Preliminary Full wwPDB EM Validation Report ⓘ

Nov 17, 2025 – 08:07 AM EST

This wwPDB validation report is NOT for manuscript review

This is a Preliminary Full wwPDB EM Validation Report.

This report is produced by the standalone wwPDB validation server.
The structure in question has not been deposited to the wwPDB.
This report should not be submitted to journals.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
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)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

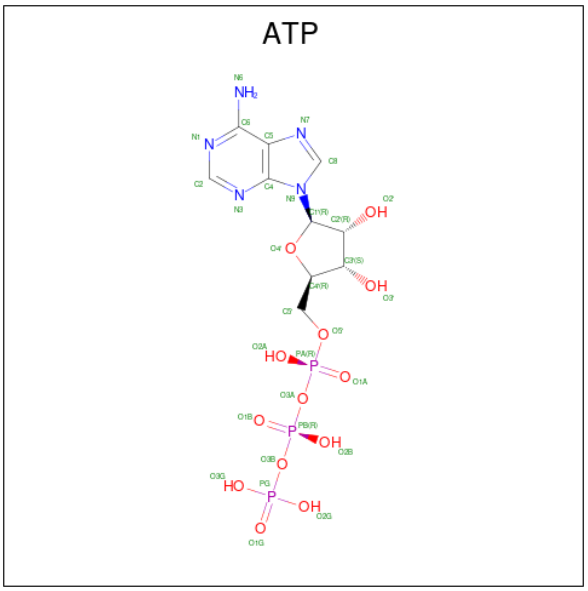
There are no overall percentile quality scores available for this entry.

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 186 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
1	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
1	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
1	F	1	Total	C	N	O	P	0
			31	10	5	13	3	
1	X	1	Total	C	N	O	P	0
			31	10	5	13	3	
1	e	1	Total	C	N	O	P	0
			31	10	5	13	3	
1	f	1	Total	C	N	O	P	0
			31	10	5	13	3	

3 Residue-property plots (i)

There is no protein, DNA or RNA chain in this entry to show sequence plots.

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	
Number of images used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	Not provided	
Voltage (kV)	Not provided	
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	Not provided	

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein molecules in this entry.

5.3.2 Protein sidechains

There are no protein molecules in this entry.

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 (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are 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	$\#\|Z\| > 2$
1	ATP	F	501	-	28,33,33	0.97	0	34,52,52	1.40	4 (11%)
1	ATP	D	501	-	28,33,33	1.06	0	34,52,52	1.30	2 (5%)
1	ATP	E	401	-	28,33,33	0.96	0	34,52,52	1.24	5 (14%)
1	ATP	f	501	-	28,33,33	1.00	1 (3%)	34,52,52	1.26	2 (5%)
1	ATP	e	401	-	28,33,33	0.87	0	34,52,52	1.30	5 (14%)
1	ATP	X	501	-	28,33,33	0.87	0	34,52,52	1.23	2 (5%)

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
1	ATP	F	501	-	-	4/18/38/38	0/3/3/3
1	ATP	D	501	-	-	6/18/38/38	0/3/3/3
1	ATP	E	401	-	-	4/18/38/38	0/3/3/3
1	ATP	f	501	-	-	5/18/38/38	0/3/3/3
1	ATP	e	401	-	-	3/18/38/38	0/3/3/3
1	ATP	X	501	-	-	5/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	f	501	ATP	PA-O3A	-2.04	1.57	1.59

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	501	ATP	N3-C2-N1	-4.64	122.37	128.67
1	D	501	ATP	N3-C2-N1	-4.08	123.14	128.67
1	f	501	ATP	N3-C2-N1	-4.02	123.21	128.67
1	e	401	ATP	N3-C2-N1	-3.83	123.48	128.67
1	X	501	ATP	N3-C2-N1	-3.70	123.65	128.67
1	E	401	ATP	N3-C2-N1	-3.61	123.77	128.67
1	e	401	ATP	C4-C5-N7	-2.74	106.44	109.34
1	e	401	ATP	C4'-O4'-C1'	-2.55	107.59	109.92
1	D	501	ATP	C4-C5-N7	-2.49	106.71	109.34
1	X	501	ATP	C4-C5-N7	-2.34	106.86	109.34
1	E	401	ATP	C4-C5-N7	-2.26	106.95	109.34
1	F	501	ATP	O3G-PG-O2G	2.21	116.09	107.80
1	e	401	ATP	O3A-PA-O1A	-2.20	104.09	110.70
1	F	501	ATP	C4-C5-N7	-2.16	107.06	109.34
1	E	401	ATP	O3G-PG-O2G	2.15	115.86	107.80
1	f	501	ATP	C4-C5-N7	-2.14	107.07	109.34
1	E	401	ATP	O3A-PA-O1A	-2.05	104.55	110.70
1	E	401	ATP	O2B-PB-O1B	2.02	121.83	112.44
1	F	501	ATP	C5'-C4'-C3'	-2.02	107.95	115.21
1	e	401	ATP	O3G-PG-O2G	2.01	115.35	107.80

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	501	ATP	C5'-O5'-PA-O1A
1	D	501	ATP	C5'-O5'-PA-O2A
1	D	501	ATP	C5'-O5'-PA-O3A
1	E	401	ATP	C5'-O5'-PA-O2A
1	E	401	ATP	C5'-O5'-PA-O3A
1	F	501	ATP	PB-O3B-PG-O3G
1	X	501	ATP	C5'-O5'-PA-O2A
1	X	501	ATP	C5'-O5'-PA-O3A
1	X	501	ATP	O4'-C4'-C5'-O5'
1	e	401	ATP	C4'-C5'-O5'-PA
1	f	501	ATP	C5'-O5'-PA-O2A
1	f	501	ATP	C5'-O5'-PA-O3A
1	D	501	ATP	O4'-C4'-C5'-O5'
1	D	501	ATP	C3'-C4'-C5'-O5'
1	X	501	ATP	C3'-C4'-C5'-O5'
1	f	501	ATP	C3'-C4'-C5'-O5'

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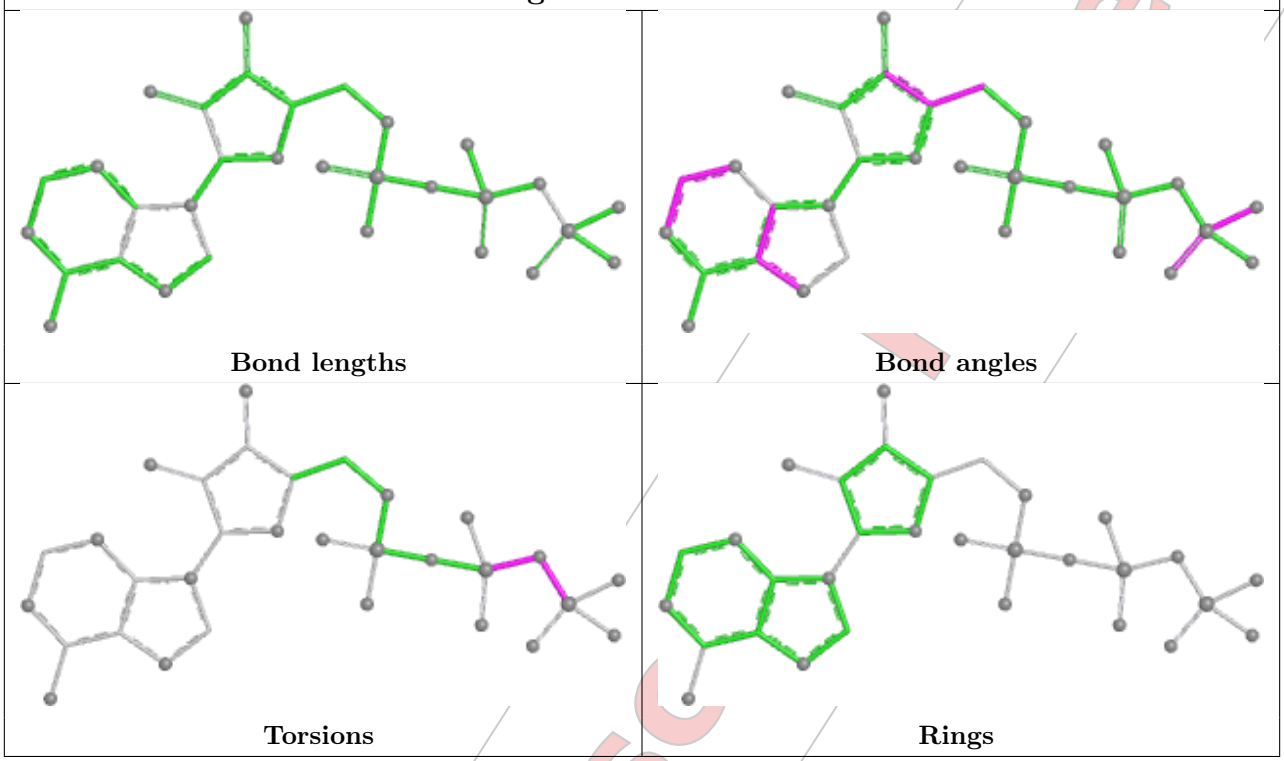
Mol	Chain	Res	Type	Atoms
1	f	501	ATP	O4'-C4'-C5'-O5'
1	X	501	ATP	C4'-C5'-O5'-PA
1	F	501	ATP	PG-O3B-PB-O1B
1	e	401	ATP	PG-O3B-PB-O1B
1	e	401	ATP	C5'-O5'-PA-O3A
1	F	501	ATP	PG-O3B-PB-O2B
1	F	501	ATP	PB-O3B-PG-O1G
1	D	501	ATP	PG-O3B-PB-O2B
1	E	401	ATP	PB-O3A-PA-O1A
1	E	401	ATP	PB-O3A-PA-O2A
1	f	501	ATP	PG-O3B-PB-O1B

There are no ring outliers.

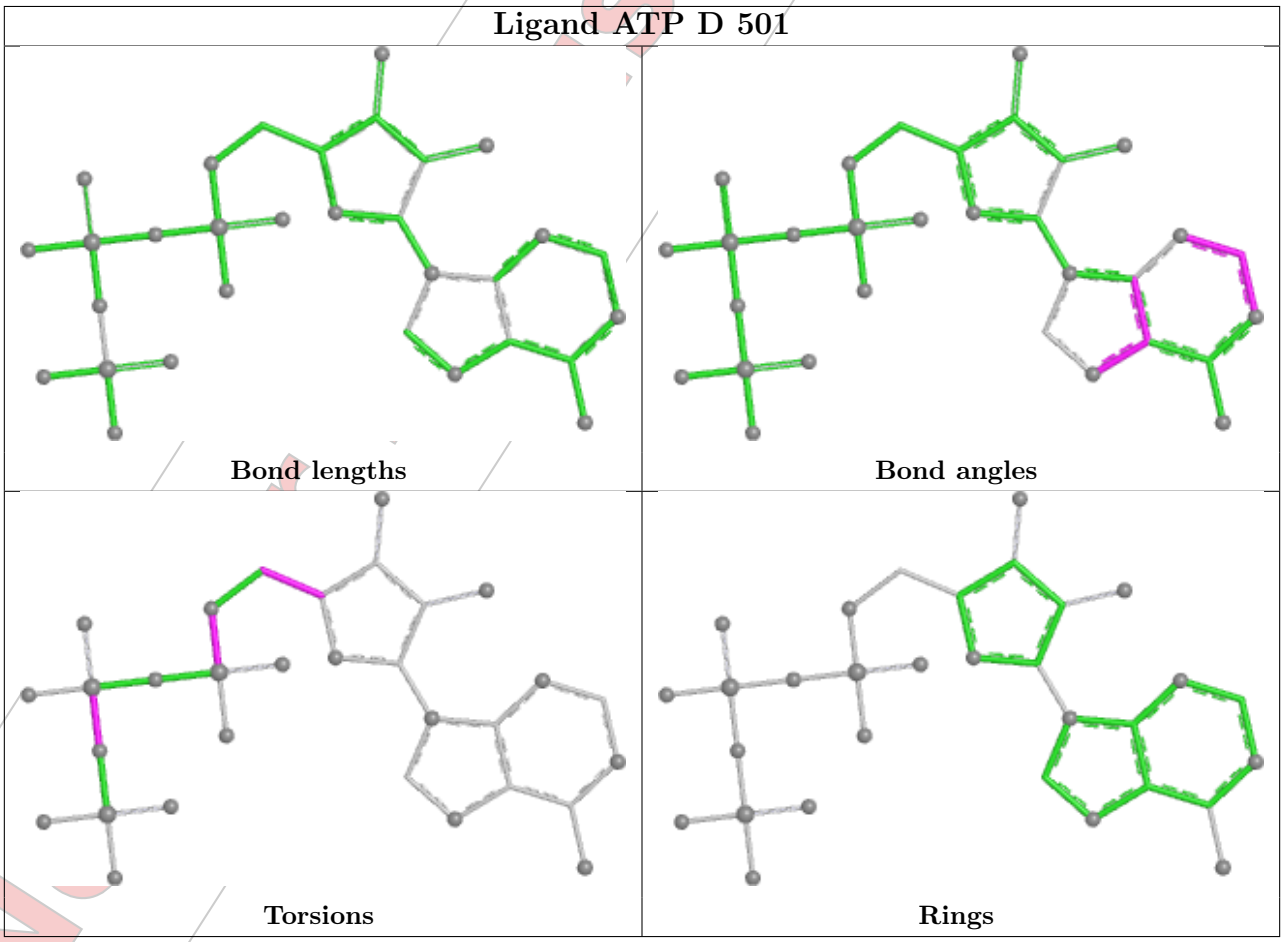
No monomer is involved in short contacts.

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 then 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.

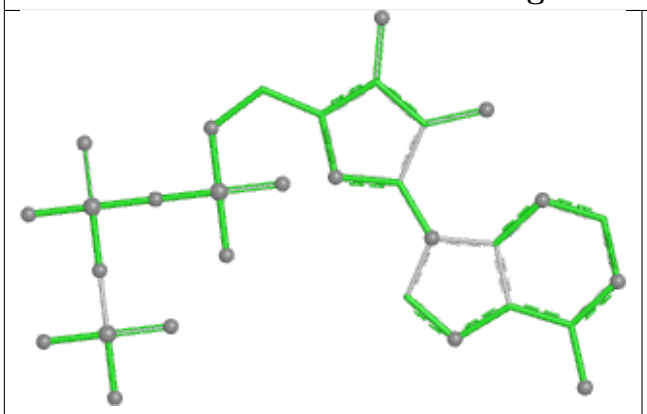
Ligand ATP F 501



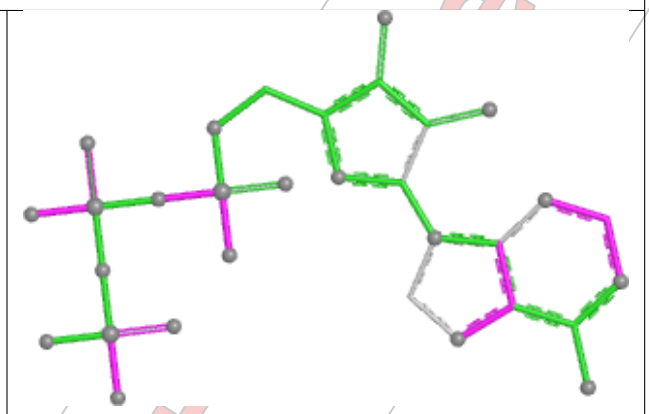
Ligand ATP D 501



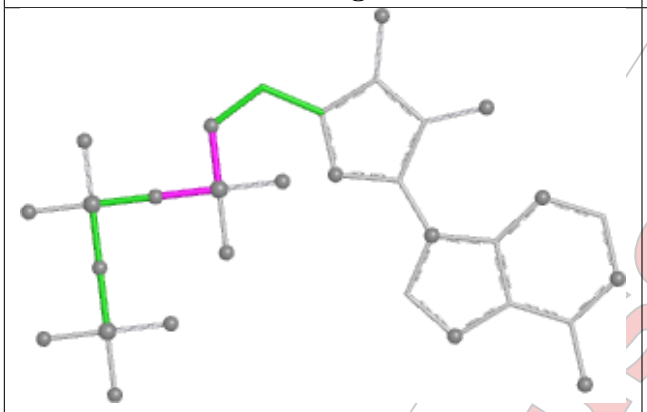
Ligand ATP E 401



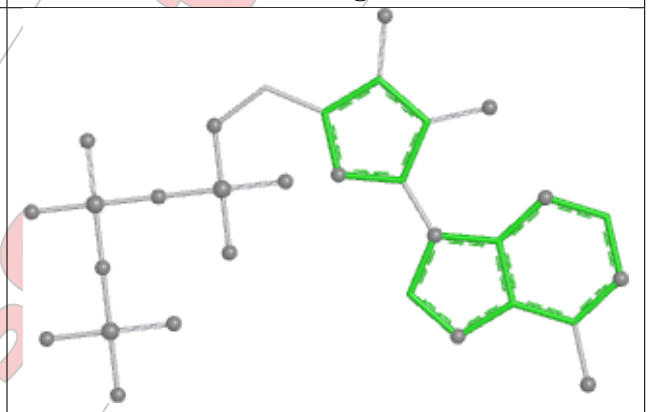
Bond lengths



Bond angles

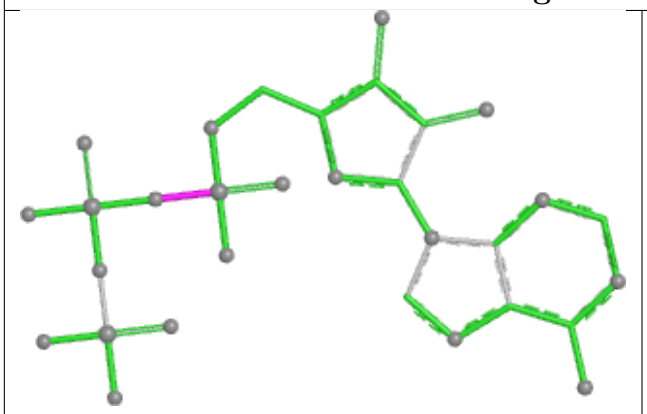


Torsions

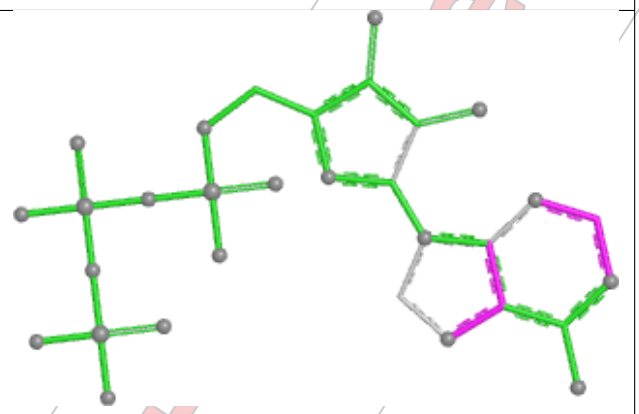


Rings

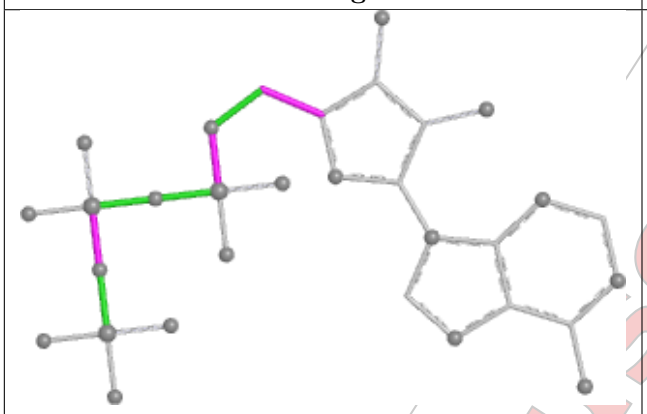
Ligand ATP f 501



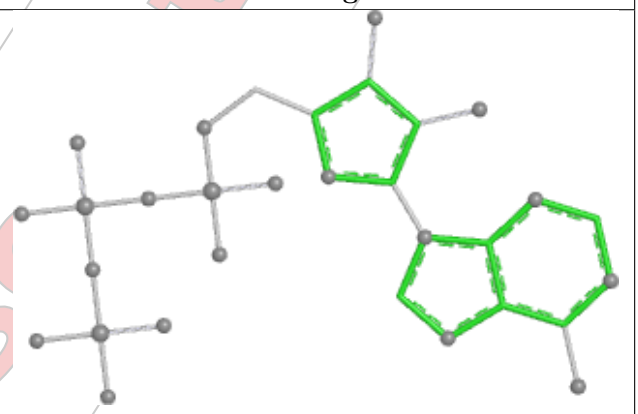
Bond lengths



Bond angles

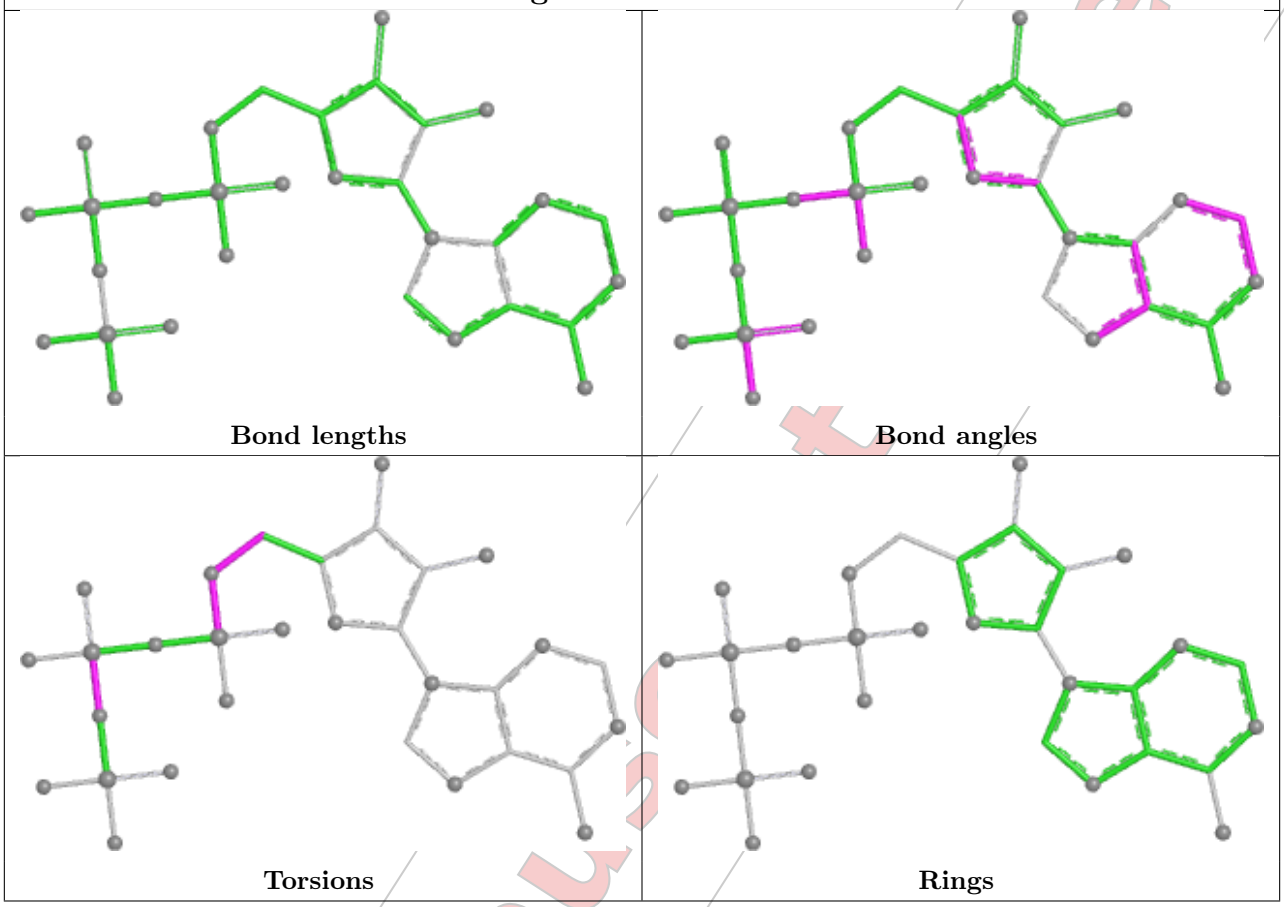


Torsions

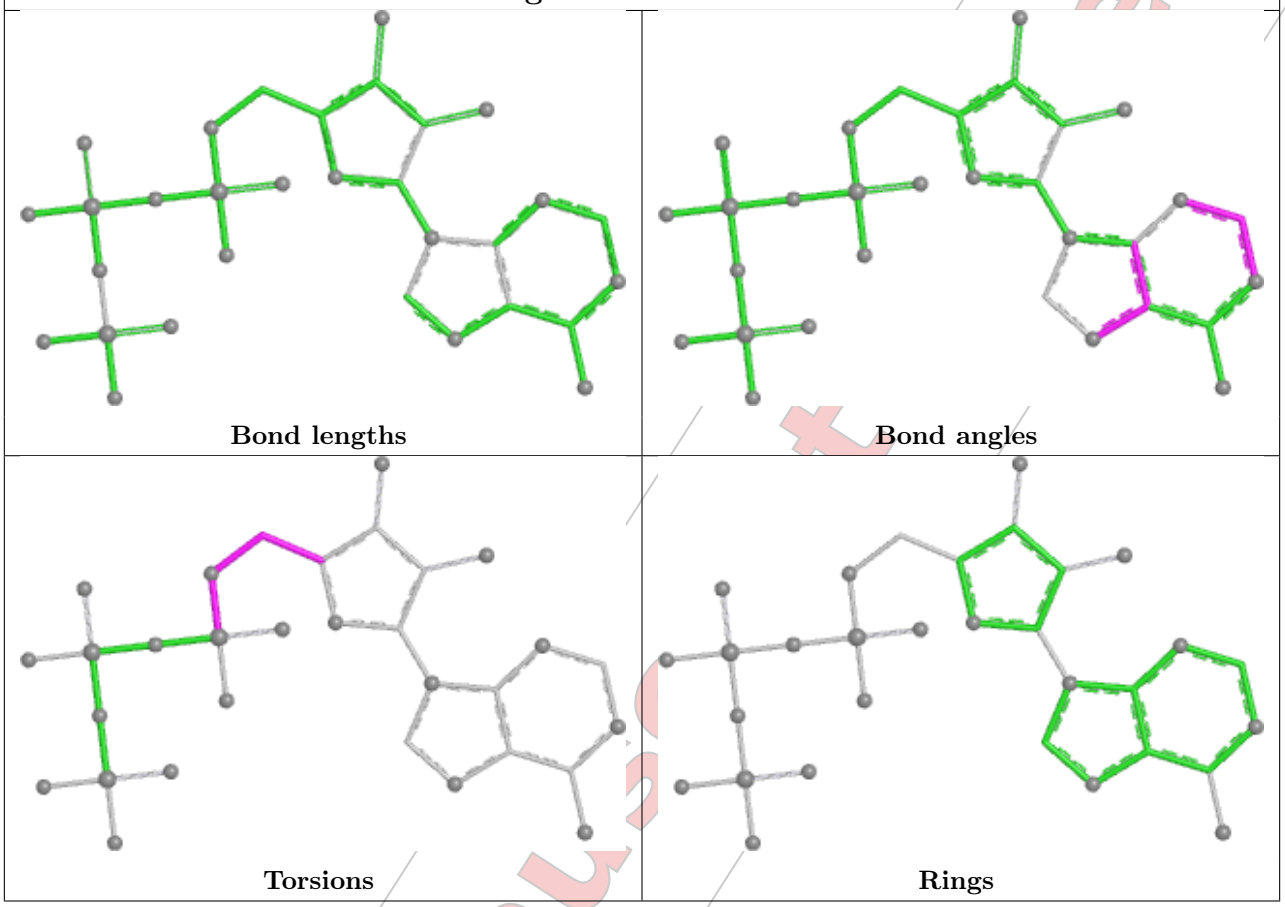


Rings

Ligand ATP e 401



Ligand ATP X 501



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.

Preliminary Full wwPDB EM Validation Report ⓘ

Nov 17, 2025 – 09:13 AM EST

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with specific help available everywhere you see the ⓘ symbol.

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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	:	FAILED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 109455 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	0	49	414	251	64	99	0	0

- Molecule 2 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	411	3237	2038	554	630	15	0	0

- Molecule 3 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	389	3098	1947	552	582	17	0	0

- Molecule 4 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	413	3246	2044	570	614	18	0	0

- Molecule 5 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	H	396	3119	1961	558	582	18	0	0

- Molecule 6 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	I	380	3040	1923	524	580	13	0	0

- Molecule 7 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	K	395	3099	1952	533	596	18	0	0

- Molecule 8 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	L	238	1850	1159	334	346	11	0	0
			Total	C	N	O	S		
8	l	238	1850	1159	334	346	11	0	0

- Molecule 9 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	M	240	1856	1178	314	353	11	0	0
			Total	C	N	O	S		
9	m	240	1856	1178	314	353	11	0	0

- Molecule 10 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	N	191	1430	893	245	280	12	0	0
			Total	C	N	O	S		
10	n	191	1430	893	245	280	12	0	0

- Molecule 11 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	O	220	1643	1033	280	318	12	0	0
			Total	C	N	O	S		
11	o	220	1643	1033	280	318	12	0	0

- Molecule 12 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	P	204	1585	1010	262	294	19	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	p	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		

- Molecule 13 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		
13	q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		

- Molecule 14 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		
14	r	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		

- Molecule 15 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		
15	s	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		

- Molecule 16 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		
16	t	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		

- Molecule 17 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	872	Total	C	N	O	S	0	0
			6829	4328	1157	1299	45		

- Molecule 18 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	480	Total 3853	C 2444	N 684	O 711	S 14	0	0

- Molecule 19 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	456	Total 3703	C 2339	N 635	O 704	S 25	0	0

- Molecule 20 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	380	Total 3009	C 1918	N 509	O 570	S 12	0	0

- Molecule 21 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Y	378	Total 3115	C 1987	N 533	O 578	S 17	0	0

- Molecule 22 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Z	286	Total 2282	C 1457	N 392	O 428	S 5	0	0

- Molecule 23 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	a	373	Total 2995	C 1911	N 510	O 559	S 15	0	0

- Molecule 24 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	b	191	Total 1459	C 910	N 261	O 280	S 8	0	0

- Molecule 25 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	c	287	Total 2260	C 1430	N 389	O 422	S 19	0	0

- Molecule 26 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	d	257	Total 2116	C 1371	N 346	O 390	S 9	0	0

- Molecule 27 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	e	433	Total 3380	C 2160	N 557	O 641	S 22	0	0

- Molecule 28 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	f	889	Total 6867	C 4315	N 1174	O 1332	S 46	0	0

- Molecule 29 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	g	240	Total 1826	C 1160	N 305	O 348	S 13	0	0
29	v	240	Total 1826	C 1160	N 305	O 348	S 13	0	0

- Molecule 30 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	h	232	Total 1708	C 1081	N 289	O 333	S 5	0	0
30	w	232	Total 1708	C 1081	N 289	O 333	S 5	0	0

- Molecule 31 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	i	250	Total 1912	C 1204	N 329	O 371	S 8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
31	x	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

- Molecule 32 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	j	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		
32	y	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		

- Molecule 33 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	k	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		
33	z	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		

- Molecule 34 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	u	125	Total	C	N	O	S	0	0
			1010	643	177	187	3		

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	
Number of images used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	Not provided	
Voltage (kV)	Not provided	
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	Not provided	

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no oligosaccharides in this entry.

4.6 Ligand geometry

There are no ligands in this entry.

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
17	U	1
33	k	1
27	e	1
33	z	1
7	K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	270:THR	C	320:ASP	N	14.64
1	k	127:ASP	C	134:SER	N	8.71
1	e	298:LYS	C	309:SER	N	8.40
1	z	127:ASP	C	134:SER	N	8.33
1	K	99:VAL	C	120:LYS	N	6.68

Preliminary Full wwPDB EM Validation Report ⓘ

Nov 17, 2025 – 06:22 PM EST

This wwPDB validation report is NOT for manuscript review

This is a Preliminary Full wwPDB EM Validation Report.

This report is produced by the standalone wwPDB validation server.
The structure in question has not been deposited to the wwPDB.
This report should not be submitted to journals.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
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	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 109044 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	441	3453	2201	570	659	23	0	0

- Molecule 2 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	125	1010	643	177	187	3	0	0

- Molecule 3 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	380	3004	1892	536	558	18	0	0

- Molecule 4 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	380	3040	1923	524	580	13	0	0

- Molecule 5 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	389	3098	1947	552	582	17	0	0

- Molecule 6 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	395	3099	1952	533	596	18	0	0

- Molecule 7 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	411	3225	2031	567	609	18	0	0

- Molecule 8 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	411	3237	2038	554	630	15	0	0

- Molecule 9 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	246	1872	1180	319	365	8	0	0

- Molecule 10 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	239	1704	1056	308	335	5	0	0
10	j	239	Total 1704	C 1056	N 308	O 335	S 5	0	0

- Molecule 11 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	228	1722	1080	284	348	10	0	0
11	k	228	Total 1722	C 1080	N 284	O 348	S 10	0	0

- Molecule 12 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	238	1850	1159	334	346	11	0	0
12	l	238	Total 1850	C 1159	N 334	O 346	S 11	0	0

- Molecule 13 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		
13	m	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		

- Molecule 14 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		
14	n	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		

- Molecule 15 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		
15	o	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		

- Molecule 16 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		
16	p	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		

- Molecule 17 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		
17	q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		

- Molecule 18 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
18	r	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		

- Molecule 19 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		
19	s	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		

- Molecule 20 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		
20	t	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		

- Molecule 21 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	872	Total	C	N	O	S	0	0
			6829	4328	1157	1299	45		

- Molecule 22 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	480	Total	C	N	O	S	0	0
			3853	2444	684	711	14		

- Molecule 23 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	456	Total	C	N	O	S	0	0
			3703	2339	635	704	25		

- Molecule 24 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	380	Total 3009	C 1918	N 509	O 570	S 12	0	0

- Molecule 25 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	378	Total 3115	C 1987	N 533	O 578	S 17	0	0

- Molecule 26 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	286	Total 2282	C 1457	N 392	O 428	S 5	0	0

- Molecule 27 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	373	Total 2995	C 1911	N 510	O 559	S 15	0	0

- Molecule 28 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	191	Total 1459	C 910	N 261	O 280	S 8	0	0

- Molecule 29 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	287	Total 2260	C 1430	N 389	O 422	S 19	0	0

- Molecule 30 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	257	Total 2116	C 1371	N 346	O 390	S 9	0	0

- Molecule 31 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	237	Total	C	N	O	S	0	0
			1809	1151	302	343	13		

- Molecule 32 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	889	Total	C	N	O	S	0	0
			6867	4315	1174	1332	46		

- Molecule 33 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		

- Molecule 34 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		

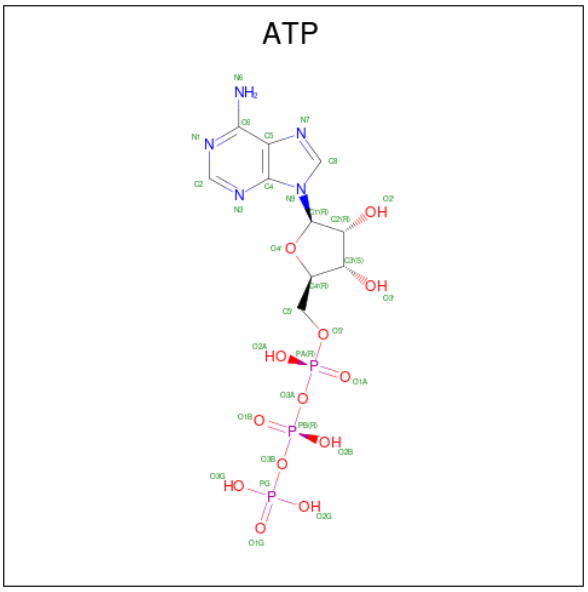
- Molecule 35 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

- Molecule 36 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	u	225	Total	C	N	O	S	0	0
			1649	1044	279	321	5		

- Molecule 37 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
37	v	1	Total	C	N	O	P	0
			31	10	5	13	3	
37	v	1	Total	C	N	O	P	0
			31	10	5	13	3	
37	w	1	Total	C	N	O	P	0
			31	10	5	13	3	
37	x	1	Total	C	N	O	P	0
			31	10	5	13	3	
37	y	1	Total	C	N	O	P	0
			31	10	5	13	3	
37	1	1	Total	C	N	O	P	0
			27	10	5	10	2	

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	
Number of images used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	Not provided	
Voltage (kV)	Not provided	
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	Not provided	

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no oligosaccharides in this entry.

4.6 Ligand geometry

6 ligands are 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	$\#\|Z\|>2$
37	ATP	v	505	7	28,33,33	0.61	0	34,52,52	0.69	1 (2%)
37	ATP	w	504	8	28,33,33	0.59	0	34,52,52	1.04	3 (8%)
37	ATP	1	501	3	24,29,33	0.67	0	29,45,52	0.76	1 (3%)
37	ATP	y	502	5	28,33,33	0.60	0	34,52,52	0.81	2 (5%)
37	ATP	v	506	7,6	28,33,33	0.66	0	34,52,52	0.61	0
37	ATP	x	503	-	28,33,33	0.61	0	34,52,52	0.73	2 (5%)

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
37	ATP	v	505	7	-	13/18/38/38	0/3/3/3
37	ATP	w	504	8	-	4/18/38/38	0/3/3/3
37	ATP	1	501	3	-	4/12/32/38	0/3/3/3
37	ATP	y	502	5	-	4/18/38/38	0/3/3/3
37	ATP	v	506	7,6	-	6/18/38/38	0/3/3/3
37	ATP	x	503	-	-	6/18/38/38	0/3/3/3

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	w	504	ATP	C4'-O4'-C1'	-3.90	106.36	109.92
37	y	502	ATP	C4'-O4'-C1'	-3.16	107.03	109.92
37	w	504	ATP	C1'-N9-C4	3.10	132.08	126.64
37	x	503	ATP	C4'-O4'-C1'	-2.47	107.66	109.92
37	x	503	ATP	C5-C6-N6	2.34	123.87	120.31
37	1	501	ATP	C5-C6-N6	2.31	123.83	120.31
37	y	502	ATP	C5-C6-N6	2.29	123.80	120.31
37	w	504	ATP	C5-C6-N6	2.26	123.76	120.31
37	v	505	ATP	C5-C6-N6	2.25	123.75	120.31

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	v	505	ATP	PB-O3B-PG-O2G
37	v	505	ATP	C5'-O5'-PA-O1A
37	v	505	ATP	C5'-O5'-PA-O2A
37	v	505	ATP	C5'-O5'-PA-O3A
37	w	504	ATP	C5'-O5'-PA-O2A
37	w	504	ATP	C5'-O5'-PA-O3A
37	w	504	ATP	C4'-C5'-O5'-PA
37	x	503	ATP	C5'-O5'-PA-O1A
37	x	503	ATP	C5'-O5'-PA-O2A
37	x	503	ATP	C5'-O5'-PA-O3A
37	y	502	ATP	O4'-C4'-C5'-O5'
37	1	501	ATP	C5'-O5'-PA-O2A
37	1	501	ATP	C5'-O5'-PA-O3A
37	y	502	ATP	C3'-C4'-C5'-O5'
37	v	505	ATP	O4'-C4'-C5'-O5'
37	v	505	ATP	C3'-C4'-C5'-O5'
37	v	506	ATP	C3'-C4'-C5'-O5'
37	v	506	ATP	PB-O3B-PG-O1G
37	v	506	ATP	PA-O3A-PB-O3B
37	v	506	ATP	PB-O3B-PG-O3G
37	v	505	ATP	PG-O3B-PB-O1B
37	v	506	ATP	O4'-C4'-C5'-O5'
37	v	505	ATP	C4'-C5'-O5'-PA
37	x	503	ATP	C4'-C5'-O5'-PA
37	1	501	ATP	PA-O3A-PB-O1B
37	x	503	ATP	PB-O3A-PA-O1A
37	x	503	ATP	PB-O3A-PA-O2A
37	v	505	ATP	PA-O3A-PB-O2B
37	y	502	ATP	C4'-C5'-O5'-PA
37	1	501	ATP	C4'-C5'-O5'-PA
37	v	505	ATP	PB-O3B-PG-O1G
37	v	505	ATP	PB-O3B-PG-O3G
37	w	504	ATP	C3'-C4'-C5'-O5'
37	v	506	ATP	PA-O3A-PB-O1B
37	v	505	ATP	PG-O3B-PB-O2B
37	y	502	ATP	PA-O3A-PB-O2B
37	v	505	ATP	PA-O3A-PB-O1B

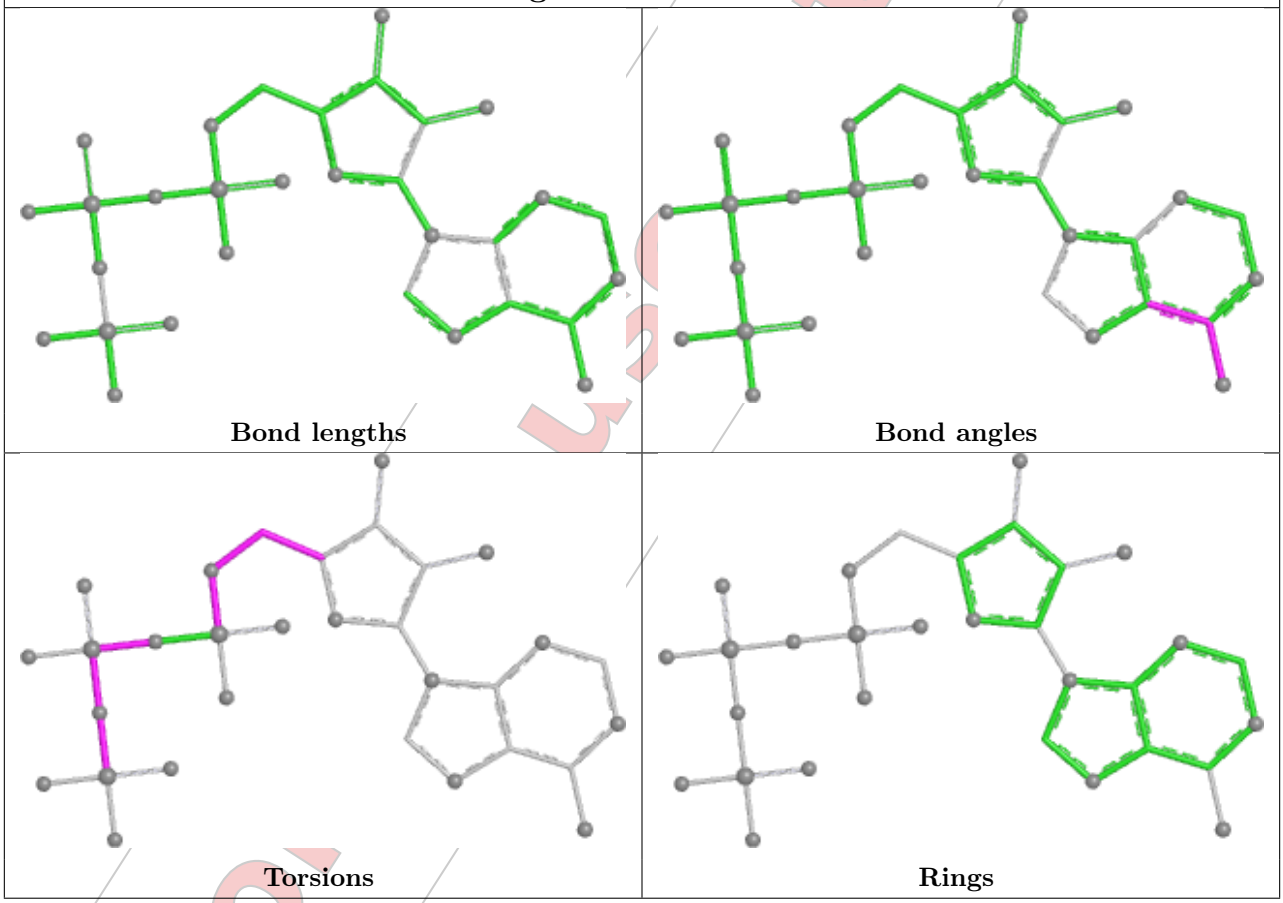
There are no ring outliers.

