



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 08:42 am BST

PDB ID : 1TWH
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

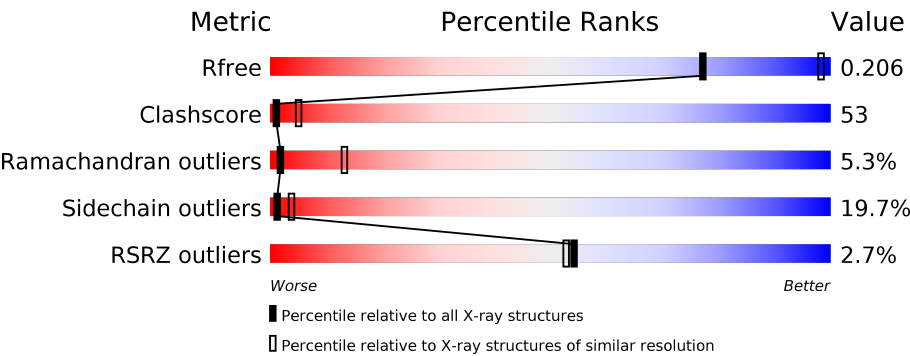
1 Overall quality at a glance i

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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 on 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	<div><div>2%</div><div><div></div><div>7%</div><div>32%</div><div>28%</div><div>11%</div><div>22%</div></div></div>
2	B	1224	<div><div>4%</div><div><div></div><div>6%</div><div>37%</div><div>34%</div><div>12%</div><div>11%</div></div></div>
3	C	318	<div><div></div><div><div></div><div>7%</div><div>30%</div><div>34%</div><div>14%</div><div>16%</div></div></div>
4	E	215	<div><div>2%</div><div><div></div><div>5%</div><div>35%</div><div>40%</div><div>20%</div></div></div>
5	F	155	<div><div></div><div><div></div><div>%</div><div>22%</div><div>23%</div><div>5%</div><div>46%</div></div></div>
6	H	146	<div><div>5%</div><div><div></div><div>•</div><div>19%</div><div>36%</div><div>34%</div><div>9%</div></div></div>

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Mol	Chain	Length	Quality of chain
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

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 (three-letter code: MN) (formula: Mn).

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

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

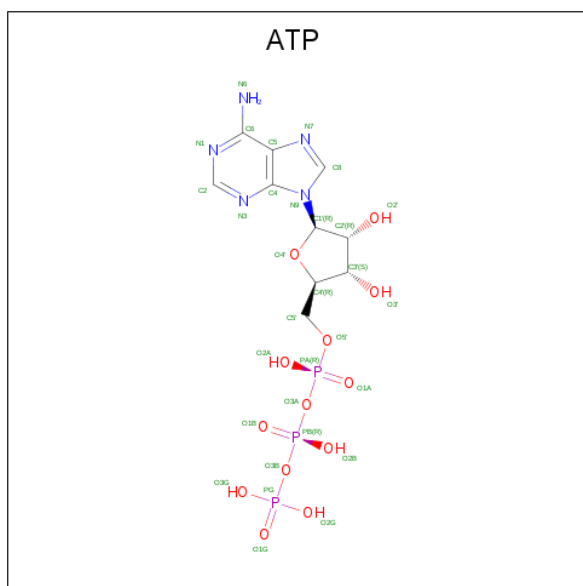
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	J	1	Total	Zn	0	0
			1	1		
12	B	1	Total	Zn	0	0
			1	1		

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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

