



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 14, 2023 – 11:43 PM EDT

PDB ID : 1R9T
Title : RNA POLYMERASE II STRAND SEPARATED ELONGATION COM-
PLEX, MISMATCHED NUCLEOTIDE
Authors : Westover, K.D.; Bushnell, D.A.; Kornberg, R.D.
Deposited on : 2003-10-30
Resolution : 3.50 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

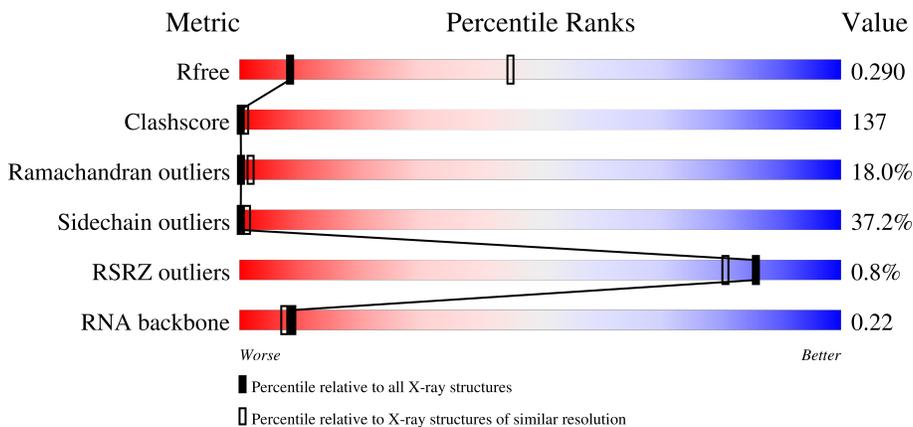
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	R	10	
2	T	28	
3	N	14	
4	A	1733	

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Mol	Chain	Length	Quality of chain
5	B	1224	 % • 15% 40% 34% 10%
6	C	318	 • 14% 39% 29% 16%
7	E	215	 • 12% 39% 47%
8	F	155	 6% 30% 19% 46%
9	H	146	 • 10% 42% 38% 9%
10	I	122	 • 11% 37% 46% 6%
11	J	70	 6% 13% 41% 33% 7%
12	K	120	 • 16% 44% 33% 5%
13	L	70	 % 6% 33% 27% 34%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	MG	A	2002	-	-	-	X

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 29248 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 strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	R	10	217	98	45	65	9	0	0	0

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

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

- Molecule 3 is a DNA chain called DNA nontemplate strand.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	A	1395	10969	6917	1923	2068	61	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	B	1106	8792	5568	1538	1631	55	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	F	84	679	434	115	127	3	0	0	0

- 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
			Total	C	N	O	S			
9	H	133	1068	673	180	211	4	0	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerase II 14.2 kDa polypeptide.

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

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	L	46	363	224	72	63	4	0	0	0

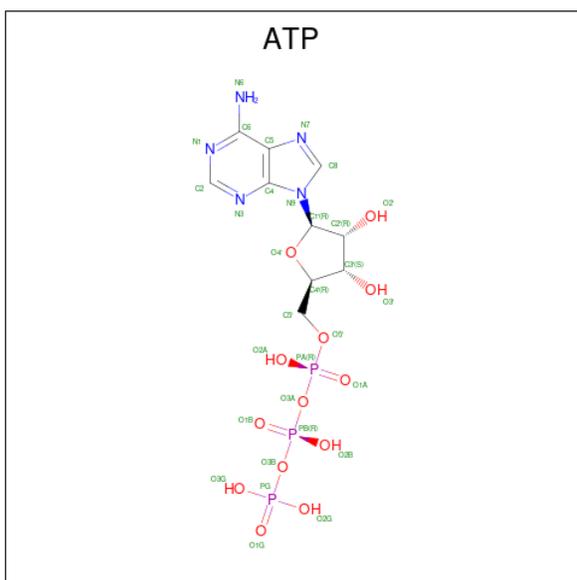
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 16 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
16	B	1	31	10	5	13	3	0	0

