



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 04:22 AM UTC

PDB ID : 1TWH / pdb_00001twh
Title : RNA polymerase II complexed with 2'dATP
Authors : Westover, K.D.; Bushnell, D.A.; Kornberg, R.D.
Deposited on : 2004-06-30
Resolution : 3.40 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:

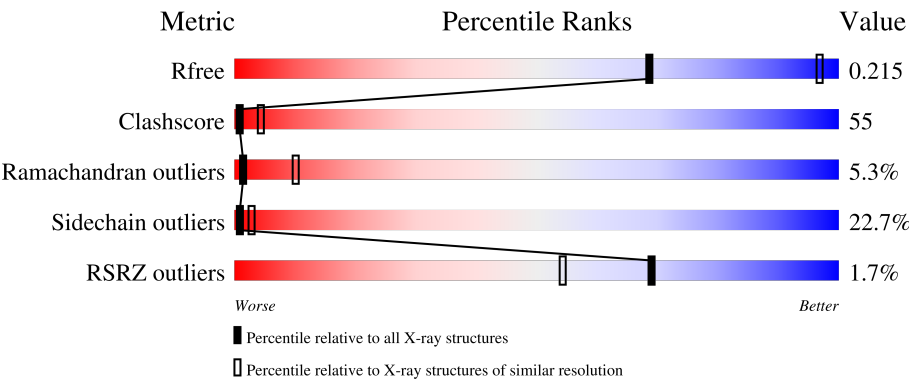
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	1733	% 32% 31% 13% 22%
2	B	1224	2% 35% 37% 15% 11%
3	C	318	31% 37% 15% 16%
4	E	215	32% 43% 24%
5	F	155	22% 24% 7% 46%

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Mol	Chain	Length	Quality of chain
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	

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
12	ZN	C	3002	-	-	X	-
12	ZN	J	3001	-	-	X	-
13	ATP	A	3011	X	-	-	-

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 27728 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 II largest subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1349	Total	C	N	O	S	0	0	0
			10606	6692	1839	2017	58			

- Molecule 2 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1091	Total	C	N	O	S	0	0	0
			8690	5511	1516	1610	53			

- Molecule 3 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

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

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	215	Total	C	N	O	S	0	0	0
			1760	1116	310	322	12			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	83	Total	C	N	O	S	0	0	0
			670	428	114	125	3			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 7 is a protein called DNA-directed RNA polymerase II 14.2 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	121	Total	C	N	O	S	0	0	0
			990	610	181	188	11			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	64	Total	C	N	O	S	0	0	0
			525	334	92	93	6			

- Molecule 9 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

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

- Molecule 11 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	2	Total	Mn	0	0
			2	2		

- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn).

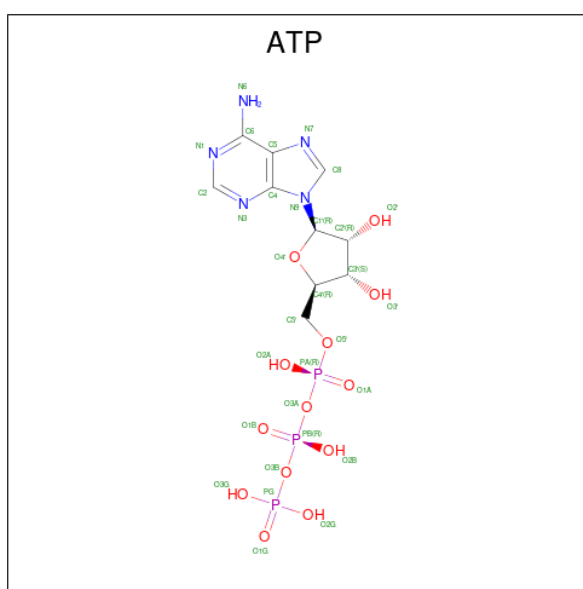
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	2	Total	Zn	0	0
			2	2		
12	B	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	1	Total	Zn	0	0
			1	1		
12	I	2	Total	Zn	0	0
			2	2		
12	J	1	Total	Zn	0	0
			1	1		
12	L	1	Total	Zn	0	0
			1	1		

