



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 09:38 pm BST

PDB ID : 2NVX
Title : RNA polymerase II elongation complex in 5 mM Mg+2 with 2'-dUTP
Authors : Wang, D.; Bushnell, D.A.; Westover, K.D.; Kaplan, C.D.; Kornberg, R.D.
Deposited on : 2006-11-13
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

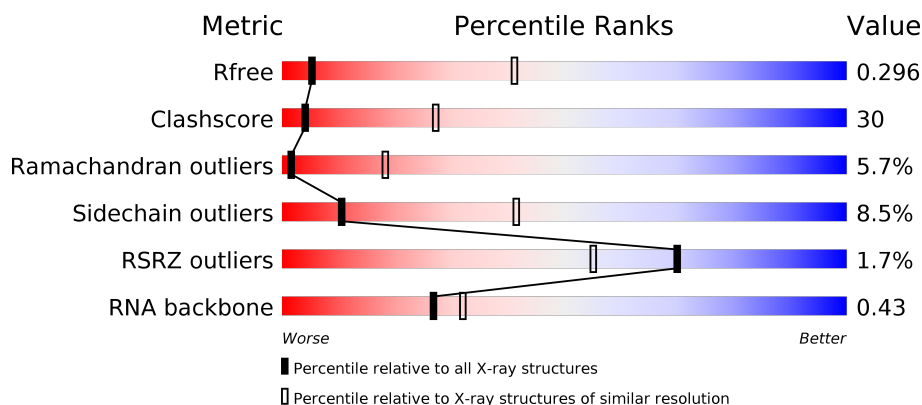
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)
RNA backbone	3102	1017 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	R	10	 20% 70% 10%
2	N	14	 21% 93% 7%
3	T	28	 25% 46% 32% 21%
4	A	1733	 44% 29% 6% 19%

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Mol	Chain	Length	Quality of chain
5	B	1224	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>48%35%7%9%</div></div>
6	C	318	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>48%30%5%16%</div></div>
7	E	215	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>72%27%</div></div>
8	F	155	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>38%15%43%</div></div>
9	H	146	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>3%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>55%31%6%8%</div></div>
10	I	122	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>71%24%</div></div>
11	J	70	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>53%33%7%7%</div></div>
12	K	120	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>67%27%5%</div></div>
13	L	70	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>3%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>40%21%34%</div></div>

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 29436 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 5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	10	Total	C	N	O	P	0	0	0
			216	98	45	64	9			

- Molecule 2 is a DNA chain called 5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3'.

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

- Molecule 3 is a DNA chain called 28-MER DNA template strand.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1402	Total	C	N	O	S	0	0	0
			11028	6950	1934	2083	61			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1114	Total	C	N	O	S	0	0	0
			8856	5605	1553	1644	54			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	88	Total	C	N	O	S	0	0	0
			712	455	120	134	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	134	Total	C	N	O	S	0	0	0
			1076	678	181	212	5			

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit 9.

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

- Molecule 11 is a protein called DNA-directed RNA polymerases I/II/III subunit 10.

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

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

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

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

tide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

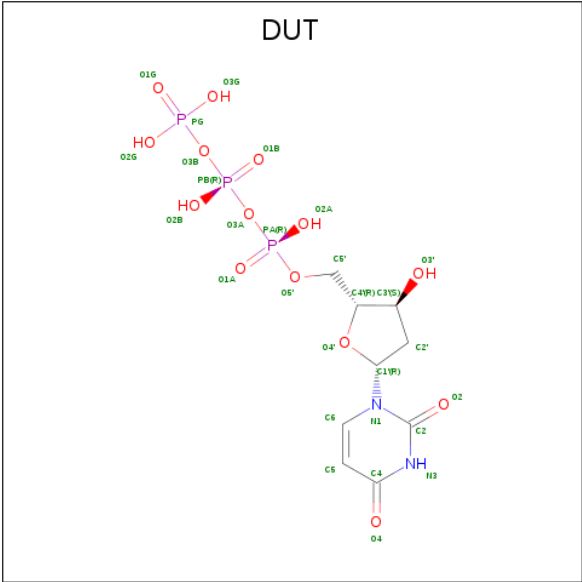
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

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

- Molecule 16 is DEOXYURIDINE-5'-TRIPHOSPHATE (three-letter code: DUT) (formula: C₉H₁₅N₂O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
16	B	1	56	18	4	28	6	0	1

