



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 01:43 PM UTC

PDB ID : 7RIY / pdb\_00007riy  
Title : RNA polymerase II elongation complex with hairpin polyamide Py-Im 1, scaffold 2 soaked with UTP  
Authors : Oh, J.; Dervan, P.B.; Wang, D.  
Deposited on : 2021-07-20  
Resolution : 3.70 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.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

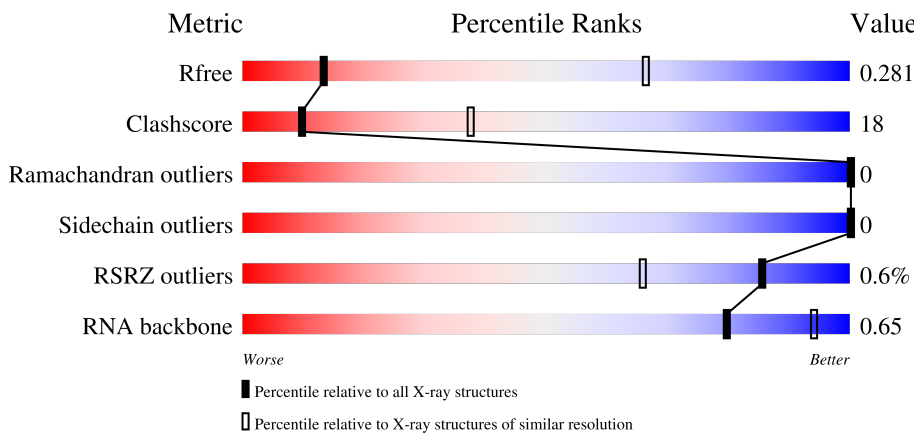
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.70 Å.

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






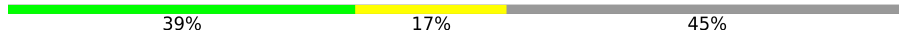


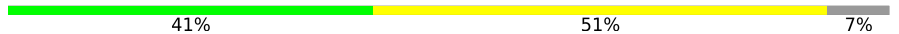

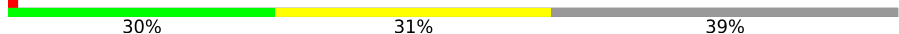
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)
RNA backbone	3983	1007 (4.30-3.08)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	R	11	
2	T	30	
3	N	20	
4	A	1733	

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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	

## 2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 29168 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	R	11	235	106	45	74	10	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	T	26	525	252	84	163	26	0	0	0

- Molecule 3 is a DNA chain called Non-template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	N	14	293	138	63	78	14	0	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	A	1384	10828	6831	1896	2041	60	0	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	B	1123	8859	5607	1552	1647	53	0	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	C	267	2101	1320	349	419	13	0	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	E	212	1731	1100	305	315	11	0	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	F	86	684	437	115	129	3	0	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	H	133	1064	670	179	211	4	0	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	I	118	952	585	173	184	10	0	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

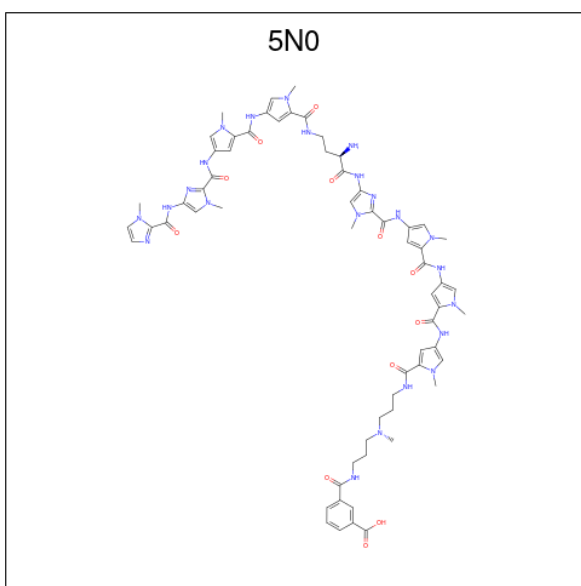
- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	L	43	337	208	66	59	4	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	R	1	Total Mg 1 1	0	0

- Molecule 15 is 3-({3-[(3-[(4-({4-[(4-({(2R)-2-amino-4-[(1-methyl-4-[[1-methyl-4-({1-methyl-4-[(1-methyl-1H-imidazole-2-carbonyl)amino]-1H-imidazole-2-carbonyl}amino)-1H-pyrrole-2-carbonyl]amino)-1H-pyrrole-2-carbonyl)amino]butanoyl}amino)-1-methyl-1H-imidazole-2-carbonyl]amino)-1-methyl-1H-pyrrole-2-carbonyl)amino]-1-methyl-1H-pyrrole-2-carbonyl]amino}propyl)(methyl)amino]propyl}carbamoyl)benzoic acid (CCD ID: 5N0) (formula: C<sub>64</sub>H<sub>75</sub>N<sub>23</sub>O<sub>12</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	T	1	Total C N O 99 64 23 12	0	0

