



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:02 PM UTC

PDB ID : 8W8P / pdb_00008w8p
Title : Thermus thermophilus initiation transcription complex containing CMPcPP
in the post-translocated state
Authors : Li, L.; Zhang, Y.
Deposited on : 2023-09-04
Resolution : 3.17 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

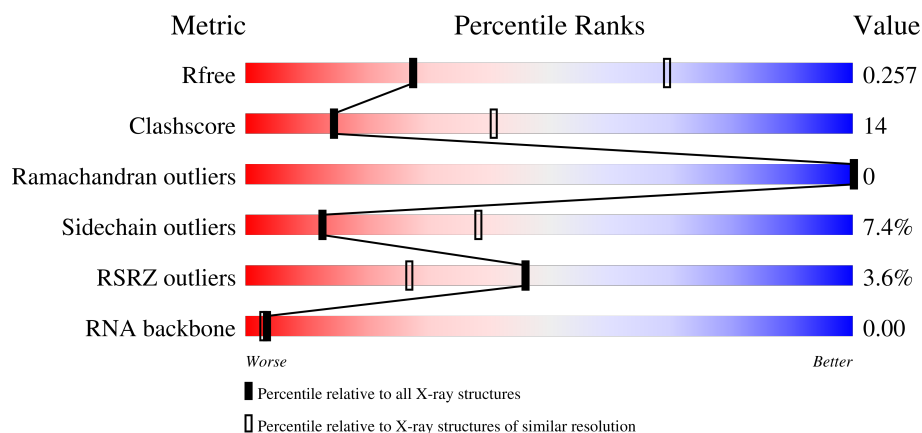
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.17 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)
RNA backbone	3983	1113 (3.42-2.90)

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	A	315	3% 49% 22% . 27%
1	B	315	3% 46% 24% . 28%
2	C	1119	3% 63% 33% ..
3	D	1524	4% 63% 33% ..

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Mol	Chain	Length	Quality of chain
4	E	99	% 72% 20% • 5%
5	F	443	4% 55% 22% • 22%
6	G	21	5% 43% 33% 19%
7	H	27	4% 15% 41% 33% 11%
8	I	3	33% 67%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 28769 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 protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1809	1155	315	337	2			
1	B	227	Total	C	N	O	S	0	0	0
			1789	1143	310	334	2			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1112	Total	C	N	O	S	0	0	0
			8771	5547	1565	1635	24			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1497	Total	C	N	O	S	0	1	0
			11817	7488	2085	2208	36			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2804	1769	509	522	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	expression tag	UNP Q5SKW1
F	-18	GLY	-	expression tag	UNP Q5SKW1
F	-17	SER	-	expression tag	UNP Q5SKW1
F	-16	SER	-	expression tag	UNP Q5SKW1
F	-15	HIS	-	expression tag	UNP Q5SKW1
F	-14	HIS	-	expression tag	UNP Q5SKW1
F	-13	HIS	-	expression tag	UNP Q5SKW1
F	-12	HIS	-	expression tag	UNP Q5SKW1
F	-11	HIS	-	expression tag	UNP Q5SKW1
F	-10	HIS	-	expression tag	UNP Q5SKW1
F	-9	SER	-	expression tag	UNP Q5SKW1
F	-8	SER	-	expression tag	UNP Q5SKW1
F	-7	GLY	-	expression tag	UNP Q5SKW1
F	-6	LEU	-	expression tag	UNP Q5SKW1
F	-5	VAL	-	expression tag	UNP Q5SKW1
F	-4	PRO	-	expression tag	UNP Q5SKW1
F	-3	ARG	-	expression tag	UNP Q5SKW1
F	-2	GLY	-	expression tag	UNP Q5SKW1
F	-1	SER	-	expression tag	UNP Q5SKW1
F	0	HIS	-	expression tag	UNP Q5SKW1

- Molecule 6 is a DNA chain called DNA (21-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	17	Total	C	N	O	P	0	0	0
			347	165	66	100	16			

- Molecule 7 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	24	Total	C	N	O	P	0	0	0
			495	236	94	142	23			

- Molecule 8 is a RNA chain called RNA (5'-(GTP)GA-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	3	Total	C	N	O	P	0	0	0
			77	30	15	27	5			

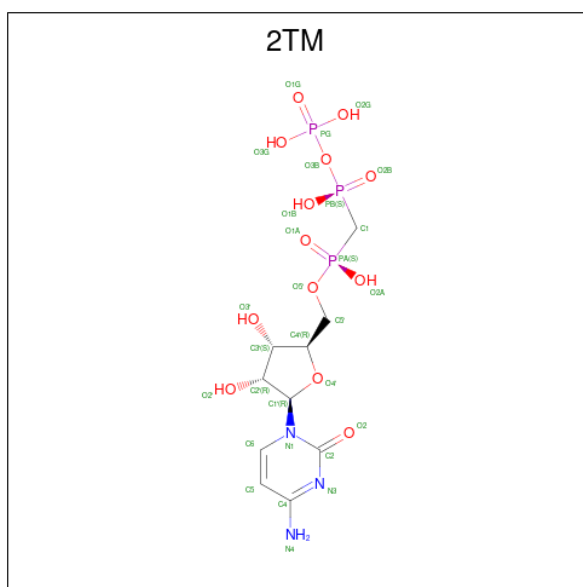
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	2	Total Mg 2 2	0	0
9	D	3	Total Mg 3 3	0	0
9	F	1	Total Mg 1 1	0	0