M1202	T1142	ASN	L1022	L982	V842	R782	L722	R662	D602	E542	F482	G422	D362	T302	P242
M1203	L1143	THR	R1023	R903	K843	T783	N723	S863	M603	L943	D883	G423	Q363	Y303	P243
D1204	K1144	PRE	S1024	T904	A844	L784	E724	G484	G604	D544	G484	L424	Q363	R304	P244
K1205	S1145	HIS	R1025	D905	B845	P785	A725	G665	M605	Q545	G485	Q425	G365	D305	P245
L1206	V1146	PRE	L1026	H906	E846	H786	R726	G666	L606	V546	A486	L426	G366	N306	V246
D1207	T1147	ALA	A1027	T907	D847	F787	D727	G667	I607	L547	M487	Q427	V367	D307	V247
L1208	L1148	GLY	T1028	L908	I848	S788	K728	D668	L608	N548	M488	Y428	K368	L308	P248
M1209	A1149	VAL	R1029	D909	M849	K789	A729	T669	D609	M949	L489	G429	S369	A309	S249
S1150	S1150	ALA	R1030	P910	V849	D790	R729	I670	G609	L550	H490	Q430	S369	G310	L250
E1151	E1151	SER	V1031	S911	H851	D791	L731	A671	Q611	Y551	V491	K431	R311	R311	S251
L1152	L1152	THR	L1032	H912	R852	F792	R732	D672	L612	M552	P492	V432	K372	P312	F252
Y1153	Y1153	K1093	Q1033	L913	D853	S793	A733	G673	I613	V553	Q493	E433	T373	Q313	M253
E1154	E1154	V1094	E1034	L914	N854	F794	E734	G674	F614	P554	A494	L434	L374	A314	E254
D1155	D1155	T1095	Y1035	S915	T855	E795	V735	T675	G515	D555	E495	H435	T375	L315	S255
P1156	P1156	S1096	R1036	G916	H856	S796	N736	M676	V616	M556	E496	L436	Y376	Q316	Q256
L1157	L1157	G1097	L1037	S917	R857	K797	V737	F677	V616	D557	T497	N437	F377	K317	R257
R1158	R1158	V1098	T1038	E918	N858	F798	K738	E678	E618	G558	R498	D438	E378	S318	E258
L1159	L1159	P1099	K1039	I919	S859	F799	D739	I679	K619	V559	A499	N439	E379	G319	E259
F1200	S1160	R1100	Q1040	L920	L860	V800	L740	T680	K620	L560	E500	D440	V380	R320	D260
K1221	T1161	L1101	A1041	G921	G861	E801	N741	E881	T621	P661	L501	P441	T381	P321	D261
V1162	V1162	K1102	F1042	D922	H862	N802	M742	F682	V622	L562	F382	V442	T381	V322	L262
L1163	L1163	E1103	D1043	L923	V863	S803	V743	I683	G623	Q603	K503	L443	Y383	K323	T263
L1224	P1164	L1104	K1044	K924	I864	R804	K744	A684	S624	A564	L504	F444	S324	S324	F264
F1225	E1165	L1105	V1045	L925	Q865	L805	Q745	E885	S625	I565	C505	N445	I385	I325	K265
V1226	D1166	M1106	L1046	Q926	F866	R806	M746	A686	N626	I566	A506	R446	D386	R326	L266
I1227	E1167	V1107	S1047	V927	I867	C807	V747	K687	G627	K667	V507	Q447	R387	A327	A267
E1168	E1168	A1108	M1048	L928	Y868	L808	M748	K688	G628	P668	P508	P448	L388	R328	D268
L1169	L1169	K1109	I1049	L929	G869	T809	A749	K689	L629	K569	L509	S449	L388	L329	T269
L1170	L1170	M1110	E1050	D930	E870	P810	G750	V690	P630	P570	Q510	L450	Q390	K330	L270
D1231	Q1171	M1111	A1051	E931	R871	Q811	S751	I671	H631	L571	I511	H451	Q390	G331	K271
L1172	L1172	K1112	Q1052	E932	G872	F812	K752	D692	V632	M672	V512	K452	V392	K332	A272
L1173	L1173	L1113	F1053	E933	M873	F813	G753	V693	V633	S573	S513	K453	R383	E333	N273
F1174	F1174	P1114	L1054	R934	D874	F814	S754	G694	T634	G574	P514	N454	N394	G334	L274
S1175	S1175	E1115	Q1055	Q935	A875	F815	I755	K695	R635	K575	Q515	N455	G395	R335	S275
L1176	L1176	L1116	S1056	L936	E876	H816	F756	E696	E636	Q576	S516	N456	R396	L336	L276
LEU	LEU	T1117	V1057	L937	H877	A817	N757	A697	K637	L577	N517	A457	N397	R337	E277
ASP	ASP	V1118	K1058	K938	I878	M818	V758	Q698	G638	L578	K518	H458	E398	G338	T278
GLU	GLU	Y1119	H1059	D939	E879	G819	A759	A699	P639	S579	P519	R459	I399	N339	L279
GLU	GLU	L1120	P1060	R940	K880	G820	Q760	T700	Q640	V580	C520	V460	P400	L340	E280
ALA	ALA	E1121	G1061	K941	R881	R821	M761	L701	V641	A581	N521	K461	G401	K341	H281
GLN	GLN	P1122	E1062	F942	S882	G822	A762	T702	C642	I582	G522	V462	A402	G342	N282
GLN	GLN	G1123	M1063	L943	L883	G823	A763	T703	A643	P583	I523	L463	K403	G283	G283
SER	SER	H1124	V1064	R944	D884	L824	C764	A704	K644	N584	V524	P464	Y404	K344	A284
PHE	PHE	A1125	G1065	E945	H885	I825	V765	A705	L645	G585	G525	Y465	V405	K345	P285
ASP	ASP	A1126	V1066	V946	I886	D826	G766	H706	F646	I586	D526	S466	L406	D346	H286
GLU	GLU	D1127	L1067	F947	G887	T827	Q767	G707	G647	H887	T527	T467	R407	F347	H287
LEU	LEU	Q1128	A1068	V948	G888	A828	Q768	R708	N648	L588	L528	F468	D408	S348	A288
ASP	ASP	E1129	M1069	D949	S889	V829	S769	T709	I649	Q589	C529	R469	S409	A349	I289
ALA	ALA	P1190	Q1070	G950	D890	K830	V770	L710	Q650	R590	G530	L470	O410	R350	E290
GLU	GLU	W1191	S1071	E951	A891	T831	E771	R711	K651	F591	I531	N471	D411	T351	E291
L1192	L1192	K1132	L1072	A952	H892	A832	G772	E712	V652	D592	R532	L472	K412	V352	A292
THR	THR	L1133	D1013	N953	F893	E833	K773	S713	V653	E593	K533	S473	L413	L353	E293
L1194	L1194	L1134	E1074	A954	E894	T834	F714	F714	N654	G594	L534	V474	D414	S354	S294
E1255	L1195	R1135	P1075	P955	K895	G835	I775	E715	G655	T595	T535	T475	L415	G355	L295
E1196	E1196	S1136	A1076	L956	R896	Y836	D716	N716	M656	T596	L536	S476	L416	G356	L296
D1257	L1197	T1077	L1017	P957	Y897	I837	F777	D717	L657	T597	R537	P477	V417	P357	Q297
L1198	L1198	L1138	Q1078	V958	R898	Q838	G778	V718	L658	L598	D538	Y478	S418	N358	F288
R1199	R1199	E1139	M1079	N959	F899	R839	F779	V719	H659	S599	T539	N479	R419	L359	H299
L1200	L1200	C1019	C1020	I960	D900	R840	V780	R720	M660	P600	F540	N479	R419	E360	V300
A1201	A1201	L1211	L1021	R961	L901	L841	D781	F721	G661	K601	L541	D481	A421	L361	A301

