
8	F	155	
9	H	146	
10	I	122	
11	J	70	
12	K	120	
13	L	70	

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
15	MG	A	2002	-	-	-	X

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 29248 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 RNA chain called RNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	10	Total	C	N	O	P	0	0	0
			217	98	45	65	9			

- Molecule 2 is a DNA chain called DNA template strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	28	Total	C	N	O	P	0	0	0
			566	271	104	164	27			

- Molecule 3 is a DNA chain called DNA nontemplate strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	14	Total	C	N	O	P	0	0	0
			284	137	49	85	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1395	Total	C	N	O	S	0	0	0
			10969	6917	1923	2068	61			

- Molecule 5 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1106	Total	C	N	O	S	0	0	0
			8792	5568	1538	1631	55			

- Molecule 6 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

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

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

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

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

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

- Molecule 10 is a protein called DNA-directed RNA polymerase II 14.2 kDa polypeptide.

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

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

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

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

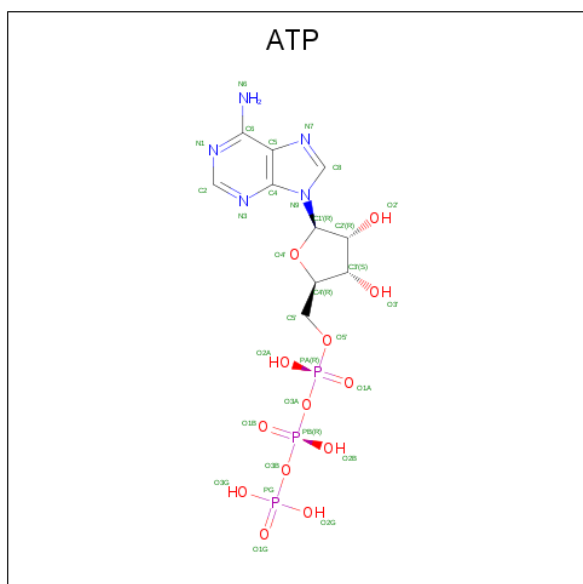
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	J	1	Total	Zn	0	0
			1	1		
14	B	1	Total	Zn	0	0
			1	1		
14	I	2	Total	Zn	0	0
			2	2		
14	C	1	Total	Zn	0	0
			1	1		
14	A	2	Total	Zn	0	0
			2	2		
14	L	1	Total	Zn	0	0
			1	1		

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	2	Total	Mg	0	0
			2	2		

- Molecule 16 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

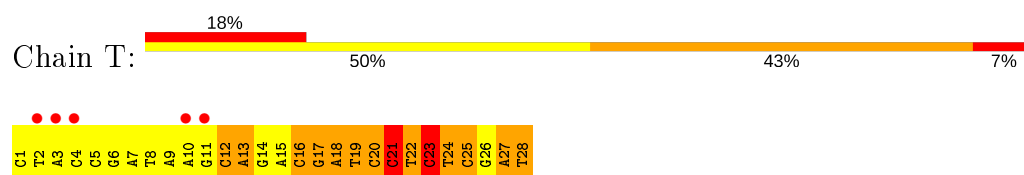
3 Residue-property plots [i](#)

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.