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	2	Total Zn 2 2	0	0

- Molecule 11 is 5'-O-[(S)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]methyl}phosphoryl]cytidine (CCD ID: 2TM) (formula: C₁₀H₁₈N₃O₁₃P₃).



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

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	3	Total O 3 3	0	0
12	B	4	Total O 4 4	0	0

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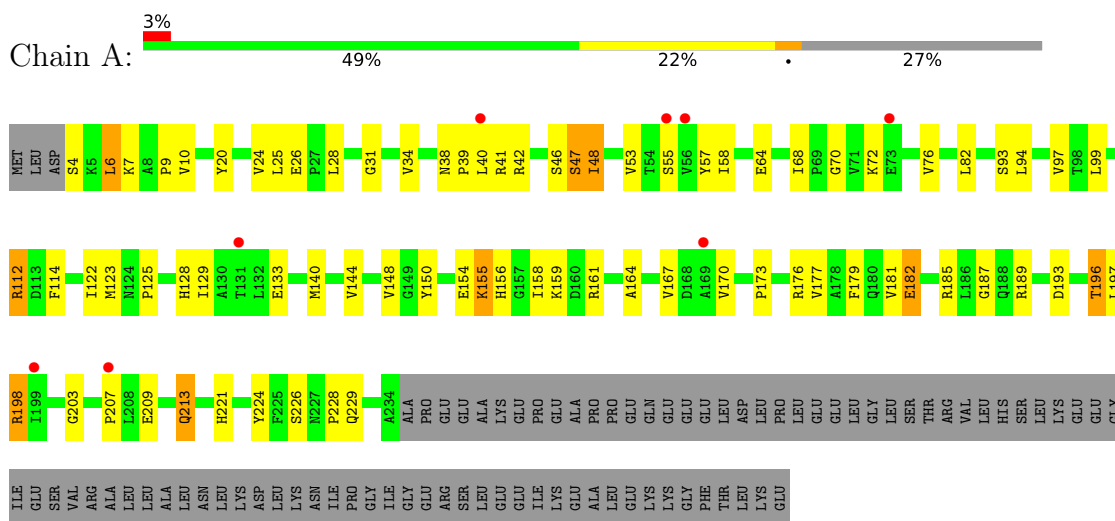
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	19	Total 19	O 19	0	0
12	D	24	Total 24	O 24	0	0
12	E	2	Total 2	O 2	0	0
12	F	1	Total 1	O 1	0	0
12	G	5	Total 5	O 5	0	0
12	H	1	Total 1	O 1	0	0
12	I	3	Total 3	O 3	0	0

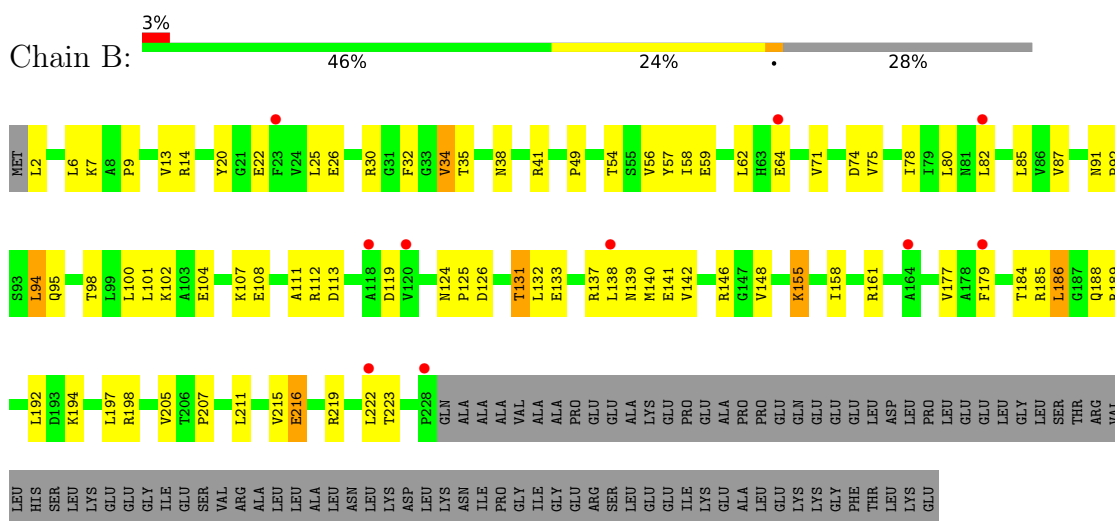
3 Residue-property plots [i](#)

