



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2025 – 10:10 AM EDT

PDB ID : 9N5C / pdb_00009n5c
Title : RNA polymerase II elongation complex with 8-oxoG at +1 site, CMPCPP-bound
Authors : Oh, J.; Wang, D.
Deposited on : 2025-02-04
Resolution : 3.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

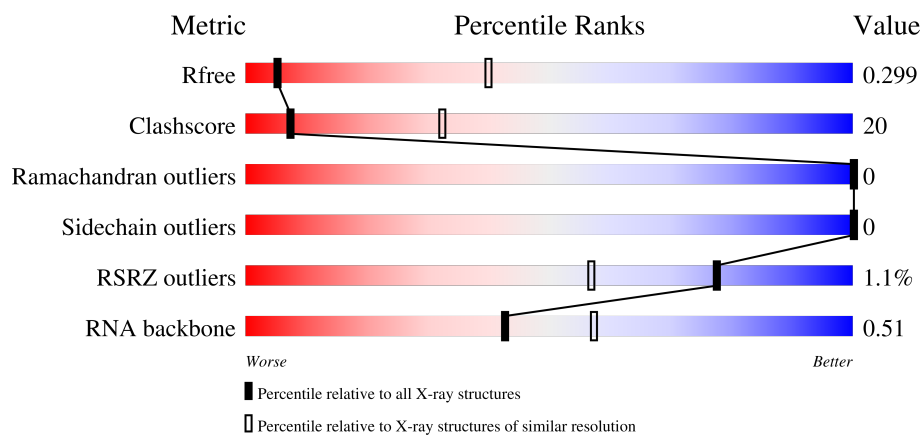
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	164625	1563 (3.70-3.50)
Clashscore	180529	1665 (3.70-3.50)
Ramachandran outliers	177936	1641 (3.70-3.50)
Sidechain outliers	177891	1640 (3.70-3.50)
RSRZ outliers	164620	1562 (3.70-3.50)
RNA backbone	3690	1108 (4.20-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	R	9	 33% 56% 11%
2	T	29	 31% 59% 10%
3	N	18	 28% 56% 17%
4	A	1733	 45% 35% 20%

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Mol	Chain	Length	Quality of chain
5	B	1224	<div> <div>%</div> <div> <div></div> <div>53%</div> <div>38%</div> <div>8%</div> </div> </div>
6	C	318	<div> <div>%</div> <div> <div></div> <div>47%</div> <div>37%</div> <div>16%</div> </div> </div>
7	E	215	<div> <div></div> <div> <div>67%</div> <div>32%</div> <div>.</div> </div> </div>
8	F	155	<div> <div></div> <div> <div>32%</div> <div>23%</div> <div>45%</div> </div> </div>
9	H	146	<div> <div>%</div> <div> <div></div> <div>51%</div> <div>40%</div> <div>9%</div> </div> </div>
10	I	122	<div> <div></div> <div> <div>54%</div> <div>42%</div> <div>..</div> </div> </div>
11	J	70	<div> <div>3%</div> <div> <div></div> <div>46%</div> <div>47%</div> <div>7%</div> </div> </div>
12	K	120	<div> <div></div> <div> <div>61%</div> <div>34%</div> <div>5%</div> </div> </div>
13	L	70	<div> <div>%</div> <div> <div></div> <div>30%</div> <div>31%</div> <div>39%</div> </div> </div>

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 29046 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
1	R	9	Total	C	N	O	P	0	0	0
			199	88	40	62	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	26	Total	C	N	O	P	0	0	0
			521	250	80	165	26			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	15	Total	C	N	O	P	0	0	0
			317	148	71	83	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1385	Total	C	N	O	S	0	0	0
			10817	6824	1890	2043	60			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1121	Total	C	N	O	S	0	0	0
			8843	5598	1547	1645	53			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	213	Total	C	N	O	S	0	0	0
			1740	1105	307	317	11			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	133	Total	C	N	O	S	0	0	0
			1052	664	173	211	4			

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

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

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

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 subunit RPB11.