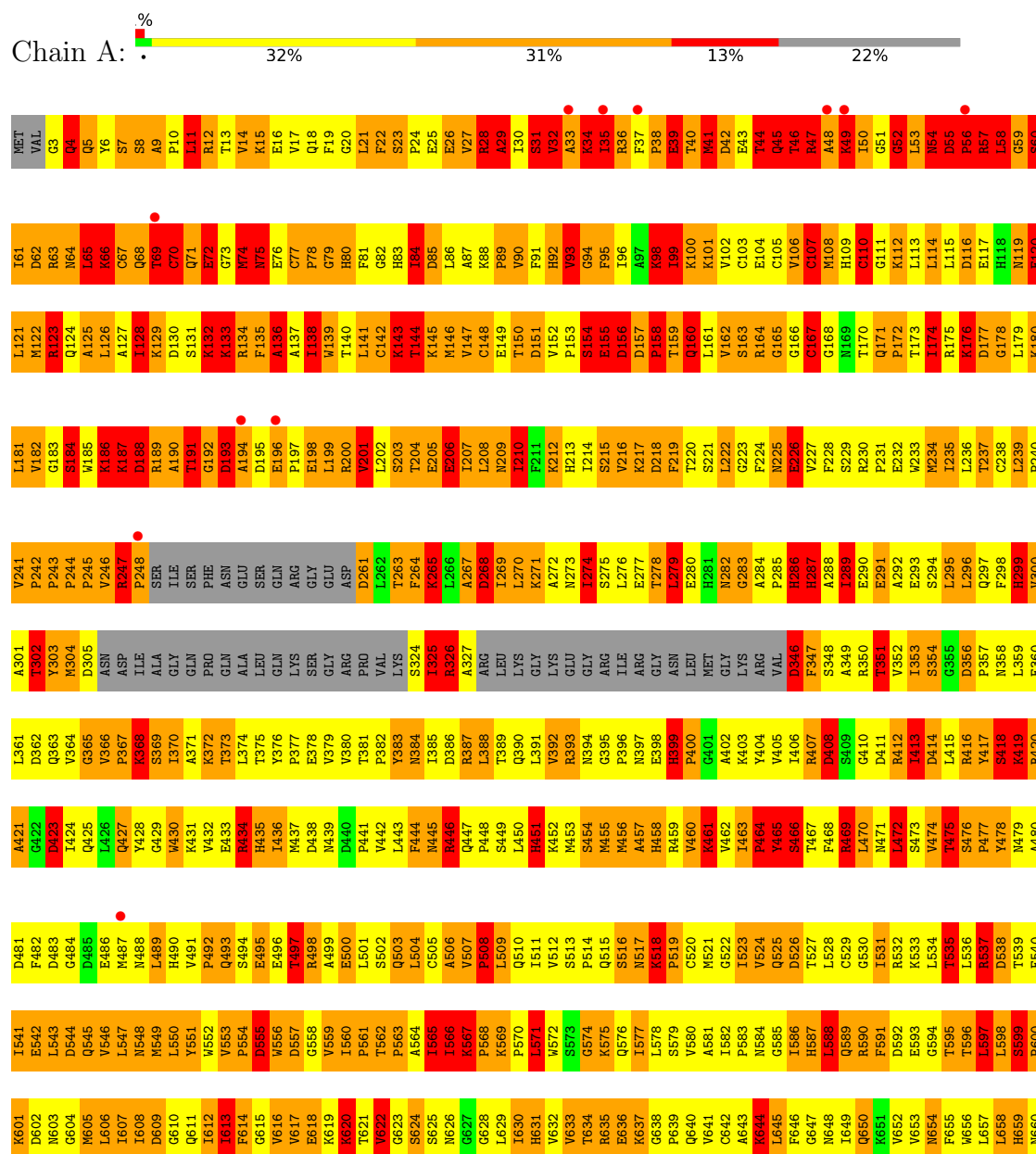
- Molecule 13 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