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

- Molecule 1: DNA-directed RNA polymerase subunit alpha

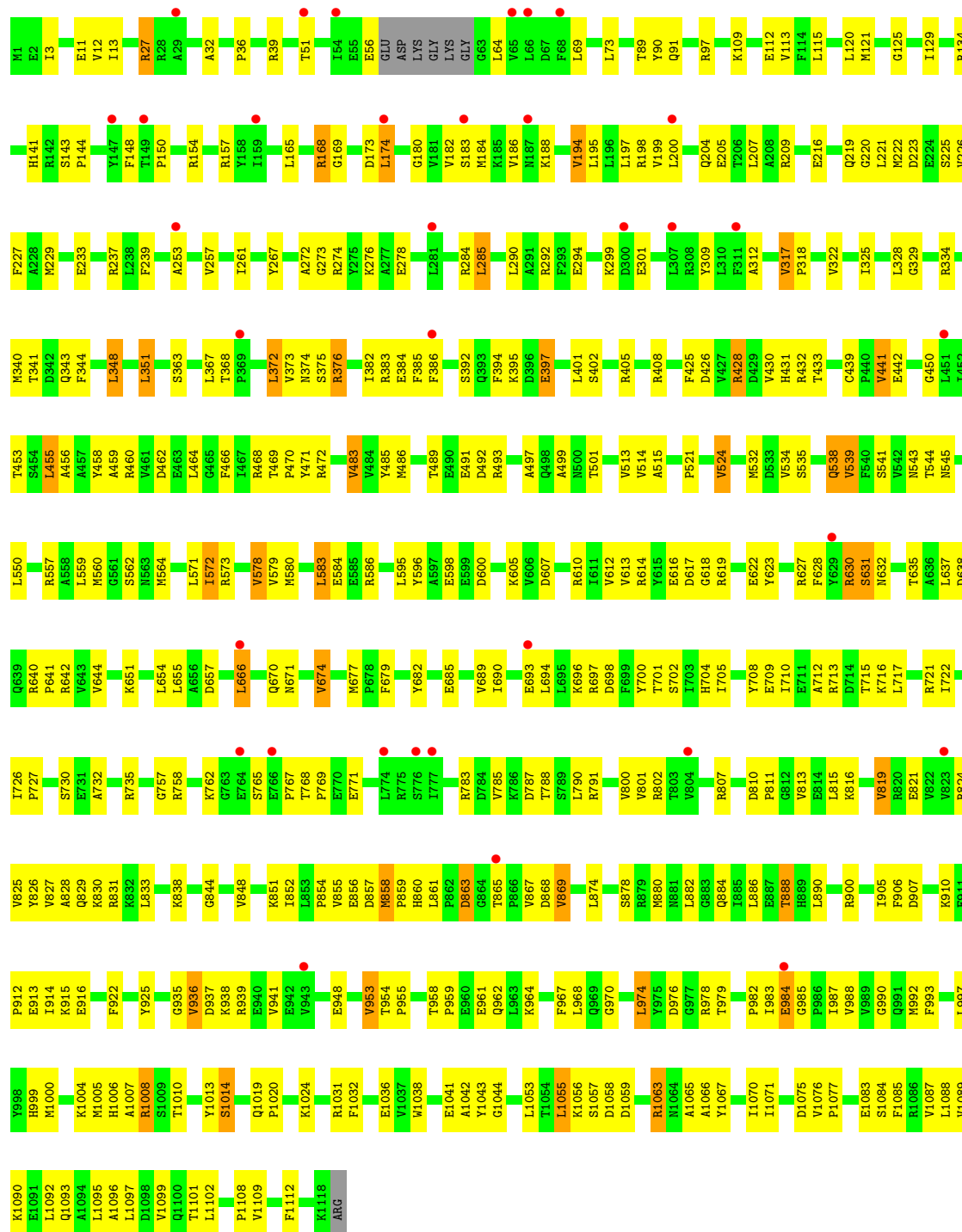


- Molecule 1: DNA-directed RNA polymerase subunit alpha

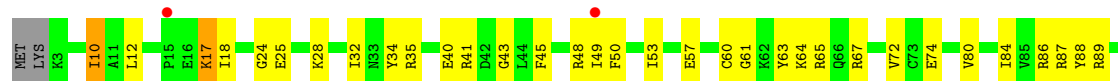


- Molecule 2: DNA-directed RNA polymerase subunit beta

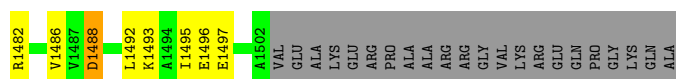




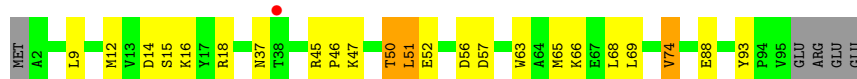
• Molecule 3: DNA-directed RNA polymerase subunit beta'