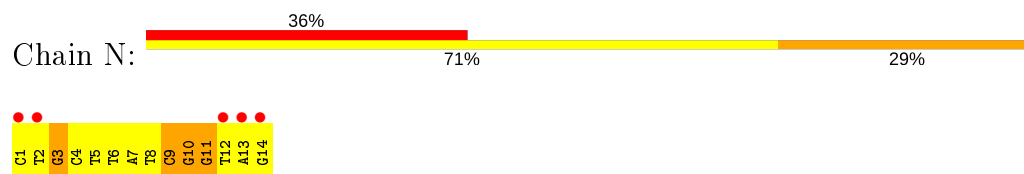
- Molecule 1: RNA strand



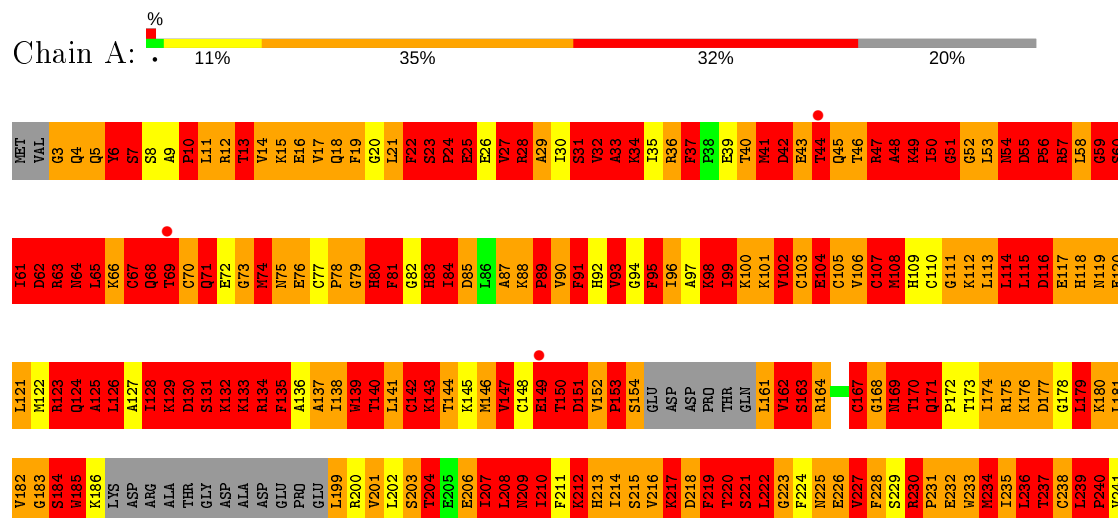
- Molecule 2: DNA template strand



- Molecule 3: DNA nontemplate strand



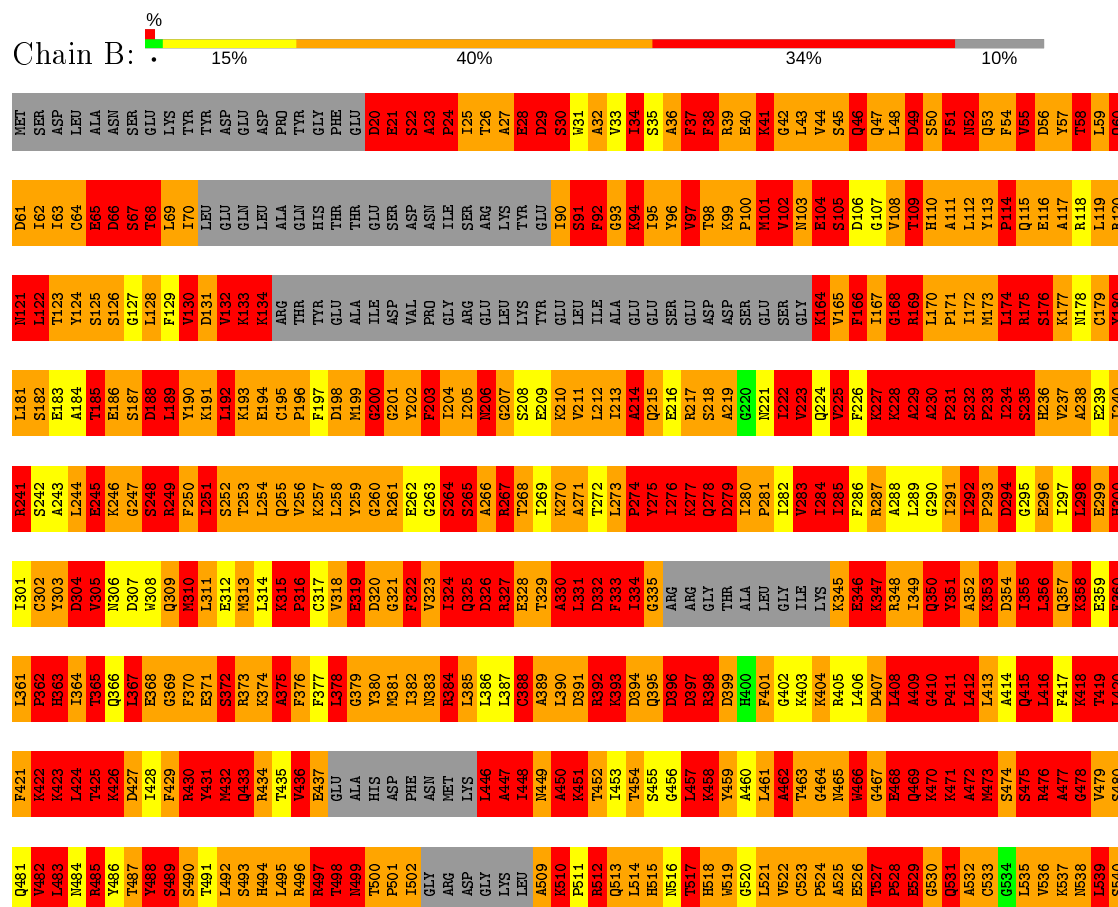
- Molecule 4: DNA-directed RNA polymerase II largest subunit



