



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 23, 2026 – 09:57 AM EDT

PDB ID : 8UKR / pdb_00008ukr
Title : RNA polymerase II elongation complex with Fapy-dG lesion soaking with ATP before chemistry
Authors : Hou, P.; Oh, J.; Wang, D.
Deposited on : 2023-10-15
Resolution : 3.78 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

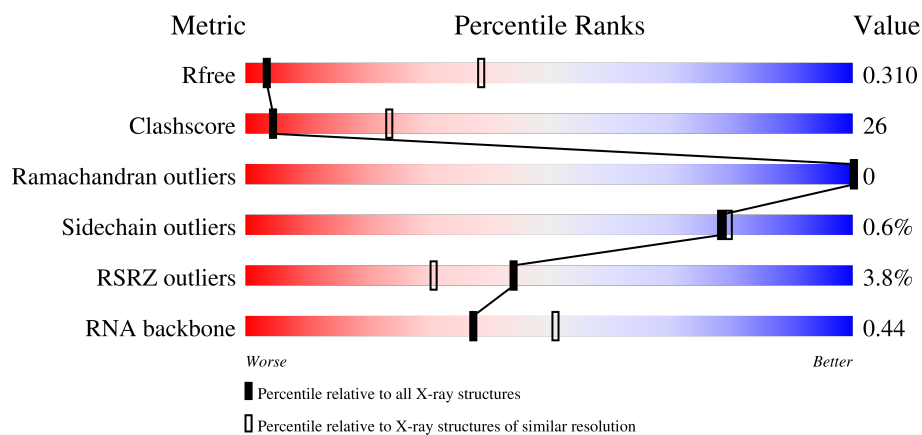
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.78 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	1085 (3.94-3.62)
Clashscore	190562	1029 (3.92-3.64)
Ramachandran outliers	187476	1064 (3.94-3.62)
Sidechain outliers	187428	1059 (3.94-3.62)
RSRZ outliers	180081	1084 (3.94-3.62)
RNA backbone	3983	1002 (4.46-3.10)

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	9	
2	T	29	
3	N	18	
4	A	1733	

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Mol	Chain	Length	Quality of chain
5	B	1224	
6	C	318	
7	E	215	
8	F	155	
9	H	146	
10	I	122	
11	J	70	
12	K	120	
13	L	70	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 28985 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	9	Total	C	N	O	P	0	0	0
			194	88	40	58	8			

- Molecule 2 is a DNA chain called tsDNA with Fapy-dG lesion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	24	Total	C	N	O	P	0	0	0
			481	230	76	151	24			

- Molecule 3 is a DNA chain called ntsDNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	13	Total	C	N	O	P	0	0	0
			275	128	61	73	13			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1384	Total	C	N	O	S	0	0	0
			10828	6831	1896	2041	60			

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1123	Total	C	N	O	S	0	0	0
			8859	5607	1552	1647	53			

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	267	Total	C	N	O	S	0	0	0
			2101	1320	349	419	13			

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	212	Total	C	N	O	S	0	0	0
			1724	1094	305	314	11			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	86	Total	C	N	O	S	0	0	0
			684	437	115	129	3			

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	133	Total	C	N	O	S	0	0	0
			1064	670	179	211	4			

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	118	Total	C	N	O	S	0	0	0
			952	585	173	184	10			

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	43	Total	C	N	O	S	0	0	0
			332	205	64	59	4			

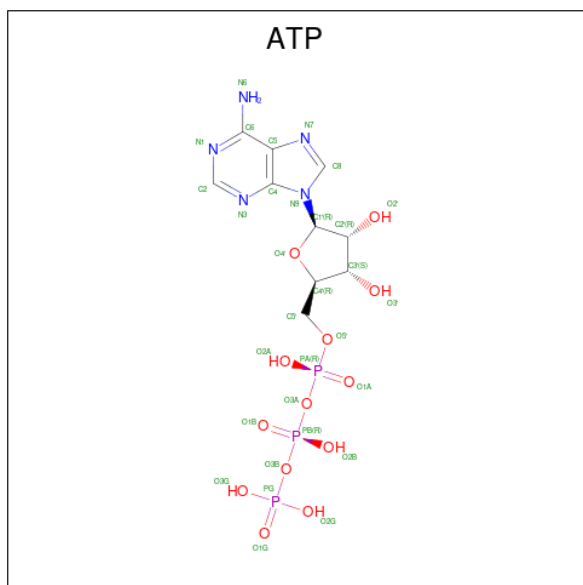
- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 16 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



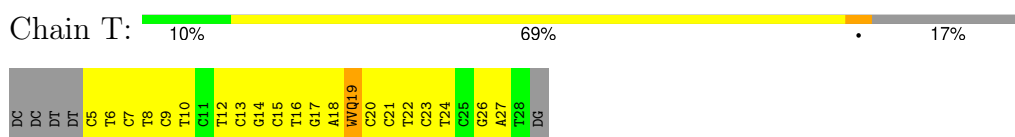
3 Residue-property plots

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.