L541	L542	S543	S544	I545	S546	V547	G548	T549	D550	P551	M552	P553	L554	I555	T556	F557	L558	S559	E560	M561	G562	M563	E564	P565	L566	E567	D568	V569	A570	P571	H572	O573	S574	P575	D576	A577	T578	V579	V580	F581	D582	M583	G584	V585	M586	H587	G588	V589	H590	R591	M592	P593	A594	R595	L596	M597	E598	T599	L600																																																																																											
R601	T602	L603	R604	R605	K606	G607	D608	L609	N610	G611	G612	P613	L614	M615	V616	R617	L618	L619	R620	M621	G622	E623	L624	K625	L626	F627	D628	D629	A630	G631	R632	V633	Y634	R635	P636	L637	F638	L639	V640	E641	D642	D643	G644	S645	L646	G647	H648	K649	E650	L651	M652	V653	A654	R655	L656	M657	L658	A659	K660																																																																																											
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L722	F723	D724	F725	A726	K727	R728	R729	R730	R731	S732	H733	H734	A735	T736	F737	F738	T739	H740	C741	E742	S743	H744	F745	L746	S747	E748	L749	G750	V751	A752	A753	D754	I755	I756	F757	F758	F759	D760	H761	L762	T763	Q764	F765	R766	N767	L768	R769	K770	L771	S772	M773	G774	R775	K776	A777	M778	G779	V780																																																																																												
L781	L782	T783	R784	T785	R786	V787	R788	R789	D790	R791	M792	A793	R794	R795	L796	Y797	F798	P799	Q800	R801	F802	L803	G804	H805	T806	R807	A808	M809	E810	E811	L812	R813	R814	R815	E816	L817	R818	R819	G820	N821	N822	A823	L824	R825	A826	L827	A828	C829	X830	S831	G832	Y833	N834	O835	E836	R837	S838	M839	L840																																																																																											
M841	N842	Q843	S844	S845	I846	D847	R848	G849	L850	F851	R852	G853	L854	R855	F856	Y857	S858	Y859	M860	R861	ASP	GLU	E863	K864	L865	Y866	G867	A868	S869	L870	A871	T872	R873	E874	E875	K876	P877	Q878	R879	T880	L881	H882	R883	L884	M885	K886	H887	G888	T889	V890	D891	Q892	L893	L894	E895	L896	D897	L898	I899	G900																																																																																										
G901	G902	V903	R904	V905	S906	G907	E908	D909	V910	F911	R912	G913	R914	T915	F916	P917	I918	S919	PRO	A921	GLU	E923	H924	L925	G926	G927	A928	THR	ALA	T929	H930	S933	K934	R935	R936	A937	S938	T939	P940	L941	R942	S943	A1003	E1004	E945	N946	G947	I948	V949	D950	Q951	R952	L953	D954	V955	D956	R957	Q958	D959	I960	G960																																																																																									
L981	K982	F983	V984	K985	V986	R987	V988	R989	T990	T991	K992	I993	P994	Q995	L996	G997	D998	K999	F980	A981	GLU	R983	H984	L985	Q986	R987	G988	T989	L990	G991	I992	F993	Y994	R995	R996	E997	D998	R999	P1000	F1001	T982	L983	A1003	E1004	G1005	I1006	V1007	I1008	D1009	L1010	L1011	I1012	M1013	P1014	T985	H1015	D986	I1017	P1018	L989	R1020																																																																																									
M1021	T1022	V1023	A1024	H1025	L1026	L1027	E1028	C1029	L1030	L1031	K972	K1033	V1034	A1035	L1036	L1037	L1038	G1039	M1040	E1041	D1042	D1043	H1044	A1045	P1046	F1047	L1048	D1049	L1050	T1051	V1052	I1053	Y994	I1055	R1056	K1057	L1058	L1059	R1060	E1061	H1062	G1063	Q1065	S1066	I1067	G1068	F1069	E1070	V1071	M1072	Y1073	N1074	G1075	H1076	T1077	G1078	K1079	A1080																																																																																												
L1081	M1082	A1083	Q1084	I1085	F1086	L1087	G1088	P1089	T1090	L1091	L1092	Q1093	R1094	L1095	R1096	H1097	M1098	V1099	D1100	E1101	K1102	L1103	H1104	A1105	R1106	A1107	R1108	G1109	P1110	M1111	G1112	V1113	L1114	T1115	R1116	Q1117	P1118	V1119	E1120	G1121	R1122	S1123	R1124	D1125	G1126	L1127	L1128	R1129	F1130	G1131	E1132	M1133	E1134	R1135	L1136	C1137	M1138	I1139	A1140																																																																																											
H1141	G1142	A1143	A1144	S1145	F1146	L1147	K1148	E1149	R1150	L1151	M1152	E1153	A1154	S1155	L1156	F1157	A1158	R1159	V1160	H1161	I1162	C1163	L1164	I1165	C1166	L1167	L1168	M1169	L1170	V1171	I1172	A1173	K1174	L1175	N1176	H1177	N1178	Q1179	F1180	E1181	C1182	K1183	G1184	C1185	D1186	N1187	K1188	L1189	D1190	I1191	Y1192	Q1193	L1194	S1195	H1196	L1197	Y1198	A1199	A1200																																																																																											
K1201	L1202	L1203	F1204	Q1205	E1206	L1207	M1208	A1209	M1210	M1211	I1212	L1213	F1214	L1215	D1216	Y1217	L1218	D1219	A1220	S1221	R1222	S223	N224	Y225	D226	L227	A228	E229	A300	N301	H302	L303	R304	C305	V306	M307	L308	A309	E400	L401	P402	T403	L404	A405	L406	D407	S408	R409	V409	E500	V501	M502	L503	A504	L505	L506	L507	L508	L509	L510	L511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600