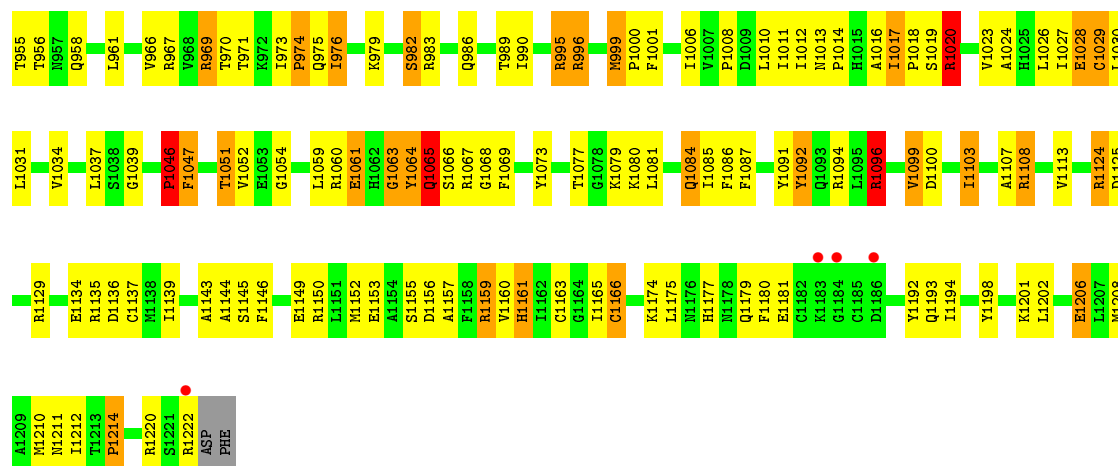
- Molecule 1: 5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*A)-3'