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 subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	43	Total	C	N	O	S	0	0	0
			331	205	63	59	4			

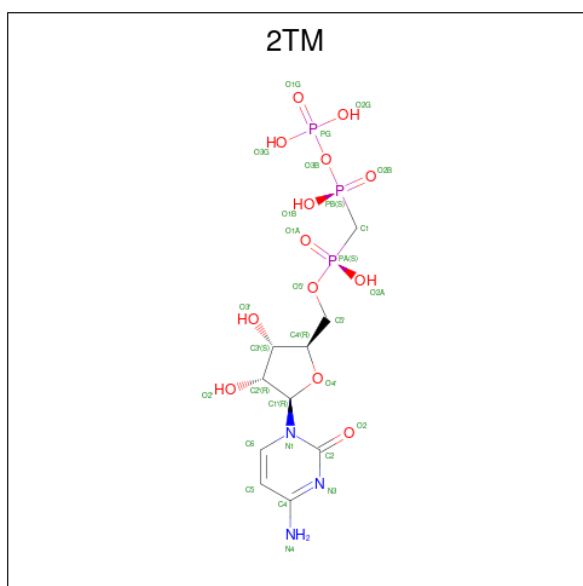
- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total 1	Mg 1	0	0

- Molecule 16 is 5'-O-[(S)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]methyl}phosphoryl]cytidine (CCD ID: 2TM) (formula: C₁₀H₁₈N₃O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



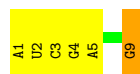
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
16	B	1	Total 29	C 10	N 3	O 13	P 3	0	0

3 Residue-property plots

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

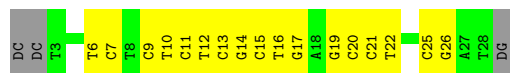
• Molecule 1: RNA

Chain R: 



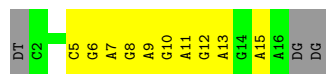
• Molecule 2: Template strand DNA

Chain T: 



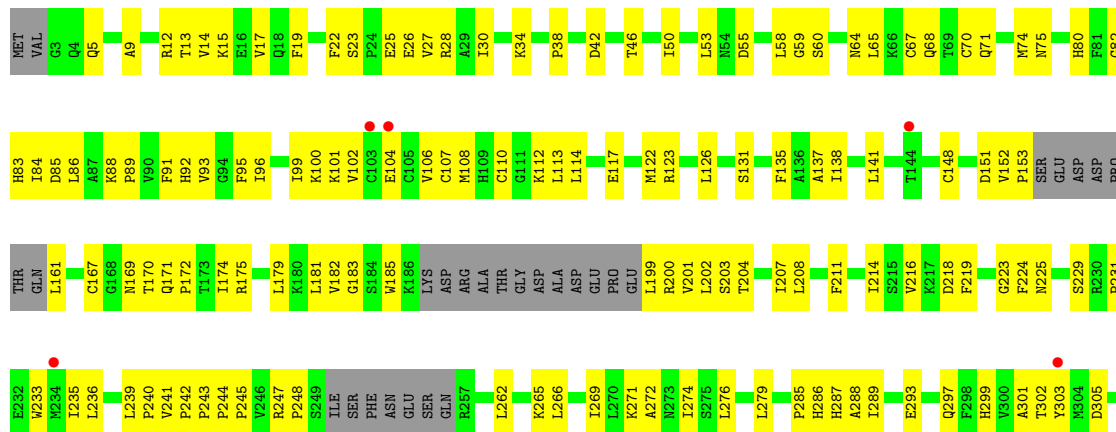
• Molecule 3: Non-template strand DNA

Chain N: 

