



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:17 PM UTC

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 Phenix2.0
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

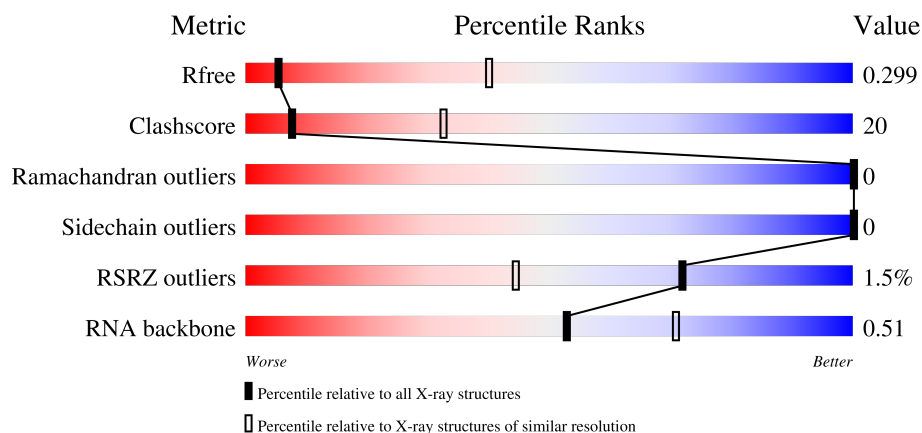
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)
RNA backbone	3983	1014 (4.14-3.06)

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	 2% 53% 38% 8%
6	C	318	 % 47% 37% 16%
7	E	215	 67% 32% .
8	F	155	 32% 23% 45%
9	H	146	 % 51% 40% 9%
10	I	122	 54% 42% . .
11	J	70	 3% 46% 47% 7%
12	K	120	 % 61% 34% 5%
13	L	70	 % 30% 31% 39%

2 Entry composition [i](#)

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			

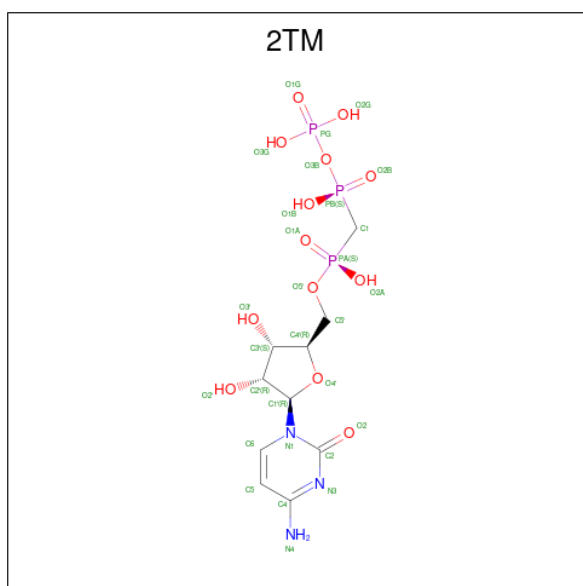
- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

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).

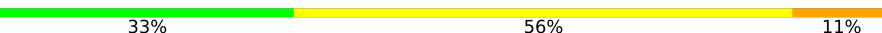


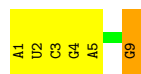
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	B	1	Total 29	C 10	N 3	O 13	P 3	0	0

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.

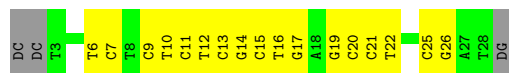
• Molecule 1: RNA

Chain R: 

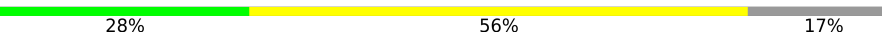


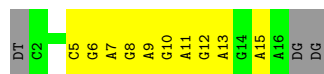
• Molecule 2: Template strand DNA

Chain T: 



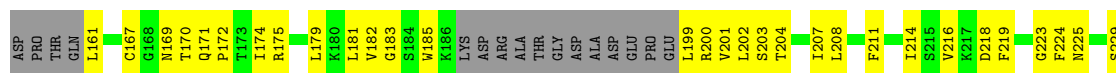
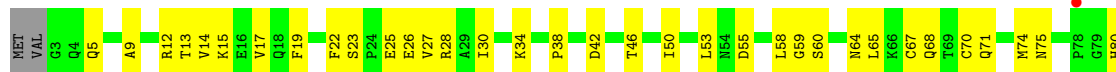
• Molecule 3: Non-template strand DNA