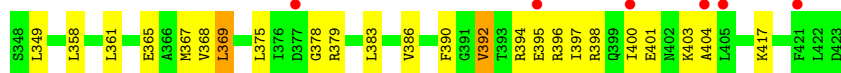
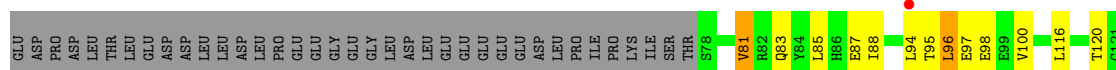
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ALA	ALA	D1261	T1262	T1263	G1264	G1265	P1267	P1268	M1269	I1270	F1263	I1274	I1283	E1284	E1285	L1290	S1291	S1296	E1297	G1298	F1299	K1304	L1305	A1309	L1312	V1313	K1314	D1315	Q1334	K1339	G1340	P1341	E1342	A1343	V1344	E1345	E1350	Q1353	K1354	R1357	Y1361	K1362	L1363	H1364																				
L1156	G1157	V1158	L1166	S1167	M1168	D1169	D1170	V1171	H1172	I1175	E1185	V1188	R1189	L1192	T1193	C1194	R1197	Y1198	G1199	V1200	K1203	C1204	Y1205	D1208	L1209	S1210	M1211	S1216	A1220	V1221	G1222	I1223	V1224	P1232	G1233	T1234	Q1235	L1236	T1237	M1238	R1239	T1240	F1241	H1242	V1246	A1247	GLY																	
P846	A849	L850	L851	A852	V853	A854	H855	G856	I857	V858	D859	D862	V863	V864	V670	S771	S774	S782	R783	D784	I785	T786	S790	Y790	G797	I792	T793	L880	F881	F882	F883	A883	R884	I885	V886	A889	V890	D891	E892	K894	V895	E1012	Y1021	V1022	R1029	G1030	N1031	Q906	E907	K908	L909	I1035	S910	R1036	Q1037	L1038								
L731	F736	F740	D741	G742	D743	Q744	M745	A746	V747	F754	M763	S771	S774	L778	S782	R783	D784	I785	T786	S790	Y791	I792	T793	L880	F881	F882	F883	A883	R884	I885	V886	A889	V890	D891	E892	K894	V895	E1012	Y1021	V1022	R1029	G1030	N1031	Q1034	I1035	S910	R1036	Q1037	L1038															
P846	A849	L850	L851	A852	V853	A854	H855	G856	I857	V858	D859	D862	V863	V864	V670	S771	S774	S782	R783	D784	I785	T786	S790	Y790	G797	I792	T793	L880	F881	F882	F883	A883	R884	I885	V886	A889	V890	D891	E892	K894	V895	E1012	Y1021	V1022	R1029	G1030	N1031	Q906	E907	K908	L909	I1035	S910	R1036	Q1037	L1038								
V915	Y916	L920	R921	L922	G923	K926	T927	A928	R929	L930	K936	F939	T940	F941	T944	S945	G946	I947	T951	D952	K960	P977	K970	E975	E979	T984	L995	T999	V1003	V1007	E1012	Y1021	V1022	R1029	G1030	N1031	Q1034	I1035	S910	R1036	Q1037	L1038																						
C1039	G1040	L1041	R1042	G1043	L1044	M1045	Q1046	K1047	P1048	F1053	P1056	V1057	R1062	V1067	L1068	E1069	I1072	S1073	K1079	G1080	D1083	T1084	A1085	L1086	Y1093	L1094	T1095	V1099	D1100	V1101	T1102	V1107	A1110	D1111	C1112	G1113	T1114	S1119	I1140	L1144	R1147	V1148	L1149																					
L1156	G1157	V1158	L1166	S1167	M1168	D1169	D1170	V1171	H1172	I1175	E1185	V1188	R1189	L1192	T1193	C1194	R1197	Y1198	G1199	V1200	K1203	C1204	Y1205	D1208	L1209	S1210	M1211	S1216	A1220	V1221	G1222	I1223	V1224	P1232	G1233	T1234	Q1235	L1236	T1237	M1238	R1239	T1240	F1241	H1242	V1246	A1247	GLY																	
ALA	ALA	D1261	T1262	T1263	G1264	G1265	P1267	P1268	M1269	I1270	F1263	I1274	I1283	E1284	E1285	L1290	S1291	S1296	E1297	G1298	F1299	K1304	L1305	A1309	L1312	V1313	K1314	D1315	Q1334	K1339	G1340	P1341	E1342	A1343	V1344	E1345	E1350	Q1353	K1354	R1357	Y1361	K1362	L1363	H1364																				
H92	I93	E94	L95	A96	T97	A100	F104	D107	T114	L115	L116	D117	L118	E122	L123	E124	L127	Y128	F129	I133	V134	L135	K138	G222	L223	L227	Y236	K237	P238	L242	A243	D244	L245	P248	V258	L262	G267	A268	P269	L270	R273	D274	E275																					
G182	E183	V184	E185	V186	K187	L191	A192	P193	S197	R198	L199	G201	D202	L204	Y205	R206	F207	R209	R210	V211	V216	K217	L218	E219	G222	L223	L227	Y236	K237	P238	L242	A243	D244	L245	P248	V258	L262	G267	A268	P269	L270	R273	D274	E275																				
