



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:26 PM UTC

PDB ID : 8U9X / pdb_00008u9x
Title : STRUCTURAL BASIS OF TRANSCRIPTION: RNA POLYMERASE II
SUBSTRATE BINDING AND METAL COORDINATION AT 3.0 Å OF
T834P MUTANT USING A FREE-ELECTRON LASER
Authors : Arjunan, P.; Calero, G.; Kaplan, C.D.
Deposited on : 2023-09-20
Resolution : 3.05 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

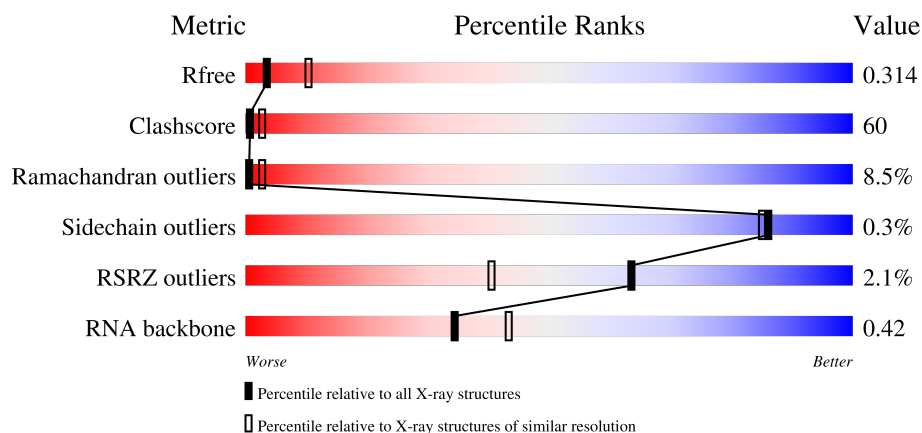
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)
RNA backbone	3983	1079 (3.30-2.82)

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	
2	B	1224	
3	C	318	

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Mol	Chain	Length	Quality of chain
4	D	221	
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	R	10	
14	T	13	

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	ZN	L	101	-	-	X	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 30893 atoms, of which 8 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 subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1398	Total	C	N	O	S	0	0	0
			10987	6934	1918	2073	62			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	834	PRO	THR	conflict	UNP P04050

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1060	Total	C	N	O	S	0	0	0
			8424	5346	1475	1549	54			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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 polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	162	Total	C	N	O	S	0	0	0
			1287	799	224	262	2			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	208	Total	C	N	O	S	0	0	0
			1713	1089	303	312	9			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	117	Total	C	N	O	S	0	0	0
			951	605	158	184	4			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases II subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	65	Total	C	N	O	S	0	0	0
			526	336	90	94	6			

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	115	Total	C	N	O	S	0	0	1
			920	590	157	171	2			

- Molecule 12 is a protein called DNA-directed RNA polymerases II subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	43	Total	C	N	O	S	0	0	0
			343	211	69	59	4			

- Molecule 13 is a RNA chain called MOL_ID: 13.

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

- Molecule 14 is a DNA chain called MOL_ID: 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	13	Total	C	N	O	P	0	0	0
			260	124	44	79	13			

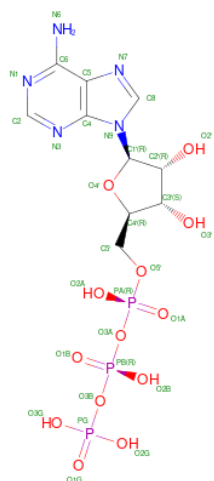
- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 16 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

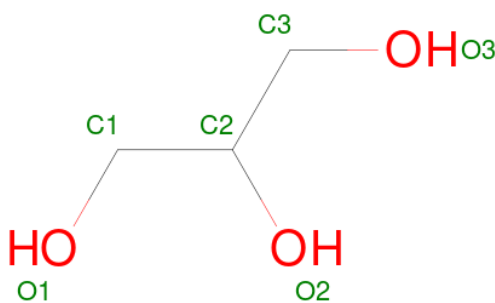
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	2	Total	Mn	0	0
			2	2		
16	B	1	Total	Mn	0	0
			1	1		

- Molecule 17 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 18 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	E	1	Total	C	H	O	0	0
			14	3	8	3		

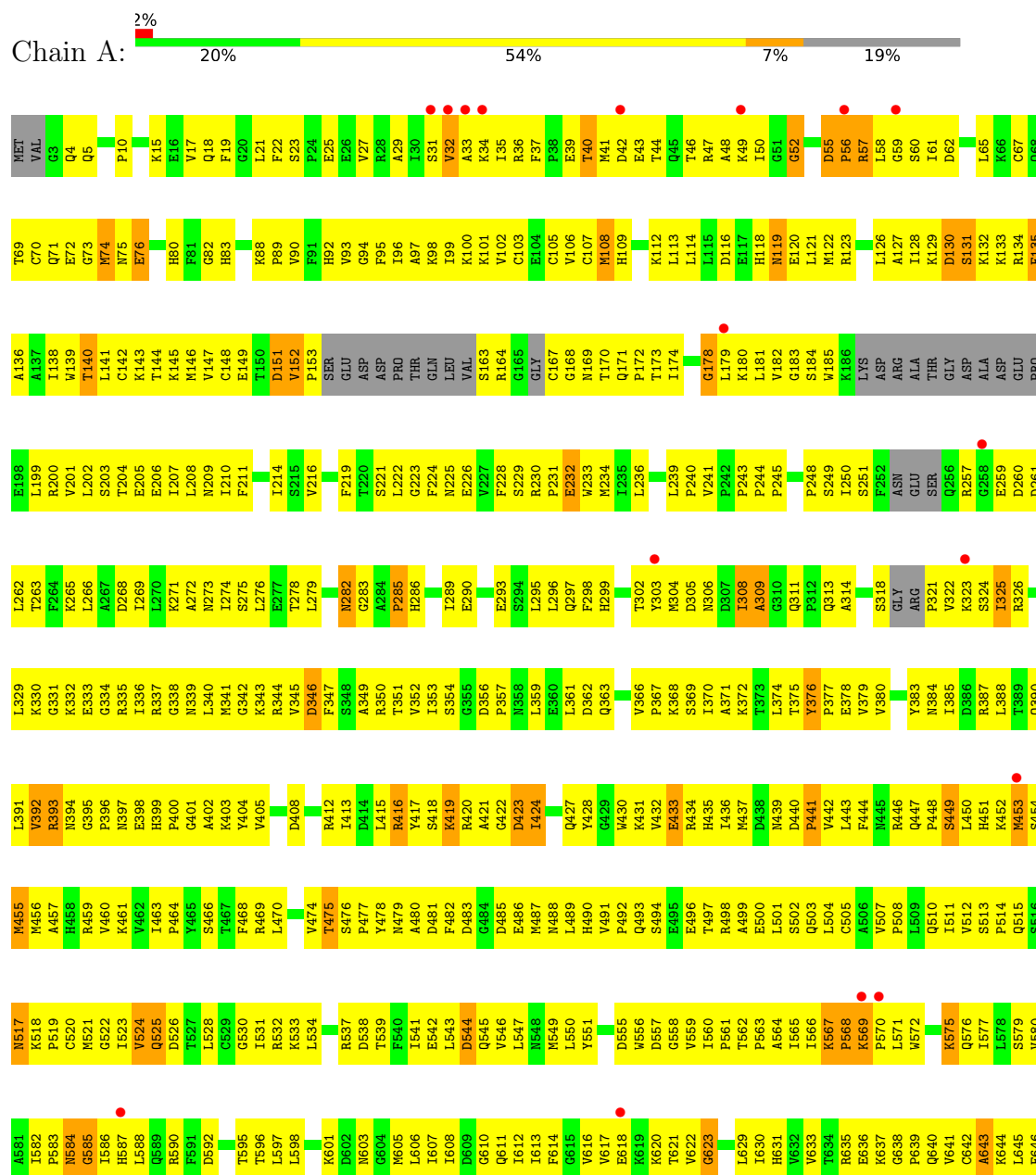
- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	46	Total 46	O 46	0	0
19	B	38	Total 38	O 38	0	0
19	C	6	Total 6	O 6	0	0
19	D	5	Total 5	O 5	0	0
19	E	7	Total 7	O 7	0	0
19	F	3	Total 3	O 3	0	0
19	G	4	Total 4	O 4	0	0
19	H	3	Total 3	O 3	0	0
19	J	2	Total 2	O 2	0	0
19	K	5	Total 5	O 5	0	0
19	L	2	Total 2	O 2	0	0
19	R	1	Total 1	O 1	0	0
19	T	2	Total 2	O 2	0	0

