



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 1, 2026 – 12:12 PM EDT

PDB ID : 9PVV / pdb_00009pvv
Title : RNA polymerase II elongation complex with dC at +1 site, 8-oxo-GTP bound in A-site.
Authors : Hou, P.; Oh, J.; Wang, D.
Deposited on : 2025-08-03
Resolution : 3.48 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

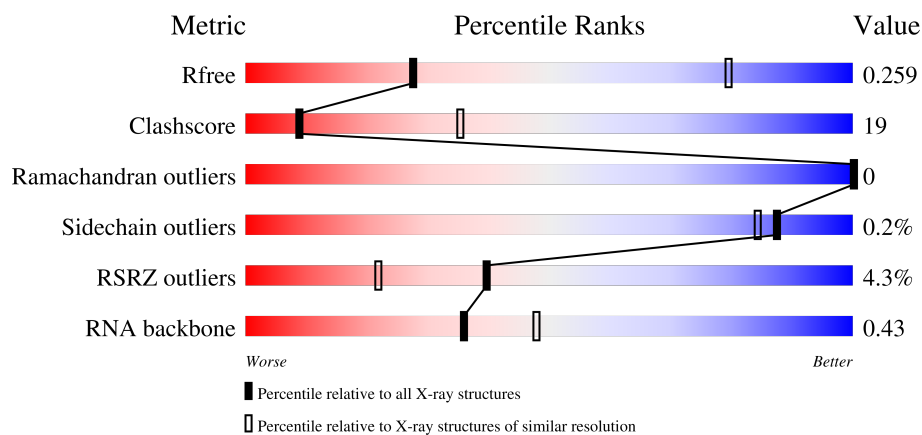
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.48 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	1083 (3.52-3.44)
Clashscore	190562	1139 (3.52-3.44)
Ramachandran outliers	187476	1111 (3.52-3.44)
Sidechain outliers	187428	1112 (3.52-3.44)
RSRZ outliers	180081	1082 (3.52-3.44)
RNA backbone	3983	1001 (3.94-3.02)

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	<div> <div>5%</div> <div>33% 56% 11%</div> </div>
2	T	29	<div> <div>48% 38% 14%</div> </div>
3	N	18	<div> <div>17% 61% 22%</div> </div>
4	A	1733	<div> <div>5% 47% 34% 20%</div> </div>

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

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 29102 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
			193	88	40	57	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	25	Total	C	N	O	P	0	0	0
			497	239	76	157	25			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	14	Total	C	N	O	P	0	0	0
			296	138	66	78	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1393	Total	C	N	O	S	0	0	0
			10894	6875	1908	2051	60			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1123	Total	C	N	O	S	0	0	0
			8859	5607	1552	1647	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	212	Total	C	N	O	S	0	0	0
			1731	1100	305	315	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
			1064	670	179	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.

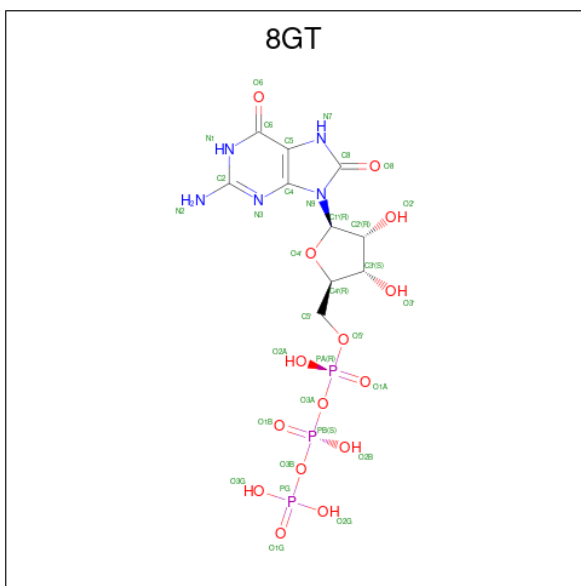
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- 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
			337	208	66	59	4			

- Molecule 14 is 8-OXO-GUANOSINE-5'-TRIPHOSPHATE (CCD ID: 8GT) (formula:

C₁₀H₁₆N₅O₁₅P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	T	1	Total	C	N	O	P	0	0
			33	10	5	15	3		

- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

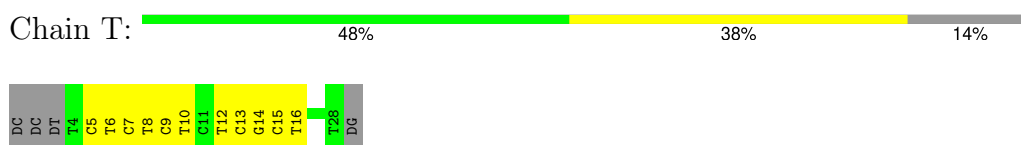
3 Residue-property plots

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.