Chain N: 

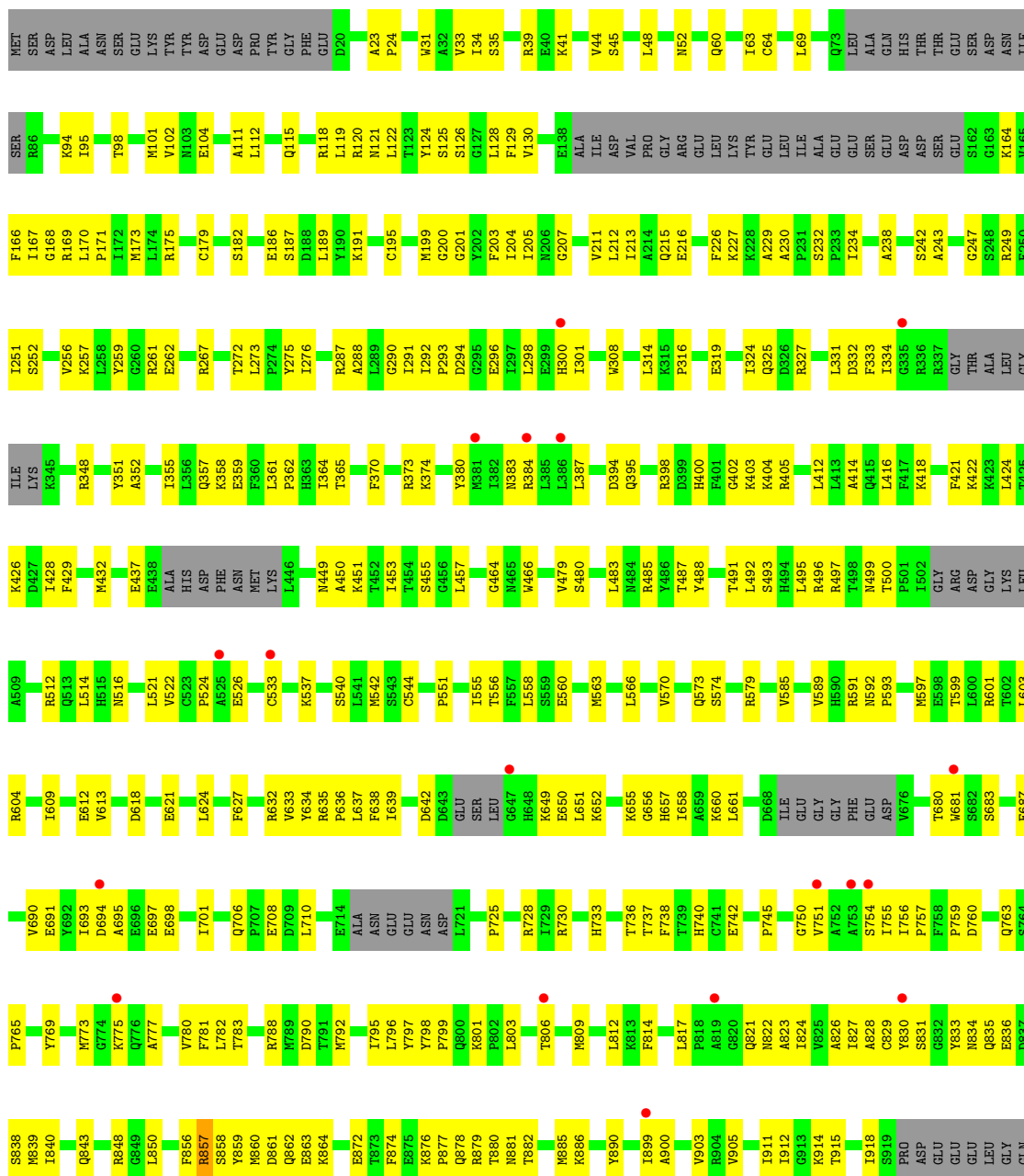


• Molecule 4: DNA-directed RNA polymerase II subunit RPB1

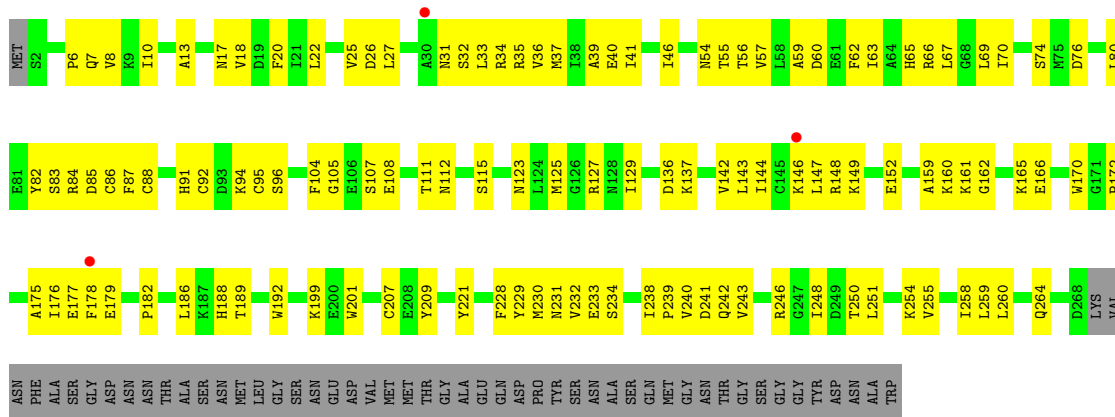
Chain A: 