3 Residue-property plots

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

- Molecule 1: DNA-directed RNA polymerase II largest subunit



PRO	ASN	F1441	L1381	G1321	K1261	A1201	T1141	L1021	R961	L901	L841	D781	F721	G661
SER	ASP	D1442	T1382	I1322	K1262	M1202	T1142	L1022	R962	L902	V842	R782	L722	F662
TYR	ALA	V1443	D1323	D1323	E1263	N1203	L1143	R1023	I963	R903	R843	T783	L723	S663
SER	MET	M1444	P1324	P1324	E1264	D1204	K1144	S1024	I964	T904	A844	T784	E724	T664
PRO	ALA	I1445	T1385	T1325	M1265	K1205	S1145	R1025	Q965	D905	R845	F785	A725	G665
THR	GLY	D1446	R1326	R1326	T1266	D1206	V1146	L1026	N966	H906	E846	H786	R726	R666
SER	GLY	E1447	I1327	I1327	M1267	L1207	T1147	A1027	A967	T907	D847	F787	D727	G667
PRO	PHE	E1448	V1328	L1268	L1268	T1208	I1148	T1028	Q968	L908	R848	S788	K728	D668
SER	THR	L1449	T1329	M1209	L1269	M1209	A1149	T1029	Q969	D909	R849	K789	A729	T669
TYR	ALA	L1450	N1330	N1270	N1270	G1210	S1150	R1030	T970	P910	V850	D790	G730	P670
SER	TYR	VAL	S1331	Q1211	E1151	Q1211	E1151	V1031	F971	S911	H851	D791	R731	A671
PRO	GLY	LYS	V1332	V1212	T1271	V1212	I1152	L1032	H972	L912	X852	V792	L732	D672
THR	ASN	I1333	I1273	G1213	L1273	G1213	V1153	Q1033	I973	R913	D853	S793	A733	G673
SER	ALA	D1334	R1274	E1214	A1274	E1214	V1154	E1034	D974	E914	N854	P794	E734	P674
PRO	ASP	I1335	G1275	R1215	D1275	R1215	D1155	Y1035	H975	S915	T855	E795	V735	T675
SER	TYR	E1337	E1277	K1217	V1277	K1217	P1156	R1036	T976	G916	T856	S796	W736	M676
TYR	GLN	L1337	L1278	P1158	G1278	P1158	D1158	L1037	K977	S917	R857	K797	L737	R677
SER	GLY	LYS	N1278	K1218	N1278	K1218	P1159	T1038	P978	E918	N858	G798	K738	E678
PRO	ALA	I1339	T1279	T1219	T1279	T1219	R1159	K1039	S979	T919	S859	F799	D739	T679
THR	THR	G1340	E1280	F1220	E1280	F1220	S1160	Q1040	D980	L920	R860	V800	L740	T680
SER	GLU	I1341	R1281	K1221	R1281	K1221	T1161	A1041	L981	G921	E861	E801	R741	E681
PRO	ILE	E1342	V1282	D1222	V1282	D1222	V1162	F1042	T982	D922	N862	N802	N742	T682
SER	PHE	A1343	V1283	D1223	V1283	D1223	I1163	D1043	I983	L923	V863	S803	V743	T683
TYR	GLY	G1344	M1284	L1224	M1284	L1224	P1164	V1044	K984	X924	T864	H804	K744	A684
SER	ALA	R1345	E1285	F1225	E1285	F1225	E1165	V1045	D985	L925	D865	L805	G745	E685
PRO	TYR	A1346	K1286	V1226	K1286	V1226	D1166	L1046	I986	Q926	F866	R806	M746	A686
THR	GLY	A1347	Y1287	I1227	Y1287	I1227	E1167	S1047	V987	V927	T867	G807	V747	K687
SER	GLU	L1348	L1288	W1228	L1288	W1228	E1168	N1048	L988	L928	R868	L808	M748	K688
PRO	ALA	V1349	R1289	S1229	R1289	S1229	I1169	I1049	G989	L929	C869	T809	A749	K689
SER	PRO	K1350	K1290	E1230	K1290	E1230	T1170	E1050	V990	D930	E870	P810	G750	V690
TYR	THR	E1351	V1291	D1231	V1291	D1231	O1171	A1051	K991	E931	D871	O811	K751	L691
SER	PRO	A1412	P1292	M1232	P1292	M1232	L1172	Q1052	D992	E932	C872	S812	K752	D692
PRO	PRO	G1413	S1293	D1233	S1293	D1233	H1173	F1053	L993	T933	R873	F813	G753	V693
THR	SER	M1354	E1234	E1234	E1234	E1234	PHE	L1054	Q994	R934	D874	F814	S754	T694
SER	PHE	S1415	T1295	K1235	T1295	K1235	SER	R1055	E995	Q935	A875	F815	V755	K695
PRO	GLY	A1416	G1296	L1236	G1296	L1236	L1176	S1056	N996	L936	A876	H816	I756	E696
SER	VAL	E1417	E1297	I1237	E1297	I1237	LEU	T1117	L997	V937	H877	A817	N757	A697
TYR	SER	S1358	Y1298	I1238	Y1298	I1238	ASP	V1057	L998	K938	T878	M818	I758	Q698
SER	LEU	D1359	V1299	R1239	V1299	R1239	GLU	H1059	V999	D939	E879	G819	A759	A699
PRO	PRO	G1360	K1300	C1240	K1300	C1240	GLU	P1060	L1000	R940	R880	G820	Q760	M700
THR	GLY	S1361	E1301	R1241	E1301	R1241	ALA	G1061	R1001	R821	Q881	R821	M761	L701
SER	PHE	A1362	P1302	V1242	P1302	V1242	GLU	E1062	G1002	F942	S882	E822	S762	L702
PRO	SER	V1363	E1303	V1243	E1303	V1243	GLN	M1063	K1003	L943	L883	G823	A763	T703
SER	PRO	M1364	V1304	ARG	V1304	ARG	SER	V1064	M1004	R944	D884	L824	C764	A704
TYR	THR	Y1365	V1305	PRO	V1305	PRO	PHE	G1065	E1005	E945	T885	I825	V765	K705
SER	VAL	R1366	L1306	LYS	L1306	LYS	ASP	V1066	I1006	V946	I886	D826	G766	H706
PRO	PRO	H1367	E1307	SER	E1307	SER	Q1187	L1067	I1007	F947	C887	T827	Q767	G707
THR	ASP	M1368	T1308	LEU	T1308	LEU	Q1188	A1068	Q1008	V948	G888	A828	Q768	X708
SER	TYR	A1369	D1309	ASP	D1309	ASP	S1189	E1129	N1009	D949	S889	V829	S769	T709
PRO	LEU	L1370	G1310	ALA	G1310	ALA	P1190	Q1070	A1010	G950	D890	K830	V770	L710
SER	PRO	L1371	V1311	GLU	V1311	GLU	V1191	S1071	Q1011	E951	A891	T831	E771	R711
TYR	THR	V1372	N1312	THR	N1312	THR	L1192	I1072	R1012	A952	A892	A832	G772	E712
SER	SER	D1373	L1313	GLU	L1313	GLU	L1193	G1073	D1013	N953	F893	E833	K773	S713
PRO	PRO	V1374	S1314	A1254	S1314	A1254	R1194	E1074	A1014	N954	E894	T834	R774	F714
THR	ALA	M1375	E1315	L1195	E1315	L1195	L1195	P1075	V1015	P955	K895	G835	I775	E715
SER	TYR	T1376	V1316	E1256	V1316	E1256	E1196	A1076	T1016	L956	R896	V836	A776	D716
PRO	SER	T1377	M1317	D1257	M1317	D1257	L1197	T1077	L1017	P957	V897	I837	F777	N717
SER	THR	Q1378	T1318	H1258	T1318	H1258	D1198	Q1078	F1018	V958	R898	Q838	G778	V718
TYR	GLY	G1379	V1319	M1259	V1319	M1259	R1199	M1079	C1019	N959	R899	R839	F779	W719
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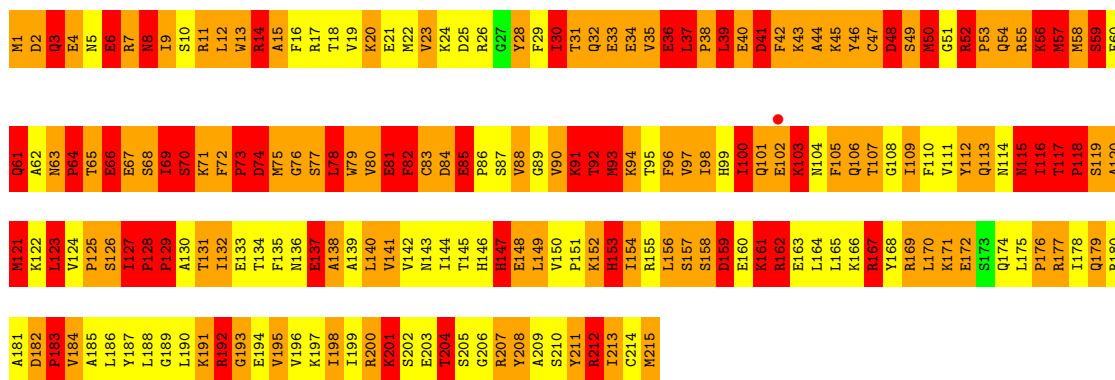
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- Molecule 2: DNA-directed RNA polymerase II 140 kDa polypeptide