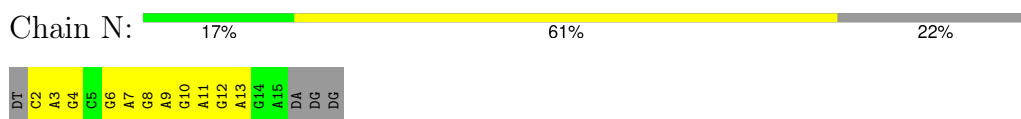
- Molecule 1: RNA



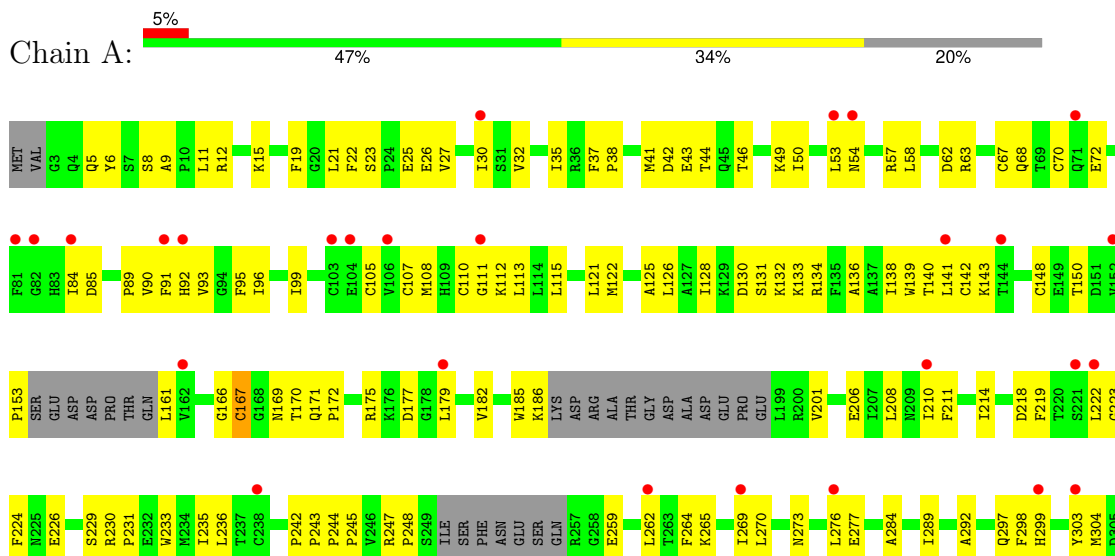
- Molecule 2: Template strand DNA



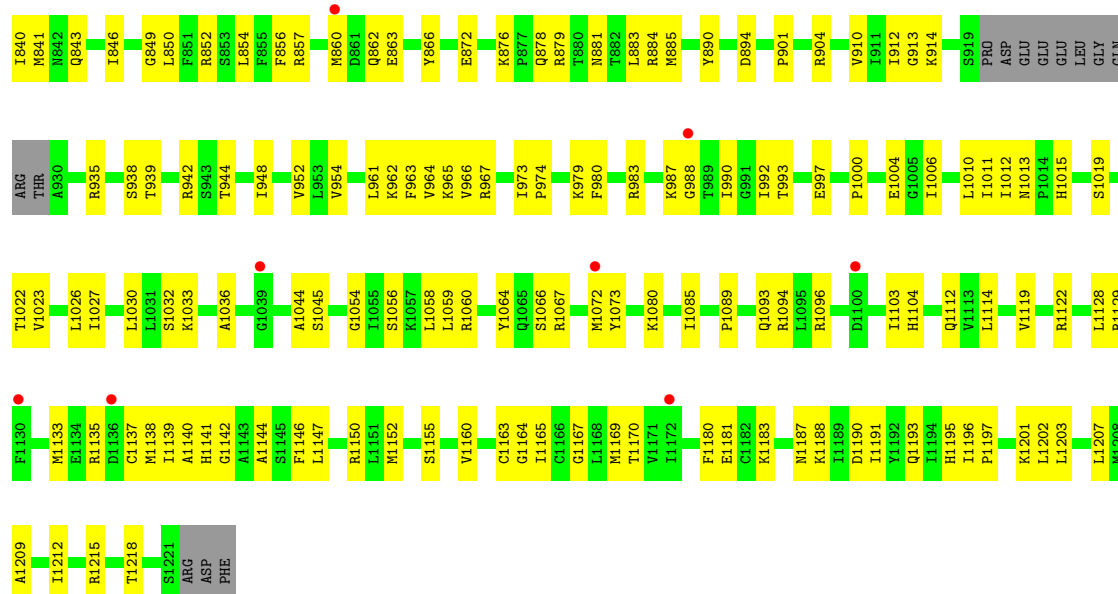
- Molecule 3: Non-template strand DNA



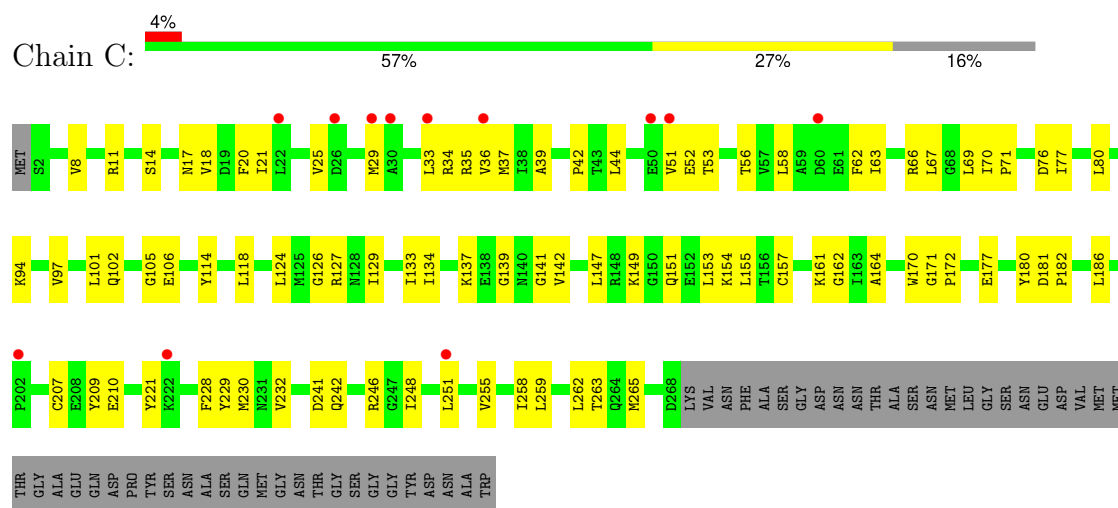
- Molecule 4: DNA-directed RNA polymerase II subunit RPB1