M1202	T1142	ASN	L1022	R982	L902	V942	R782	L722	R662	D602	E542	F482	G422	D862	T302	P242
M1203	L1143	THR	R1023	R983	R903	K943	T783	M723	S663	M603	L943	D483	D423	Q663	T303	P243
D1204	K1144	PRO	R1024	R964	T904	A944	L784	E724	T664	G604	D544	G484	L424	Q664	R304	P244
M1205	S1145	HIS	R1025	Q965	D905	L845	P785	A725	G665	M605	Q545	G485	Q425	G365	D305	P245
L1206	V1146	PRE	L1026	N966	H906	E946	H786	R726	T666	L606	V546	E486	L426	P366	D306	P246
L1207	T1147	ALA	A1027	A967	T907	D947	S787	D727	G667	L607	L547	M487	Q427	P367	D307	P247
T1208	I1148	GLY	T1028	Q968	L908	L848	S788	R728	K668	L608	N548	N488	Y428	K368	L308	P248
M1209	A1149	VAL	R1029	Q969	D909	M949	R789	A729	T669	D609	M549	L489	G429	S369	A309	S249
G1210	S1150	ALA	R1030	T970	P910	M850	D790	G730	L670	G610	L550	H490	N430	L370	G310	L260
Q1211	E1151	SER	V1031	F971	S911	H851	D791	R731	A671	Q611	N551	P492	K431	K372	Q312	S251
Q1212	L1152	LEU	L1032	H972	L912	H852	T792	L732	D672	L612	N552	V492	K432	K373	P313	P252
G1213	Y1153	K1093	Q1033	R973	L913	D853	S793	A733	G673	L613	V553	Q493	B433	T373	Q314	I253
E1214	Y1154	V1094	E1034	D974	E914	N854	R794	E734	D674	F614	P554	S494	B434	L374	A314	E254
R1215	D1155	T1095	T1035	H975	S915	T855	E795	V735	T675	G615	D555	E495	N435	T375	L315	S255
P1216	P1156	S1096	R1036	T976	G916	T856	S796	M736	M676	V616	N556	E496	L436	V376	Q316	Q256
K1217	L1157	G1097	L1037	R977	S917	R857	T797	V737	T677	V617	D557	T497	N437	P377	K317	R257
Q1218	P1158	V1098	T1038	S978	E918	N858	G798	K738	E678	E618	G458	R498	D438	S378	S318	G258
L1219	R1159	K1039	R1039	S979	I919	S859	F799	D739	M679	M619	V559	A499	N439	V379	Q319	E259
F1220	S1160	R1100	Q1040	D980	L920	L860	V800	L740	T680	M620	L560	E500	D440	V380	R320	D660
K1221	T1161	L1101	A1041	L981	G921	G861	E801	M741	E681	T621	P661	L501	P441	T381	P321	D261
R1222	V1162	K1102	F1042	T982	D922	N862	N802	M742	T682	V622	S602	S502	V442	T382	V322	L262
D1223	L1163	L1103	D1043	R983	L923	V863	S803	V743	L683	G623	P563	L503	L443	T383	K323	T263
L1224	P1164	T1104	M1044	K984	K924	L864	Y804	K744	A684	S624	A564	L504	F444	N384	S324	F264
F1225	E1165	V1045	V1045	D985	L925	Q865	L805	Q745	E685	S625	V565	C505	N445	I385	I325	R265
V1226	D1166	L1106	L1046	R986	Q926	F866	R806	M746	A686	N626	A506	E506	D446	D386	R326	L266
I1227	E1167	N1107	S1047	V987	V927	L867	G807	V747	K687	G627	V567	V507	Q447	K387	A327	A267
E1228	E1168	A1108	M1048	L988	L928	Y868	L808	M748	K688	G628	P568	P508	P448	L388	R328	D268
S1229	L1169	K1109	T1049	G989	L929	K869	T809	A749	K689	E629	K569	L509	S449	T389	L329	L269
E1230	K1170	N1110	E1050	V990	D930	E870	P810	G750	V690	L630	P570	Q510	L450	Q390	K330	L270
D1231	Q1171	M1111	A1051	K991	R931	D871	Q811	S751	L691	H631	L571	T511	H451	Q391	G331	K271
L1232	L1172	T1112	F1052	D992	E932	G872	E812	K752	D692	V632	N672	V512	K452	V392	K332	A272
D1233	R1173	T1113	F1053	L993	R933	M873	F813	G753	V693	V633	S573	S513	N453	K393	E333	I273
E1234	F1174	P1114	L1054	Q994	R934	D874	F814	S754	G694	T634	S454	S454	N455	P396	K335	S275
K1235	S1175	S1115	S1055	E995	Q935	A875	F815	I756	E696	N636	K575	S516	N456	P396	L336	L276
L1236	L1176	L1116	L1056	N996	L936	K876	H816	T756	E696	E636	Q576	S516	N456	P396	L336	L276
I1237	LEU	T1117	V1057	V997	V937	H877	A817	N757	A697	K637	N517	N517	A457	K397	K337	E277
L1238	ASP	V1118	V1058	L998	K938	L878	M818	I758	Q698	G638	L578	K518	R458	K398	T278	T278
R1239	GLU	Y1119	H1059	V999	D939	E879	G819	A759	A699	P639	S579	P519	R459	K399	I339	L279
G1240	GLU	L1120	P1060	R940	R940	K880	G820	Q760	N700	Q640	V580	G520	V460	P400	L340	E280
R1241	ALA	E1121	G1061	R1001	R941	Q881	R821	M761	L701	V641	A581	N521	K461	G401	L341	E281
V1242	GLN	P1122	E1062	G1002	F942	S882	E822	S762	L702	C642	L582	G522	V462	A402	G342	I282
V1243	GLN	M1063	K1003	L943	L943	L883	G823	A763	T703	A643	P583	L523	L463	K403	G343	Q283
ARG	SER	H1124	V1064	R944	R944	D884	L824	V764	A704	K644	N584	V524	P464	Y404	K344	A284
PRO	PHE	A1125	G1065	E945	E945	T885	L825	C765	K705	L645	G585	G525	V465	Y405	V345	P285
LYS	ASP	A1126	V1066	V946	V946	L886	D826	G766	H706	P646	L586	D526	S466	L406	D346	E286
SER	LEU	L1127	L1067	V947	F947	G887	T827	Q767	G707	G647	H667	T527	T467	R407	F347	E287
LEU	Q1188	Q1128	A1068	V948	V948	G888	A828	Q768	L708	M648	L588	L528	F468	D408	S348	A288
ASP	S1189	E1129	A1069	D949	D949	S889	V829	T709	R709	I649	R469	C529	R469	S409	A349	I289
ALA	P1190	Q1130	Q1070	G950	G950	D890	K830	V770	L710	Q650	R590	G530	L470	Q410	R350	E290
GLU	W1191	A1131	S1071	E951	E951	A891	T831	E771	R711	M651	F591	L531	D471	D411	T351	E291
L1192	L1192	K1132	L1072	A952	A952	A892	A832	G772	E712	V652	D592	R532	L472	K412	V352	A292
A1254	L1193	L1133	G1073	N953	N953	F893	E833	K773	S713	V653	E593	R533	S473	L413	I353	E293
E1255	R1194	T1134	E1074	M954	M954	E894	T834	R774	F714	M654	G594	L534	V474	D414	S354	S294
L1195	L1195	R1135	P1075	P955	P955	K895	G835	I775	E715	P655	T595	T535	V475	L415	G355	L295
E1256	E1196	S1136	A1076	L1016	L956	R896	Y836	D716	M656	L536	S476	L536	P476	R416	D356	L296
D1257	L1197	T1077	T1017	P957	P957	H897	I837	F777	N717	L657	V597	R537	P477	V417	P357	Q297
D1198	L1198	T1138	Q1078	N958	N958	R898	Q838	G778	V718	L658	L598	D538	V478	S418	I358	E298
R1199	R1199	E1139	M1079	I959	I959	H899	R839	F779	V719	H659	S599	T539	N479	R419	L359	E299
L1260	A1200	H1140	T1080	C1020	C1020	D900	R840	V780	R720	M660	P540	F540	R479	R420	E360	V300
K1261	A1201	T1141	L1081	L1021	R961	L901	L841	D781	F721	G661	K601	L541	D481	A421	L361	A301