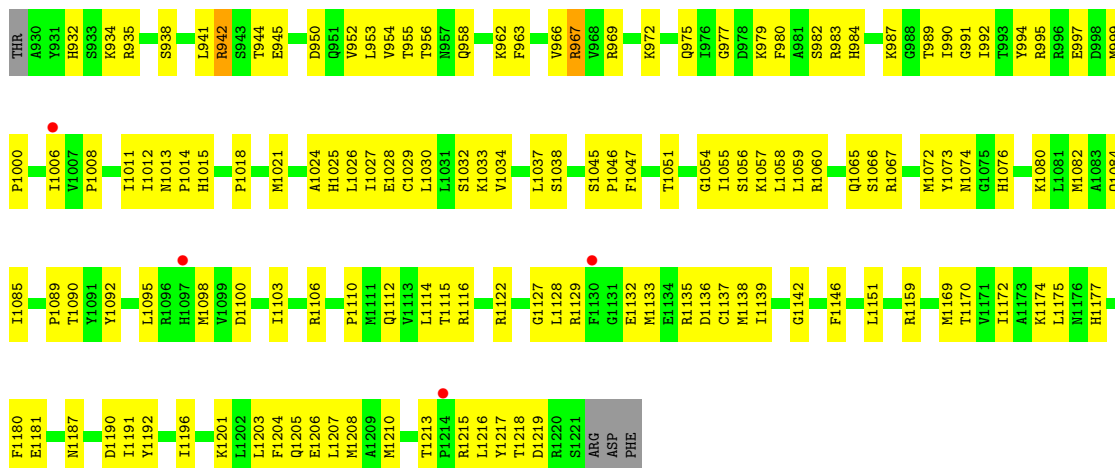


• Molecule 4: DNA-directed RNA polymerase II subunit RPB1

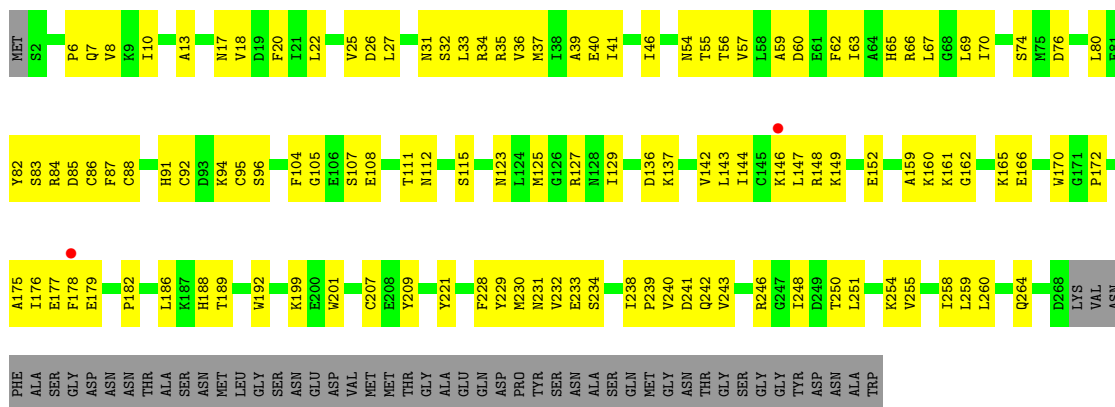
Chain A: 