No monomer is involved in short contacts.

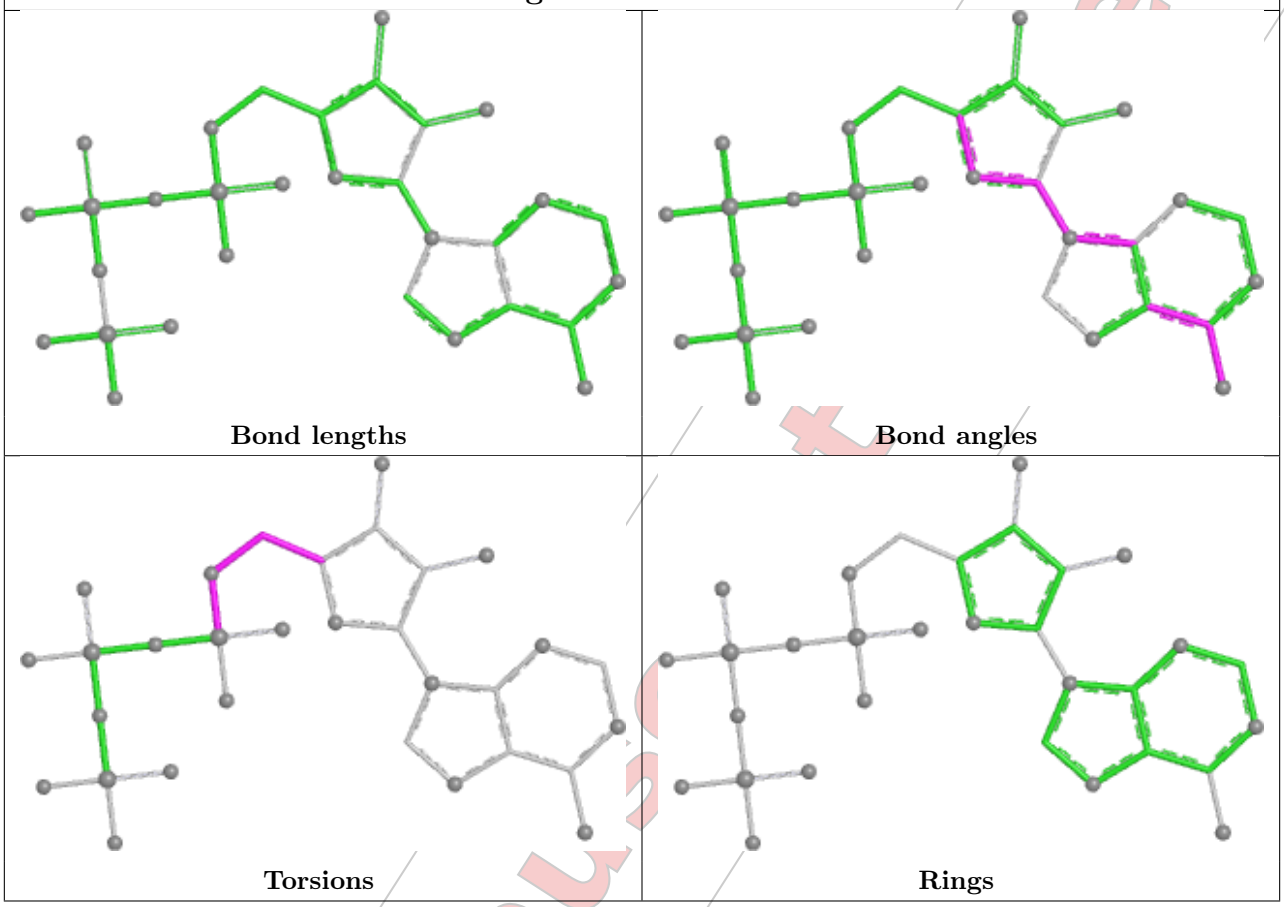
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 then 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.

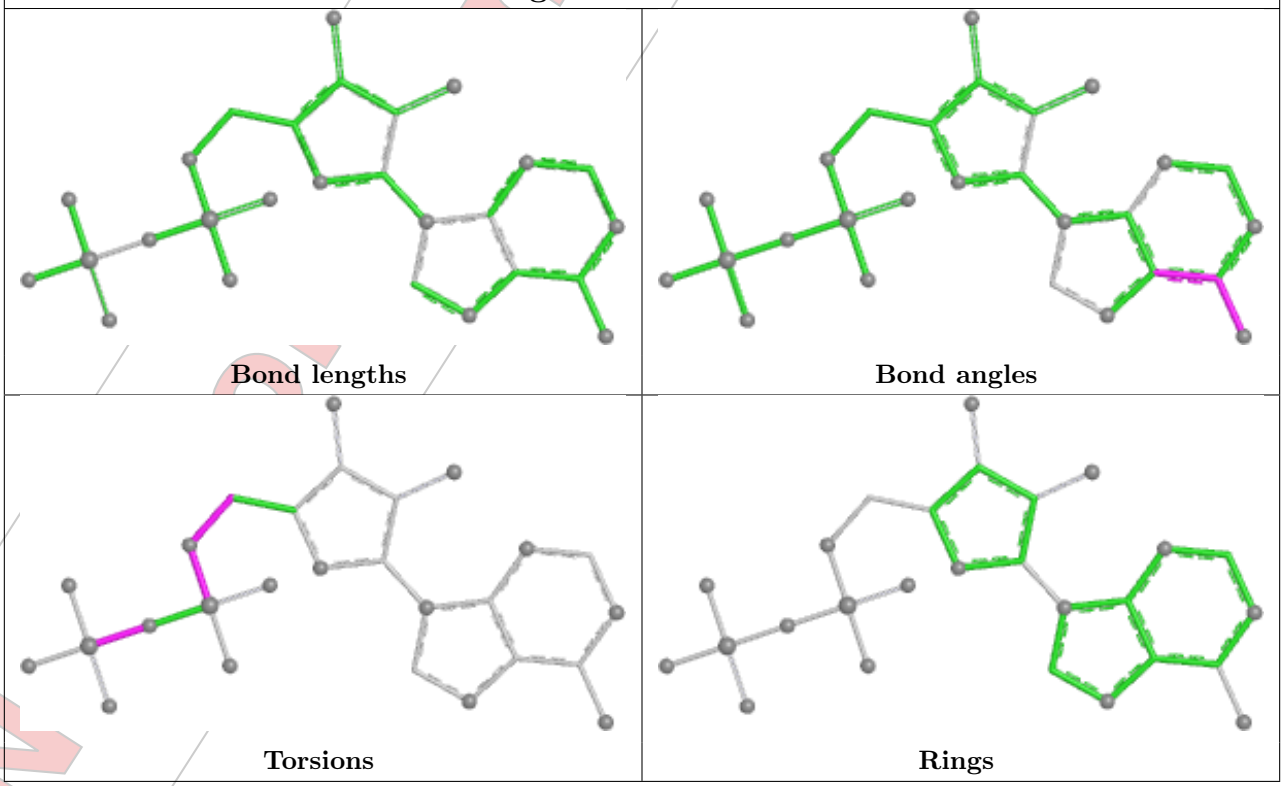
Ligand ATP v 505



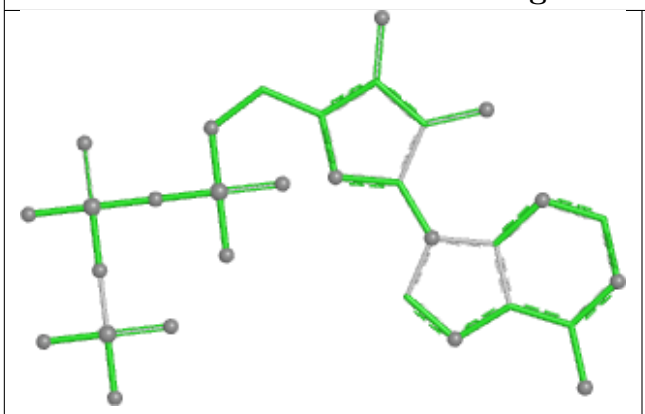
Ligand ATP w 504



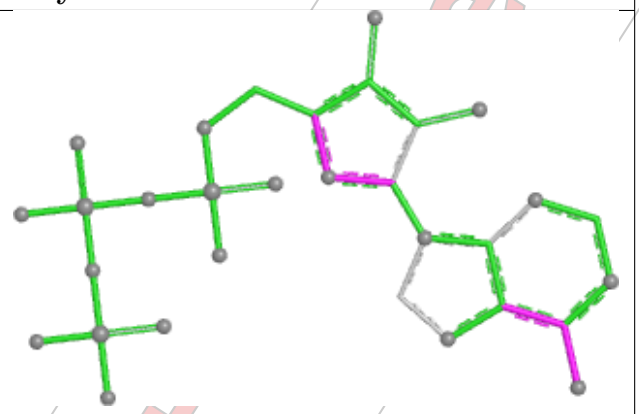
Ligand ATP 1 501



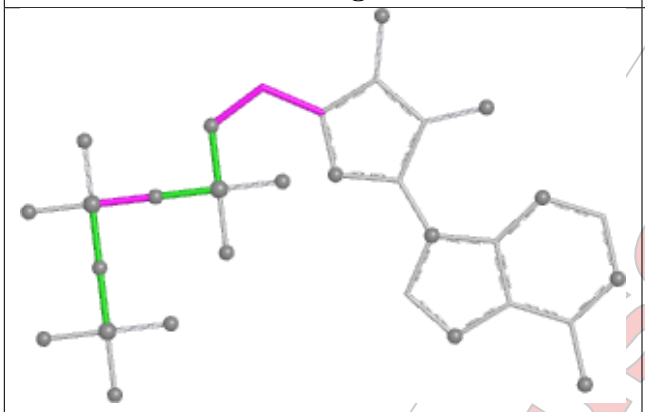
Ligand ATP y 502



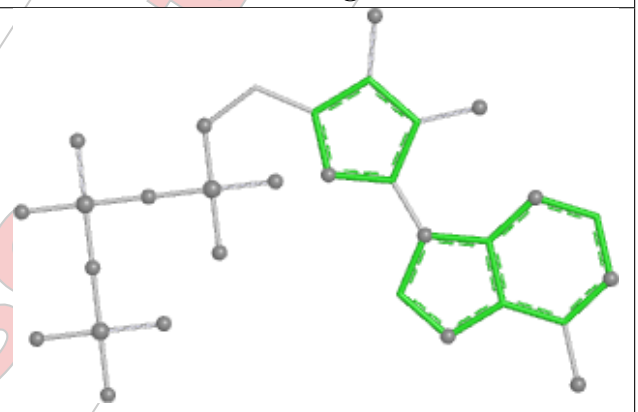
Bond lengths



Bond angles

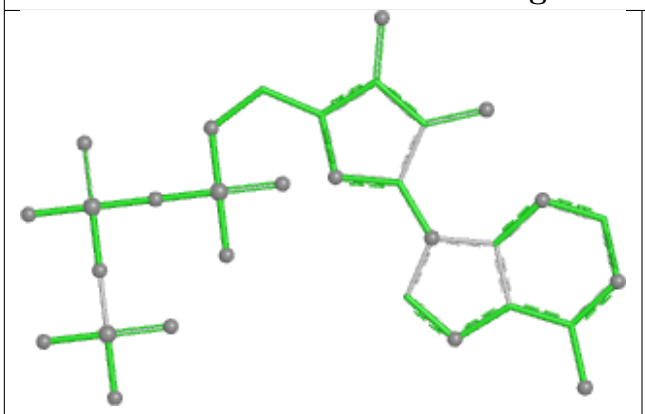


Torsions

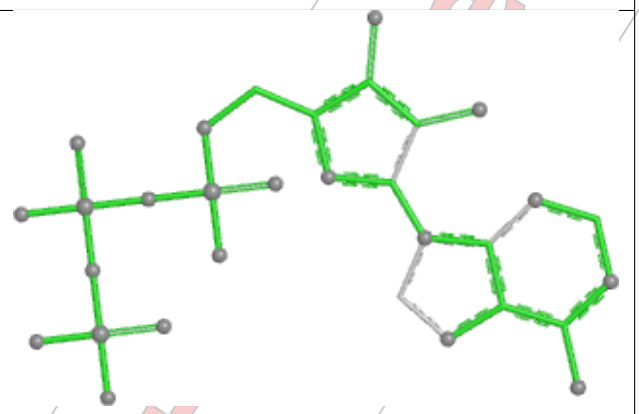


Rings

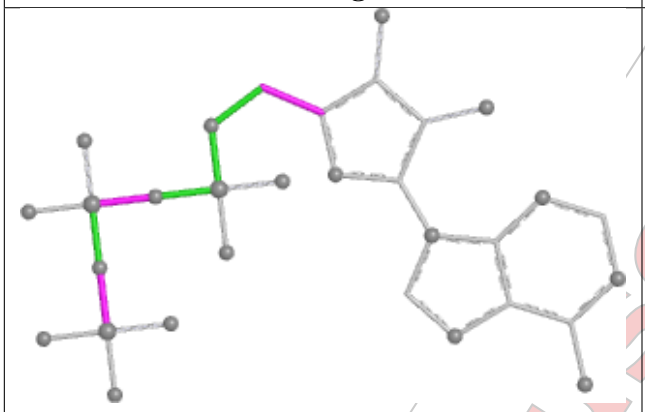
Ligand ATP v 506



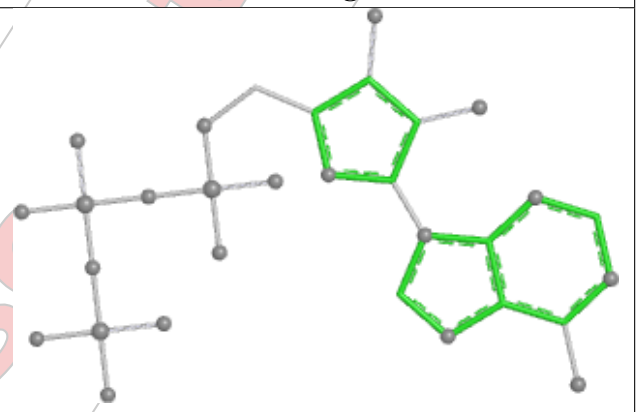
Bond lengths



Bond angles

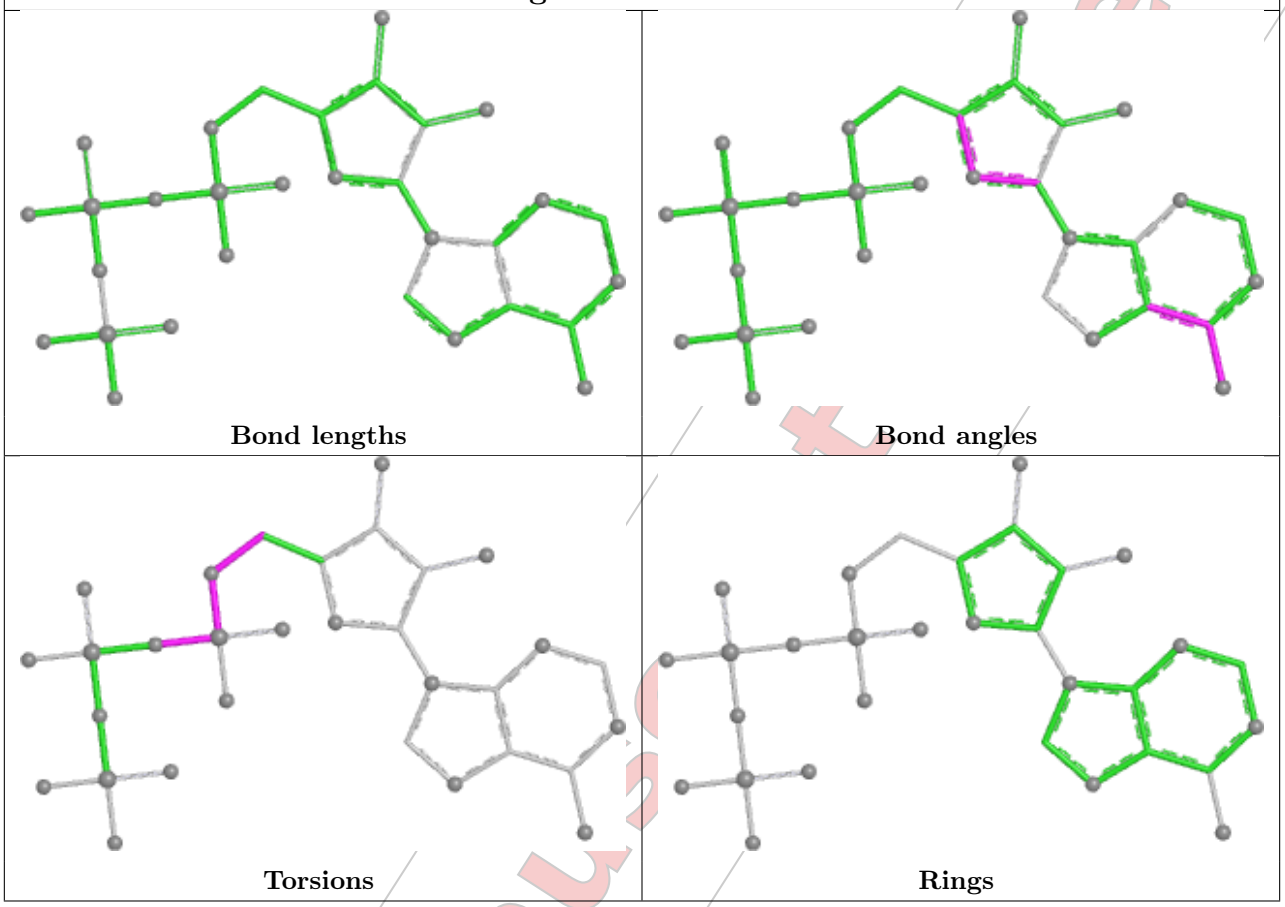


Torsions



Rings

Ligand ATP x 503



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	F	2
21	U	1
11	K	1
3	C	1
11	k	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	270:THR	C	320:ASP	N	14.90
1	K	127:ASP	C	134:SER	N	11.74
1	C	254:ILE	C	267:SER	N	10.10
1	k	127:ASP	C	134:SER	N	8.90
1	A	300:GLN	C	306:GLU	N	7.73
1	F	99:VAL	C	120:LYS	N	7.60
1	F	231:THR	C	232:GLY	N	5.86

Preliminary Full wwPDB EM Validation Report ⓘ

Nov 18, 2025 – 08:01 AM EST

This wwPDB validation report is NOT for manuscript review

This is a Preliminary Full wwPDB EM Validation Report.

This report is produced by the standalone wwPDB validation server.
The structure in question has not been deposited to the wwPDB.
This report should not be submitted to journals.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
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	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 39 unique types of molecules in this entry. The entry contains 108932 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	441	3458	2205	577	653	23	0	0

- Molecule 2 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	125	1010	643	177	187	3	0	0

- Molecule 3 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	396	3119	1961	558	582	18	0	0

- Molecule 4 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	380	3040	1923	524	580	13	0	0

- Molecule 5 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	389	3098	1947	552	582	17	0	0

- Molecule 6 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	368	2883	1822	497	547	17	0	0

- Molecule 7 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	411	3225	2031	567	609	18	0	0

- Molecule 8 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	403	3174	1998	540	621	15	0	0

- Molecule 9 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	248	1895	1195	324	368	8	0	0

- Molecule 10 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	239	1704	1056	308	335	5	0	0
10	j	239	Total 1704	C 1056	N 308	O 335	S 5	0	0

- Molecule 11 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	225	1696	1066	281	339	10	0	0

- Molecule 12 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	238	1850	1159	334	346	11	0	0
12	l	238	Total 1850	C 1159	N 334	O 346	S 11	0	0

- Molecule 13 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		
13	m	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		

- Molecule 14 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		
14	n	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		

- Molecule 15 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		
15	o	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		

- Molecule 16 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		
16	p	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		

- Molecule 17 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		
17	q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		

- Molecule 18 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
18	r	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		

- Molecule 19 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		
19	s	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		

- Molecule 20 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		
20	t	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		

- Molecule 21 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	872	Total	C	N	O	S	0	0
			6829	4328	1157	1299	45		

- Molecule 22 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	480	Total	C	N	O	S	0	0
			3853	2444	684	711	14		

- Molecule 23 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	456	Total	C	N	O	S	0	0
			3703	2339	635	704	25		

- Molecule 24 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	380	Total 3009	C 1918	N 509	O 570	S 12	0	0

- Molecule 25 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	378	Total 3115	C 1987	N 533	O 578	S 17	0	0

- Molecule 26 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	286	Total 2282	C 1457	N 392	O 428	S 5	0	0

- Molecule 27 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	373	Total 2995	C 1911	N 510	O 559	S 15	0	0

- Molecule 28 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	191	Total 1459	C 910	N 261	O 280	S 8	0	0

- Molecule 29 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	287	Total 2260	C 1430	N 389	O 422	S 19	0	0

- Molecule 30 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	257	Total 2116	C 1371	N 346	O 390	S 9	0	0

- Molecule 31 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	237	Total 1809	C 1151	N 302	O 343	S 13	0	0

- Molecule 32 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	889	Total 6867	C 4315	N 1174	O 1332	S 46	0	0

- Molecule 33 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	240	Total 1826	C 1160	N 305	O 348	S 13	0	0

- Molecule 34 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	232	Total 1708	C 1081	N 289	O 333	S 5	0	0

- Molecule 35 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	250	Total 1912	C 1204	N 329	O 371	S 8	0	0

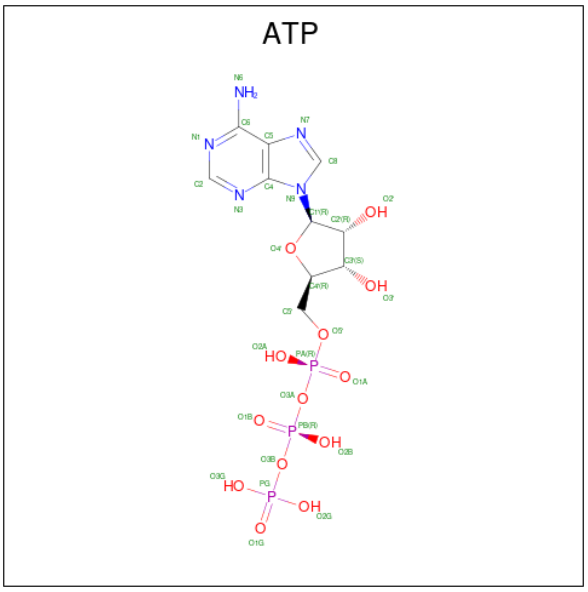
- Molecule 36 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	228	Total 1722	C 1080	N 284	O 348	S 10	0	0

- Molecule 37 is a protein.

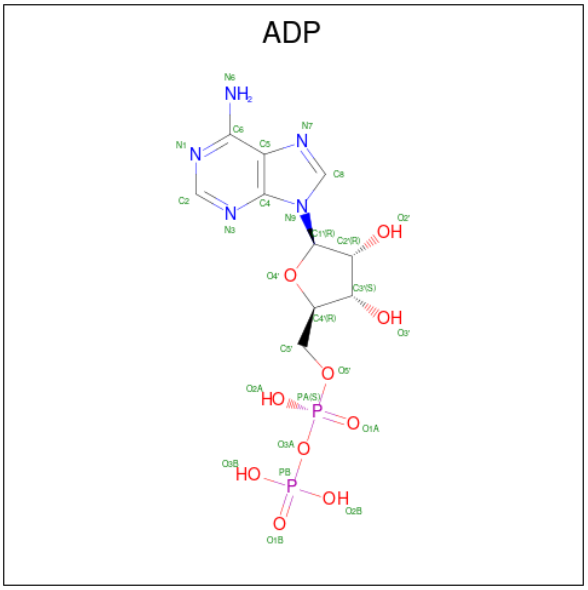
Mol	Chain	Residues	Atoms					AltConf	Trace
37	u	231	Total 1699	C 1076	N 288	O 330	S 5	0	0

- Molecule 38 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
38	v	1	Total	C	N	O	P	0
			31	10	5	13	3	
38	w	1	Total	C	N	O	P	0
			31	10	5	13	3	
38	x	1	Total	C	N	O	P	0
			31	10	5	13	3	
38	y	1	Total	C	N	O	P	0
			31	10	5	13	3	
38	z	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 39 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
39	0	1	Total	C	N	O	P	0
			27	10	5	10	2	

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	
Number of images used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	Not provided	
Voltage (kV)	Not provided	
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	Not provided	

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no oligosaccharides in this entry.

4.6 Ligand geometry

6 ligands are 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	$\#\|Z\| > 2$
39	ADP	0	419	5	24,29,29	1.22	2 (8%)	29,45,45	1.48	3 (10%)
38	ATP	y	408	8,7	28,33,33	0.63	0	34,52,52	0.66	1 (2%)
38	ATP	v	408	8	28,33,33	0.62	0	34,52,52	0.61	1 (2%)
38	ATP	w	407	6	28,33,33	0.74	0	34,52,52	1.60	5 (14%)
38	ATP	x	409	3	28,33,33	0.66	0	34,52,52	0.84	2 (5%)
38	ATP	z	440	4	28,33,33	0.63	0	34,52,52	0.62	1 (2%)

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
39	ADP	0	419	5	-	4/12/32/32	0/3/3/3
38	ATP	y	408	8,7	-	3/18/38/38	0/3/3/3
38	ATP	v	408	8	-	5/18/38/38	0/3/3/3
38	ATP	w	407	6	-	4/18/38/38	0/3/3/3
38	ATP	x	409	3	-	7/18/38/38	0/3/3/3
38	ATP	z	440	4	-	7/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	0	419	ADP	PA-O3A	3.95	1.63	1.59
39	0	419	ADP	O4'-C1'	2.41	1.44	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	w	407	ATP	C5-C6-N6	6.57	130.31	120.31
39	0	419	ADP	N3-C2-N1	-4.21	122.95	128.67
38	w	407	ATP	C4-C5-N7	-3.75	105.37	109.34
38	x	409	ATP	C4'-O4'-C1'	-3.35	106.86	109.92
39	0	419	ADP	O3B-PB-O2B	3.16	119.67	107.80
38	w	407	ATP	N6-C6-N1	-2.90	112.14	118.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	v	408	ATP	C5-C6-N6	2.40	123.97	120.31
38	x	409	ATP	C5-C6-N6	2.33	123.86	120.31
38	z	440	ATP	C5-C6-N6	2.27	123.77	120.31
38	y	408	ATP	C5-C6-N6	2.23	123.71	120.31
38	w	407	ATP	C1'-N9-C4	2.19	130.49	126.64
39	0	419	ADP	O4'-C4'-C5'	2.06	115.93	109.33
38	w	407	ATP	C6-C5-C4	-2.06	113.90	117.90

There are no chirality outliers.

All (30) torsion outliers are listed below:

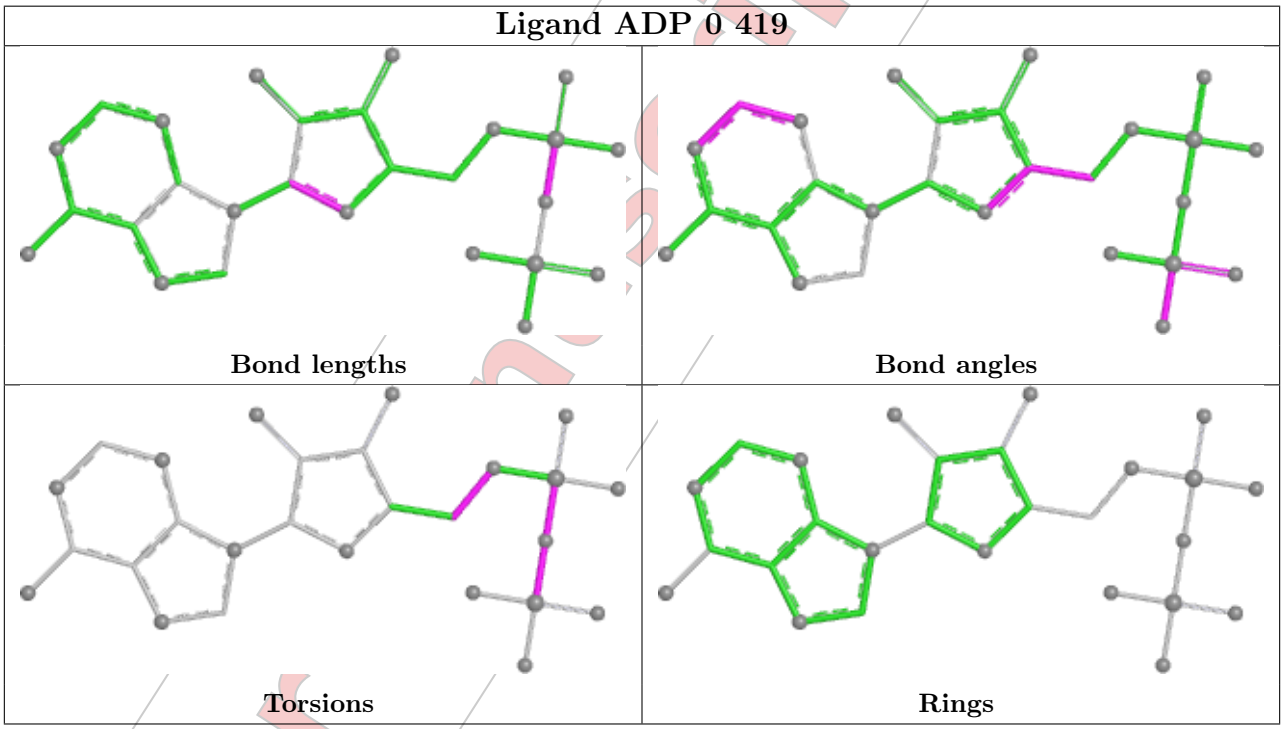
Mol	Chain	Res	Type	Atoms
38	x	409	ATP	C5'-O5'-PA-O2A
38	x	409	ATP	C5'-O5'-PA-O3A
38	x	409	ATP	C4'-C5'-O5'-PA
38	x	409	ATP	O4'-C4'-C5'-O5'
38	y	408	ATP	PB-O3B-PG-O2G
38	z	440	ATP	C5'-O5'-PA-O2A
38	z	440	ATP	C5'-O5'-PA-O3A
39	0	419	ADP	PA-O3A-PB-O3B
38	x	409	ATP	C3'-C4'-C5'-O5'
38	z	440	ATP	C3'-C4'-C5'-O5'
38	z	440	ATP	O4'-C4'-C5'-O5'
38	w	407	ATP	PA-O3A-PB-O1B
38	x	409	ATP	PB-O3A-PA-O1A
38	w	407	ATP	C5'-O5'-PA-O1A
38	z	440	ATP	C5'-O5'-PA-O1A
38	z	440	ATP	C4'-C5'-O5'-PA
39	0	419	ADP	PB-O3A-PA-O2A
38	y	408	ATP	PB-O3B-PG-O1G
38	v	408	ATP	O4'-C4'-C5'-O5'
38	y	408	ATP	C4'-C5'-O5'-PA
39	0	419	ADP	C4'-C5'-O5'-PA
38	v	408	ATP	PG-O3B-PB-O2B
38	v	408	ATP	PA-O3A-PB-O1B
38	v	408	ATP	PA-O3A-PB-O2B
38	w	407	ATP	PA-O3A-PB-O2B
38	x	409	ATP	PB-O3A-PA-O2A
38	w	407	ATP	PB-O3A-PA-O2A
38	z	440	ATP	PG-O3B-PB-O2B
39	0	419	ADP	PB-O3A-PA-O1A
38	v	408	ATP	PG-O3B-PB-O3A

There are no ring outliers.

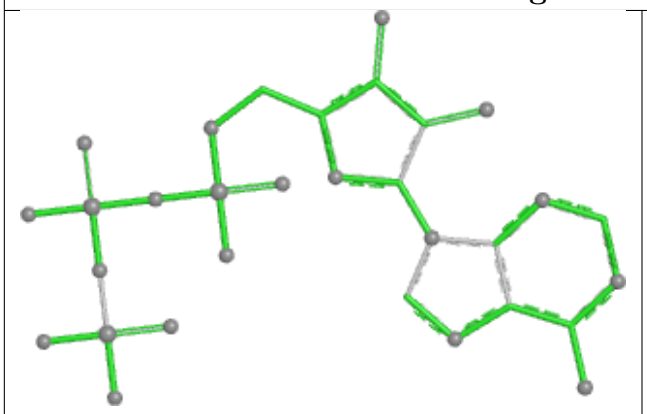
No monomer is involved in short contacts.

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 then 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.