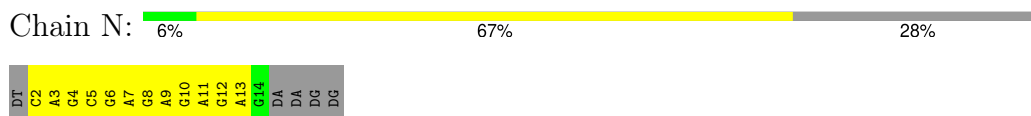
- Molecule 1: RNA



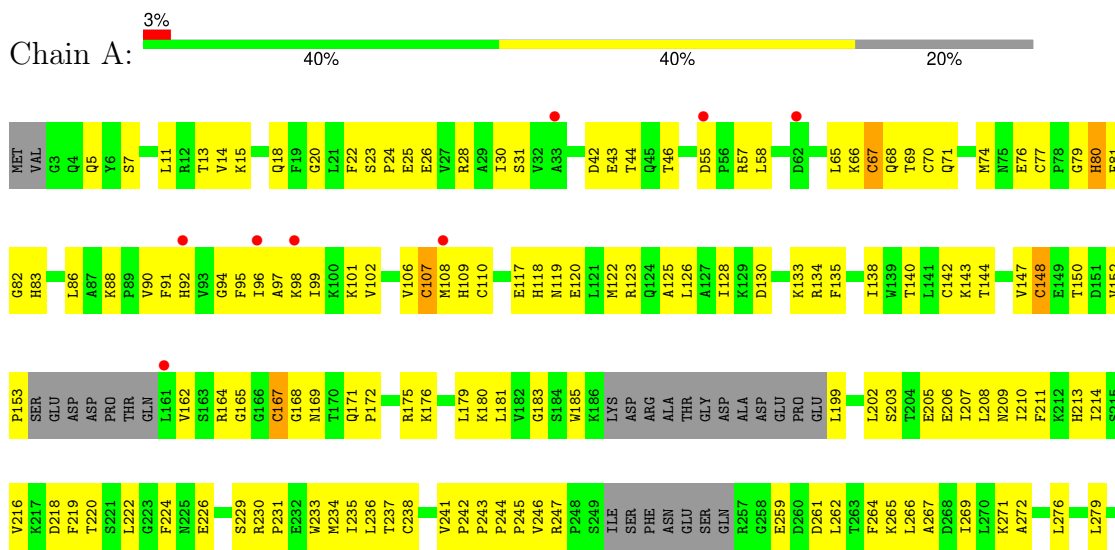
- Molecule 2: tsDNA with Fapy-dG lesion



- Molecule 3: ntsDNA

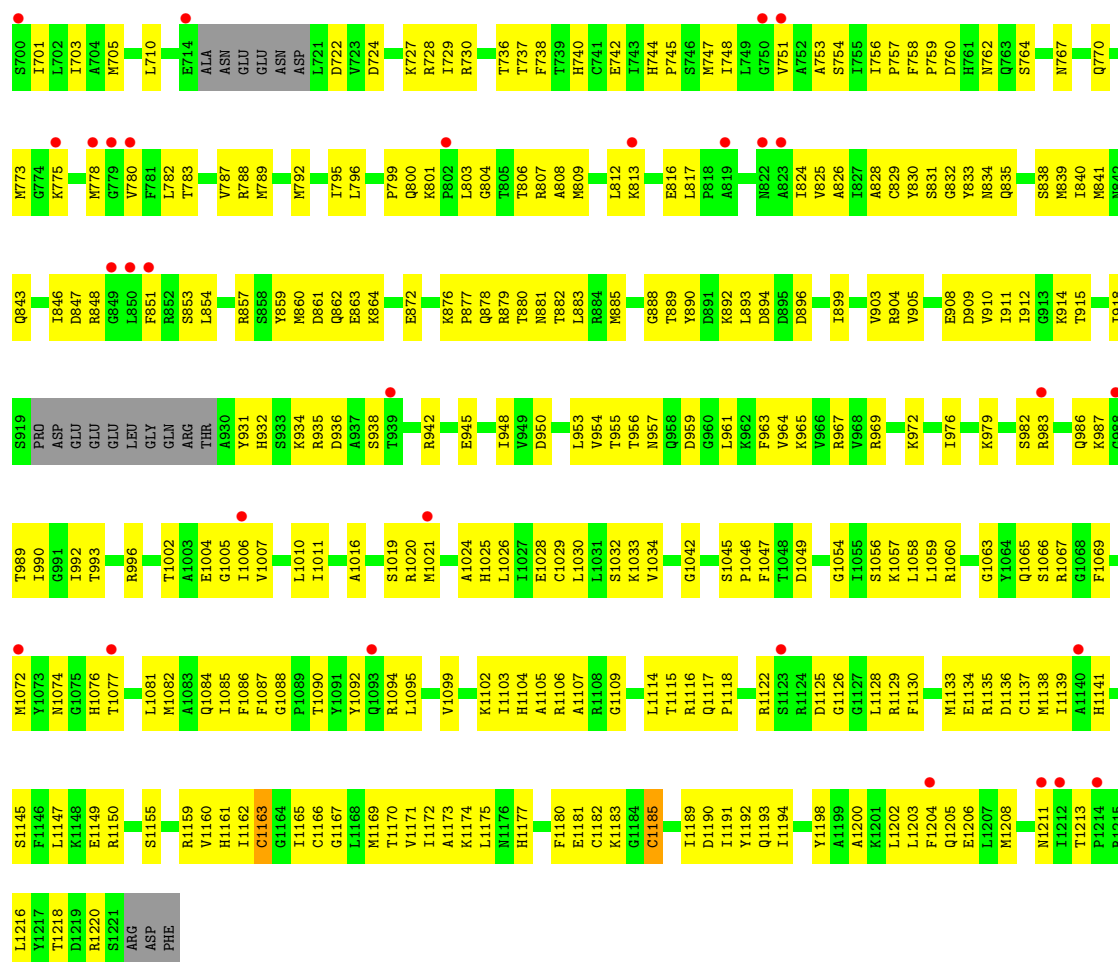


- Molecule 4: DNA-directed RNA polymerase II subunit RPB1

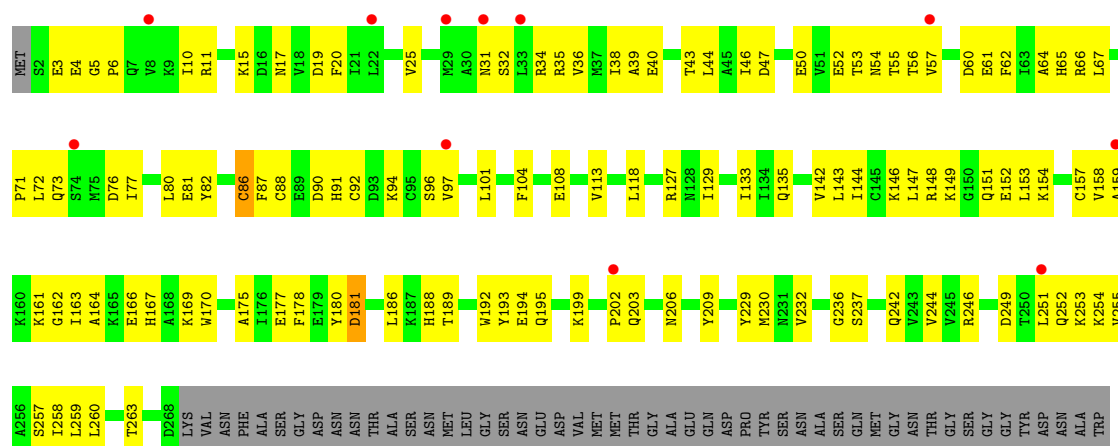


K1290	V1291	P1292	K1300	E1303	L1306	T1307	T1308	T1309	G1310	V1311	M1312	L1313	S1314	E1315	V1316	M1317	D1323	P1324	T1325	R1326	I1327	Y1328	T1329	D1334	I1335	M1336	E1337	V1338	G1339	I1340	I1341	E1342	R1345	A1346	Y1349	K1350	V1355	S1358	D1359	V1363	M1364	Y1365	R1366	H1367	M1368	A1369	L1370	L1371	K1286	