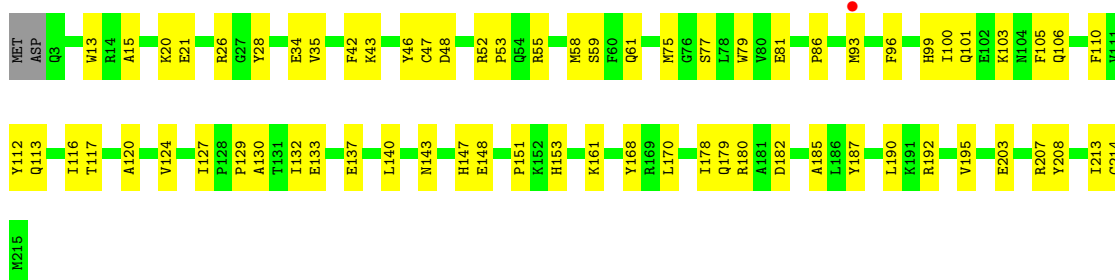
GLY	HI367	M1267	W1191	A1108	L1021	H906	K830	K744	N648	P561	Y478	V392	D305
PHE	M1368	L1268	L1192	K1109	L1022	T907	T834	Q745	I649	P561	M479	G395	I308
THR	E1269	E1269	L1193	M1110	R1023	T907	T834	M746	Q850	P561	M479	G396	A309
ALA	L1370	N1270	L1193	M1111	S1024	E914	T834	M747	K651	P561	M479	G396	G310
TYR	L1371	L1271	E1196	K1112	R1025	S915	Y836	M748	V653	P561	M479	G396	A314
GLY	L1372	T1272	L1197	T1113	R1030	G916	I837	S751	N654	P561	M479	G396	A314
MET	D1373	L1273	D1198	L1116	V1031	G916	Q838	S751	N654	P561	M479	G396	A314
ASP	V1374	L1274	D1198	L1117	V1031	G916	Q838	S751	N654	P561	M479	G396	A314
GLY	M1375	G1275	M1202	V1118	E1034	T919	R839	S754	F662	P561	M479	G396	A314
GLY	T1376	E1276	K1205	V1119	Y1035	G921	R840	I756	S663	P561	M479	G396	A314
GLY	S1383	L1277	D1206	L1132	R1036	G921	L841	I756	S663	P561	M479	G396	A314
ILE	V1384	L1278	L1207	L1133	L1037	G921	V842	I758	G665	P561	M479	G396	A314
THR	T1385	V1282	T1208	A1131	L1037	G921	V842	I758	G665	P561	M479	G396	A314
SER	K1386	K1290	M1209	L1134	M1048	E932	D847	Q760	A671	P561	M479	G396	A314
PRO	H1387	T1295	G1213	L1135	T1049	E932	D847	Q760	A671	P561	M479	G396	A314
PHE	H1387	T1295	G1213	L1135	T1049	E932	D847	Q760	A671	P561	M479	G396	A314
GLY	N1390	K1300	E1214	R1135	S1056	Y933	M849	A763	T675	P561	M479	G396	A314
ALA	R1391	K1300	E1214	S1136	V1057	Y933	M849	A763	T675	P561	M479	G396	A314
TYR	A1396	E1303	I1216	A1137	V1058	Y933	M849	A763	T675	P561	M479	G396	A314
ASP	L1397	K1217	E1139	I1138	M1063	K941	Y852	Q767	T680	P561	M479	G396	A314
GLY	M1398	Q1218	H1140	E1139	V1064	P942	D853	Q767	T680	P561	M479	G396	A314
ALA	T1308	T1219	E1140	E1139	G1065	P942	D853	Q767	T680	P561	M479	G396	A314
PRO	R1399	F1220	K1144	K1144	V1066	E945	R857	I775	I683	P561	M479	G396	A314
THR	F1402	K1221	I1148	I1148	L1067	E945	R857	I775	I683	P561	M479	G396	A314
SER	E1403	N1222	I1148	I1148	L1067	E945	R857	I775	I683	P561	M479	G396	A314
PRO	E1403	N1222	I1148	I1148	L1067	E945	R857	I775	I683	P561	M479	G396	A314
GLY	V1406	D1223	I1148	I1148	Q1070	A952	V863	D781	K688	P561	M479	G396	A314
ASN	E1407	L1224	E1151	E1151	S1071	A952	V863	D781	K688	P561	M479	G396	A314
GLY	E1407	L1224	E1151	E1151	S1071	A952	V863	D781	K688	P561	M479	G396	A314
VAL	I1408	V1225	I1152	I1152	A1076	Q954	F866	T783	T694	P561	M479	G396	A314