THR	ALA	SER	L1369	E1269	L1193	M1110	R1023	T907	T834	M746	Q650		M479	G395	I308
LEU	VAL	LEU	L1370	M1270	E1196	M1111	S1024	E914	T835	V747	R651		F482	F396	A309
GLY	GLY	LYS	L1371	T1271	L1197	T1112	R1025	E915	G835	M748	V652		D483		G310
GLY	GLY	TYR	L1372	T1272	L1198	T1113		G916	G836		V653		P400		A314
ALA	GLY	TYR	L1373	L1273	D1198	L1116	R1030	G917	Q837	S751	N654		D485	C401	
ASP	PRO	PRO	M1374	R1274	M1202	T1117	V1031		Q838	S752			M487	A402	I325
TYR	GLY	GLY	M1375	G1275	M1203	T1118	E1034	L920	R839	S753	F662		M488		R326
GLY	GLY	GLN	L1276	K1205	K1206	V1119	Y1035	G921	R840	F755	S663			V405	R335
GLY	GLY	LYS	D1206	D1206	L1207	E1129	R1036	L922	L841	I756	G574			I406	I336
ALA	ALA	ILE	L1207	V1282	V1282	E1130	R1037	L925	V842	M757	G665		V491		R337
THR	THR	THR	T1208	M1208	M1209	A1131	L1037	Q926	L845	A759	I666		P492		G338
PRO	ILE	GLU	M1209	M1209		L1132	M1048		E846	Q760	D672				M341
GLU	GLU	GLU	V1212	V1212		L1133	I1049	E932	D847						G342
GLY	GLY	ASP	G1213	G1213		R1135	S1056	Y933	I848	A763	T675		E496		K343
ALA	ALA	GLY	E1214	E1214		S1136	V1057	L936	M849	C764	M676				R344
TYR	TYR	GLN	R1215	R1215		A1137	V1058	L937	M849	A765					S348
GLY	GLY	ASP	L1216	L1216		I1138		K941	V851	G766					A349
GLY	GLY	ASP	K1217	K1217		E1139	M1063	F942	H851	G767					R350
ALA	ALA	GLY	Q1218	Q1218		H1140	V1064	L943	V852						T351
PRO	PRO	VAL	T1219	T1219		K1144	G1065	R944	H857	I775					V352
THR	THR	THR	F1220	F1220			V1066	E945	H858	A776					S354
SER	SER	PRO	K1221	K1221		I1148	L1067	D949	S859	F777					G355
PRO	PRO	TYR	N1222	N1222											D356
GLY	GLY	SER	D1223	D1223		E1151	Q1070	A952	V863	D781	K688				P357
PHE	GLY	ASN	L1224	L1224		I1152	S1071	A953	F866	R782	T694				E360
VAL	VAL	GLY	F1225	F1225		V1153	A1076	G954	I867	I783					L361
SER	SER	GLY	I1226	I1226		Y1154	T1077	P955	Y868	P785	Q698				D362
SER	SER	LEU	W1228	W1228		P1155	M1078	L956	G869	H786	L701				V364
PRO	PRO	VAL	K1235	K1235		D1157	M1079		E870		R711				G365
GLY	PHE	ASN	L1236	L1236		S1160	T1080	T960	D871	K789					D366
PRO	PRO	LEU	T1237	T1237		T1161	ASN	R961	G872		F714				P367
THR	THR	LEU	I1238	I1238		V1162	THR	R962	D874	Y792	E715				K368
PRO	PRO	ASP	R1239	R1239		I1163	PHE	I963	A875	K797					S369
SER	SER	VAL	C1240	C1240		P1164	HIS	I964	A876	G798	V718				Q363
PRO	PRO	LYS	R1241	R1241		E1165	PHE	Q965	H877	F799					V364
ASP	ASP	ASP	V1242	V1242		D1166	ALA	Q968	I878	V800	L722				P367
THR	THR	LEU	V1243	V1243		I1169	VAL	H975	E879	R806	R726				K368
PRO	PRO	MET	ARG	ARG		I1170	VAL	H975	K880	R727					I370
THR	THR	PHE	LYS	LYS		L1176	ALA	I986	Q881	T809	G623				A371
PRO	PRO	SER	LEU	LEU		LEU	SER	I986	S882		A457				K372
ALA	ALA	LEU	ASP	ASP		ASP	T1095	V990	D884	E812	A729				T373
SER	SER	VAL	ALA	ALA		GLY	V1098	K991	T885	F813	G730				T374
ASP	ASP	ASP	GLY	GLY		GLY	P1099	D992	T886	F814	R731				T375
PRO	PRO	GLY	THR	THR		GLY	R1100	Q994	I886	F815	L732				V380
SER	SER	GLY	GLY	GLY		ALA	R1101	E995	S889	M818	N736				T381
SER	SER	ASN	ALA	ALA		GLY	L1102	R996	R896	G819	L737				P382
THR	THR	ASN	GLY	GLY		GLY	E1103	L997	R898	G820	K738				Y383
PRO	PRO	ALA	THR	THR		PHE	L1104	R1001	R821	L740	D739				R387
ALA	ALA	ALA	D1257	D1257		ASP	L1105		L824	N741					L388
PRO	PRO	ALA	I1263	I1263		Q1187	M1106	D1013	L825	I825	N742				L391
THR	THR	GLY	M1267	M1267		W1191	V1107	L1021	N903	D826	V743				V392
PHE	PHE	PHE	L1268	L1268		L1192	K1109	L1022	H906	K830	Q745				



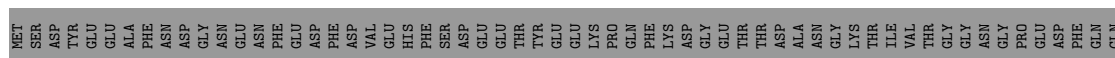
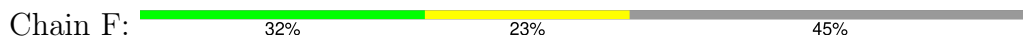
• Molecule 6: DNA-directed RNA polymerase II subunit RPB3

