



## wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Dec 10, 2019 – 04:15 PM EST

PDB ID : 6RKD  
EMDB ID: : EMD-4907  
Title : Molybdenum storage protein under turnover conditions  
Authors : Bruenle, S.; Mills, D.J.; Vonck, J.; Ermler, U.  
Deposited on : 2019-04-30  
Resolution : 3.20 Å(reported)  
Based on PDB ID : 4F6T

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

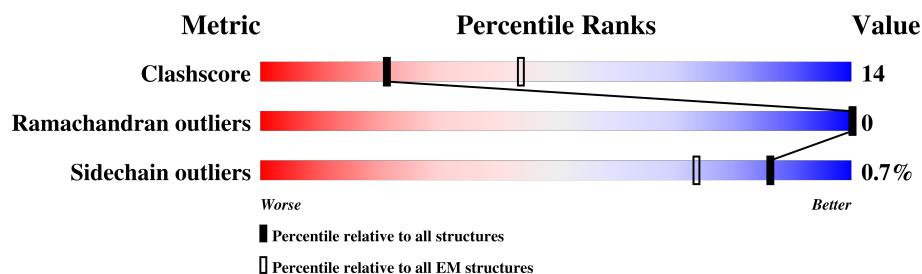
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	276	83% 15% .
1	C	276	83% 15% .
1	E	276	83% 15% .
1	G	276	83% 15% .
1	I	276	83% 15% .
1	K	276	83% 15% .
2	B	270	81% 18% .
2	D	270	81% 19% .
2	F	270	80% 19% .

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Mol	Chain	Length	Quality of chain
2	H	270	 80% 19%
2	J	270	 80% 19%
2	L	270	 81% 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ATP	B	805	-	-	X	-
3	ATP	D	906	-	-	X	-
3	ATP	F	905	-	-	X	-
3	ATP	H	805	-	-	X	-
3	ATP	J	804	-	-	X	-
3	ATP	L	905	-	-	X	-
5	8M0	B	806	-	-	X	-
5	8M0	D	907	-	-	X	-
5	8M0	F	906	-	-	X	-
5	8M0	H	806	-	-	X	-
5	8M0	J	805	-	-	X	-
5	8M0	L	906	-	-	X	-
7	MOO	A	305	-	-	X	-
7	MOO	A	306	-	-	X	-
7	MOO	A	308	-	-	X	-
7	MOO	B	801	-	-	X	-
7	MOO	B	802	-	-	X	-
7	MOO	B	803	-	-	X	-
7	MOO	B	804	-	-	X	-
7	MOO	B	807	-	-	X	-
7	MOO	C	305	-	-	X	-
7	MOO	C	306	-	-	X	-
7	MOO	D	902	-	-	X	-
7	MOO	D	903	-	-	X	-
7	MOO	D	904	-	-	X	-
7	MOO	D	905	-	-	X	-
7	MOO	D	908	-	-	X	-
7	MOO	E	306	-	-	X	-
7	MOO	E	307	-	-	X	-
7	MOO	F	902	-	-	X	-
7	MOO	F	903	-	-	X	-
7	MOO	F	904	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	MOO	F	907	-	-	X	-
7	MOO	G	305	-	-	X	-
7	MOO	G	306	-	-	X	-
7	MOO	G	307	-	-	X	-
7	MOO	H	801	-	-	X	-
7	MOO	H	802	-	-	X	-
7	MOO	H	803	-	-	X	-
7	MOO	H	804	-	-	X	-
7	MOO	H	807	-	-	X	-
7	MOO	I	306	-	-	X	-
7	MOO	I	307	-	-	X	-
7	MOO	I	308	-	-	X	-
7	MOO	J	801	-	-	X	-
7	MOO	J	802	-	-	X	-
7	MOO	J	803	-	-	X	-
7	MOO	J	806	-	-	X	-
7	MOO	K	306	-	-	X	-
7	MOO	K	307	-	-	X	-
7	MOO	L	902	-	-	X	-
7	MOO	L	903	-	-	X	-
7	MOO	L	904	-	-	X	-
7	MOO	L	907	-	-	X	-
8	OMO	A	307	-	-	X	-
8	OMO	C	307	-	-	X	-
8	OMO	E	301	-	-	X	-
8	OMO	G	308	-	-	X	-
8	OMO	I	301	-	-	X	-
8	OMO	K	301	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 25290 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.