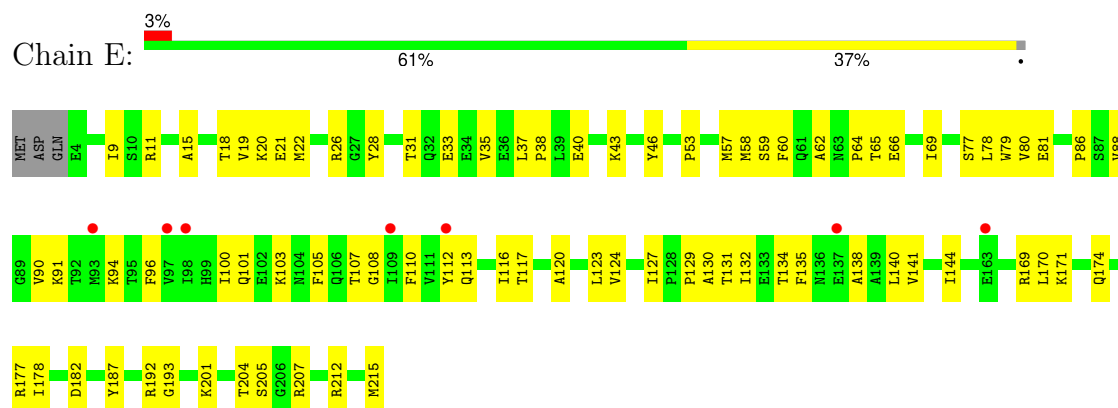
VAL	L1348	L1193	V1107	V948	V863	D781	I683	F591	L501	R407	N306
LYS	N1270	R1194	A1108	D949	T867	R762	K687	D592	L501	R407	P312
TYR	I1271	E1195	N1109	G950	T868	T783	L784	E593	V507	I413	L315
MET	L1272	E1196	M1111	E951	G869	P785	D692	G594	L511	D414	L325
PRO	L1273	D1198	L1115	N953	E870	H786	L702	T596	V512	L415	P321
GLU	R1274	R1199	S1116	P955	D871	F787	L702	L597	S513	R420	V322
GLN	G1275	R1199	L1117	L956	G872	S788	L702	L598	P519	R420	K323
LYS	V1276	M1202	T1119	P957	H873	K789	K705	L598	C520	R420	S324
ILE	G1360	N1203	V1119	V958	D874	S796	H706	D602	N603	I424	I325
THR	S1361	D1206	Y1118	L958	H877	K797	G707	L598	N521	I424	R328
GLU	R1366	L1207	L1120	N959	L878	G798	M708	G504	G522	Q427	R336
ILE	V1281	L1207	E1121	I960	E879	F799	L710	G605	Y428	Q427	R336
ASP	V1283	T1208	P1122	R961	E881	V800	R711	L806	G429	Q427	R336
GLY	M1284	G1210	D1127	R962	D882	R806	S713	I613	R430	Q427	R336
GLN	K1286	Q1211	Q1130	I964	L883	R806	S713	I613	R430	Q427	R336
ASP	K1287	G1212	Q1131	I964	L883	R806	S713	I613	R430	Q427	R336
GLY	V1288	G1213	A1131	I964	L883	R806	S713	I613	R430	Q427	R336
VAL	R1288	E1214	K1132	Q968	T885	T809	D716	I613	R430	Q427	R336
THR	K1290	A1215	L1133	Q969	L886	P810	R720	V616	L531	Q427	R336
PRO	N1393	I1216	I1134	I973	D890	E812	F721	L534	L534	Q427	R336
TYR	P1292	I1216	R1135	I973	D890	F813	L722	T621	L534	Q427	R336
SER	G1395	T1219	S1136	D974	K895	F814	L722	T621	L534	Q427	R336
ASN	T1236	F1220	A1137	H975	K896	R815	R726	V622	L534	Q427	R336
GLU	K1221	K1221	I1138	V1088	R896	H816	D727	V622	L534	Q427	R336
SER	Y1298	L1224	E1139	P978	T897	A817	K728	G628	L534	Q427	R336
GLY	P1302	L1224	H1140	S979	R898	M818	A729	L629	L534	Q427	R336
LEU	E1303	V1226	T1141	D980	V899	G819	G730	I630	L534	Q427	R336
VAL	V1304	I1227	K1144	L981	D900	G820	R731	H631	L534	Q427	R336
ASN	V1305	I1227	K1144	T982	L901	L732	L732	V632	L534	Q427	R336