3 Residue-property plots

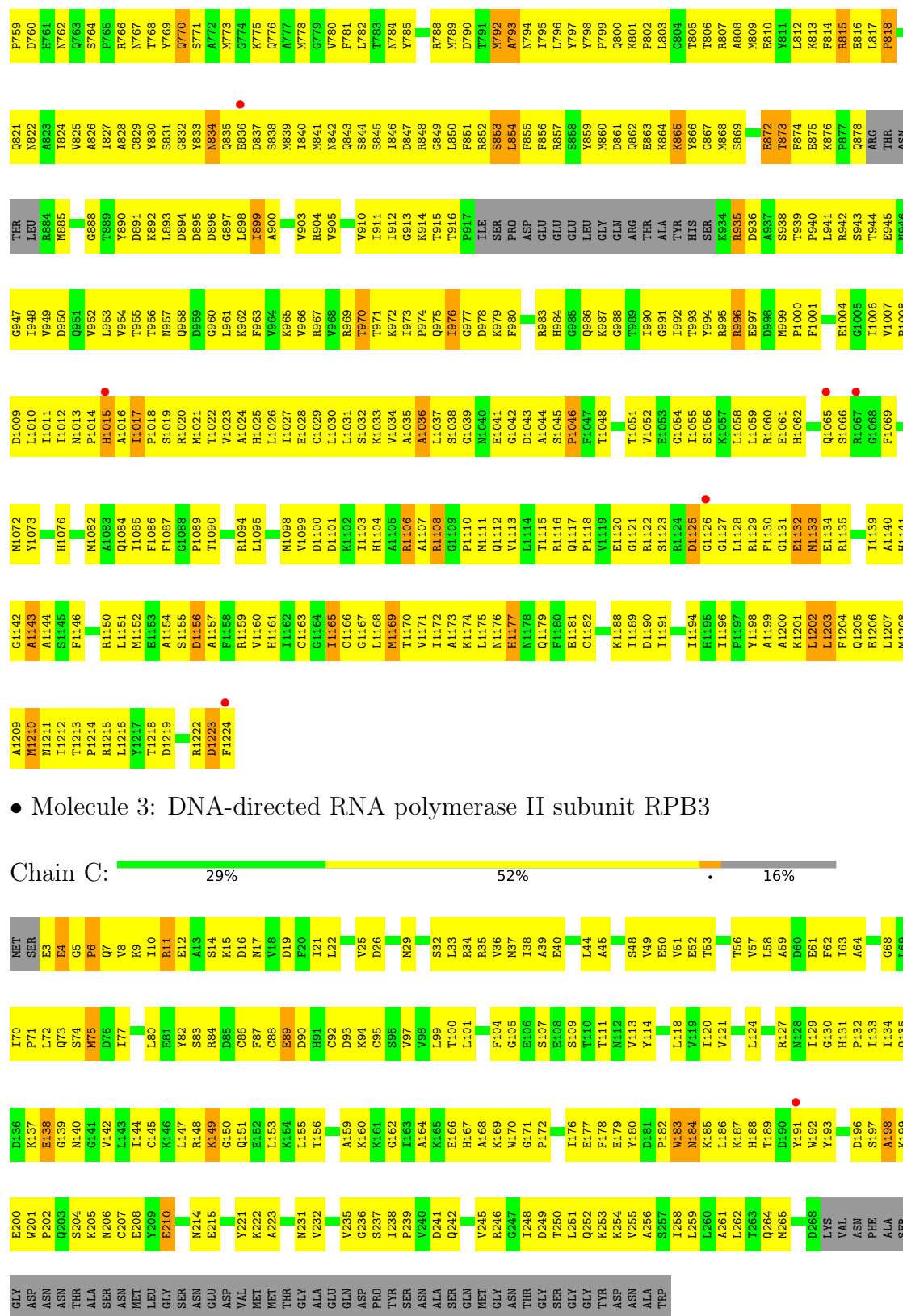
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 subunit RPB1