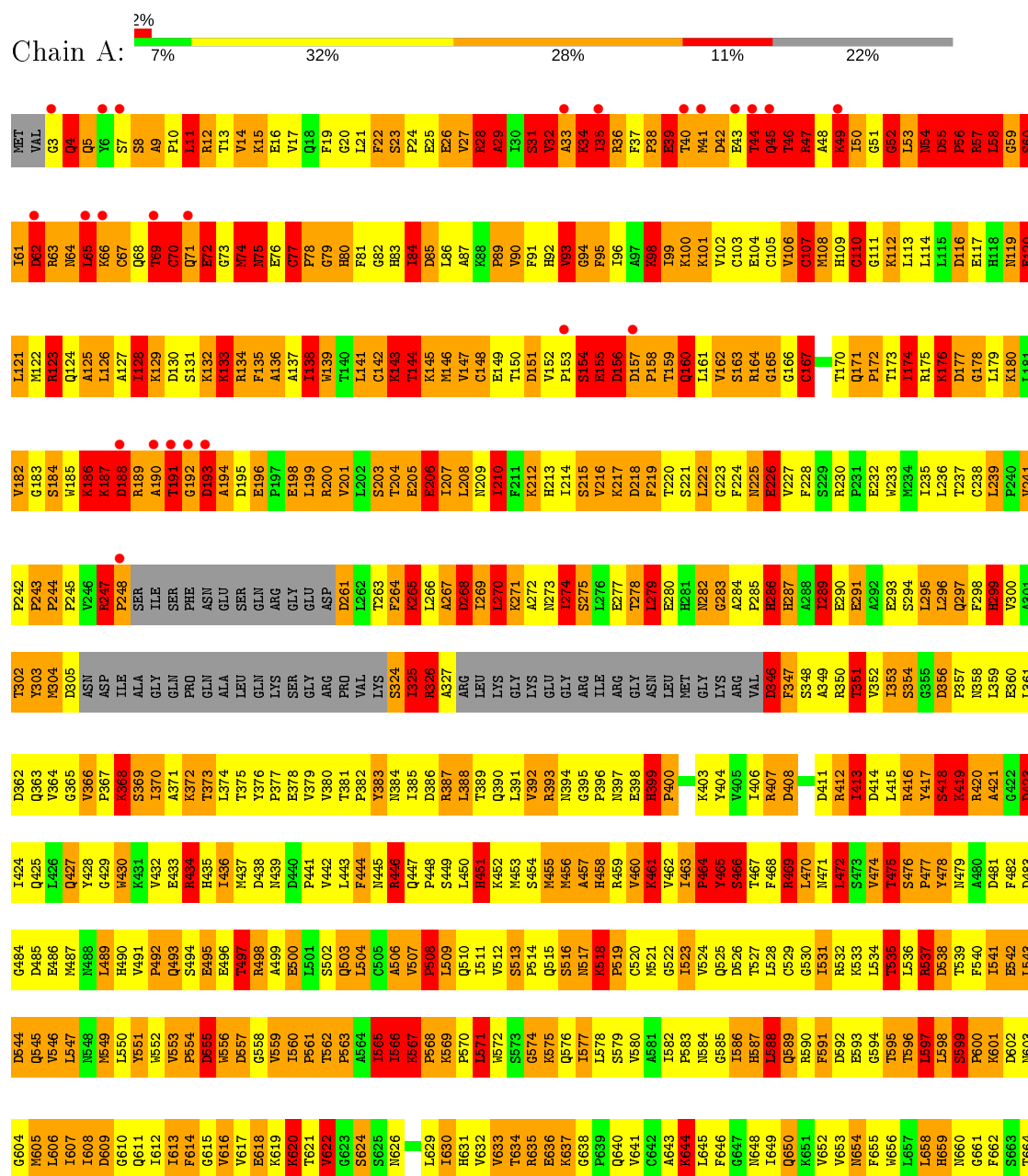
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	B	1	Total	O	0	0
			1	1		

3 Residue-property plots

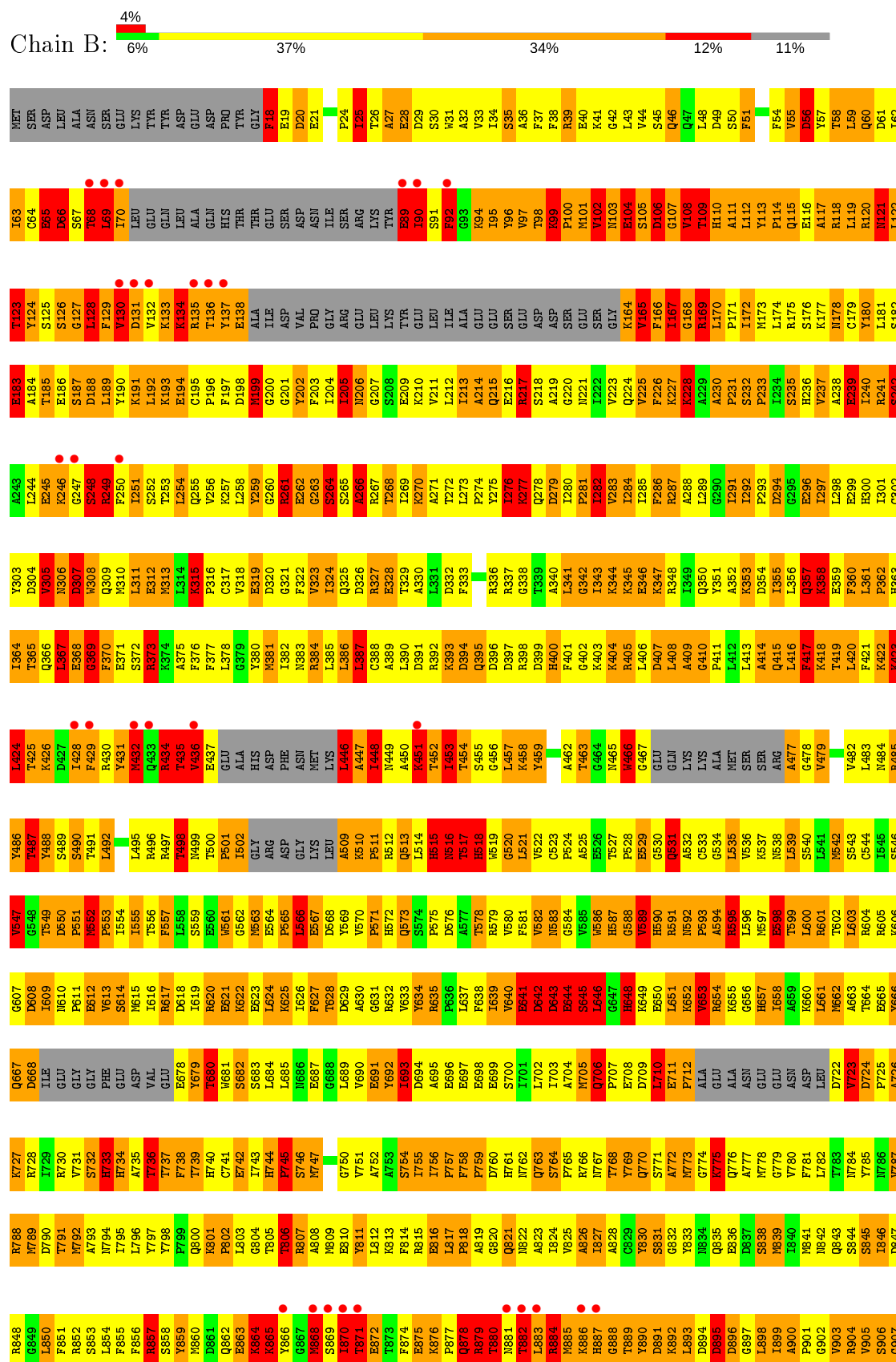
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