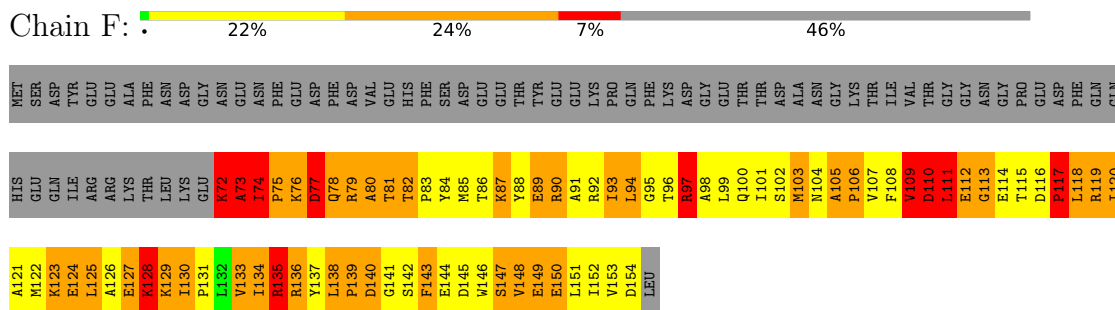


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W722	M652	T602	M542	V482	K422	P362	C302	S242	S182	L122	I62
V723	A663	L603	S443	L483	K423	H363	Y303	A243	E183	T123	I63
D724	T664	R604	C544	N484	L424	L364	D304	A184	L184	Y124	C64
F725	E665	R605	I545	N485	T425	T365	V305	E245	T185	S125	E65
A726	Y666	K606	S546	Y486	K426	O366	N306	K246	S126	D66	ASN
K727	Q667	G607	V547	T487	D427	L387	D307	G247	S187	G127	S67
R728	D668	D608	G488	L488	T428	E368	W308	S248	D188	L128	T68
L729	ILE	I609	T459	S489	F429	O369	Q309	R249	L189	F129	L69
R730	GLU	N610	D550	S490	R430	F370	M310	Y190	V130	I70	LYR
V731	GLY	P611	P551	T491	Y431	E371	L311	I251	K191	D131	LEU
S732	GLY	P612	M552	L492	K432	S372	E312	S252	L192	Y132	LYR
R733	PHE	V613	P553	S493	Q433	R373	M313	T253	K193	X133	GLU
A735	GLU	S614	L554	H494	R434	K374	L314	Q255	E194	K134	ASP
T736	ASP	M615	I555	L495	T435	A375	K315	Q256	C195	R135	PRO
L737	VAL	I616	T556	R496	V436	F376	P316	V256	T136	GLM	TYR
T738	GLU	R617	F557	R497	E437	F377	C317	K257	F197	Y137	GLY
F738	E678	D618	L558	T498	GLU	L378	V318	L258	D198	E138	F18
L739	Y679	I619	S559	N499	ALA	G379	E319	Y259	M199	ALA	E19
H740	T690	R620	E560	H500	HIS	Y380	D320	G260	G200	I1E	D20
C741	M681	E621	M561	P501	ASP	M381	G321	R261	G201	ASP	E21
E742	S682	K622	G562	I502	PHE	L382	F322	E262	Y202	VAL	S22
L743	S683	E623	M563	GLY	ASN	N383	V323	G263	F203	PRO	ASN
I744	L684	L624	E564	ARG	WET	R384	L324	S264	I204	GLY	P24
F745	L685	K625	P565	ASP	LYS	L385	Q325	S265	I205	ARG	I25
T746	M686	I626	L566	GLY	L446	L386	D326	A266	M206	GLU	T26
M747	G687	F627	E567	LYS	A447	L387	R327	R267	G207	LEU	A27
L748	G688	T628	D568	LEU	N448	C388	E328	T268	S208	LYS	E28
L749	L689	D629	Y569	A509	R449	A389	T329	I269	E209	TYR	D29
G750	V690	A630	V570	K510	A450	L390	A330	K270	K210	GLU	S30
V751	E691	B631	P571	R511	K451	D391	L331	A271	V211	LEU	I90
A752	E692	R632	H572	R512	T452	R392	D332	T272	L212	I1E	W31
S753	L693	G633	Q573	Q513	L453	K393	F333	L273	T213	ALA	A32
A754	D694	Y634	S574	L514	T454	D394	I334	P274	A214	GLU	X34
L755	E695	R635	P575	H515	S455	O395	G335	Y275	Q215	GLU	S35
L756	E696	P636	D576	N516	G456	D396	R336	I276	E216	Y96	A36
F757	G697	L637	A577	T517	L457	D397	R337	K277	R217	GLU	F37
F758	E698	F638	T578	H518	K458	R398	T339	Q278	S218	ASP	F38
E699	E699	I639	R579	W519	Y459	D399	T339	D279	A219	ASP	R39
D700	S700	V640	V580	G520	H400	H400	A340	I280	G220	SER	E40
H761	I701	E641	F581	L521	L461	F401	L341	P281	N221	GLU	K41
N762	L702	D642	V582	V522	A462	G402	G342	I282	I222	SER	Q42
I703	G763	D643	N583	C523	T463	K403	I343	V283	V223	GLY	L43
A764	A704	E644	G584	P524	G464	K404	K344	I284	E104	X164	V44
R765	M705	S645	W585	A525	V465	R405	K345	I285	V225	S105	S45
G766	Q706	L646	V586	E526	V466	L406	E346	F286	F226	D106	Q46
N767	T707	G647	H587	T527	G467	D407	K347	R287	K227	I167	Q47
T768	E708	R648	G588	P528	GLU	A408	R348	A288	K228	V108	L48
L709	K649	E589	V589	E529	GLU	L409	I349	L289	R169	T109	D49
W710	L710	E590	H590	G530	LYS	G410	Q350	G290	A230	L170	H10
S771	E711	L651	R591	Q531	LYS	Y351	I291	P231	P171	A111	F51
A772	P712	K652	N592	A532	MET	L412	K352	I292	S232	I172	N12
M773	ALA	E653	P593	C533	WET	L413	K353	P293	M173	Y113	O53
G774	GLU	R654	A594	Q534	SER	A414	D354	D294	I234	L174	F54
R775	ALA	K655	R595	L535	SER	Q415	I355	G295	S235	Q115	V55
Q776	ASN	G656	L596	V536	ARG	L416	L356	E296	H236	S176	D56
A777	GLU	H657	M597	F417	A477	F417	Q357	I297	V237	K177	V57
M778	GLU	E658	E598	N538	Q478	K418	K358	L298	M178	R118	T58
G779	ASN	A659	T599	L539	V479	T419	E359	E299	E239	G179	L59
L780	ASN	K660	L600	E540	S480	L420	P360	H260	X120	X120	O60