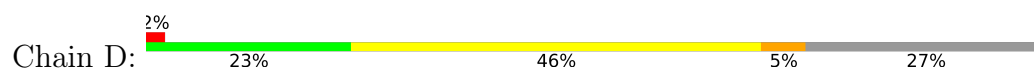


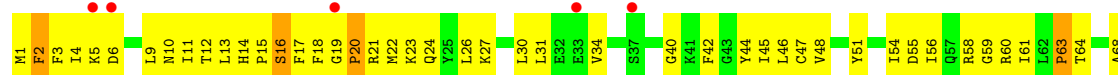
PRO	THR	LYS	S1425	S1361	V1299	S1229	P1156	K1092	V1031	I964	D900	1837	1775	L710	G647
THR	ASP	ASP	E1426	Y1362	K1300	S1229	ASP	K1093	L1032	Q965	L901	Q836	A776	L710	M648
TYR	GLU	PRO	N1427	V1363	E1301	D1233	ARG	V1094	Q1033	N966	L902	R839	F777	R711	M649
SER	LEU	ARG	V1428	P1302	P1302	L1236	SER	S1095	Y1035	A967	T904	R840	G778	R711	Q650
PRO	MET	SER	I1429	Y1365	W1303	L1237	T1161	G1097	Y1036	T970	D905	L841	F779	E715	K651
THR	PHE	LEU	I1430	R1366	W1304	I1238	V1162	G1098	R1036	F971	H906	K843	W780	E716	V652
SER	SER	LEU	G1431	H1367	V1305	R1239	I1163	P1099	L1037	H972	T907	K844	W781	D716	V653
PRO	PRO	LEU		M1368	L1306			R1100	Y1038	N973	L908	R845	W782	W717	M654
ALA	LEU	LEU	A1434	A1369	E1307	V1242	I1170	R1101	K1039	P978	L908	L846	W783	W718	F655
TYR	VAL	VAL	P1435	L1370	T1308	V1243	K1171	K1102	F1042	S979	D909	E846	W784	W719	F656
SER	ASP	ASP	I1436	L1371	D1309	L1243	E1103	E1101	D1043	D980	P910	R847	W785	W720	L657
THR	SER	THR	G1437	D1372	G1310	ARG	H1372	E1104	L1044	L981	L912	R848	W786	W721	L658
THR	GLY	GLY	T1438	D1373	V1311	P80	PHE	L1105	V1045	L981	L913	R849	W787	L722	H659
SER	SER	SER	V1374	N1312	N1312	LVS	SER	M1106	L1046	L981	L913	W850	W788	W723	M660
PRO	ASN	ASN	A1440	M1375	L1313	SER	SER	V1107	L1047	L982	L914	R851	W789	E724	G661
SER	ASP	ASP	F1441	T1376	S1314	LEU	LEU	A1108	S1047	I983	S915	W852	D790	A725	F662
TYR	ALA	ALA	D1442	T1377	E1315	ASP	ASP	A1109	N1048	D985	G916	D853	W793	W726	S663
SER	MET	GLY	V1443	Q1378	V1316	ALA	GLU	K1109	I1049	I986	T919	N854	W794	D727	G665
PRO	ALA	ALA	M1444	L1381	M1317	THR	GLU	N1110	E1050	I987	L920	R857	W795	K728	G666
THR	GLY	GLY	I1445		GLU	THR	ALA	M1111	A1051	L988	L920	R858	W796	A729	L666
SER	GLY	GLY	D1446	V1384	V1319	GLU	ALA	S1115	Q1052	L988	G921	N858	W797	G730	G667
PRO	PHE	PHE	E1447	T1385	P1320	ALA	GLU	L1116	F1053	G989	D922	R859	W798	L737	D668
SER	THR	THR		R1386	G1321	E1255	GLN	L1117	L1054	V990	L923	L860	G798	L732	T669
TYR	ALA	ALA	L1450	R1387	D1323	M1259	SER	T1118	R1055	K991	K924	C861	W799	A733	1670
SER	TYR	TYR	V1451	G1388	P1324	L1260	ASP	Y1119	S1056	D982	L925	N862	W800	W734	A671
PRO	GLY	GLY	K1452	F1389	P1325	K1261	ASP		I1057	L993	Q926	W863	E801	W735	D672
THR	GLY	GLY	M1453	M1390	T1326	K1262	GLU	L1120	H1058		V927	R864		N736	G673
SER	ALA	ALA	M1454	R1391	R1327	I1263	GLN	P1122	L1059	L997	L928	Q865	W798	L737	G674
PRO	ASP	ASP	P1455	S1392	I1327	E1264	SER	G1123	G1061	N999	L929	F866	W799	K738	T675
SER	TYR	TYR	GLU	Y1328	Y1328	I1265	PHE	G1124	E1062	W987	L932	W868	D739	L740	R677
GLY	GLY	GLY	GLN	M1393	N1329	N1266	THR	H1124	M1063	L1000	E932	C869	L808	N741	E678
SER	GLY	GLY	LVS	T1394	N1330	T1267		A1125	M1063	L1001	Y933	E870	L809	N742	1679
PRO	ALA	ALA	I1456	G1395	S1331	M1267	R1194	A1126	V1064		K934	C872	D810	W743	T680
THR	THR	THR	THR	L1396	F1332	L1268	E1196	D1127	G1065	N1004		N873	Q811	K744	E681
SER	GLU	SER	GLU	L1397	I1333	E1269	E1197	Q1128	V1066	E1005	V937	D874	E812	Q745	T682
PRO	ILE	PRO	ILE	D1334	D1334	N1270	L1197	E1129	L1067	I1006	D939	D874	F813	W746	T683
SER	PHE	PRO	GLU	M1398	M1335	I1271	D1198	Q1130	A1068	I1007	D939	A875	F814	W747	A684
TYR	ASP	GLY	ASP	G1400	M1336	I1271		A1131	A1069	I1007	R940		F815	A748	E686
SER	ALA	ALA	GLN	S1401	E1337	R1274	A1201	K1132	Q1070	Q1008	F941		H816	K748	K687
PRO	TYR	TYR	GLN	F1402	V1338	G1275	M1202	L1133	S1071	N1009	F942		H817	K752	K688
THR	GLY	GLY	ASP	E1403	L1339	E1276	K1205	T1134	G1072	A1010	L943		N818	G753	K689
SER	GLY	GLY	GLY	E1404	G1340	E1277	D1206	R1135	G1073	Q1011	E879		G820	W754	V690
PRO	ALA	ALA	VAL	T1405	I1341	N1278	L1207	S1136	E1074	D1012	Y946		G820	F755	L691
SER	THR	THR	THR	W1406	E1342	I1279	L1207	A1137	P1075	R1013	F947		R821	W756	D692
PRO	SER	SER	PRO	E1407	A1343	V1282	T1208	L1138	A1076	A1014	V948		E822	N757	T694
SER	PRO	PRO	PRO	L1408	G1344	V1283	M1209	E1139	Q1077	V1015	D949		G823		K695
THR	GLY	GLY	THR	F1410	R1345	M1284	G1210	H1140	T1078	L1016	G950		L824		F693
SER	PHE	ASN	SER	A1346	A1346			T1141	M1079	L1017	E951		L825	W761	
GLY	GLY	GLY	GLY	A1347	A1347	D1213	G1213	T1142	T1080	F1018	A952		R826	S762	E696
VAL	SER	VAL	SER	L1348	L1348	R1214	R1214	L1143	H1082	L1021	N954		T827	A763	A697
TYR	GLY	SER	GLY	Y1349	Y1349	K1288	E1215		T1083	L1022	P955		A828		Q698
SER	SER	SER	LEU	K1350	K1350	R1289	T1216	V1146	P955	R1023	D890		W829	G766	A699
PRO	PRO	PRO	VAL	E1351	P1291	P1291	T1147	T1148	A891	S1024	L956		K830	Q767	N700
THR	GLY	GLY	ASN	V1352	P1292	S1293	T1219	H1085	P957	S1024	L956		T831		L701
SER	PHE	PHE	ALA	S1293	S1293	K1221	F1220	F1086	Y958	R893	N959		W770		T702
PRO	ASP	ASP	ASP	T1295	T1295			F1087	L1026	A1027	N960		E833	E771	T703
SER	LEU	LEU	LEU	T1296	T1296			G1088	A1027	R1028	R961		P834	G772	A704
THR	THR	THR	ASP	E1297	E1297			V1089	R1029	R1029	R962		W897	K773	K705
SER	SER	SER	VAL	G1298	G1298			S1091	R1030				W899	R774	H706