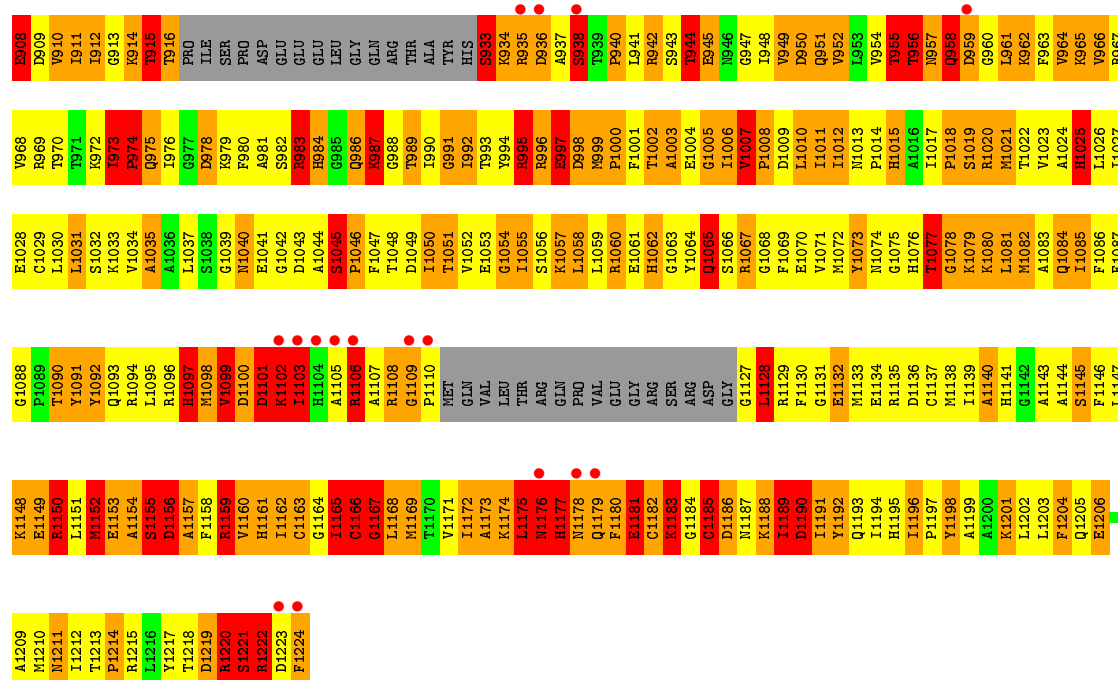
- Molecule 1: DNA-directed RNA polymerase II largest subunit