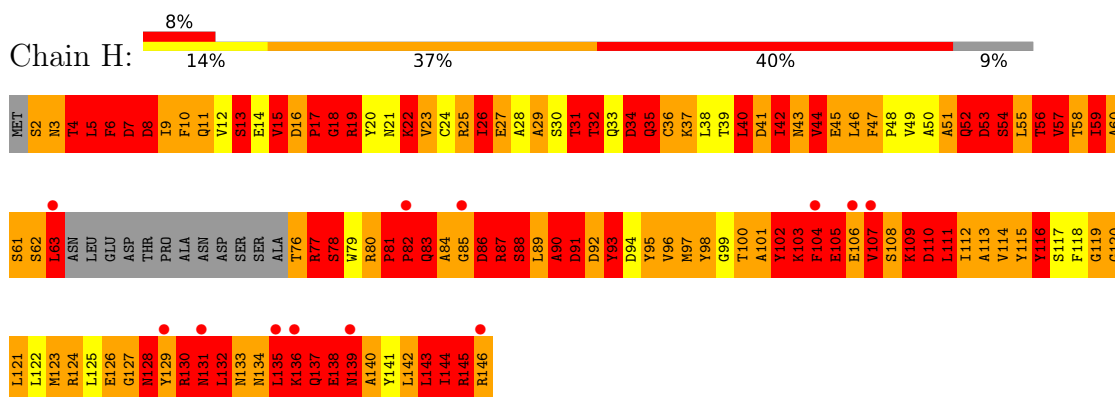




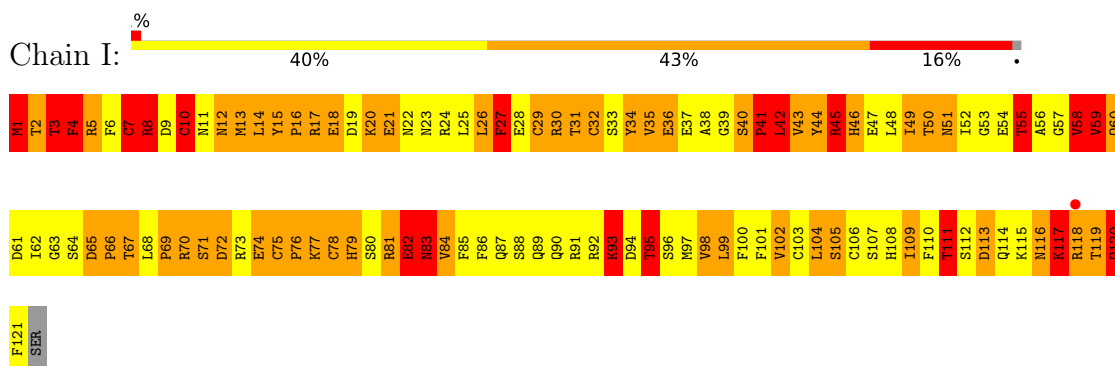
- Molecule 5: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide



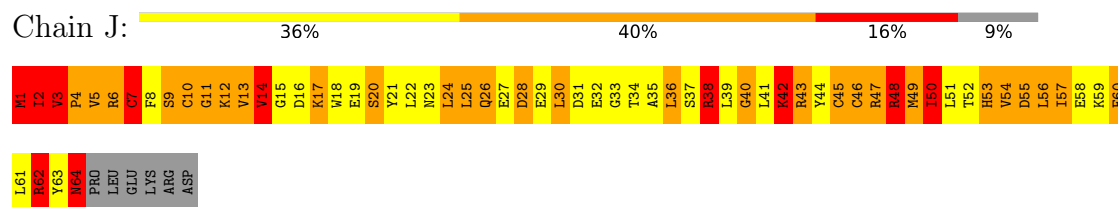
- Molecule 6: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



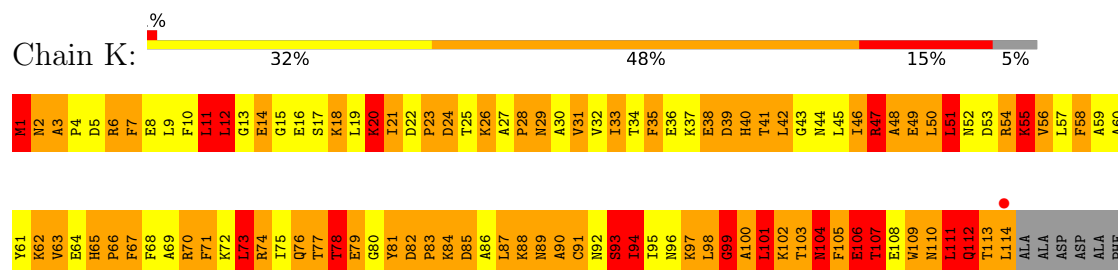
- Molecule 7: DNA-directed RNA polymerase II 14.2 kDa polypeptide