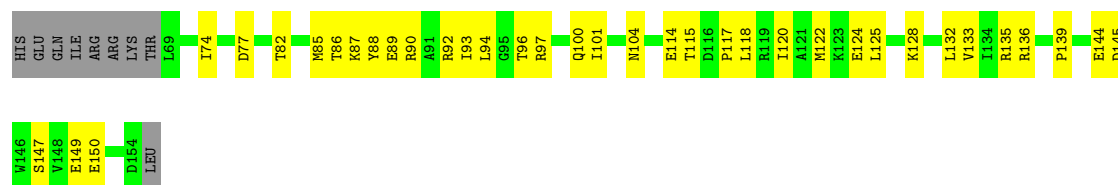


• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1

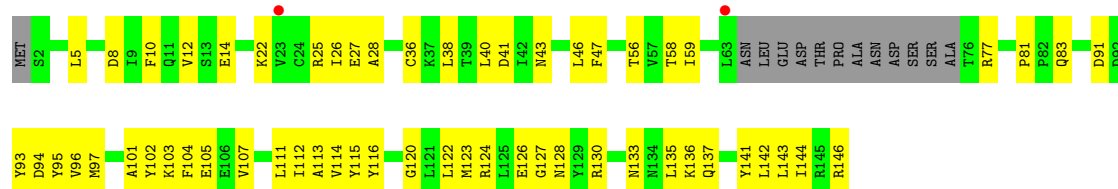


• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2

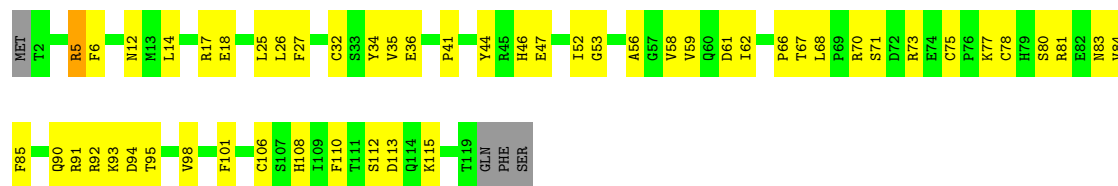




- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3



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



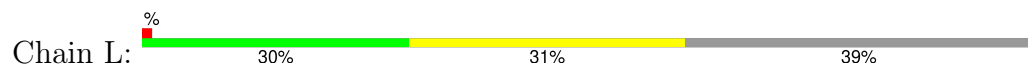
- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5



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



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



MET	SER	ARG	GLU	GLY	PHE	GLN	ILE	PRO	THR	ASN	LEU	ASP	ALA	ALA	ALA	GLY	THR	SER	GLN	ALA	ARG	THR	ALA	THR	LEU	K28	Y29	I30	C31	A32	E33	C34	K37	L38	S39	L40	D44	A45	V46	R47	C48	C51	G52	H53	R54	I55	L56	T61	E68	A69	R70
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.64Å 222.99Å 192.26Å 90.00° 98.55° 90.00°	Depositor
Resolution (Å)	48.77 – 3.60 48.77 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.77-3.60) 99.4 (48.77-3.60)	Depositor EDS
R_{merge}	0.51	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 3.57Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.252 , 0.297 0.253 , 0.299	Depositor DCC
R_{free} test set	2000 reflections (2.41%)	wwPDB-VP
Wilson B-factor (Å ²)	103.1	Xtriage
Anisotropy	0.582	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 117.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	29046	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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, 8OG, 2TM, 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	R	0.18	0/223	0.39	0/345
2	T	0.22	0/551	0.48	0/843
3	N	0.22	0/359	0.42	0/553
4	A	0.17	0/11009	0.41	0/14897
5	B	0.15	0/9014	0.37	0/12165
6	C	0.16	0/2139	0.39	0/2899
7	E	0.14	0/1776	0.36	0/2390
8	F	0.12	0/696	0.35	0/943
9	H	0.16	0/1070	0.45	0/1452
10	I	0.17	0/970	0.45	0/1308
11	J	0.19	0/541	0.48	0/727
12	K	0.17	0/937	0.42	0/1265
13	L	0.13	0/333	0.46	0/443
All	All	0.16	0/29618	0.40	0/40230

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
4	A	0	2
5	B	0	3
9	H	0	1
10	I	0	1
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	412	ARG	Sidechain
4	A	726	ARG	Sidechain
5	B	857	ARG	Sidechain
5	B	942	ARG	Sidechain
5	B	967	ARG	Sidechain

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	199	0	98	8	0
2	T	521	0	297	14	0
3	N	317	0	166	12	0
4	A	10817	0	10839	521	0
5	B	8843	0	8799	363	0
6	C	2101	0	2058	102	0
7	E	1740	0	1766	48	0
8	F	684	0	692	29	0
9	H	1052	0	1007	56	0
10	I	952	0	904	48	1
11	J	532	0	543	38	0
12	K	919	0	929	41	0
13	L	331	0	343	16	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	1	0	0	0	0
16	B	29	0	14	1	0
All	All	29046	0	28455	1157	1

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 20.