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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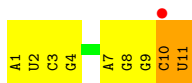
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
16	L	1	Total	Zn	0	0
			1	1		

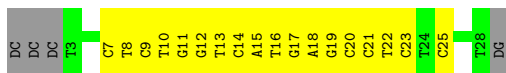
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

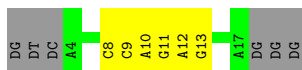
- Molecule 1: RNA



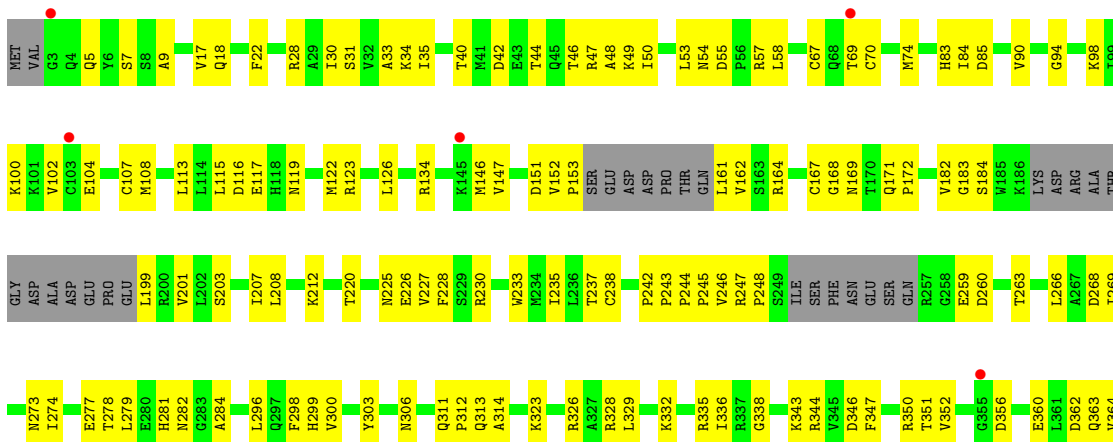
- Molecule 2: Template strand DNA



- Molecule 3: Non-template strand DNA



- Molecule 4: DNA-directed RNA polymerase II subunit RPB1



SER	PRO	SER	PRO	TYR	PRO	R1345	D1287	Q1171	M1079	K984	E879	I775	L645	P563	L470	G365
THR	THR	GLY	GLY	GLY	ASP	E1351	L1280	L1176	T1080	D985	K890	E795	F646	K567	M471	V386
PRO	PRO	GLU	THR	GLU	GLU	V1352	I1263	LEU	ASN	K991	Q881	E786	T649	P368	M472	P367
THR	THR	GLU	THR	GLU	GLU	V1355	M1287	ASP	THR	D992	S882	K797	Q650	K368	S473	K368
PRO	PRO	VAL	ALA	ALA	ALA	V1356	I1271	GLU	PHE	L993	D884	V800	V653	K569	V474	S369
PRO	PRO	VAL	THR	GLU	GLU	I1357	T1272	GLU	ALA	L998	G888	W800	Y478	K372	I370	A371
PRO	PRO	VAL	THR	GLU	GLU	V1358	L1273	GLN	ALA	R1001	S889	E807	M479	K372	K372	K372
PRO	PRO	VAL	THR	GLU	GLU	V1359	T1274	GLN	ALA	R1002	D890	S573	A490	Y376	A490	A490
PRO	PRO	VAL	THR	GLU	GLU	V1360	R1274	GLN	VAL	G1002	F662	G574	D483	P377	D483	P377
PRO	PRO	VAL	THR	GLU	GLU	V1361	G1275	GLN	ALA	K1003	R898	Y804	E378	E378	E378	E378
PRO	PRO	VAL	THR	GLU	GLU	V1362	V1276	GLN	SER	M1004	D900	L806	M487	V379	V379	V379
PRO	PRO	VAL	THR	GLU	GLU	V1363	I1277	GLN	K1092	Q1008	L901	G807	M488	V380	V380	V380
PRO	PRO	VAL	THR	GLU	GLU	V1364	M1278	GLN	T1095	L902	L902	L808	V491	D386	D386	D386
PRO	PRO	VAL	THR	GLU	GLU	V1365	I1279	GLN	L1095	R1012	L903	T809	S494	R387	R387	R387
PRO	PRO	VAL	THR	GLU	GLU	V1366	E1280	GLN	M1106	T1016	T907	P810	S494	L388	L388	L388
PRO	PRO	VAL	THR	GLU	GLU	V1367	R1281	GLN	V1107	L1016	T907	E811	E496	V392	V392	V392
PRO	PRO	VAL	THR	GLU	GLU	V1368	K1286	GLN	L1021	L1021	Q926	H816	E500	P396	P396	P396
PRO	PRO	VAL	THR	GLU	GLU	V1369	E1291	GLN	L1022	L1022	L929	T809	E500	K403	K403	K403
PRO	PRO	VAL	THR	GLU	GLU	V1370	P1292	GLN	R1023	R1023	L929	T809	E500	R407	R407	R407
PRO	PRO	VAL	THR	GLU	GLU	V1371	G1296	GLN	S1024	S1024	D930	P810	E500	D408	D408	D408
PRO	PRO	VAL	THR	GLU	GLU	V1372	E1297	GLN	L1025	L1025	E931	E822	E500	S409	S409	S409
PRO	PRO	VAL	THR	GLU	GLU	V1373	I1297	GLN	L1026	L1026	D939	G823	E500	R407	R407	R407
PRO	PRO	VAL	THR	GLU	GLU	V1374	E1303	GLN	A1027	A1027	D939	G823	E500	D408	D408	D408
PRO	PRO	VAL	THR	GLU	GLU	V1375	M1304	GLN	R940	R940	L929	T809	E500	S409	S409	S409
PRO	PRO	VAL	THR	GLU	GLU	V1376	V1305	GLN	L1120	L1120	L929	T809	E500	S409	S409	S409