ALA	L1306	L1236	I1148	K983	H906	L824	A733	V632	L534	Q427	R336
ASP	L1307	L1236	I1148	K984	H906	I825	A733	V632	L534	Q427	R336
ASP	T1308	I1237	I1152	D985	T907	V829	L737	R635	L534	Q427	R336
VAL	D1309	V1153	Y1153	V987	L908	K830	N741	C642	L534	Q427	R336
LYS	G1310	G1240	Y1154	L988	L913	N742	N742	L645	L534	Q427	R336
ASP	V1311	R1241	D1155	L988	L913	N742	N742	L645	L534	Q427	R336
LEU	N1312	V1242	D1166	V996	S915	S761	S761	Q650	L534	Q427	R336
LEU	L1313	V1243	D1166	L997	G916	K762	K762	Q650	L534	Q427	R336
MET	S1314	ARG	L1169	L998	Y836	F755	F755	W656	L534	Q427	R336
PHE	V1428	PRO	I1169	L998	Y836	F755	F755	W656	L534	Q427	R336
SER	V1316	LYS	I1170	L1000	R938	Q760	Q760	L658	L534	Q427	R336
PRO	V1319	SER	L1176	R1001	R840	Q760	Q760	L658	L534	Q427	R336
LEU	M1433	LEU	L1176	F1084	L841	A763	A763	F662	L534	Q427	R336
VAL	A1434	ASP	ASP	N1004	L841	A763	A763	F662	L534	Q427	R336
ASP	P1435	ALA	ASP	E1005	V842	C764	C764	I666	L534	Q427	R336
SER	I1436	GLU	GLU	I1006	K843	V765	V765	G667	L534	Q427	R336
GLY	G1437	THR	GLU	I1007	A844	G766	G766	G667	L534	Q427	R336
SER	T1438	ALA	ALA	Q1008	L845	Q767	Q767	G667	L534	Q427	R336
ASN	Y1327	GLU	GLN	D1013	T848	Q768	Q768	G673	L534	Q427	R336
ASP	Y1328	GLU	GLN	I1013	T848	Q768	Q768	G673	L534	Q427	R336
ALA	T1329	GLU	GLN	F1018	R940	S769	S769	T675	L534	Q427	R336
ALA	N1330	GLU	SER	F1018	R940	S769	S769	T675	L534	Q427	R336
MET	S1331	GLU	PHE	F1018	R940	S769	S769	T675	L534	Q427	R336
ALA	F1332	D1257	ASP	F1018	R940	S769	S769	T675	L534	Q427	R336
GLY	F1446	L1260	GLN	C1020	R943	R857	R774	E678	L534	Q427	R336
GLY	GLU	L1266	GLN	L1021	R944	R857	R774	E678	L534	Q427	R336
PHE	M1336	T1266	GLU	L1021	R944	R857	R774	E678	L534	Q427	R336
THR	S1341	M1267	W1191	L1021	R944	R857	R774	E678	L534	Q427	R336
ALA	L1268	L1268	L1105	S1024	V946	L860	G778	T680	L534	Q427	R336
			L1106	R1025	F947	N862	V780	T682	L534	Q427	R336