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



NET	SER	E3	E4	O5	P6	O7	V8	R9	I10	R11	R12	E13	S14	K15	D16	M17	R18	D19	F20	I21	L22	S23	N24	Y25	D26	L27	A28	E29	A30	N31	H32	L33	R34	C35	V36	M37	L38	A39	E40	L41	P42	T43	L44	A45	L46	D47	S48	V49	E50	V51	E52	T53	N54	S55	L56	V57	L58	A59	D60
E61	F62	I63	A64	H65	R66	L67	G68	L69	G70	R71	L72	O73	S74	M75	D76	F77	E78	O79	L80	E81	G82	L83	R84	D85	C86	F87	C88	R89	E90	G91	H92	D93	K94	C95	S96	Y97	V98	L99	T100	L101	Q102	A103	F104	G105	E106	S107	A108	S109	T110	T111	M112	V113	H114	S115	L116	T117	L118	V119	L120
V121	S122	M123	L124	M125	G126	R127	N128	L129	G130	H131	P132	L133	L134	Q135	D136	K137	E138	G139	N140	G141	L142	L143	I144	C145	K146	L147	R148	K149	G150	O151	E152	L153	K154	L155	T156	C157	V158	A159	L160	K161	G162	I163	A164	K165	E166	H167	A168	K169	H170	G171	P172	A173	A174	A175	L176	E177	F178	E179	L180
D181	P182	M183	N184	K185	L186	K187	H188	L189	D190	V191	M192	V193	E194	Q195	D196	S197	A198	K199	E200	W201	Q202	Q203	S204	X205	N206	C207	E208	E209	E210	D211	P212	F213	N214	E215	G216	D217	D220	Y221	K222	A223	Q224	A225	D226	T227	F228	Y229	W230	N231	V232	E233	S234	V235	G236	Q237	L238	P239	V240	D241	