SER	PRO	ALA	V1443	T1382	I1322	K1262
	PRO	SER	M1444	S1383	D1323	I1263
	THR	ALA	V1445	V1384	P1324	E1264
	SER	GLY	ASP	T1385	T1325	N1265
	PRO	GLY	GLU	E1386	R1326	T1266
	PRO	PHE	GLU	H1387	I1327	M1267
	SER	THR	SER	G1388	Y1328	L1268
	SER	ALA	LEU	F1389	T1329	E1269
	PRO	THR	VAL	N1390	M1330	N1270
	THR	GLY	LYS	R1391	S1331	I1271
SER	THR	GLY	TYR	S1392	F1332	T1272
	SER	ALA	MET	N1393	I1333	L1273
	PRO	ASP	PRO	T1394	D1334	R1274
	TYR	THR	GLY	G1395	I1335	G1275
	SER	GLY	GLN	A1396	M1336	V1276
	PRO	SER	GLU	L1397	E1337	E1277
	THR	ALA	ILE	M1398	V1338	N1278
	THR	THR	THR	R1399	L1339	I1279
	PRO	SER	GLU	C1400	G1340	E1280
	PRO	PRO	ILE	S1401	I1341	R1281
SER	PRO	PHE	GLY	F1402	E1342	V1282
	TYR	GLY	ASP	E1403	A1343	I1283
	SER	ALA	GLY	E1404	G1344	M1284
	PRO	THR	GLN	T1405	R1345	M1285
	THR	GLY	ASP	V1406	A1346	K1286
	PRO	GLY	GLY	E1407	A1347	Y1287
	PRO	ALA	GLY	I1408	L1348	D1288
	THR	PRO	VAL	L1409	Y1349	R1289
	THR	THR	THR	F1410	K1350	K1290
	PRO	SER	PRO	E1411	E1351	V1291
SER	THR	PRO	T1412	Y1352	P1292	S1293
	SER	GLY	G1413	Y1353	I1354	P1294
	SER	PHE	ASN	M1354	N1355	G1296
	PRO	GLY	VAL	A1416	V1355	T1295
	THR	VAL	GLY	E1417	I1356	E1297
	SER	SER	GLY	L1418	A1357	Y1298
	PRO	SER	LEU	D1419	S1358	V1299
	ALA	PRO	VAL	D1420	D1359	K1300
	GLN	THR	GLY	C1421	G1360	R1301
	ASP	SER	PHE	A1422	S1361	P1302
SER	PRO	SER	ASP	G1423	Y1362	E1303
	THR	PRO	LEU	V1424	V1363	E1304
	SER	THR	ASP	S1425	N1364	V1305
	PRO	SER	VAL	E1426	Y1365	L1306
	ASN	SER	PRO	LYS	N1427	E1307
	GLU	THR	THR	ASP	F1428	T1308
	ASN	SER	THR	GLY	I1429	D1309
	PRO	SER	LEU	L1430	M1368	G1310
	THR	THR	GLY	G1431	L1370	V1311
	SER	THR	PHE	G1432	L1371	N1312
SER	PRO	SER	M1433	Y1372	L1372	L1313
	THR	PRO	ALA	A1434	D1373	S1314
	THR	THR	LEU	P1435	V1374	E1315
	SER	THR	VAL	T1436	M1375	E1316
	PRO	SER	ASP	G1437	T1376	V1317
	PRO	SER	PRO	T1438	M1377	T1318
	THR	THR	GLY	A1439	Q1378	V1319
	PRO	SER	GLY	G1440	G1379	P1320
	PRO	ASN	ASN	F1441	G1380	E1321
	THR	THR	THR	D1442	T1381	N1322

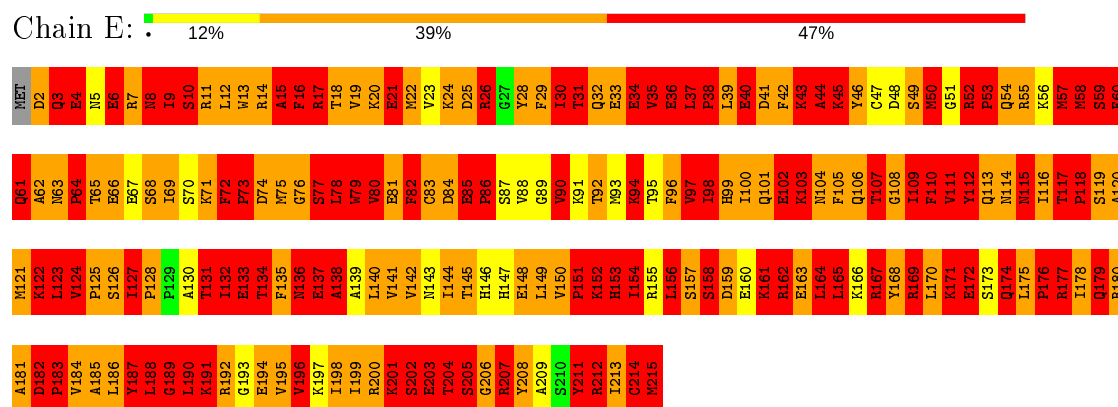
- Molecule 5: DNA-directed RNA polymerase II 140 kDa polypeptide



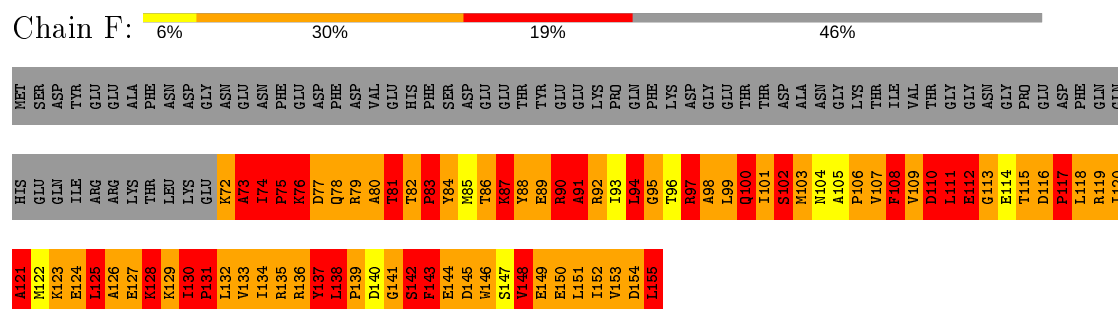
- Molecule 6: DNA-directed RNA polymerase II 45 kDa polypeptide