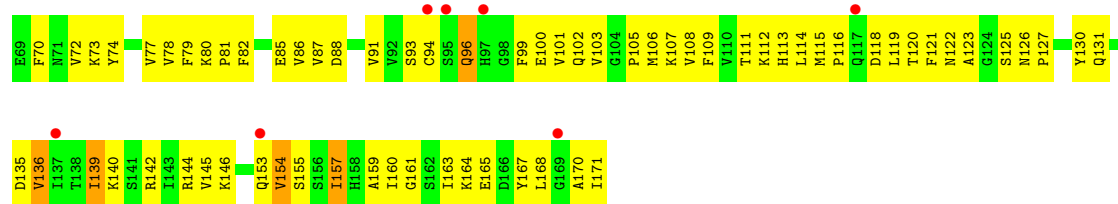




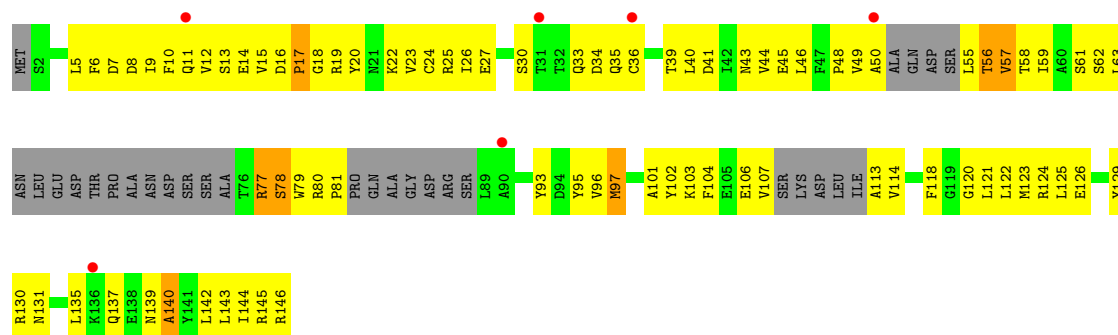
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4



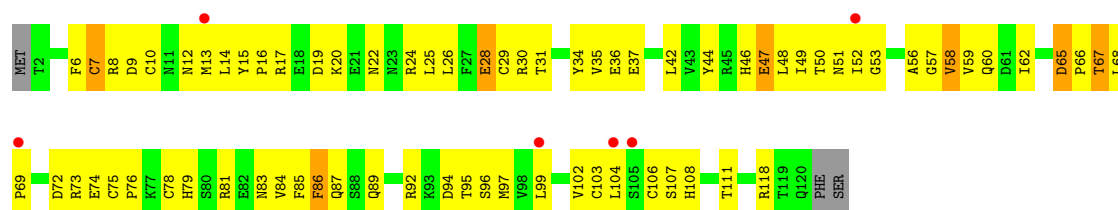




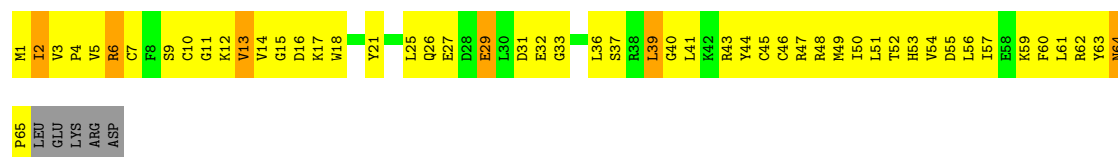
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

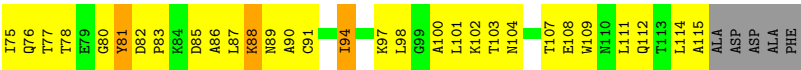


• Molecule 10: DNA-directed RNA polymerases II subunit RPABC5



• Molecule 11: DNA-directed RNA polymerase II subunit RPB11

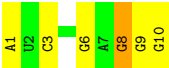




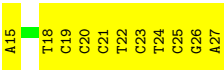
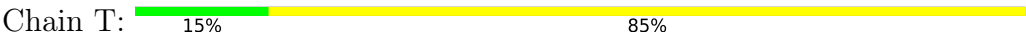
● Molecule 12: DNA-directed RNA polymerases II subunit RPABC4



● Molecule 13: MOL_ID: 13



● Molecule 14: MOL_ID: 14



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	220.17Å 392.60Å 280.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.00 – 3.05 18.00 – 3.05	Depositor EDS
% Data completeness (in resolution range)	98.0 (18.00-3.05) 99.2 (18.00-3.05)	Depositor EDS
R_{merge}	0.67	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 3.00Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.283 , 0.307 0.293 , 0.314	Depositor DCC
R_{free} test set	7379 reflections (3.06%)	wwPDB-VP
Wilson B-factor (Å ²)	76.8	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 27.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.073 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.078 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	30893	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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: MN, ZN, ATP, GOL