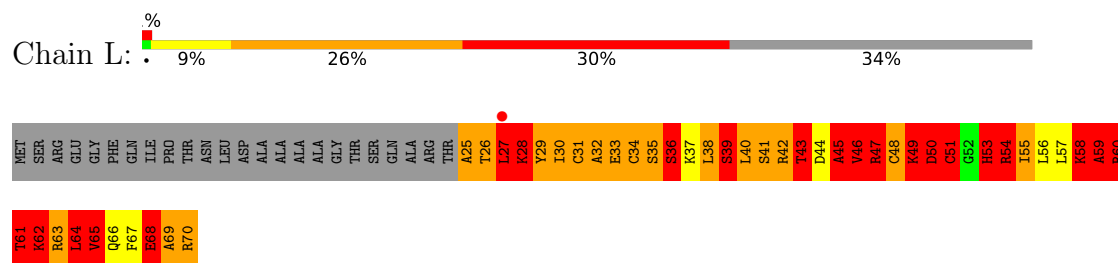
- Molecule 8: DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide



• Molecule 9: DNA-directed RNA polymerase II 13.6 kDa polypeptide



• Molecule 10: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	123.00Å 223.00Å 374.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.40 40.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.40) 97.2 (40.00-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 3.32Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.262 0.207 , 0.215	Depositor DCC
R_{free} test set	2319 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	57.9	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 61.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	27728	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% 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, MN, 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	A	5.43	3403/10792 (31.5%)	3.43	1848/14601 (12.7%)
2	B	5.33	2843/8860 (32.1%)	3.33	1486/11945 (12.4%)
3	C	5.40	695/2133 (32.6%)	3.41	398/2891 (13.8%)
4	E	5.37	555/1796 (30.9%)	3.35	301/2416 (12.5%)
5	F	4.96	183/682 (26.8%)	3.37	110/922 (11.9%)
6	H	5.31	306/1086 (28.2%)	3.19	178/1470 (12.1%)
7	I	5.54	343/1009 (34.0%)	3.55	203/1357 (15.0%)
8	J	5.10	165/533 (31.0%)	3.58	95/715 (13.3%)
9	K	5.19	305/937 (32.6%)	3.31	161/1265 (12.7%)
10	L	6.23	141/366 (38.5%)	3.65	81/485 (16.7%)
All	All	5.38	8939/28194 (31.7%)	3.39	4861/38067 (12.8%)

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	A	0	57
2	B	0	55
3	C	0	15
4	E	1	9
5	F	0	1
6	H	0	12
7	I	0	6
9	K	0	2
10	L	0	2
All	All	1	159

The worst 5 of 8939 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1064	VAL	CA-C	64.08	2.34	1.52
1	A	1064	VAL	C-O	53.64	1.88	1.24
4	E	57	MET	SD-CE	47.96	2.99	1.79
4	E	50	MET	SD-CE	39.00	2.77	1.79
2	B	552	MET	SD-CE	35.62	2.68	1.79

The worst 5 of 4861 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1064	VAL	CA-C-O	-60.75	44.85	120.78
1	A	1064	VAL	O-C-N	-42.11	69.93	122.57
1	A	1064	VAL	CB-CA-C	22.66	148.46	111.29
1	A	1064	VAL	N-CA-CB	-21.45	75.83	111.23
7	I	43	VAL	N-CA-CB	-18.76	83.56	112.07

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	E	204	THR	CB

5 of 159 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	31	SER	Peptide
1	A	44	THR	Peptide
1	A	52	GLY	Peptide
1	A	60	SER	Peptide
1	A	74	MET	Peptide

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	10606	0	10668	1112	0
2	B	8690	0	8714	954	0
3	C	2095	0	2054	240	0
4	E	1760	0	1788	230	0
5	F	670	0	690	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	1068	0	1040	233	0
7	I	990	0	948	102	0
8	J	525	0	538	63	0
9	K	919	0	929	114	0
10	L	364	0	387	92	0
11	A	2	0	0	0	0
12	A	2	0	0	1	0
12	B	1	0	0	0	0
12	C	1	0	0	3	0
12	I	2	0	0	0	0
12	J	1	0	0	2	0
12	L	1	0	0	1	0
13	A	30	0	9	0	0
14	B	1	0	0	0	0
All	All	27728	0	27765	3057	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 55.

The worst 5 of 3057 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:B:137:TYR:CB	2:B:137:TYR:CG	1.77	1.66
9:K:26:LYS:CD	9:K:26:LYS:CE	1.74	1.66
1:A:1225:PHE:CB	1:A:1225:PHE:CG	1.78	1.65
1:A:977:LYS:CG	1:A:977:LYS:CD	1.74	1.64
2:B:884:ARG:CD	2:B:884:ARG:CG	1.75	1.64

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	
1	A	1332/1733 (77%)	1173 (88%)	93 (7%)	66 (5%)	1	10
2	B	1071/1224 (88%)	914 (85%)	110 (10%)	47 (4%)	2	13
3	C	264/318 (83%)	230 (87%)	22 (8%)	12 (4%)	2	12
4	E	213/215 (99%)	182 (85%)	20 (9%)	11 (5%)	1	10
5	F	81/155 (52%)	72 (89%)	7 (9%)	2 (2%)	4	21
6	H	129/146 (88%)	82 (64%)	21 (16%)	26 (20%)	0	0
7	I	119/122 (98%)	107 (90%)	11 (9%)	1 (1%)	16	44
8	J	62/70 (89%)	58 (94%)	3 (5%)	1 (2%)	7	29
9	K	112/120 (93%)	99 (88%)	9 (8%)	4 (4%)	2	16
10	L	44/70 (63%)	24 (54%)	9 (20%)	11 (25%)	0	0
All	All	3427/4173 (82%)	2941 (86%)	305 (9%)	181 (5%)	1	10