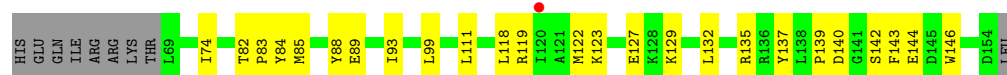
• Molecule 6: DNA-directed RNA polymerase II subunit RPB3



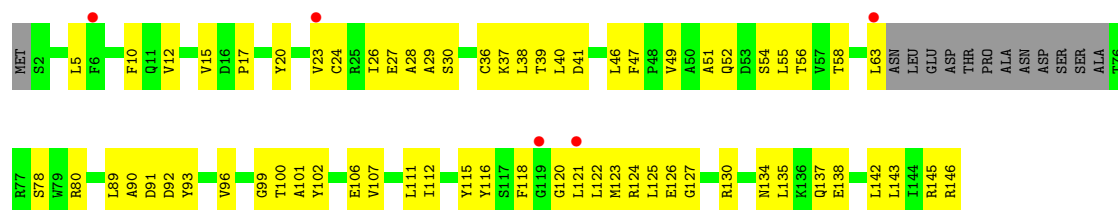
• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1



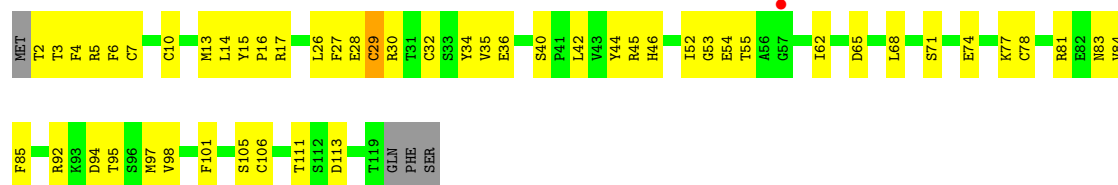
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2



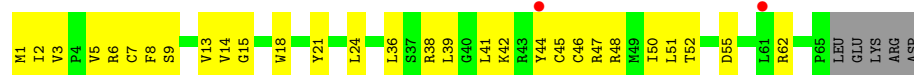
- Chain H: 