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	0.66	1/11181 (0.0%)	0.97	12/15114 (0.1%)
2	B	0.55	0/8589	0.87	6/11581 (0.1%)
3	C	0.56	0/2133	0.87	3/2891 (0.1%)
4	D	0.44	0/1296	0.74	1/1741 (0.1%)
5	E	0.89	0/1747	1.27	2/2349 (0.1%)
6	F	0.66	0/691	0.94	0/933
7	G	1.04	0/1368	1.32	1/1844 (0.1%)
8	H	0.48	0/965	0.72	0/1302
9	I	0.47	0/989	0.75	1/1331 (0.1%)
10	J	0.52	0/535	0.83	1/720 (0.1%)
11	K	0.51	0/938	0.75	0/1267
12	L	0.84	0/345	1.01	0/457
13	R	0.35	0/244	0.55	0/380
14	T	0.61	0/289	0.75	0/442
All	All	0.64	1/31310 (0.0%)	0.94	27/42352 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	ASP	N-CA	5.01	1.50	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1079	MET	N-CA-C	-10.79	100.11	113.28
1	A	295	LEU	N-CA-C	-7.04	105.22	113.88
1	A	1081	LEU	N-CA-C	-6.92	103.12	112.26
1	A	1080	THR	CA-CB-OG1	-6.79	99.42	109.60
10	J	39	LEU	N-CA-C	-6.72	103.00	113.02

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	56	PRO	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10987	0	11060	1499	0
2	B	8424	0	8455	1150	0
3	C	2095	0	2052	244	0
4	D	1287	0	1296	159	0
5	E	1713	0	1739	196	0
6	F	679	0	701	93	0
7	G	1340	0	1357	183	0
8	H	951	0	926	135	0
9	I	971	0	930	117	0
10	J	526	0	533	95	0
11	K	920	0	929	113	0
12	L	343	0	364	70	0
13	R	217	0	109	15	0
14	T	260	0	147	20	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	2	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	B	31	0	12	3	0
18	E	6	8	8	2	0
19	A	46	0	0	0	0
19	B	38	0	0	1	0
19	C	6	0	0	0	0
19	D	5	0	0	0	0
19	E	7	0	0	0	0
19	F	3	0	0	0	0
19	G	4	0	0	0	0
19	H	3	0	0	1	0
19	J	2	0	0	0	0
19	K	5	0	0	0	0
19	L	2	0	0	0	0
19	R	1	0	0	0	0
19	T	2	0	0	0	0
All	All	30885	8	30618	3681	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 60.

The worst 5 of 3681 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)
12:L:48:CYS:SG	12:L:51:CYS:HB2	1.92	1.09
12:L:48:CYS:SG	12:L:51:CYS:CB	2.41	1.09
2:B:1082:MET:HA	3:C:189:THR:HA	1.38	1.05
12:L:30:ILE:HG22	12:L:31:CYS:H	1.23	1.04
2:B:963:PHE:HE2	2:B:965:LYS:HE2	1.22	1.03

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	1380/1733 (80%)	959 (70%)	290 (21%)	131 (10%)	0	2
2	B	1036/1224 (85%)	726 (70%)	220 (21%)	90 (9%)	0	2
3	C	264/318 (83%)	205 (78%)	48 (18%)	11 (4%)	2	10
4	D	156/221 (71%)	113 (72%)	29 (19%)	14 (9%)	0	2
5	E	202/215 (94%)	164 (81%)	29 (14%)	9 (4%)	2	9
6	F	82/155 (53%)	56 (68%)	24 (29%)	2 (2%)	4	18
7	G	169/171 (99%)	132 (78%)	27 (16%)	10 (6%)	1	6
8	H	107/146 (73%)	73 (68%)	26 (24%)	8 (8%)	1	3
9	I	117/122 (96%)	82 (70%)	24 (20%)	11 (9%)	0	2
10	J	63/70 (90%)	51 (81%)	6 (10%)	6 (10%)	0	2
11	K	113/120 (94%)	77 (68%)	27 (24%)	9 (8%)	1	3
12	L	41/70 (59%)	15 (37%)	10 (24%)	16 (39%)	0	0
All	All	3730/4565 (82%)	2653 (71%)	760 (20%)	317 (8%)	0	3

5 of 317 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	57	ARG
1	A	76	GLU
1	A	119	ASN
1	A	128	ILE

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	1218/1520 (80%)	1214 (100%)	4 (0%)	86	85
2	B	917/1061 (86%)	913 (100%)	4 (0%)	84	84
3	C	234/274 (85%)	234 (100%)	0	100	100
4	D	144/200 (72%)	144 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	192/197 (98%)	192 (100%)	0	100	100
6	F	74/137 (54%)	74 (100%)	0	100	100
7	G	152/152 (100%)	152 (100%)	0	100	100
8	H	104/128 (81%)	103 (99%)	1 (1%)	68	77
9	I	113/116 (97%)	112 (99%)	1 (1%)	70	78
10	J	59/65 (91%)	59 (100%)	0	100	100
11	K	99/102 (97%)	99 (100%)	0	100	100
12	L	38/57 (67%)	38 (100%)	0	100	100
All	All	3344/4009 (83%)	3334 (100%)	10 (0%)	86	85

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1106	ARG
8	H	97	MET
9	I	74	GLU
1	A	658	LEU
2	B	527	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
8	H	128	ASN
8	H	137	GLN
11	K	52	ASN
2	B	306	ASN
2	B	121	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	R	8/10 (80%)	1 (12%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	R	8	G

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 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
17	ATP	B	2501	16	32,33,33	0.86	2 (6%)	48,52,52	1.44	4 (8%)
18	GOL	E	301	-	5,5,5	1.38	0	5,5,5	1.02	0

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
17	ATP	B	2501	16	-	2/22/38/38	0/3/3/3
18	GOL	E	301	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	2501	ATP	PG-O2G	-2.81	1.44	1.54
17	B	2501	ATP	PB-O2B	-2.25	1.44	1.55

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	2501	ATP	O2G-PG-O3B	-5.73	85.43	104.64
17	B	2501	ATP	O2B-PB-O3B	-5.62	92.07	107.27
17	B	2501	ATP	O3G-PG-O3B	2.71	113.72	104.64
17	B	2501	ATP	O3A-PA-O1A	-2.09	104.42	110.70

There are no chirality outliers.