SER	L1409	V1226	Y1153	Y1153	A1076	Q954	F866	T783	T694	P561	M479	G396	A314
LEU	F1410	I1227	Y1154	Y1154	T1077	P955	Y868	P785	Q698	P561	M479	G396	A314
PRO	A1416	W1228	D1155	D1155	Q1078	L956	G869	H786	L701	P561	M479	G396	A314
GLY	A1416	K1235	P1156	P1156	M1079	L956	G869	H786	L701	P561	M479	G396	A314
ASN	S1331	L1236	L1081	L1081	T1081	R961	G872	K789	R711	P561	M479	G396	A314
ASP	F1332	L1236	ASN	ASN	THR	R961	G872	K789	R711	P561	M479	G396	A314
LEU	I1333	T1237	THR	THR	THR	R961	G872	K789	R711	P561	M479	G396	A314
PRO	D1420	I1238	T1161	T1161	ASN	R961	G872	K789	R711	P561	M479	G396	A314
THR	C1421	R1239	V1162	V1162	PHE	P963	D874	Y792	F714	P561	M479	G396	A314
SER	R1422	C1240	I1163	I1163	HIS	P965	A876	K797	E715	P561	M479	G396	A314
PRO	M1336	L1241	P1164	P1164	PHE	Q965	A876	K797	E715	P561	M479	G396	A314
TYR	E1426	V1242	E1165	E1165	ALA	Q968	I878	V718	L722	P561	M479	G396	A314
GLY	N1427	V1243	D1166	D1166	GLY	Q968	I878	V718	L722	P561	M479	G396	A314
SER	V1428	V1243	D1166	D1166	VAL	Q968	I878	V718	L722	P561	M479	G396	A314
PRO	T1429	ARG	I1169	I1169	ALA	H975	K880	R806	R726	P561	M479	G396	A314
THR	G1430	PRO	I1170	I1170	ALA	H975	K880	R806	R726	P561	M479	G396	A314
SER	G1431	LYS	I1170	I1170	SER	H975	K880	R806	R726	P561	M479	G396	A314
PRO	R1345	LEU	L1176	L1176	K1092	H975	K880	R806	R726	P561	M479	G396	A314
ALA	L1348	ASP	L1176	L1176	T1095	H975	K880	R806	R726	P561	M479	G396	A314
VAL	P1435	ALA	LEU	LEU	T1095	H975	K880	R806	R726	P561	M479	G396	A314
ASP	T1436	GLY	ASP	ASP	T1095	H975	K880	R806	R726	P561	M479	G396	A314
PRO	G1437	THR	GLU	GLU	P1099	H975	K880	R806	R726	P561	M479	G396	A314
THR	T1438	GLY	GLU	GLU	R1100	H975	K880	R806	R726	P561	M479	G396	A314
SER	V1352	ALA	GLU	GLU	L1101	H975	K880	R806	R726	P561	M479	G396	A314
SER	V1355	ALA	GLN	GLN	K1102	H975	K880	R806	R726	P561	M479	G396	A314
ASN	I1356	GLY	SER	SER	E1103	H975	K880	R806	R726	P561	M479	G396	A314
ASP	D1442	GLY	PHE	PHE	L1104	H975	K880	R806	R726	P561	M479	G396	A314
ALA	V1443	ASP	ASP	ASP	L1104	H975	K880	R806	R726	P561	M479	G396	A314
THR	M1444	M1364	ASP	ASP	L1106	H975	K880	R806	R726	P561	M479	G396	A314
SER	I1445	Y1365	ALA	ALA	L1106	H975	K880	R806	R726	P561	M479	G396	A314
PRO	I1445	Y1365	ALA	ALA	L1106	H975	K880	R806	R726	P561	M479	G396	A314
THR	D1446	R1366	GLY	GLY	V1107	H975	K880	R806	R726	P561	M479	G396	A314