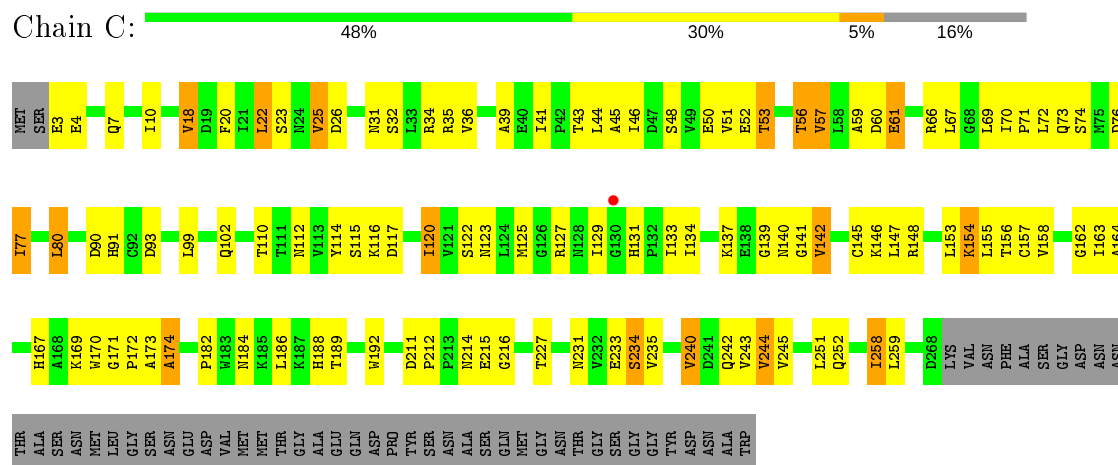
SER	VAL	SER	C1400	Y1298	I1227	R1135	T1028	E918	H850	V785	V653	G574	E495	L415	K332
TTR	SER	GLY	S1401	V1299	W1228	S1136	R1029	I919	H851	R774	T664	K575	E496	R416	E333
PRO	SER	VAL	F1402	K1300	A1137	T1138	V1031	G921	D853	R775	G685	Q576	T497	S418	G334
THR	GLY	ASN	V1406	V1305	D1230	K1144	Y1035	D922	H854	A776	I666	L578	R498	R335	R335
SER	PRO	ASP	E1407	L1306	N1232	D1281	R1036	Q926	T855	G777	D688	S579	A499	I336	R337
PRO	SER	ASP	I1408	E1307	N1232	K1144	R1036	Q926	T856	G778	T669	S579	E500	R344	R344
THR	THR	ASP	L1409	T1308	D1233	S1150	L1037	L929	R857	F779	D672	I586	L504	F347	F347
THR	ASP	ASP	F1410	D1309	E1234	E1151	L1046	L929	S859	D781	D672	I586	C505	T351	T351
PRO	VAL	VAL	A1411	K1235	E1234	E1152	L1046	Y933	S859	R782	T675	Q589	A506	V352	V352
PRO	LYS	LYS	A1412	V1311	L1236	Y1153	L1046	Y933	S859	R782	T675	Q589	A506	I353	I353
THR	THR	ASP	L1418	N1312	I1237	Y1154	N1048	D839	G861	T783	T676	F591	V507	S354	S354
PRO	GLU	GLU	D1419	I1313	I1238	D1155	L1084	R940	H862	T785	T679	D592	P508	G355	G355
SER	LEU	LEU		S1314	R1239	D1155	L1084	R940	H863	H786	I679	D592	P508	E360	E360
SER	MET	MET		E1315		T1161	V1243	L943	K864	D790	T682	T596	L511	L370	L370
THR	THR	PHE	V1424	V1316	V1243	T1162	V1058	L943	K865	D790	T682	T596	L511	L374	L374
PRO	PRO	PRO	V1428	M1317	R1244	I1163	H1059	V946	F866	D790	T682	T596	L511	T375	T375
THR	ALA	LEU			LVS	D1166	P1060	F947	F866	D790	T682	T596	L511	Y376	Y376
SER	VAL	VAL	Q1432	I1322	SER	E1167	M1063	E951	G869	S793	E685	D602	C520	P377	P377
PRO	ASP	ASP	M1433	D1323	LEU	E1168	V1064	E951	G869	S793	E685	D602	C520	V380	V380
SER	PRO	PRO	A1434	P1324	ASP	I1169	G1065	A952	D871	S796	V690	M605	V524	T381	T381
THR	THR	GLY	P1435	T1325	ALA	I1170	Y1066	N953	G872	K787	T694	M605	V524	P382	P382
SER	SER	SER	I1436	R1326	GLU	Q1171	L1067	W954	H873	G798	T694	M605	V524	Y383	Y383
PRO	ASN	ASN	G1437	I1327	THR	L1172	A1068	P955	D874	F799	T703	I607	D526	G366	G366
THR	ASP	ASP			GLU	H1173	A1069	L956	A875	V800	T703	I607	D526	P367	P367
SER	ALA	ALA	F1441	G1340	A1254	F1174	A1069	L956	A875	V800	T703	I607	D526	I370	I370
PRO	MET	MET		I1341	S1175	S1175	E1074	V958	H877	E801	G707	G610	C529	L374	L374
PRO	ALA	ALA	I1445	H1258	L1176	L1176	M1079	R961	R878	L805	T709	Q611	M455	A457	A457
THR	GLY	GLY	ASP	LEU	ASP	LEU	M1079	R961	R878	L805	T709	Q611	M455	H458	H458
SER	GLY	GLY	GLU	GLU	GLU	GLU	T1080	R962	G807	R806	F714	V617	T535	R459	R459
PRO	PHE	PHE	GLU	GLU	GLU	GLU	L1081	I963	G807	R806	F714	V617	T535	V462	V462
THR	THR	THR	SER	ASN	ASN	ASN	ASN	Q969	H884	G807	F714	V617	T535	I463	I463
SER	THR	THR	LEU	ALA	ALA	ALA	PHE	T809	H885	T809	D716	K619	L536	P464	P464
PRO	VAL	VAL	VAL	THR	THR	THR	THR	G117	I886	P810	D716	K619	L536	Y465	Y465
PRO	LYS	LYS	VAL	GLN	HIS	GLN	HIS	H972	G887	E812	V718	V622	T539	S466	S466
THR	GLY	GLY	THR	SER	PHE	SER	PHE	R972	G887	E812	V718	V622	T539	T467	T467
THR	GLY	GLY	THR	SER	PHE	SER	PHE	R972	G887	E812	V718	V622	T539	P468	P468
SER	ALA	ALA	MET	PHE	ALA	PHE	ALA	L881	S889	F814	F721	G623	I541	L470	L470
PRO	ASP	ASP	PRO	ASP	GLY	ASP	GLY	T982	D890	F814	F721	G623	I541	L470	L470
THR	THR	THR	GLU	Q1187	VAL	Q1187	VAL	I953	D890	F814	F721	G623	I541	L470	L470
SER	GLY	GLY	GLN	ALA	ALA	ALA	ALA	I953	D890	F814	F721	G623	I541	L470	L470
PRO	LYS	LYS	V1363	L1193	SER	L1193	SER	I956	K895	R821	R731	G628	D544	L391	L391
PRO	LYS	LYS	N1364	R1194	K1092	R1194	K1092	I956	K895	R821	R731	G628	D544	L391	L391
THR	THR	THR	Y1365	L1195	K1093	L1195	K1093	L983	R896	R821	R731	G628	D544	L391	L391
SER	THR	THR	R1298	E1196	K1093	E1196	K1093	L983	R896	R821	R731	G628	D544	L391	L391
PRO	PRO	PRO	E1280	L1197	V1094	L1197	V1094	L983	R896	R821	R731	G628	D544	L391	L391
THR	THR	THR	R1281	D1198	V1098	D1198	V1098	Q1011	R896	R821	R731	G628	D544	L391	L391
SER	GLY	GLY	ASP	R1199	P1099	R1199	P1099	Q1011	R896	R821	R731	G628	D544	L391	L391
PRO	ALA	ALA	GLY	R1199	R1100	R1199	R1100	Q1011	R896	R821	R731	G628	D544	L391	L391
PRO	GLN	GLN	GLN	M1284	L1101	M1284	L1101	Q1011	R896	R821	R731	G628	D544	L391	L391
THR	THR	THR	ASP	D1206	L1101	D1206	L1101	Q1011	R896	R821	R731	G628	D544	L391	L391
SER	GLY	GLY	GLY	L1207	L1105	L1207	L1105	F1018	R907	R839	K744	C642	I565	P482	P482
PRO	ALA	ALA	GLY	T1208	L1105	T1208	L1105	F1018	R907	R839	K744	C642	I565	Y403	Y403
PRO	VAL	VAL	VAL	M1209	L1116	M1209	L1116	C1019	R908	R840	S754	C642	I565	Y404	Y404
THR	THR	THR	VAL	V1291	L1117	V1291	L1117	C1020	R909	R841	S754	C642	I565	V405	V405
SER	THR	THR	THR	P1292	T1117	P1292	T1117	L1021	R910	R841	S754	C642	I565	I406	I406
PRO	SER	SER	PRO	S1293	T1118	S1293	T1118	L1022	S911	R842	F755	L645	K567	G484	G484
PRO	PRO	PRO	THR	P1294	T1118	P1294	T1118	L1022	S911	R842	F755	L645	K567	P568	P568
THR	THR	THR	THR	T1295	T1118	T1295	T1118	L1022	S911	R842	F755	L645	K567	D485	D485
SER	GLY	GLY	SER	T1295	T1118	T1295	T1118	L1022	S911	R842	F755	L645	K567	S409	S409
THR	PHE	PHE	THR	T1295	T1118	T1295	T1118	L1022	S911	R842	F755	L645	K567	R412	R412
PRO	GLY	GLY	GLY	T1295	T1118	T1295	T1118	L1022	S911	R842	F755	L645	K567	I413	I413
PRO	GLY	GLY	GLY	T1295	T1118	T1295	T1118	L1022	S911	R842	F755	L645	K567	D485	D485
PRO	GLY	GLY	GLY	T1295	T1118	T1295	T1118	L1022	S911	R842	F755	L645	K567	H490	H490