5 of 181 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	38	PRO
1	A	45	GLN
1	A	47	ARG
1	A	59	GLY

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	1181/1520 (78%)	936 (79%)	245 (21%)	1	4
2	B	947/1061 (89%)	756 (80%)	191 (20%)	1	4
3	C	234/274 (85%)	186 (80%)	48 (20%)	1	4
4	E	197/197 (100%)	138 (70%)	59 (30%)	0	1
5	F	73/137 (53%)	61 (84%)	12 (16%)	2	10
6	H	117/128 (91%)	65 (56%)	52 (44%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	I	115/116 (99%)	85 (74%)	30 (26%)	0	1
8	J	59/65 (91%)	43 (73%)	16 (27%)	0	1
9	K	99/102 (97%)	76 (77%)	23 (23%)	1	2
10	L	40/57 (70%)	21 (52%)	19 (48%)	0	0
All	All	3062/3657 (84%)	2367 (77%)	695 (23%)	1	3

5 of 695 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	184	ASN
6	H	53	ASP
3	C	242	GLN
3	C	163	ILE
4	E	117	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 104 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	706	GLN
2	B	1179	GLN
8	J	26	GLN
2	B	763	GLN
2	B	1065	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry

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	$\# Z > 2$
13	ATP	A	3011	11	31,32,33	1.08	2 (6%)	46,50,52	1.92	6 (13%)

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
13	ATP	A	3011	11	1/1/6/7	5/22/34/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	3011	ATP	C4-N3	3.32	1.40	1.34
13	A	3011	ATP	PA-O3A	2.03	1.61	1.59

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	3011	ATP	O4'-C1'-N9	9.59	125.18	107.96
13	A	3011	ATP	C1'-N9-C8	-4.72	110.45	126.95
13	A	3011	ATP	O4'-C1'-C2'	3.66	113.08	106.25
13	A	3011	ATP	C4-N9-C1'	2.89	138.10	126.50
13	A	3011	ATP	C2'-C1'-N9	2.47	120.42	114.63

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	3011	ATP	C1'

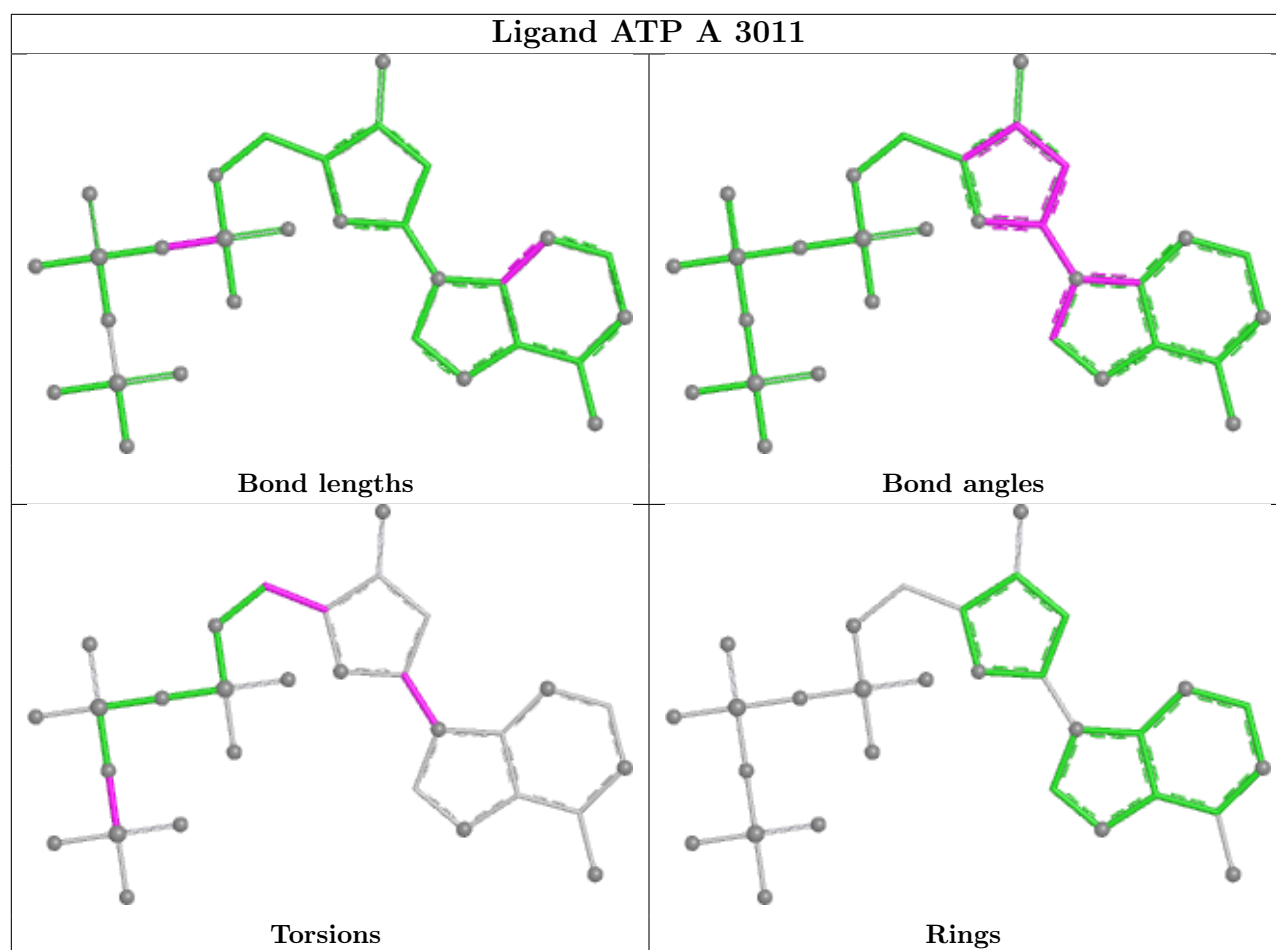
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	3011	ATP	O4'-C4'-C5'-O5'
13	A	3011	ATP	C3'-C4'-C5'-O5'
13	A	3011	ATP	C2'-C1'-N9-C4
13	A	3011	ATP	PB-O3B-PG-O2G
13	A	3011	ATP	PB-O3B-PG-O3G