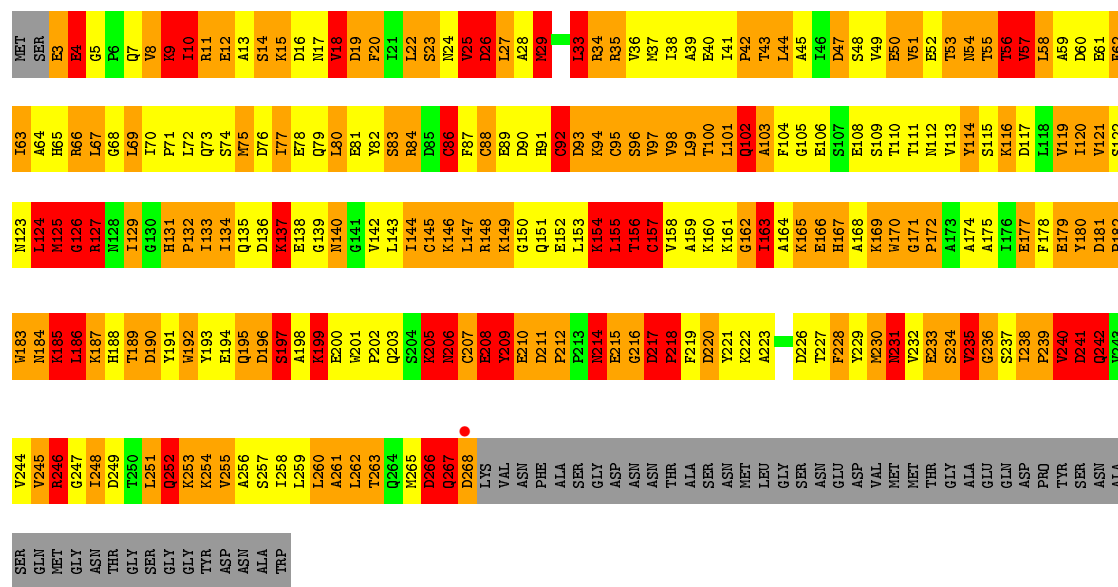
● Molecule 2: DNA-directed RNA polymerase II 140 kDa polypeptide