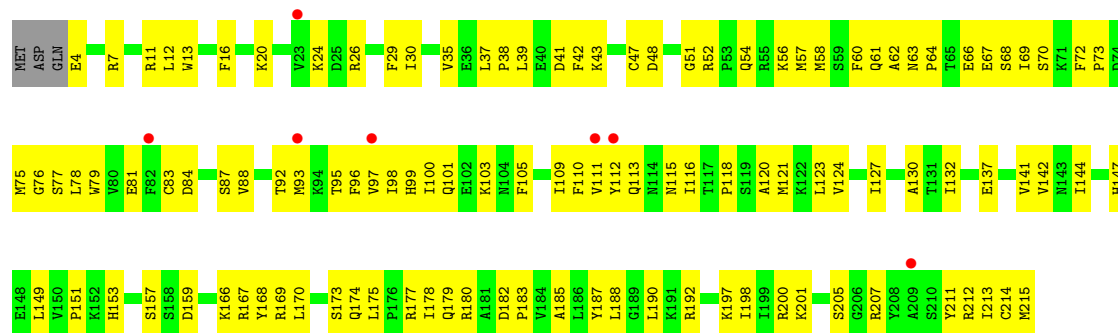


● Molecule 6: DNA-directed RNA polymerase II subunit RPB3

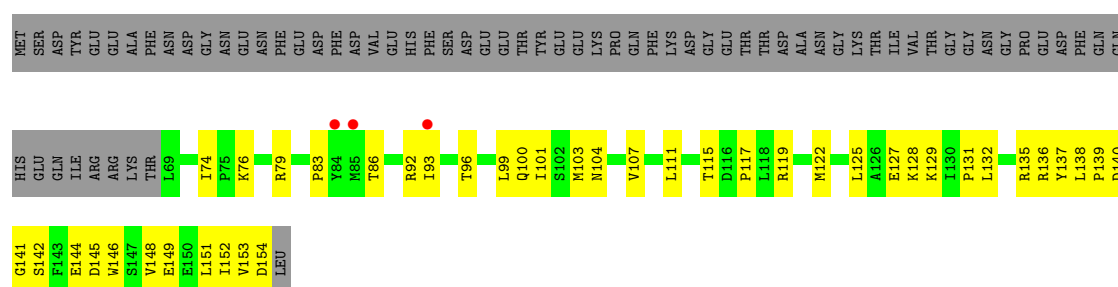
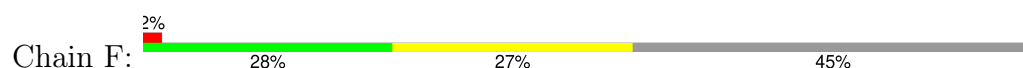


● Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1

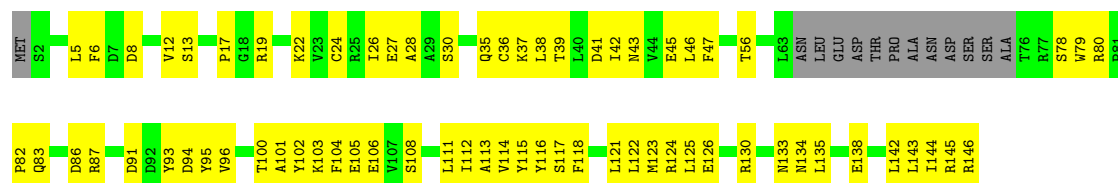




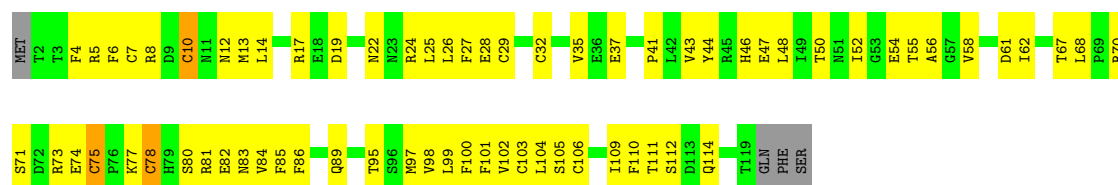
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2



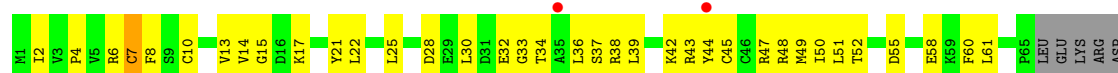
• Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3



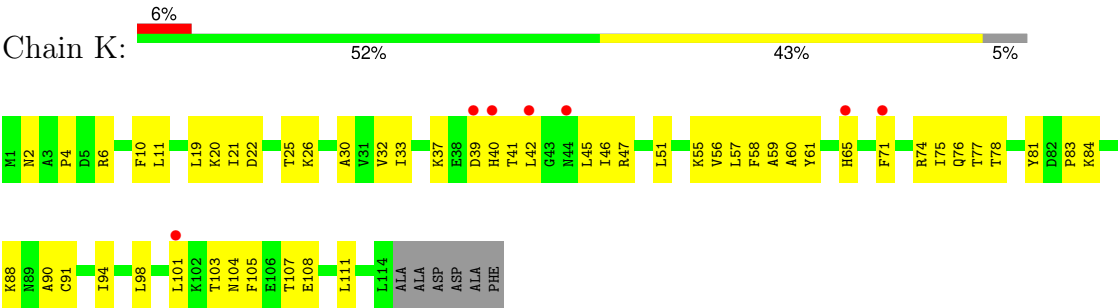
• Molecule 10: DNA-directed RNA polymerase II subunit RPB9