All (4) torsion outliers are listed below:

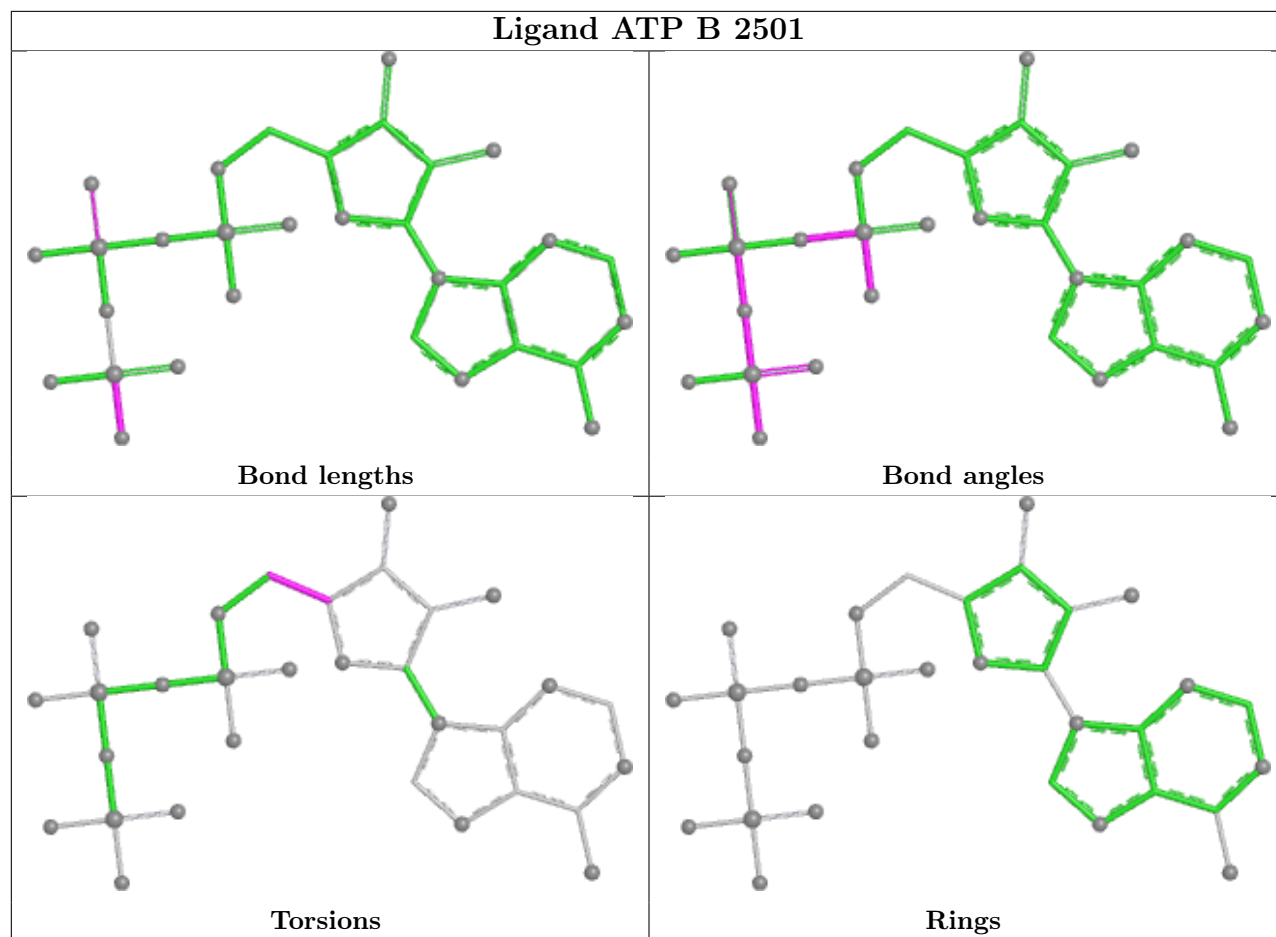
Mol	Chain	Res	Type	Atoms
17	B	2501	ATP	O4'-C4'-C5'-O5'
18	E	301	GOL	O1-C1-C2-C3
17	B	2501	ATP	C3'-C4'-C5'-O5'
18	E	301	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	2501	ATP	3	0
18	E	301	GOL	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1398/1733 (80%)	-0.12	33 (2%) 59 37	38, 100, 164, 286	0
2	B	1060/1224 (86%)	-0.10	15 (1%) 73 51	40, 103, 172, 273	0
3	C	266/318 (83%)	-0.20	1 (0%) 88 75	50, 102, 153, 197	0
4	D	162/221 (73%)	-0.06	4 (2%) 58 35	73, 118, 163, 198	0
5	E	208/215 (96%)	0.03	4 (1%) 66 43	59, 132, 186, 293	0
6	F	84/155 (54%)	-0.17	0 100 100	44, 77, 116, 167	0
7	G	171/171 (100%)	0.28	12 (7%) 22 11	61, 103, 153, 189	0
8	H	117/146 (80%)	0.28	6 (5%) 33 17	93, 133, 189, 235	0
9	I	119/122 (97%)	0.19	6 (5%) 34 17	92, 147, 208, 248	0
10	J	65/70 (92%)	-0.14	0 100 100	68, 106, 148, 186	0
11	K	115/120 (95%)	-0.33	0 100 100	54, 95, 154, 175	0
12	L	43/70 (61%)	0.35	1 (2%) 61 38	78, 120, 181, 202	0
13	R	10/10 (100%)	0.07	0 100 100	117, 161, 213, 218	0
14	T	13/13 (100%)	0.44	0 100 100	128, 140, 169, 212	0
All	All	3831/4588 (83%)	-0.07	82 (2%) 63 40	38, 106, 173, 293	0

The worst 5 of 82 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	95	SER	6.8
2	B	728	ARG	5.4
7	G	5	LYS	5.2
7	G	153	GLN	5.2
1	A	1084	PHE	5.1

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](#)