• Molecule 3: DNA-directed RNA polymerase II 45 kDa polypeptide

Chain C: 7% 30% 34% 14% 16%

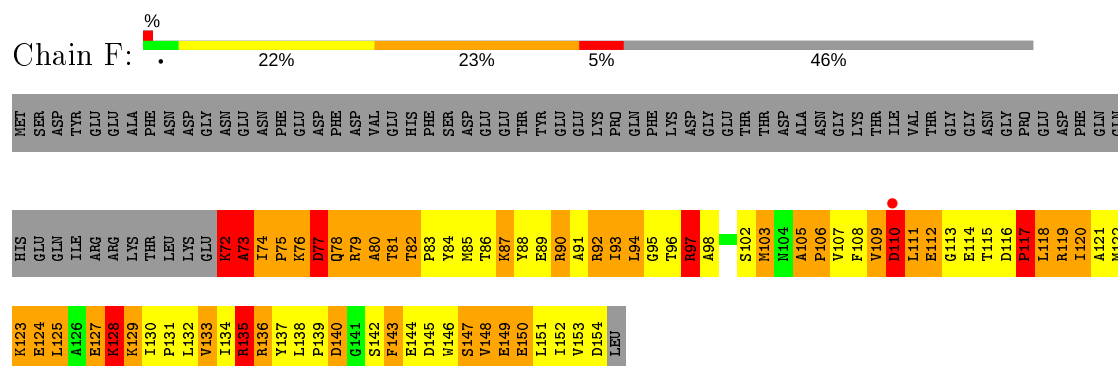


• Molecule 4: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

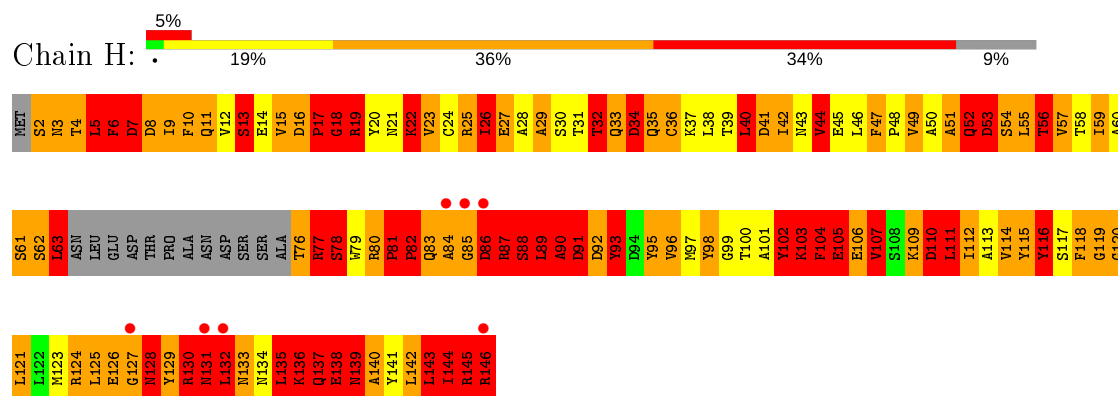
Chain E: 2% 5% 35% 40% 20%



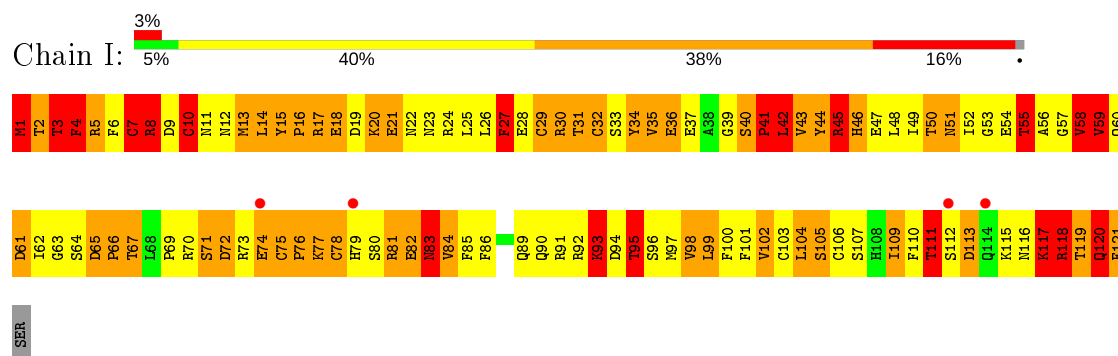
- Molecule 5: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide



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

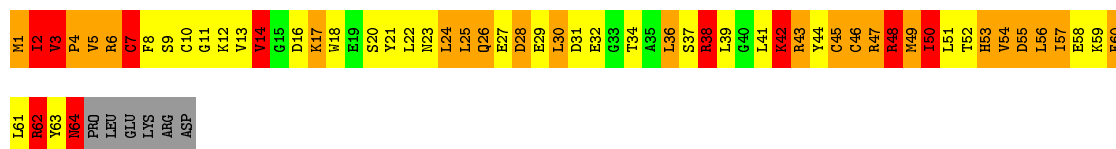


- Molecule 7: DNA-directed RNA polymerase II 14.2 kDa polypeptide



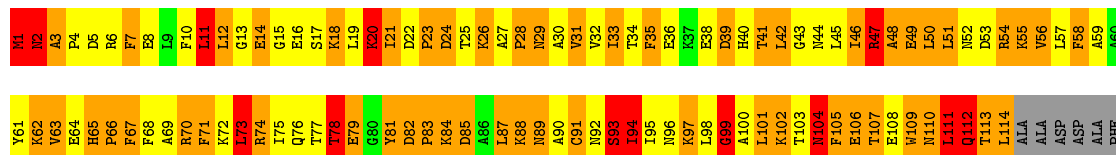
- Molecule 8: DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide





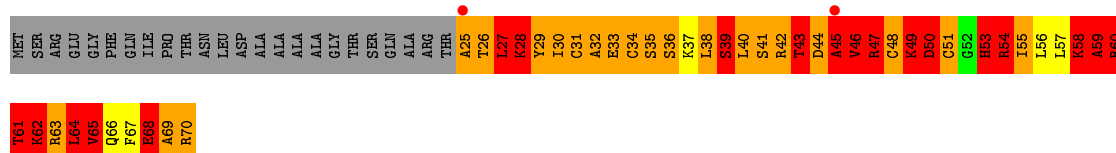
- Molecule 9: DNA-directed RNA polymerase II 13.6 kDa polypeptide

Chain K: . 35% 45% 11% 5%



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

Chain L: . 3% 7% 30% 27% 34%



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	123.00 Å 223.00 Å 374.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.40 39.69 – 3.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.40) 97.3 (39.69-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 3.32 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.262 0.191 , 0.206	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)	0.26 , 50.1	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	4.62	2331/10792 (21.6%)	3.06	1145/14601 (7.8%)
2	B	4.57	1918/8860 (21.6%)	3.01	930/11945 (7.8%)
3	C	4.57	476/2133 (22.3%)	2.99	227/2891 (7.9%)
4	E	4.64	405/1796 (22.6%)	2.92	193/2416 (8.0%)
5	F	4.01	117/682 (17.2%)	3.01	56/922 (6.1%)
6	H	4.54	246/1086 (22.7%)	2.94	113/1470 (7.7%)
7	I	5.00	250/1009 (24.8%)	3.19	124/1357 (9.1%)
8	J	4.42	116/533 (21.8%)	3.66	79/715 (11.0%)
9	K	4.36	210/937 (22.4%)	3.12	108/1265 (8.5%)
10	L	5.55	101/366 (27.6%)	3.72	71/485 (14.6%)
All	All	4.60	6170/28194 (21.9%)	3.05	3046/38067 (8.0%)