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

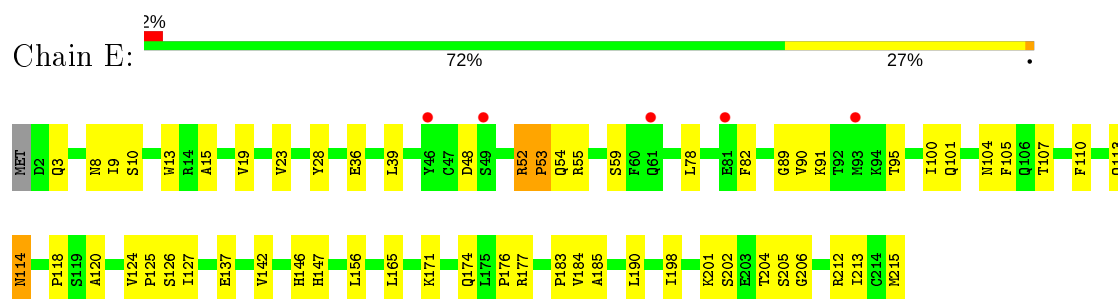




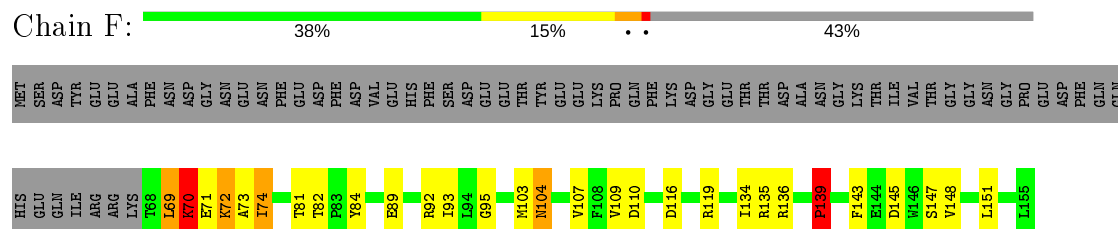
• Molecule 6: DNA-directed RNA polymerase II 45 kDa polypeptide



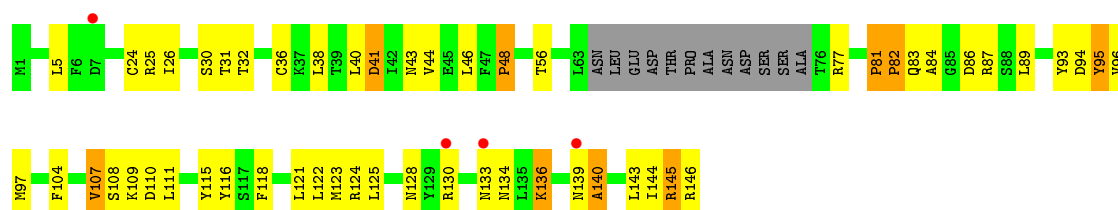
• Molecule 7: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide



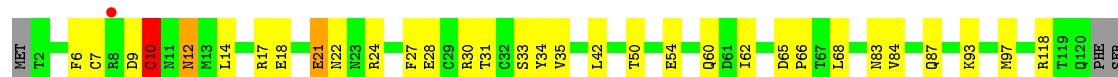
• Molecule 8: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide