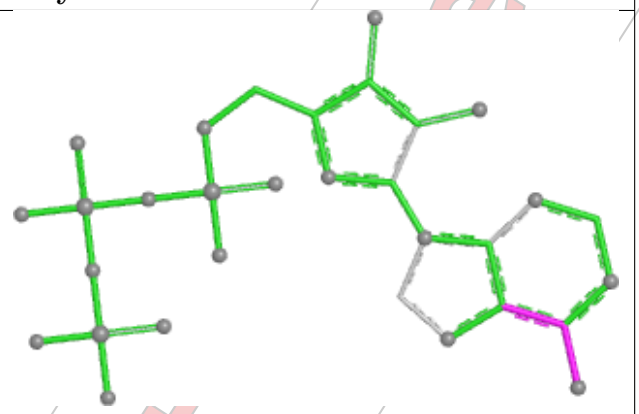
Ligand ADP 0 419



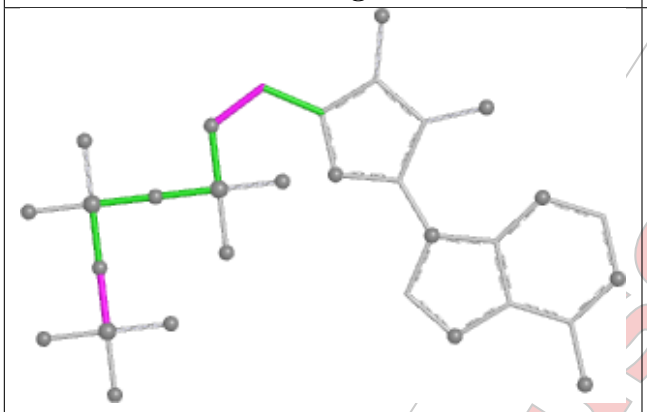
Ligand ATP y 408



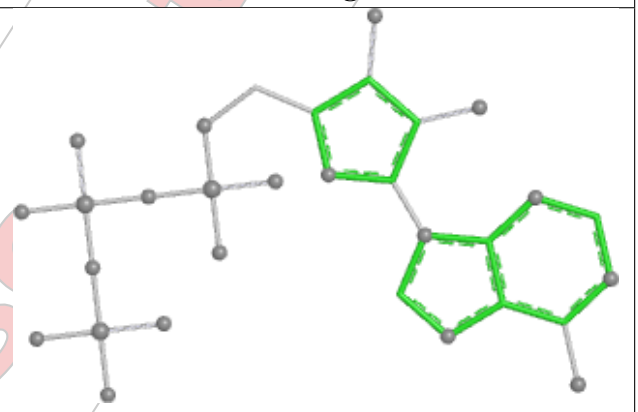
Bond lengths



Bond angles

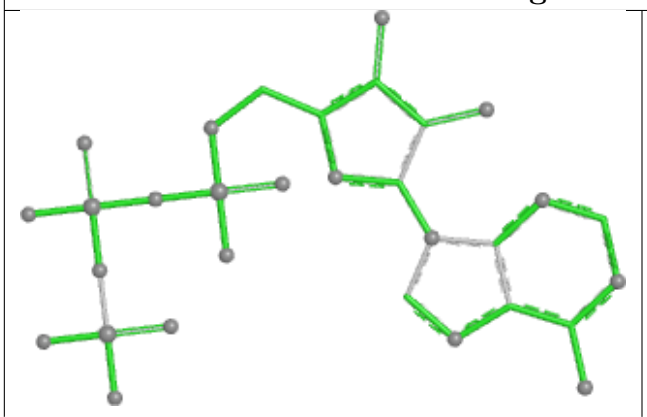


Torsions

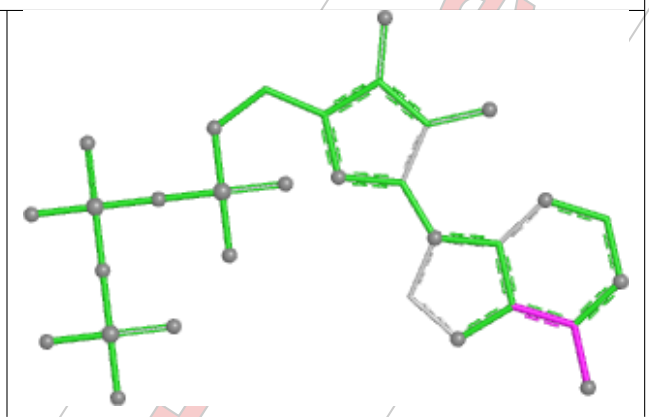


Rings

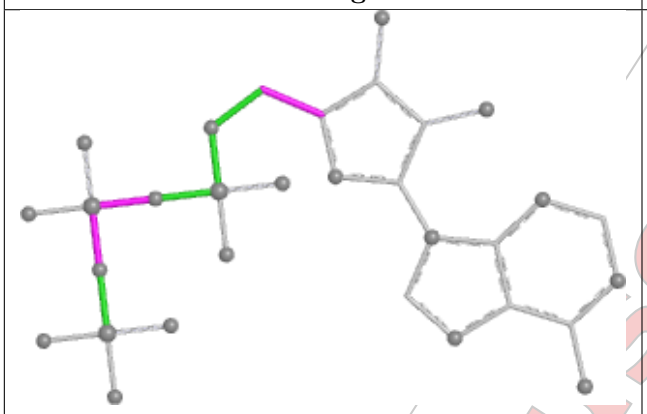
Ligand ATP v 408



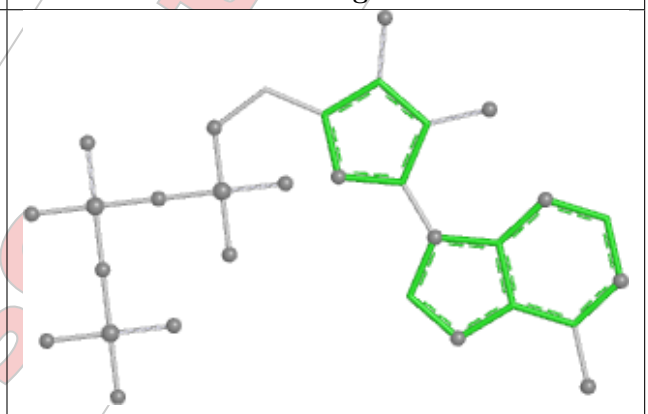
Bond lengths



Bond angles

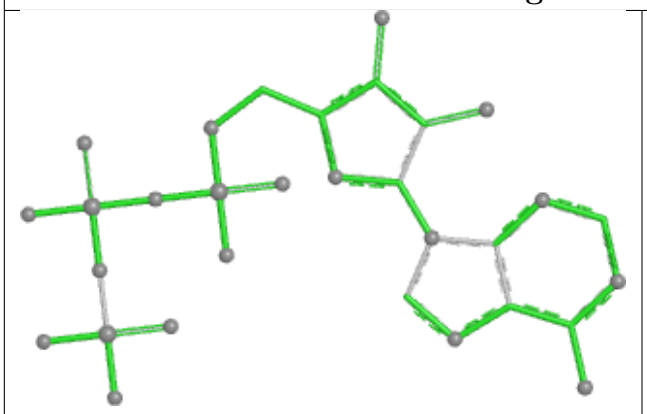


Torsions

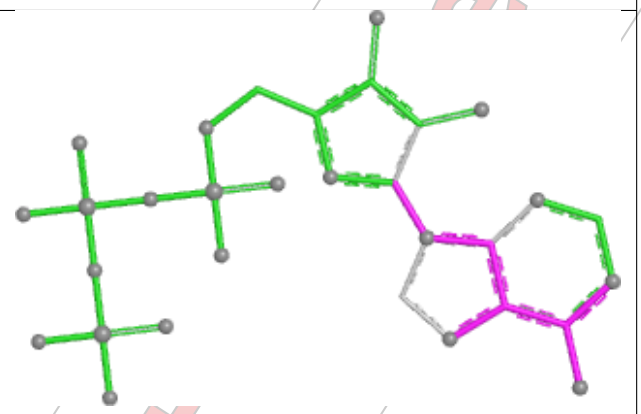


Rings

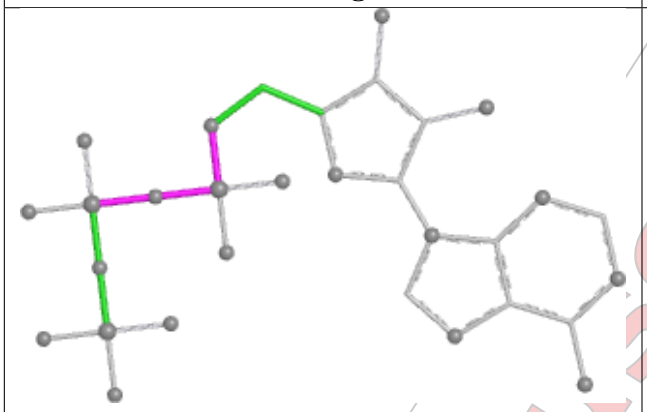
Ligand ATP w 407



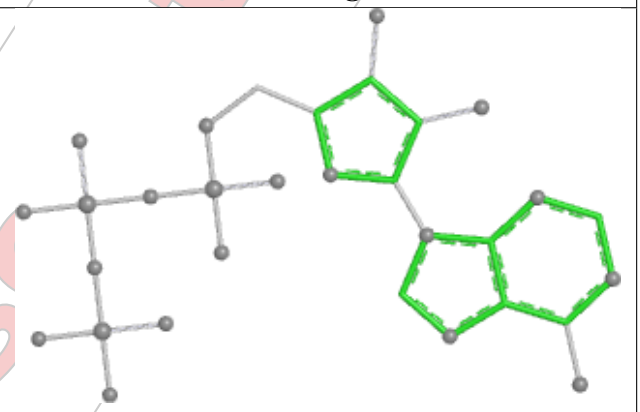
Bond lengths



Bond angles

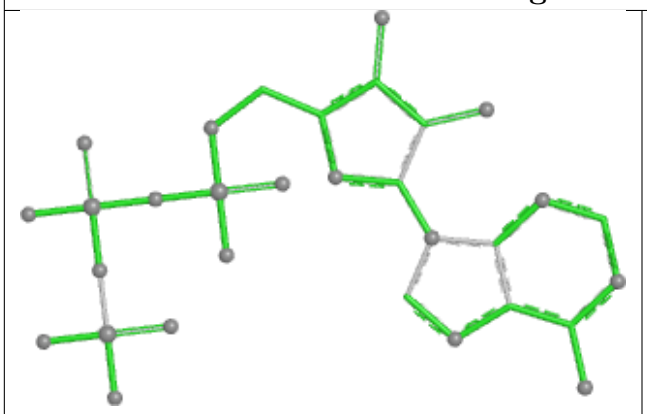


Torsions

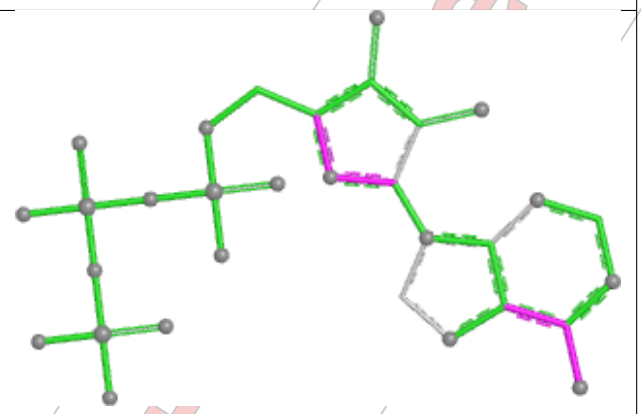


Rings

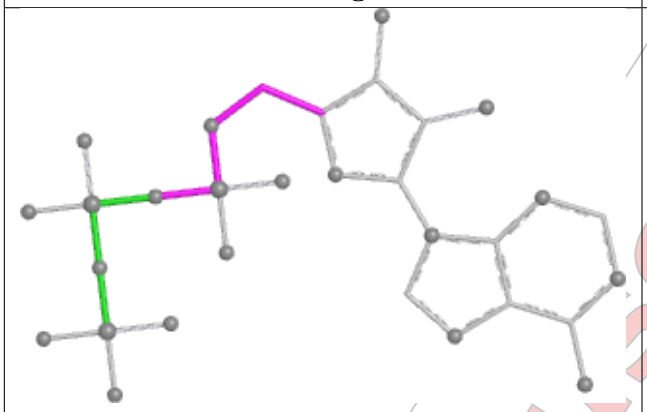
Ligand ATP x 409



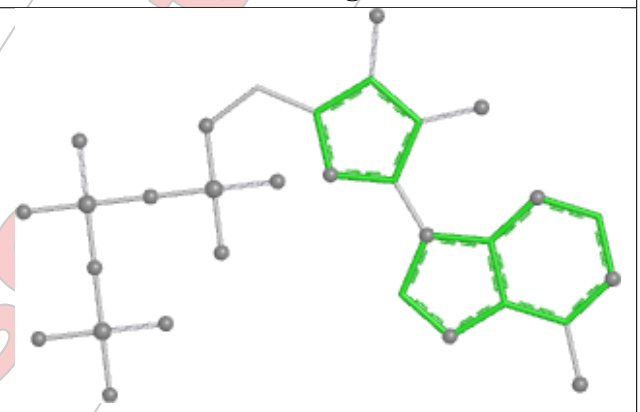
Bond lengths



Bond angles

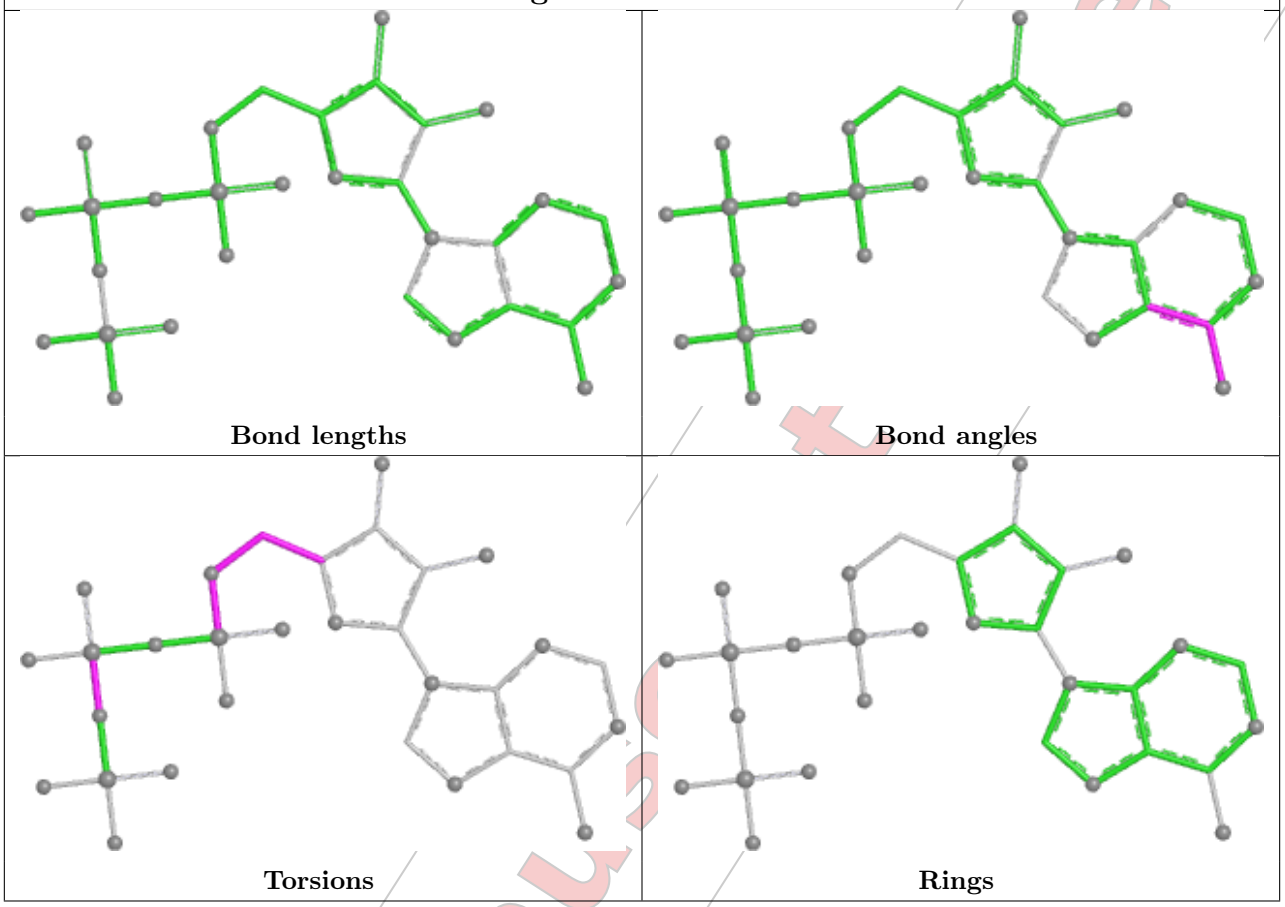


Torsions



Rings

Ligand ATP z 440



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
21	U	1
1	A	1
36	k	1
11	K	1
12	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	270:THR	C	320:ASP	N	14.44

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	300:GLN	C	309:SER	N	9.89
1	k	127:ASP	C	134:SER	N	8.70
1	K	124:GLY	C	134:SER	N	5.50
1	L	31:GLN	C	32:GLY	N	1.61

Preliminary Full wwPDB EM Validation Report ⓘ

Nov 19, 2025 – 07:34 AM EST

This wwPDB validation report is NOT for manuscript review

This is a Preliminary Full wwPDB EM Validation Report.

This report is produced by the standalone wwPDB validation server.
The structure in question has not been deposited to the wwPDB.
This report should not be submitted to journals.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
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	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 39 unique types of molecules in this entry. The entry contains 108978 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	238	1814	1154	303	344	13	0	0

- Molecule 2 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	125	1010	643	177	187	3	0	0

- Molecule 3 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	413	3246	2044	570	614	18	0	0

- Molecule 4 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	403	3174	1998	540	621	15	0	0

- Molecule 5 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	380	3040	1923	524	580	13	0	0

- Molecule 6 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	385	3062	1922	547	576	17	0	0

- Molecule 7 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	I	872	6829	4328	1157	1299	45	0	0

- Molecule 8 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	L	446	3485	2218	575	669	23	0	0

- Molecule 9 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	M	240	1856	1178	314	353	11	0	0
9	m	240	Total 1856	C 1178	N 314	O 353	S 11	0	0

- Molecule 10 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	N	191	1430	893	245	280	12	0	0
10	n	191	Total 1430	C 893	N 245	O 280	S 12	0	0

- Molecule 11 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	O	220	1643	1033	280	318	12	0	0
11	o	220	Total 1643	C 1033	N 280	O 318	S 12	0	0

- Molecule 12 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	P	204	1585	1010	262	294	19	0	0
12	p	204	Total 1585	C 1010	N 262	O 294	S 19	0	0

- Molecule 13 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		
13	q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		

- Molecule 14 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		
14	r	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		

- Molecule 15 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		
15	s	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		

- Molecule 16 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		
16	t	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		

- Molecule 17 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		
17	h	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		

- Molecule 18 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	480	Total 3853	C 2444	N 684	O 711	S 14	0	0

- Molecule 19 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	456	Total 3703	C 2339	N 635	O 704	S 25	0	0

- Molecule 20 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	380	Total 3009	C 1918	N 509	O 570	S 12	0	0

- Molecule 21 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Y	378	Total 3115	C 1987	N 533	O 578	S 17	0	0

- Molecule 22 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Z	286	Total 2282	C 1457	N 392	O 428	S 5	0	0

- Molecule 23 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	a	373	Total 2995	C 1911	N 510	O 559	S 15	0	0

- Molecule 24 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	b	191	Total 1459	C 910	N 261	O 280	S 8	0	0

- Molecule 25 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	c	287	Total 2260	C 1430	N 389	O 422	S 19	0	0

- Molecule 26 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	d	257	Total 2116	C 1371	N 346	O 390	S 9	0	0

- Molecule 27 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	e	368	Total 2883	C 1822	N 497	O 547	S 17	0	0

- Molecule 28 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	f	889	Total 6867	C 4315	N 1174	O 1332	S 46	0	0

- Molecule 29 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	g	240	Total 1826	C 1160	N 305	O 348	S 13	0	0

- Molecule 30 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	i	250	Total 1912	C 1204	N 329	O 371	S 8	0	0

- Molecule 31 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	j	239	Total 1704	C 1056	N 308	O 335	S 5	0	0
31	x	239	Total 1704	C 1056	N 308	O 335	S 5	0	0

- Molecule 32 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	k	228	Total 1722	C 1080	N 284	O 348	S 10	0	0

- Molecule 33 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	l	238	Total 1850	C 1159	N 334	O 346	S 11	0	0
33	z	238	Total 1850	C 1159	N 334	O 346	S 11	0	0

- Molecule 34 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	u	396	Total 3119	C 1961	N 558	O 582	S 18	0	0

- Molecule 35 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	v	249	Total 1906	C 1201	N 328	O 369	S 8	0	0

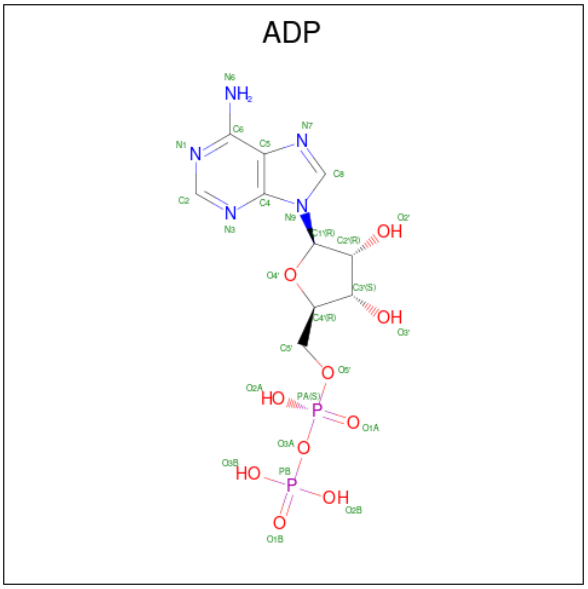
- Molecule 36 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	y	229	Total 1731	C 1085	N 288	O 348	S 10	0	0

- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

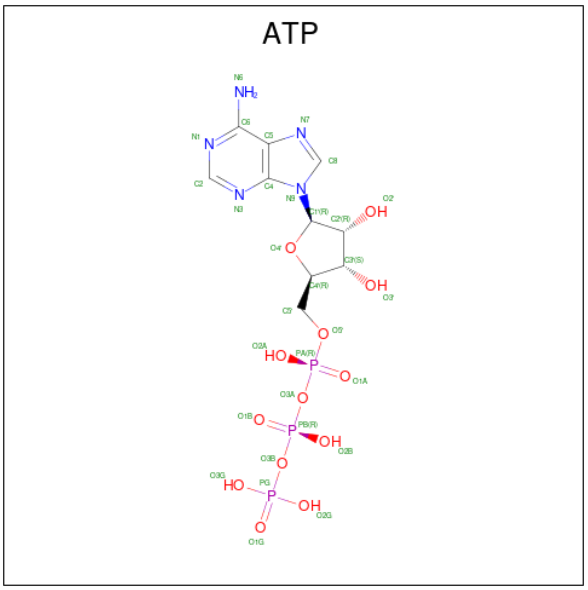
Mol	Chain	Residues	Atoms		AltConf
37	G	1	Total 1	Mg 1	0
37	H	1	Total 1	Mg 1	0
37	J	1	Total 1	Mg 1	0
37	K	1	Total 1	Mg 1	0
37	w	1	Total 1	Mg 1	0

- Molecule 38 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
38	0	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 39 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
39	1	1	Total	C	N	O	P	0
			31	10	5	13	3	
39	2	1	Total	C	N	O	P	0
			31	10	5	13	3	

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Mol	Chain	Residues	Atoms					AltConf
39	3	1	Total	C	N	O	P	0
			31	10	5	13	3	
39	4	1	Total	C	N	O	P	0
			31	10	5	13	3	

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	
Number of images used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	Not provided	
Voltage (kV)	Not provided	
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	Not provided	

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no oligosaccharides in this entry.

4.6 Ligand geometry

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
39	ATP	3	501	37	28,33,33	0.62	0	34,52,52	0.71	2 (5%)
39	ATP	1	1	37,4	28,33,33	0.62	0	34,52,52	0.79	2 (5%)
39	ATP	4	501	37,34	28,33,33	0.63	0	34,52,52	0.63	1 (2%)
38	ADP	0	502	37,5	24,29,29	0.91	0	29,45,45	1.28	3 (10%)
39	ATP	2	501	37	28,33,33	0.63	0	34,52,52	0.64	1 (2%)

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
39	ATP	3	501	37	-	6/18/38/38	0/3/3/3
39	ATP	1	1	37,4	-	8/18/38/38	0/3/3/3
39	ATP	4	501	37,34	-	3/18/38/38	0/3/3/3
38	ADP	0	502	37,5	-	3/12/32/32	0/3/3/3
39	ATP	2	501	37	-	4/18/38/38	0/3/3/3

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	0	502	ADP	N3-C2-N1	-3.63	123.75	128.67
38	0	502	ADP	O4'-C1'-N9	3.04	112.77	108.75
39	1	1	ATP	C4'-O4'-C1'	-2.98	107.20	109.92
38	0	502	ADP	C4-C5-N7	-2.45	106.75	109.34
39	1	1	ATP	C5-C6-N6	2.32	123.85	120.31
39	3	501	ATP	C5-C6-N6	2.32	123.84	120.31
39	2	501	ATP	C5-C6-N6	2.30	123.82	120.31
39	4	501	ATP	C5-C6-N6	2.26	123.75	120.31
39	3	501	ATP	C4'-O4'-C1'	-2.13	107.97	109.92

There are no chirality outliers.

All (24) torsion outliers are listed below:

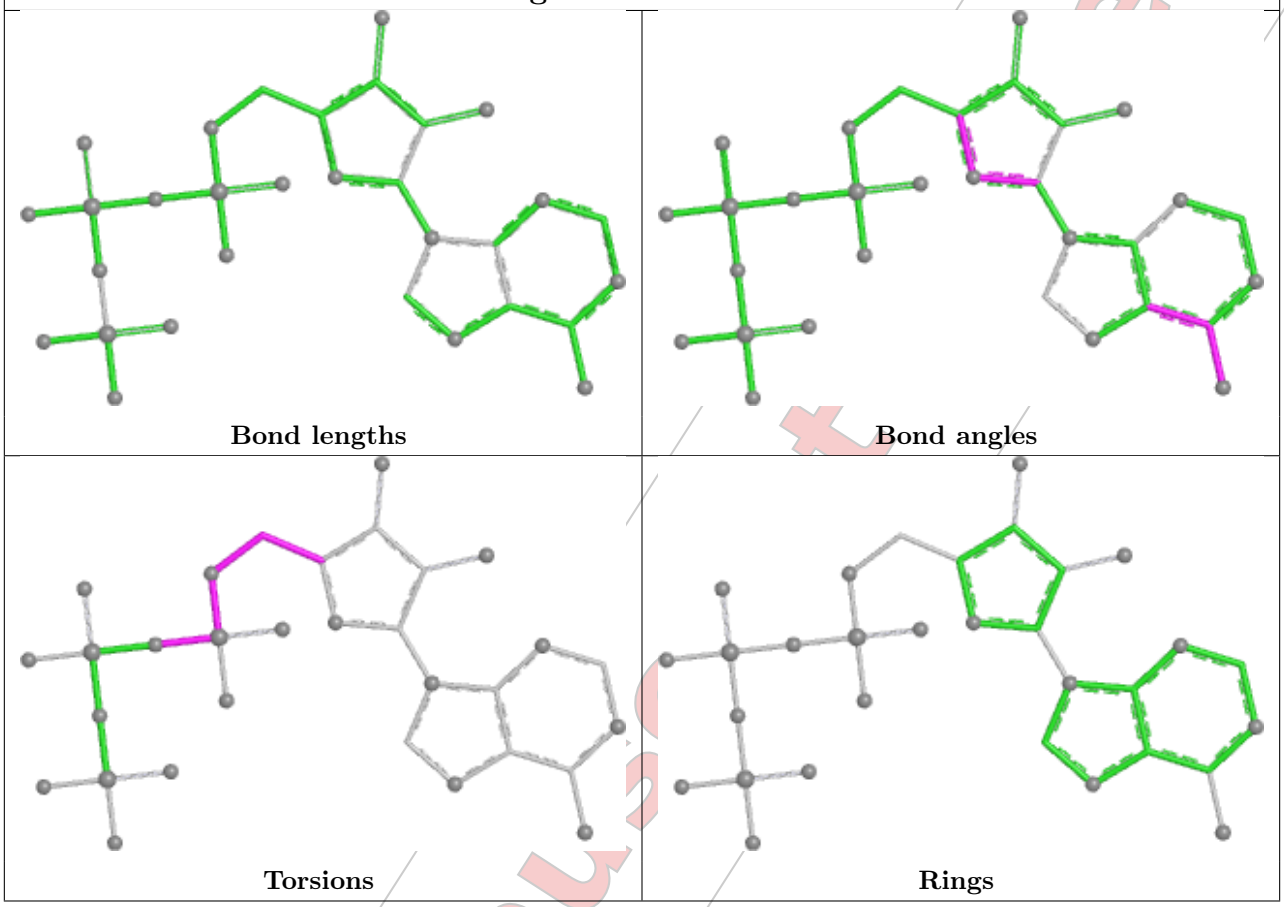
Mol	Chain	Res	Type	Atoms
38	0	502	ADP	C5'-O5'-PA-O3A
39	1	1	ATP	C5'-O5'-PA-O1A
39	1	1	ATP	C5'-O5'-PA-O3A
39	3	501	ATP	PB-O3A-PA-O5'
39	3	501	ATP	C5'-O5'-PA-O1A
39	3	501	ATP	C5'-O5'-PA-O3A
39	2	501	ATP	O4'-C4'-C5'-O5'
39	1	1	ATP	O4'-C4'-C5'-O5'
39	2	501	ATP	C3'-C4'-C5'-O5'
39	4	501	ATP	PB-O3A-PA-O5'
38	0	502	ADP	C5'-O5'-PA-O1A
39	1	1	ATP	C5'-O5'-PA-O2A
39	3	501	ATP	C5'-O5'-PA-O2A
39	1	1	ATP	C4'-C5'-O5'-PA
39	3	501	ATP	C4'-C5'-O5'-PA
39	4	501	ATP	C4'-C5'-O5'-PA
39	1	1	ATP	C3'-C4'-C5'-O5'
39	1	1	ATP	PB-O3A-PA-O1A
39	2	501	ATP	PB-O3B-PG-O1G
39	4	501	ATP	PB-O3B-PG-O3G
39	3	501	ATP	O4'-C4'-C5'-O5'
38	0	502	ADP	PB-O3A-PA-O1A
39	1	1	ATP	PB-O3A-PA-O2A
39	2	501	ATP	PG-O3B-PB-O2B

There are no ring outliers.

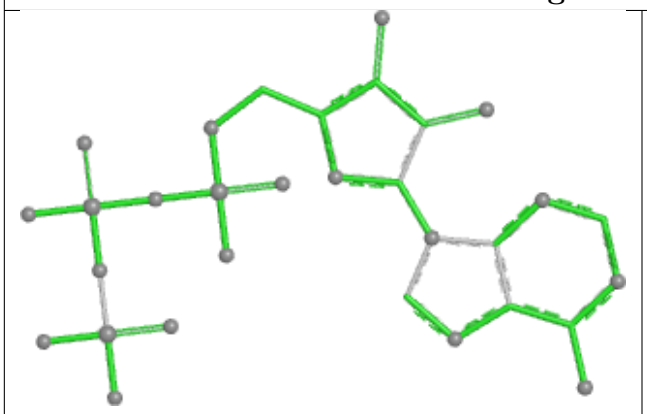
No monomer is involved in short contacts.

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 then 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.

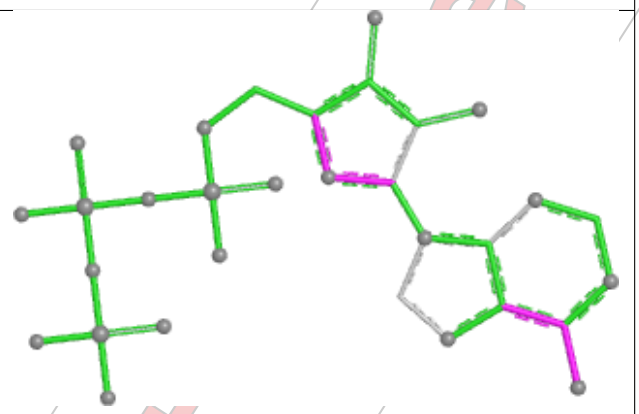
Ligand ATP 3 501



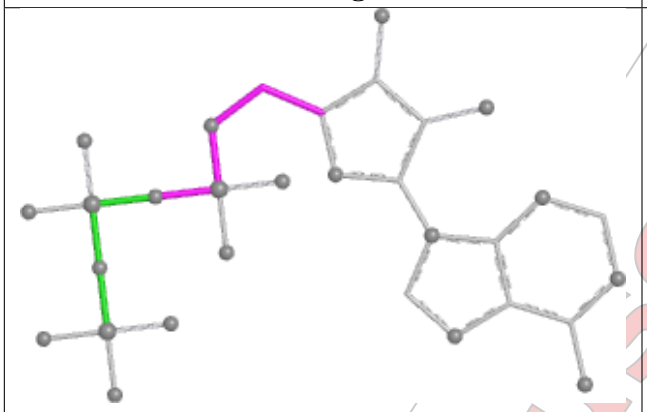
Ligand ATP 1 1



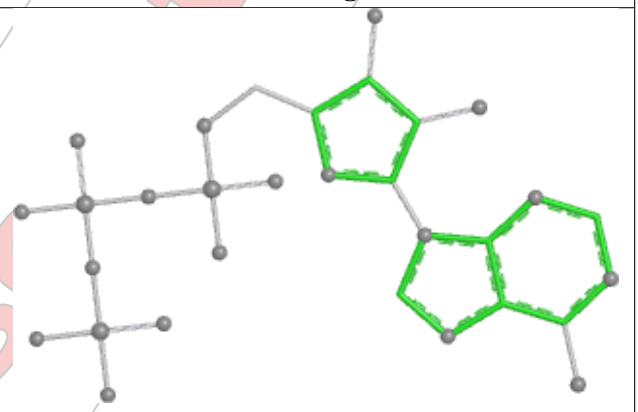
Bond lengths



Bond angles

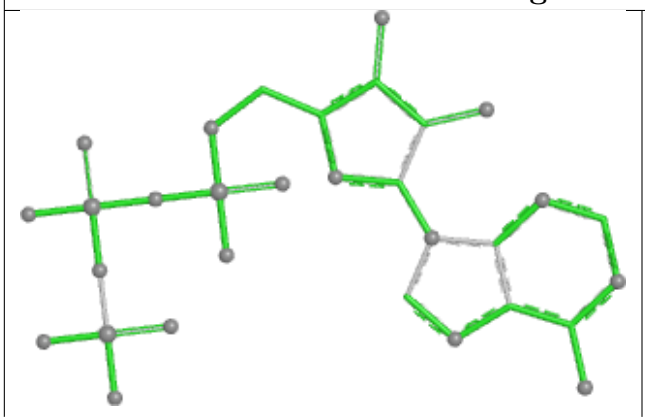


Torsions

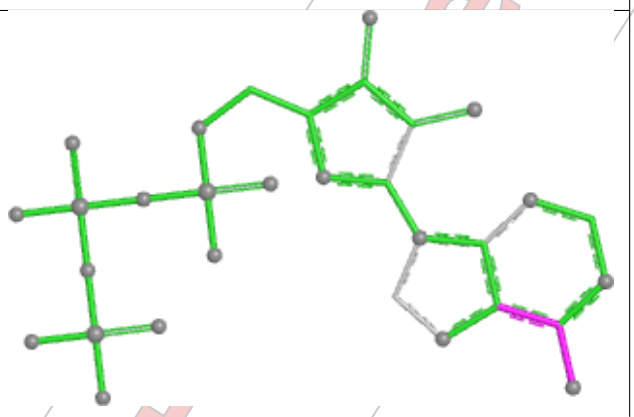


Rings

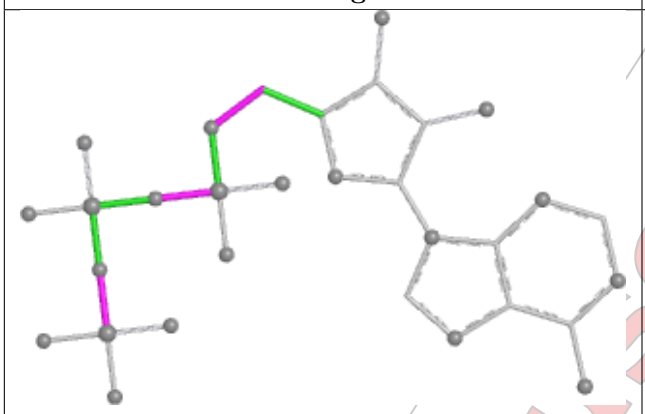
Ligand ATP 4 501



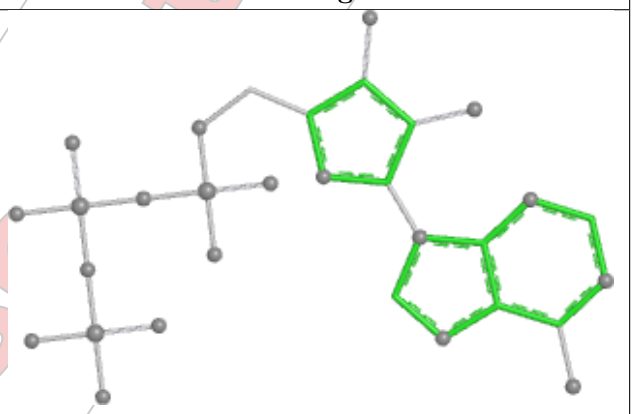
Bond lengths



Bond angles

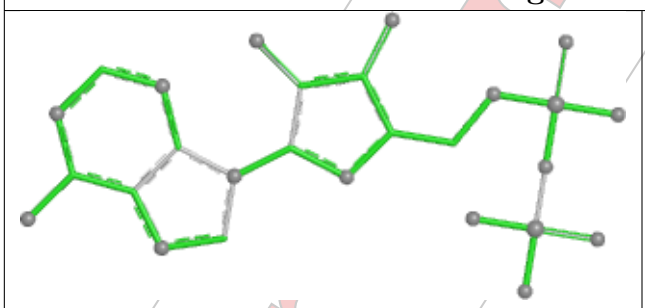


Torsions

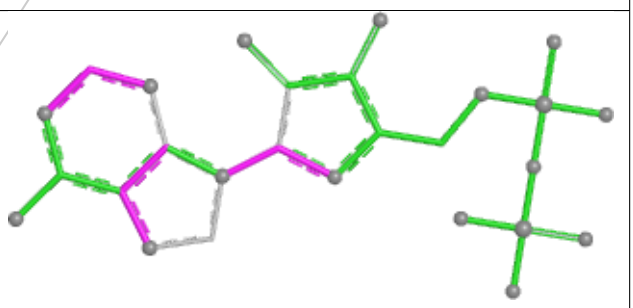


Rings

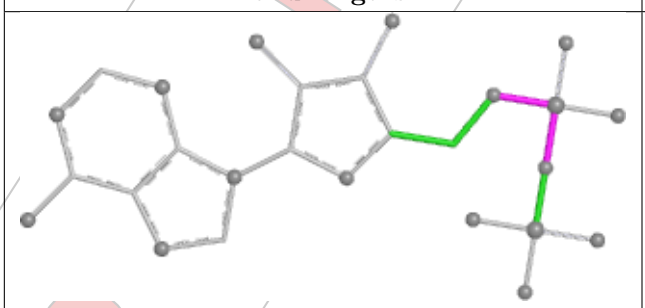
Ligand ADP 0 502



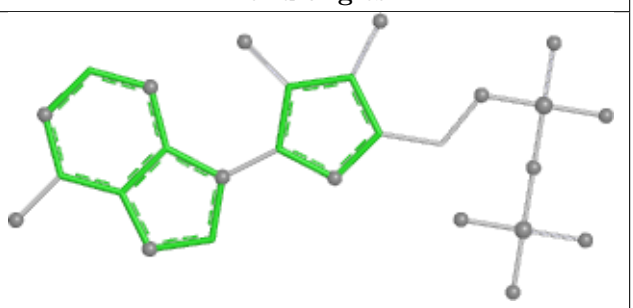
Bond lengths



Bond angles

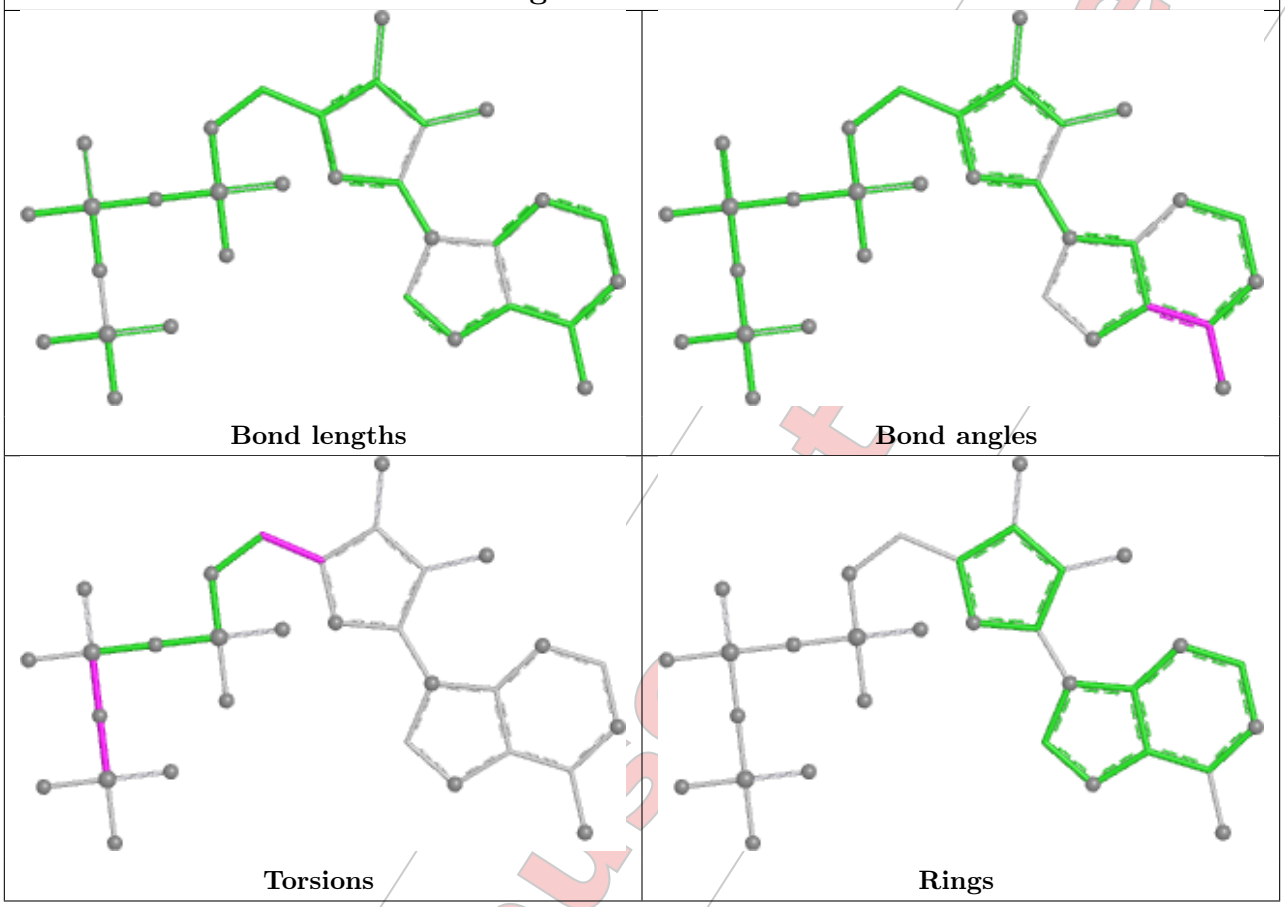


Torsions



Rings

Ligand ATP 2 501



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	I	1
36	y	1
32	k	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	270:THR	C	320:ASP	N	14.16
1	y	125:GLU	C	134:SER	N	10.28
1	k	127:ASP	C	134:SER	N	8.51

Preliminary Full wwPDB EM Validation Report ⓘ

Nov 19, 2025 – 08:23 AM EST

This wwPDB validation report is NOT for manuscript review

This is a Preliminary Full wwPDB EM Validation Report.

This report is produced by the standalone wwPDB validation server.
The structure in question has not been deposited to the wwPDB.
This report should not be submitted to journals.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
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	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 105990 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	250	1971	1245	339	377	10	0	0
1	i	250	Total	C	N	O	S	0	0
			1971	1245	339	377	10		

- Molecule 2 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	413	3246	2044	570	614	18	0	0

- Molecule 3 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	403	3174	1998	540	621	15	0	0

- Molecule 4 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	380	3040	1923	524	580	13	0	0

- Molecule 5 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	389	3098	1947	552	582	17	0	0

- Molecule 6 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	240	Total 1871	C 1189	N 310	O 359	S 13	0	0
6	g	240	Total 1871	C 1189	N 310	O 359	S 13	0	0

- Molecule 7 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	232	Total 1813	C 1158	N 307	O 342	S 6	0	0
7	h	232	Total 1813	C 1158	N 307	O 342	S 6	0	0

- Molecule 8 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	872	Total 6829	C 4328	N 1157	O 1299	S 45	0	0

- Molecule 9 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	239	Total 1887	C 1183	N 334	O 365	S 5	0	0
9	j	239	Total 1887	C 1183	N 334	O 365	S 5	0	0

- Molecule 10 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	228	Total 1753	C 1103	N 289	O 351	S 10	0	0
10	k	228	Total 1753	C 1103	N 289	O 351	S 10	0	0

- Molecule 11 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	238	Total 1873	C 1172	N 337	O 353	S 11	0	0
11	l	238	Total 1873	C 1172	N 337	O 353	S 11	0	0

- Molecule 12 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	240	1881	1193	321	356	11	0	0
12	m	240	Total	C	N	O	S	0	0
			1881	1193	321	356	11		

- Molecule 13 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	191	1430	893	245	280	12	0	0
13	n	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		

- Molecule 14 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O	220	1659	1044	283	320	12	0	0
14	o	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		

- Molecule 15 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	P	204	1591	1013	265	294	19	0	0
15	p	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

- Molecule 16 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q	199	1596	1022	272	293	9	0	0
16	q	199	Total	C	N	O	S	0	0
			1596	1022	272	293	9		

- Molecule 17 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		
17	r	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		

- Molecule 18 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	213	Total	C	N	O	S	0	0
			1654	1047	284	313	10		
18	s	213	Total	C	N	O	S	0	0
			1654	1047	284	313	10		

- Molecule 19 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	215	Total	C	N	O	S	0	0
			1681	1061	290	318	12		
19	t	215	Total	C	N	O	S	0	0
			1681	1061	290	318	12		

- Molecule 20 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	480	Total	C	N	O	S	0	0
			3853	2444	684	711	14		

- Molecule 21 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	456	Total	C	N	O	S	0	0
			3703	2339	635	704	25		

- Molecule 22 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	422	Total	C	N	O	S	0	0
			3335	2116	567	639	13		

- Molecule 23 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	378	Total 3115	C 1987	N 533	O 578	S 17	0	0

- Molecule 24 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	286	Total 2282	C 1457	N 392	O 428	S 5	0	0

- Molecule 25 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	373	Total 2995	C 1911	N 510	O 559	S 15	0	0

- Molecule 26 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	191	Total 1459	C 910	N 261	O 280	S 8	0	0

- Molecule 27 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	287	Total 2260	C 1430	N 389	O 422	S 19	0	0

- Molecule 28 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	257	Total 2116	C 1371	N 346	O 390	S 9	0	0

- Molecule 29 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	e	368	Total 2883	C 1822	N 497	O 547	S 17	0	0

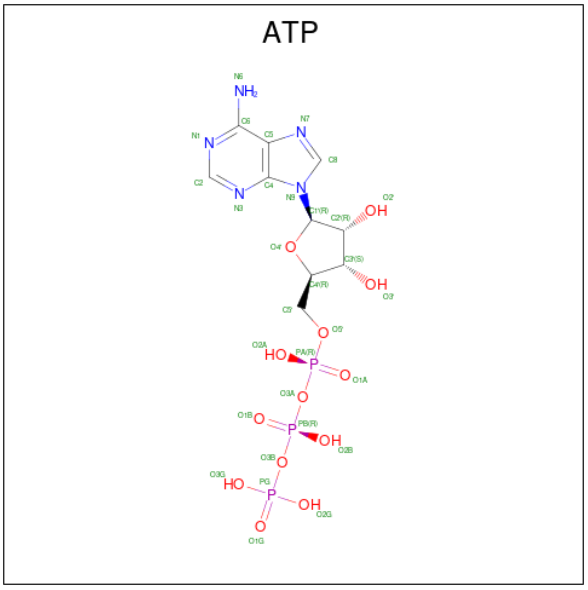
- Molecule 30 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	f	889	6867	4315	1174	1332	46	0	0

- Molecule 31 is a protein.

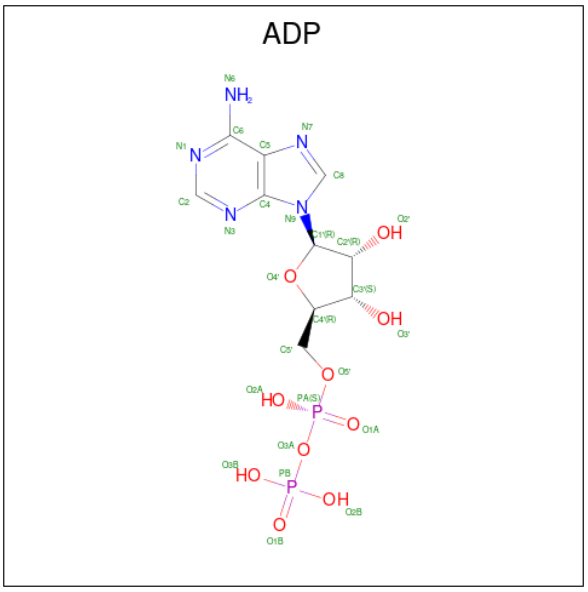
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	u	396	3119	1961	558	582	18	0	0

- Molecule 32 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
32	B	1	31	10	5	13	3	0
32	v	1	Total 31	C 10	N 5	O 13	P 3	0
32	z	1	Total 31	C 10	N 5	O 13	P 3	0
32	1	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 33 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
33	U	1	Total	C	N	O	P	0
			27	10	5	10	2	
33	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	
Number of images used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	Not provided	
Voltage (kV)	Not provided	
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	Not provided	

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no oligosaccharides in this entry.