PRO	PRO	VAL	THR	GLU	GLU	V1377	L1306	GLN	R941	R941	L929	T809	E500	S409	S409	S409
PRO	PRO	VAL	THR	GLU	GLU	V1378	E1307	GLN	R1029	R1029	L929	T809	E500	S409	S409	S409
PRO	PRO	VAL	THR	GLU	GLU	V1379	L1308	GLN	R1030	R1030	L929	T809	E500	S409	S409	S409
PRO	PRO	VAL	THR	GLU	GLU	V1380	V1312	GLN	P1122	P1122	L929	T809	E500	S409	S409	S409
PRO	PRO	VAL	THR	GLU	GLU	V1381	E1315	GLN	V1031	V1031	L929	T809	E500	S409	S409	S409
PRO	PRO	VAL	THR	GLU	GLU	V1382	V1316	GLN	A1125	A1125	L929	T809	E500	S409	S409	S409
PRO	PRO	VAL	THR	GLU	GLU	V1383	V1319	GLN	E1034	E1034	L929	T809	E500	S409	S409	S409
PRO	PRO	VAL	THR	GLU	GLU	V1384	I1322	GLN	A1041	A1041	L929	T809	E500	S409	S409	S409
PRO	PRO	VAL	THR	GLU	GLU	V1385	P1324	GLN	A1041	A1041	L929	T809	E500	S409	S409	S409
PRO	PRO	VAL	THR	GLU	GLU	V1386	T1325	GLN	W1044	W1044	L929	T809	E500	S409	S409	S409
PRO	PRO	VAL	THR	GLU	GLU	V1387	R1326	GLN	V1045	V1045	L929	T809	E500	S409	S409	S409
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PRO	PRO	VAL	THR	GLU	GLU	V1389	Y1328	GLN	A1051	A1051	L929	T809	E500	S409	S409	S409
PRO	PRO	VAL	THR	GLU	GLU	V1390	T1329	GLN	R1055	R1055	L929	T809	E500	S409	S409	S409
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PRO	PRO	VAL	THR	GLU	GLU	V1408		GLN	G1061	G1061	L929	T809	E500	S409	S409	S409
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PRO	PRO	VAL	THR	GLU	GLU	V1411		GLN	G1061	G1061	L929	T809	E500	S409	S409	S409
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PRO	PRO	VAL	THR	GLU	GLU	V1423		GLN	G1061	G1061	L929	T809	E500	S409	S409	S409
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PRO	PRO	VAL	THR	GLU	GLU	V1431		GLN	G1061	G1061	L929	T809	E500	S409	S409	S409
PRO	PRO	VAL	THR	GLU	GLU	V1432		GLN	G1061	G1061	L929	T809	E500	S409	S409	S409
PRO	PRO	VAL	THR	GLU	GLU	V1433		GLN	G1061	G1061	L929	T809	E500	S409	S409	S409
PRO	PRO	VAL	THR	GLU	GLU	V1434		GLN	G1061	G1061	L929	T809	E500	S409	S409	S409
PRO	PRO	VAL	THR	GLU	GLU	V1435		GLN	G1061	G1061	L929	T809	E500	S409	S409	S409
PRO	PRO	VAL	THR	GLU	GLU	V1436		GLN	G1061	G1061	L929	T809	E500	S409	S409	S409
PRO	PRO	VAL	THR	GLU	GLU	V1437		GLN	G1061	G1061	L929	T809	E500	S409	S409	S409
PRO	PRO	VAL	THR	GLU	GLU	V1438		GLN	G1061	G1061	L929	T809	E500	S409	S409	S409
PRO	PRO	VAL	THR	GLU	GLU	V1439		GLN	G1061	G1061	L929	T809	E500	S409	S409	S409
PRO	PRO	VAL	THR	GLU	GLU	V1440		GLN	G1061	G1061	L929	T809	E500	S409	S409	S409
PRO	PRO	VAL	THR	GLU	GLU	V1441		GLN	G1061	G1061	L929	T809	E500	S409	S409	S409
PRO	PRO	VAL	THR	GLU	GLU	V1442		GLN	G1061	G1061	L929	T809	E500	S409	S409	S409
PRO	PRO	VAL	THR	GLU	GLU	V1443		GLN	G1061	G1061	L929	T809	E500	S409	S409	S409
PRO	PRO	VAL	THR	GLU	GLU	V1444		GLN	G1061	G1061	L929	T809	E500	S409	S409	S409
PRO	PRO	VAL														