D181	D182	D183	D184	D185	D186	D187	D188	D189	D190	D191	D192	D193	D194	D195	D196	D197	D198	D199	D200	D201	D202	D203	D204	D205	D206	D207	D208	D209	D210	D211	D212	D213	D214	D215	D216	D217	D218	D219	D220	D221	D222	D223	D224	D225	D226	D227	D228	D229	D230	D231	D232	D233	D234	D235	D236	D237	D238	D239	D240	D241	D242	D243	D244	D245	D246	D247	D248	D249	D250	D251	D252	D253	D254	D255	D256	D257	D258	D259	D260	D261	D262	D263	D264	D265	D266	D267	D268	D269	D270	D271	D272	D273	D274	D275	D276	D277	D278	D279	D280	D281	D282	D283	D284	D285	D286	D287	D288	D289	D290	D291	D292	D293	D294	D295	D296	D297	D298	D299	D300	D301	D302	D303	D304	D305	D306	D307	D308	D309	D310	D311	D312	D313	D314	D315	D316	D317	D318	D319	D320	D321	D322	D323	D324	D325	D326	D327	D328	D329	D330	D331	D332	D333	D334	D335	D336	D337	D338	D339	D340	D341	D342	D343	D344	D345	D346	D347	D348	D349	D350	D351	D352	D353	D354	D355	D356	D357	D358	D359	D360	D361	D362	D363	D364	D365	D366	D367	D368	D369	D370	D371	D372	D373	D374	D375	D376	D377	D378	D379	D380	D381	D382	D383	D384	D385	D386	D387	D388	D389	D390	D391	D392	D393	D394	D395	D396	D397	D398	D399	D400	D401	D402	D403	D404	D405	D406	D407	D408	D409	D410	D411	D412	D413	D414	D415	D416	D417	D418	D419	D420	D421	D422	D423	D424	D425	D426	D427	D428	D429	D430	D431	D432	D433	D434	D435	D436	D437	D438	D439	D440	D441	D442	D443	D444	D445	D446	D447	D448	D449	D450	D451	D452	D453	D454	D455	D456	D457	D458	D459	D460	D461	D462	D463	D464	D465	D466	D467	D468	D469	D470	D471	D472	D473	D474	D475	D476	D477	D478	D479	D480	D481	D482	D483	D484	D485	D486	D487	D488	D489	D490	D491	D492	D493	D494	D495	D496	D497	D498	D499	D500	D501	D502	D503	D504	D505	D506	D507	D508	D509	D510	D511	D512	D513	D514	D515	D516	D517	D518	D519	D520	D521	D522	D523	D524	D525	D526	D527	D528	D529	D530	D531	D532	D533	D534	D535	D536	D537	D538	D539	D540	D541	D542	D543	D544	D545	D546	D547	D548	D549	D550	D551	D552	D553	D554	D555	D556	D557	D558	D559	D560	D561	D562	D563	D564	D565	D566	D567	D568	D569	D570	D571	D572	D573	D574	D575	D576	D577	D578	D579	D580	D581	D582	D583	D584	D585	D586	D587	D588	D589	D590	D591	D592	D593	D594	D595	D596	D597	D598	D599	D600	D601	D602	D603	D604	D605	D606	D607	D608	D609	D610	D611	D612	D613	D614	D615	D616	D617	D618	D619	D620	D621	D622	D623	D624	D625	D626	D627	D628	D629	D630	D631	D632	D633	D634	D635	D636	D637	D638	D639	D640	D641	D642	D643	D644	D645	D646	D647	D648	D649	D650	D651	D652	D653	D654	D655	D656	D657	D658	D659	D660	D661	D662	D663	D664	D665	D666	D667	D668	D669	D670	D671	D672	D673	D674	D675	D676	D677	D678	D679	D680	D681	D682	D683	D684	D685	D686	D687	D688	D689	D690	D691	D69
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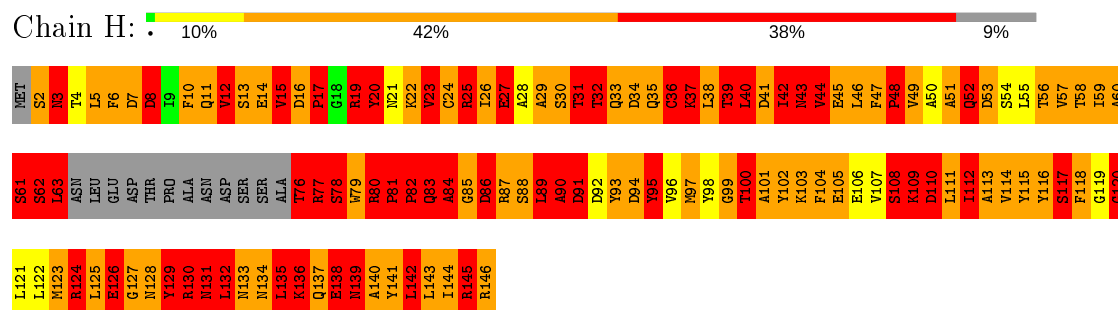
- Molecule 7: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide



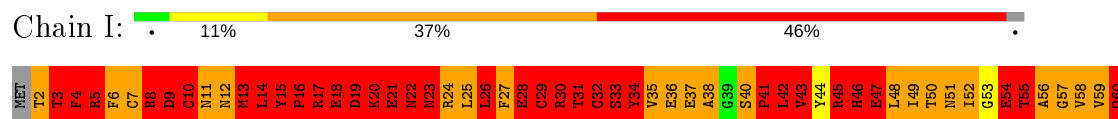
- Molecule 8: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide



- Molecule 9: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



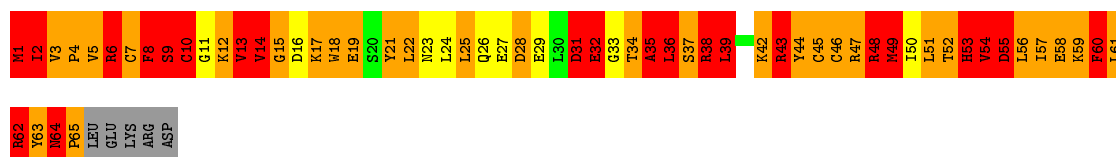
- Molecule 10: DNA-directed RNA polymerase II 14.2 kDa polypeptide





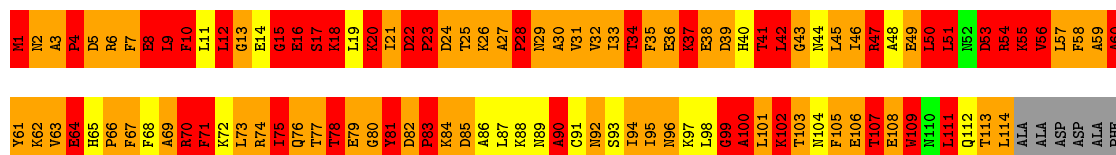
- Molecule 11: DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide

Chain J: 6% 13% 41% 33% 7%



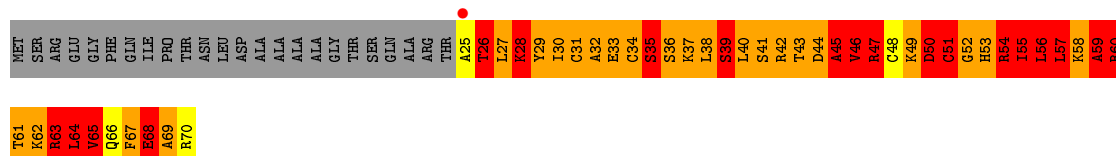
- Molecule 12: DNA-directed RNA polymerase II 13.6 kDa polypeptide