4.6 Ligand geometry

6 ligands are 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	$\#\|Z\|>2$
32	ATP	v	501	2	28,33,33	0.68	0	34,52,52	0.70	1 (2%)
32	ATP	B	501	29,2	28,33,33	0.58	0	34,52,52	1.05	2 (5%)
32	ATP	1	1	3,31	28,33,33	0.65	0	34,52,52	0.82	2 (5%)
33	ADP	U	502	4	24,29,29	0.98	2 (8%)	29,45,45	1.54	3 (10%)
32	ATP	z	501	31	28,33,33	0.63	0	34,52,52	0.78	2 (5%)
33	ADP	w	503	5	24,29,29	0.87	0	29,45,45	1.91	8 (27%)

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
32	ATP	v	501	2	-	5/18/38/38	0/3/3/3
32	ATP	B	501	29,2	-	5/18/38/38	0/3/3/3
32	ATP	1	1	3,31	-	8/18/38/38	0/3/3/3
33	ADP	U	502	4	-	2/12/32/32	0/3/3/3
32	ATP	z	501	31	-	6/18/38/38	0/3/3/3
33	ADP	w	503	5	-	7/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	U	502	ADP	C2-N3	2.31	1.35	1.32
33	U	502	ADP	O4'-C1'	2.19	1.43	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	U	502	ADP	O4'-C1'-N9	5.36	115.86	108.75
33	w	503	ADP	C4'-O4'-C1'	5.15	114.64	109.92
33	w	503	ADP	N3-C2-N1	-3.62	123.77	128.67
32	B	501	ATP	C1'-N9-C4	3.56	132.90	126.64
33	w	503	ADP	C5'-C4'-C3'	-3.35	103.15	115.21
32	1	1	ATP	C4'-O4'-C1'	-3.20	107.00	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	U	502	ADP	N3-C2-N1	-3.01	124.58	128.67
33	w	503	ADP	C2'-C3'-C4'	3.01	108.42	102.61
33	U	502	ADP	C4-C5-N7	-2.85	106.33	109.34
32	z	501	ATP	C4'-O4'-C1'	-2.81	107.35	109.92
33	w	503	ADP	O3A-PA-O1A	-2.64	102.77	110.70
33	w	503	ADP	O4'-C4'-C3'	-2.52	100.14	105.15
32	1	1	ATP	C5-C6-N6	2.29	123.80	120.31
32	z	501	ATP	C5-C6-N6	2.27	123.77	120.31
33	w	503	ADP	C4-C5-N7	-2.25	106.96	109.34
32	v	501	ATP	C5-C6-N6	2.24	123.72	120.31
32	B	501	ATP	C5-C6-N6	2.22	123.69	120.31
33	w	503	ADP	O3'-C3'-C4'	2.00	116.84	111.08

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	B	501	ATP	PB-O3B-PG-O2G
32	v	501	ATP	PB-O3B-PG-O2G
32	z	501	ATP	C5'-O5'-PA-O1A
32	z	501	ATP	O4'-C4'-C5'-O5'
32	1	1	ATP	C5'-O5'-PA-O1A
32	1	1	ATP	C5'-O5'-PA-O2A
32	1	1	ATP	C5'-O5'-PA-O3A
33	U	502	ADP	PA-O3A-PB-O2B
33	U	502	ADP	C5'-O5'-PA-O1A
33	w	503	ADP	PA-O3A-PB-O2B
33	w	503	ADP	C5'-O5'-PA-O1A
33	w	503	ADP	C5'-O5'-PA-O2A
33	w	503	ADP	C5'-O5'-PA-O3A
32	B	501	ATP	C3'-C4'-C5'-O5'
32	z	501	ATP	C3'-C4'-C5'-O5'
33	w	503	ADP	O4'-C4'-C5'-O5'
32	B	501	ATP	O4'-C4'-C5'-O5'
32	1	1	ATP	O4'-C4'-C5'-O5'
32	1	1	ATP	C3'-C4'-C5'-O5'
32	z	501	ATP	PB-O3A-PA-O1A
32	z	501	ATP	C4'-C5'-O5'-PA
32	z	501	ATP	PB-O3A-PA-O5'
32	B	501	ATP	PB-O3A-PA-O1A
32	1	1	ATP	C4'-C5'-O5'-PA
32	B	501	ATP	C5'-O5'-PA-O1A

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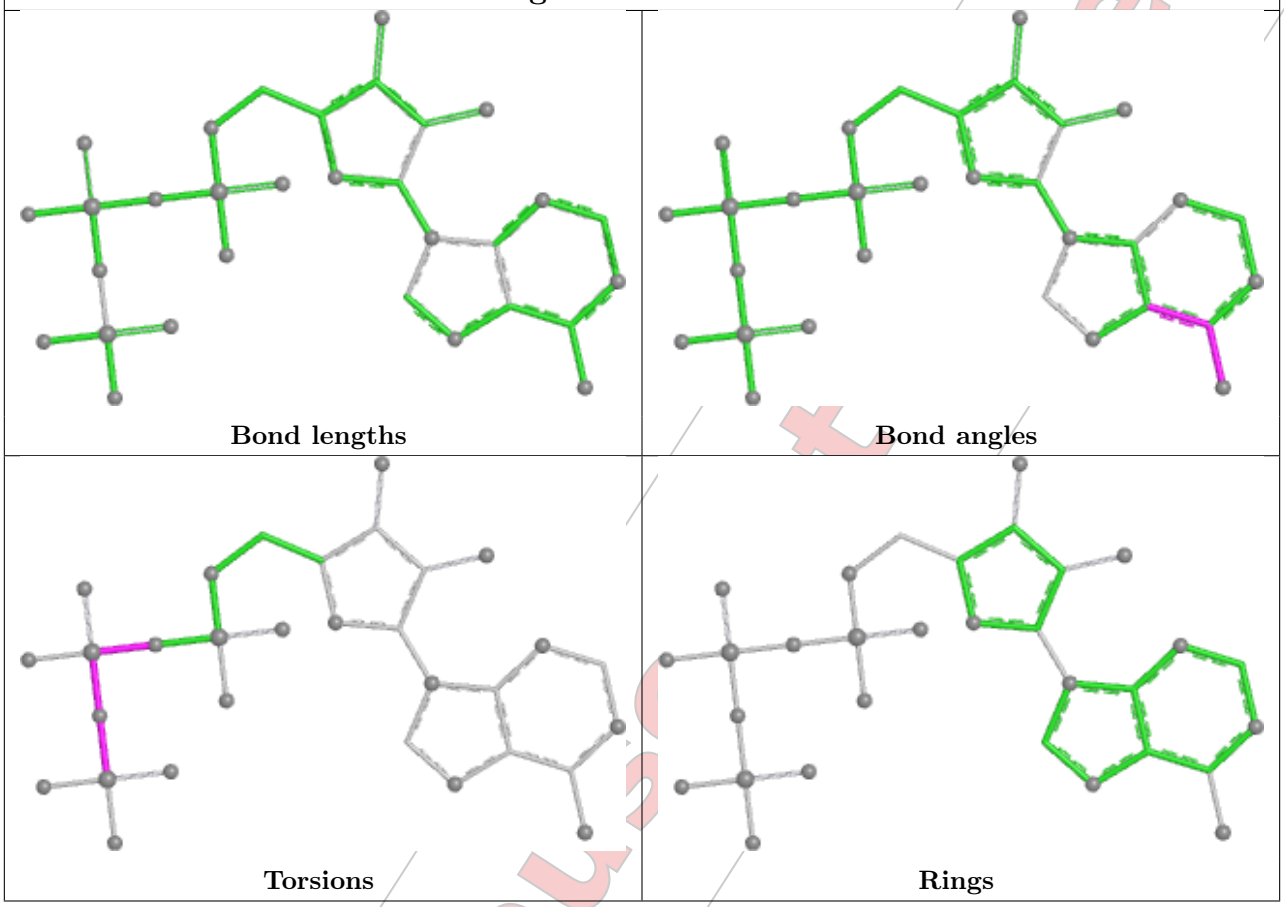
Mol	Chain	Res	Type	Atoms
32	1	1	ATP	PA-O3A-PB-O1B
32	v	501	ATP	PB-O3B-PG-O1G
32	v	501	ATP	PB-O3B-PG-O3G
33	w	503	ADP	PA-O3A-PB-O3B
32	1	1	ATP	PA-O3A-PB-O2B
33	w	503	ADP	PA-O3A-PB-O1B
32	v	501	ATP	PG-O3B-PB-O2B
32	v	501	ATP	PA-O3A-PB-O2B

There are no ring outliers.

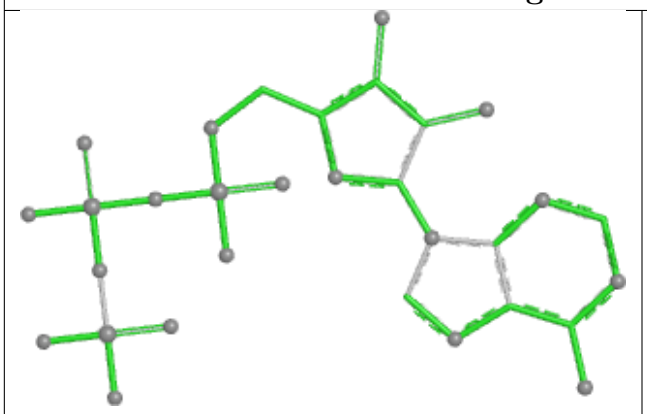
No monomer is involved in short contacts.

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 then 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.

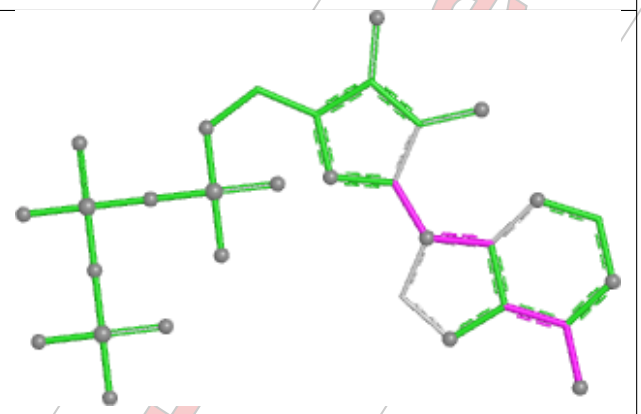
Ligand ATP v 501



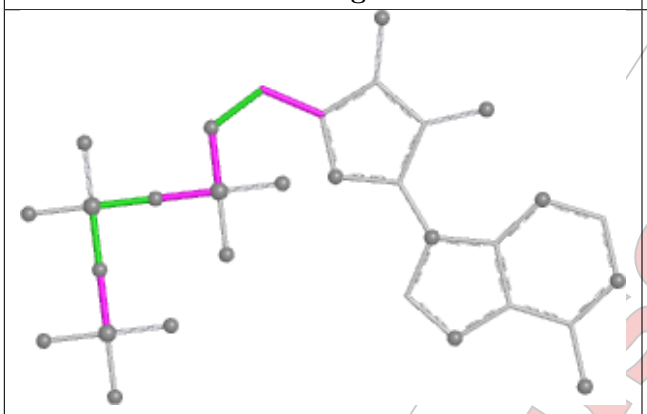
Ligand ATP B 501



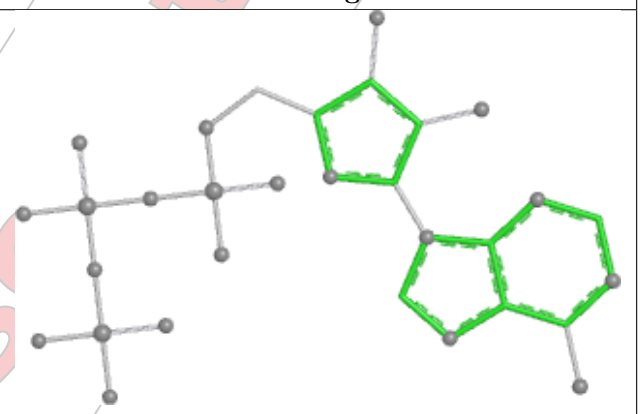
Bond lengths



Bond angles

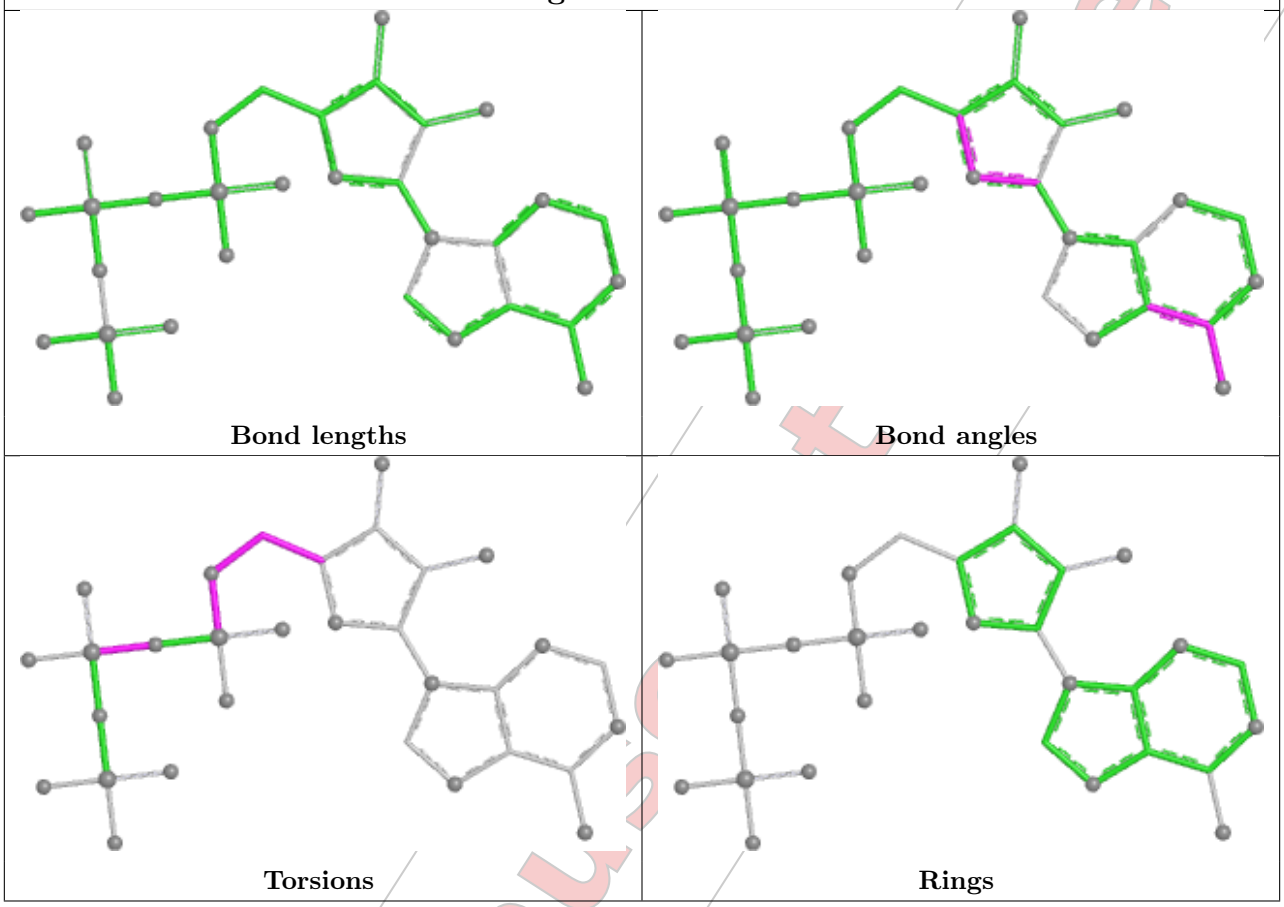


Torsions

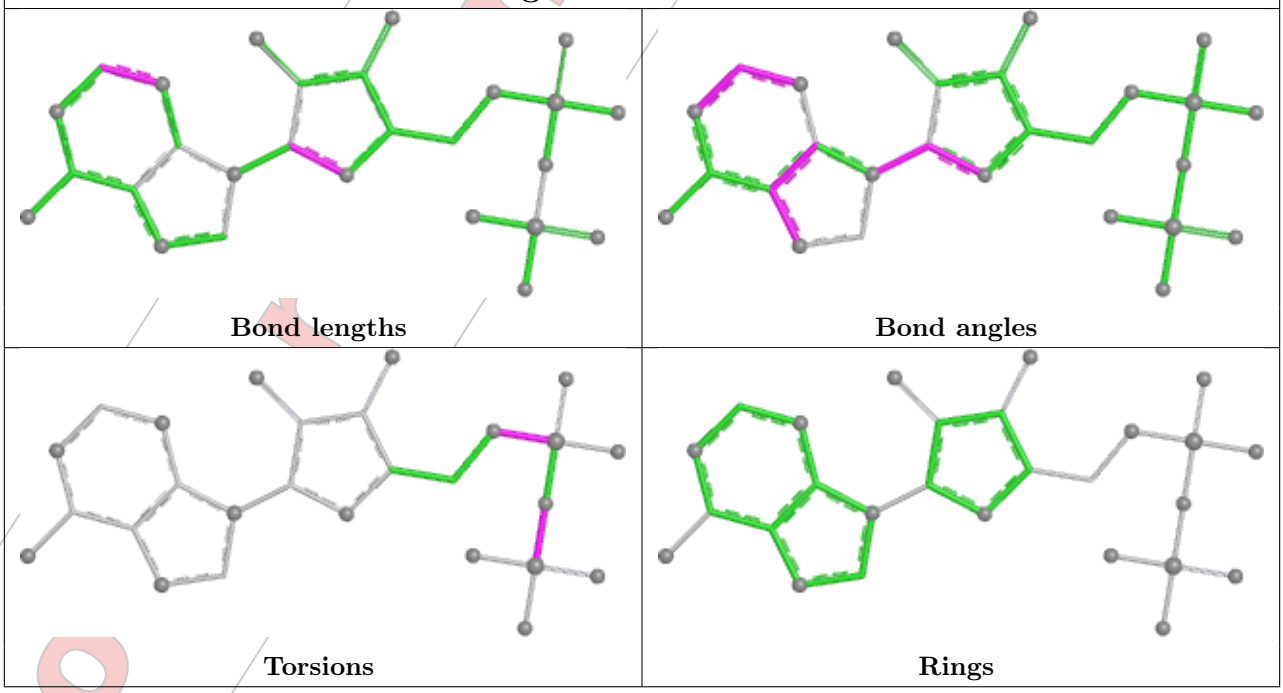


Rings

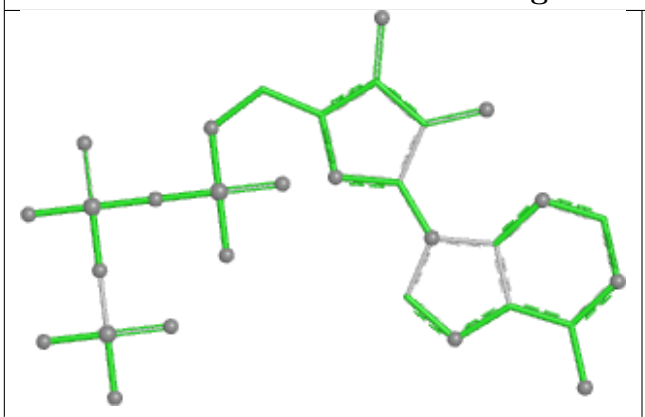
Ligand ATP 1 1



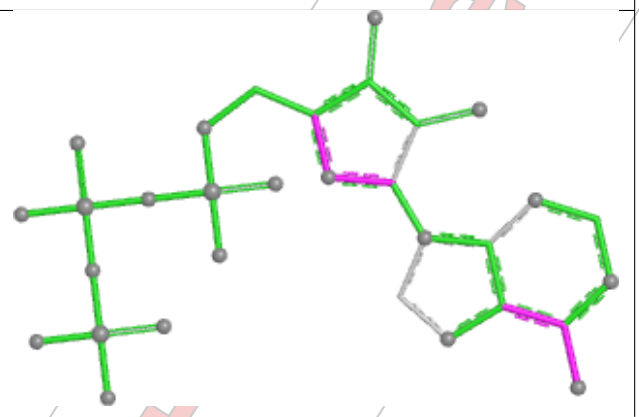
Ligand ADP U 502



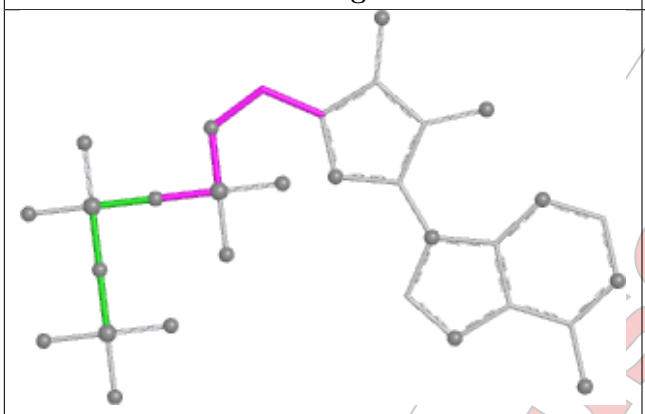
Ligand ATP z 501



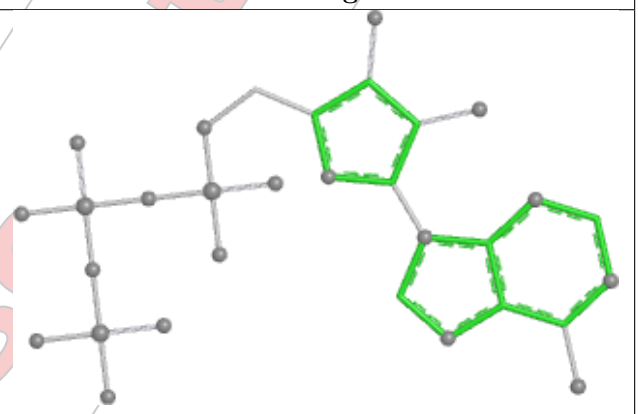
Bond lengths



Bond angles

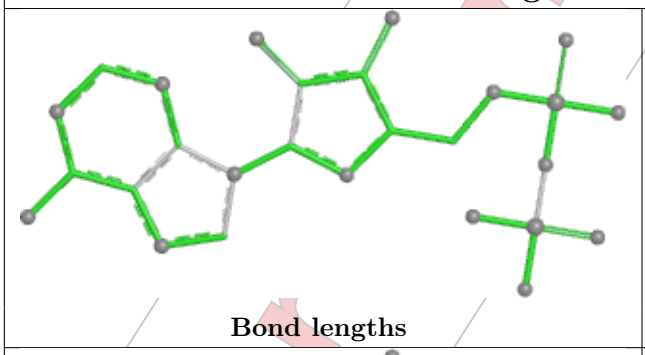


Torsions

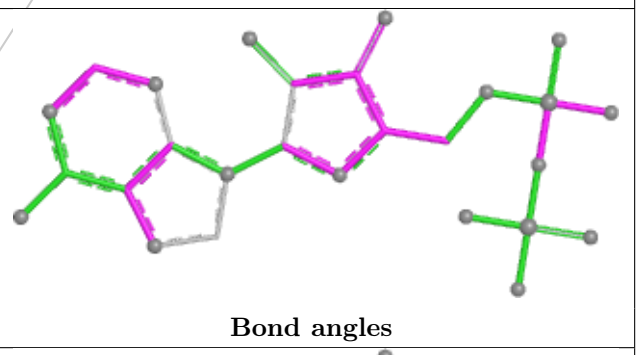


Rings

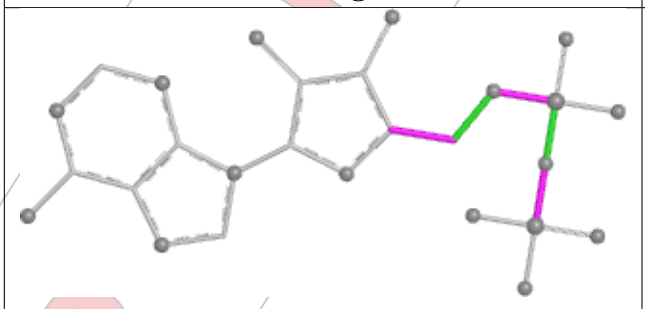
Ligand ADP w 503



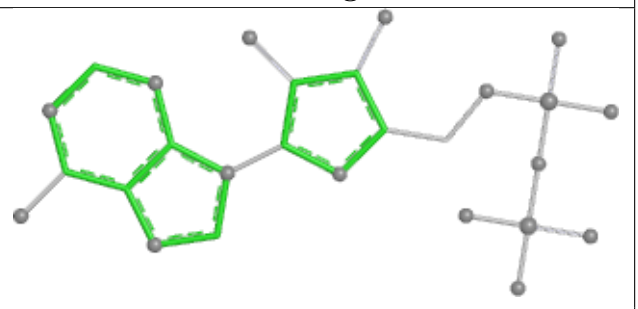
Bond lengths



Bond angles



Torsions



Rings

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	I	1
10	k	1
10	K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	270:THR	C	320:ASP	N	13.97
1	k	127:ASP	C	134:SER	N	9.33
1	K	127:ASP	C	134:SER	N	6.50

Preliminary Full wwPDB EM Validation Report ⓘ

Nov 20, 2025 – 06:44 PM EST

This wwPDB validation report is NOT for manuscript review

This is a Preliminary Full wwPDB EM Validation Report.

This report is produced by the standalone wwPDB validation server.
The structure in question has not been deposited to the wwPDB.
This report should not be submitted to journals.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
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	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 109115 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	381	3037	1911	540	570	16	0	0

- Molecule 2 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	125	1010	643	177	187	3	0	0

- Molecule 3 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	837	6479	4097	1096	1241	45	0	0

- Molecule 4 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	380	3040	1923	524	580	13	0	0

- Molecule 5 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	387	3037	1914	525	581	17	0	0

- Molecule 6 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	387	3040	1914	534	574	18	0	0

- Molecule 7 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	421	3293	2097	545	629	22	0	0

- Molecule 8 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	365	2882	1810	489	569	14	0	0

- Molecule 9 is a protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	I	48	409	249	63	97	0	0

- Molecule 10 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	358	2838	1789	507	525	17	0	0

- Molecule 11 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	228	1753	1103	289	351	10	0	0
			Total	C	N	O	S		
11	k	228	1753	1103	289	351	10	0	0

- Molecule 12 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	238	1874	1172	337	354	11	0	0
			Total	C	N	O	S		
12	l	238	1874	1172	337	354	11	0	0

- Molecule 13 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	240	Total	C	N	O	S	0	0
			1882	1193	321	357	11		
13	m	240	Total	C	N	O	S	0	0
			1882	1193	321	357	11		

- Molecule 14 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	191	Total	C	N	O	S	0	0
			1431	893	245	281	12		
14	n	191	Total	C	N	O	S	0	0
			1431	893	245	281	12		

- Molecule 15 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	220	Total	C	N	O	S	0	0
			1660	1044	283	321	12		
15	o	220	Total	C	N	O	S	0	0
			1660	1044	283	321	12		

- Molecule 16 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		
16	p	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

- Molecule 17 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	199	Total	C	N	O	S	0	0
			1597	1022	272	294	9		
17	q	199	Total	C	N	O	S	0	0
			1597	1022	272	294	9		

- Molecule 18 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	201	Total	C	N	O	S	0	0
			1560	982	274	295	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
18	r	201	Total	C	N	O	S	0	0
			1560	982	274	295	9		

- Molecule 19 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	213	Total	C	N	O	S	0	0
			1654	1047	284	313	10		
19	s	213	Total	C	N	O	S	0	0
			1654	1047	284	313	10		

- Molecule 20 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	215	Total	C	N	O	S	0	0
			1682	1061	290	319	12		
20	t	215	Total	C	N	O	S	0	0
			1682	1061	290	319	12		

- Molecule 21 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	806	Total	C	N	O	S	0	0
			6288	3990	1075	1179	44		

- Molecule 22 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	480	Total	C	N	O	S	0	0
			3853	2444	684	711	14		

- Molecule 23 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	456	Total	C	N	O	S	0	0
			3703	2339	635	704	25		

- Molecule 24 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	422	Total 3335	C 2116	N 567	O 639	S 13	0	0

- Molecule 25 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	378	Total 3115	C 1987	N 533	O 578	S 17	0	0

- Molecule 26 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	286	Total 2282	C 1457	N 392	O 428	S 5	0	0

- Molecule 27 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	373	Total 2995	C 1911	N 510	O 559	S 15	0	0

- Molecule 28 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	191	Total 1459	C 910	N 261	O 280	S 8	0	0

- Molecule 29 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	287	Total 2260	C 1430	N 389	O 422	S 19	0	0

- Molecule 30 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	257	Total 2116	C 1371	N 346	O 390	S 9	0	0

- Molecule 31 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	240	Total	C	N	O	S	0	0
			1872	1189	310	360	13		
31	g	240	Total	C	N	O	S	0	0
			1872	1189	310	360	13		

- Molecule 32 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	232	Total	C	N	O	S	0	0
			1813	1158	307	342	6		
32	h	232	Total	C	N	O	S	0	0
			1813	1158	307	342	6		

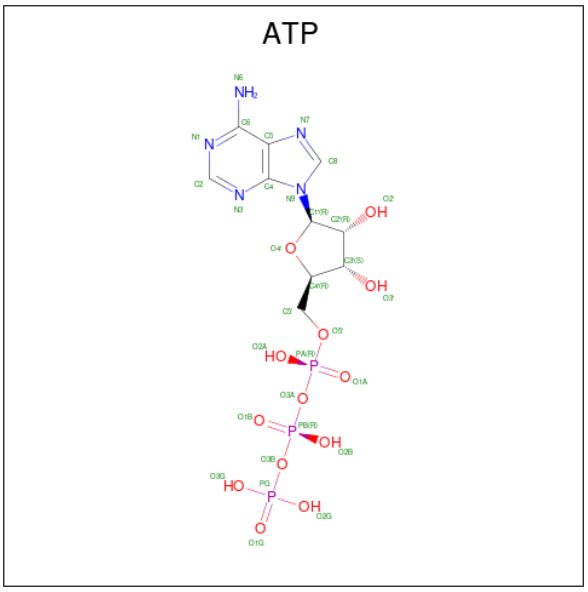
- Molecule 33 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	i	250	Total	C	N	O	S	0	0
			1972	1245	339	378	10		
33	u	250	Total	C	N	O	S	0	0
			1972	1245	339	378	10		

- Molecule 34 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	j	239	Total	C	N	O	S	0	0
			1888	1183	334	366	5		
34	v	239	Total	C	N	O	S	0	0
			1888	1183	334	366	5		

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
35	x	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	x	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	x	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	x	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	x	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	y	1	Total	C	N	O	P	0
			31	10	5	13	3	

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	
Number of images used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	Not provided	
Voltage (kV)	Not provided	
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	Not provided	

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no oligosaccharides in this entry.

4.6 Ligand geometry

6 ligands are 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	$\#\|Z\| > 2$
35	ATP	x	503	-	28,33,33	0.91	0	34,52,52	1.24	3 (8%)
35	ATP	y	501	-	28,33,33	0.67	0	34,52,52	0.63	1 (2%)
35	ATP	x	504	-	28,33,33	1.00	0	34,52,52	1.21	3 (8%)
35	ATP	x	505	-	28,33,33	0.91	0	34,52,52	1.25	2 (5%)
35	ATP	x	501	6	28,33,33	0.62	0	34,52,52	0.85	2 (5%)
35	ATP	x	502	5	28,33,33	0.87	0	34,52,52	1.21	2 (5%)

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
35	ATP	x	503	-	-	4/18/38/38	0/3/3/3
35	ATP	y	501	-	-	4/18/38/38	0/3/3/3
35	ATP	x	504	-	-	3/18/38/38	0/3/3/3
35	ATP	x	505	-	-	5/18/38/38	0/3/3/3
35	ATP	x	501	6	-	5/18/38/38	0/3/3/3
35	ATP	x	502	5	-	3/18/38/38	0/3/3/3

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	x	503	ATP	N3-C2-N1	-4.04	123.19	128.67
35	x	504	ATP	N3-C2-N1	-3.86	123.44	128.67
35	x	502	ATP	N3-C2-N1	-3.85	123.45	128.67
35	x	505	ATP	N3-C2-N1	-3.85	123.45	128.67
35	x	501	ATP	C4'-O4'-C1'	-3.54	106.69	109.92
35	x	505	ATP	C4-C5-N7	-2.91	106.26	109.34
35	x	503	ATP	C4-C5-N7	-2.52	106.67	109.34
35	x	504	ATP	C4-C5-N7	-2.38	106.82	109.34
35	x	501	ATP	C5-C6-N6	2.33	123.85	120.31
35	y	501	ATP	C5-C6-N6	2.30	123.82	120.31
35	x	504	ATP	O3G-PG-O2G	2.23	116.17	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	x	502	ATP	C4-C5-N7	-2.13	107.09	109.34
35	x	503	ATP	O3G-PG-O2G	2.04	115.44	107.80

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	x	504	ATP	C5'-O5'-PA-O2A
35	x	501	ATP	C5'-O5'-PA-O2A
35	x	501	ATP	C5'-O5'-PA-O3A
35	x	501	ATP	O4'-C4'-C5'-O5'
35	y	501	ATP	PB-O3A-PA-O5'
35	x	505	ATP	C3'-C4'-C5'-O5'
35	x	504	ATP	O4'-C4'-C5'-O5'
35	x	505	ATP	O4'-C4'-C5'-O5'
35	x	502	ATP	C3'-C4'-C5'-O5'
35	x	504	ATP	C3'-C4'-C5'-O5'
35	x	501	ATP	C3'-C4'-C5'-O5'
35	x	502	ATP	O4'-C4'-C5'-O5'
35	x	503	ATP	C3'-C4'-C5'-O5'
35	x	503	ATP	PB-O3B-PG-O1G
35	x	502	ATP	C4'-C5'-O5'-PA
35	x	501	ATP	C4'-C5'-O5'-PA
35	x	503	ATP	PB-O3B-PG-O3G
35	x	505	ATP	PG-O3B-PB-O1B
35	y	501	ATP	PG-O3B-PB-O3A
35	y	501	ATP	C5'-O5'-PA-O1A
35	x	505	ATP	PG-O3B-PB-O2B
35	x	505	ATP	C4'-C5'-O5'-PA
35	x	503	ATP	O4'-C4'-C5'-O5'
35	y	501	ATP	PG-O3B-PB-O1B

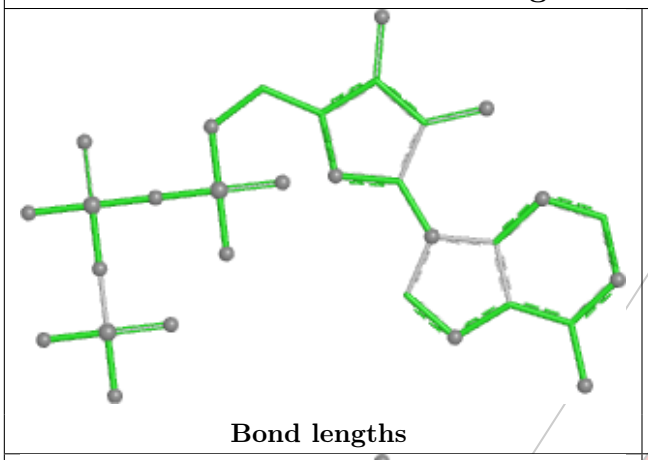
There are no ring outliers.

No monomer is involved in short contacts.

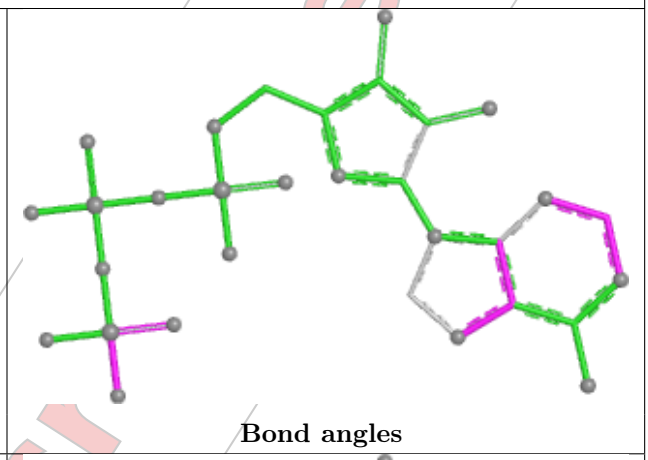
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