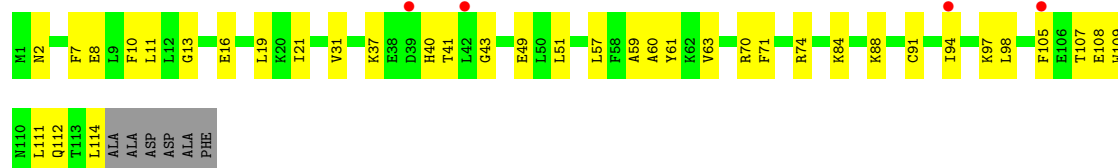
- Chain I:  %



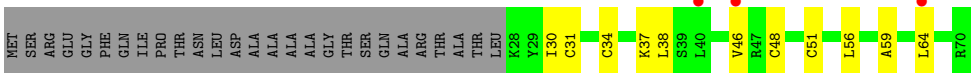
- Chain J: 



- Chain K:  3% 64% 31% 5%



- Chain L: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	159.52Å 222.70Å 191.19Å 90.00° 97.82° 90.00°	Depositor
Resolution (Å)	38.52 – 3.48 38.52 – 3.48	Depositor EDS
% Data completeness (in resolution range)	98.7 (38.52-3.48) 98.7 (38.52-3.48)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.218 , 0.258 0.218 , 0.259	Depositor DCC
R_{free} test set	2000 reflections (2.37%)	wwPDB-VP
Wilson B-factor (Å ²)	89.4	Xtriage
Anisotropy	0.842	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 116.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	29102	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, 8GT

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	0.16	0/217	0.32	0/337
2	T	0.22	0/551	0.44	0/845
3	N	0.21	0/335	0.36	0/516
4	A	0.18	0/11089	0.40	0/15001
5	B	0.17	0/9030	0.37	0/12186
6	C	0.16	0/2139	0.34	0/2899
7	E	0.17	0/1767	0.36	0/2378
8	F	0.16	0/696	0.33	0/943
9	H	0.18	0/1082	0.43	0/1466
10	I	0.16	0/970	0.41	0/1308
11	J	0.16	0/541	0.36	0/727
12	K	0.17	0/937	0.37	0/1265
13	L	0.21	0/339	0.43	0/450
All	All	0.17	0/29693	0.38	0/40321

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	193	0	98	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	T	497	0	285	10	0
3	N	296	0	155	16	0
4	A	10894	0	10937	491	0
5	B	8859	0	8816	340	0
6	C	2101	0	2056	68	0
7	E	1731	0	1758	70	0
8	F	684	0	692	22	0
9	H	1064	0	1029	58	0
10	I	952	0	897	43	0
11	J	532	0	542	24	0
12	K	919	0	929	34	0
13	L	337	0	352	9	0
14	T	33	0	11	6	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
16	A	2	0	0	0	0
All	All	29102	0	28557	1075	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 19.

The worst 5 of 1075 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)
9:H:89:LEU:HD13	9:H:91:ASP:C	1.47	1.39
9:H:89:LEU:HD13	9:H:91:ASP:O	1.28	1.31
7:E:94:LYS:HG2	7:E:123:LEU:HD13	1.30	1.08
9:H:89:LEU:CD1	9:H:91:ASP:C	2.36	0.98
4:A:705:LYS:HE3	4:A:708:MET:SD	2.06	0.95

There are no symmetry-related clashes.

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	1379/1733 (80%)	1344 (98%)	35 (2%)	0	100	100
5	B	1103/1224 (90%)	1086 (98%)	17 (2%)	0	100	100
6	C	265/318 (83%)	264 (100%)	1 (0%)	0	100	100
7	E	210/215 (98%)	207 (99%)	3 (1%)	0	100	100
8	F	84/155 (54%)	82 (98%)	2 (2%)	0	100	100
9	H	129/146 (88%)	127 (98%)	2 (2%)	0	100	100
10	I	116/122 (95%)	115 (99%)	1 (1%)	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	3502/4173 (84%)	3439 (98%)	63 (2%)	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	1200/1520 (79%)	1198 (100%)	2 (0%)	87	84
5	B	955/1061 (90%)	954 (100%)	1 (0%)	88	87
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%)	107 (97%)	3 (3%)	39	62
11	J	60/65 (92%)	59 (98%)	1 (2%)	53	69
12	K	99/102 (97%)	99 (100%)	0	100	100
13	L	37/57 (65%)	37 (100%)	0	100	100
All	All	3078/3657 (84%)	3071 (100%)	7 (0%)	87	84

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	I	7	CYS
10	I	10	CYS
11	J	7	CYS
10	I	29	CYS
5	B	1163	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
5	B	1193	GLN
5	B	1211	ASN
6	C	267	GLN
4	A	1378	GLN
4	A	1110	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	7/9 (77%)	1 (14%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	5	A

There are no RNA pucker outliers to report.