PHE
SER

- Molecule 11: DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide

Chain J: 6% 13% 41% 33% 7%



R62
T63
P65
LEU
GLU
LYS
ARG
ASP

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

Chain K: 16% 44% 33% 5%



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

Chain L: 6% 33% 27% 34%



T61
K62
R63
L64
V65
Q66
F67
E68
A69
R70

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.85Å 222.96Å 193.60Å 90.00° 101.17° 90.00°	Depositor
Resolution (Å)	40.00 – 3.50 39.98 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.50) 93.7 (39.98-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 3.48Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.230 , 0.317 0.201 , 0.290	Depositor DCC
R_{free} test set	8862 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å ²)	80.5	Xtrriage
Anisotropy	0.219	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 80.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	29248	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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, ZN, ATP

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	3.34	30/244 (12.3%)	3.47	35/380 (9.2%)
2	T	2.72	42/633 (6.6%)	2.95	63/971 (6.5%)
3	N	1.33	4/316 (1.3%)	1.10	6/484 (1.2%)
4	A	3.73	1529/11163 (13.7%)	3.57	2038/15091 (13.5%)
5	B	3.68	1206/8963 (13.5%)	3.62	1655/12086 (13.7%)
6	C	3.67	281/2133 (13.2%)	3.42	376/2891 (13.0%)
7	E	3.85	252/1788 (14.1%)	3.52	348/2406 (14.5%)
8	F	3.81	105/691 (15.2%)	3.78	136/933 (14.6%)
9	H	4.17	178/1086 (16.4%)	3.65	243/1470 (16.5%)
10	I	3.97	150/989 (15.2%)	3.89	212/1331 (15.9%)
11	J	3.68	72/541 (13.3%)	3.56	89/727 (12.2%)
12	K	3.73	149/937 (15.9%)	3.38	150/1265 (11.9%)
13	L	4.22	68/365 (18.6%)	3.67	86/485 (17.7%)
All	All	3.71	4066/29849 (13.6%)	3.55	5437/40520 (13.4%)

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
1	R	0	1
2	T	1	2
4	A	2	121
5	B	4	114
6	C	1	11
7	E	0	17
8	F	0	5
9	H	0	16
10	I	1	18
11	J	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
12	K	0	9
13	L	0	5
All	All	9	321

The worst 5 of 4066 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1110	ASN	CB-CG	39.65	2.42	1.51
4	A	820	GLY	C-O	-37.66	0.63	1.23
7	E	117	THR	CA-CB	34.64	2.43	1.53
4	A	437	MET	SD-CE	30.90	3.50	1.77
4	A	322	VAL	CA-CB	-27.33	0.97	1.54

The worst 5 of 5437 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	941	LEU	CB-CG-CD2	37.01	173.92	111.00
4	A	337	ARG	NE-CZ-NH2	-34.93	102.83	120.30
4	A	980	ASP	CB-CG-OD2	33.77	148.69	118.30
5	B	466	TRP	CA-C-N	-31.53	53.14	116.20
4	A	337	ARG	NE-CZ-NH1	31.48	136.04	120.30

5 of 9 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	T	21	DC	C3'
4	A	317	LYS	CA
4	A	324	SER	CA
5	B	636	PRO	CA
5	B	637	LEU	CA

5 of 321 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	3	GLY	Mainchain
4	A	6	TYR	Peptide
1	R	10	A	Sidechain
2	T	21	DC	Sidechain
2	T	23	DC	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	217	0	110	34	0
2	T	566	0	314	82	4
3	N	284	0	162	44	0
4	A	10969	0	11061	3443	0
5	B	8792	0	8821	2369	0
6	C	2095	0	2051	490	0
7	E	1752	0	1776	523	0
8	F	679	0	701	194	0
9	H	1068	0	1040	377	0
10	I	971	0	929	310	0
11	J	532	0	543	160	0
12	K	919	0	929	259	0
13	L	363	0	387	98	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	2	0	0	0	0
16	B	31	0	12	7	0
All	All	29248	0	28836	7970	4

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 137.