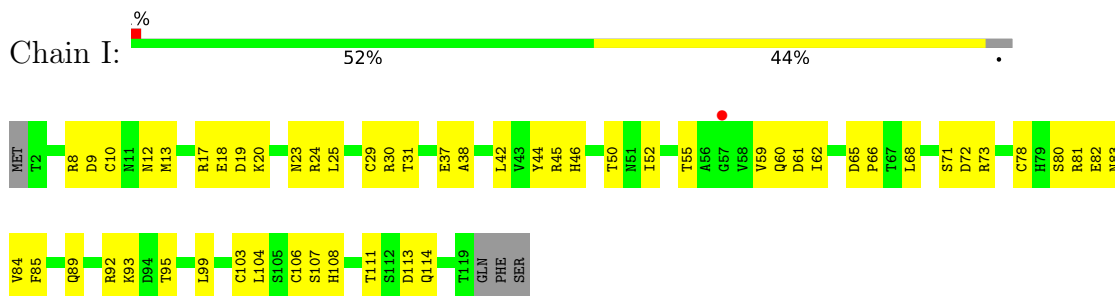
● Molecule 5: DNA-directed RNA polymerase II subunit RPB2



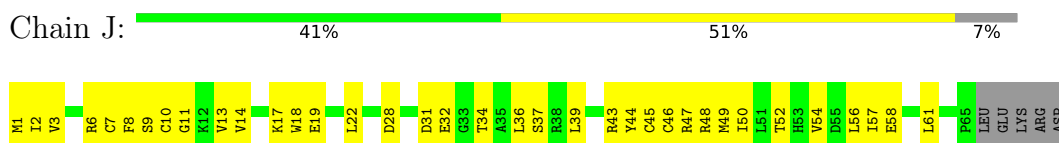
MET	SER	ASP	LEU	ALA	ASN	SER	GLY	LYS	TYR	ASP	GLU	ASP	PRO	TYR	GLY	PHE	GLY	D290	D29	E28	A27	L25	L26	L27	E28	D29	S30	W31	W31	L34	F37	E40	K41	S45	Q46	D56	Q60	T63	C64	E65	D66	S67	A76	GLN	HIS	THR	THR	THR	GLU	SER	ASP	ASN	ILE	SER																																																																									
R86	F92	M173	S176	K177	P100	N178	M179	Y180	L181	G295	E183	K193	E194	S208	E209	K210	A117	L118	L119	R120	N121	R217	L122	L128	F129	V130	N221	K227	V132	E138	ALA	ILE	ASP	GLY	VAL	PRO	ALA	GLY	ARG	GLU	LEU	LYS	T253	L254	Q255	L258	Y259	G260	R261	E262	T268	I269	F360	L361	P362	T272	L273	P274	R169	Y275	I276	G369																																																																	
E370	E371	S372	R373	F376	M381	I382	M383	R384	L385	L386	L387	R392	K393	D394	Q399	M310	L311	H400	F401	G402	K315	L314	E216	R217	L122	I324	Q325	D332	F333	I334	G335	R336	R337	THR	ALA	LEU	GLY	ILE	LYS	K345	R348	Y351	A352	I355	L356	Q357	K358	E359	I269	F360	L361	P362	T365	G467	E468	Q469	K470	L566																																																																					
S474	Q481	V482	L483	Y486	T487	T491	M383	R384	L385	S493	H494	R496	R497	T498	N499	T500	P501	F502	G503	ASP	GLY	ARG	ASP	GLY	LEU	LEU	R405	L406	D407	L408	A409	L412	F421	K422	K423	F429	Q433	E437	E438	ALA	HIS	ASP	PHE	ASN	MET	LYS	L446	A450	M552	P553	I554	F557	L558	V653	H654																																																																								
E567	D568	Y569	H572	Y582	H583	G584	Y585	Y586	H587	G588	E598	T599	L600	R601	T602	L603	R604	E612	G613	W614	S614	H615	L619	R620	E621	E622	E623	T626	T628	D629	A630	G631	R632	V633	Y634	R635	P636	F638	L641	L642	V640	H643	GLU	SER	LEU	G647	E650	L651	R652	V653	H654																																																																												