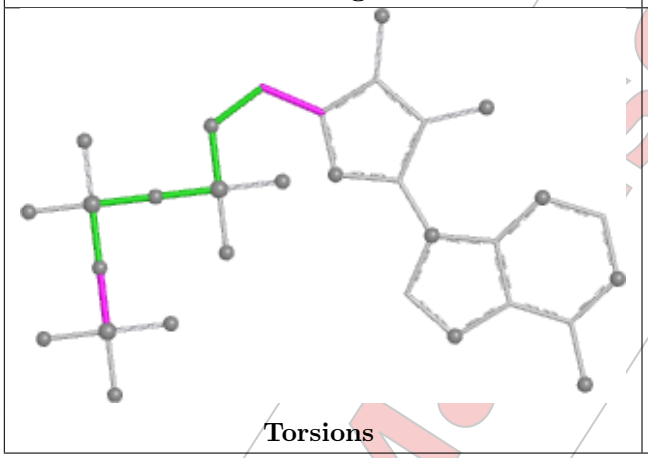
Ligand ATP x 503



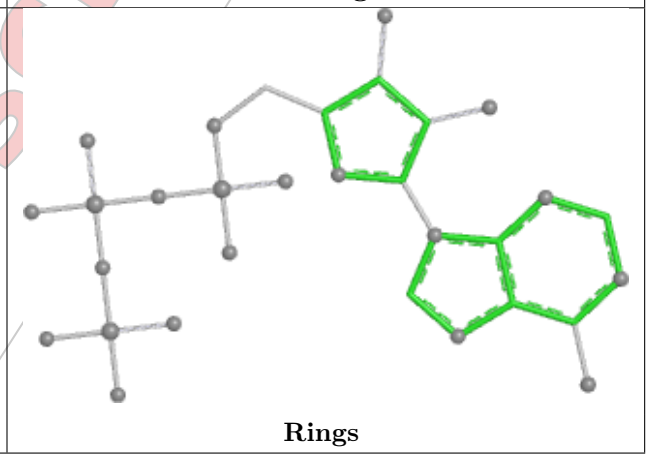
Bond lengths



Bond angles

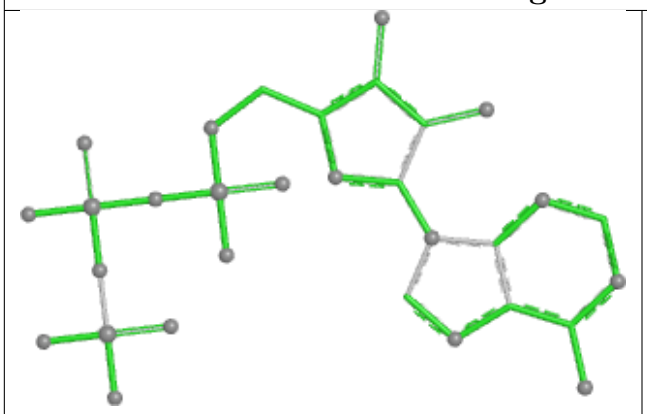


Torsions

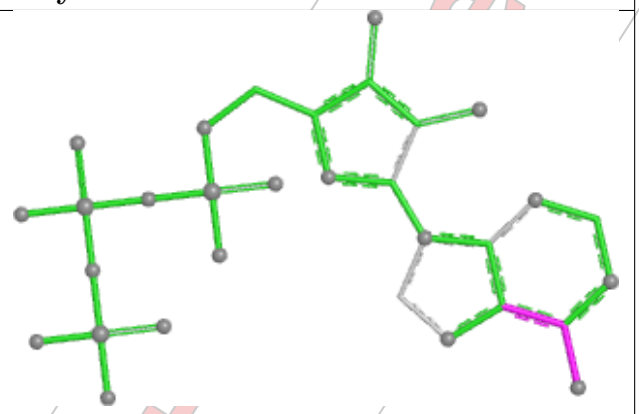


Rings

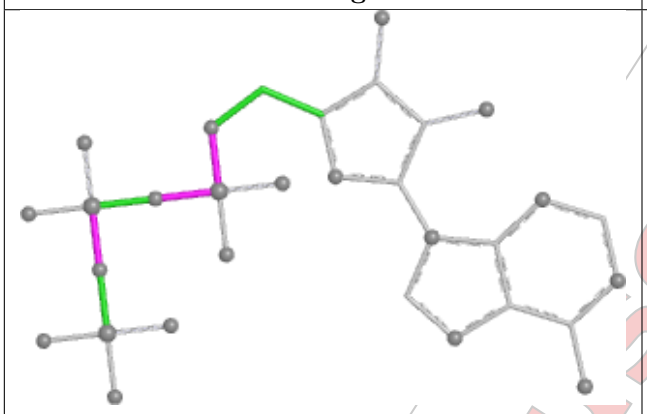
Ligand ATP y 501



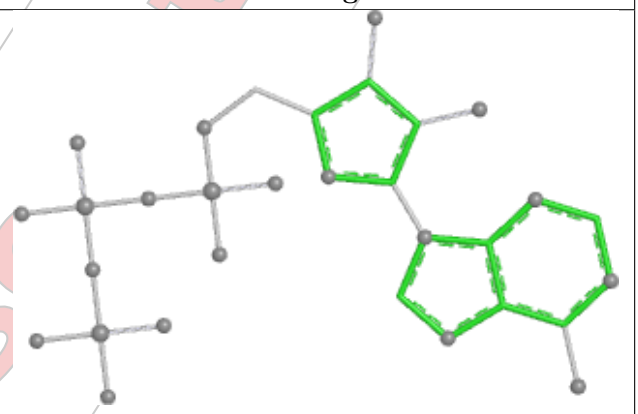
Bond lengths



Bond angles

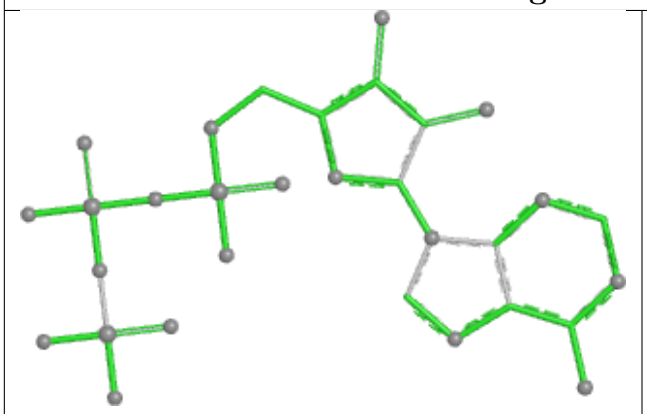


Torsions

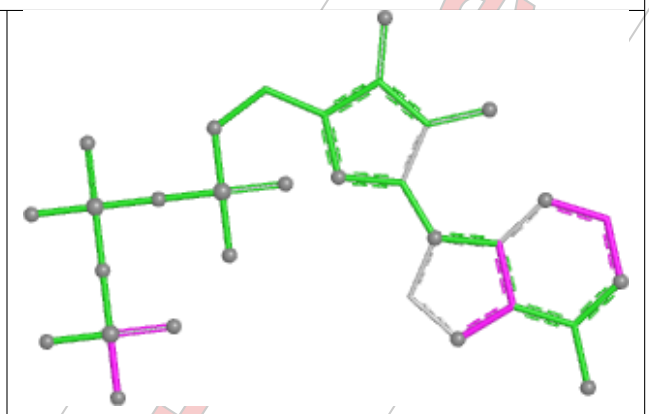


Rings

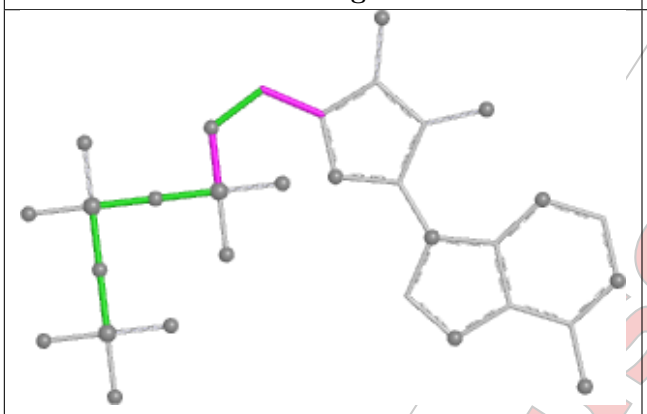
Ligand ATP x 504



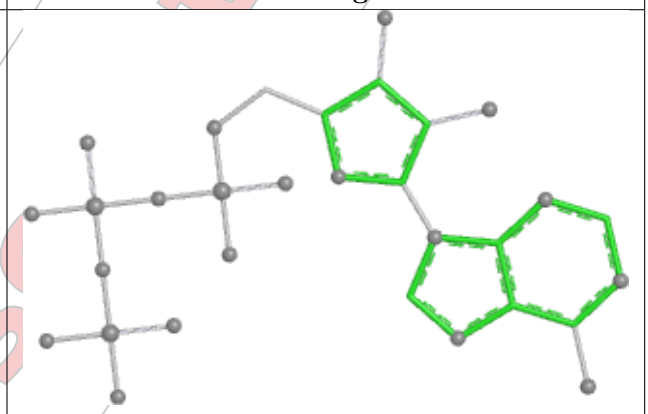
Bond lengths



Bond angles

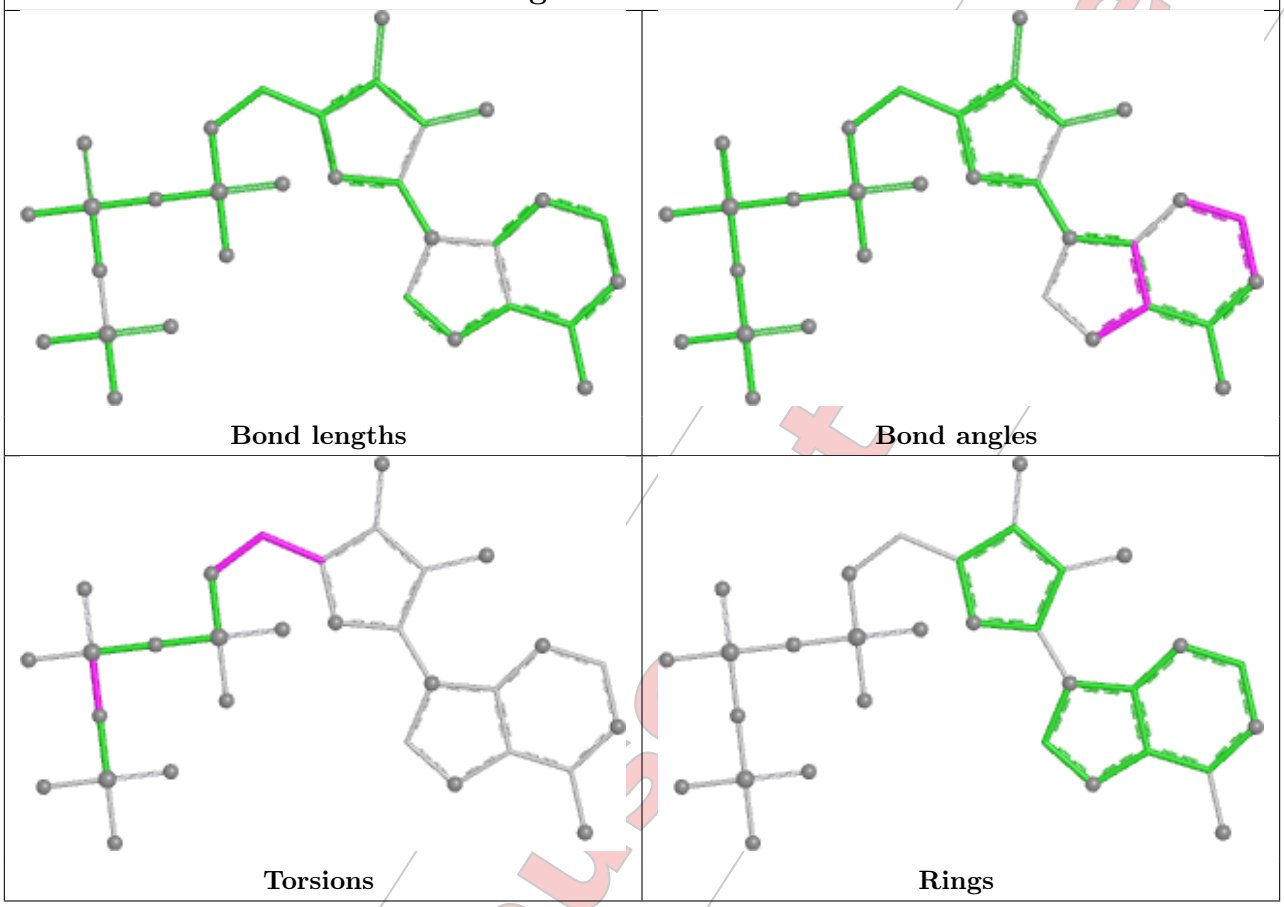


Torsions

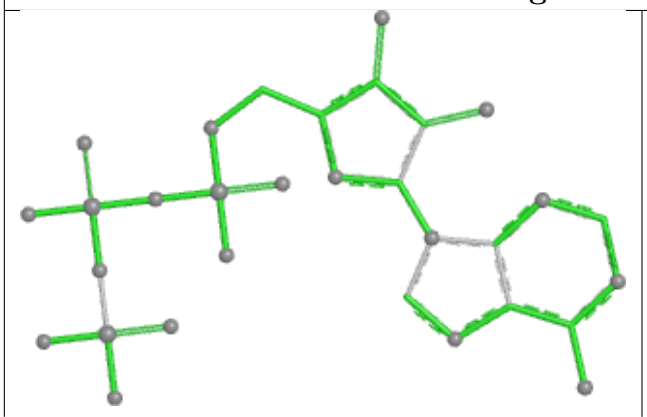


Rings

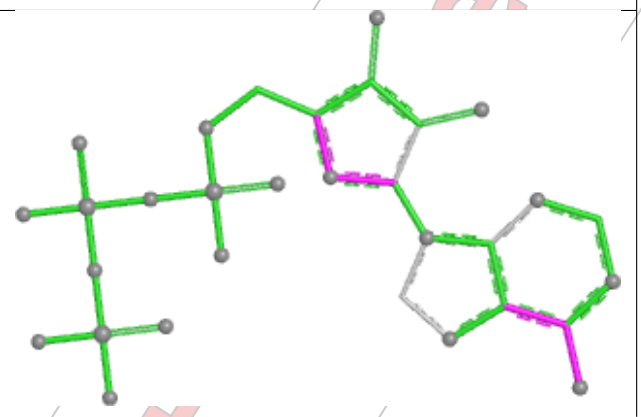
Ligand ATP x 505



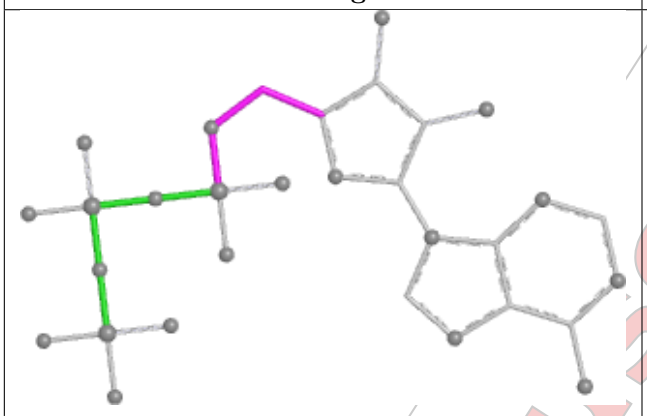
Ligand ATP x 501



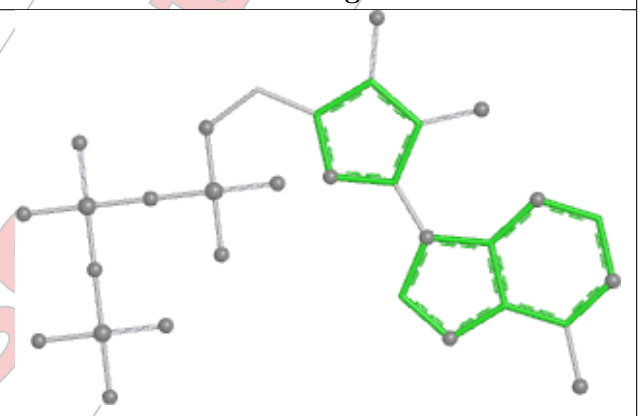
Bond lengths



Bond angles

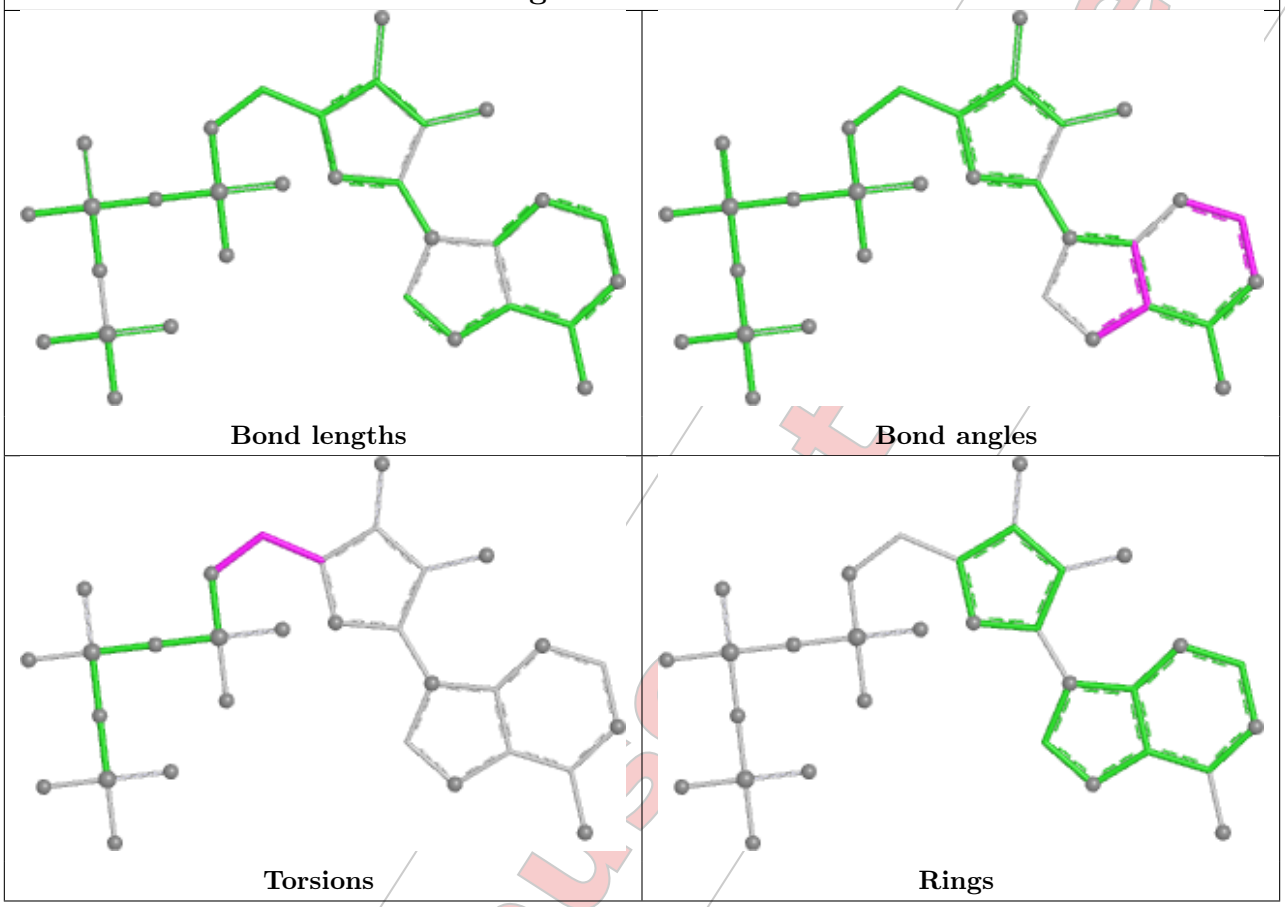


Torsions



Rings

Ligand ATP x 502



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
21	U	3
3	C	2
11	k	1
11	K	1
10	J	1
5	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	814:PRO	C	836:THR	N	18.95
1	C	356:ASN	C	366:ASP	N	17.54
1	U	270:THR	C	320:ASP	N	14.39
1	C	621:ASP	C	641:GLU	N	12.25
1	k	127:ASP	C	134:SER	N	8.94
1	K	127:ASP	C	134:SER	N	8.28
1	J	250:GLU	C	267:SER	N	8.05
1	E	102:ASN	C	118:LYS	N	7.52
1	U	844:LYS	C	880:ASN	N	6.61

Preliminary Full wwPDB EM Validation Report ⓘ

Nov 21, 2025 – 06:18 AM EST

This wwPDB validation report is NOT for manuscript review

This is a Preliminary Full wwPDB EM Validation Report.

This report is produced by the standalone wwPDB validation server.
The structure in question has not been deposited to the wwPDB.
This report should not be submitted to journals.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
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	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 107831 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	421	3292	2095	545	630	22	0	0

- Molecule 2 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	125	1010	643	177	187	3	0	0

- Molecule 3 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	358	2838	1789	507	525	17	0	0

- Molecule 4 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	380	3040	1923	524	580	13	0	0

- Molecule 5 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	376	2989	1881	531	561	16	0	0

- Molecule 6 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	390	3066	1930	533	586	17	0	0

- Molecule 7 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	240	1872	1189	310	360	13	0	0
7	g	240	Total	C	N	O	S	0	0
			1872	1189	310	360	13		

- Molecule 8 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	232	1813	1158	307	342	6	0	0
8	h	232	Total	C	N	O	S	0	0
			1813	1158	307	342	6		

- Molecule 9 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	250	1972	1245	339	378	10	0	0
9	i	250	Total	C	N	O	S	0	0
			1972	1245	339	378	10		

- Molecule 10 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	239	1888	1183	334	366	5	0	0
10	j	239	Total	C	N	O	S	0	0
			1888	1183	334	366	5		

- Molecule 11 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	228	1753	1103	289	351	10	0	0
11	k	228	Total	C	N	O	S	0	0
			1753	1103	289	351	10		

- Molecule 12 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	238	Total	C	N	O	S	0	0
			1874	1172	337	354	11		
12	l	238	Total	C	N	O	S	0	0
			1874	1172	337	354	11		

- Molecule 13 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	240	Total	C	N	O	S	0	0
			1882	1193	321	357	11		
13	m	240	Total	C	N	O	S	0	0
			1882	1193	321	357	11		

- Molecule 14 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	191	Total	C	N	O	S	0	0
			1431	893	245	281	12		
14	n	191	Total	C	N	O	S	0	0
			1431	893	245	281	12		

- Molecule 15 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	220	Total	C	N	O	S	0	0
			1660	1044	283	321	12		
15	o	220	Total	C	N	O	S	0	0
			1660	1044	283	321	12		

- Molecule 16 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		
16	p	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

- Molecule 17 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	199	Total	C	N	O	S	0	0
			1597	1022	272	294	9		

Continued on next page...

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Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	199	Total	C	N	O	S	0	0
			1597	1022	272	294	9		

- Molecule 18 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	201	Total	C	N	O	S	0	0
			1560	982	274	295	9		
18	r	201	Total	C	N	O	S	0	0
			1560	982	274	295	9		

- Molecule 19 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	213	Total	C	N	O	S	0	0
			1654	1047	284	313	10		
19	s	213	Total	C	N	O	S	0	0
			1654	1047	284	313	10		

- Molecule 20 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	215	Total	C	N	O	S	0	0
			1682	1061	290	319	12		
20	t	215	Total	C	N	O	S	0	0
			1682	1061	290	319	12		

- Molecule 21 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	806	Total	C	N	O	S	0	0
			6288	3990	1075	1179	44		

- Molecule 22 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	480	Total	C	N	O	S	0	0
			3853	2444	684	711	14		

- Molecule 23 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	456	Total 3703	C 2339	N 635	O 704	S 25	0	0

- Molecule 24 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	422	Total 3335	C 2116	N 567	O 639	S 13	0	0

- Molecule 25 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	378	Total 3115	C 1987	N 533	O 578	S 17	0	0

- Molecule 26 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	286	Total 2282	C 1457	N 392	O 428	S 5	0	0

- Molecule 27 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	373	Total 2995	C 1911	N 510	O 559	S 15	0	0

- Molecule 28 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	191	Total 1459	C 910	N 261	O 280	S 8	0	0

- Molecule 29 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	287	Total 2260	C 1430	N 389	O 422	S 19	0	0

- Molecule 30 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	257	Total	C	N	O	S	0	0
			2116	1371	346	390	9		

- Molecule 31 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	380	Total	C	N	O	S	0	0
			2986	1877	526	565	18		

- Molecule 32 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	689	Total	C	N	O	S	0	0
			5320	3343	904	1038	35		

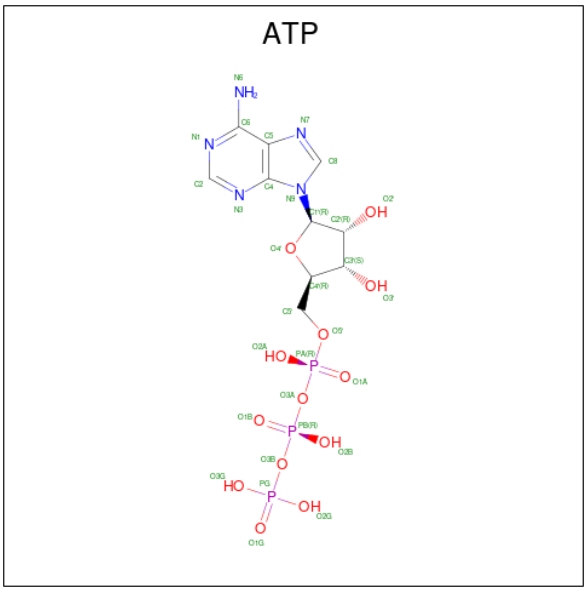
- Molecule 33 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	u	359	Total	C	N	O	S	0	0
			2831	1778	481	559	13		

- Molecule 34 is a protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	v	48	Total	C	N	O	0	0
			409	249	63	97		

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
35	x	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	x	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	x	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	x	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	x	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	y	1	Total	C	N	O	P	0
			31	10	5	13	3	

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	
Number of images used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	Not provided	
Voltage (kV)	Not provided	
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	Not provided	

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no oligosaccharides in this entry.

4.6 Ligand geometry

6 ligands are 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	$\#\|Z\| > 2$
35	ATP	x	502	4	28,33,33	0.83	0	34,52,52	1.40	4 (11%)
35	ATP	x	505	-	28,33,33	0.91	0	34,52,52	1.53	6 (17%)
35	ATP	x	503	-	28,33,33	0.92	0	34,52,52	1.17	2 (5%)
35	ATP	y	501	-	28,33,33	0.60	0	34,52,52	0.73	2 (5%)
35	ATP	x	504	-	28,33,33	0.80	0	34,52,52	1.29	2 (5%)
35	ATP	x	501	-	28,33,33	0.60	0	34,52,52	1.09	3 (8%)

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
35	ATP	x	502	4	-	6/18/38/38	0/3/3/3
35	ATP	x	505	-	-	3/18/38/38	0/3/3/3
35	ATP	x	503	-	-	0/18/38/38	0/3/3/3
35	ATP	y	501	-	-	5/18/38/38	0/3/3/3
35	ATP	x	504	-	-	7/18/38/38	0/3/3/3
35	ATP	x	501	-	-	3/18/38/38	0/3/3/3

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	x	501	ATP	C4'-O4'-C1'	-4.49	105.81	109.92
35	x	505	ATP	N3-C2-N1	-4.07	123.15	128.67
35	x	504	ATP	N3-C2-N1	-4.01	123.23	128.67
35	x	502	ATP	N3-C2-N1	-3.99	123.25	128.67
35	x	503	ATP	N3-C2-N1	-3.69	123.66	128.67
35	x	505	ATP	O3'-C3'-C2'	3.02	121.49	111.82
35	x	501	ATP	C1'-N9-C4	2.78	131.53	126.64
35	x	504	ATP	C4-C5-N7	-2.75	106.43	109.34
35	x	502	ATP	C1'-N9-C4	-2.65	121.98	126.64
35	x	502	ATP	C4-C5-N7	-2.65	106.54	109.34
35	x	505	ATP	C4'-O4'-C1'	-2.55	107.59	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	x	505	ATP	C2'-C3'-C4'	2.53	107.51	102.61
35	x	505	ATP	C4-C5-N7	-2.46	106.74	109.34
35	x	503	ATP	C4-C5-N7	-2.28	106.93	109.34
35	y	501	ATP	C5-C6-N6	2.28	123.78	120.31
35	x	501	ATP	C5-C6-N6	2.27	123.76	120.31
35	y	501	ATP	C4'-O4'-C1'	-2.23	107.88	109.92
35	x	505	ATP	O4'-C1'-N9	2.20	111.66	108.75
35	x	502	ATP	O3G-PG-O2G	2.02	115.39	107.80

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	x	502	ATP	C5'-O5'-PA-O1A
35	x	502	ATP	C5'-O5'-PA-O2A
35	x	502	ATP	C5'-O5'-PA-O3A
35	x	502	ATP	C4'-C5'-O5'-PA
35	x	502	ATP	O4'-C4'-C5'-O5'
35	x	502	ATP	C3'-C4'-C5'-O5'
35	x	501	ATP	C5'-O5'-PA-O2A
35	x	505	ATP	C5'-O5'-PA-O3A
35	x	504	ATP	C5'-O5'-PA-O1A
35	x	504	ATP	C5'-O5'-PA-O3A
35	x	504	ATP	C3'-C4'-C5'-O5'
35	x	505	ATP	C4'-C5'-O5'-PA
35	x	504	ATP	O4'-C4'-C5'-O5'
35	y	501	ATP	O4'-C4'-C5'-O5'
35	x	501	ATP	C4'-C5'-O5'-PA
35	x	504	ATP	PB-O3A-PA-O5'
35	y	501	ATP	PB-O3B-PG-O1G
35	x	504	ATP	PG-O3B-PB-O3A
35	x	501	ATP	C5'-O5'-PA-O3A
35	x	505	ATP	C5'-O5'-PA-O1A
35	x	504	ATP	C5'-O5'-PA-O2A
35	y	501	ATP	PA-O3A-PB-O1B
35	y	501	ATP	PB-O3B-PG-O2G
35	y	501	ATP	PB-O3B-PG-O3G

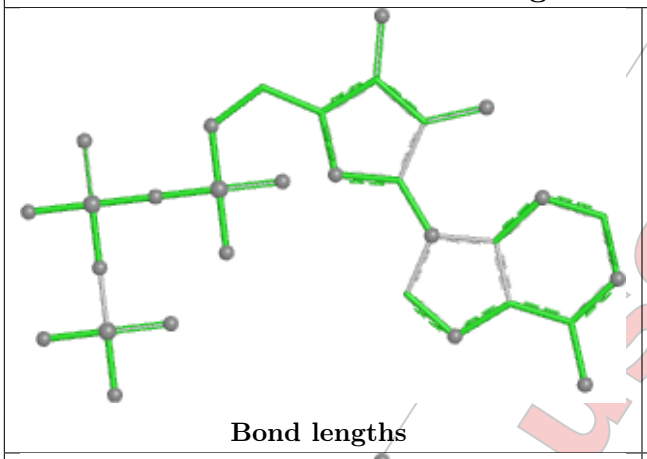
There are no ring outliers.

No monomer is involved in short contacts.

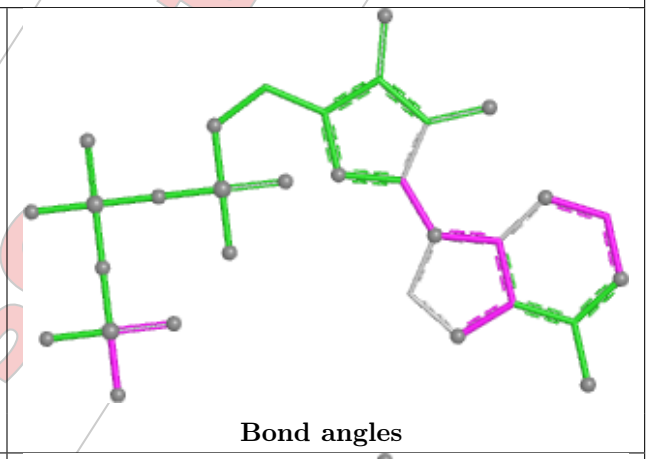
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 then 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.

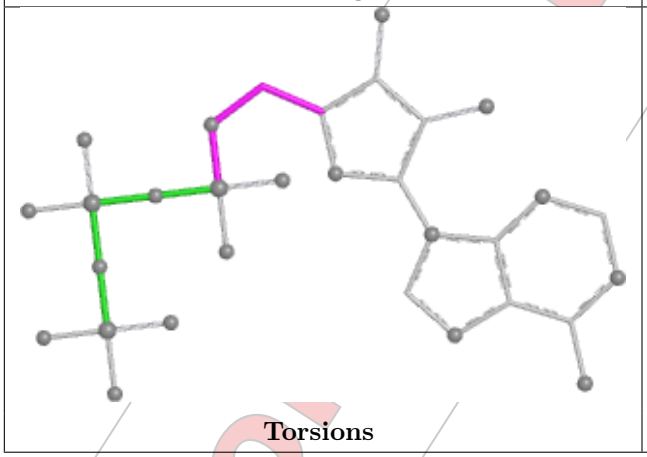
Ligand ATP x 502



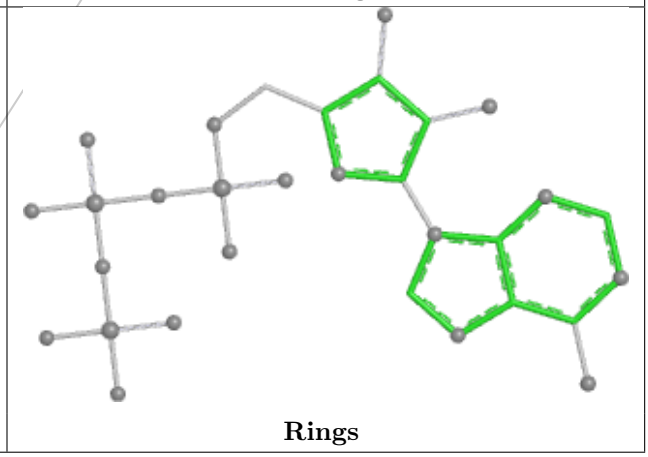
Bond lengths



Bond angles

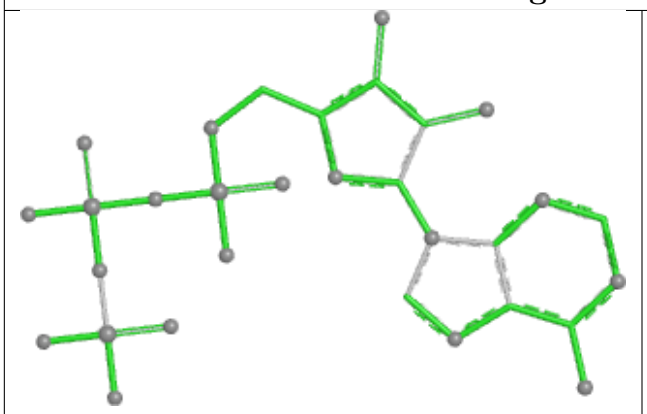


Torsions

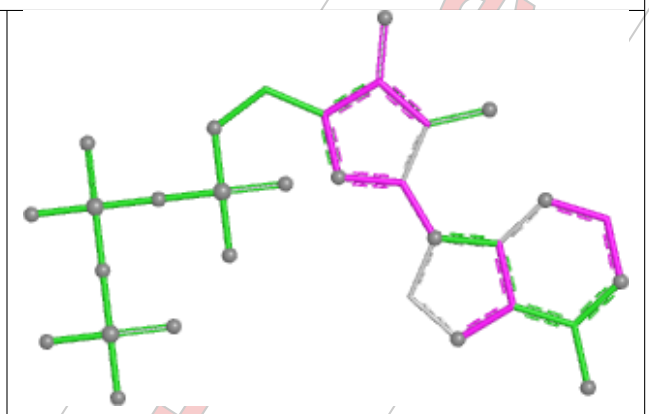


Rings

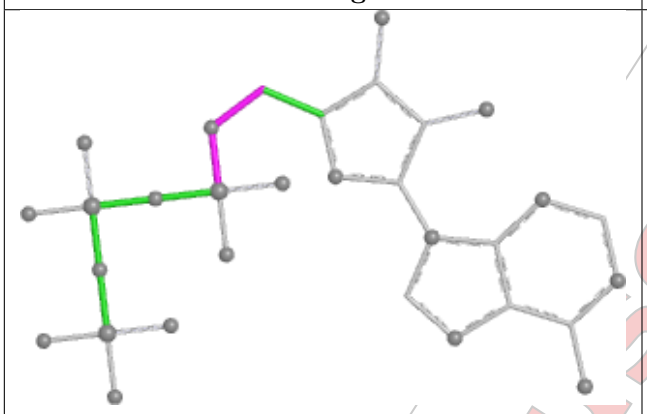
Ligand ATP x 505



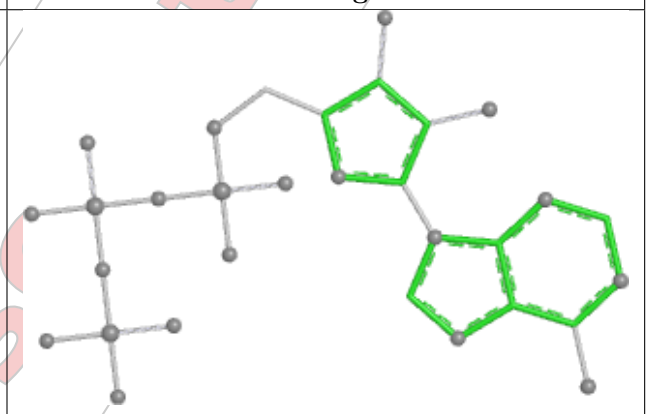
Bond lengths



Bond angles

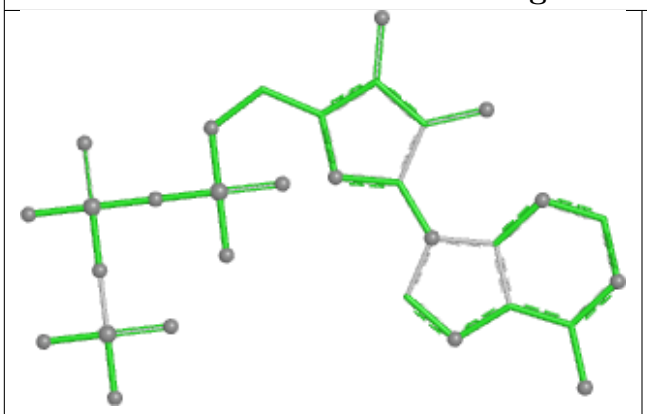


Torsions

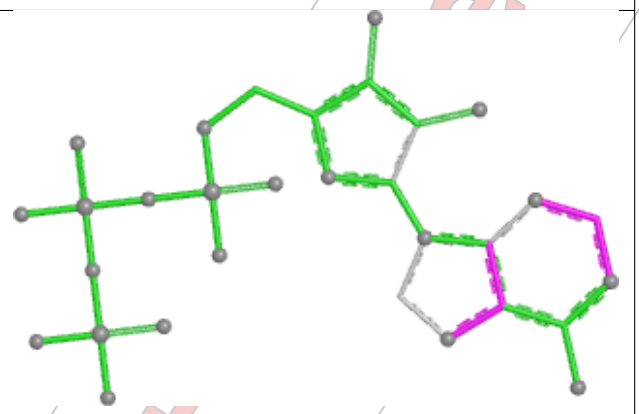


Rings

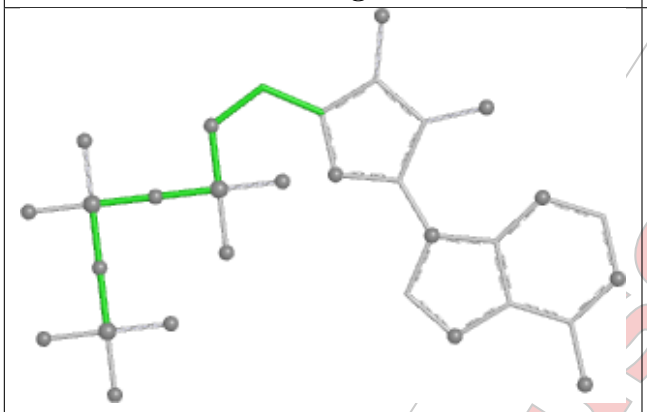
Ligand ATP x 503



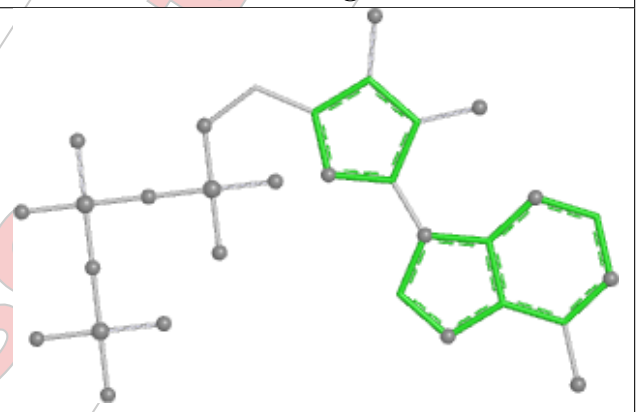
Bond lengths



Bond angles

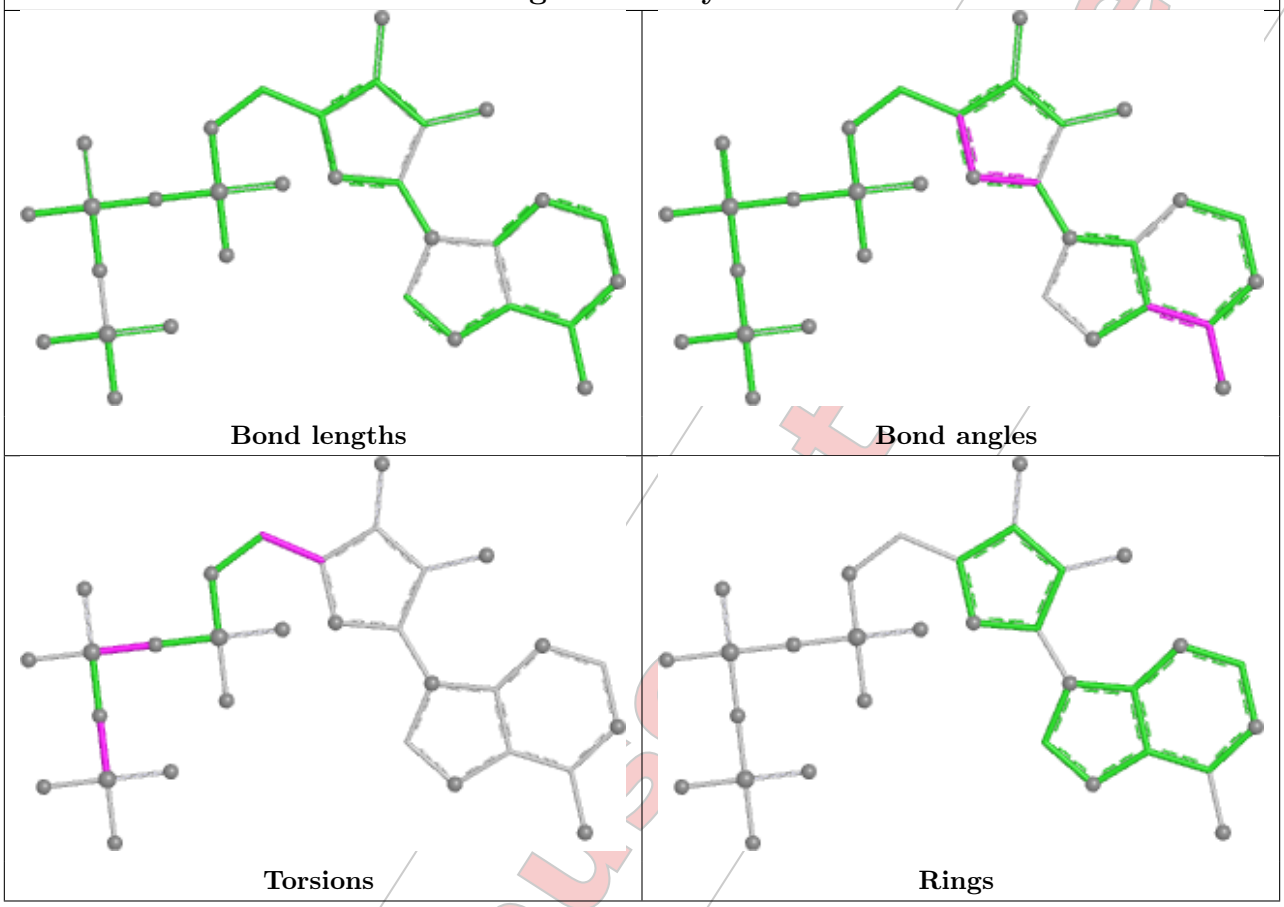


Torsions

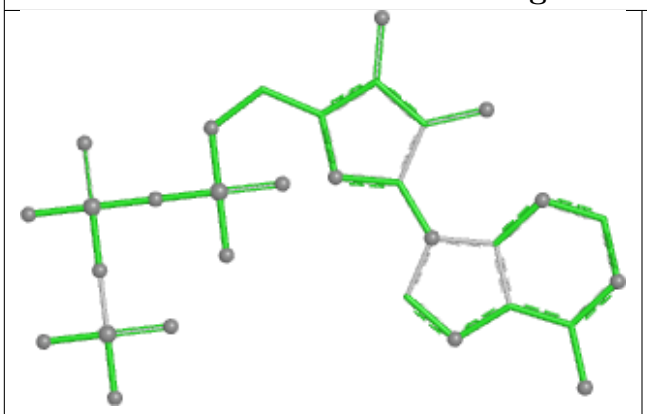


Rings

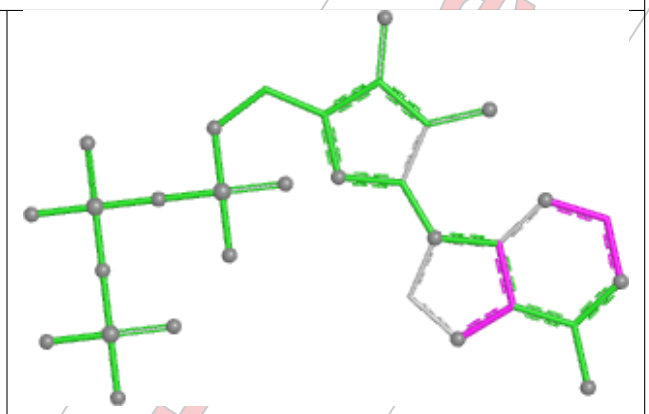
Ligand ATP y 501



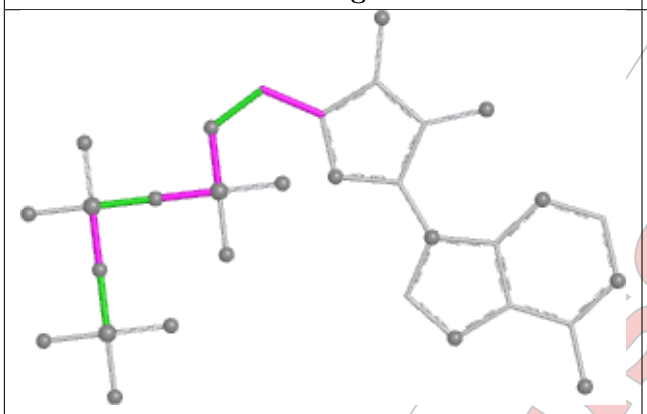
Ligand ATP x 504



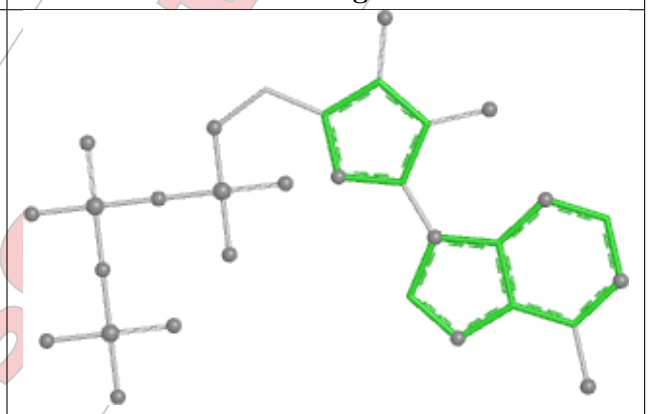
Bond lengths



Bond angles

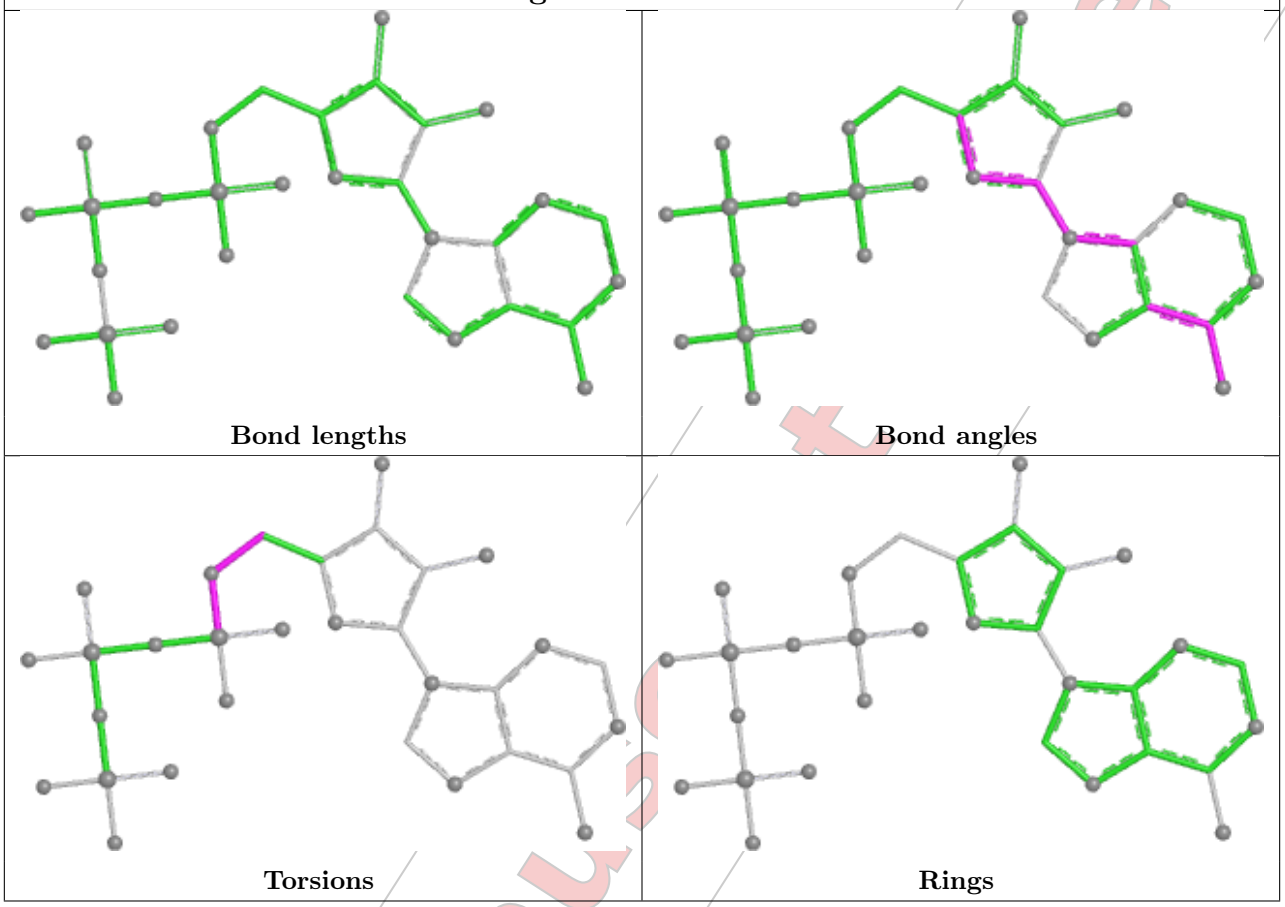


Torsions



Rings

Ligand ATP x 501



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
32	f	9
21	U	3
6	F	2
31	e	1
33	u	1
11	K	1
3	C	1
11	k	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	f	754:LYS	C	773:LYS	N	22.95
1	U	814:PRO	C	836:THR	N	20.30
1	e	72:LEU	C	80:LEU	N	17.26
1	f	699:VAL	C	714:SER	N	15.76
1	U	270:THR	C	320:ASP	N	14.84
1	u	84:GLN	C	91:LYS	N	14.76
1	f	103:TYR	C	118:ASN	N	13.07
1	F	104:GLN	C	116:GLN	N	11.32
1	f	193:PRO	C	207:LEU	N	10.43
1	f	728:ALA	C	739:ALA	N	9.80
1	f	382:ASN	C	387:GLN	N	9.79
1	K	127:ASP	C	134:SER	N	9.19
1	f	146:GLY	C	163:ALA	N	9.07
1	C	250:GLU	C	267:SER	N	8.07
1	k	127:ASP	C	134:SER	N	7.84
1	f	289:VAL	C	297:MET	N	7.10
1	f	55:GLU	C	70:LEU	N	6.17
1	U	844:LYS	C	880:ASN	N	5.72
1	F	317:LEU	C	319:GLY	N	3.42

Preliminary Full wwPDB EM Validation Report ⓘ

Dec 9, 2025 – 07:16 AM EST

This wwPDB validation report is NOT for manuscript review

This is a Preliminary Full wwPDB EM Validation Report.