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



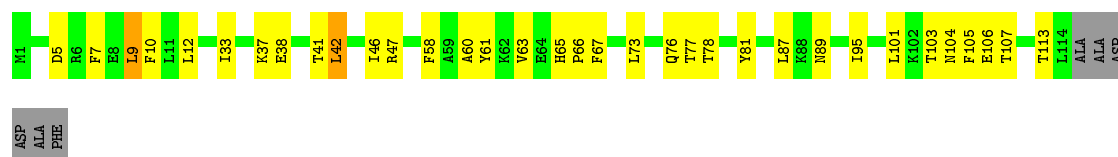
- Molecule 10: DNA-directed RNA polymerase II subunit 9



- Molecule 11: DNA-directed RNA polymerases I/II/III subunit 10



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.72Å 222.41Å 193.07Å 90.00° 101.29° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60 44.25 – 3.60	Depositor EDS
% Data completeness (in resolution range)	91.5 (50.00-3.60) 91.6 (44.25-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.285 , 0.304 0.282 , 0.296	Depositor DCC
R_{free} test set	3721 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	104.2	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 59.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	29436	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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, DUT, 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	1.16	1/243 (0.4%)	1.75	6/378 (1.6%)
2	N	0.74	0/317	1.27	0/488
3	T	1.18	4/634 (0.6%)	1.76	18/975 (1.8%)
4	A	0.68	8/11224 (0.1%)	0.67	2/15176 (0.0%)
5	B	0.82	11/9027 (0.1%)	0.73	3/12172 (0.0%)
6	C	0.71	0/2133	0.69	0/2891
7	E	0.58	1/1788 (0.1%)	0.61	0/2406
8	F	0.60	0/724	0.72	0/977
9	H	0.57	0/1094	0.65	0/1480
10	I	0.75	2/989 (0.2%)	0.68	0/1331
11	J	0.69	0/541	0.68	0/727
12	K	0.66	0/937	0.65	0/1265
13	L	0.70	0/366	0.78	0/485
All	All	0.74	27/30017 (0.1%)	0.76	29/40751 (0.1%)

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	32
5	B	0	12
8	F	0	1
All	All	0	45

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	764	SER	CB-OG	13.86	1.60	1.42
5	B	490	SER	CB-OG	9.83	1.55	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	879	GLU	CD-OE1	7.99	1.34	1.25
3	T	19	DT	C5-C7	7.74	1.54	1.50
5	B	404	LYS	CE-NZ	7.54	1.67	1.49

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	19	DT	C4-C5-C7	10.26	125.16	119.00
3	T	19	DT	C6-C5-C7	-9.91	116.95	122.90
3	T	19	DT	N3-C2-O2	-9.91	116.36	122.30
3	T	16	DC	O4'-C1'-N1	9.72	114.80	108.00
3	T	28	DT	O4'-C1'-N1	8.42	113.89	108.00

There are no chirality outliers.

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	153	PRO	Peptide
4	A	70	CYS	Peptide
4	A	71	GLN	Peptide
4	A	79	GLY	Peptide
4	A	80	HIS	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	216	0	109	7	0
2	N	284	0	161	1	0
3	T	566	0	316	11	0
4	A	11028	0	11120	901	0
5	B	8856	0	8897	724	0
6	C	2095	0	2051	80	0
7	E	1752	0	1776	33	0
8	F	712	0	738	47	0
9	H	1076	0	1052	40	0
10	I	971	0	930	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	J	532	0	542	41	0
12	K	919	0	929	20	0
13	L	364	0	387	20	0
14	A	2	0	0	1	0
14	B	1	0	0	1	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	56	0	22	1	0
All	All	29436	0	29030	1745	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 30.

The worst 5 of 1745 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:404:LYS:NZ	5:B:404:LYS:CE	1.67	1.52
4:A:1287:TYR:CD2	4:A:1305:VAL:HB	1.59	1.36
4:A:1229:SER:HB2	4:A:1236:LEU:CD1	1.59	1.33
4:A:1229:SER:CB	4:A:1236:LEU:HD12	1.64	1.27
5:B:203:PHE:CA	5:B:204:ILE:HD12	1.63	1.27

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	A	1392/1733 (80%)	1118 (80%)	182 (13%)	92 (7%)	1 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	B	1096/1224 (90%)	897 (82%)	124 (11%)	75 (7%)	1	15
6	C	264/318 (83%)	229 (87%)	28 (11%)	7 (3%)	5	35
7	E	212/215 (99%)	190 (90%)	15 (7%)	7 (3%)	4	31
8	F	86/155 (56%)	75 (87%)	6 (7%)	5 (6%)	1	18
9	H	130/146 (89%)	105 (81%)	18 (14%)	7 (5%)	2	19
10	I	117/122 (96%)	96 (82%)	18 (15%)	3 (3%)	5	35
11	J	63/70 (90%)	53 (84%)	8 (13%)	2 (3%)	4	31
12	K	112/120 (93%)	107 (96%)	5 (4%)	0	100	100
13	L	44/70 (63%)	29 (66%)	13 (30%)	2 (4%)	2	23
All	All	3516/4173 (84%)	2899 (82%)	417 (12%)	200 (6%)	1	18