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	8GT	T	101	16	34,35,35	4.96	21 (61%)	48,56,56	1.96	10 (20%)

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
14	8GT	T	101	16	-	8/22/38/38	0/3/3/3

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	101	8GT	C4-N3	10.02	1.57	1.34
14	T	101	8GT	C6-N1	9.55	1.56	1.38
14	T	101	8GT	C3'-C4'	-9.39	1.29	1.53
14	T	101	8GT	C2'-C1'	-9.08	1.24	1.53
14	T	101	8GT	O4'-C1'	8.69	1.62	1.42

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	101	8GT	O6-C6-C5	-5.63	113.68	127.26
14	T	101	8GT	N9-C4-N3	5.49	132.99	126.13
14	T	101	8GT	C5-C6-N1	4.71	125.08	112.13
14	T	101	8GT	C2-N3-C4	4.20	119.54	112.30
14	T	101	8GT	C2'-C1'-N9	-3.76	110.86	115.90

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

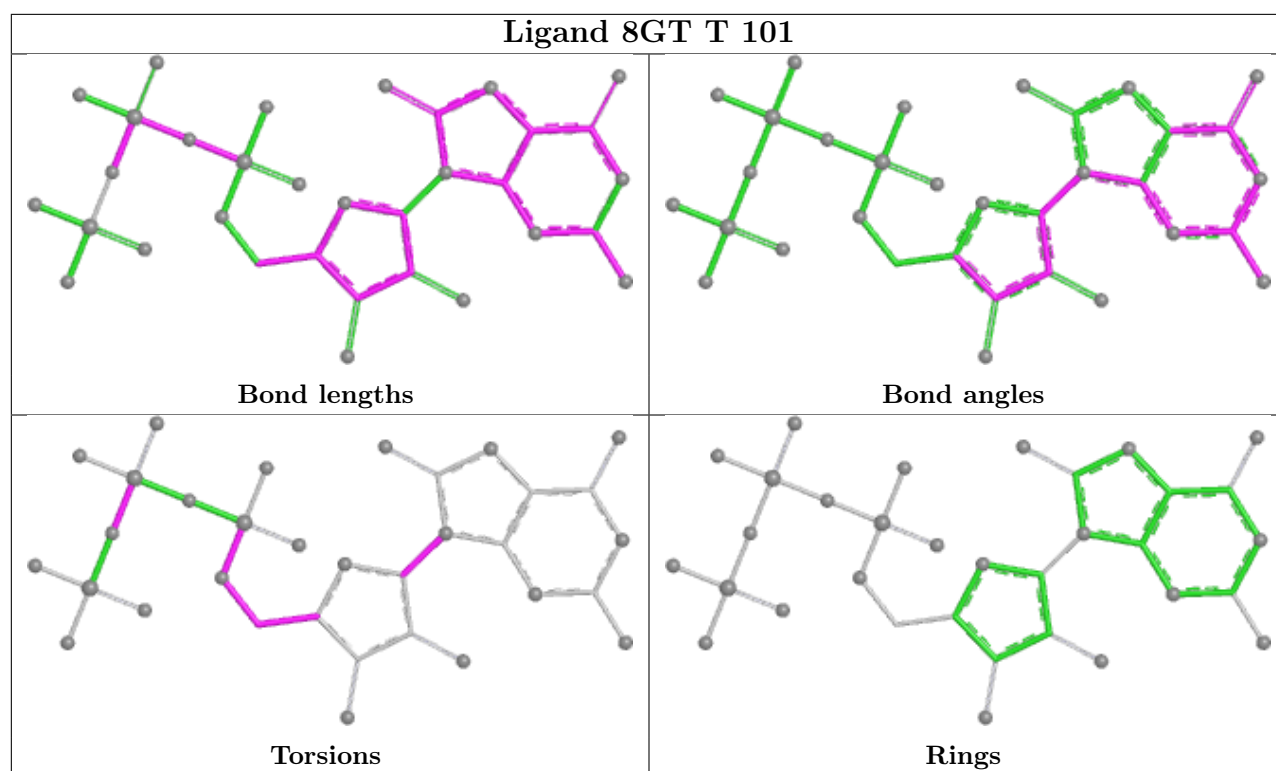
Mol	Chain	Res	Type	Atoms
14	T	101	8GT	C5'-O5'-PA-O3A
14	T	101	8GT	C5'-O5'-PA-O2A
14	T	101	8GT	C4'-C5'-O5'-PA
14	T	101	8GT	O4'-C1'-N9-C8
14	T	101	8GT	O4'-C1'-N9-C4