This report is produced by the standalone wwPDB validation server.
The structure in question has not been deposited to the wwPDB.
This report should not be submitted to journals.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
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	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.47

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 35 unique types of molecules in this entry. The entry contains 109403 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	358	2838	1789	507	525	17	0	0

- Molecule 2 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	125	1010	643	177	187	3	0	0

- Molecule 3 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	857	6635	4190	1126	1274	45	0	0

- Molecule 4 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	380	3040	1923	524	580	13	0	0

- Molecule 5 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	383	3051	1920	543	572	16	0	0

- Molecule 6 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	387	3040	1914	534	574	18	0	0

- Molecule 7 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	421	3291	2097	544	629	21	0	0

- Molecule 8 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	365	2882	1810	489	569	14	0	0

- Molecule 9 is a protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	I	49	414	251	64	99	0	0

- Molecule 10 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	402	3152	1982	543	609	18	0	0

- Molecule 11 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	228	1753	1103	289	351	10	0	0
			Total	C	N	O	S		
11	k	228	1753	1103	289	351	10	0	0

- Molecule 12 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	238	1874	1172	337	354	11	0	0
			Total	C	N	O	S		
12	l	238	1874	1172	337	354	11	0	0

- Molecule 13 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	240	Total	C	N	O	S	0	0
			1882	1193	321	357	11		
13	m	240	Total	C	N	O	S	0	0
			1882	1193	321	357	11		

- Molecule 14 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	191	Total	C	N	O	S	0	0
			1431	893	245	281	12		
14	n	191	Total	C	N	O	S	0	0
			1431	893	245	281	12		

- Molecule 15 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	220	Total	C	N	O	S	0	0
			1660	1044	283	321	12		
15	o	220	Total	C	N	O	S	0	0
			1660	1044	283	321	12		

- Molecule 16 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		
16	p	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

- Molecule 17 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	199	Total	C	N	O	S	0	0
			1597	1022	272	294	9		
17	q	199	Total	C	N	O	S	0	0
			1597	1022	272	294	9		

- Molecule 18 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	201	Total	C	N	O	S	0	0
			1560	982	274	295	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
18	r	201	Total	C	N	O	S	0	0
			1560	982	274	295	9		

- Molecule 19 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	213	Total	C	N	O	S	0	0
			1654	1047	284	313	10		
19	s	213	Total	C	N	O	S	0	0
			1654	1047	284	313	10		

- Molecule 20 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	215	Total	C	N	O	S	0	0
			1682	1061	290	319	12		
20	t	215	Total	C	N	O	S	0	0
			1682	1061	290	319	12		

- Molecule 21 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	806	Total	C	N	O	S	0	0
			6288	3990	1075	1179	44		

- Molecule 22 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	480	Total	C	N	O	S	0	0
			3853	2444	684	711	14		

- Molecule 23 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	456	Total	C	N	O	S	0	0
			3703	2339	635	704	25		

- Molecule 24 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	422	Total 3335	C 2116	N 567	O 639	S 13	0	0

- Molecule 25 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	378	Total 3115	C 1987	N 533	O 578	S 17	0	0

- Molecule 26 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	286	Total 2282	C 1457	N 392	O 428	S 5	0	0

- Molecule 27 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	373	Total 2995	C 1911	N 510	O 559	S 15	0	0

- Molecule 28 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	191	Total 1459	C 910	N 261	O 280	S 8	0	0

- Molecule 29 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	287	Total 2260	C 1430	N 389	O 422	S 19	0	0

- Molecule 30 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	257	Total 2116	C 1371	N 346	O 390	S 9	0	0

- Molecule 31 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	240	Total	C	N	O	S	0	0
			1872	1189	310	360	13		
31	g	240	Total	C	N	O	S	0	0
			1872	1189	310	360	13		

- Molecule 32 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	232	Total	C	N	O	S	0	0
			1813	1158	307	342	6		
32	h	232	Total	C	N	O	S	0	0
			1813	1158	307	342	6		

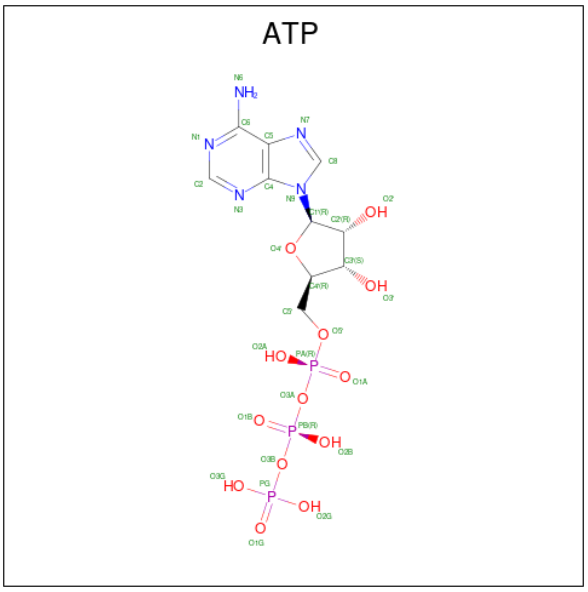
- Molecule 33 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	i	250	Total	C	N	O	S	0	0
			1972	1245	339	378	10		
33	u	250	Total	C	N	O	S	0	0
			1972	1245	339	378	10		

- Molecule 34 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	j	239	Total	C	N	O	S	0	0
			1888	1183	334	366	5		
34	v	239	Total	C	N	O	S	0	0
			1888	1183	334	366	5		

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
35	x	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	x	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	x	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	y	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	y	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	y	1	Total	C	N	O	P	0
			31	10	5	13	3	

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	
Number of images used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	Not provided	
Voltage (kV)	Not provided	
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	Not provided	

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no oligosaccharides in this entry.

4.6 Ligand geometry

6 ligands are 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	$\#\|Z\| > 2$
35	ATP	y	503	1	28,33,33	1.02	1 (3%)	34,52,52	1.65	9 (26%)
35	ATP	x	504	-	28,33,33	0.80	0	34,52,52	1.29	2 (5%)
35	ATP	x	503	10,5	28,33,33	0.82	0	34,52,52	1.28	3 (8%)
35	ATP	x	501	6	28,33,33	0.63	0	34,52,52	1.18	2 (5%)
35	ATP	y	501	8	28,33,33	0.59	0	34,52,52	0.64	1 (2%)
35	ATP	y	502	5,4	28,33,33	1.52	4 (14%)	34,52,52	1.54	7 (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
35	ATP	y	503	1	-	8/18/38/38	0/3/3/3
35	ATP	x	504	-	-	7/18/38/38	0/3/3/3
35	ATP	x	503	10,5	-	0/18/38/38	0/3/3/3
35	ATP	x	501	6	-	7/18/38/38	0/3/3/3
35	ATP	y	501	8	-	5/18/38/38	0/3/3/3
35	ATP	y	502	5,4	-	4/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	y	502	ATP	PB-O3B	5.41	1.65	1.59
35	y	503	ATP	PB-O3B	3.06	1.62	1.59
35	y	502	ATP	PA-O3A	3.03	1.62	1.59
35	y	502	ATP	O4'-C1'	2.41	1.44	1.40
35	y	502	ATP	PB-O3A	2.37	1.62	1.59

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	x	501	ATP	C4'-O4'-C1'	-5.60	104.80	109.92
35	y	503	ATP	N3-C2-N1	-4.64	122.37	128.67
35	x	503	ATP	N3-C2-N1	-4.16	123.03	128.67
35	y	502	ATP	N3-C2-N1	-4.08	123.13	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	x	504	ATP	N3-C2-N1	-4.01	123.23	128.67
35	y	503	ATP	C4-C5-N7	-3.34	105.81	109.34
35	y	502	ATP	O4'-C1'-N9	-3.08	104.67	108.75
35	y	503	ATP	O3'-C3'-C2'	3.06	121.62	111.82
35	y	502	ATP	C1'-N9-C4	-2.87	121.61	126.64
35	x	504	ATP	C4-C5-N7	-2.75	106.43	109.34
35	x	503	ATP	C4-C5-N7	-2.60	106.59	109.34
35	y	502	ATP	C4-C5-N7	-2.53	106.66	109.34
35	y	502	ATP	C4'-O4'-C1'	2.29	112.03	109.92
35	y	501	ATP	C5-C6-N6	2.29	123.80	120.31
35	x	501	ATP	C5-C6-N6	2.25	123.75	120.31
35	y	503	ATP	C5'-C4'-C3'	-2.25	107.11	115.21
35	y	502	ATP	O4'-C4'-C5'	2.22	116.44	109.33
35	y	503	ATP	C1'-N9-C4	-2.18	122.82	126.64
35	y	503	ATP	O3'-C3'-C4'	2.18	117.33	111.08
35	y	503	ATP	O3G-PG-O2G	2.12	115.76	107.80
35	y	503	ATP	O4'-C4'-C5'	2.09	116.03	109.33
35	y	502	ATP	O3A-PB-O1B	-2.04	104.56	110.70
35	y	503	ATP	C2'-C3'-C4'	2.04	106.54	102.61
35	x	503	ATP	O2A-PA-O3A	2.03	112.76	107.27

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	x	504	ATP	C5'-O5'-PA-O1A
35	x	504	ATP	C5'-O5'-PA-O3A
35	x	504	ATP	C3'-C4'-C5'-O5'
35	x	501	ATP	PB-O3B-PG-O2G
35	y	503	ATP	C5'-O5'-PA-O1A
35	y	503	ATP	O4'-C4'-C5'-O5'
35	y	501	ATP	C5'-O5'-PA-O2A
35	y	502	ATP	C5'-O5'-PA-O3A
35	x	504	ATP	O4'-C4'-C5'-O5'
35	y	503	ATP	C3'-C4'-C5'-O5'
35	x	501	ATP	C3'-C4'-C5'-O5'
35	y	502	ATP	PB-O3A-PA-O1A
35	x	501	ATP	C4'-C5'-O5'-PA
35	x	504	ATP	PB-O3A-PA-O5'
35	x	504	ATP	PG-O3B-PB-O3A
35	x	501	ATP	PB-O3B-PG-O3G
35	y	503	ATP	PB-O3A-PA-O2A

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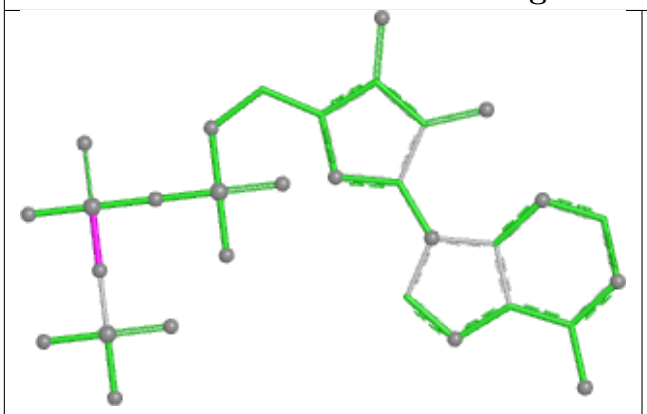
Mol	Chain	Res	Type	Atoms
35	y	503	ATP	C4'-C5'-O5'-PA
35	x	501	ATP	O4'-C4'-C5'-O5'
35	x	504	ATP	C5'-O5'-PA-O2A
35	y	501	ATP	C5'-O5'-PA-O1A
35	y	502	ATP	C5'-O5'-PA-O1A
35	y	503	ATP	PB-O3A-PA-O1A
35	y	502	ATP	PB-O3A-PA-O2A
35	y	501	ATP	C4'-C5'-O5'-PA
35	y	503	ATP	PB-O3B-PG-O1G
35	y	503	ATP	PB-O3B-PG-O2G
35	y	501	ATP	PB-O3B-PG-O2G
35	x	501	ATP	PB-O3A-PA-O1A
35	x	501	ATP	PB-O3A-PA-O2A
35	y	501	ATP	PA-O3A-PB-O2B

There are no ring outliers.

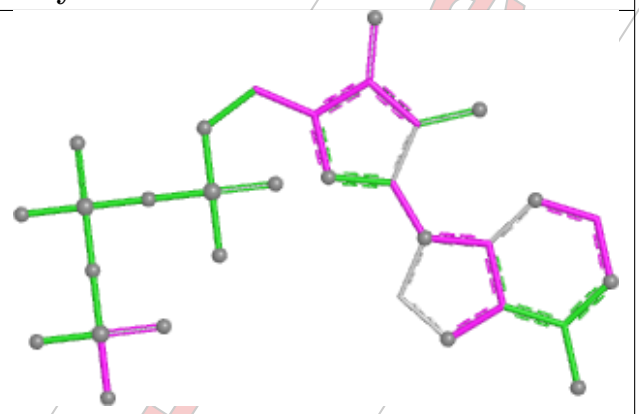
No monomer is involved in short contacts.

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 then 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.

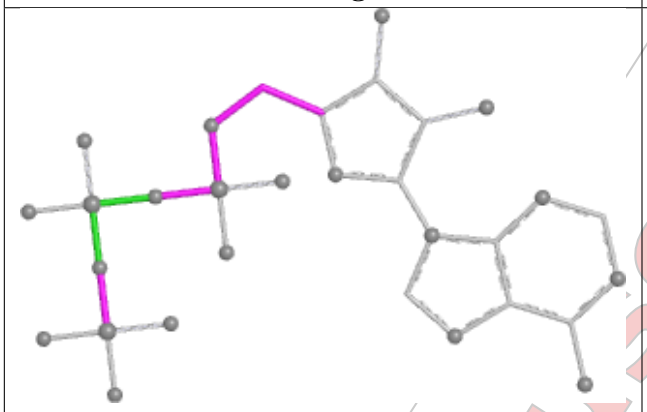
Ligand ATP y 503



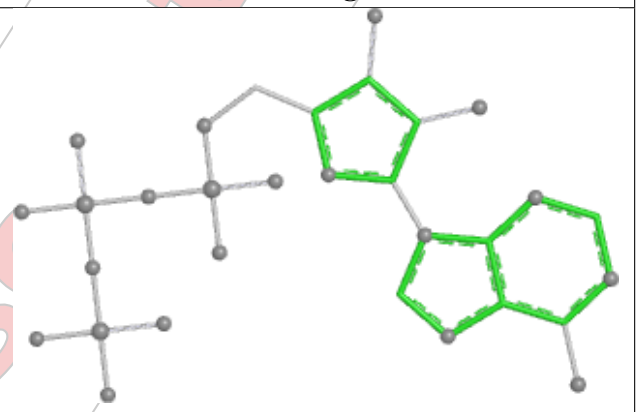
Bond lengths



Bond angles

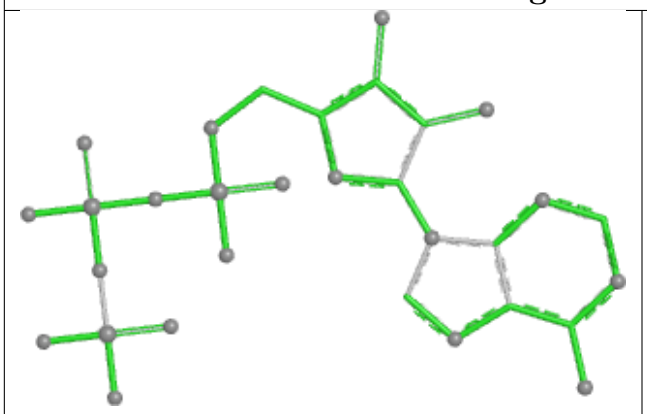


Torsions

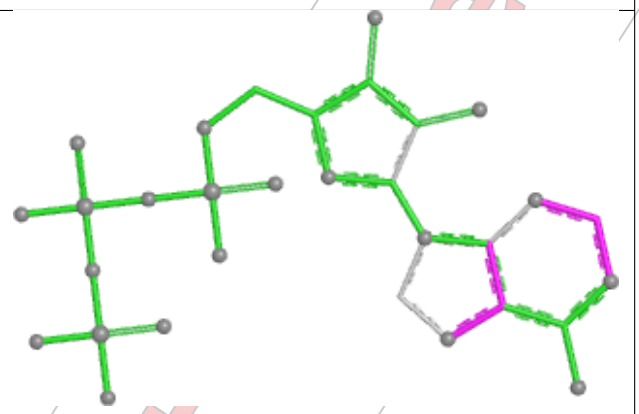


Rings

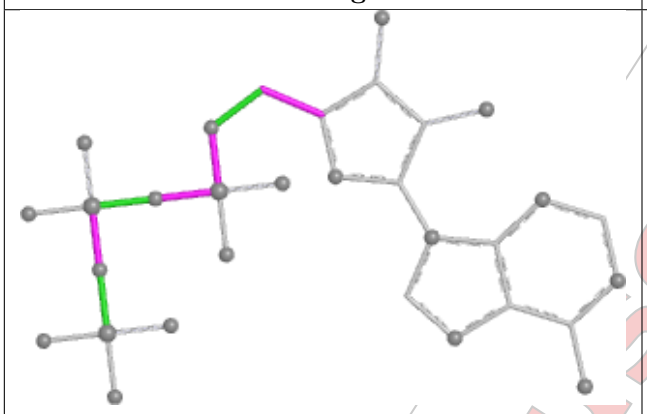
Ligand ATP x 504



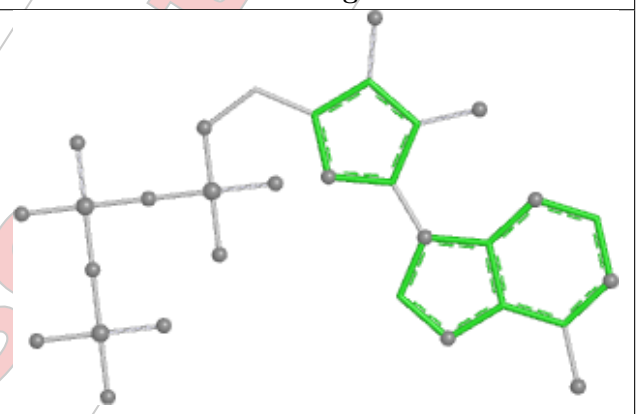
Bond lengths



Bond angles

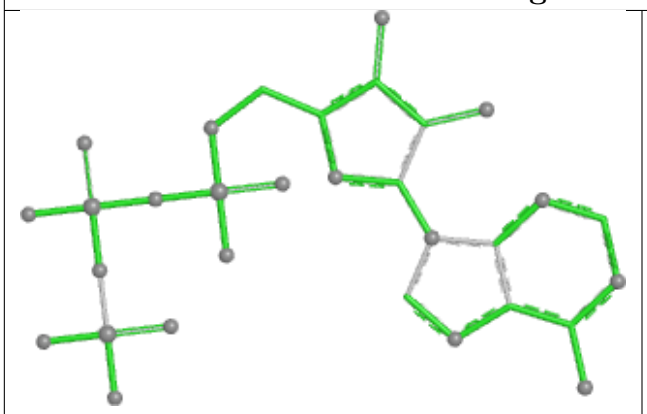


Torsions

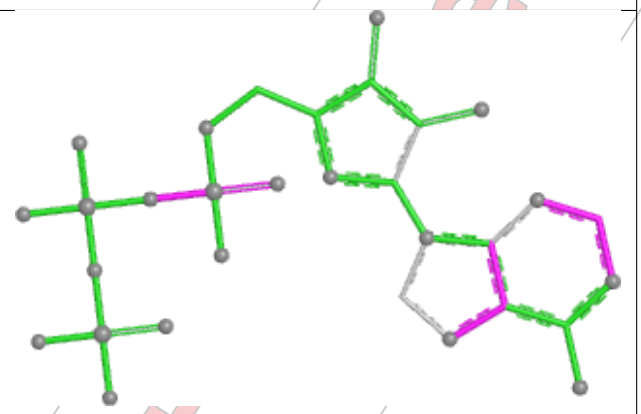


Rings

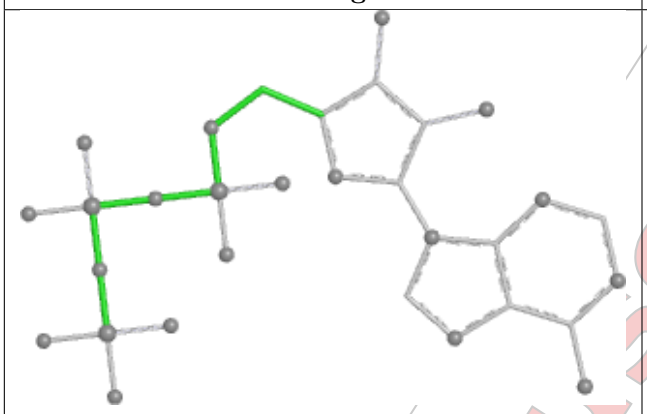
Ligand ATP x 503



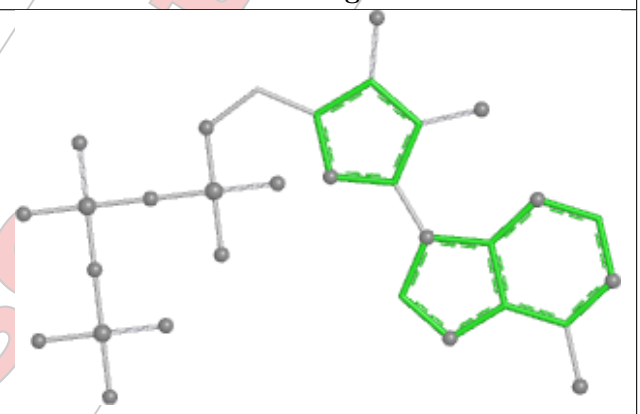
Bond lengths



Bond angles

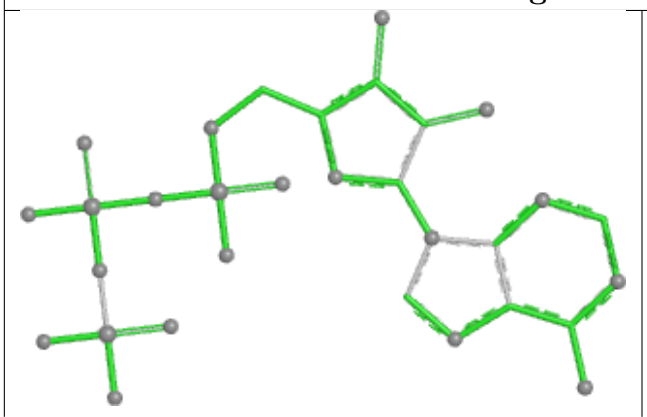


Torsions

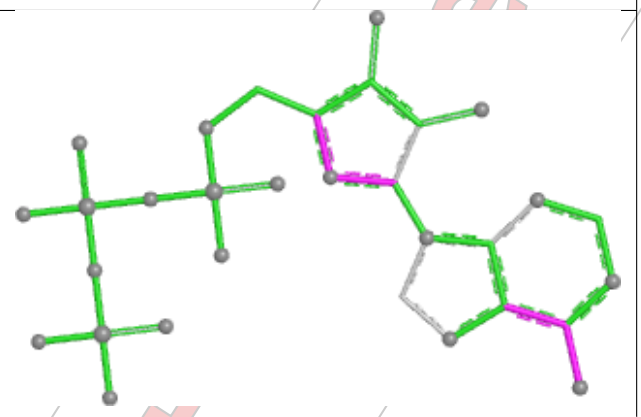


Rings

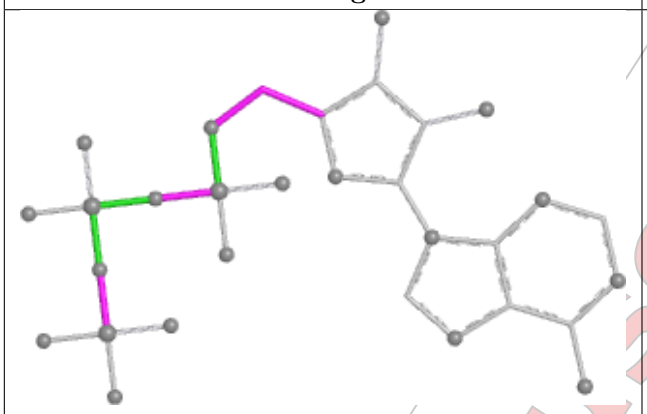
Ligand ATP x 501



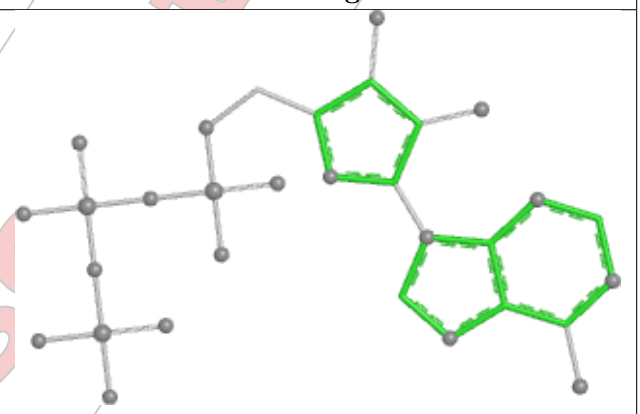
Bond lengths



Bond angles

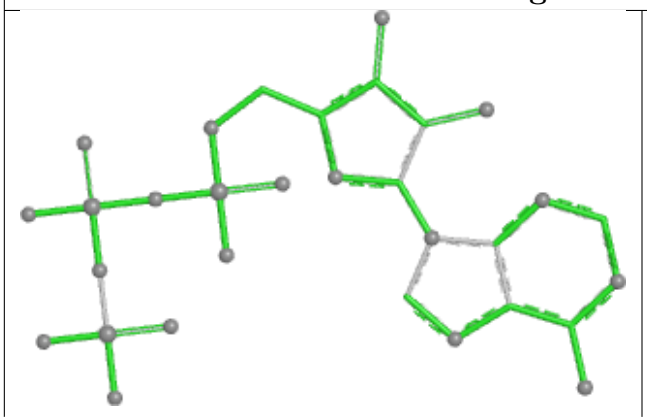


Torsions

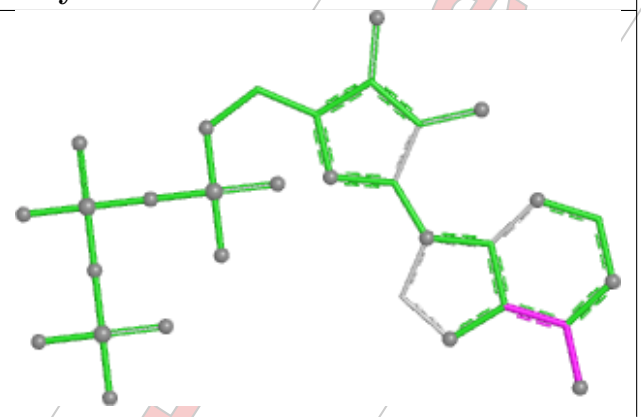


Rings

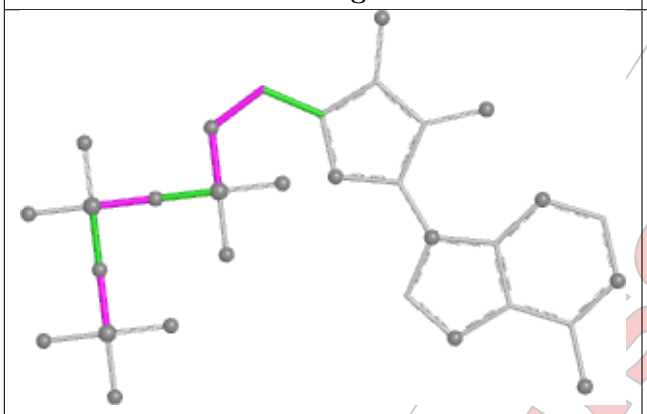
Ligand ATP y 501



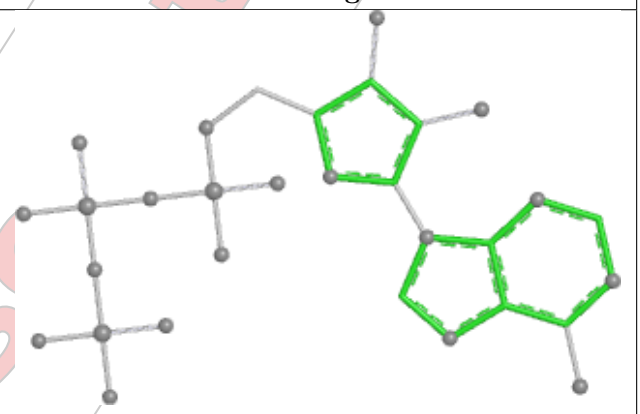
Bond lengths



Bond angles

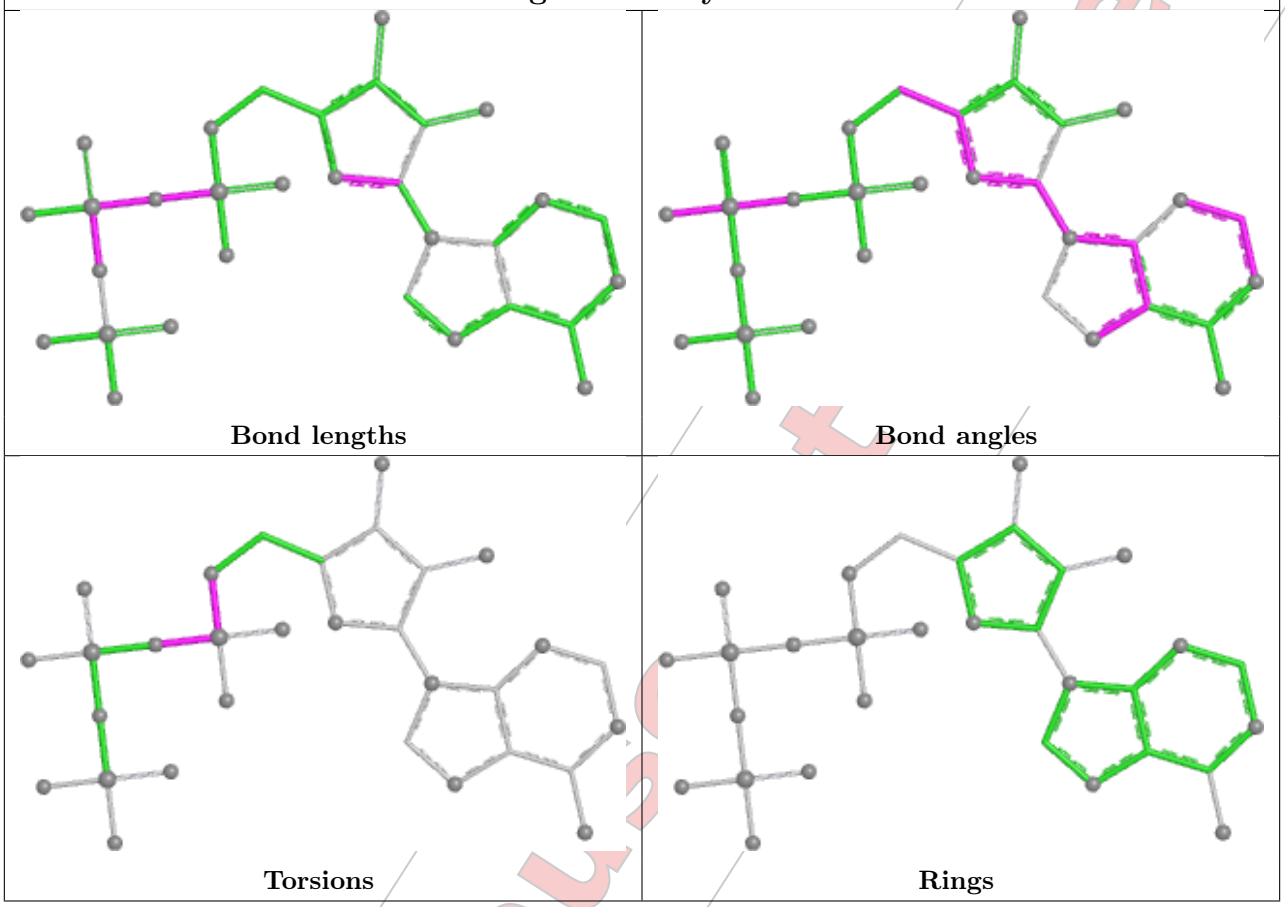


Torsions



Rings

Ligand ATP y 502



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
21	U	3
3	C	1
10	J	1
11	k	1
11	K	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	814:PRO	C	836:THR	N	21.65
1	C	624:GLU	C	637:LYS	N	19.47
1	U	270:THR	C	320:ASP	N	14.67
1	J	104:GLN	C	118:LYS	N	12.05
1	k	127:ASP	C	134:SER	N	9.13
1	K	127:ASP	C	134:SER	N	8.10
1	A	250:GLU	C	267:SER	N	7.32
1	U	844:LYS	C	880:ASN	N	5.62

Preliminary Full wwPDB EM Validation Report ⓘ

Nov 17, 2025 – 09:37 AM EST

This wwPDB validation report is NOT for manuscript review

This is a Preliminary Full wwPDB EM Validation Report.

This report is produced by the standalone wwPDB validation server.
The structure in question has not been deposited to the wwPDB.
This report should not be submitted to journals.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
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	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 32 unique types of molecules in this entry. The entry contains 97945 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	49	414	251	64	99	0	0

- Molecule 2 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	387	3035	1913	524	581	17	0	0

- Molecule 3 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	358	2838	1789	507	525	17	0	0

- Molecule 4 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	380	3040	1923	524	580	13	0	0

- Molecule 5 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	380	2986	1877	526	565	18	0	0

- Molecule 6 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	359	2831	1778	481	559	13	0	0

- Molecule 7 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	240	1872	1189	310	360	13	0	0
7	g	240	Total	C	N	O	S	0	0
			1872	1189	310	360	13		

- Molecule 8 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	232	1813	1158	307	342	6	0	0
8	h	232	Total	C	N	O	S	0	0
			1813	1158	307	342	6		

- Molecule 9 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	250	1972	1245	339	378	10	0	0
9	i	250	Total	C	N	O	S	0	0
			1972	1245	339	378	10		

- Molecule 10 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	239	1888	1183	334	366	5	0	0
10	j	239	Total	C	N	O	S	0	0
			1888	1183	334	366	5		

- Molecule 11 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	228	1753	1103	289	351	10	0	0
11	k	228	Total	C	N	O	S	0	0
			1753	1103	289	351	10		

- Molecule 12 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	238	Total	C	N	O	S	0	0
			1874	1172	337	354	11		
12	l	238	Total	C	N	O	S	0	0
			1874	1172	337	354	11		

- Molecule 13 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	240	Total	C	N	O	S	0	0
			1882	1193	321	357	11		
13	m	240	Total	C	N	O	S	0	0
			1882	1193	321	357	11		

- Molecule 14 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	191	Total	C	N	O	S	0	0
			1431	893	245	281	12		
14	n	191	Total	C	N	O	S	0	0
			1431	893	245	281	12		

- Molecule 15 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	220	Total	C	N	O	S	0	0
			1660	1044	283	321	12		
15	o	220	Total	C	N	O	S	0	0
			1660	1044	283	321	12		

- Molecule 16 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		
16	p	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

- Molecule 17 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	199	Total	C	N	O	S	0	0
			1597	1022	272	294	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	199	Total	C	N	O	S	0	0
			1597	1022	272	294	9		

- Molecule 18 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	201	Total	C	N	O	S	0	0
			1560	982	274	295	9		
18	r	201	Total	C	N	O	S	0	0
			1560	982	274	295	9		

- Molecule 19 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	213	Total	C	N	O	S	0	0
			1654	1047	284	313	10		
19	s	213	Total	C	N	O	S	0	0
			1654	1047	284	313	10		

- Molecule 20 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	215	Total	C	N	O	S	0	0
			1682	1061	290	319	12		
20	t	215	Total	C	N	O	S	0	0
			1682	1061	290	319	12		

- Molecule 21 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	806	Total	C	N	O	S	0	0
			6288	3990	1075	1179	44		

- Molecule 22 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	480	Total	C	N	O	S	0	0
			3853	2444	684	711	14		

- Molecule 23 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	456	Total 3703	C 2339	N 635	O 704	S 25	0	0

- Molecule 24 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	380	Total 3009	C 1918	N 509	O 570	S 12	0	0

- Molecule 25 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	378	Total 3115	C 1987	N 533	O 578	S 17	0	0

- Molecule 26 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	286	Total 2282	C 1457	N 392	O 428	S 5	0	0

- Molecule 27 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	373	Total 2995	C 1911	N 510	O 559	S 15	0	0

- Molecule 28 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	191	Total 1459	C 910	N 261	O 280	S 8	0	0

- Molecule 29 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	287	Total 2260	C 1430	N 389	O 422	S 19	0	0

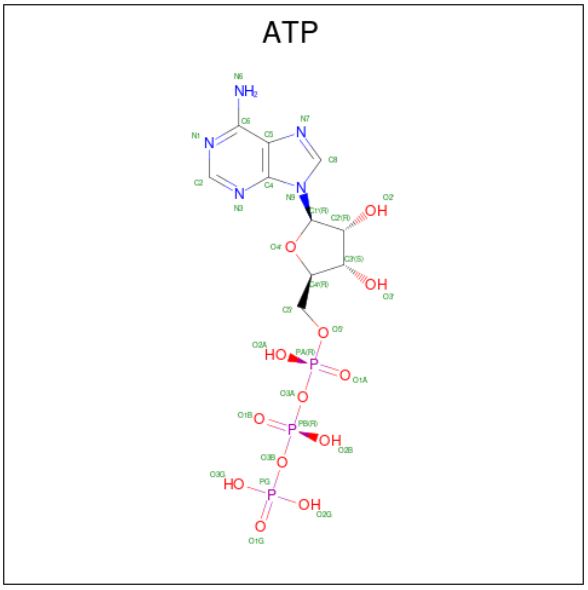
- Molecule 30 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	257	Total	C	N	O	S	0	0
			2116	1371	346	390	9		

- Molecule 31 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	386	Total	C	N	O	S	0	0
			3077	1935	549	577	16		

- Molecule 32 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
32	f	1	Total	C	N	O	P	0
			31	10	5	13	3	
32	f	1	Total	C	N	O	P	0
			31	10	5	13	3	
32	f	1	Total	C	N	O	P	0
			31	10	5	13	3	
32	u	1	Total	C	N	O	P	0
			31	10	5	13	3	
32	v	1	Total	C	N	O	P	0
			31	10	5	13	3	
32	w	1	Total	C	N	O	P	0
			31	10	5	13	3	

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	
Number of images used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	Not provided	
Voltage (kV)	Not provided	
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	Not provided	

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no oligosaccharides in this entry.