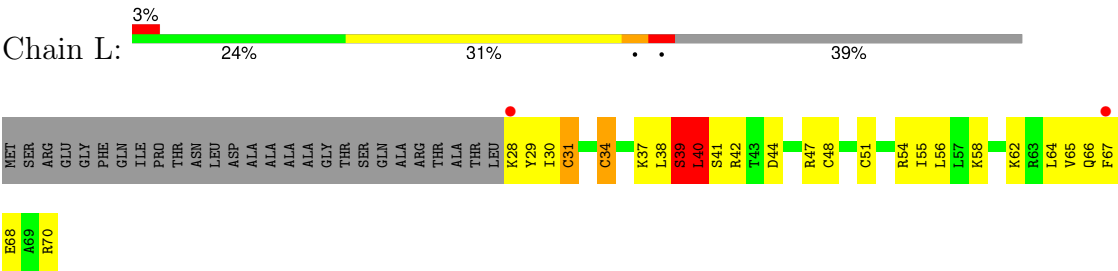
• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5



● Molecule 12: DNA-directed RNA polymerase II subunit RPB11



● Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC4



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	159.62Å 222.63Å 190.70Å 90.00° 97.69° 90.00°	Depositor
Resolution (Å)	47.96 – 3.78 47.96 – 3.78	Depositor EDS
% Data completeness (in resolution range)	97.6 (47.96-3.78) 97.5 (47.96-3.78)	Depositor EDS
R_{merge}	0.57	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 3.77Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.261 , 0.310 0.261 , 0.310	Depositor DCC
R_{free} test set	2000 reflections (2.61%)	wwPDB-VP
Wilson B-factor (Å ²)	112.7	Xtriage
Anisotropy	0.584	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 135.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	28985	wwPDB-VP
Average B, all atoms (Å ²)	148.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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: ZN, MG, ATP, WVQ

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	0.19	0/218	0.41	0/339
2	T	0.30	0/507	0.62	0/775
3	N	0.32	0/311	0.50	0/479
4	A	0.23	0/11020	0.51	1/14907 (0.0%)
5	B	0.21	0/9030	0.49	1/12186 (0.0%)
6	C	0.24	1/2139 (0.0%)	0.47	0/2899
7	E	0.26	0/1759	0.51	0/2367
8	F	0.19	0/696	0.46	0/943
9	H	0.21	0/1082	0.53	0/1466
10	I	0.23	0/970	0.55	0/1308
11	J	0.23	0/541	0.48	0/727
12	K	0.25	0/937	0.53	0/1265
13	L	0.97	2/333 (0.6%)	1.05	3/442 (0.7%)
All	All	0.25	3/29543 (0.0%)	0.51	5/40103 (0.0%)

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
13	L	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L	39	SER	C-O	-8.31	1.12	1.24
13	L	40	LEU	CG-CD2	-8.29	1.25	1.52
6	C	181	ASP	C-O	-5.40	1.21	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	39	SER	CA-C-O	-8.54	109.13	120.15
13	L	40	LEU	CB-CG-CD1	8.00	134.70	110.70
13	L	39	SER	CB-CA-C	7.37	122.48	111.06
4	A	622	VAL	N-CA-C	-6.09	106.56	112.29
5	B	1167	GLY	N-CA-C	-5.14	108.74	115.47

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	L	39	SER	Peptide
13	L	40	LEU	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	R	194	0	98	7	0
2	T	481	0	262	28	0
3	N	275	0	144	20	0
4	A	10828	0	10875	629	0
5	B	8859	0	8816	486	0
6	C	2101	0	2056	113	0
7	E	1724	0	1751	100	0
8	F	684	0	692	36	0
9	H	1064	0	1029	69	0
10	I	952	0	897	69	0
11	J	532	0	542	33	0
12	K	919	0	929	59	0
13	L	332	0	347	40	1
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	1	0	0	0	0
16	B	31	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	28985	0	28450	1505	1

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 26.