K655	L661	Y666	D668	ILE	GLY	GLY	PHE	GLU	ASP	V676	L689	V690	E691	Y692	L693	D694	R695	E696	D790	E699	M705	E714	ALA	ASN	GLU	GLU	ASN	L721	P725	A726	K727	R728	I729	R730	V731	T737	C741	E742	I743	H744	Q835	H834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	D891	K892	L893	L894	L895	L896	L897	L898	L899	L900	Y903	R904	Y910	L911	L912	G913	K914	L915	L916	S919	PRO	ASP	GLU	GLU	GLU	LEU	GLY	GLN	L1010
THR	A930	Y931	H932	D936	A937	S938	T939	R942	S943	T944	E945	N946	V952	L953	V954	Q958	L961	V964	R967	V968	R969	T970	T971	K972	Q975	I976	G977	D978	R983	H984	K987	G988	T989	I990	G991	Y994	R995	R996	E997	D998	M999	P1000	I1006	V1007	P1008	D1009	L1010																																																																																
I1011	I1012	P1013	P1014	H1015	P1018	S1019	R1020	M1021	T1022	V1023	A1024	I1027	L1030	M1033	V1034	L1037	S1038	S1045	P1046	E1053	R1054	R1055	R1056	M1072	Y1073	M1074	G1075	H1076	L1081	M1082	A1083	Q1084	I1085	F1086	F1087	Y1092	Q1093	R1094	M1098	V1099	D1100	D1101	R1108	R1109	R1110	R1111	R1112	R1113	R1114	R1115	R1116	R1117	R1118	R1119	R1120	R1121	R1122																																																																						
L1128	R1129	E1134	R1135	D1136	C1137	M1138	A1143	A1144	F1146	R1150	L1151	M1152	E1153	D1156	A1157	F1158	R1159	V1160	H1161	I1162	C1163	G1164	I1165	L1168	M1169	I1172	A1173	K1174	L1175	Q1179	C1182	K1183	D1186	M1187	K1188	I1189	D1190	Q1193	P1197	Y1198	K1201	E1206	L1207	M1208																																																																																			
I1212	T1213	P1214	R1215	L1216	Y1217	S1221	ARG	ASP	PHE																																																																																																																						



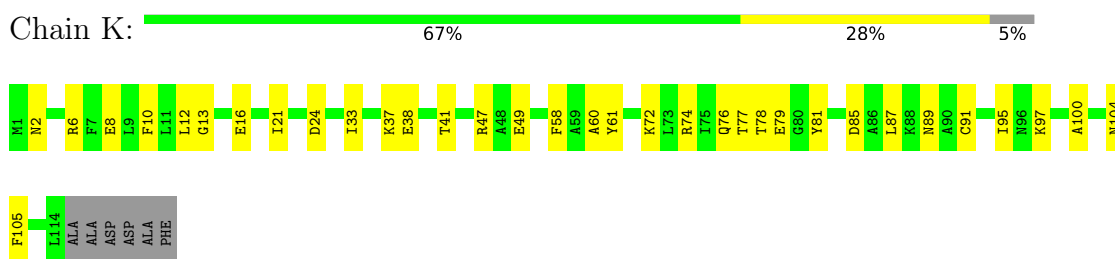
- Molecule 10: DNA-directed RNA polymerase II subunit RPB9



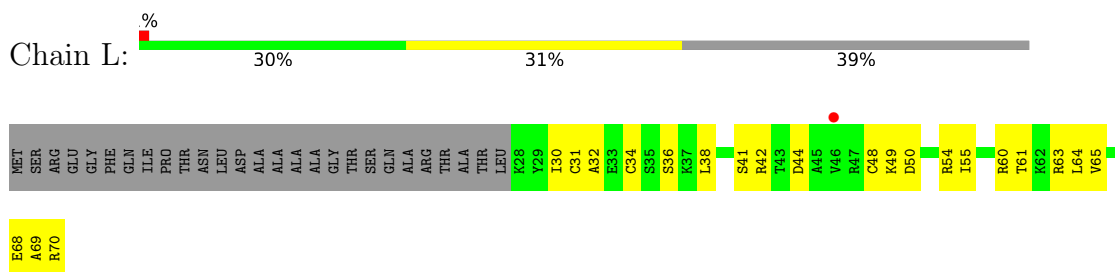
- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 12: DNA-directed RNA polymerase II subunit RPB11



- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC4



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	167.78Å 222.76Å 192.96Å 90.00° 100.54° 90.00°	Depositor
Resolution (Å)	49.53 – 3.70 49.53 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.53-3.70) 99.8 (49.53-3.70)	Depositor EDS
$R_{merge}$	0.52	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 3.67Å)	Xtrriage
Refinement program	PHENIX 1.13	Depositor
R, $R_{free}$	0.232 , 0.281 0.234 , 0.281	Depositor DCC
$R_{free}$ test set	2000 reflections (2.55%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	106.3	Xtrriage
Anisotropy	0.319	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 89.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	29168	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	119.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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: 5N0, MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	R	0.20	0/263	0.48	0/409
2	T	0.30	0/584	0.51	0/898
3	N	0.19	0/331	0.35	0/509
4	A	0.23	0/11020	0.42	0/14907
5	B	0.22	0/9030	0.42	0/12186
6	C	0.22	0/2139	0.41	0/2899
7	E	0.21	0/1767	0.41	0/2378
8	F	0.21	0/696	0.40	0/943
9	H	0.20	0/1082	0.44	0/1466
10	I	0.22	0/970	0.43	0/1308
11	J	0.23	0/541	0.43	0/727
12	K	0.23	0/937	0.41	0/1265
13	L	0.19	0/339	0.45	0/450
All	All	0.22	0/29699	0.42	0/40345

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	235	0	121	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	T	525	0	297	31	0
3	N	293	0	156	9	0
4	A	10828	0	10876	399	0
5	B	8859	0	8816	356	0
6	C	2101	0	2056	91	0
7	E	1731	0	1758	51	0
8	F	684	0	692	29	0
9	H	1064	0	1029	42	0
10	I	952	0	897	45	0
11	J	532	0	542	36	0
12	K	919	0	929	30	0
13	L	337	0	352	16	0
14	R	1	0	0	0	0
15	T	99	0	0	5	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
All	All	29168	0	28521	1011	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 18.

The worst 5 of 1011 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:446:ARG:NH2	4:A:480:ALA:HA	1.53	1.23
4:A:446:ARG:HH21	4:A:480:ALA:CA	1.76	0.98
4:A:446:ARG:HH21	4:A:480:ALA:HA	0.79	0.94
11:J:10:CYS:SG	11:J:43:ARG:NH2	2.46	0.89
4:A:1224:LEU:HD11	4:A:1240:CYS:HB3	1.57	0.84

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	
4	A	1370/1733 (79%)	1264 (92%)	106 (8%)	0	100	100
5	B	1103/1224 (90%)	1030 (93%)	73 (7%)	0	100	100
6	C	265/318 (83%)	245 (92%)	20 (8%)	0	100	100
7	E	210/215 (98%)	196 (93%)	14 (7%)	0	100	100
8	F	84/155 (54%)	78 (93%)	6 (7%)	0	100	100
9	H	129/146 (88%)	119 (92%)	10 (8%)	0	100	100
10	I	116/122 (95%)	104 (90%)	12 (10%)	0	100	100
11	J	63/70 (90%)	57 (90%)	6 (10%)	0	100	100
12	K	112/120 (93%)	107 (96%)	5 (4%)	0	100	100
13	L	41/70 (59%)	39 (95%)	2 (5%)	0	100	100
All	All	3493/4173 (84%)	3239 (93%)	254 (7%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	1194/1520 (79%)	1194 (100%)	0	100	100
5	B	955/1061 (90%)	955 (100%)	0	100	100
6	C	235/274 (86%)	235 (100%)	0	100	100
7	E	193/197 (98%)	193 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	F	73/137 (53%)	73 (100%)	0	100	100
9	H	116/128 (91%)	116 (100%)	0	100	100
10	I	110/116 (95%)	110 (100%)	0	100	100
11	J	60/65 (92%)	60 (100%)	0	100	100
12	K	99/102 (97%)	99 (100%)	0	100	100
13	L	37/57 (65%)	37 (100%)	0	100	100
All	All	3072/3657 (84%)	3072 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
10	I	46	HIS
10	I	90	GLN
12	K	112	GLN
5	B	325	GLN
5	B	60	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	10/11 (90%)	2 (20%)	1 (10%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	10	C
1	R	11	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	R	9	G