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
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 6170 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1064	VAL	C-O	33.98	1.88	1.23
10	L	68	GLU	CG-CD	32.08	2.00	1.51
1	A	1064	VAL	CA-C	31.22	2.34	1.52
1	A	734	GLU	CD-OE2	30.34	1.59	1.25
2	B	552	MET	CG-SD	28.64	2.55	1.81

The worst 5 of 3046 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1064	VAL	CA-C-O	-35.84	44.85	120.10
5	F	136	ARG	NE-CZ-NH1	-34.13	103.24	120.30
1	A	774	ARG	NE-CZ-NH1	32.04	136.32	120.30
1	A	1064	VAL	O-C-N	-31.34	69.93	123.20
1	A	821	ARG	NE-CZ-NH2	-29.52	105.54	120.30

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

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	10662	1054	0
2	B	8690	0	8707	918	0
3	C	2095	0	2054	226	0
4	E	1760	0	1788	222	0
5	F	670	0	689	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	1068	0	1040	220	0
7	I	990	0	948	101	0
8	J	525	0	537	61	0
9	K	919	0	928	108	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	27749	2914	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 53.

The worst 5 of 2914 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:CG	2:B:137:TYR:CB	1.77	1.66
9:K:26:LYS:CE	9:K:26:LYS:CD	1.74	1.66
1:A:1225:PHE:CG	1:A:1225:PHE:CB	1.78	1.65
2:B:884:ARG:CG	2:B:884:ARG:CD	1.75	1.64
1:A:977:LYS:CD	1:A:977:LYS:CG	1.74	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%)	2	14
2	B	1071/1224 (88%)	914 (85%)	110 (10%)	47 (4%)	2	16
3	C	264/318 (83%)	230 (87%)	22 (8%)	12 (4%)	2	16
4	E	213/215 (99%)	182 (85%)	20 (9%)	11 (5%)	2	13
5	F	81/155 (52%)	72 (89%)	7 (9%)	2 (2%)	5	26
6	H	129/146 (88%)	82 (64%)	21 (16%)	26 (20%)	0	0
7	I	119/122 (98%)	107 (90%)	11 (9%)	1 (1%)	19	51
8	J	62/70 (89%)	58 (94%)	3 (5%)	1 (2%)	9	34
9	K	112/120 (93%)	99 (88%)	9 (8%)	4 (4%)	3	21
10	L	44/70 (63%)	24 (54%)	9 (20%)	11 (25%)	0	0
All	All	3427/4173 (82%)	2941 (86%)	305 (9%)	181 (5%)	2	13

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%)	971 (82%)	210 (18%)	2	6
2	B	947/1061 (89%)	788 (83%)	159 (17%)	2	8
3	C	234/274 (85%)	194 (83%)	40 (17%)	2	8
4	E	197/197 (100%)	145 (74%)	52 (26%)	0	1
5	F	73/137 (53%)	62 (85%)	11 (15%)	3	12
6	H	117/128 (91%)	71 (61%)	46 (39%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	I	115/116 (99%)	82 (71%)	33 (29%)	0	1
8	J	59/65 (91%)	45 (76%)	14 (24%)	1	2
9	K	99/102 (97%)	81 (82%)	18 (18%)	1	6
10	L	40/57 (70%)	21 (52%)	19 (48%)	0	0
All	All	3062/3657 (84%)	2460 (80%)	602 (20%)	1	4

5 of 602 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	463	THR
2	B	996	ARG
8	J	20	SER
2	B	531	GLN
2	B	802	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	366	GLN
2	B	590	HIS
7	I	46	HIS
2	B	395	GLN
2	B	516	ASN

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 carbohydrates 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	26,32,33	1.05	2 (7%)	30,50,52	1.51	6 (20%)

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	5/18/34/38	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	3.60	1.40	1.35
13	A	3011	ATP	C8-N7	-2.60	1.30	1.34

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'-C2'	3.62	113.08	106.25
13	A	3011	ATP	PA-O3A-PB	-3.55	120.63	132.83
13	A	3011	ATP	PB-O3B-PG	-3.43	121.06	132.83
13	A	3011	ATP	C2'-C1'-N9	2.67	120.42	114.27
13	A	3011	ATP	C4-C5-N7	2.59	112.10	109.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	3011	ATP	C1'