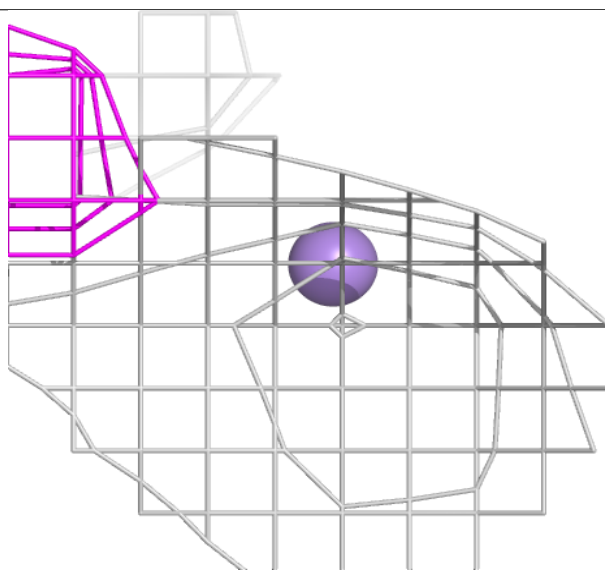
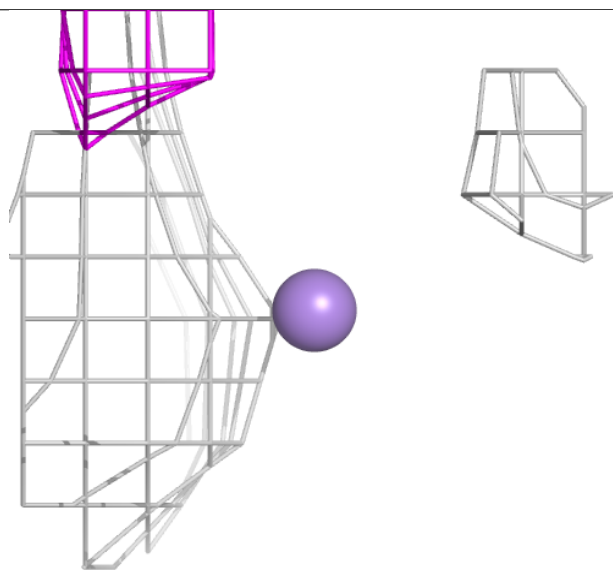
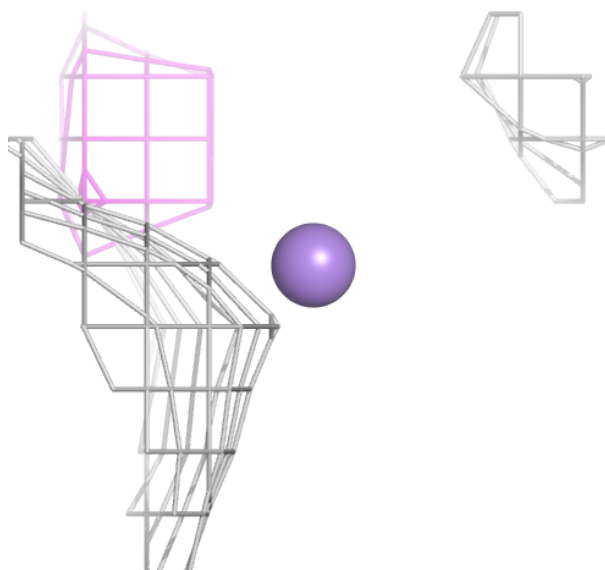
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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
16	MN	B	2503	1/1	0.85	0.17	138,138,138,138	1
18	GOL	E	301	6/6	0.89	0.16	113,136,158,158	0
15	ZN	L	101	1/1	0.91	0.06	153,153,153,153	0
17	ATP	B	2501	31/31	0.94	0.11	117,141,170,172	0
15	ZN	I	202	1/1	0.97	0.03	182,182,182,182	0
15	ZN	A	1801	1/1	0.98	0.06	139,139,139,139	0
15	ZN	B	2502	1/1	0.99	0.02	77,77,77,77	0
16	MN	A	1803	1/1	0.99	0.04	69,69,69,69	0
16	MN	A	1804	1/1	0.99	0.05	78,78,78,78	0
15	ZN	C	401	1/1	0.99	0.04	69,69,69,69	0
15	ZN	I	201	1/1	0.99	0.05	119,119,119,119	0
15	ZN	A	1802	1/1	0.99	0.05	65,65,65,65	0
15	ZN	J	101	1/1	1.00	0.04	85,85,85,85	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.

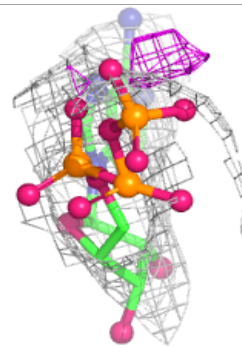
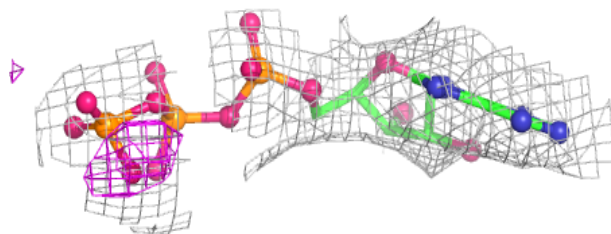
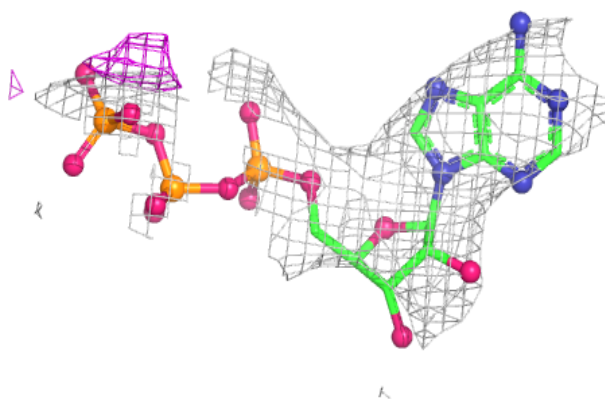
Electron density around MN B 2503:

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



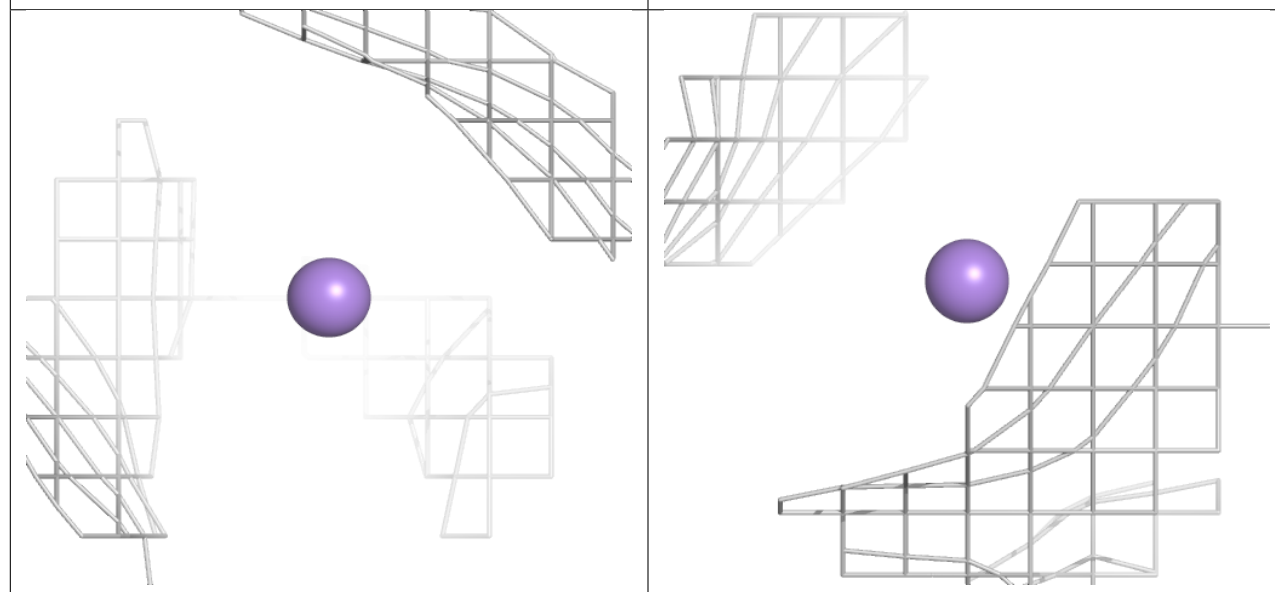
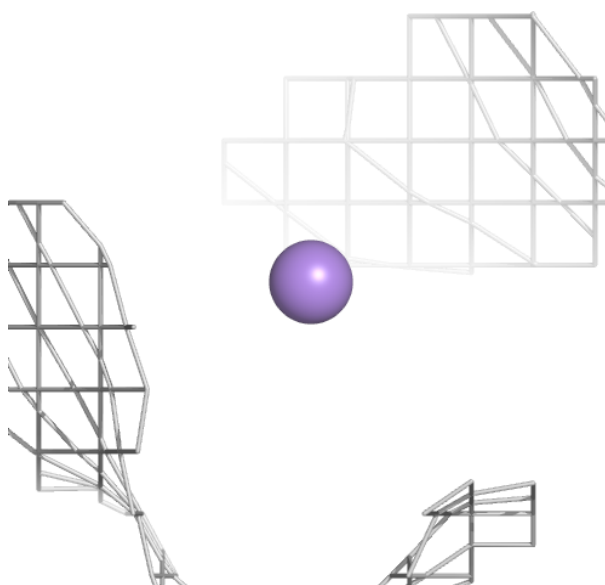
Electron density around ATP B 2501:

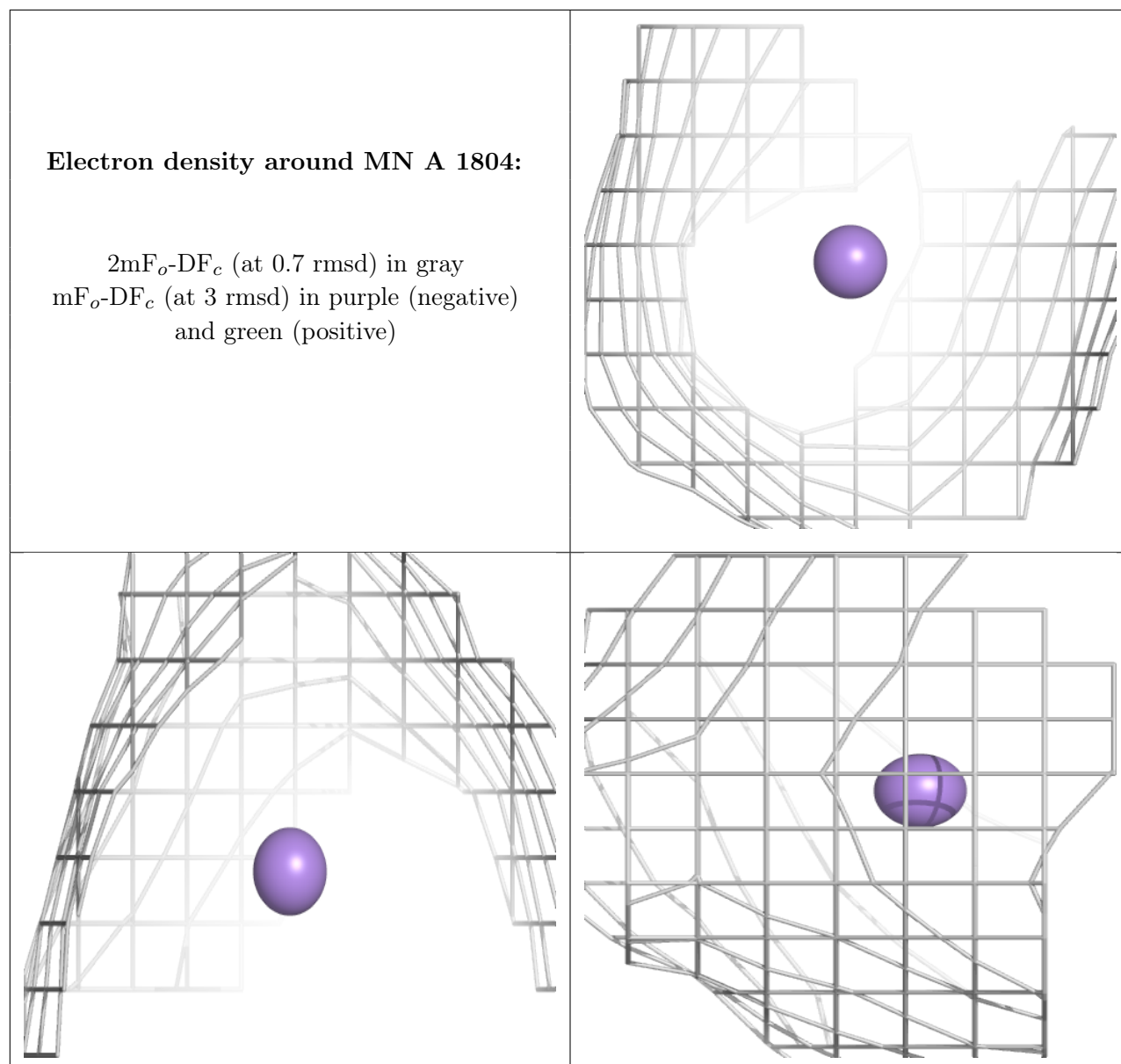
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MN A 1803:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.