5 of 200 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	55	ASP
4	A	56	PRO
4	A	74	MET
4	A	157	ASP
4	A	158	PRO

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	1225/1520 (81%)	1128 (92%)	97 (8%)	12	44
5	B	967/1061 (91%)	886 (92%)	81 (8%)	11	42
6	C	234/274 (85%)	211 (90%)	23 (10%)	8	36
7	E	196/197 (100%)	181 (92%)	15 (8%)	13	45
8	F	78/137 (57%)	74 (95%)	4 (5%)	24	58
9	H	118/128 (92%)	107 (91%)	11 (9%)	9	38
10	I	113/116 (97%)	103 (91%)	10 (9%)	10	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	J	60/65 (92%)	52 (87%)	8 (13%)	4	23
12	K	99/102 (97%)	87 (88%)	12 (12%)	5	26
13	L	40/57 (70%)	36 (90%)	4 (10%)	7	35
All	All	3130/3657 (86%)	2865 (92%)	265 (8%)	10	41

5 of 265 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	B	388	CYS
5	B	806	THR
11	J	13	VAL
5	B	465	ASN
5	B	567	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
5	B	363	HIS
5	B	592	ASN
9	H	137	GLN
5	B	366	GLN
5	B	494	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	8/10 (80%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 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	DUT	B	1308[A]	-	22,29,29	0.71	1 (4%)	27,45,45	1.06	1 (3%)
16	DUT	B	1308[B]	15	22,29,29	0.67	0	27,45,45	1.31	2 (7%)

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	DUT	B	1308[A]	-	-	6/19/34/34	0/2/2/2
16	DUT	B	1308[B]	15	-	4/19/34/34	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	1308[A]	DUT	C4-N3	2.22	1.36	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	1308[B]	DUT	PB-O3B-PG	-2.88	122.94	132.83
16	B	1308[B]	DUT	C2'-C1'-N1	-2.39	108.75	114.27
16	B	1308[A]	DUT	O3G-PG-O2G	2.14	115.81	107.64

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

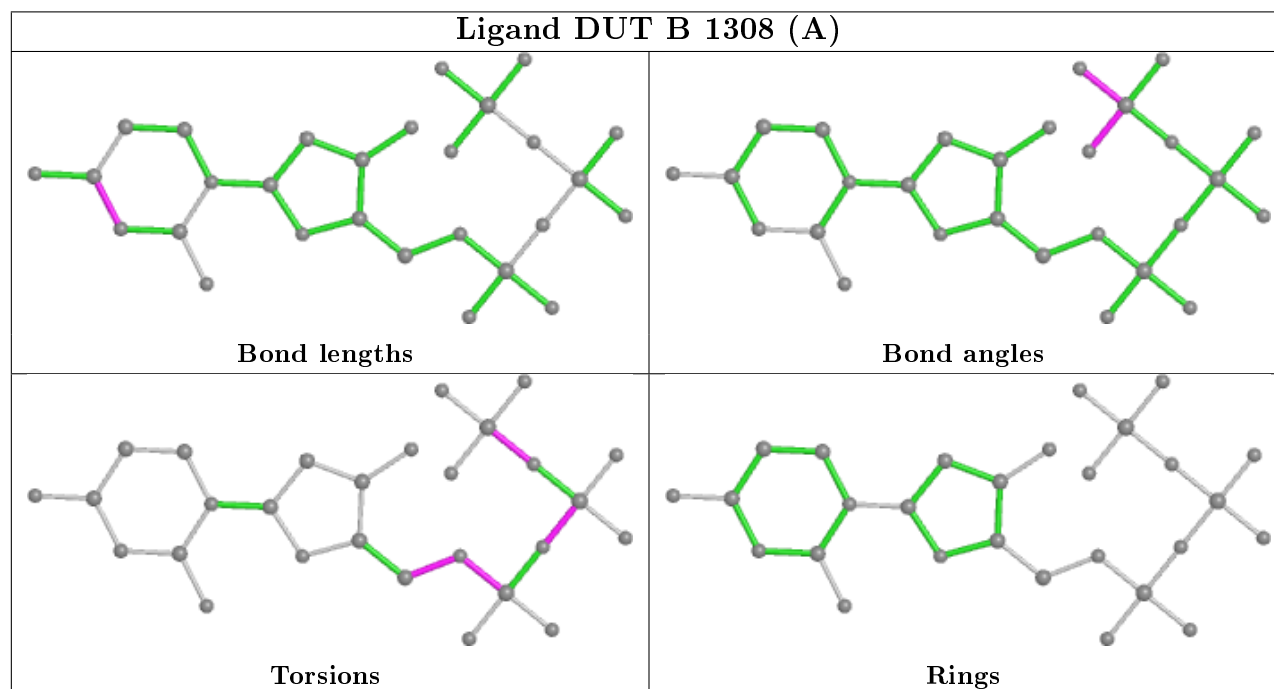
Mol	Chain	Res	Type	Atoms
16	B	1308[B]	DUT	C5'-O5'-PA-O1A
16	B	1308[B]	DUT	C5'-O5'-PA-O2A
16	B	1308[A]	DUT	PB-O3B-PG-O1G
16	B	1308[A]	DUT	C4'-C5'-O5'-PA
16	B	1308[A]	DUT	PB-O3B-PG-O2G