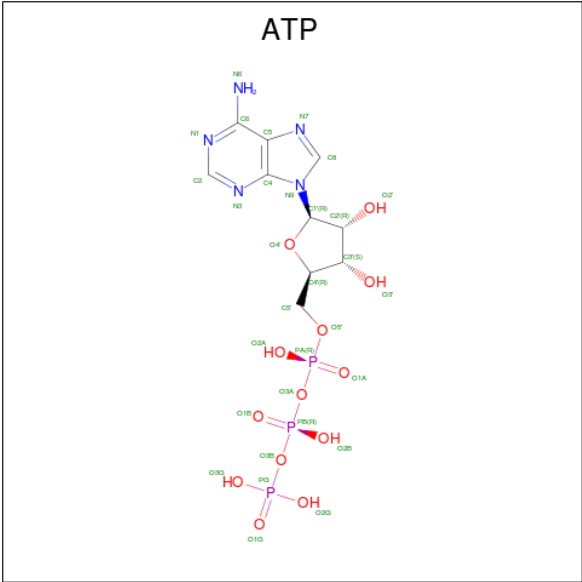
- Molecule 1 is a protein called Molybdenum storage protein subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	271	Total 2033	C 1283	N 382	O 365	S 3	1	0
1	C	271	Total 2033	C 1283	N 382	O 365	S 3	1	0
1	E	271	Total 2033	C 1283	N 382	O 365	S 3	1	0
1	G	271	Total 2033	C 1283	N 382	O 365	S 3	1	0
1	I	271	Total 2033	C 1283	N 382	O 365	S 3	1	0
1	K	271	Total 2033	C 1283	N 382	O 365	S 3	1	0

- Molecule 2 is a protein called Molybdenum storage protein subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	268	Total 1982	C 1258	N 347	O 369	S 8	3	0
2	D	268	Total 1982	C 1258	N 347	O 369	S 8	3	0
2	F	268	Total 1982	C 1258	N 347	O 369	S 8	3	0
2	H	268	Total 1982	C 1258	N 347	O 369	S 8	3	0
2	J	268	Total 1982	C 1258	N 347	O 369	S 8	3	0
2	L	268	Total 1982	C 1258	N 347	O 369	S 8	3	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).

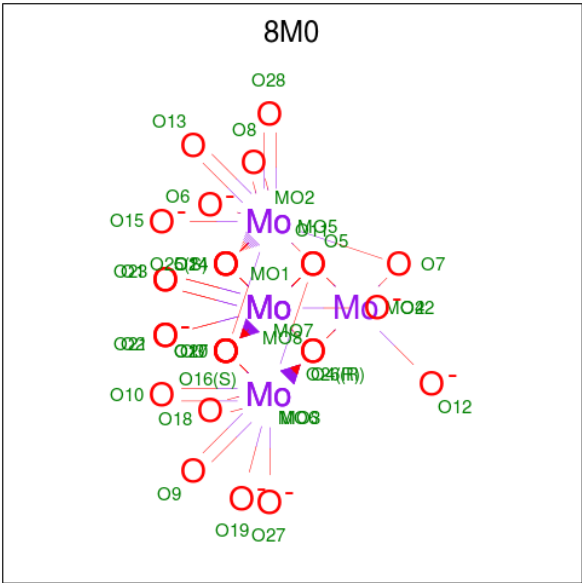


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	F	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	G	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	H	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	J	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	K	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	L	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	G	1	Total	Mg	0
			1	1	
4	K	1	Total	Mg	0
			1	1	
4	E	1	Total	Mg	0
			1	1	
4	I	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	
4	A	1	Total	Mg	0
			1	1	

- Molecule 5 is bis(mu4-oxo)-tetrakis(mu3-oxo)-hexakis(mu2-oxo)-hexadeca-oxo-octamolybdenum (VI) (three-letter code: 8M0) (formula: Mo<sub>8</sub>O<sub>28</sub>).