Chain K: 16% 44% 33% 5%



- Molecule 13: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide

Chain L: 6% 33% 27% 34%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.85Å 222.96Å 193.60Å 90.00° 101.17° 90.00°	Depositor
Resolution (Å)	40.00 – 3.50 39.98 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.50) 93.7 (39.98-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 3.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.230 , 0.317 0.201 , 0.290	Depositor DCC
R_{free} test set	8862 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å ²)	80.5	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 80.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	29248	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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, ATP

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	R	3.34	30/244 (12.3%)	3.47	35/380 (9.2%)
2	T	2.72	42/633 (6.6%)	2.95	63/971 (6.5%)
3	N	1.33	4/316 (1.3%)	1.10	6/484 (1.2%)
4	A	3.73	1529/11163 (13.7%)	3.57	2038/15091 (13.5%)
5	B	3.68	1206/8963 (13.5%)	3.62	1655/12086 (13.7%)
6	C	3.67	281/2133 (13.2%)	3.42	376/2891 (13.0%)
7	E	3.85	252/1788 (14.1%)	3.52	348/2406 (14.5%)
8	F	3.81	105/691 (15.2%)	3.78	136/933 (14.6%)
9	H	4.17	178/1086 (16.4%)	3.65	243/1470 (16.5%)
10	I	3.97	150/989 (15.2%)	3.89	212/1331 (15.9%)
11	J	3.68	72/541 (13.3%)	3.56	89/727 (12.2%)
12	K	3.73	149/937 (15.9%)	3.38	150/1265 (11.9%)
13	L	4.22	68/365 (18.6%)	3.67	86/485 (17.7%)
All	All	3.71	4066/29849 (13.6%)	3.55	5437/40520 (13.4%)

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
1	R	0	1
2	T	1	2
4	A	2	121
5	B	4	114
6	C	1	11
7	E	0	17
8	F	0	5
9	H	0	16
10	I	1	18
11	J	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
12	K	0	9
13	L	0	5
All	All	9	321

The worst 5 of 4066 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1110	ASN	CB-CG	39.65	2.42	1.51
4	A	820	GLY	C-O	-37.66	0.63	1.23
7	E	117	THR	CA-CB	34.64	2.43	1.53
4	A	437	MET	SD-CE	30.90	3.50	1.77
4	A	322	VAL	CA-CB	-27.33	0.97	1.54

The worst 5 of 5437 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	941	LEU	CB-CG-CD2	37.01	173.92	111.00
4	A	337	ARG	NE-CZ-NH2	-34.93	102.83	120.30
4	A	980	ASP	CB-CG-OD2	33.77	148.69	118.30
5	B	466	TRP	CA-C-N	-31.53	53.14	116.20
4	A	337	ARG	NE-CZ-NH1	31.48	136.04	120.30

5 of 9 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	T	21	DC	C3'
4	A	317	LYS	CA
4	A	324	SER	CA
5	B	636	PRO	CA
5	B	637	LEU	CA

5 of 321 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	3	GLY	Mainchain
4	A	6	TYR	Peptide
1	R	10	A	Sidechain
2	T	21	DC	Sidechain
2	T	23	DC	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	R	217	0	110	34	0
2	T	566	0	314	82	4
3	N	284	0	162	44	0
4	A	10969	0	11061	3443	0
5	B	8792	0	8821	2369	0
6	C	2095	0	2051	490	0
7	E	1752	0	1776	523	0
8	F	679	0	701	194	0
9	H	1068	0	1040	377	0
10	I	971	0	929	310	0
11	J	532	0	543	160	0
12	K	919	0	929	259	0
13	L	363	0	387	98	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	2	0	0	0	0
16	B	31	0	12	7	0
All	All	29248	0	28836	7970	4

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 137.

The worst 5 of 7970 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)
3:N:12:DT:P	7:E:117:THR:HG21	1.32	1.67
4:A:128:ILE:CB	4:A:128:ILE:CA	1.74	1.66
5:B:422:LYS:CB	5:B:422:LYS:CG	1.74	1.65
5:B:866:TYR:CB	5:B:866:TYR:CG	1.80	1.65
4:A:37:PHE:CG	4:A:37:PHE:CB	1.74	1.65

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:1:DC:C4'	2:T:1:DC:C4'[2_656]	1.63	0.57
2:T:1:DC:C5'	2:T:1:DC:O4'[2_656]	1.69	0.51
2:T:1:DC:O4'	2:T:1:DC:O4'[2_656]	1.78	0.42
2:T:1:DC:C4'	2:T:1:DC:O4'[2_656]	1.80	0.40

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	
4	A	1383/1733 (80%)	816 (59%)	306 (22%)	261 (19%)	0	2
5	B	1088/1224 (89%)	708 (65%)	199 (18%)	181 (17%)	0	2
6	C	264/318 (83%)	170 (64%)	58 (22%)	36 (14%)	0	4
7	E	212/215 (99%)	119 (56%)	47 (22%)	46 (22%)	0	1
8	F	82/155 (53%)	45 (55%)	22 (27%)	15 (18%)	0	2
9	H	129/146 (88%)	75 (58%)	28 (22%)	26 (20%)	0	1
10	I	117/122 (96%)	60 (51%)	32 (27%)	25 (21%)	0	1
11	J	63/70 (90%)	41 (65%)	10 (16%)	12 (19%)	0	2
12	K	112/120 (93%)	78 (70%)	18 (16%)	16 (14%)	0	3
13	L	44/70 (63%)	21 (48%)	11 (25%)	12 (27%)	0	0
All	All	3494/4173 (84%)	2133 (61%)	731 (21%)	630 (18%)	0	2

5 of 630 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	34	LYS
4	A	44	THR
4	A	48	ALA
4	A	51	GLY

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Mol	Chain	Res	Type
4	A	55	ASP