The worst 5 of 1157 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)
5:B:863:GLU:HG3	5:B:962:LYS:HB2	1.46	0.97
9:H:36:CYS:HA	9:H:126:GLU:O	1.67	0.94
11:J:21:TYR:HB2	11:J:39:LEU:HD11	1.50	0.92
4:A:1364:ASN:OD1	4:A:1366:ARG:NH1	2.03	0.91
5:B:101:MET:HG2	5:B:111:ALA:HA	1.57	0.87

All (1) 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)
10:I:81:ARG:O	10:I:81:ARG:NH2[2_556]	2.14	0.06

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	1371/1733 (79%)	1326 (97%)	45 (3%)	0	100	100
5	B	1101/1224 (90%)	1081 (98%)	20 (2%)	0	100	100
6	C	265/318 (83%)	259 (98%)	6 (2%)	0	100	100
7	E	211/215 (98%)	198 (94%)	13 (6%)	0	100	100
8	F	84/155 (54%)	83 (99%)	1 (1%)	0	100	100
9	H	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
10	I	116/122 (95%)	113 (97%)	3 (3%)	0	100	100
11	J	63/70 (90%)	63 (100%)	0	0	100	100
12	K	112/120 (93%)	111 (99%)	1 (1%)	0	100	100
13	L	41/70 (59%)	40 (98%)	1 (2%)	0	100	100
All	All	3493/4173 (84%)	3397 (97%)	96 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	1191/1520 (78%)	1191 (100%)	0	100	100
5	B	954/1061 (90%)	954 (100%)	0	100	100
6	C	235/274 (86%)	235 (100%)	0	100	100
7	E	194/197 (98%)	194 (100%)	0	100	100
8	F	73/137 (53%)	73 (100%)	0	100	100
9	H	114/128 (89%)	114 (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	36/57 (63%)	36 (100%)	0	100	100
All	All	3066/3657 (84%)	3066 (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 32 such sidechains are listed below:

Mol	Chain	Res	Type
9	H	33	GLN
9	H	134	ASN
4	A	1222	ASN
4	A	1187	GLN
10	I	46	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	8/9 (88%)	1 (12%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	9	G

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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
2	8OG	T	19	2	22,25,26	3.97	18 (81%)	26,37,40	1.50	5 (19%)

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
2	8OG	T	19	2	-	4/7/21/22	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	19	8OG	C8-N7	7.26	1.51	1.38
2	T	19	8OG	C8-N9	6.14	1.51	1.40
2	T	19	8OG	C2-N3	5.78	1.47	1.33
2	T	19	8OG	C4-N3	5.61	1.47	1.34
2	T	19	8OG	C2-N2	4.74	1.45	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	19	8OG	C2-N3-C4	3.63	118.55	112.30
2	T	19	8OG	C5-N7-C8	-2.77	105.65	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	19	8OG	O6-C6-C5	-2.57	121.06	127.26
2	T	19	8OG	C4-C5-N7	2.46	110.57	106.06
2	T	19	8OG	C5-C6-N1	2.24	118.29	112.13

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	19	8OG	O4'-C4'-C5'-O5'
2	T	19	8OG	C3'-C4'-C5'-O5'
2	T	19	8OG	C4'-C5'-O5'-P
2	T	19	8OG	C2'-C1'-N9-C8

There are no ring outliers.

No monomer is involved in short contacts.

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
16	2TM	B	2101	-	26,30,30	3.98	15 (57%)	39,47,47	0.96	2 (5%)

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	2TM	B	2101	-	-	4/19/38/38	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	2101	2TM	PB-O3B	7.73	1.67	1.58
16	B	2101	2TM	C2'-C3'	-7.14	1.34	1.53
16	B	2101	2TM	C2-N3	6.50	1.49	1.36
16	B	2101	2TM	O4'-C4'	6.38	1.59	1.45
16	B	2101	2TM	C6-C5	6.10	1.49	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	2101	2TM	C3'-C2'-C1'	2.53	106.25	101.46
16	B	2101	2TM	PB-O3B-PG	-2.35	124.02	132.45

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	B	2101	2TM	C3'-C4'-C5'-O5'
16	B	2101	2TM	O4'-C4'-C5'-O5'
16	B	2101	2TM	C5'-O5'-PA-O1A
16	B	2101	2TM	C4'-C5'-O5'-PA