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 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
15	5N0	T	101	-	100,107,107	2.82	51 (51%)	115,153,153	2.05	26 (22%)

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
15	5N0	T	101	-	-	13/92/92/92	0/9/9/9

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	101	5N0	C49-N23	8.35	1.47	1.33
15	T	101	5N0	C22-N10	7.97	1.47	1.33
15	T	101	5N0	C56-N25	6.25	1.47	1.33
15	T	101	5N0	C26-N14	6.13	1.47	1.36
15	T	101	5N0	C9-N3	6.08	1.49	1.39

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	101	5N0	C16-C11-N7	6.27	129.57	122.78
15	T	101	5N0	C37-C32-N18	5.55	128.80	122.78
15	T	101	5N0	C4-C5-N3	5.44	121.26	113.08
15	T	101	5N0	C22-C17-N9	5.36	128.59	122.78
15	T	101	5N0	N1-C4-N2	-5.31	108.41	111.40

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

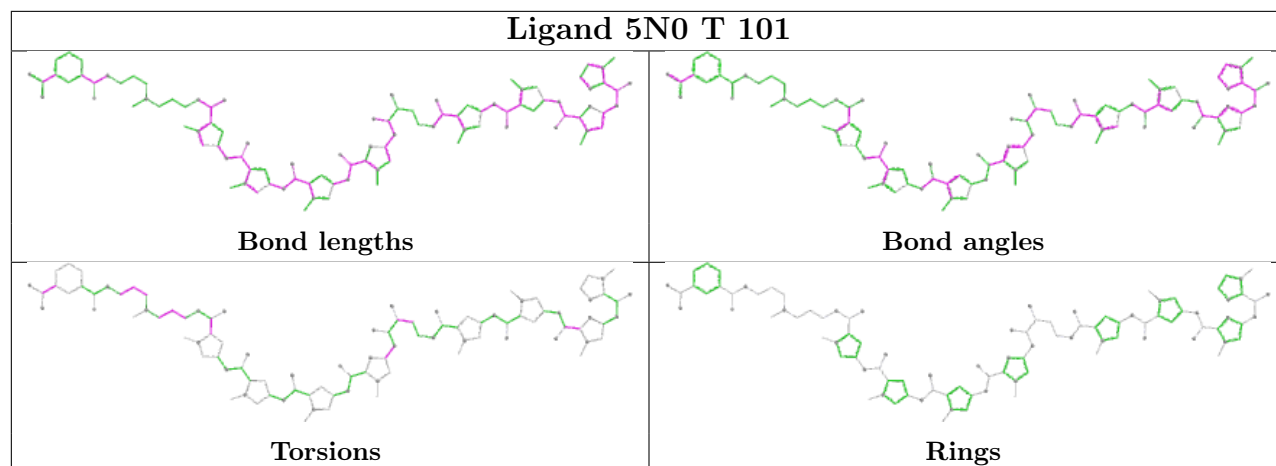
Mol	Chain	Res	Type	Atoms
15	T	101	5N0	C23-C24-C25-C26
15	T	101	5N0	N22-C44-C49-O9
15	T	101	5N0	N22-C44-C49-N23
15	T	101	5N0	C58-C59-C63-O11
15	T	101	5N0	C60-C59-C63-O12

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	T	101	5N0	5	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](#)

There are no chain breaks in this entry.

## 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, 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	R	11/11 (100%)	0.21	1 (9%) 15 13	116, 132, 191, 198	0
2	T	26/30 (86%)	0.41	0 100 100	118, 225, 252, 258	0
3	N	14/20 (70%)	0.20	0 100 100	229, 244, 260, 264	0
4	A	1384/1733 (79%)	0.02	9 (0%) 84 63	52, 113, 188, 236	0
5	B	1123/1224 (91%)	0.01	5 (0%) 88 72	55, 99, 153, 196	0
6	C	267/318 (83%)	-0.05	1 (0%) 88 72	67, 99, 136, 165	0
7	E	212/215 (98%)	-0.06	2 (0%) 81 58	96, 154, 209, 231	0
8	F	86/155 (55%)	-0.18	0 100 100	82, 114, 147, 186	0
9	H	133/146 (91%)	0.07	2 (1%) 72 46	106, 137, 170, 202	0
10	I	118/122 (96%)	-0.07	1 (0%) 82 60	83, 117, 150, 162	0
11	J	65/70 (92%)	0.02	0 100 100	73, 93, 151, 161	0
12	K	114/120 (95%)	-0.18	0 100 100	78, 105, 131, 153	0
13	L	43/70 (61%)	0.27	1 (2%) 61 38	92, 158, 222, 258	0
All	All	3596/4234 (84%)	-0.00	22 (0%) 85 66	52, 111, 185, 264	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	E	83	CYS	3.5
9	H	63	LEU	3.3
10	I	57	GLY	3.2
13	L	46	VAL	3.0
5	B	620	ARG	2.9