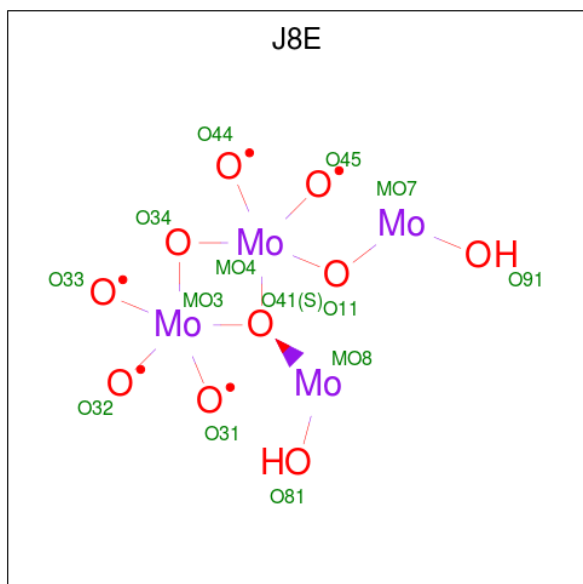
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	Mo	O	0
			34	8	26	
5	B	1	Total	Mo	O	0
			36	8	28	
5	C	1	Total	Mo	O	0
			34	8	26	
5	D	1	Total	Mo	O	0
			36	8	28	
5	E	1	Total	Mo	O	0
			34	8	26	

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Mol	Chain	Residues	Atoms			AltConf
5	F	1	Total	Mo	O	0
			36	8	28	
5	G	1	Total	Mo	O	0
			34	8	26	
5	H	1	Total	Mo	O	0
			36	8	28	
5	I	1	Total	Mo	O	0
			34	8	26	
5	J	1	Total	Mo	O	0
			36	8	28	
5	K	1	Total	Mo	O	0
			34	8	26	
5	L	1	Total	Mo	O	0
			36	8	28	

- Molecule 6 is oxidanyl-[[2,2,4,4,4-pentakis( $\text{O}^{\wedge}\{1\}$ -oxidanyl)-1-(oxidanylmolybdenio)-1 $\text{O}^{\wedge}\{3\}$ ,3-dioxa-2 $\text{O}^{\wedge}\{5\}$ ,4 $\text{O}^{\wedge}\{5\}$ -dimolybdacyclobut-2-yl]oxy]molybdenum (three-letter code: J8E) (formula:  $\text{H}_2\text{Mo}_4\text{O}_{10}$ ).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	Mo	O	0
			14	4	10	
6	B	1	Total	Mo	O	0
			14	4	10	
6	C	1	Total	Mo	O	0
			14	4	10	

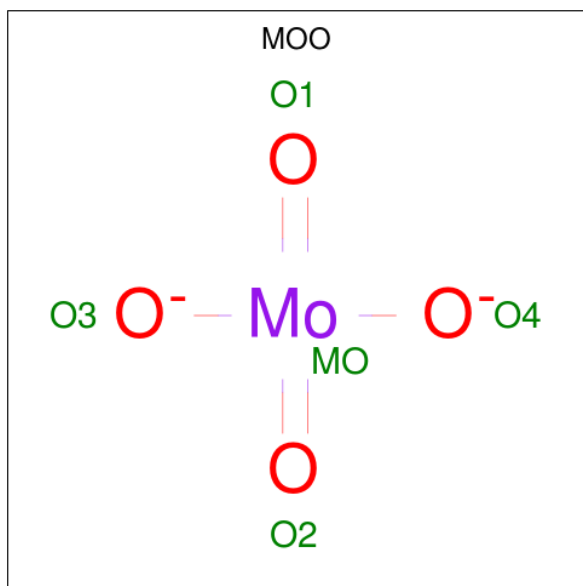
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Mol	Chain	Residues	Atoms			AltConf
6	D	1	Total	Mo	O	0
			14	4	10	
6	E	1	Total	Mo	O	0
			14	4	10	
6	F	1	Total	Mo	O	0
			14	4	10	
6	G	1	Total	Mo	O	0
			14	4	10	
6	H	1	Total	Mo	O	0
			14	4	10	
6	I	1	Total	Mo	O	0
			14	4	10	
6	J	1	Total	Mo	O	0
			14	4	10	
6	K	1	Total	Mo	O	0
			14	4	10	
6	L	1	Total	Mo	O	0
			14	4	10	

- Molecule 7 is MOLYBDATE ION (three-letter code: MOO) (formula:  $\text{MoO}_4$ ).



Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	Mo	O	0
			15	3	12	
7	A	1	Total	Mo	O	0
			15	3	12	

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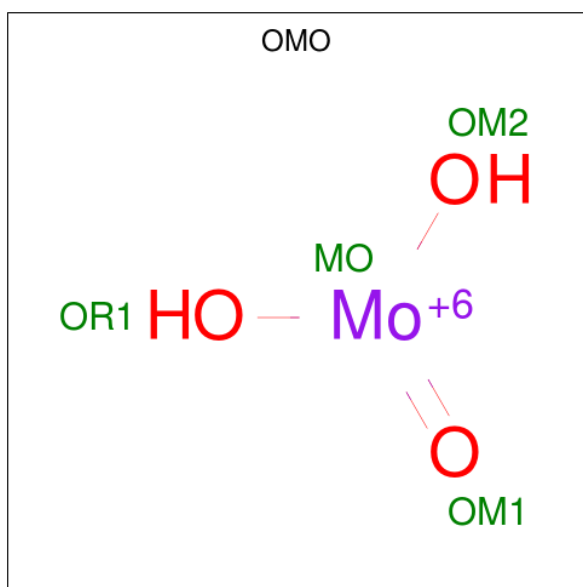
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total 15	Mo 3	O 12	0
7	B	1	Total 25	Mo 5	O 20	0
7	B	1	Total 25	Mo 5	O 20	0
7	B	1	Total 25	Mo 5	O 20	0
7	B	1	Total 25	Mo 5	O 20	0
7	B	1	Total 25	Mo 5	O 20	0
7	C	1	Total 10	Mo 2	O 8	0
7	C	1	Total 10	Mo 2	O 8	0
7	D	1	Total 25	Mo 5	O 20	0
7	D	1	Total 25	Mo 5	O 20	0
7	D	1	Total 25	Mo 5	O 20	0
7	D	1	Total 25	Mo 5	O 20	0
7	D	1	Total 25	Mo 5	O 20	0
7	D	1	Total 25	Mo 5	O 20	0
7	E	1	Total 10	Mo 2	O 8	0
7	E	1	Total 10	Mo 2	O 8	0
7	F	1	Total 20	Mo 4	O 16	0
7	F	1	Total 20	Mo 4	O 16	0
7	F	1	Total 20	Mo 4	O 16	0
7	F	1	Total 20	Mo 4	O 16	0
7	F	1	Total 20	Mo 4	O 16	0
7	G	1	Total 15	Mo 3	O 12	0
7	G	1	Total 15	Mo 3	O 12	0

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Mol	Chain	Residues	Atoms			AltConf
7	G	1	Total	Mo	O	0
			15	3	12	
7	H	1	Total	Mo	O	0
			25	5	20	
7	H	1	Total	Mo	O	0
			25	5	20	
7	H	1	Total	Mo	O	0
			25	5	20	
7	H	1	Total	Mo	O	0
			25	5	20	
7	H	1	Total	Mo	O	0
			25	5	20	
7	I	1	Total	Mo	O	0
			15	3	12	
7	I	1	Total	Mo	O	0
			15	3	12	
7	I	1	Total	Mo	O	0
			15	3	12	
7	J	1	Total	Mo	O	0
			20	4	16	
7	J	1	Total	Mo	O	0
			20	4	16	
7	J	1	Total	Mo	O	0
			20	4	16	
7	J	1	Total	Mo	O	0
			20	4	16	
7	K	1	Total	Mo	O	0
			10	2	8	
7	K	1	Total	Mo	O	0
			10	2	8	
7	L	1	Total	Mo	O	0
			20	4	16	
7	L	1	Total	Mo	O	0
			20	4	16	
7	L	1	Total	Mo	O	0
			20	4	16	
7	L	1	Total	Mo	O	0
			20	4	16	

- Molecule 8 is MO(VI)(=O)(OH)<sub>2</sub> CLUSTER (three-letter code: OMO) (formula: H<sub>2</sub>MoO<sub>3</sub>).