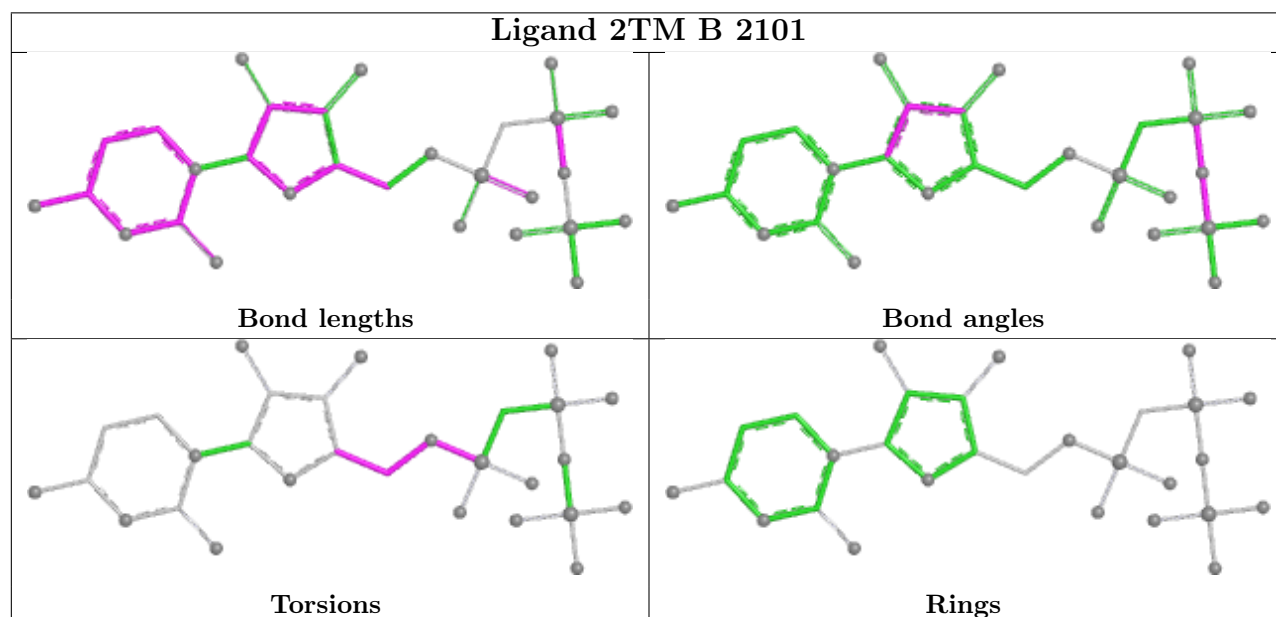
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	2101	2TM	1	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	R	9/9 (100%)	0.00	0 100 100	76, 86, 172, 223	0
2	T	25/29 (86%)	0.15	0 100 100	90, 188, 241, 268	0
3	N	15/18 (83%)	0.19	0 100 100	143, 205, 241, 253	0
4	A	1385/1733 (79%)	-0.07	16 (1%) 76 55	74, 121, 184, 241	0
5	B	1121/1224 (91%)	0.02	18 (1%) 70 49	52, 106, 170, 250	0
6	C	267/318 (83%)	-0.17	2 (0%) 84 67	73, 111, 158, 195	0
7	E	213/215 (99%)	-0.33	0 100 100	83, 144, 211, 252	0
8	F	86/155 (55%)	-0.25	0 100 100	76, 110, 158, 178	0
9	H	133/146 (91%)	-0.03	2 (1%) 71 51	106, 146, 202, 220	0
10	I	118/122 (96%)	-0.06	0 100 100	88, 137, 194, 229	0
11	J	65/70 (92%)	0.14	2 (3%) 51 33	65, 99, 134, 165	0
12	K	114/120 (95%)	-0.23	0 100 100	63, 103, 147, 185	0
13	L	43/70 (61%)	0.08	1 (2%) 61 41	93, 195, 256, 274	0
All	All	3594/4229 (84%)	-0.06	41 (1%) 77 57	52, 118, 188, 274	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	B	775	LYS	4.7
4	A	103	CYS	3.6
5	B	899	ILE	3.6
13	L	32	ALA	3.5
5	B	819	ALA	3.5

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	8OG	T	19	23/24	0.88	0.11	88,96,112,144	0