The worst 5 of 1505 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)
4:A:70:CYS:SG	4:A:80:HIS:CE1	2.58	0.96
4:A:613:ILE:HG21	9:H:102:TYR:HB3	1.49	0.93
4:A:881:GLN:HB2	4:A:956:LEU:HD12	1.52	0.92
5:B:892:LYS:NZ	5:B:904:ARG:O	2.07	0.88
4:A:1325:THR:HA	7:E:147:HIS:HA	1.57	0.87

All (1) 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)
13:L:39:SER:O	13:L:39:SER:O[2_555]	1.95	0.25

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	1370/1733 (79%)	1337 (98%)	33 (2%)	0	100	100
5	B	1103/1224 (90%)	1085 (98%)	18 (2%)	0	100	100
6	C	265/318 (83%)	261 (98%)	4 (2%)	0	100	100
7	E	210/215 (98%)	207 (99%)	3 (1%)	0	100	100
8	F	84/155 (54%)	81 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	H	129/146 (88%)	128 (99%)	1 (1%)	0	100	100
10	I	116/122 (95%)	112 (97%)	4 (3%)	0	100	100
11	J	63/70 (90%)	63 (100%)	0	0	100	100
12	K	112/120 (93%)	110 (98%)	2 (2%)	0	100	100
13	L	41/70 (59%)	37 (90%)	4 (10%)	0	100	100
All	All	3493/4173 (84%)	3421 (98%)	72 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	1194/1520 (79%)	1189 (100%)	5 (0%)	84	83
5	B	955/1061 (90%)	952 (100%)	3 (0%)	86	84
6	C	235/274 (86%)	234 (100%)	1 (0%)	84	83
7	E	192/197 (98%)	192 (100%)	0	100	100
8	F	73/137 (53%)	73 (100%)	0	100	100
9	H	116/128 (91%)	116 (100%)	0	100	100
10	I	110/116 (95%)	106 (96%)	4 (4%)	31	53
11	J	60/65 (92%)	59 (98%)	1 (2%)	53	67
12	K	99/102 (97%)	99 (100%)	0	100	100
13	L	36/57 (63%)	33 (92%)	3 (8%)	10	34
All	All	3070/3657 (84%)	3053 (99%)	17 (1%)	78	79

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	L	31	CYS
13	L	51	CYS

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Mol	Chain	Res	Type
5	B	1185	CYS
6	C	86	CYS
10	I	10	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
9	H	21	ASN
12	K	92	ASN
9	H	35	GLN
11	J	64	ASN
5	B	236	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	7/9 (77%)	3 (42%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	2	U
1	R	5	A
1	R	8	G

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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
2	WVQ	T	19	2	19,24,25	3.63	7 (36%)	18,33,36	1.58	4 (22%)

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
2	WVQ	T	19	2	-	4/6/40/41	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	19	WVQ	C5-N7	12.79	1.46	1.28
2	T	19	WVQ	C4-N9	4.65	1.45	1.35
2	T	19	WVQ	C2-N2	4.18	1.45	1.34
2	T	19	WVQ	C6-C5	-4.05	1.36	1.47
2	T	19	WVQ	C6-N1	-3.11	1.32	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	19	WVQ	N3-C2-N1	-4.45	119.39	126.44
2	T	19	WVQ	N2-C2-N3	2.34	120.30	116.57
2	T	19	WVQ	N9-C4-N3	-2.08	116.60	119.70
2	T	19	WVQ	N2-C2-N1	2.08	120.31	117.09

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	19	WVQ	C3'-C4'-C5'-O5'
2	T	19	WVQ	O4'-C4'-C5'-O5'
2	T	19	WVQ	O4'-C1'-N9-C4
2	T	19	WVQ	C4'-C5'-O5'-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	19	WVQ	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 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	1302	-	32,33,33	0.28	0	48,52,52	0.37	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
16	ATP	B	1302	-	-	6/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