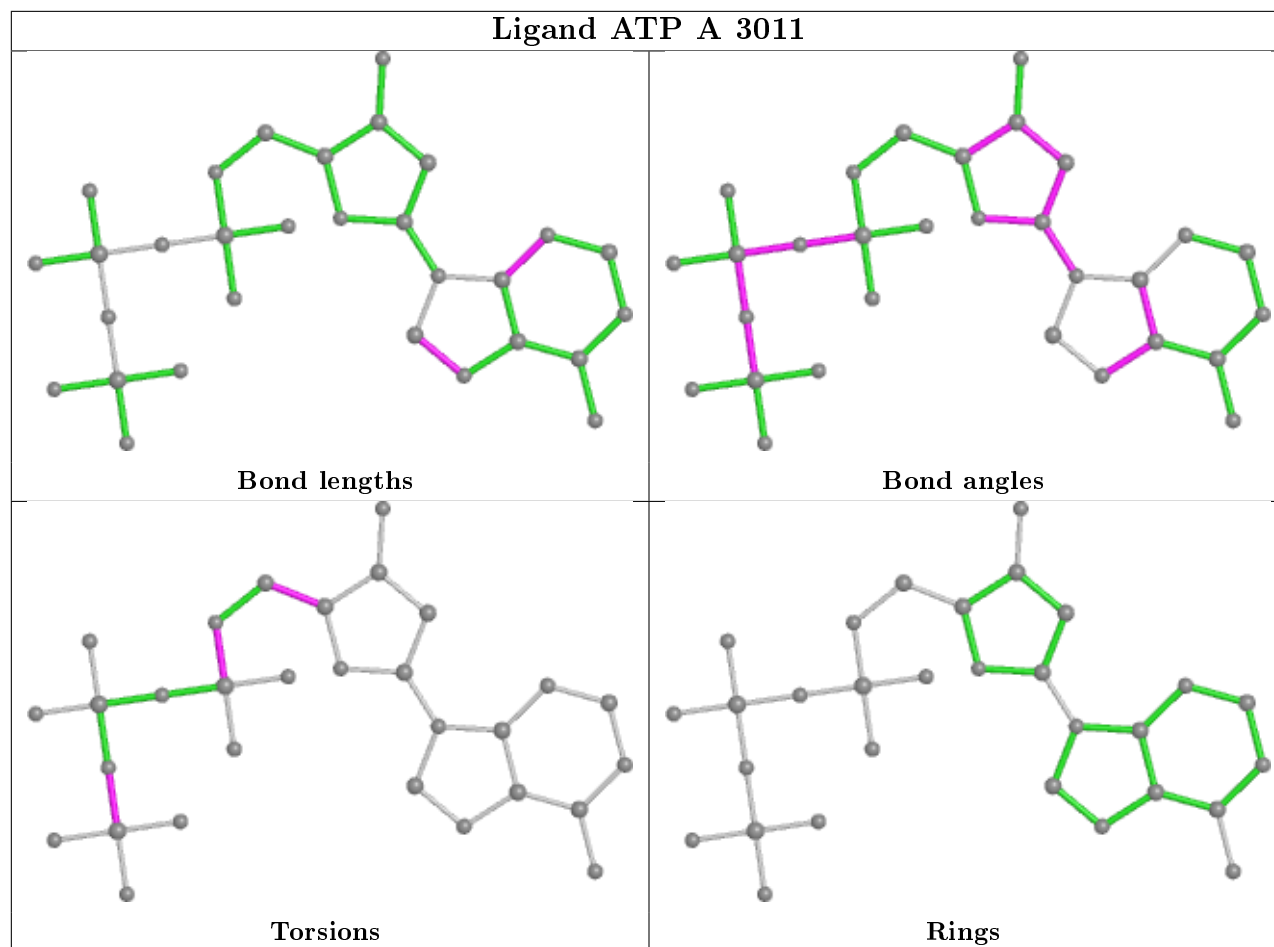
All (5) torsion outliers are listed below:

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	PB-O3B-PG-O2G
13	A	3011	ATP	PB-O3B-PG-O3G
13	A	3011	ATP	C5'-O5'-PA-O3A

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
7	I	2
3	C	2
8	J	1
9	K	1
5	F	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 ⓘ

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	1349/1733 (77%)	-0.34	27 (2%) 65 64	1, 22, 99, 165	0
2	B	1091/1224 (89%)	-0.31	47 (4%) 35 35	1, 22, 107, 155	0
3	C	266/318 (83%)	-0.53	1 (0%) 92 92	1, 22, 72, 145	0
4	E	215/215 (100%)	-0.30	4 (1%) 66 65	1, 40, 102, 138	0
5	F	83/155 (53%)	-0.33	1 (1%) 79 77	1, 21, 63, 89	0
6	H	133/146 (91%)	0.17	7 (5%) 26 27	14, 65, 120, 167	0
7	I	121/122 (99%)	-0.17	4 (3%) 46 45	1, 30, 79, 120	0
8	J	64/70 (91%)	-0.50	0 100 100	3, 18, 64, 91	0
9	K	114/120 (95%)	-0.32	0 100 100	1, 32, 72, 103	0
10	L	46/70 (65%)	0.10	2 (4%) 35 35	16, 72, 123, 140	0
All	All	3482/4173 (83%)	-0.31	93 (2%) 54 53	1, 25, 103, 167	0