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	
4	A	1218/1520 (80%)	759 (62%)	459 (38%)	0	1
5	B	960/1061 (90%)	614 (64%)	346 (36%)	0	1
6	C	234/274 (85%)	151 (64%)	83 (36%)	0	1
7	E	196/197 (100%)	116 (59%)	80 (41%)	0	1
8	F	74/137 (54%)	47 (64%)	27 (36%)	0	1
9	H	117/128 (91%)	71 (61%)	46 (39%)	0	1
10	I	113/116 (97%)	70 (62%)	43 (38%)	0	1
11	J	60/65 (92%)	38 (63%)	22 (37%)	0	1
12	K	99/102 (97%)	63 (64%)	36 (36%)	0	1
13	L	40/57 (70%)	24 (60%)	16 (40%)	0	1
All	All	3111/3657 (85%)	1953 (63%)	1158 (37%)	0	1

5 of 1158 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	B	257	LYS
5	B	682	SER
10	I	79	HIS
5	B	319	GLU
5	B	436	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
4	A	1364	ASN
5	B	383	ASN

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Mol	Chain	Res	Type
10	I	60	GLN
4	A	1390	ASN
5	B	115	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	10/10 (100%)	4 (40%)	3 (30%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	2	U
1	R	5	A
1	R	6	G
1	R	10	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	R	1	A
1	R	4	G
1	R	5	A

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 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	ATP	B	1308	-	26,33,33	2.38	7 (26%)	31,52,52	3.10	10 (32%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	ATP	B	1308	-	-	7/18/38/38	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	1308	ATP	O5'-C5'	-5.93	1.22	1.44
16	B	1308	ATP	C2'-C1'	5.11	1.61	1.53
16	B	1308	ATP	PA-O5'	-4.73	1.40	1.59
16	B	1308	ATP	O4'-C1'	4.63	1.47	1.41
16	B	1308	ATP	C2-N3	4.15	1.38	1.32

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	1308	ATP	O5'-C5'-C4'	10.76	146.02	108.99
16	B	1308	ATP	PA-O5'-C5'	5.59	154.49	121.68
16	B	1308	ATP	N3-C2-N1	-5.51	120.07	128.68
16	B	1308	ATP	C5'-C4'-C3'	-5.29	95.35	115.18
16	B	1308	ATP	O4'-C4'-C3'	4.06	113.16	105.11

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	B	1308	ATP	C5'-O5'-PA-O1A
16	B	1308	ATP	C5'-O5'-PA-O3A
16	B	1308	ATP	C4'-C5'-O5'-PA
16	B	1308	ATP	PB-O3A-PA-O5'

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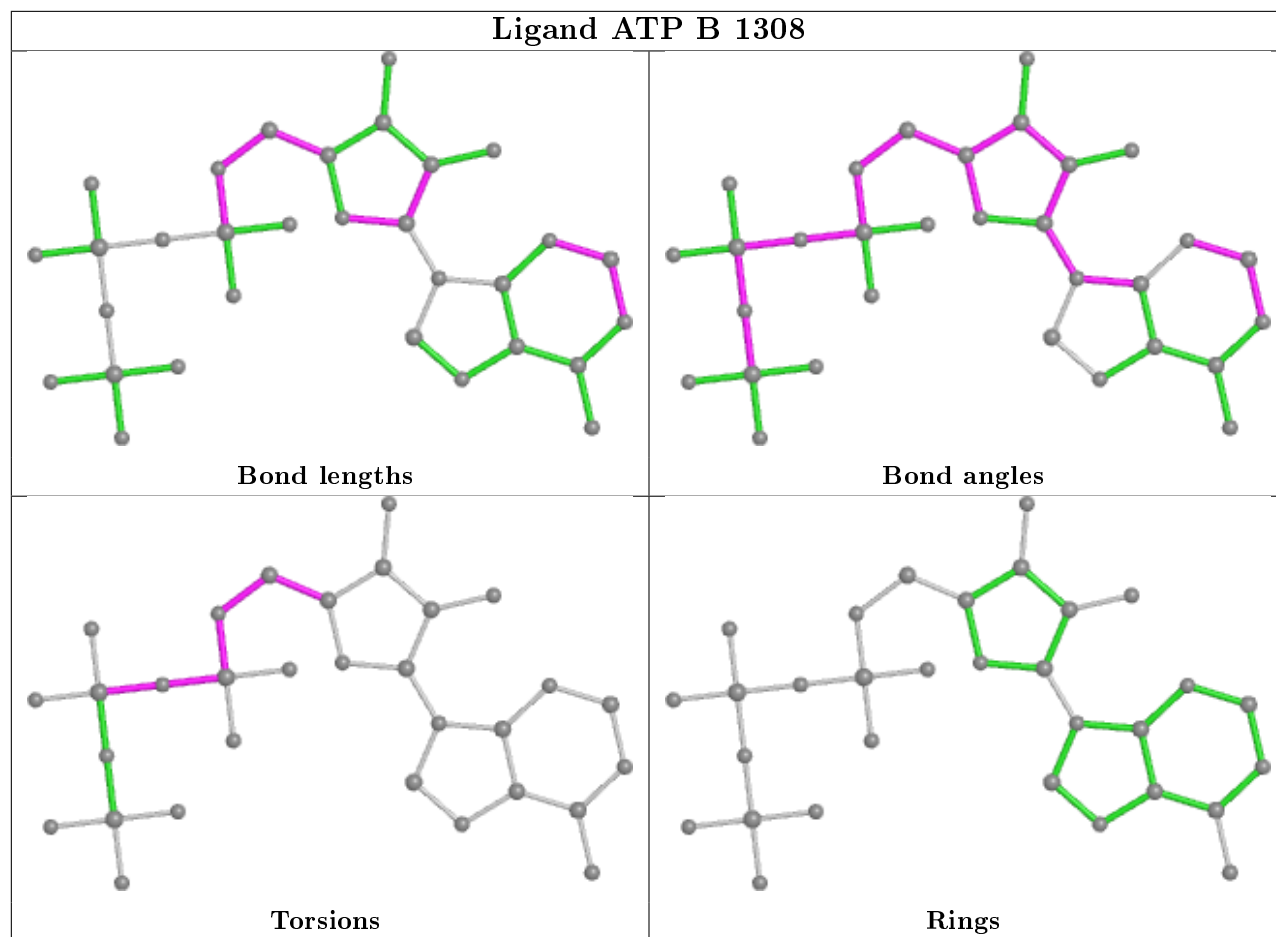
Mol	Chain	Res	Type	Atoms
16	B	1308	ATP	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	1308	ATP	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	A	2
2	T	2
1	R	1
3	N	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	T	15:DA	O3'	16:DC	P	2.98
1	N	2:DT	O3'	3:DG	P	2.67