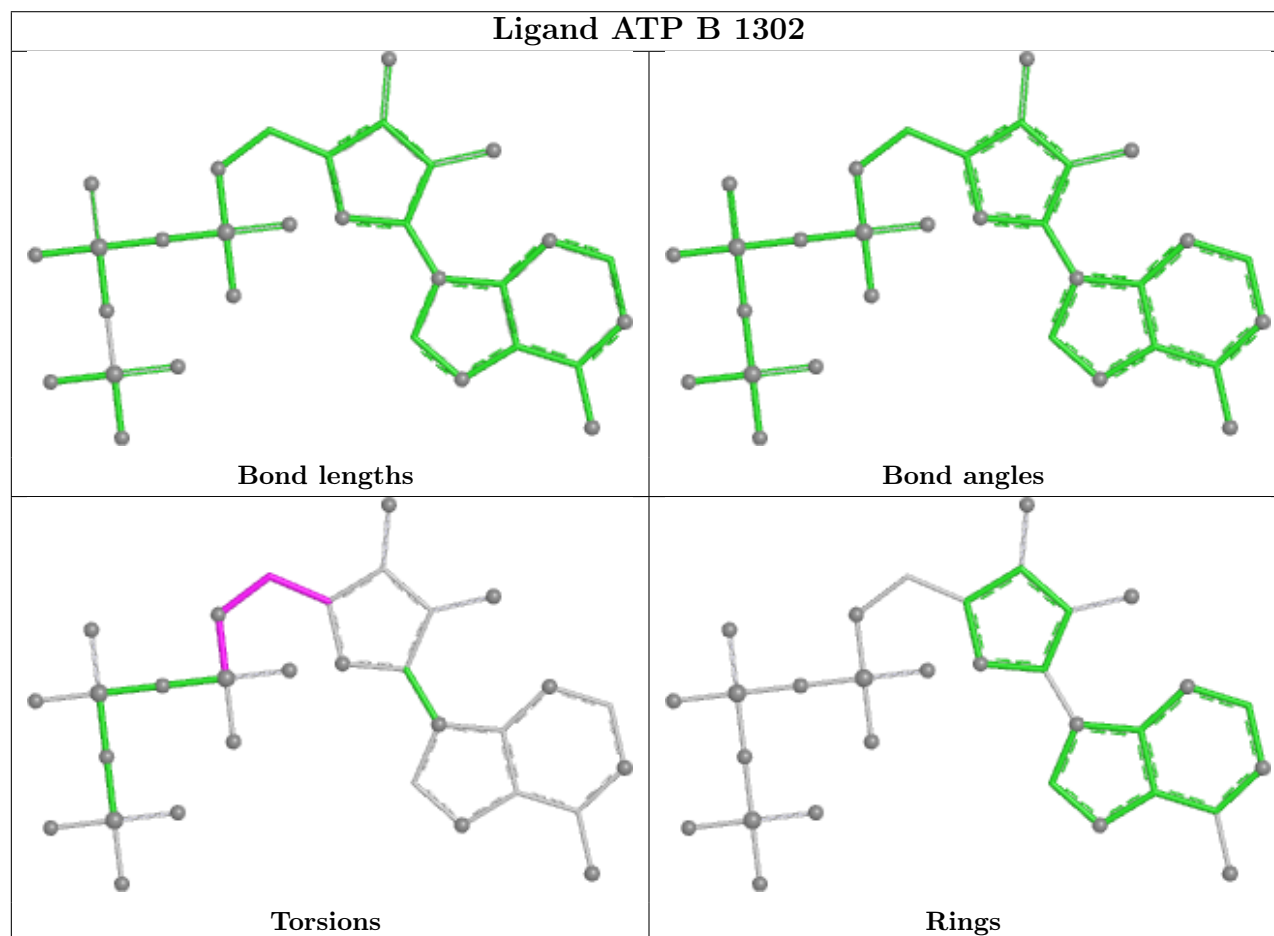
Mol	Chain	Res	Type	Atoms
16	B	1302	ATP	C5'-O5'-PA-O1A
16	B	1302	ATP	C5'-O5'-PA-O2A
16	B	1302	ATP	C5'-O5'-PA-O3A
16	B	1302	ATP	O4'-C4'-C5'-O5'
16	B	1302	ATP	C4'-C5'-O5'-PA

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	1302	ATP	3	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	R	9/9 (100%)	-0.11	0	100	100	111, 134, 207, 245	0
2	T	23/29 (79%)	0.20	0	100	100	113, 216, 300, 320	0
3	N	13/18 (72%)	0.19	0	100	100	215, 252, 297, 312	0
4	A	1384/1733 (79%)	0.25	51 (3%)	45	31	81, 142, 221, 332	0
5	B	1123/1224 (91%)	0.34	54 (4%)	35	26	61, 131, 197, 288	0
6	C	267/318 (83%)	0.31	11 (4%)	41	29	58, 119, 186, 246	0
7	E	212/215 (98%)	0.10	7 (3%)	49	33	126, 174, 259, 319	0
8	F	86/155 (55%)	0.02	3 (3%)	47	32	90, 134, 191, 258	0
9	H	133/146 (91%)	0.06	0	100	100	96, 162, 229, 346	0
10	I	118/122 (96%)	0.14	0	100	100	114, 171, 225, 258	0
11	J	65/70 (92%)	0.38	2 (3%)	51	34	68, 118, 167, 225	0
12	K	114/120 (95%)	0.10	7 (6%)	27	22	72, 122, 173, 199	0
13	L	43/70 (61%)	0.52	2 (4%)	36	26	112, 255, 330, 400	0
All	All	3590/4229 (84%)	0.26	137 (3%)	44	31	58, 139, 227, 400	0

The worst 5 of 137 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	B	543	SER	6.3
5	B	779	GLY	6.2
5	B	775	LYS	5.8
4	A	1010	ALA	4.9
7	E	93	MET	4.7

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	WVQ	T	19	23/24	0.84	0.11	171,184,201,215	0