The worst 5 of 7970 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)
3:N:12:DT:P	7:E:117:THR:HG21	1.32	1.67
4:A:128:ILE:CB	4:A:128:ILE:CA	1.74	1.66
5:B:422:LYS:CB	5:B:422:LYS:CG	1.74	1.65
5:B:866:TYR:CG	5:B:866:TYR:CB	1.80	1.65
4:A:37:PHE:CB	4:A:37:PHE:CG	1.74	1.65

All (4) 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)
2:T:1:DC:C4'	2:T:1:DC:C4'[2_656]	1.63	0.57
2:T:1:DC:C5'	2:T:1:DC:O4'[2_656]	1.69	0.51
2:T:1:DC:O4'	2:T:1:DC:O4'[2_656]	1.78	0.42
2:T:1:DC:C4'	2:T:1:DC:O4'[2_656]	1.80	0.40

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	1383/1733 (80%)	816 (59%)	306 (22%)	261 (19%)	0	2
5	B	1088/1224 (89%)	708 (65%)	199 (18%)	181 (17%)	0	2
6	C	264/318 (83%)	170 (64%)	58 (22%)	36 (14%)	0	4
7	E	212/215 (99%)	119 (56%)	47 (22%)	46 (22%)	0	1
8	F	82/155 (53%)	45 (55%)	22 (27%)	15 (18%)	0	2
9	H	129/146 (88%)	75 (58%)	28 (22%)	26 (20%)	0	1
10	I	117/122 (96%)	60 (51%)	32 (27%)	25 (21%)	0	1
11	J	63/70 (90%)	41 (65%)	10 (16%)	12 (19%)	0	2
12	K	112/120 (93%)	78 (70%)	18 (16%)	16 (14%)	0	3
13	L	44/70 (63%)	21 (48%)	11 (25%)	12 (27%)	0	0
All	All	3494/4173 (84%)	2133 (61%)	731 (21%)	630 (18%)	0	2

5 of 630 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	34	LYS
4	A	44	THR
4	A	48	ALA
4	A	51	GLY

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Mol	Chain	Res	Type
4	A	55	ASP

5.3.2 Protein sidechains [i](#)

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	1218/1520 (80%)	759 (62%)	459 (38%)	0	1
5	B	960/1061 (90%)	614 (64%)	346 (36%)	0	1
6	C	234/274 (85%)	151 (64%)	83 (36%)	0	1
7	E	196/197 (100%)	116 (59%)	80 (41%)	0	1
8	F	74/137 (54%)	47 (64%)	27 (36%)	0	1
9	H	117/128 (91%)	71 (61%)	46 (39%)	0	1
10	I	113/116 (97%)	70 (62%)	43 (38%)	0	1
11	J	60/65 (92%)	38 (63%)	22 (37%)	0	1
12	K	99/102 (97%)	63 (64%)	36 (36%)	0	1
13	L	40/57 (70%)	24 (60%)	16 (40%)	0	1
All	All	3111/3657 (85%)	1953 (63%)	1158 (37%)	0	1

5 of 1158 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	E	105	PHE
13	L	38	LEU
7	E	182	ASP
7	E	103	LYS
9	H	145	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
5	B	686	ASN
5	B	1193	GLN

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Mol	Chain	Res	Type
5	B	744	HIS
5	B	975	GLN
6	C	123	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	10/10 (100%)	4 (40%)	3 (30%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	2	U
1	R	5	A
1	R	6	G
1	R	10	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	R	1	A
1	R	4	G
1	R	5	A

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 monosaccharides 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
16	ATP	B	1308	-	26,33,33	2.38	7 (26%)	31,52,52	3.10	10 (32%)

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	ATP	B	1308	-	-	7/18/38/38	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	1308	ATP	O5'-C5'	-5.93	1.22	1.44
16	B	1308	ATP	C2'-C1'	5.11	1.61	1.53
16	B	1308	ATP	PA-O5'	-4.73	1.40	1.59
16	B	1308	ATP	O4'-C1'	4.63	1.47	1.41
16	B	1308	ATP	C2-N3	4.15	1.38	1.32

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	1308	ATP	O5'-C5'-C4'	10.76	146.02	108.99
16	B	1308	ATP	PA-O5'-C5'	5.59	154.49	121.68
16	B	1308	ATP	N3-C2-N1	-5.51	120.07	128.68
16	B	1308	ATP	C5'-C4'-C3'	-5.29	95.35	115.18
16	B	1308	ATP	O4'-C4'-C3'	4.06	113.16	105.11

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	B	1308	ATP	C5'-O5'-PA-O1A
16	B	1308	ATP	C5'-O5'-PA-O3A
16	B	1308	ATP	C4'-C5'-O5'-PA
16	B	1308	ATP	PB-O3A-PA-O5'