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	320:ARG	C	321:PRO	N	1.75
1	A	820:GLY	C	821:ARG	N	1.68
1	T	21:DC	O3'	22:DT	P	1.39

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	R	10/10 (100%)	0.36	0 100 100	70, 83, 159, 164	0
2	T	28/28 (100%)	0.90	5 (17%) 1 1	84, 188, 200, 200	0
3	N	14/14 (100%)	1.68	5 (35%) 0 0	185, 198, 200, 200	0
4	A	1395/1733 (80%)	-0.71	11 (0%) 86 81	1, 51, 137, 186	0
5	B	1106/1224 (90%)	-0.73	7 (0%) 89 86	1, 43, 119, 194	0
6	C	266/318 (83%)	-0.83	0 100 100	6, 44, 95, 151	0
7	E	214/215 (99%)	-0.54	0 100 100	13, 79, 141, 165	0
8	F	84/155 (54%)	-0.62	0 100 100	17, 58, 105, 114	0
9	H	133/146 (91%)	-0.60	0 100 100	19, 74, 132, 154	0
10	I	119/122 (97%)	-0.73	0 100 100	4, 56, 105, 146	0
11	J	65/70 (92%)	-0.81	0 100 100	11, 40, 92, 116	0
12	K	114/120 (95%)	-0.74	0 100 100	8, 43, 88, 131	0
13	L	46/70 (65%)	-0.44	1 (2%) 62 56	17, 84, 143, 163	0
All	All	3594/4225 (85%)	-0.69	29 (0%) 86 81	1, 50, 133, 200	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	316	GLN	5.4
4	A	255	SER	4.0
4	A	44	THR	3.7
3	N	14	DG	3.6
5	B	866	TYR	3.6

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 ⓘ

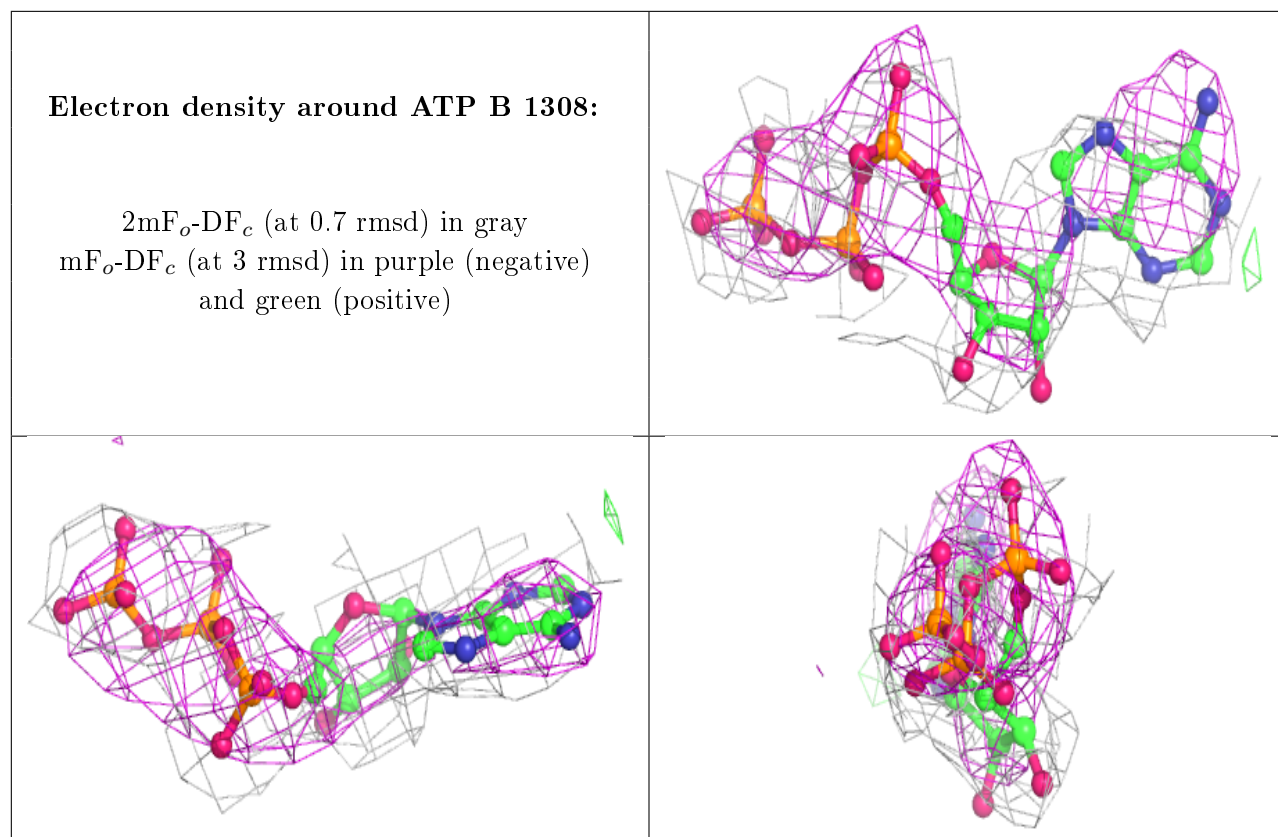
There are no carbohydrates in this entry.

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(\AA^2)	Q<0.9
15	MG	A	2002	1/1	0.71	0.49	63,63,63,63	0
16	ATP	B	1308	31/31	0.75	0.35	64,71,77,78	0
14	ZN	A	1734	1/1	0.79	0.05	115,115,115,115	0
15	MG	A	2001	1/1	0.95	0.56	55,55,55,55	0
14	ZN	J	101	1/1	0.97	0.10	39,39,39,39	0
14	ZN	I	203	1/1	0.98	0.05	98,98,98,98	0
14	ZN	L	105	1/1	0.98	0.03	76,76,76,76	0
14	ZN	A	1735	1/1	0.98	0.04	75,75,75,75	0
14	ZN	B	1307	1/1	0.99	0.05	80,80,80,80	0
14	ZN	C	319	1/1	0.99	0.02	31,31,31,31	0
14	ZN	I	204	1/1	0.99	0.05	31,31,31,31	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.