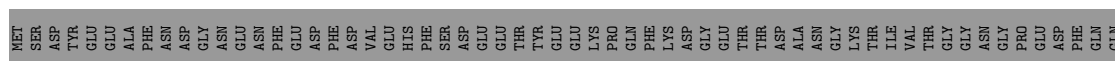
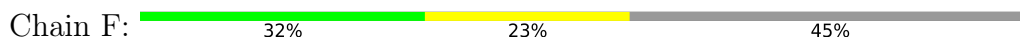
- Molecule 6: DNA-directed RNA polymerase II subunit RPB3

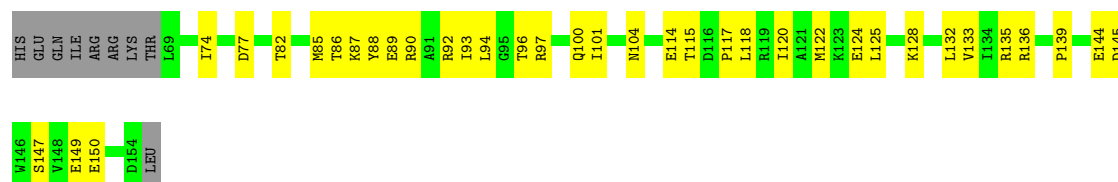


- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1

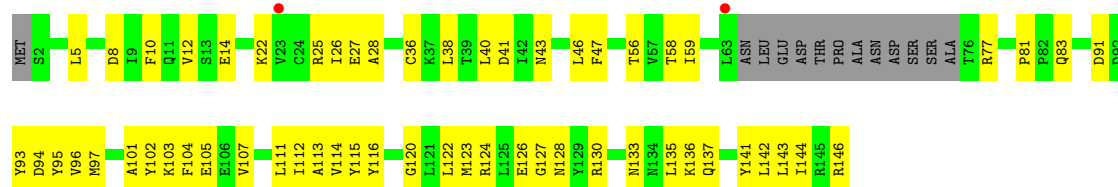


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2

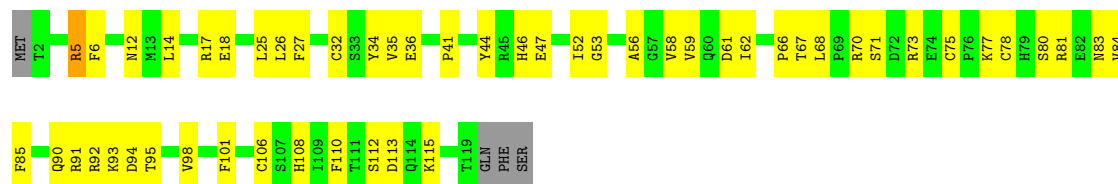




- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3



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



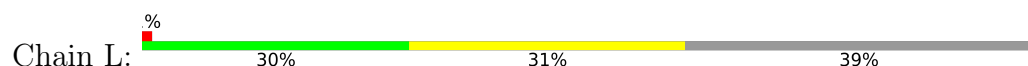
- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- 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	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 , 117.4	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, 2TM, 8OG, 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