D276	L284	P285	G287	V288	T289	L288	T289	V292	V293	V298	V298	Q302	K303	L304	P305	A306	K308	G309	L310	L311	Q316	R317	R318	A319	V322	V331	G332	L333	T334	L335	V336	L337	E338	V339	P349	V353	V354	V355	P356	A359	R360	K366	I367	A368	V369	A370	I371	D372	P373															
E376	V377	I378	A379	V384	V385	H386	L387	H388	E389	P390	A391	I393	L394	V395	V396	K397	Y400	Y401	V407	E408	V409	S410	A319	V412	V415	D419	V420	L421	A422	K428	S429	D430	V431	Y432	V437	V440	R441	N442	V443	V444	E448	D453	A454	R455	K456	L457	P458	D459	E460	G461	L462	K463	E464	N465	V466	I467	L468	G469	L470	L471	L472	P473	T476	D479
L464	L465	L470	A471	A472	L473	E476	L477	L478	E479	F480	M481	K482	H483	P484	A487	R488	K491	D492	R493	K494	R495	L496	E497	R500	L503	I513	P518	R519	L520	P521	P522	D523	L524	R525	P526	M527	V530	D531	R534	T537	N541	D542	L543	Y544	R545	P546	K547																	
I548	R549	R550	R553	L554	Q560	G561	I566	I567	R568	N569	E570	R571	R572	M573	L574	V578	D579	A580	L581	L582	D583	N584	R587	R601	L607	R613	R614	R615	G616	M617	L618	L619	G620	V623	D624	Y625	R628	S629	V630	I631	V632	V633	G723	Q724	S725	L726	Q727	G643	L644	H645	K646													
K648	A649	L650	E651	K654	P655	F656	L657	L658	H661	K664	V670	R674	L677	E678	R679	G680	R681	D682	L683	K684	D685	E686	V687	V688	E692	R693	V694	L695	H696	L702	R703	R704	A705	P706	T707	L708	H709	R710	L711	P718	G723	Q724	S725	L726	Q727	G643	L644	H645	K646															
L731	F736	F740	D741	G742	D743	Q744	M745	A746	V747	F754	M763	S771	S774	L778	S782	R783	D784	I785	T786	S790	Y791	I792	T793	L880	F881	F882	F883	A883	R884	I885	V886	A889	V890	D891	E892	K894	V895	E1012	Y1021	V1022	R1029	G1030	N1031	Q1034	I1035	S910	R1036	Q1037	L1038															
P846	A849	L850	L851	A852	V853	A854	H855	G856	I857	V858	D859	D862	V863	V864	V670	S771	S774	S782	R783	D784	I785	T786	S790	Y790	G797	I792	T793	L880	F881	F882	F883	A883	R884	I885	V886	A889	V890	D891	E892	K894	V895	E1012	Y1021	V1022	R1029	G1030	N1031	Q906	E907	K908	L909	I1035	S910	R1036	Q1037	L1038								
V915	Y916	L920	R921	L922	G923	K926	T927	A928	R929	L930	K936	F939	T940	F941	T944	S945	G946	I947	T951	D952	K960	P977	K970	E975	E979	T984	L995	T999	V1003	V1007	E1012	Y1021	V1022	R1029	G1030	N1031	Q1034	I1035	S910	R1036	Q1037	L1038																						
C1039	G1040	L1041	R1042	G1043	L1044	M1045	Q1046	K1047	P1048	F1053	P1056	V1057	R1062	V1067	L1068	E1069	I1072	S1073	K1079	G1080	D1083	T1084	A1085	L1086	Y1093	L1094	T1095	V1099	D1100	V1101	T1102	V1107	A1110	D1111	C1112	G1113	T1114	S1119	I1140	L1144	R1147	V1148	L1149																					
L1156	G1157	V1158	L1166	S1167	M1168	D1169	D1170	V1171	H1172	I1175	E1185	V1188	R1189	L1192	T1193	C1194	R1197	Y1198	G1199	V1200	K1203	C1204	Y1205	D1208	L1209	S1210	M1211	S1216	A1220	V1221	G1222	I1223	V1224	P1232	G1233	T1234	Q1235	L1236	T1237	M1238	R1239	T1240	F1241	H1242	V1246	A1247	GLY																	
ALA	ALA	D1261	T1262	T1263	G1264	G1265	P1267	P1268	M1269	I1270	F1263	I1274	I1283	E1284	E1285	L1290	S1291	S1296	E1297	G1298	F1299	K1304	L1305	A1309	L1312	V1313	K1314	D1315	Q1334	K1339	G1340	P1341	E1342	A1343	V1344	E1345	E1350	Q1353	K1354	R1357	Y1361	K1362	L1363	H1364																				