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	T	101	8GT	6	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, 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%)	-0.27	0	100	100	78, 84, 138, 140	0
2	T	25/29 (86%)	0.31	0	100	100	78, 121, 257, 265	0
3	N	14/18 (77%)	0.48	0	100	100	144, 231, 286, 286	0
4	A	1393/1733 (80%)	0.45	87 (6%)	26	17	52, 117, 202, 273	0
5	B	1123/1224 (91%)	0.37	34 (3%)	52	31	50, 96, 167, 297	0
6	C	267/318 (83%)	0.42	12 (4%)	38	21	45, 87, 136, 218	0
7	E	212/215 (98%)	0.36	7 (3%)	49	28	98, 149, 214, 243	0
8	F	86/155 (55%)	0.28	1 (1%)	76	53	84, 117, 166, 205	0
9	H	133/146 (91%)	0.37	5 (3%)	44	25	87, 129, 178, 267	0
10	I	118/122 (96%)	0.40	1 (0%)	82	61	80, 142, 199, 225	0
11	J	65/70 (92%)	0.52	2 (3%)	51	30	56, 78, 130, 153	0
12	K	114/120 (95%)	0.28	4 (3%)	47	27	58, 92, 134, 181	0
13	L	43/70 (61%)	0.67	3 (6%)	22	15	81, 146, 219, 305	0
All	All	3602/4229 (85%)	0.41	156 (4%)	40	22	45, 109, 193, 305	0

The worst 5 of 156 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	B	1136	ASP	5.6
7	E	97	VAL	5.1
4	A	1282	VAL	5.1
7	E	93	MET	4.5
4	A	1098	VAL	4.3

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

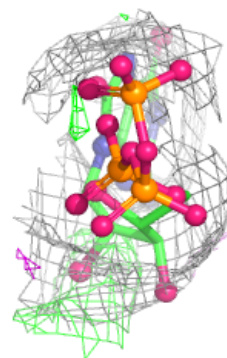
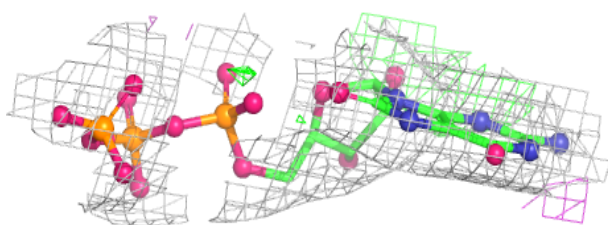
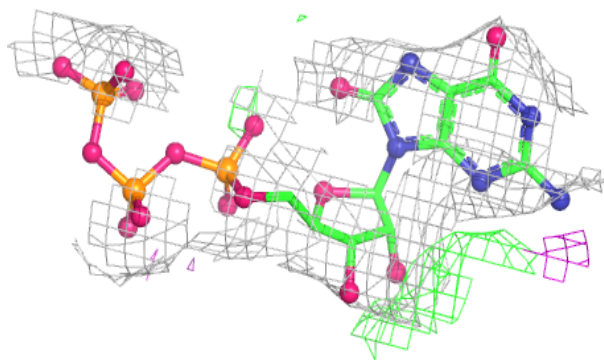
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
16	MG	A	1803	1/1	0.72	0.15	123,123,123,123	0
15	ZN	L	101	1/1	0.88	0.09	297,297,297,297	0
15	ZN	A	1801	1/1	0.88	0.08	272,272,272,272	0
14	8GT	T	101	33/33	0.93	0.09	46,68,125,132	0
15	ZN	I	202	1/1	0.93	0.09	245,245,245,245	0
16	MG	A	1804	1/1	0.97	0.05	103,103,103,103	0
15	ZN	A	1802	1/1	0.98	0.03	169,169,169,169	0
15	ZN	I	201	1/1	0.98	0.15	204,204,204,204	0
15	ZN	B	1301	1/1	0.99	0.03	191,191,191,191	0
15	ZN	C	401	1/1	0.99	0.14	154,154,154,154	0
15	ZN	J	101	1/1	0.99	0.10	104,104,104,104	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.

Electron density around 8GT T 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.