4.6 Ligand geometry

6 ligands are 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	$\#\|Z\| > 2$
32	ATP	f	501	-	28,33,33	0.61	0	34,52,52	0.70	1 (2%)
32	ATP	f	502	2	28,33,33	1.21	2 (7%)	34,52,52	1.46	4 (11%)
32	ATP	v	501	4	28,33,33	0.61	0	34,52,52	0.66	1 (2%)
32	ATP	u	501	6	28,33,33	0.62	0	34,52,52	0.69	1 (2%)
32	ATP	f	503	3	28,33,33	0.93	0	34,52,52	1.69	3 (8%)
32	ATP	w	401	31	28,33,33	0.61	0	34,52,52	0.85	2 (5%)

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
32	ATP	f	501	-	-	4/18/38/38	0/3/3/3
32	ATP	f	502	2	-	0/18/38/38	0/3/3/3
32	ATP	v	501	4	-	7/18/38/38	0/3/3/3
32	ATP	u	501	6	-	3/18/38/38	0/3/3/3
32	ATP	f	503	3	-	7/18/38/38	0/3/3/3
32	ATP	w	401	31	-	5/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	f	502	ATP	O4'-C1'	2.92	1.44	1.40
32	f	502	ATP	C8-N7	-2.24	1.30	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	f	503	ATP	C4'-O4'-C1'	-6.58	103.90	109.92
32	f	502	ATP	C4'-O4'-C1'	-5.04	105.31	109.92
32	f	502	ATP	N3-C2-N1	-4.60	122.42	128.67
32	f	503	ATP	C4-C5-N7	-3.87	105.25	109.34
32	f	503	ATP	N3-C2-N1	-3.81	123.50	128.67
32	w	401	ATP	C1'-N9-C4	3.10	132.08	126.64
32	f	502	ATP	PA-O5'-C5'	-2.54	106.79	121.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	v	501	ATP	C5-C6-N6	2.33	123.86	120.31
32	u	501	ATP	C5-C6-N6	2.32	123.84	120.31
32	f	501	ATP	C5-C6-N6	2.23	123.71	120.31
32	f	502	ATP	C4-C5-N7	-2.09	107.13	109.34
32	w	401	ATP	C5-C6-N6	2.02	123.39	120.31

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	f	501	ATP	C5'-O5'-PA-O2A
32	f	501	ATP	C5'-O5'-PA-O3A
32	f	503	ATP	C5'-O5'-PA-O1A
32	f	503	ATP	C5'-O5'-PA-O3A
32	v	501	ATP	C5'-O5'-PA-O1A
32	w	401	ATP	O4'-C4'-C5'-O5'
32	w	401	ATP	C3'-C4'-C5'-O5'
32	f	501	ATP	PB-O3A-PA-O5'
32	f	503	ATP	PB-O3A-PA-O5'
32	w	401	ATP	PB-O3B-PG-O3G
32	f	503	ATP	C5'-O5'-PA-O2A
32	u	501	ATP	C5'-O5'-PA-O1A
32	v	501	ATP	C5'-O5'-PA-O2A
32	v	501	ATP	C5'-O5'-PA-O3A
32	f	503	ATP	C4'-C5'-O5'-PA
32	v	501	ATP	PG-O3B-PB-O2B
32	w	401	ATP	PB-O3B-PG-O1G
32	f	503	ATP	PB-O3B-PG-O3G
32	u	501	ATP	PB-O3B-PG-O2G
32	w	401	ATP	PB-O3B-PG-O2G
32	v	501	ATP	O4'-C4'-C5'-O5'
32	v	501	ATP	C3'-C4'-C5'-O5'
32	f	501	ATP	C4'-C5'-O5'-PA
32	f	503	ATP	PB-O3A-PA-O2A
32	u	501	ATP	PB-O3A-PA-O2A
32	v	501	ATP	PG-O3B-PB-O1B

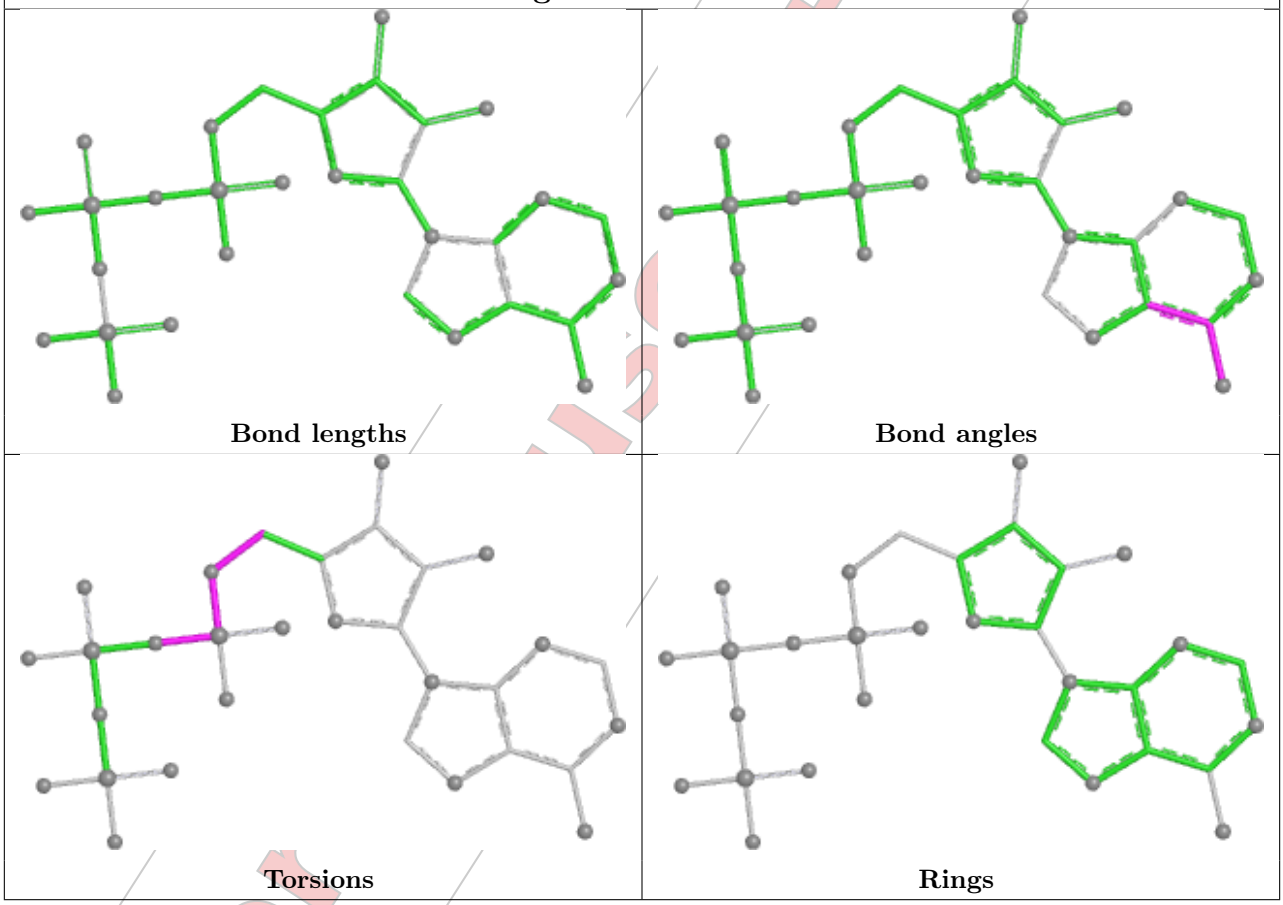
There are no ring outliers.

No monomer is involved in short contacts.

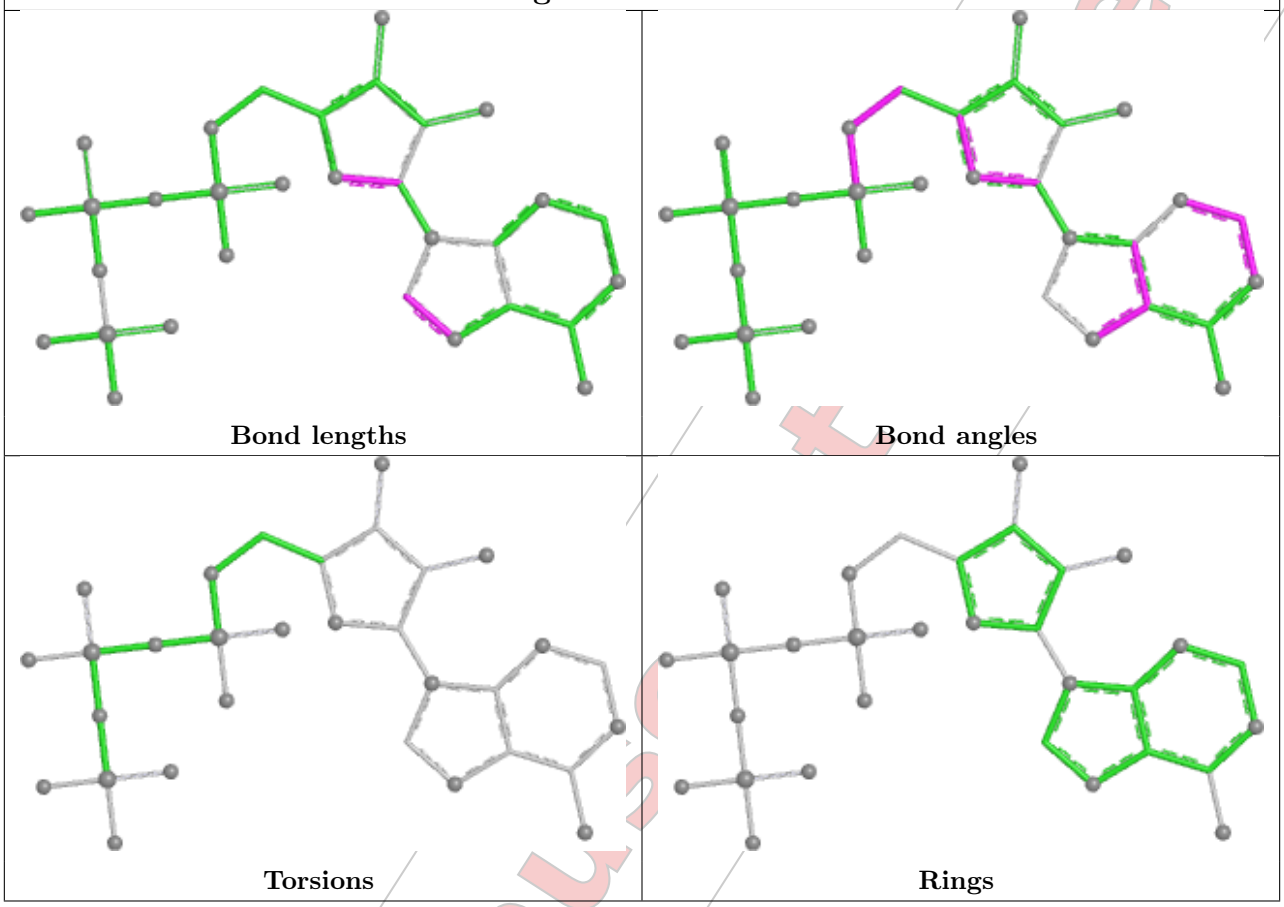
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

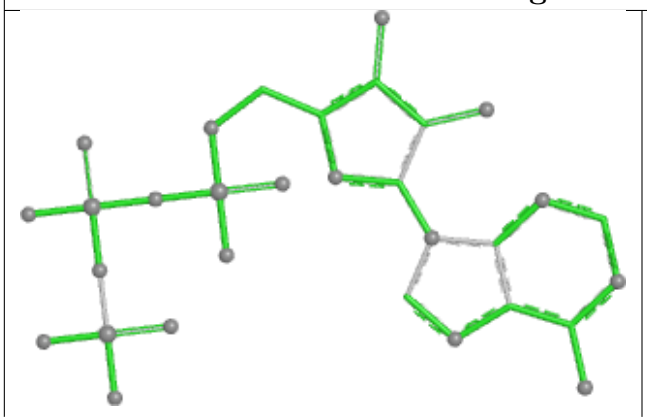
Ligand ATP f 501



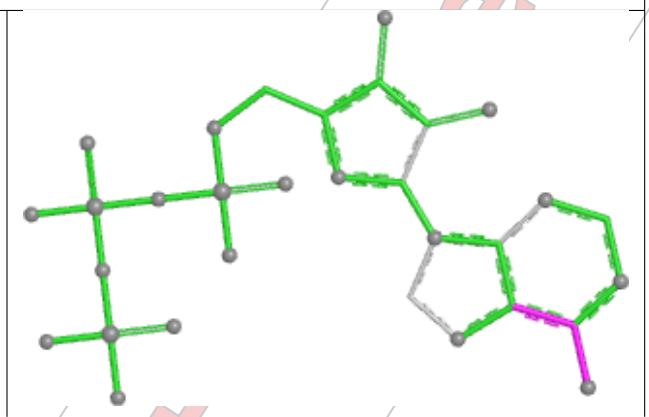
Ligand ATP f 502



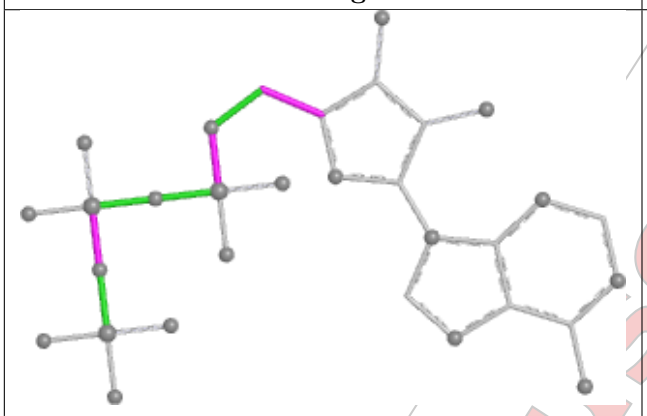
Ligand ATP v 501



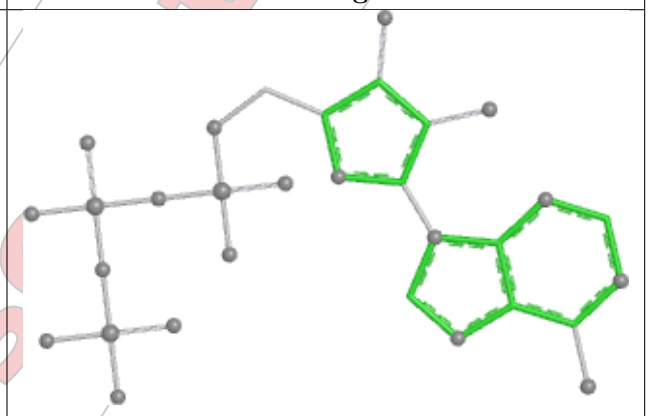
Bond lengths



Bond angles

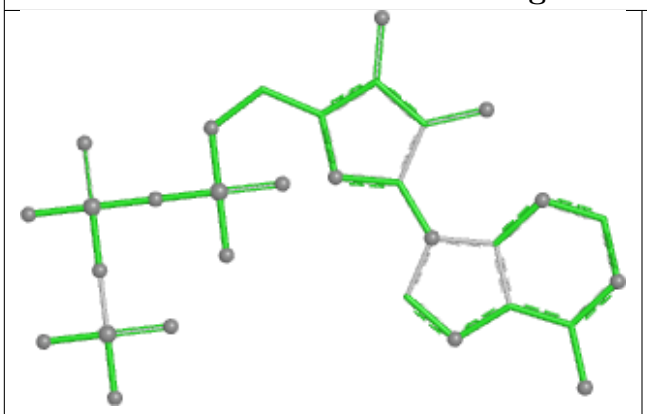


Torsions

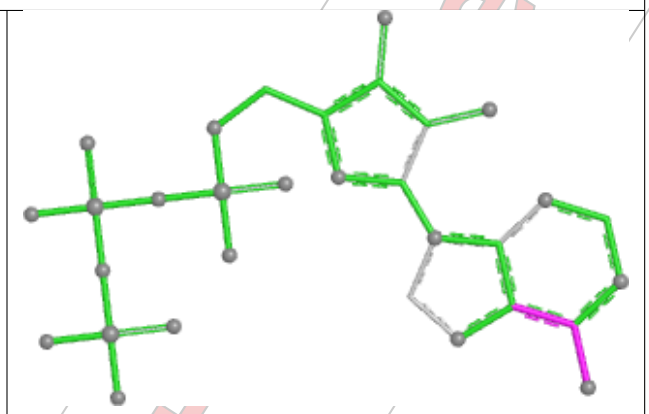


Rings

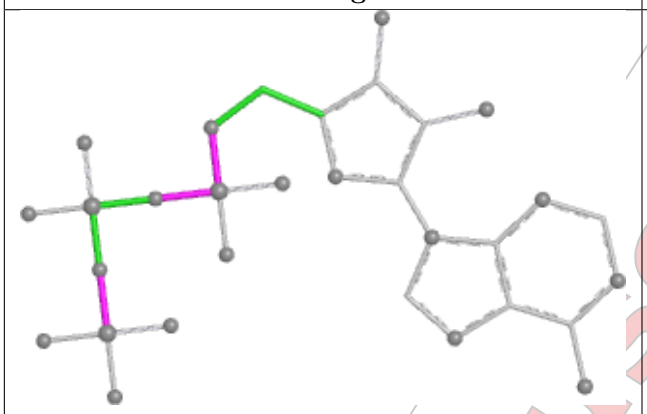
Ligand ATP u 501



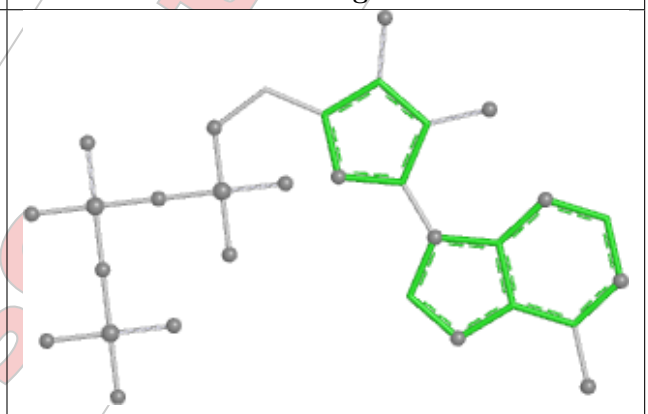
Bond lengths



Bond angles

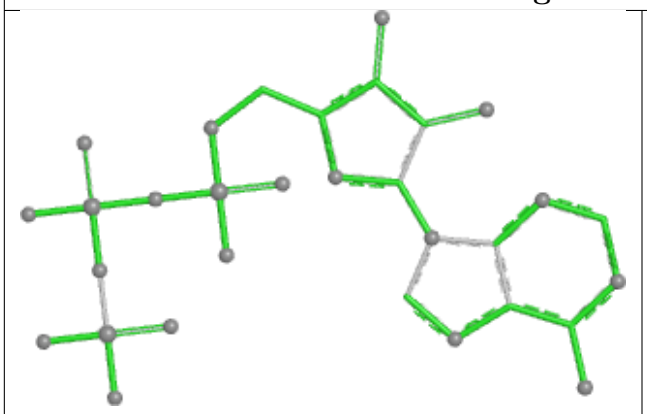


Torsions

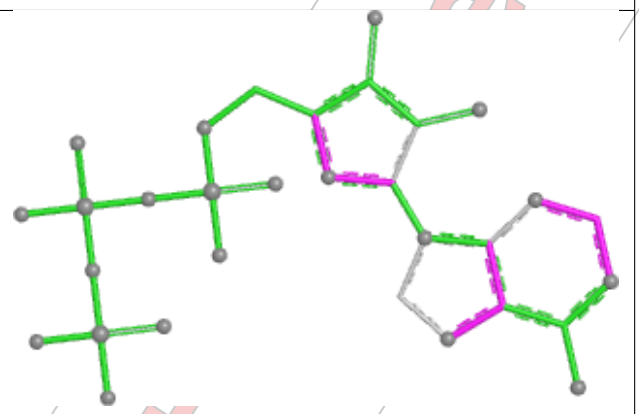


Rings

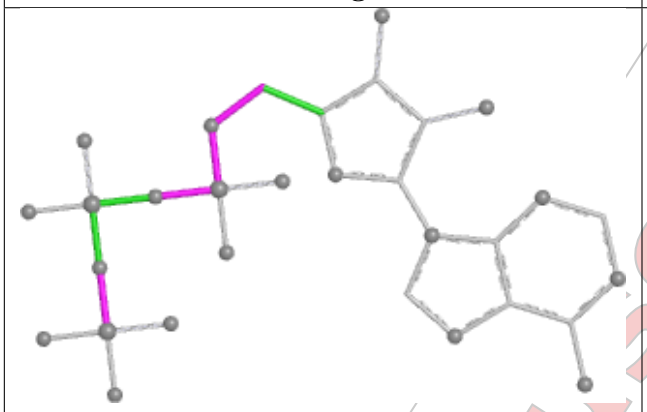
Ligand ATP f 503



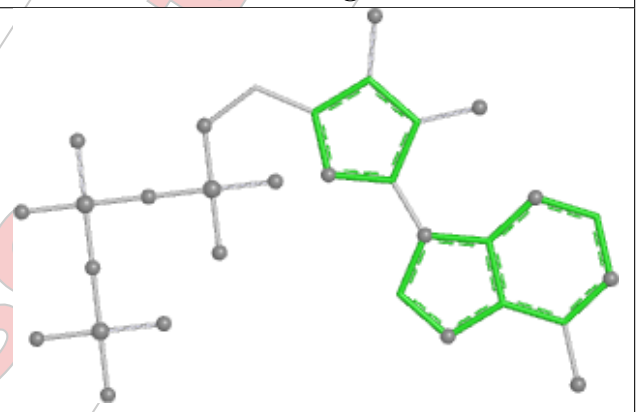
Bond lengths



Bond angles

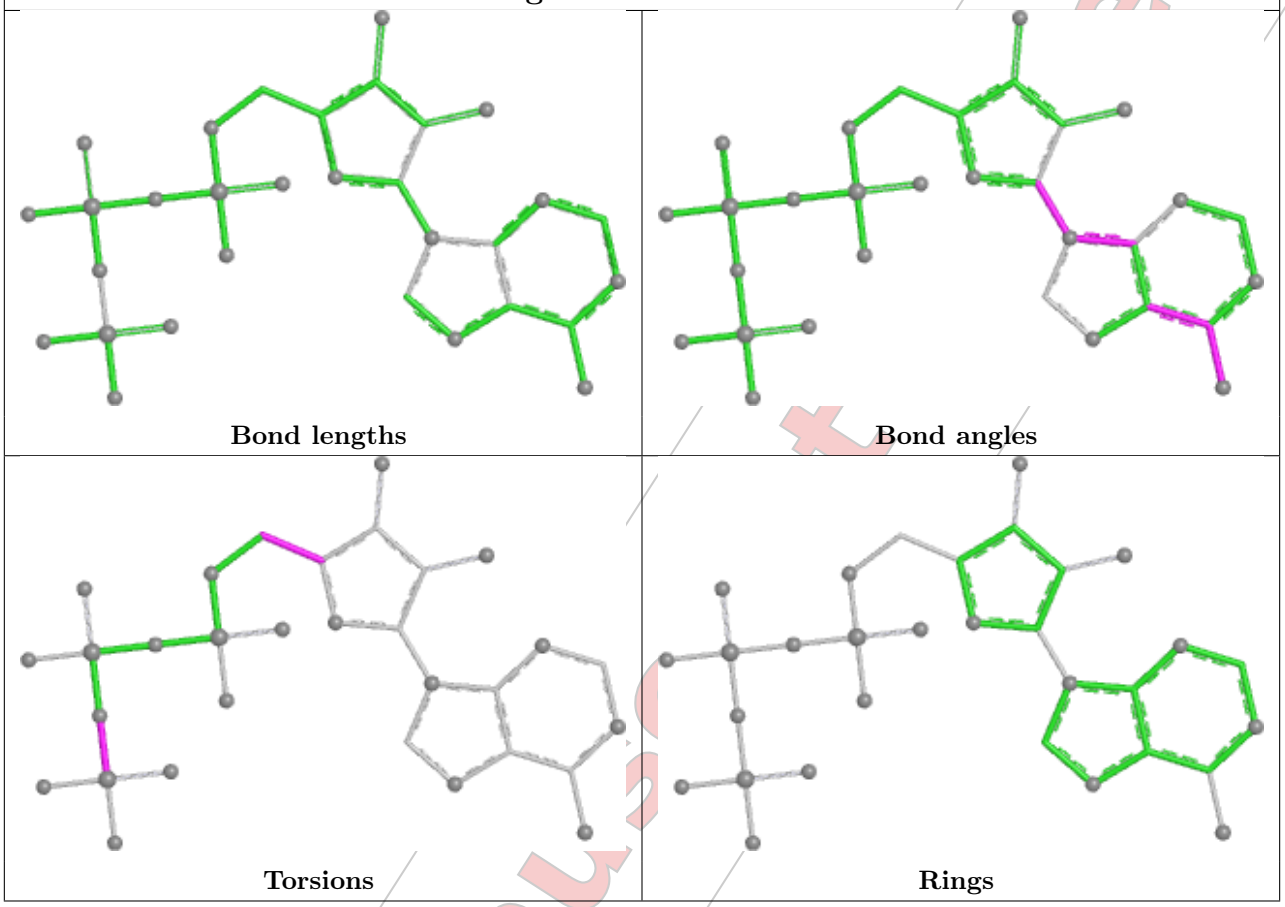


Torsions



Rings

Ligand ATP w 401



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
21	U	3
6	F	1
5	E	1
11	k	1
11	K	1
3	C	1
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	84:GLN	C	91:LYS	N	19.55
1	E	72:LEU	C	80:LEU	N	18.83
1	U	814:PRO	C	836:THR	N	18.68
1	U	270:THR	C	320:ASP	N	13.60
1	k	127:ASP	C	134:SER	N	10.52
1	K	127:ASP	C	134:SER	N	9.62
1	C	250:GLU	C	267:SER	N	8.63
1	B	101:PRO	C	118:LYS	N	7.77
1	U	844:LYS	C	880:ASN	N	5.89

Preliminary Full wwPDB EM Validation Report ⓘ

Nov 17, 2025 – 05:44 PM EST

This wwPDB validation report is NOT for manuscript review

This is a Preliminary Full wwPDB EM Validation Report.

This report is produced by the standalone wwPDB validation server.
The structure in question has not been deposited to the wwPDB.
This report should not be submitted to journals.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
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	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 35 unique types of molecules in this entry. The entry contains 108636 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	49	414	251	64	99	0	0

- Molecule 2 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	404	3169	1988	548	615	18	0	0

- Molecule 3 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	358	2838	1789	507	525	17	0	0

- Molecule 4 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	380	3040	1923	524	580	13	0	0

- Molecule 5 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	389	3098	1947	552	582	17	0	0

- Molecule 6 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	240	1871	1189	310	359	13	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	g	240	1871	1189	310	359	13	0	0

- Molecule 7 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	380	2986	1877	526	565	18	0	0

- Molecule 8 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	359	2831	1778	481	559	13	0	0

- Molecule 9 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	250	1971	1245	339	377	10	0	0
			Total	C	N	O	S		
9	i	250	1971	1245	339	377	10	0	0

- Molecule 10 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	239	1887	1183	334	365	5	0	0
			Total	C	N	O	S		
10	j	239	1887	1183	334	365	5	0	0

- Molecule 11 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	228	1753	1103	289	351	10	0	0
			Total	C	N	O	S		
11	k	228	1753	1103	289	351	10	0	0

- Molecule 12 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	238	Total	C	N	O	S	0	0
			1873	1172	337	353	11		
12	l	238	Total	C	N	O	S	0	0
			1873	1172	337	353	11		

- Molecule 13 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	240	Total	C	N	O	S	0	0
			1881	1193	321	356	11		
13	m	240	Total	C	N	O	S	0	0
			1881	1193	321	356	11		

- Molecule 14 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		
14	n	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		

- Molecule 15 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		
15	o	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		

- Molecule 16 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		
16	p	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

- Molecule 17 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	199	Total	C	N	O	S	0	0
			1596	1022	272	293	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	199	Total	C	N	O	S	0	0
			1596	1022	272	293	9		

- Molecule 18 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		
18	r	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		

- Molecule 19 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	213	Total	C	N	O	S	0	0
			1654	1047	284	313	10		
19	s	213	Total	C	N	O	S	0	0
			1654	1047	284	313	10		

- Molecule 20 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	215	Total	C	N	O	S	0	0
			1681	1061	290	318	12		
20	t	215	Total	C	N	O	S	0	0
			1681	1061	290	318	12		

- Molecule 21 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	806	Total	C	N	O	S	0	0
			6288	3990	1075	1179	44		

- Molecule 22 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	480	Total	C	N	O	S	0	0
			3853	2444	684	711	14		

- Molecule 23 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	456	Total 3703	C 2339	N 635	O 704	S 25	0	0

- Molecule 24 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	380	Total 3009	C 1918	N 509	O 570	S 12	0	0

- Molecule 25 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	232	Total 1813	C 1158	N 307	O 342	S 6	0	0
25	h	232	Total 1813	C 1158	N 307	O 342	S 6	0	0

- Molecule 26 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	286	Total 2282	C 1457	N 392	O 428	S 5	0	0

- Molecule 27 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	373	Total 2995	C 1911	N 510	O 559	S 15	0	0

- Molecule 28 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	191	Total 1459	C 910	N 261	O 280	S 8	0	0

- Molecule 29 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	287	Total 2260	C 1430	N 389	O 422	S 19	0	0

- Molecule 30 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	257	Total 2116	C 1371	N 346	O 390	S 9	0	0

- Molecule 31 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	378	Total 3115	C 1987	N 533	O 578	S 17	0	0

- Molecule 32 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	383	Total 2998	C 1920	N 500	O 558	S 20	0	0

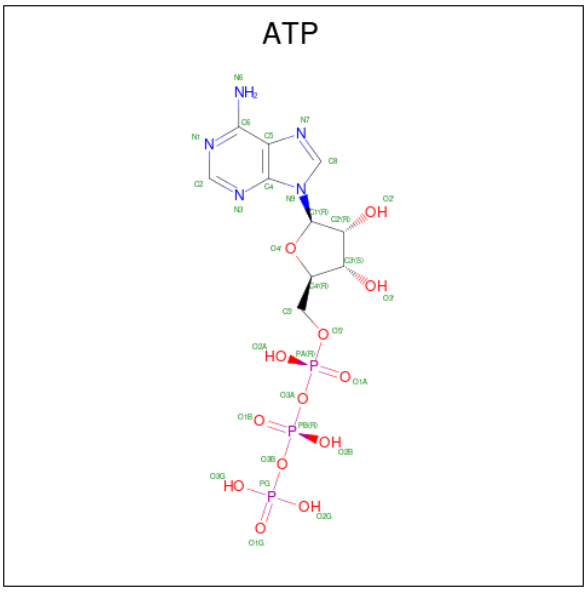
- Molecule 33 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	u	125	Total 1010	C 643	N 177	O 187	S 3	0	0

- Molecule 34 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	v	847	Total 6548	C 4138	N 1112	O 1253	S 45	0	0

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
35	x	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	x	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	x	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	x	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	x	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	y	1	Total	C	N	O	P	0
			31	10	5	13	3	

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	
Number of images used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	Not provided	
Voltage (kV)	Not provided	
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	Not provided	

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no oligosaccharides in this entry.

4.6 Ligand geometry

6 ligands are 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	$\#\|Z\| > 2$
35	ATP	x	501	7	28,33,33	0.59	0	34,52,52	0.90	2 (5%)
35	ATP	x	502	4	28,33,33	0.92	0	34,52,52	1.21	2 (5%)
35	ATP	y	501	8	28,33,33	0.63	0	34,52,52	0.67	1 (2%)
35	ATP	x	503	5,2	28,33,33	0.93	1 (3%)	34,52,52	1.19	2 (5%)
35	ATP	x	504	-	28,33,33	1.21	2 (7%)	34,52,52	1.46	4 (11%)
35	ATP	x	505	3	28,33,33	1.29	6 (21%)	34,52,52	1.87	4 (11%)

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
35	ATP	x	501	7	-	4/18/38/38	0/3/3/3
35	ATP	x	502	4	-	6/18/38/38	0/3/3/3
35	ATP	y	501	8	-	3/18/38/38	0/3/3/3
35	ATP	x	503	5,2	-	7/18/38/38	0/3/3/3
35	ATP	x	504	-	-	0/18/38/38	0/3/3/3
35	ATP	x	505	3	-	4/18/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	x	505	ATP	PB-O3B	3.08	1.62	1.59
35	x	505	ATP	PB-O3A	3.07	1.62	1.59
35	x	504	ATP	O4'-C1'	2.98	1.44	1.40
35	x	505	ATP	O4'-C1'	2.31	1.43	1.40
35	x	505	ATP	C2-N3	2.30	1.35	1.32
35	x	503	ATP	PB-O3B	2.28	1.62	1.59
35	x	504	ATP	C8-N7	-2.27	1.30	1.34
35	x	505	ATP	PA-O3A	2.08	1.61	1.59
35	x	505	ATP	C6-C5	2.02	1.50	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	x	505	ATP	C4'-O4'-C1'	-5.75	104.66	109.92
35	x	504	ATP	C4'-O4'-C1'	-5.05	105.30	109.92
35	x	505	ATP	O4'-C1'-N9	4.87	115.21	108.75
35	x	505	ATP	C4-C5-N7	-4.81	104.25	109.34
35	x	504	ATP	N3-C2-N1	-4.58	122.45	128.67
35	x	501	ATP	C4'-O4'-C1'	-3.72	106.52	109.92
35	x	502	ATP	N3-C2-N1	-3.58	123.81	128.67
35	x	503	ATP	N3-C2-N1	-3.54	123.87	128.67
35	x	505	ATP	N3-C2-N1	-3.50	123.92	128.67
35	x	503	ATP	C4-C5-N7	-3.21	105.94	109.34
35	x	502	ATP	C4-C5-N7	-3.15	106.01	109.34
35	x	504	ATP	PA-O5'-C5'	-2.54	106.79	121.35
35	x	501	ATP	C5-C6-N6	2.49	124.10	120.31
35	y	501	ATP	C5-C6-N6	2.13	123.55	120.31
35	x	504	ATP	C4-C5-N7	-2.09	107.13	109.34

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	x	503	ATP	PB-O3B-PG-O2G
35	x	503	ATP	C5'-O5'-PA-O1A
35	x	502	ATP	C3'-C4'-C5'-O5'
35	x	505	ATP	C5'-O5'-PA-O1A
35	x	505	ATP	C5'-O5'-PA-O3A
35	x	505	ATP	C4'-C5'-O5'-PA
35	x	503	ATP	O4'-C4'-C5'-O5'
35	x	502	ATP	O4'-C4'-C5'-O5'
35	x	501	ATP	O4'-C4'-C5'-O5'
35	x	502	ATP	C4'-C5'-O5'-PA
35	x	501	ATP	C3'-C4'-C5'-O5'
35	y	501	ATP	O4'-C4'-C5'-O5'
35	x	503	ATP	C3'-C4'-C5'-O5'
35	y	501	ATP	C3'-C4'-C5'-O5'
35	x	503	ATP	C4'-C5'-O5'-PA
35	x	502	ATP	C5'-O5'-PA-O1A
35	x	503	ATP	PB-O3A-PA-O2A
35	x	503	ATP	PB-O3B-PG-O1G
35	x	501	ATP	PB-O3B-PG-O1G
35	x	501	ATP	C4'-C5'-O5'-PA
35	x	502	ATP	PA-O3A-PB-O1B
35	x	505	ATP	PB-O3A-PA-O2A
35	x	502	ATP	PA-O3A-PB-O2B

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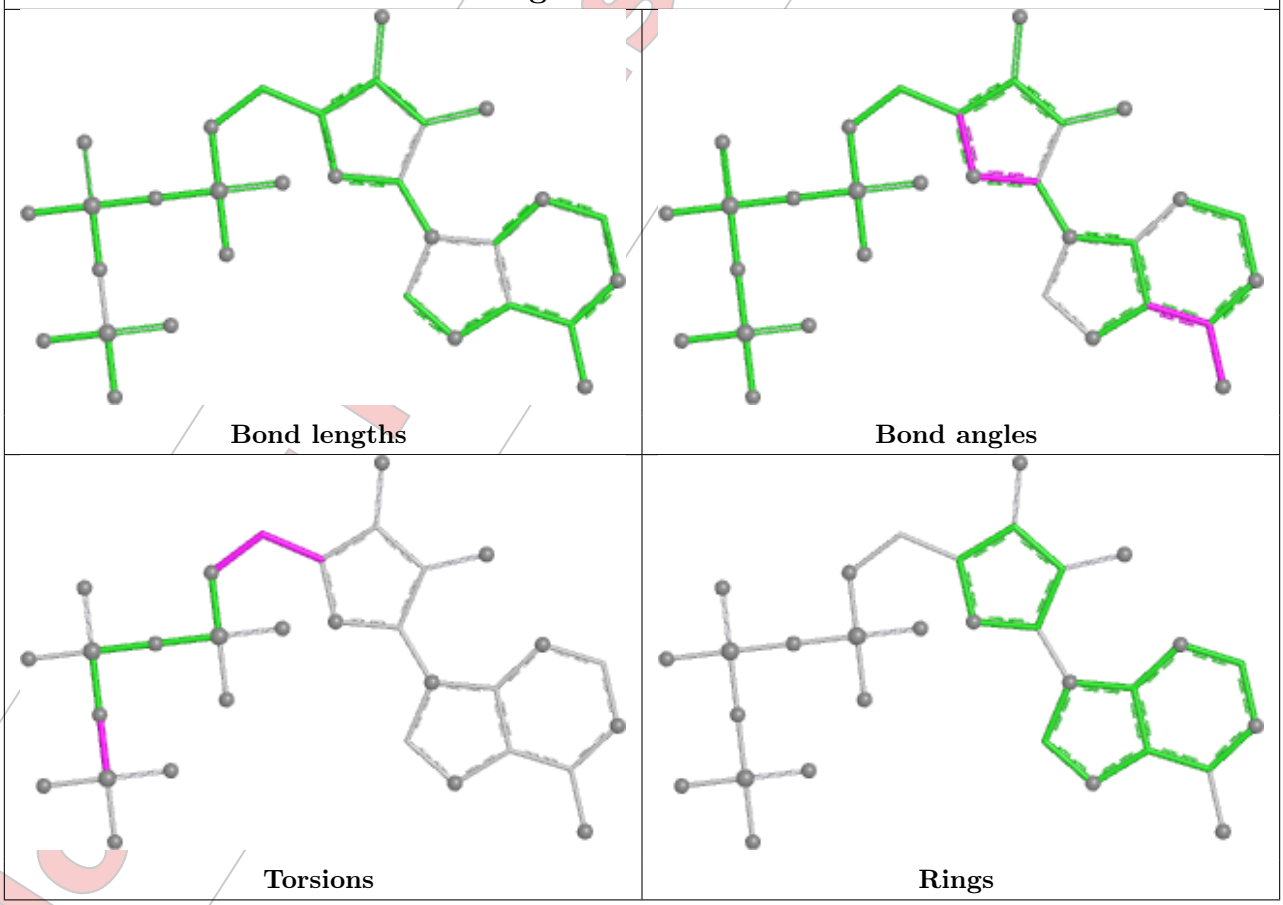
Mol	Chain	Res	Type	Atoms
35	y	501	ATP	PB-O3A-PA-O2A

There are no ring outliers.

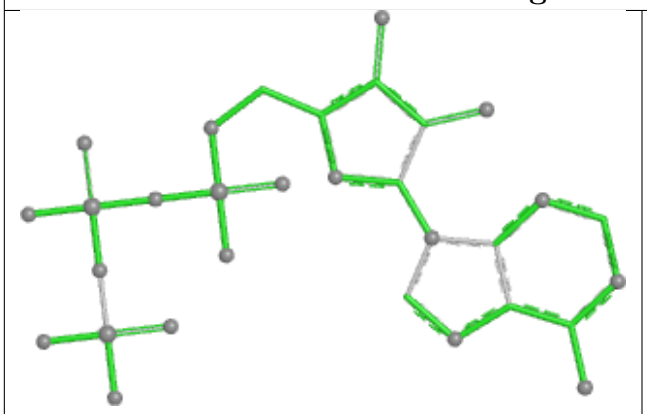
No monomer is involved in short contacts.

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 then 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.