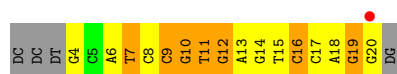
- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 5: RNA polymerase sigma factor SigA



- Molecule 6: DNA (21-MER)



- Molecule 7: DNA (27-MER)



- Molecule 8: RNA (5'-(GTP)GA-3')





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.68Å 103.89Å 294.61Å 90.00° 98.97° 90.00°	Depositor
Resolution (Å)	39.76 – 3.17 39.76 – 3.17	Depositor EDS
% Data completeness (in resolution range)	94.4 (39.76-3.17) 94.4 (39.76-3.17)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 3.18Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.211 , 0.257 0.211 , 0.257	Depositor DCC
R_{free} test set	2014 reflections (2.26%)	wwPDB-VP
Wilson B-factor (Å ²)	57.6	Xtriage
Anisotropy	0.957	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 35.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.025 for $1/2^*h-3/2^*k,-1/2^*h-1/2^*k,-1/2^*h+1/2^*k-l$ 0.025 for $1/2^*h+3/2^*k,1/2^*h-1/2^*k,-1/2^*h-1/2^*k-l$	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	28769	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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: MG, 2TM, ZN, GTP

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	A	0.42	0/1841	0.65	0/2504
1	B	0.41	0/1821	0.60	0/2476
2	C	0.43	0/8938	0.65	0/12088
3	D	0.44	0/12027	0.65	1/16261 (0.0%)
4	E	0.42	0/775	0.59	0/1045
5	F	0.40	0/2849	0.60	0/3833
6	G	0.48	0/389	1.25	12/599 (2.0%)
7	H	0.51	0/556	1.12	11/858 (1.3%)
8	I	0.54	0/50	1.13	1/76 (1.3%)
All	All	0.43	0/29246	0.67	25/39740 (0.1%)

There are no bond length outliers.

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	3	DT	P-O3'-C3'	-9.80	105.51	120.20
7	H	15	DT	P-O3'-C3'	-9.37	106.15	120.20
6	G	15	DT	P-O3'-C3'	-8.79	107.01	120.20
6	G	14	DG	P-O3'-C3'	-8.35	107.67	120.20
6	G	9	DC	P-O3'-C3'	-8.13	108.01	120.20

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	A	1809	0	1863	53	0
1	B	1789	0	1841	54	0
2	C	8771	0	8868	289	0
3	D	11817	0	12044	368	0
4	E	761	0	778	15	0
5	F	2804	0	2880	68	0
6	G	347	0	192	13	0
7	H	495	0	272	27	0
8	I	77	0	34	1	0
9	B	2	0	0	0	0
9	D	3	0	0	0	0
9	F	1	0	0	0	0
10	D	2	0	0	0	0
11	D	29	0	14	4	0
12	A	3	0	0	0	0
12	B	4	0	0	1	0
12	C	19	0	0	7	0
12	D	24	0	0	2	0
12	E	2	0	0	0	0
12	F	1	0	0	0	0
12	G	5	0	0	0	0
12	H	1	0	0	0	0
12	I	3	0	0	0	0
All	All	28769	0	28786	802	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 14.

The worst 5 of 802 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)
2:C:1057:SER:HA	12:C:1202:HOH:O	1.44	1.18
2:C:993:PHE:HB3	12:C:1201:HOH:O	1.46	1.15
3:D:236:TYR:CE2	3:D:322:VAL:HG21	1.95	1.02
2:C:579:VAL:HG23	12:C:1206:HOH:O	1.60	1.01
3:D:1102:THR:HG22	3:D:1222:GLY:CA	1.97	0.92

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	
1	A	229/315 (73%)	216 (94%)	13 (6%)	0	100	100
1	B	225/315 (71%)	212 (94%)	13 (6%)	0	100	100
2	C	1108/1119 (99%)	1050 (95%)	58 (5%)	0	100	100
3	D	1494/1524 (98%)	1411 (94%)	83 (6%)	0	100	100
4	E	92/99 (93%)	84 (91%)	8 (9%)	0	100	100
5	F	344/443 (78%)	334 (97%)	10 (3%)	0	100	100
All	All	3492/3815 (92%)	3307 (95%)	185 (5%)	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	
1	A	200/273 (73%)	184 (92%)	16 (8%)	11	35
1	B	200/273 (73%)	189 (94%)	11 (6%)	19	47
2	C	935/941 (99%)	860 (92%)	75 (8%)	11	35
3	D	1259/1279 (98%)	1168 (93%)	91 (7%)	13	39
4	E	83/88 (94%)	79 (95%)	4 (5%)	23	52
5	F	300/388 (77%)	277 (92%)	23 (8%)	12	37
All	All	2977/3242 (92%)	2757 (93%)	220 (7%)	13	38