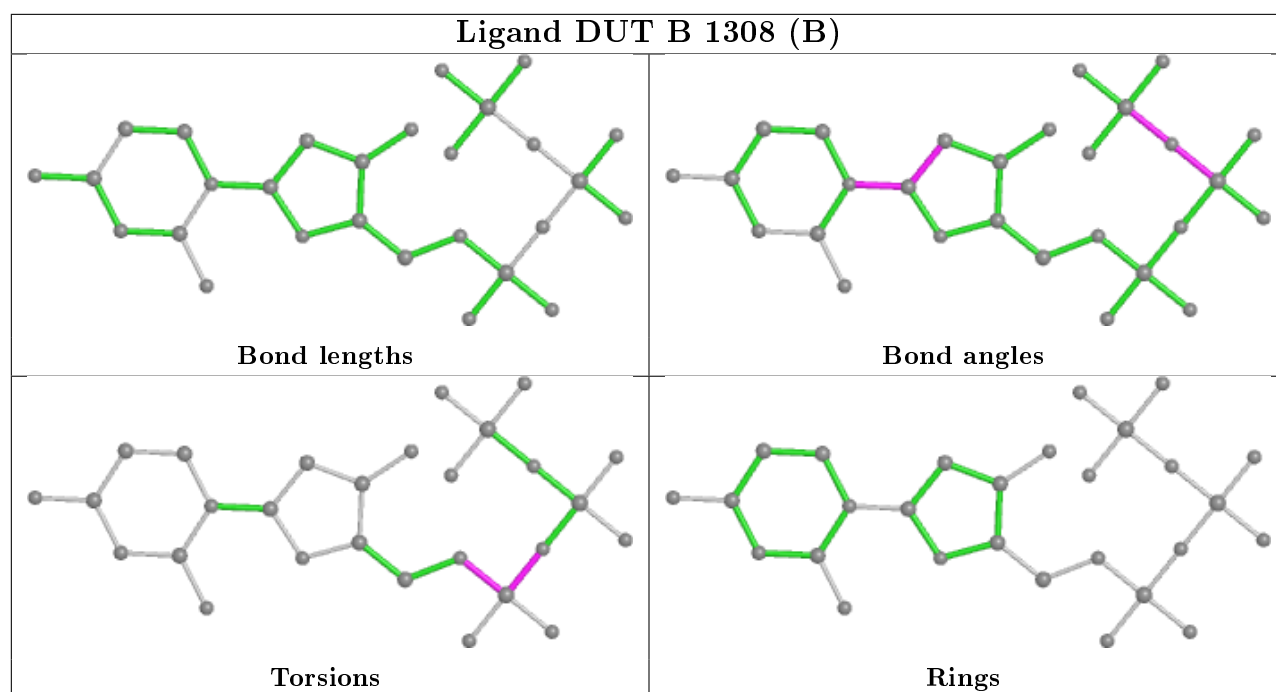
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	1308[A]	DUT	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	10/10 (100%)	-0.58	0 100 100	85, 109, 154, 170	0
2	N	14/14 (100%)	1.46	3 (21%) 0 0	178, 182, 198, 202	0
3	T	28/28 (100%)	0.74	7 (25%) 0 0	93, 173, 189, 192	0
4	A	1402/1733 (80%)	-0.04	21 (1%) 73 60	75, 103, 150, 163	0
5	B	1114/1224 (91%)	-0.05	17 (1%) 73 60	26, 102, 133, 143	0
6	C	266/318 (83%)	-0.23	1 (0%) 92 86	81, 100, 128, 144	0
7	E	214/215 (99%)	0.07	5 (2%) 60 44	91, 131, 165, 167	0
8	F	88/155 (56%)	-0.12	0 100 100	84, 104, 130, 137	0
9	H	134/146 (91%)	0.12	4 (2%) 50 34	100, 119, 152, 155	0
10	I	119/122 (97%)	-0.08	1 (0%) 86 75	87, 104, 122, 138	0
11	J	65/70 (92%)	-0.28	0 100 100	92, 102, 122, 125	0
12	K	114/120 (95%)	-0.28	0 100 100	82, 105, 119, 121	0
13	L	46/70 (65%)	0.31	2 (4%) 35 22	108, 145, 156, 157	0
All	All	3614/4225 (85%)	-0.04	61 (1%) 70 55	26, 104, 150, 202	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	69	THR	5.0
4	A	72	GLU	4.8
5	B	338	GLY	4.0
7	E	46	TYR	4.0
4	A	44	THR	3.9