6.3 Carbohydrates [i](#)

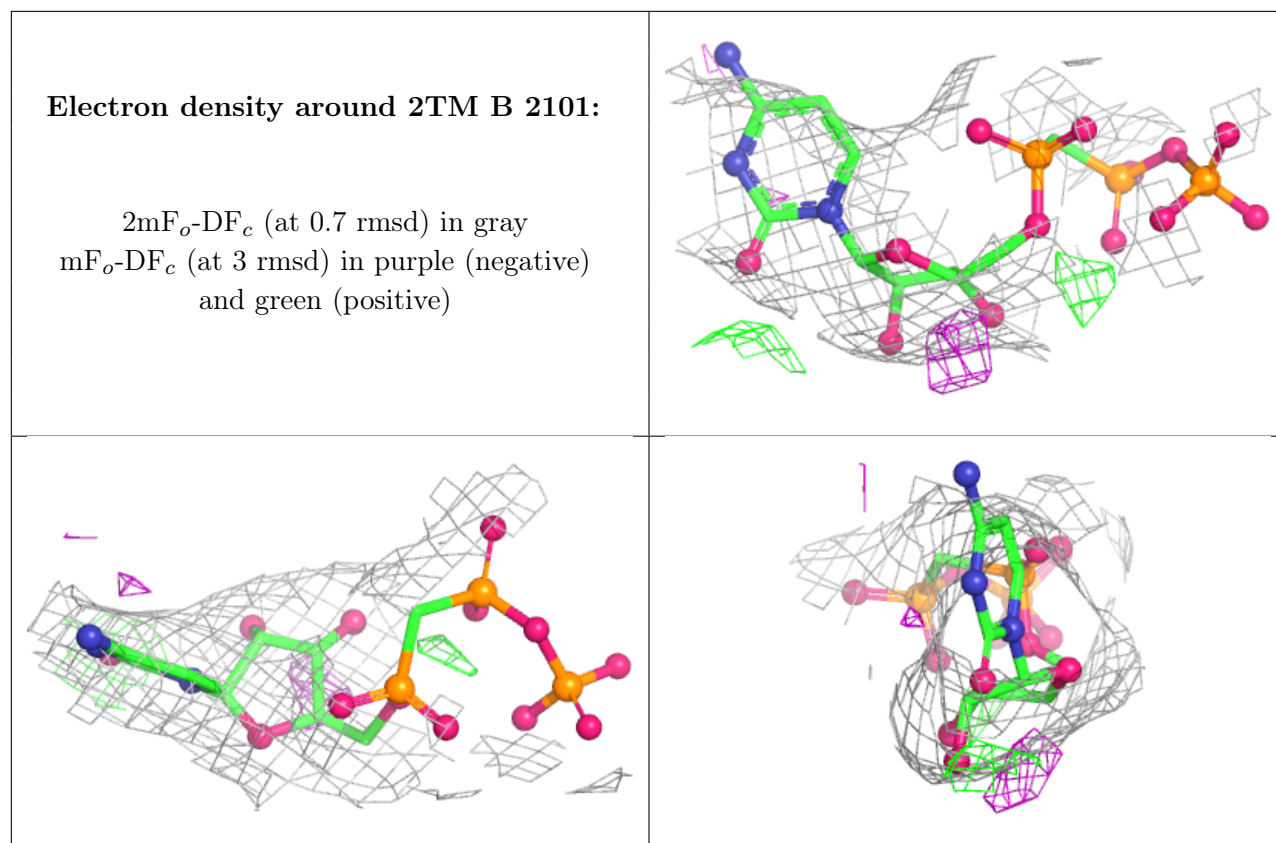
There are no oligosaccharides in this entry.

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	ZN	I	202	1/1	0.65	0.19	209,209,209,209	0
14	ZN	L	101	1/1	0.78	0.11	309,309,309,309	0
16	2TM	B	2101	29/29	0.87	0.09	38,77,133,172	0
14	ZN	A	1801	1/1	0.92	0.07	240,240,240,240	0
14	ZN	J	101	1/1	0.92	0.09	145,145,145,145	0
14	ZN	C	401	1/1	0.93	0.10	148,148,148,148	0
14	ZN	B	2102	1/1	0.98	0.04	163,163,163,163	0
15	MG	A	1803	1/1	0.98	0.05	62,62,62,62	0
14	ZN	A	1802	1/1	0.98	0.03	121,121,121,121	0
14	ZN	I	201	1/1	0.99	0.03	110,110,110,110	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.