5 of 220 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	183	GLU
3	D	615	ARG
5	F	417	LYS
5	F	94	LEU
3	D	216	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	1034	GLN
3	D	1172	HIS
3	D	1046	GLN
3	D	1227	GLN
2	C	1019	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	1/3 (33%)	1 (100%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	I	7	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 9 ligands modelled in this entry, 8 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
11	2TM	D	1606	9	26,30,30	4.03	15 (57%)	39,47,47	1.17	3 (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
11	2TM	D	1606	9	-	2/19/38/38	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)
11	D	1606	2TM	PB-O3B	8.24	1.67	1.58
11	D	1606	2TM	O4'-C1'	7.57	1.59	1.42
11	D	1606	2TM	O4'-C4'	-7.01	1.29	1.45
11	D	1606	2TM	C2-N3	6.56	1.49	1.36
11	D	1606	2TM	C2'-C1'	-5.91	1.34	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	1606	2TM	PB-O3B-PG	-3.15	121.15	132.45
11	D	1606	2TM	O2G-PG-O3B	3.06	114.91	104.64
11	D	1606	2TM	N4-C4-N3	2.36	122.13	117.91

There are no chirality outliers.

All (2) torsion outliers are listed below:

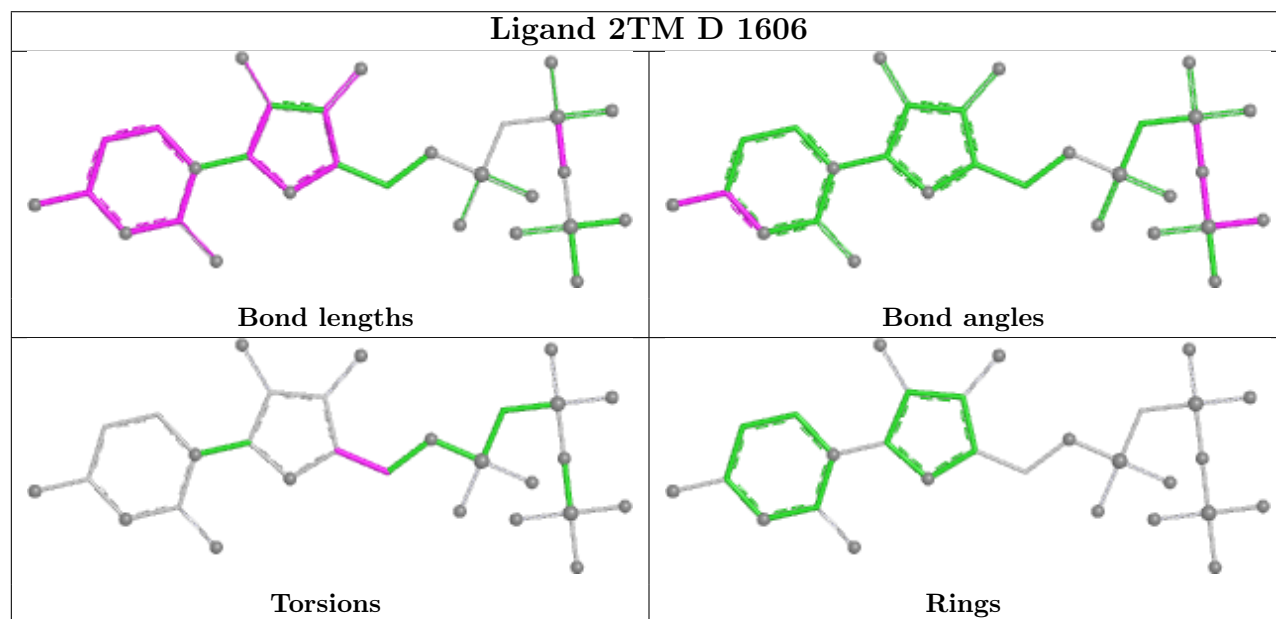
Mol	Chain	Res	Type	Atoms
11	D	1606	2TM	O4'-C4'-C5'-O5'
11	D	1606	2TM	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	1606	2TM	4	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	A	231/315 (73%)	0.43	8 (3%) 47 28	36, 54, 76, 122	0
1	B	227/315 (72%)	0.60	10 (4%) 39 22	37, 68, 91, 126	0
2	C	1112/1119 (99%)	0.46	34 (3%) 51 31	21, 54, 99, 121	0
3	D	1497/1524 (98%)	0.47	58 (3%) 43 25	20, 56, 108, 167	2 (0%)
4	E	94/99 (94%)	0.41	1 (1%) 78 60	36, 59, 90, 96	0
5	F	346/443 (78%)	0.53	16 (4%) 37 21	33, 65, 107, 125	0
6	G	17/21 (80%)	0.58	1 (5%) 28 16	36, 67, 142, 143	0
7	H	24/27 (88%)	0.65	1 (4%) 40 23	53, 84, 122, 154	0
8	I	2/3 (66%)	0.04	0 100 100	38, 38, 38, 39	0
All	All	3550/3866 (91%)	0.48	129 (3%) 46 27	20, 57, 105, 167	2 (0%)