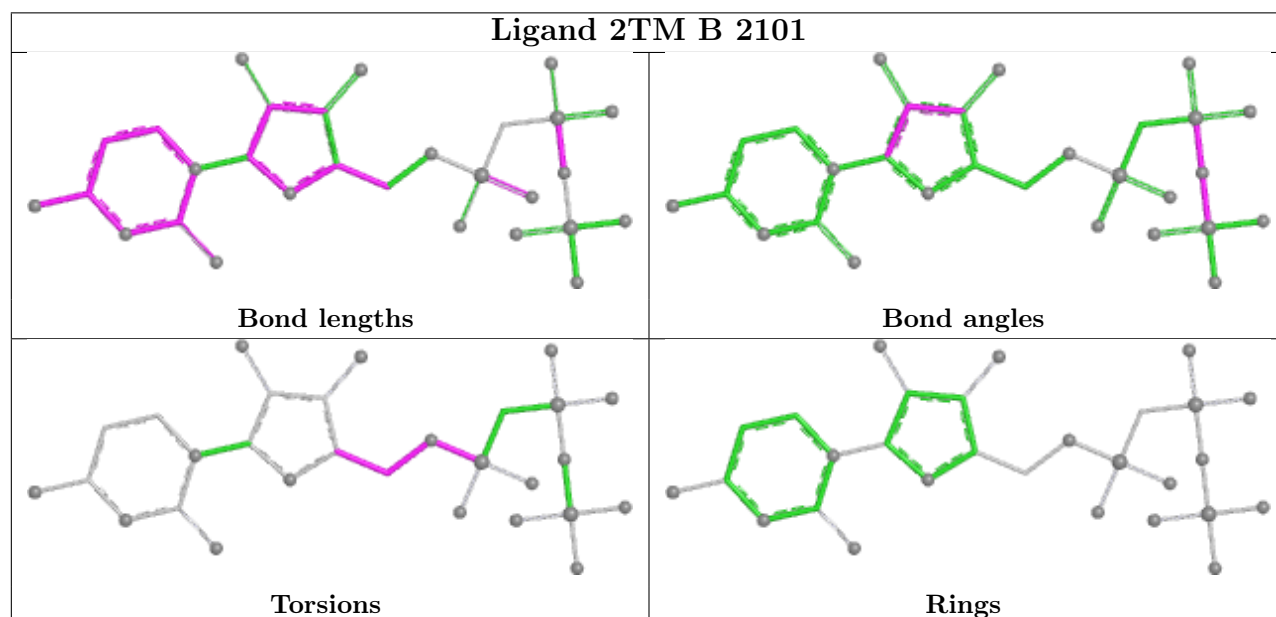
There are no ring outliers.

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	R	9/9 (100%)	0.19	0 100 100	76, 86, 172, 223	0
2	T	25/29 (86%)	0.33	0 100 100	90, 188, 241, 268	0
3	N	15/18 (83%)	0.35	0 100 100	143, 205, 241, 253	0
4	A	1385/1733 (79%)	0.09	21 (1%) 72 44	74, 121, 184, 241	0
5	B	1121/1224 (91%)	0.18	23 (2%) 63 37	52, 106, 170, 250	0
6	C	267/318 (83%)	-0.00	3 (1%) 78 52	73, 111, 158, 195	0
7	E	213/215 (99%)	-0.16	1 (0%) 87 66	83, 144, 211, 252	0
8	F	86/155 (55%)	-0.09	0 100 100	76, 110, 158, 178	0
9	H	133/146 (91%)	0.13	2 (1%) 72 44	106, 146, 202, 220	0
10	I	118/122 (96%)	0.10	0 100 100	88, 137, 194, 229	0
11	J	65/70 (92%)	0.30	2 (3%) 51 29	65, 99, 134, 165	0
12	K	114/120 (95%)	-0.07	1 (0%) 81 56	63, 103, 147, 185	0
13	L	43/70 (61%)	0.25	1 (2%) 61 35	93, 195, 256, 274	0
All	All	3594/4229 (84%)	0.10	54 (1%) 72 44	52, 118, 188, 274	0