There are no ring outliers.

No monomer is involved in short contacts.

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	B	12
1	A	8
3	C	2
7	I	2
5	F	1
9	K	1
8	J	1

The worst 5 of 27 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1014:ALA	C	1015:VAL	N	1.20
1	A	1378:GLN	C	1379:GLY	N	1.20
1	B	49:ASP	C	50:SER	N	1.20
1	B	586:TRP	C	587:HIS	N	1.20
1	B	724:ASP	C	725:PRO	N	1.20

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	1349/1733 (77%)	-0.25	21 (1%) 70 56	1, 22, 99, 165	0
2	B	1091/1224 (89%)	-0.20	22 (2%) 65 49	1, 22, 107, 155	0
3	C	266/318 (83%)	-0.20	0 100 100	1, 22, 72, 145	0
4	E	215/215 (100%)	-0.14	1 (0%) 87 78	1, 40, 102, 138	0
5	F	83/155 (53%)	-0.38	0 100 100	1, 21, 63, 88	0
6	H	133/146 (91%)	0.62	12 (9%) 15 14	14, 65, 120, 167	0
7	I	121/122 (99%)	-0.13	1 (0%) 82 71	1, 30, 79, 120	0
8	J	64/70 (91%)	-0.29	0 100 100	3, 18, 64, 91	0
9	K	114/120 (95%)	-0.17	1 (0%) 81 68	1, 32, 72, 103	0
10	L	46/70 (65%)	0.56	1 (2%) 62 47	16, 72, 123, 140	0
All	All	3482/4173 (83%)	-0.18	59 (1%) 69 54	1, 25, 103, 167	0

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	248	PRO	4.8
6	H	104	PHE	4.3
2	B	882	THR	4.1
6	H	85	GLY	3.9
1	A	33	ALA	3.8

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](#)

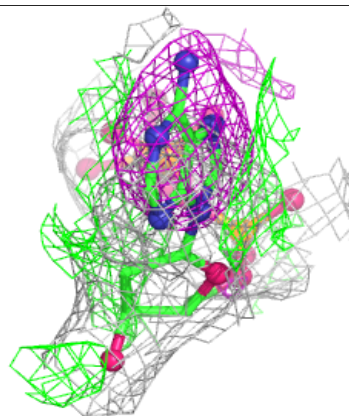
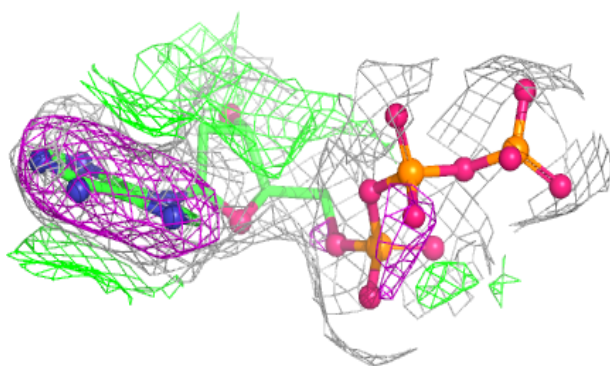
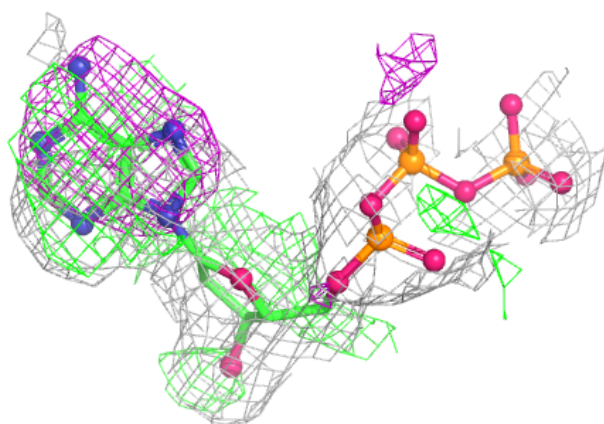
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
13	ATP	A	3011	30/31	0.80	0.16	5,46,82,85	0
12	ZN	I	3004	1/1	0.95	0.09	66,66,66,66	0
12	ZN	J	3001	1/1	0.97	0.13	34,34,34,34	0
12	ZN	A	3008	1/1	0.97	0.05	91,91,91,91	0
12	ZN	I	3003	1/1	0.98	0.07	46,46,46,46	0
12	ZN	A	3006	1/1	0.98	0.10	47,47,47,47	0
12	ZN	B	3007	1/1	0.99	0.08	57,57,57,57	0
12	ZN	C	3002	1/1	0.99	0.12	42,42,42,42	0
12	ZN	L	3005	1/1	0.99	0.12	90,90,90,90	0
11	MN	A	3010	1/1	0.99	0.05	12,12,12,12	0
11	MN	A	3009	1/1	1.00	0.02	4,4,4,4	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 ATP A 3011:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.