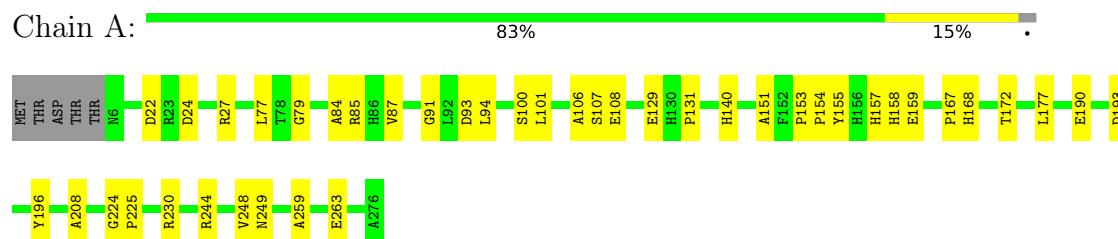


Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	Mo	O	0
			4	1	3	
8	C	1	Total	Mo	O	0
			4	1	3	
8	E	1	Total	Mo	O	0
			4	1	3	
8	G	1	Total	Mo	O	0
			4	1	3	
8	I	1	Total	Mo	O	0
			4	1	3	
8	K	1	Total	Mo	O	0
			4	1	3	

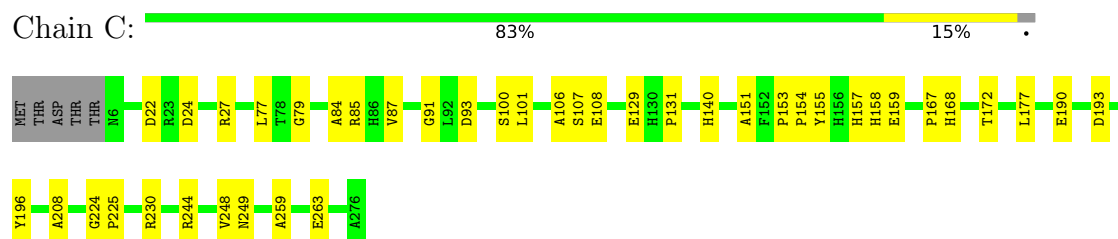
### 3 Residue-property plots [i](#)

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

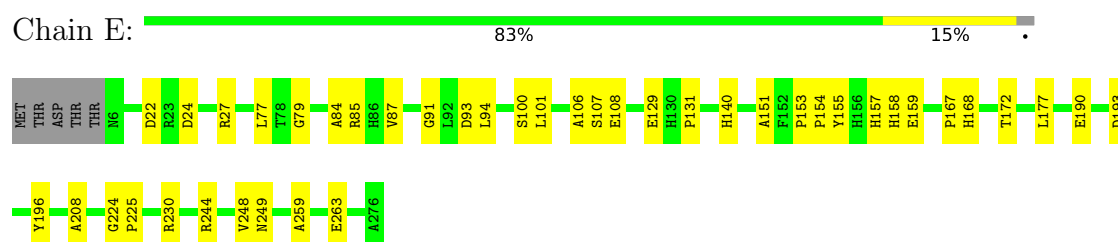
- Molecule 1: Molybdenum storage protein subunit alpha



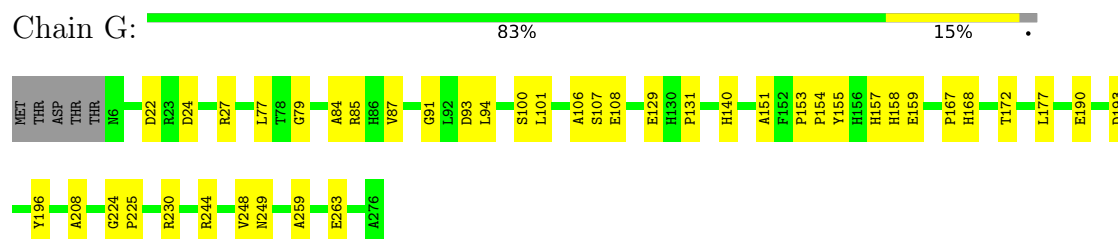
- Molecule 1: Molybdenum storage protein subunit alpha