The worst 5 of 129 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	203	ALA	7.1
3	D	412	GLY	4.8
3	D	368	VAL	4.5
2	C	764	GLU	4.3
3	D	1246	VAL	4.1

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](#)

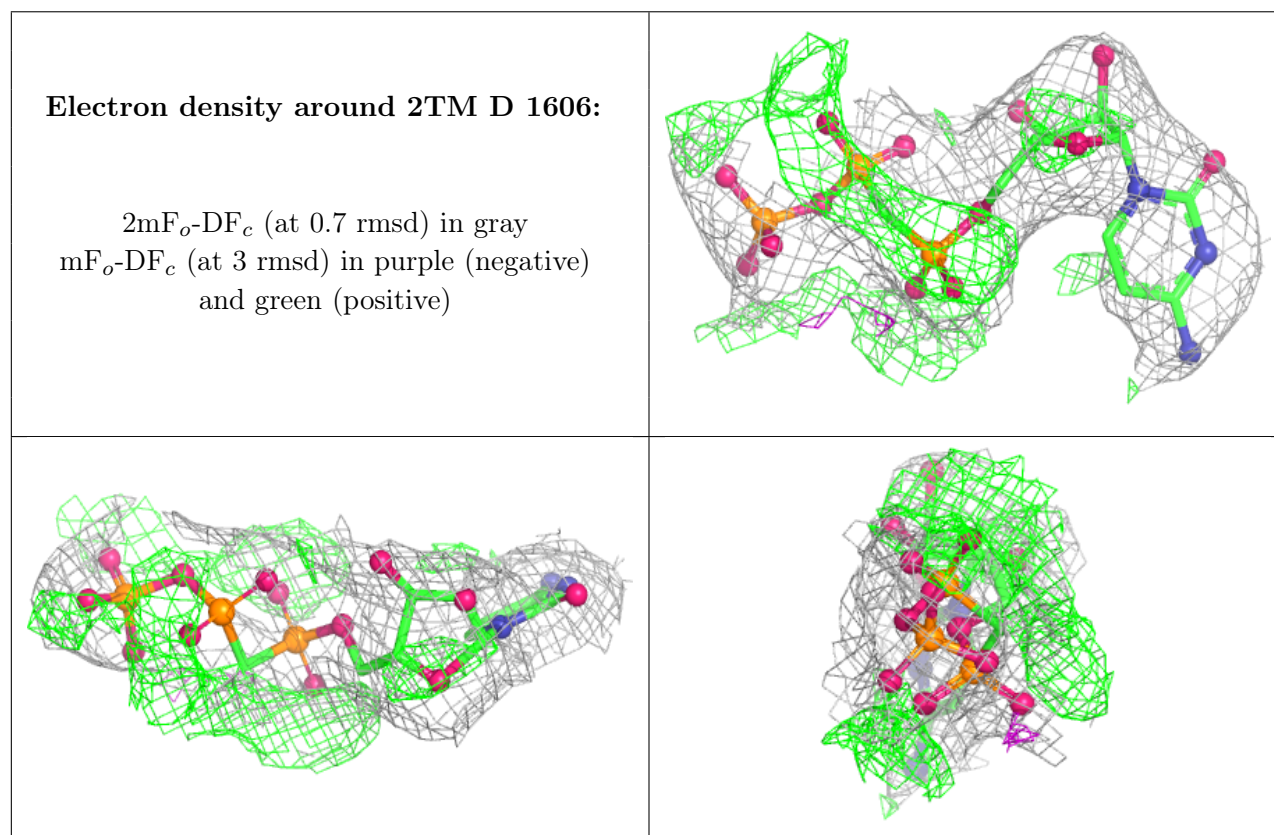
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
11	2TM	D	1606	29/29	0.81	0.15	26,37,62,75	29
9	MG	D	1605	1/1	0.86	0.15	59,59,59,59	0
9	MG	B	402	1/1	0.87	0.24	44,44,44,44	0
9	MG	B	401	1/1	0.89	0.07	73,73,73,73	0
9	MG	D	1604	1/1	0.92	0.24	42,42,42,42	0
9	MG	F	501	1/1	0.94	0.06	65,65,65,65	0
9	MG	D	1603	1/1	0.96	0.07	27,27,27,27	0
10	ZN	D	1602	1/1	0.99	0.02	57,57,57,57	0
10	ZN	D	1601	1/1	0.99	0.05	46,46,46,46	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.