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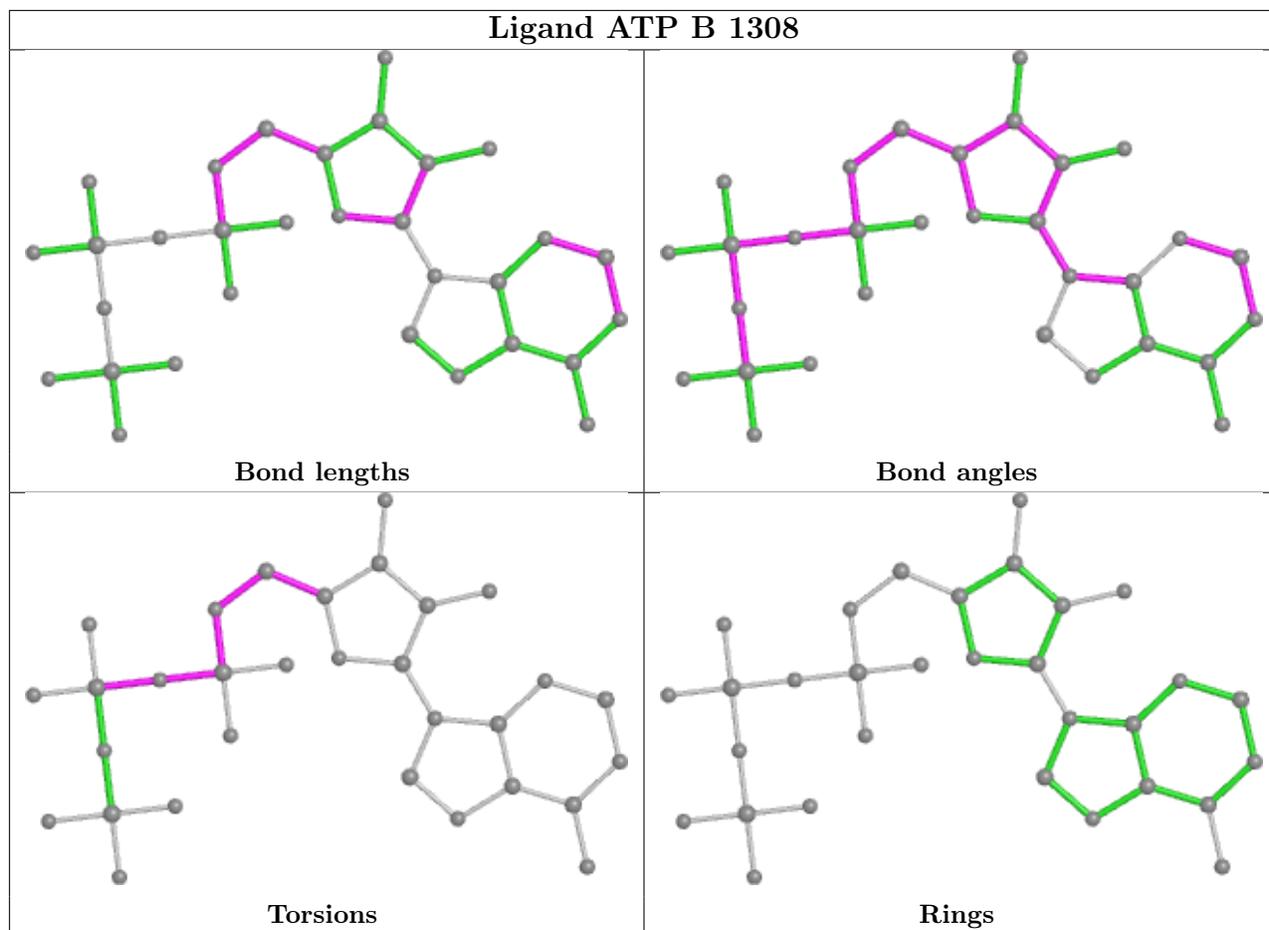
Mol	Chain	Res	Type	Atoms
16	B	1308	ATP	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	1308	ATP	7	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	T	2
4	A	2
3	N	1
1	R	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	T	15:DA	O3'	16:DC	P	2.98
1	N	2:DT	O3'	3:DG	P	2.67

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	320:ARG	C	321:PRO	N	1.75
1	A	820:GLY	C	821:ARG	N	1.68
1	T	21:DC	O3'	22:DT	P	1.39

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	10/10 (100%)	0.36	0 100 100	70, 83, 159, 164	0
2	T	28/28 (100%)	0.90	5 (17%) 1 1	84, 188, 200, 200	0
3	N	14/14 (100%)	1.68	5 (35%) 0 0	185, 198, 200, 200	0
4	A	1395/1733 (80%)	-0.71	11 (0%) 86 81	1, 51, 137, 186	0
5	B	1106/1224 (90%)	-0.73	7 (0%) 89 86	1, 43, 119, 194	0
6	C	266/318 (83%)	-0.83	0 100 100	6, 44, 95, 151	0
7	E	214/215 (99%)	-0.54	0 100 100	13, 79, 141, 165	0
8	F	84/155 (54%)	-0.62	0 100 100	17, 58, 105, 114	0
9	H	133/146 (91%)	-0.60	0 100 100	19, 74, 132, 154	0
10	I	119/122 (97%)	-0.73	0 100 100	4, 56, 105, 146	0
11	J	65/70 (92%)	-0.81	0 100 100	11, 40, 92, 116	0
12	K	114/120 (95%)	-0.74	0 100 100	8, 43, 88, 131	0
13	L	46/70 (65%)	-0.44	1 (2%) 62 56	17, 84, 143, 163	0
All	All	3594/4225 (85%)	-0.69	29 (0%) 86 81	1, 50, 133, 200	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	316	GLN	5.4
4	A	255	SER	4.0
4	A	44	THR	3.7
3	N	14	DG	3.6
5	B	866	TYR	3.6