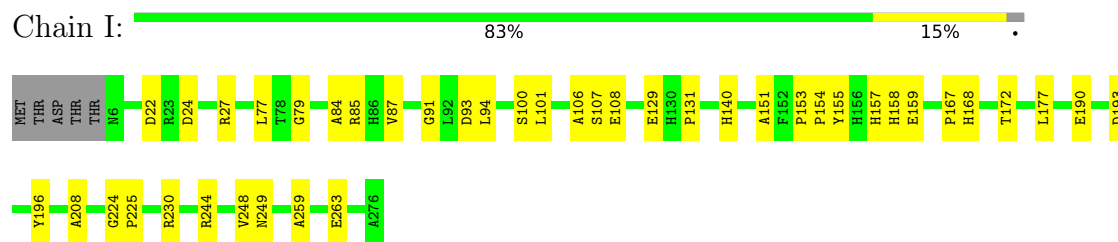
- Molecule 1: Molybdenum storage protein subunit alpha



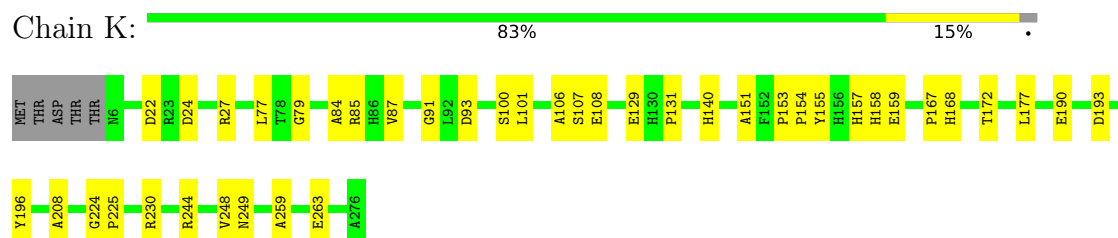
- Molecule 1: Molybdenum storage protein subunit alpha



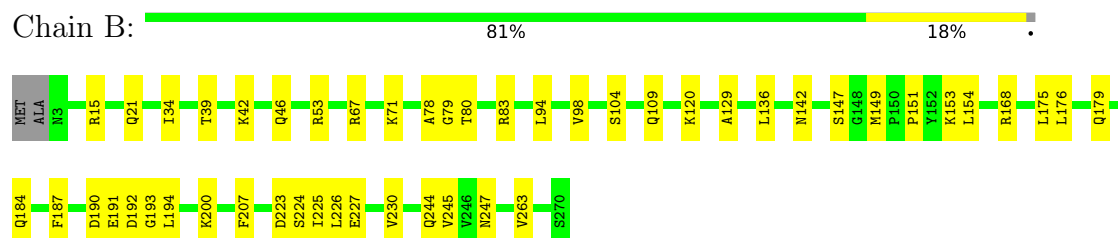
- Molecule 1: Molybdenum storage protein subunit alpha



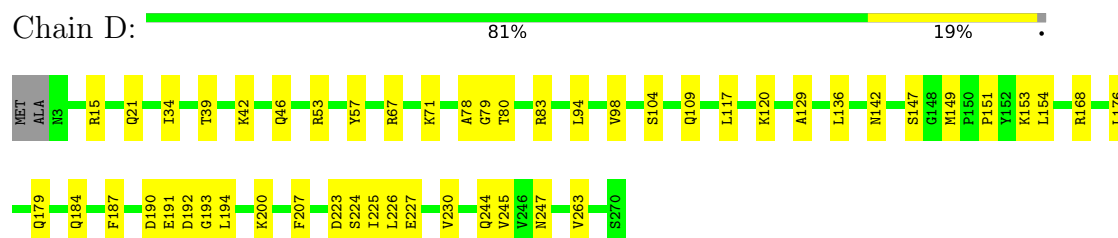
- Molecule 1: Molybdenum storage protein subunit alpha