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	B	775	LYS	4.8
4	A	103	CYS	4.0
13	L	32	ALA	3.7
5	B	819	ALA	3.7
4	A	448	PRO	3.6

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](#)

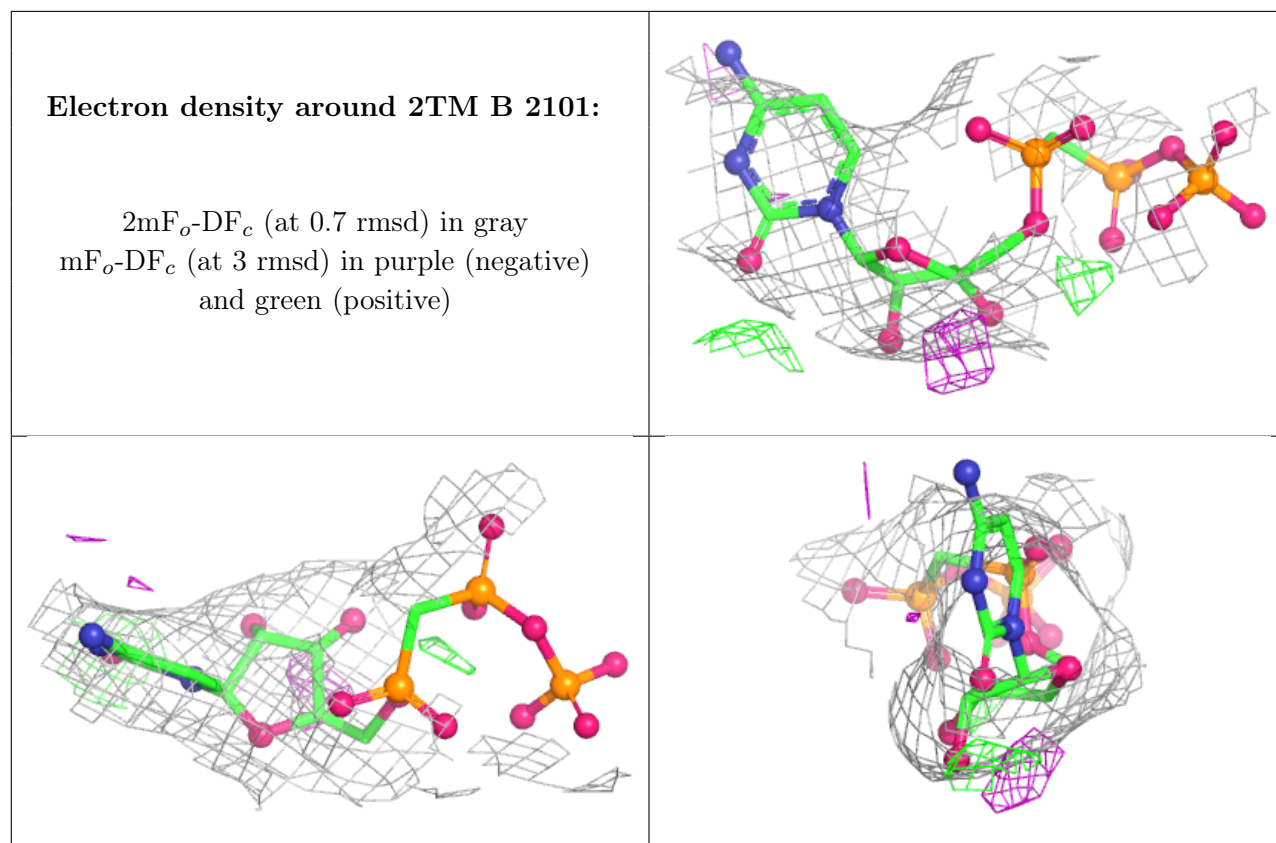
There are no oligosaccharides in this entry.

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	0.64	0.20	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	0.08	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.