### 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](#)

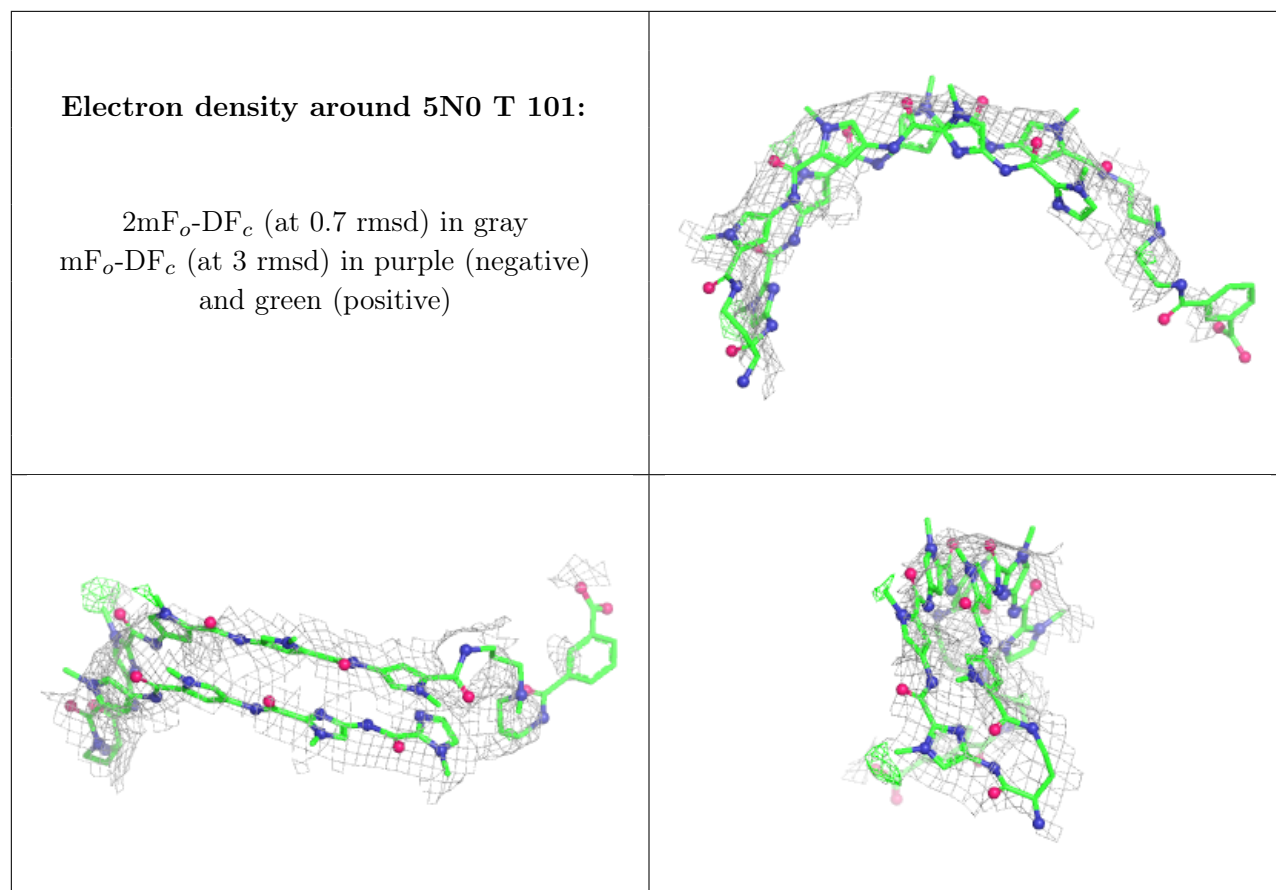
There are no oligosaccharides in this entry.

### 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
15	5N0	T	101	99/99	0.71	0.12	198,236,262,264	0
14	MG	R	2001	1/1	0.80	0.26	141,141,141,141	0
16	ZN	A	1801	1/1	0.93	0.12	242,242,242,242	0
16	ZN	B	1301	1/1	0.93	0.07	195,195,195,195	0
16	ZN	L	101	1/1	0.96	0.08	182,182,182,182	0
16	ZN	A	1802	1/1	0.97	0.04	167,167,167,167	0
16	ZN	C	401	1/1	0.99	0.02	108,108,108,108	0
16	ZN	I	202	1/1	1.00	0.03	110,110,110,110	0
16	ZN	J	101	1/1	1.00	0.02	90,90,90,90	0
16	ZN	I	201	1/1	1.00	0.03	99,99,99,99	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.