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

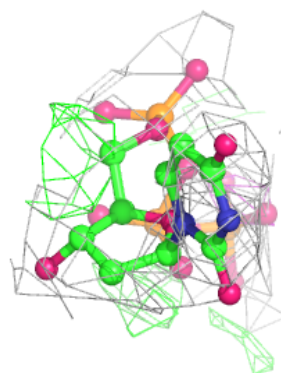
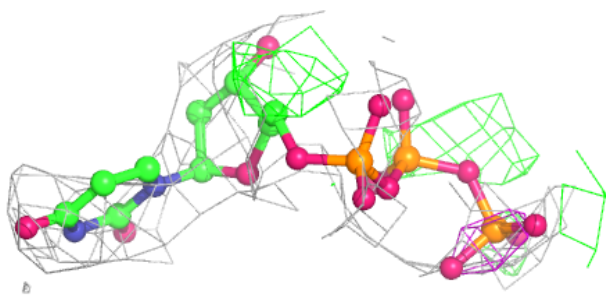
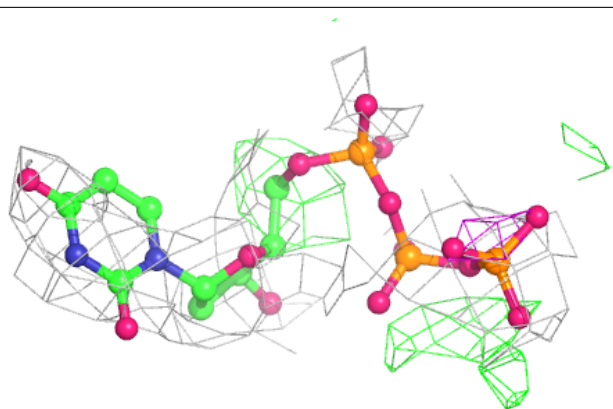
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
16	DUT	B	1308[A]	28/28	0.79	0.35	131,133,149,150	28
16	DUT	B	1308[B]	28/28	0.79	0.35	57,59,61,62	28
14	ZN	A	1734	1/1	0.89	0.05	159,159,159,159	0
14	ZN	I	203	1/1	0.93	0.07	97,97,97,97	0
14	ZN	B	1307	1/1	0.96	0.10	126,126,126,126	0
15	MG	A	2000	1/1	0.97	0.22	74,74,74,74	0
14	ZN	L	105	1/1	0.97	0.06	181,181,181,181	0
14	ZN	I	204	1/1	0.97	0.09	107,107,107,107	0
14	ZN	J	101	1/1	0.98	0.12	149,149,149,149	0
14	ZN	A	1735	1/1	0.98	0.09	142,142,142,142	0
14	ZN	C	319	1/1	0.99	0.06	104,104,104,104	0

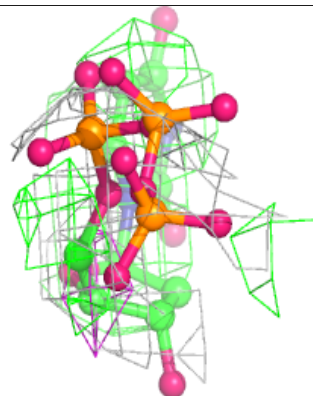
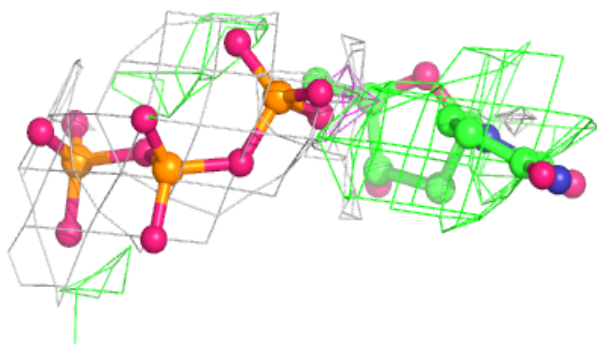
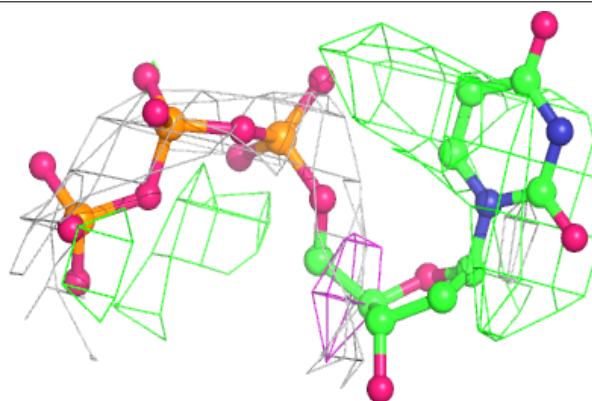
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DUT B 1308 (A):

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

**Electron density around DUT B 1308 (B):**

$2mF_o-DF_c$ (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.