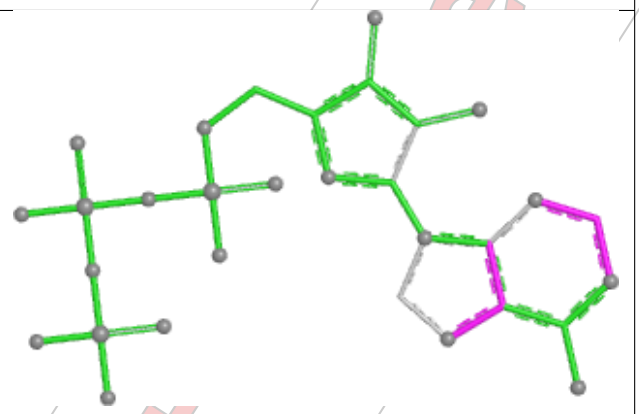
Ligand ATP x 501



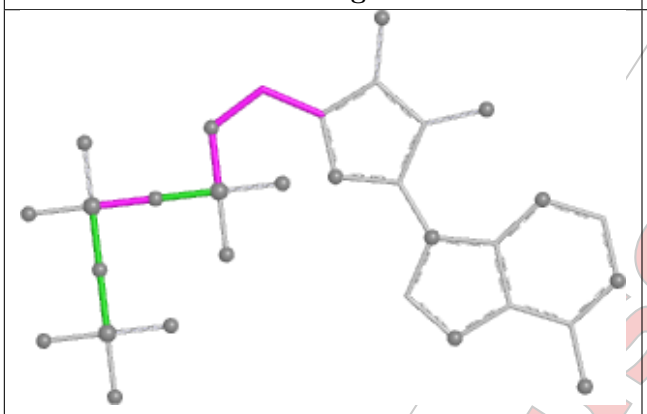
Ligand ATP x 502



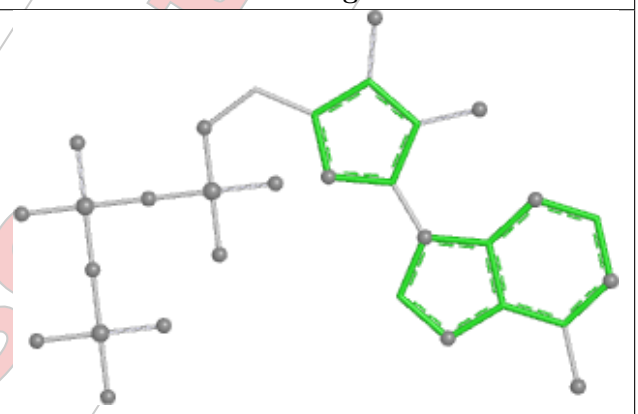
Bond lengths



Bond angles

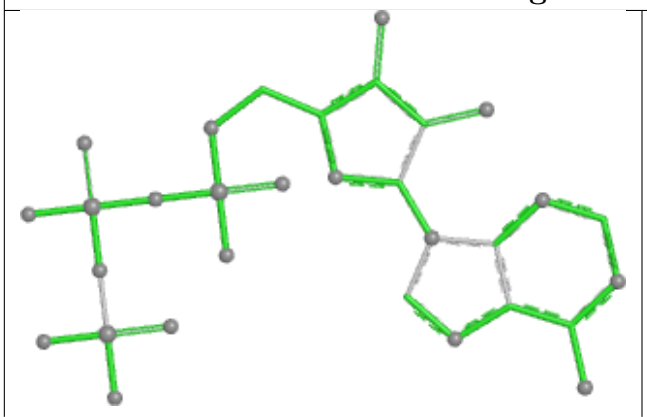


Torsions

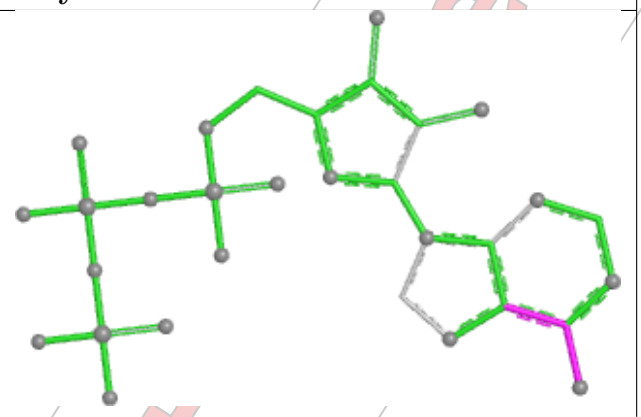


Rings

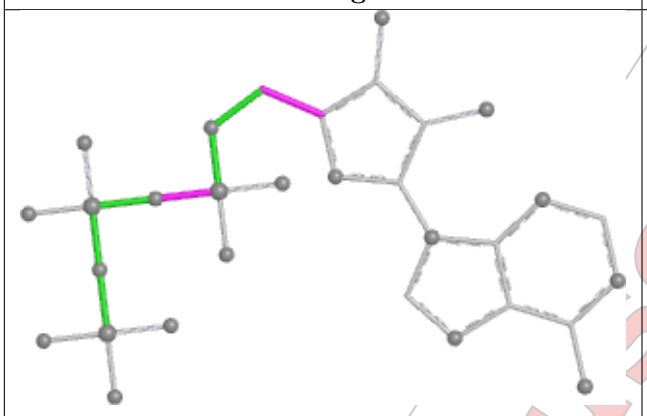
Ligand ATP y 501



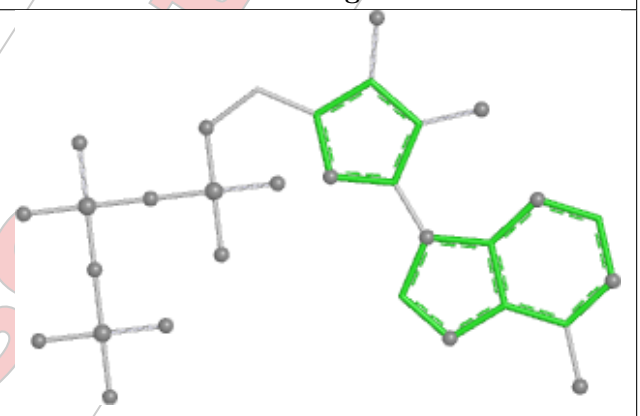
Bond lengths



Bond angles

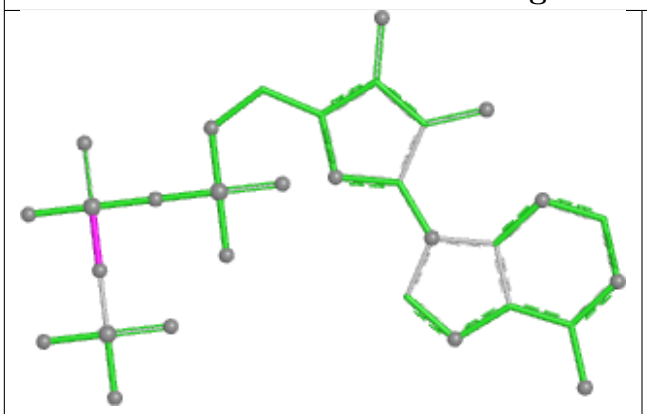


Torsions

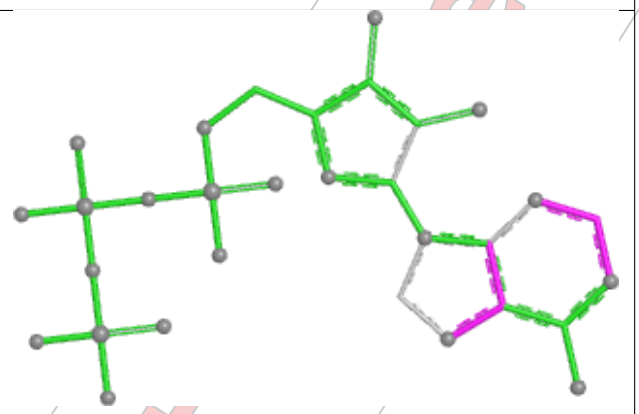


Rings

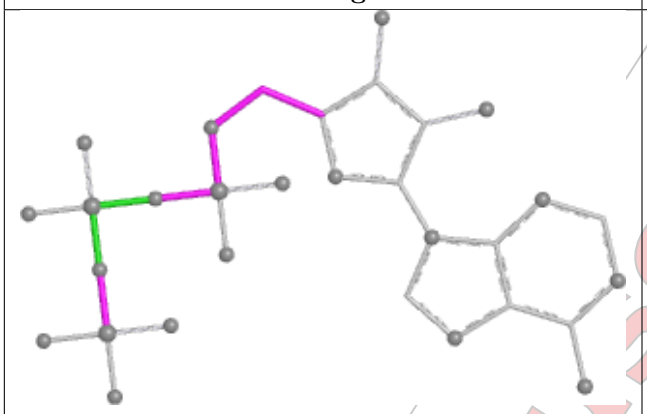
Ligand ATP x 503



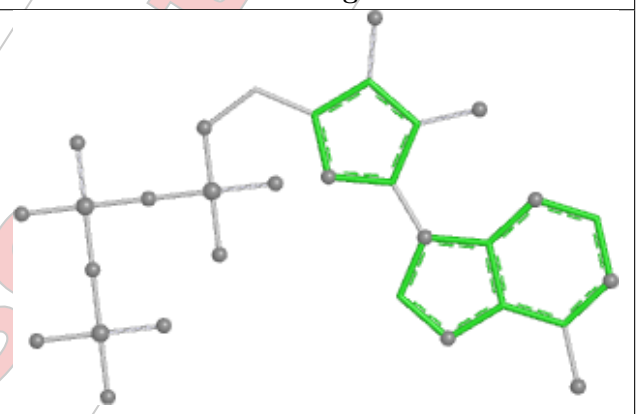
Bond lengths



Bond angles

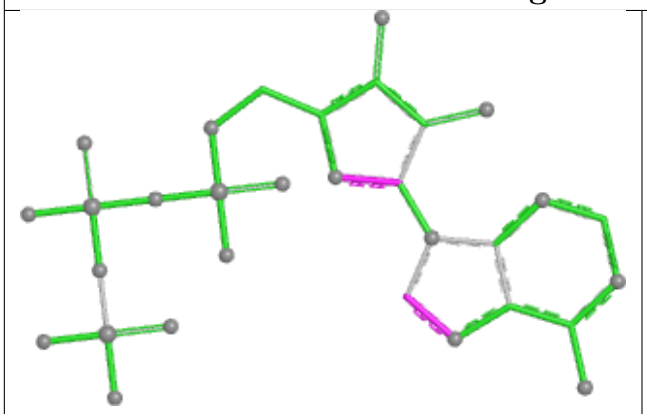


Torsions

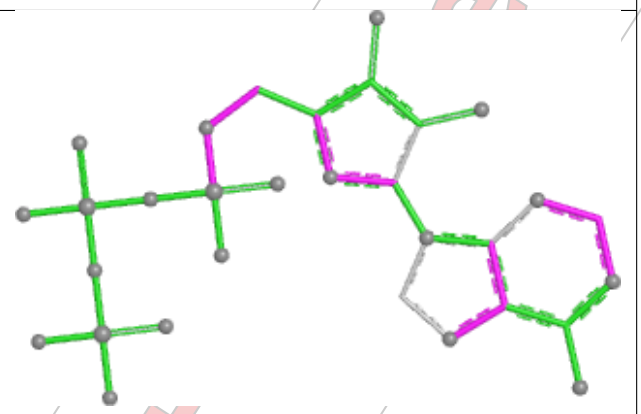


Rings

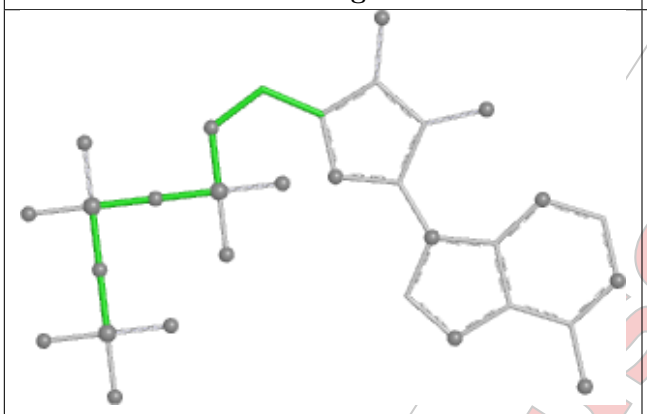
Ligand ATP x 504



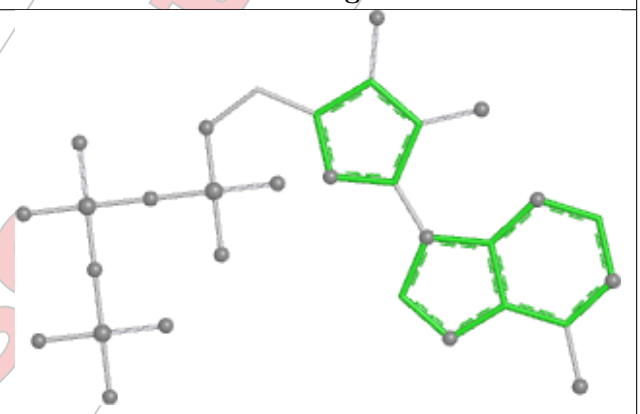
Bond lengths



Bond angles

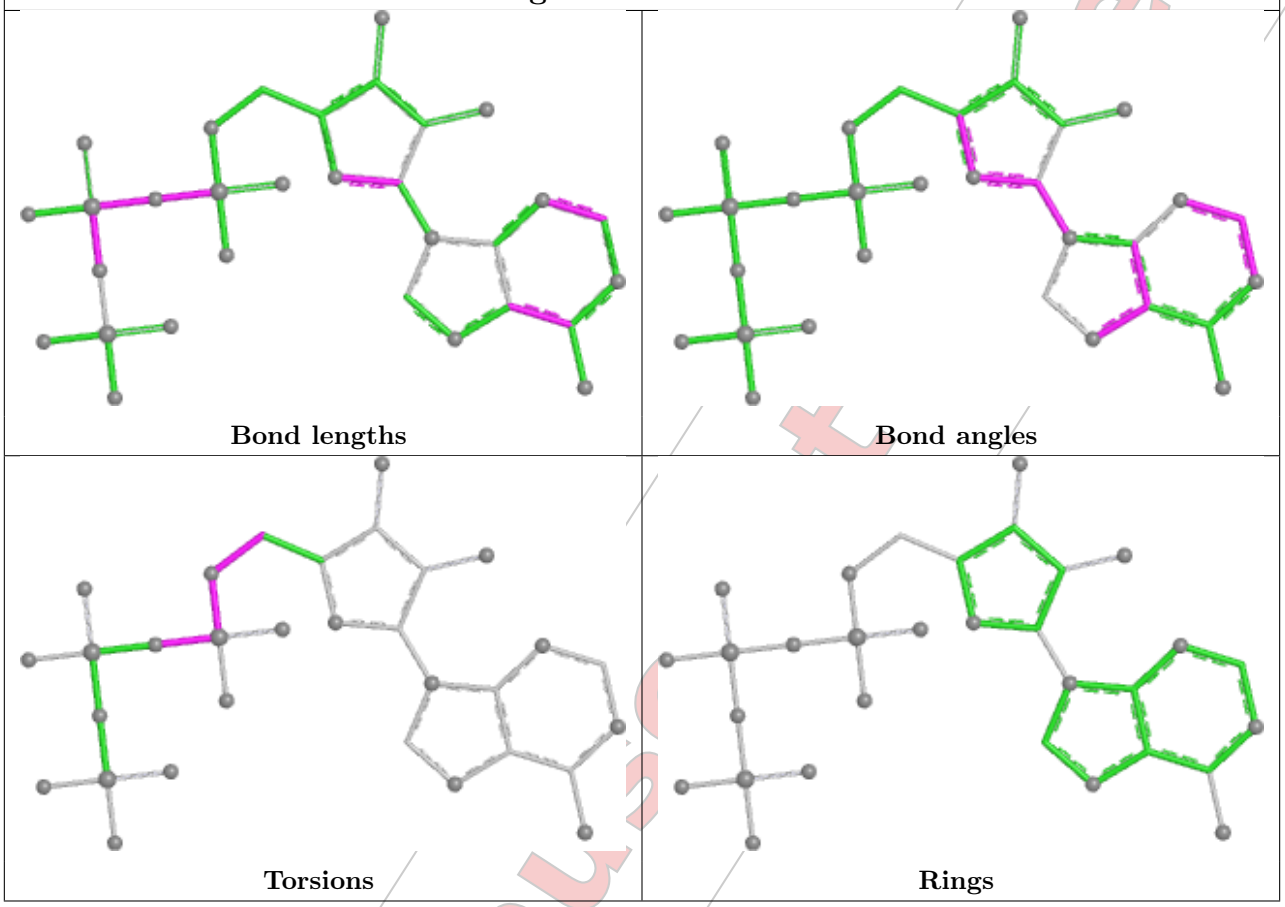


Torsions



Rings

Ligand ATP x 505



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
32	f	5
21	U	3
7	G	1
8	H	1
11	k	1
34	v	1
11	K	1
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	72:LEU	C	80:LEU	N	22.64
1	U	814:PRO	C	836:THR	N	19.38
1	H	84:GLN	C	91:LYS	N	15.61
1	U	270:THR	C	320:ASP	N	15.46
1	f	160:SER	C	164:CYS	N	10.34
1	k	127:ASP	C	134:SER	N	9.58
1	v	623:LYS	C	640:LYS	N	9.56
1	f	30:GLU	C	37:LYS	N	9.12
1	K	127:ASP	C	134:SER	N	8.83
1	C	250:GLU	C	267:SER	N	8.47
1	f	302:GLY	C	309:SER	N	7.82
1	f	344:PRO	C	348:GLU	N	6.67
1	U	844:LYS	C	880:ASN	N	6.21
1	f	392:ALA	C	395:SER	N	5.93

Preliminary Full wwPDB EM Validation Report ⓘ

Nov 17, 2025 – 08:27 AM EST

This wwPDB validation report is NOT for manuscript review

This is a Preliminary Full wwPDB EM Validation Report.

This report is produced by the standalone wwPDB validation server.
The structure in question has not been deposited to the wwPDB.
This report should not be submitted to journals.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
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:

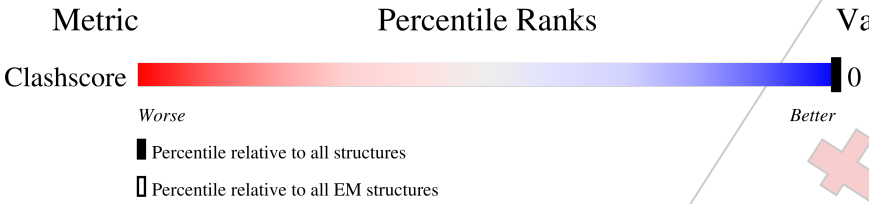
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

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.



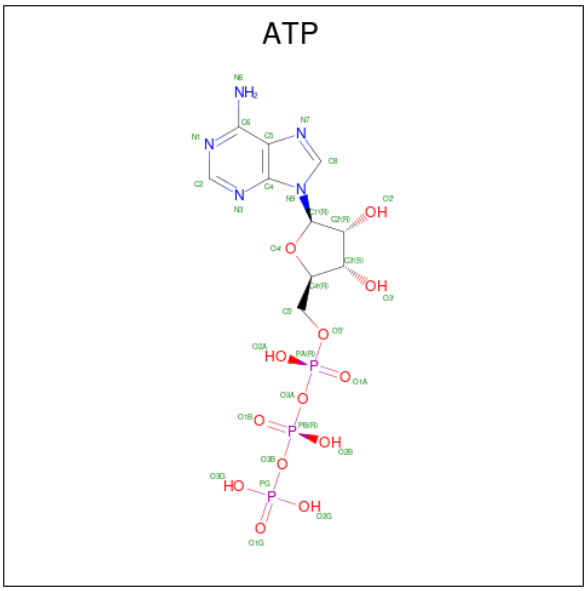
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 186 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
1	x	1	Total	C	N	O	P	0
			31	10	5	13	3	
1	x	1	Total	C	N	O	P	0
			31	10	5	13	3	
1	x	1	Total	C	N	O	P	0
			31	10	5	13	3	
1	x	1	Total	C	N	O	P	0
			31	10	5	13	3	
1	x	1	Total	C	N	O	P	0
			31	10	5	13	3	
1	y	1	Total	C	N	O	P	0
			31	10	5	13	3	

3 Residue-property plots (i)

There is no protein, DNA or RNA chain in this entry to show sequence plots.

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	
Number of images used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	Not provided	
Voltage (kV)	Not provided	
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	Not provided	

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	x	155	0	60	0	0
1	y	31	0	12	0	0
All	All	186	0	72	0	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 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein molecules in this entry.

5.3.2 Protein sidechains

There are no protein molecules in this entry.

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

6 ligands are 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	$\#\|Z\| > 2$
1	ATP	x	504	-	28,33,33	0.94	1 (3%)	34,52,52	1.53	8 (23%)
1	ATP	x	505	-	28,33,33	1.17	1 (3%)	34,52,52	1.25	2 (5%)
1	ATP	y	501	-	28,33,33	0.68	0	34,52,52	0.96	2 (5%)
1	ATP	x	503	-	28,33,33	0.91	0	34,52,52	1.23	2 (5%)
1	ATP	x	502	-	28,33,33	0.92	0	34,52,52	1.25	3 (8%)
1	ATP	x	501	-	28,33,33	0.60	0	34,52,52	0.76	2 (5%)

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
1	ATP	x	504	-	-	3/18/38/38	0/3/3/3
1	ATP	x	505	-	-	7/18/38/38	0/3/3/3
1	ATP	y	501	-	-	6/18/38/38	0/3/3/3
1	ATP	x	503	-	-	4/18/38/38	0/3/3/3
1	ATP	x	502	-	-	3/18/38/38	0/3/3/3
1	ATP	x	501	-	-	6/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	x	505	ATP	PB-O3B	4.16	1.64	1.59
1	x	504	ATP	O4'-C1'	2.01	1.43	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	x	504	ATP	N3-C2-N1	-4.00	123.25	128.67
1	y	501	ATP	C4'-O4'-C1'	-3.97	106.29	109.92
1	x	503	ATP	N3-C2-N1	-3.90	123.38	128.67
1	x	502	ATP	N3-C2-N1	-3.75	123.59	128.67
1	x	505	ATP	N3-C2-N1	-3.61	123.77	128.67
1	x	504	ATP	C4-C5-N7	-2.88	106.30	109.34
1	x	504	ATP	C4'-O4'-C1'	2.86	112.54	109.92
1	x	504	ATP	O3'-C3'-C2'	2.67	120.39	111.82
1	x	503	ATP	C4-C5-N7	-2.64	106.55	109.34
1	x	505	ATP	C4-C5-N7	-2.60	106.59	109.34
1	x	504	ATP	C2'-C3'-C4'	2.55	107.54	102.61
1	x	501	ATP	C1'-N9-C4	2.44	130.93	126.64
1	y	501	ATP	C5-C6-N6	2.38	123.93	120.31
1	x	501	ATP	C5-C6-N6	2.27	123.78	120.31
1	x	502	ATP	N6-C6-N1	2.17	122.98	118.33
1	x	504	ATP	O3G-PG-O2G	2.16	115.89	107.80
1	x	504	ATP	O3'-C3'-C4'	2.14	117.23	111.08
1	x	502	ATP	C4-C5-N7	-2.09	107.13	109.34
1	x	504	ATP	O2B-PB-O1B	2.03	121.87	112.44

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	x	502	ATP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	x	502	ATP	C3'-C4'-C5'-O5'
1	x	503	ATP	C5'-O5'-PA-O2A
1	x	503	ATP	C5'-O5'-PA-O3A
1	x	501	ATP	C5'-O5'-PA-O1A
1	x	501	ATP	C5'-O5'-PA-O3A
1	x	505	ATP	PB-O3B-PG-O2G
1	x	505	ATP	C5'-O5'-PA-O3A
1	y	501	ATP	C5'-O5'-PA-O1A
1	y	501	ATP	C5'-O5'-PA-O2A
1	y	501	ATP	C5'-O5'-PA-O3A
1	y	501	ATP	O4'-C4'-C5'-O5'
1	x	503	ATP	O4'-C4'-C5'-O5'
1	y	501	ATP	C3'-C4'-C5'-O5'
1	x	503	ATP	C3'-C4'-C5'-O5'
1	x	505	ATP	C4'-C5'-O5'-PA
1	x	502	ATP	PB-O3A-PA-O5'
1	y	501	ATP	PB-O3A-PA-O5'
1	x	504	ATP	PB-O3B-PG-O3G
1	x	501	ATP	C4'-C5'-O5'-PA
1	x	501	ATP	O4'-C4'-C5'-O5'
1	x	501	ATP	C5'-O5'-PA-O2A
1	x	505	ATP	C5'-O5'-PA-O1A
1	x	504	ATP	C5'-O5'-PA-O3A
1	x	501	ATP	C3'-C4'-C5'-O5'
1	x	505	ATP	PB-O3B-PG-O1G
1	x	505	ATP	PB-O3B-PG-O3G
1	x	504	ATP	C4'-C5'-O5'-PA
1	x	505	ATP	PG-O3B-PB-O3A

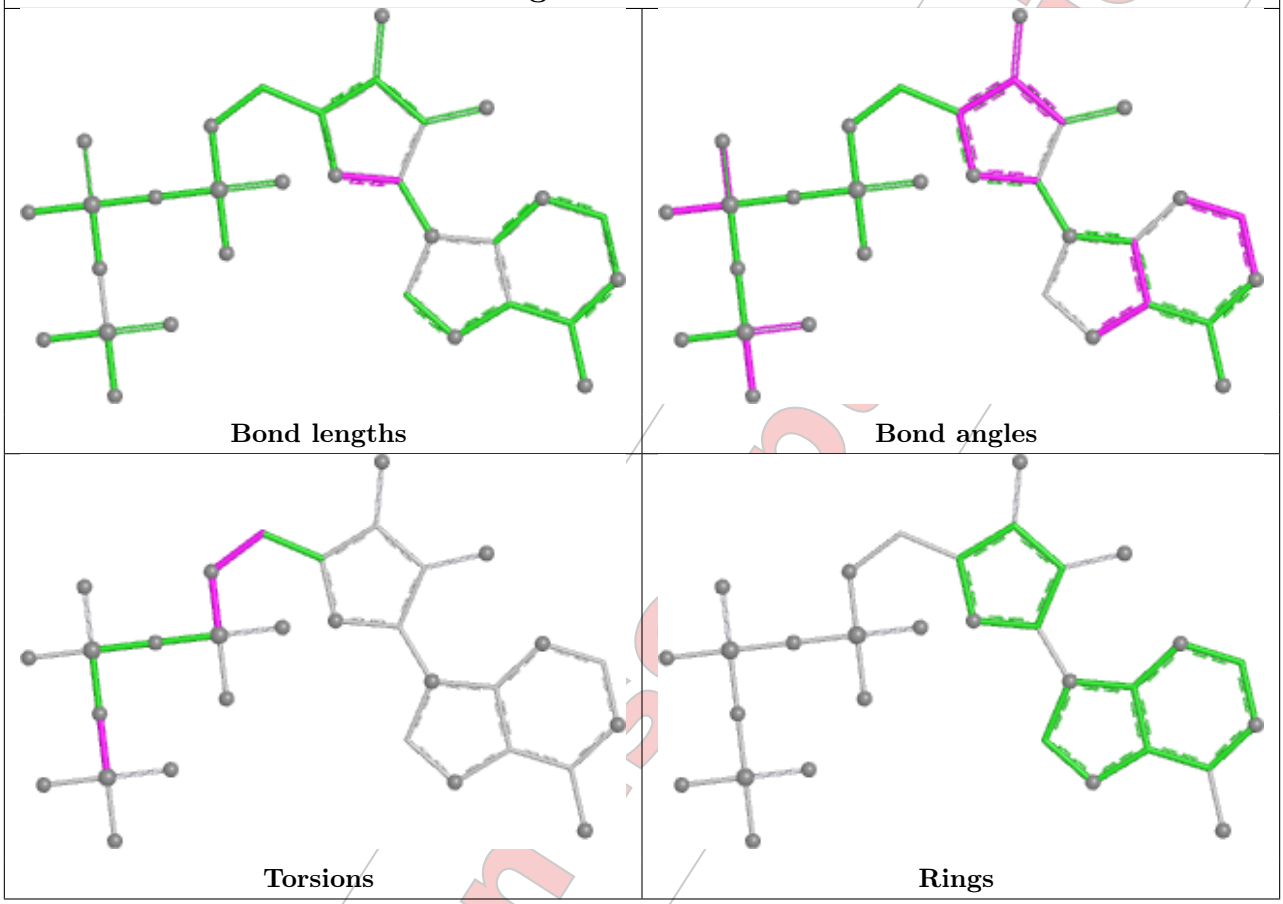
There are no ring outliers.

No monomer is involved in short contacts.

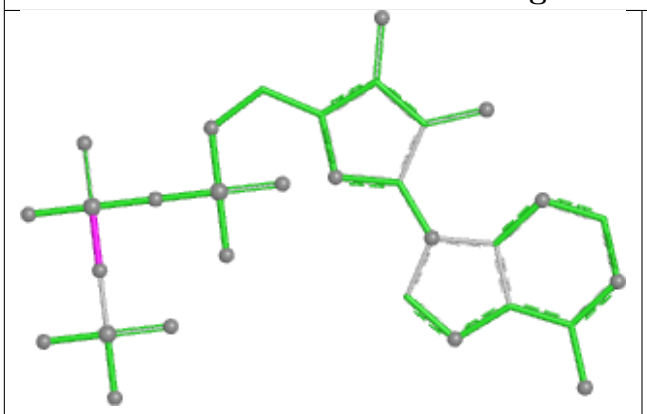
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

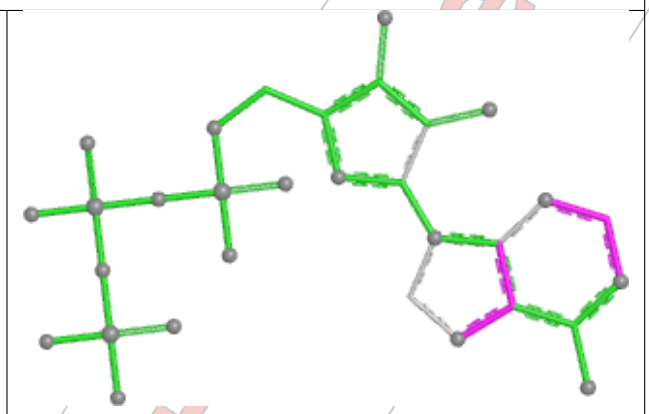
Ligand ATP x 504



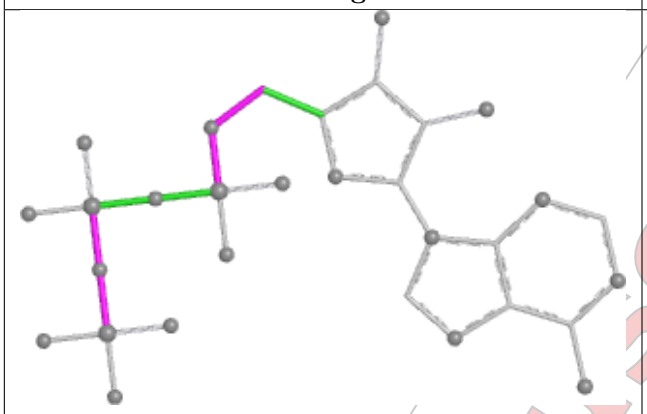
Ligand ATP x 505



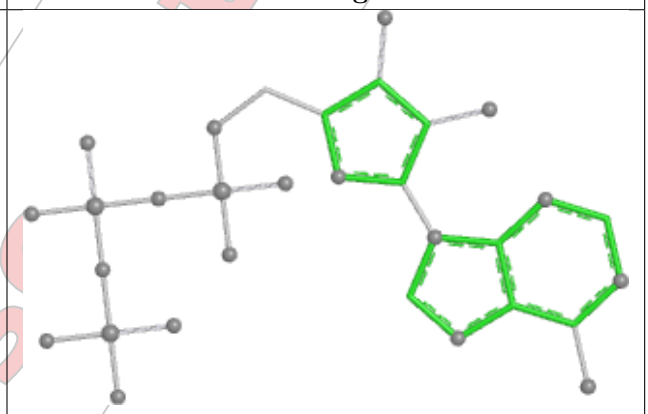
Bond lengths



Bond angles

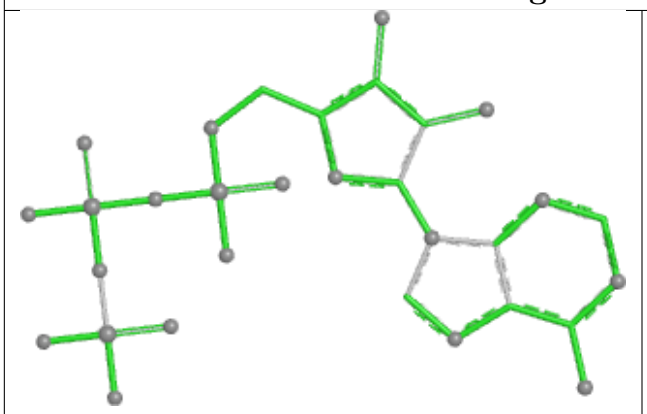


Torsions

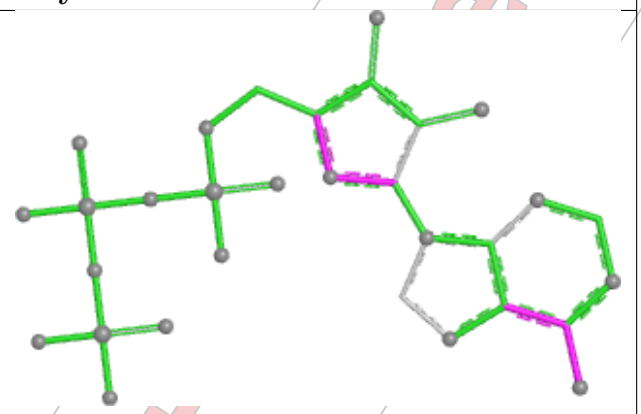


Rings

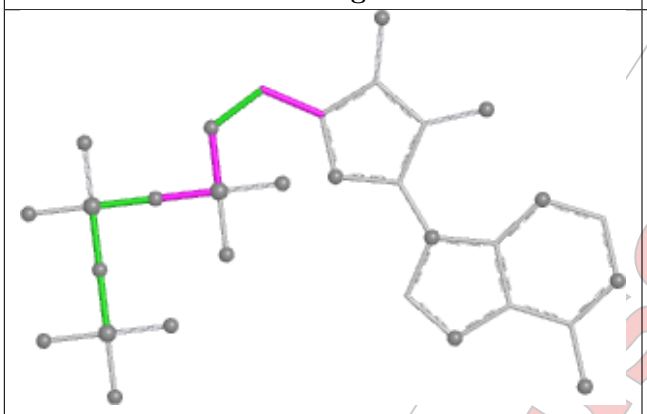
Ligand ATP y 501



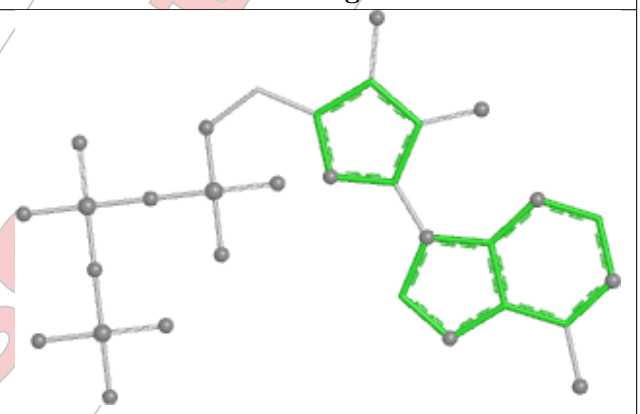
Bond lengths



Bond angles

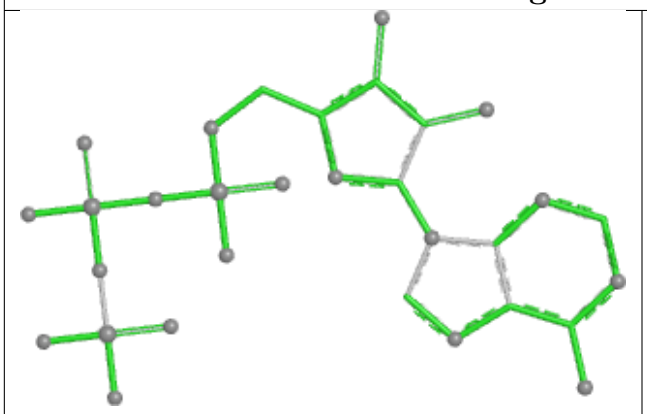


Torsions

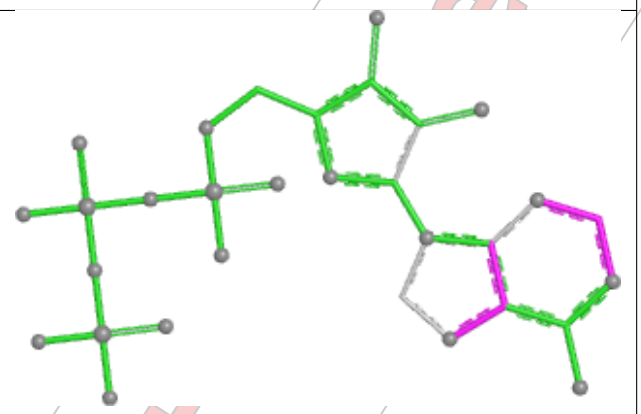


Rings

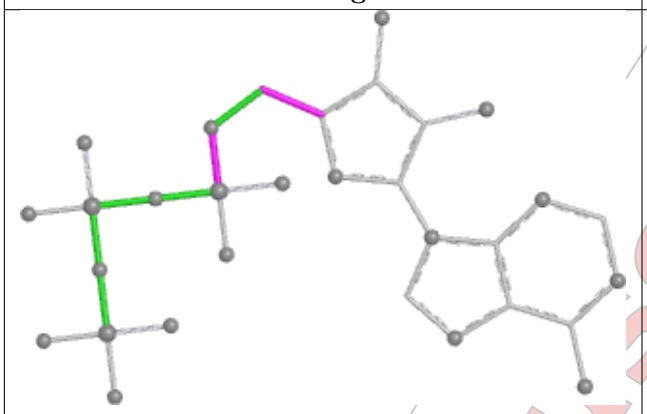
Ligand ATP x 503



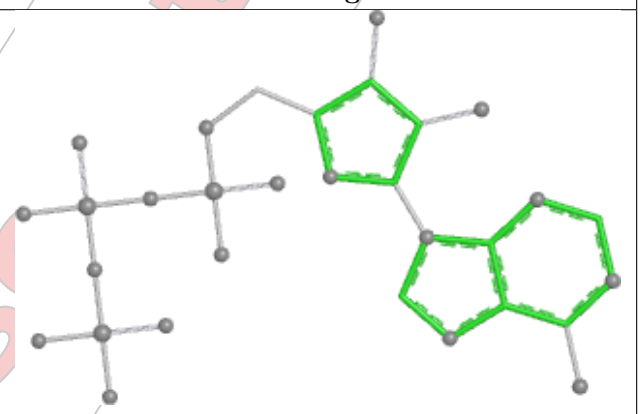
Bond lengths



Bond angles

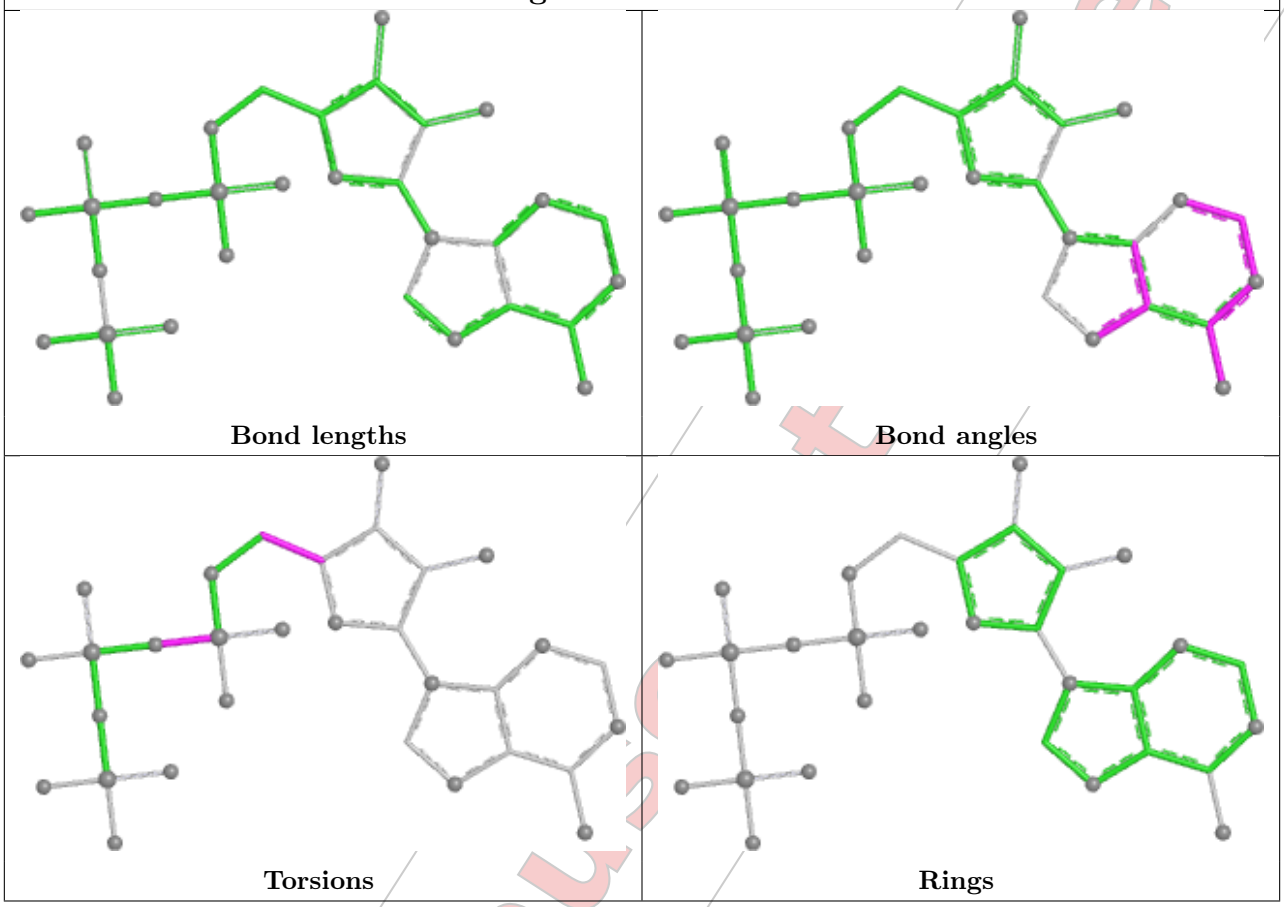


Torsions

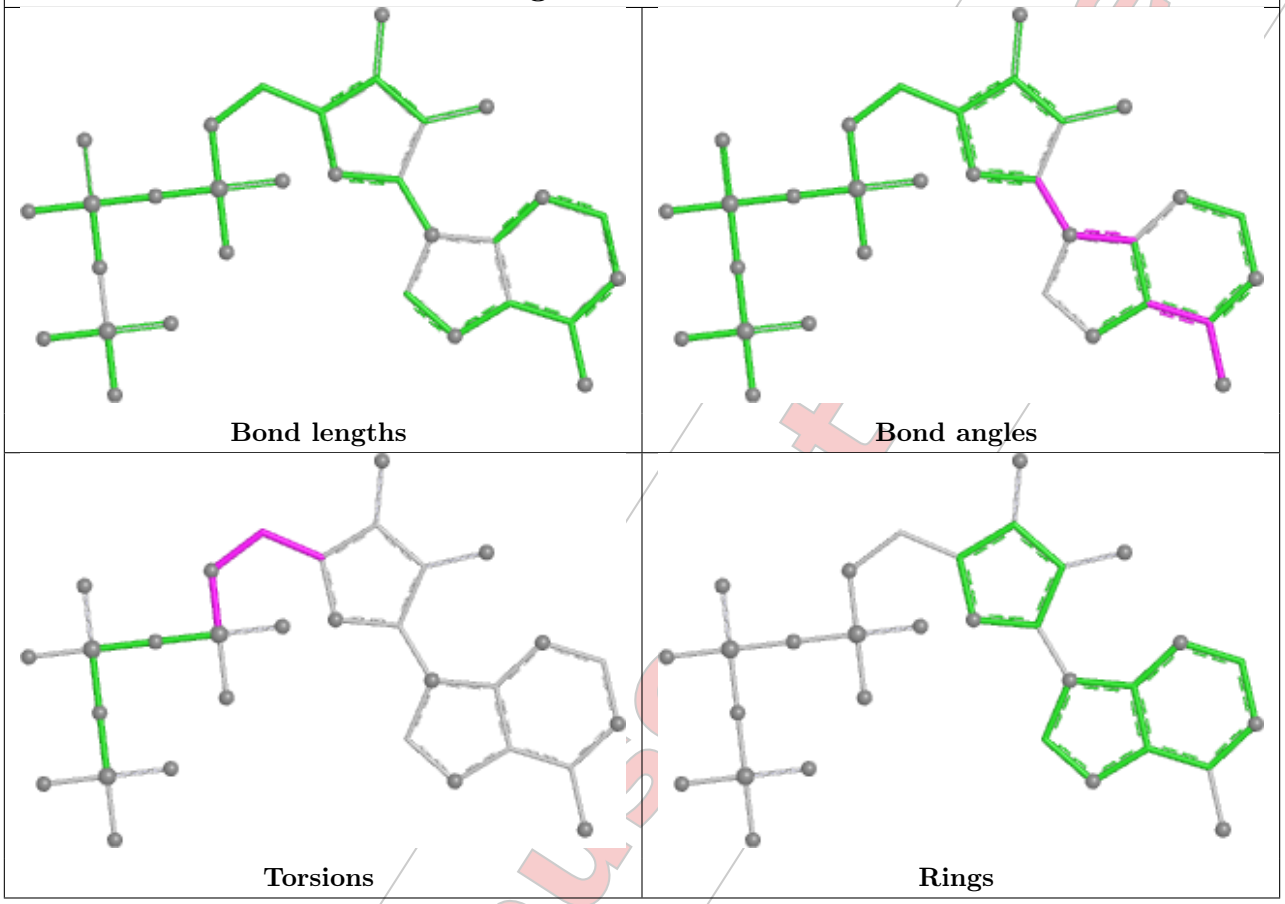


Rings

Ligand ATP x 502



Ligand ATP x 501



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.