6.3 Carbohydrates [i](#)

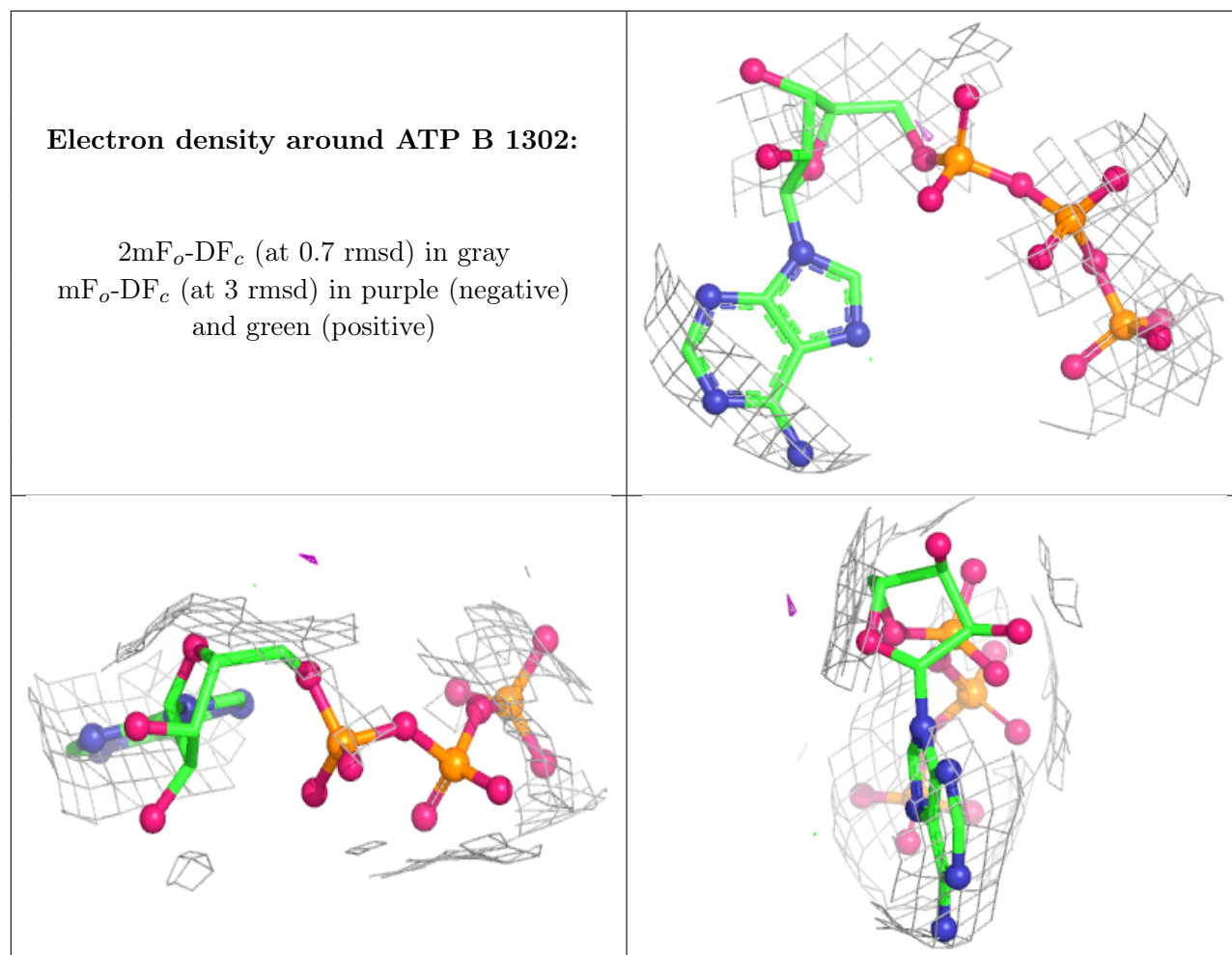
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
16	ATP	B	1302	31/31	0.72	0.10	140,168,215,232	0
15	MG	A	1803	1/1	0.88	0.05	107,107,107,107	0
14	ZN	L	101	1/1	0.88	0.09	369,369,369,369	0
14	ZN	A	1801	1/1	0.89	0.05	342,342,342,342	0
14	ZN	I	202	1/1	0.90	0.08	287,287,287,287	0
14	ZN	I	201	1/1	0.93	0.06	216,216,216,216	0
14	ZN	B	1301	1/1	0.96	0.04	216,216,216,216	0
14	ZN	A	1802	1/1	0.96	0.04	208,208,208,208	0
14	ZN	C	401	1/1	0.97	0.05	158,158,158,158	0
14	ZN	J	101	1/1	0.99	0.05	115,115,115,115	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 ⓘ

There are no such residues in this entry.