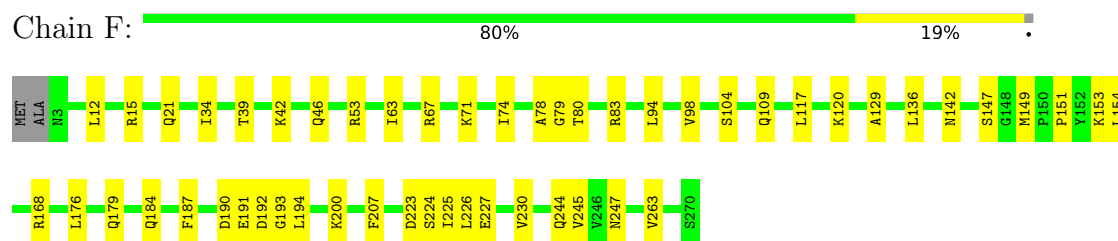
- Molecule 2: Molybdenum storage protein subunit beta



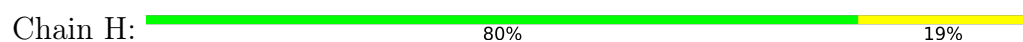
- Molecule 2: Molybdenum storage protein subunit beta

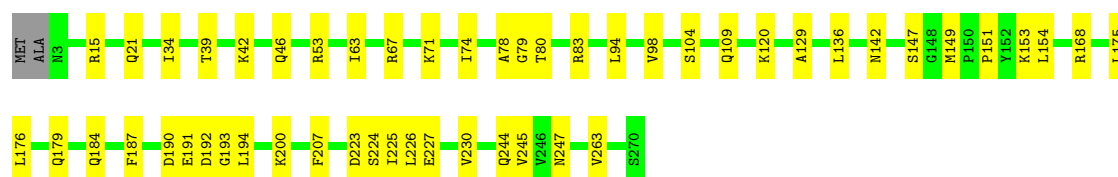


- Molecule 2: Molybdenum storage protein subunit beta



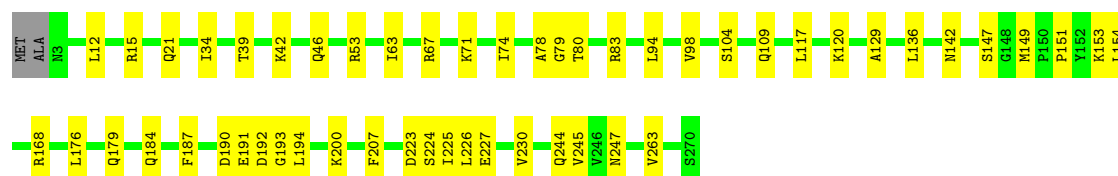
- Molecule 2: Molybdenum storage protein subunit beta





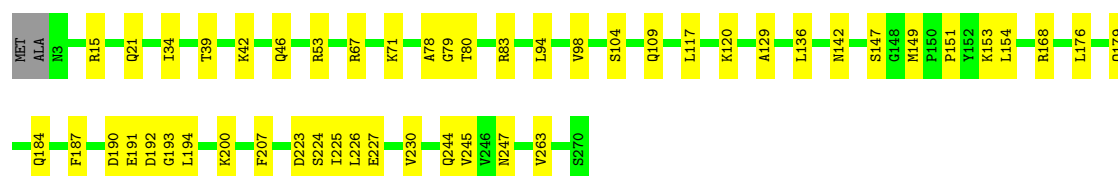
- Molecule 2: Molybdenum storage protein subunit beta

Chain J: 80% 19% .



- Molecule 2: Molybdenum storage protein subunit beta

Chain L: 81% 18% .



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	137558	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	54	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	45045	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMO, J8E, ATP, MOO, 8M0

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.48	1/2081 (0.0%)	0.63	0/2836
1	C	0.48	1/2081 (0.0%)	0.63	0/2836
1	E	0.48	1/2081 (0.0%)	0.63	0/2836
1	G	0.48	1/2081 (0.0%)	0.63	0/2836
1	I	0.48	1/2081 (0.0%)	0.63	0/2836
1	K	0.48	1/2081 (0.0%)	0.63	0/2836
2	B	0.40	0/2041	0.59	0/2773
2	D	0.40	0/2041	0.58	0/2773
2	F	0.40	0/2041	0.59	0/2773
2	H	0.40	0/2041	0.59	0/2773
2	J	0.40	0/2041	0.59	0/2773
2	L	0.40	0/2041	0.58	0/2773
All	All	0.44	6/24732 (0.0%)	0.61	0/33654