The worst 5 of 93 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	69	THR	7.8
2	B	882	THR	6.9
2	B	1109	GLY	6.6
1	A	1450	LEU	6.2
1	A	1449	SER	6.2

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

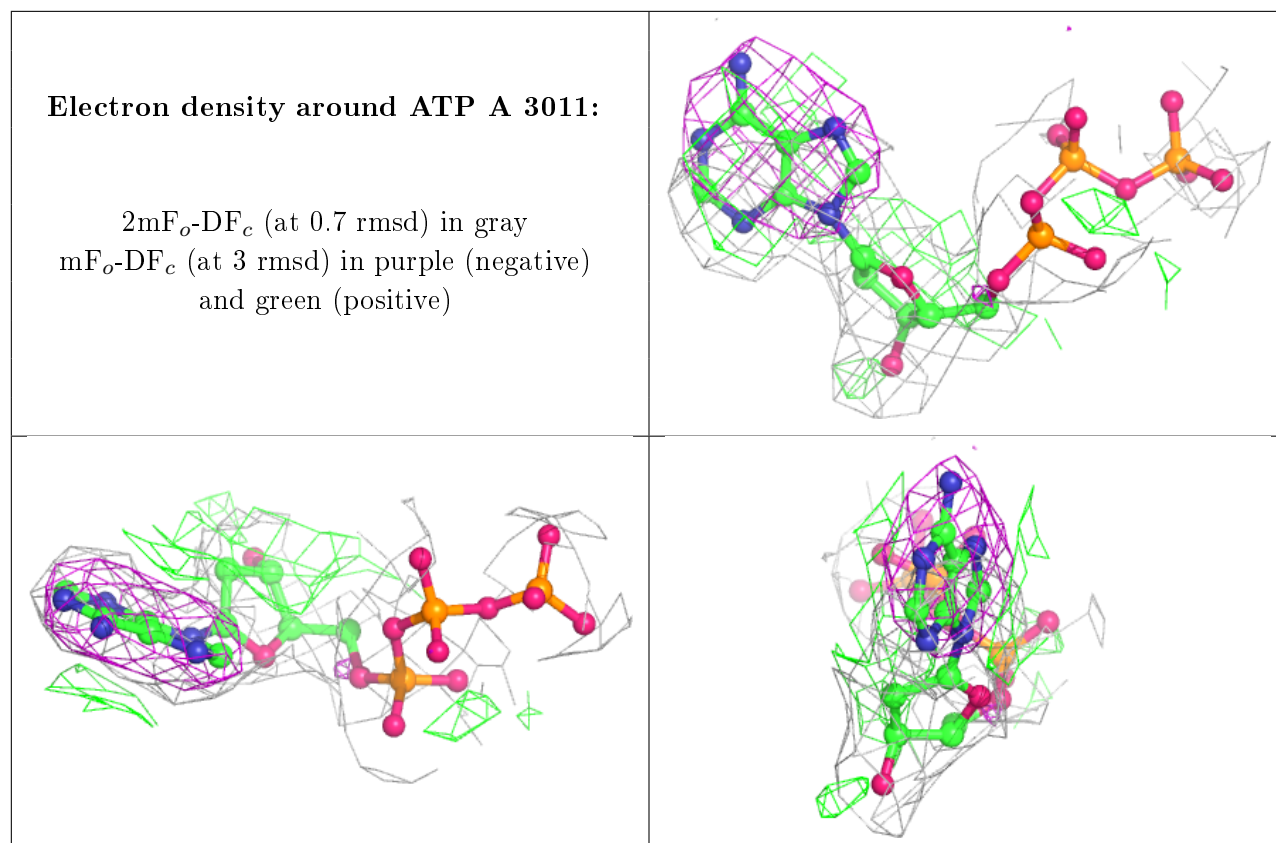
There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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(\AA^2)	Q<0.9
13	ATP	A	3011	30/31	0.80	0.30	5,46,82,85	0
12	ZN	I	3004	1/1	0.94	0.08	66,66,66,66	0
11	MN	A	3009	1/1	0.94	0.09	4,4,4,4	0
12	ZN	A	3006	1/1	0.95	0.05	47,47,47,47	0
12	ZN	J	3001	1/1	0.95	0.06	34,34,34,34	0
12	ZN	A	3008	1/1	0.95	0.05	91,91,91,91	0
12	ZN	L	3005	1/1	0.96	0.11	90,90,90,90	0
11	MN	A	3010	1/1	0.97	0.05	12,12,12,12	0
12	ZN	I	3003	1/1	0.98	0.03	46,46,46,46	0
12	ZN	C	3002	1/1	0.98	0.07	42,42,42,42	0
12	ZN	B	3007	1/1	0.98	0.06	57,57,57,57	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.