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](#)

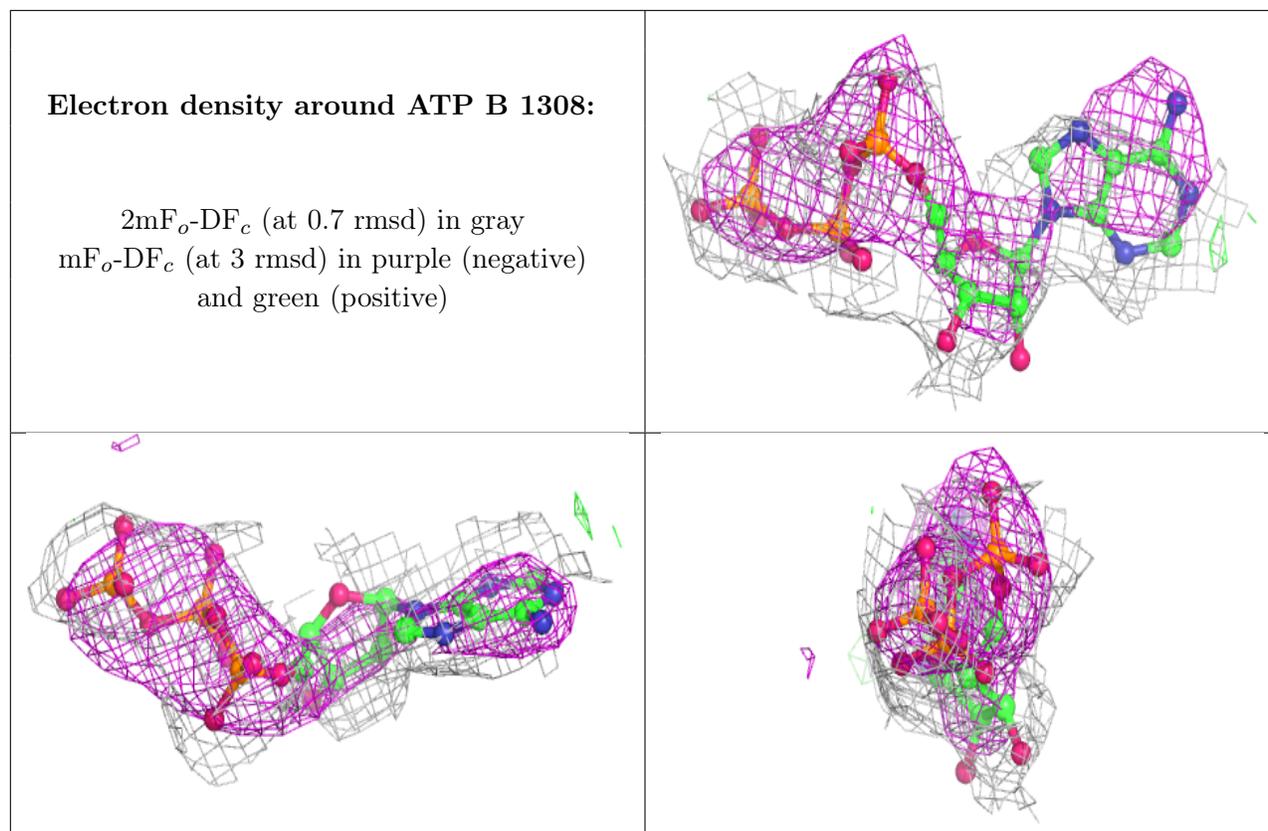
There are no monosaccharides in this entry.

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
15	MG	A	2002	1/1	0.71	0.49	63,63,63,63	0
16	ATP	B	1308	31/31	0.75	0.35	64,71,77,78	0
14	ZN	A	1734	1/1	0.79	0.05	115,115,115,115	0
15	MG	A	2001	1/1	0.95	0.56	55,55,55,55	0
14	ZN	J	101	1/1	0.97	0.10	39,39,39,39	0
14	ZN	I	203	1/1	0.98	0.05	98,98,98,98	0
14	ZN	A	1735	1/1	0.98	0.04	75,75,75,75	0
14	ZN	L	105	1/1	0.98	0.03	76,76,76,76	0
14	ZN	I	204	1/1	0.99	0.05	31,31,31,31	0
14	ZN	C	319	1/1	0.99	0.02	31,31,31,31	0
14	ZN	B	1307	1/1	0.99	0.05	80,80,80,80	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.