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	PRO	C-N	7.46	1.51	1.34
1	G	154	PRO	C-N	7.46	1.51	1.34
1	E	154	PRO	C-N	7.45	1.51	1.34
1	I	154	PRO	C-N	7.45	1.51	1.34
1	C	154	PRO	C-N	7.43	1.51	1.34

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	A	2033	0	2090	43	0
1	C	2033	0	2090	43	0
1	E	2033	0	2090	45	0
1	G	2033	0	2090	43	0
1	I	2033	0	2090	45	0
1	K	2033	0	2090	43	0
2	B	1982	0	2024	48	0
2	D	1982	0	2024	50	0
2	F	1982	0	2024	51	0
2	H	1982	0	2024	49	0
2	J	1982	0	2024	51	0
2	L	1982	0	2024	48	0
3	A	31	0	12	5	0
3	B	31	0	12	10	0
3	C	31	0	12	5	0
3	D	31	0	12	10	0
3	E	31	0	12	5	0
3	F	31	0	12	10	0
3	G	31	0	12	5	0
3	H	31	0	12	10	0
3	I	31	0	12	5	0
3	J	31	0	12	10	0
3	K	31	0	12	5	0
3	L	31	0	12	10	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
5	A	34	0	0	2	0
5	B	36	0	0	8	0
5	C	34	0	0	1	0
5	D	36	0	0	8	0
5	E	34	0	0	2	0
5	F	36	0	0	8	0
5	G	34	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	36	0	0	8	0
5	I	34	0	0	2	0
5	J	36	0	0	8	0
5	K	34	0	0	1	0
5	L	36	0	0	8	0
6	A	14	0	0	3	0
6	B	14	0	0	0	0
6	C	14	0	0	3	0
6	D	14	0	0	0	0
6	E	14	0	0	3	0
6	F	14	0	0	0	0
6	G	14	0	0	3	0
6	H	14	0	0	0	0
6	I	14	0	0	3	0
6	J	14	0	0	0	0
6	K	14	0	0	3	0
6	L	14	0	0	0	0
7	A	15	0	0	26	0
7	B	25	0	0	32	0
7	C	10	0	0	17	0
7	D	25	0	0	33	0
7	E	10	0	0	17	0
7	F	20	0	0	26	0
7	G	15	0	0	26	0
7	H	25	0	0	32	0
7	I	15	0	0	26	0
7	J	20	0	0	26	0
7	K	10	0	0	17	0
7	L	20	0	0	25	0
8	A	4	0	0	5	0
8	C	4	0	0	5	0
8	E	4	0	0	5	0
8	G	4	0	0	5	0
8	I	4	0	0	5	0
8	K	4	0	0	5	0
All	All	25290	0	24828	713	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 14.

The worst 5 of 713 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:305:MOO:O3	7:C:306:MOO:O1	1.78	1.01
7:K:306:MOO:O3	7:K:307:MOO:O1	1.78	1.01
7:A:305:MOO:O3	7:A:306:MOO:O1	1.78	1.01
7:G:305:MOO:O3	7:G:306:MOO:O1	1.78	1.01
7:E:306:MOO:O3	7:E:307:MOO:O1	1.78	1.00

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	270/276 (98%)	262 (97%)	8 (3%)	0	100	100
1	C	270/276 (98%)	261 (97%)	9 (3%)	0	100	100
1	E	270/276 (98%)	262 (97%)	8 (3%)	0	100	100
1	G	270/276 (98%)	262 (97%)	8 (3%)	0	100	100
1	I	270/276 (98%)	262 (97%)	8 (3%)	0	100	100
1	K	270/276 (98%)	261 (97%)	9 (3%)	0	100	100
2	B	269/270 (100%)	261 (97%)	8 (3%)	0	100	100
2	D	269/270 (100%)	261 (97%)	8 (3%)	0	100	100
2	F	269/270 (100%)	261 (97%)	8 (3%)	0	100	100
2	H	269/270 (100%)	261 (97%)	8 (3%)	0	100	100
2	J	269/270 (100%)	261 (97%)	8 (3%)	0	100	100
2	L	269/270 (100%)	261 (97%)	8 (3%)	0	100	100
All	All	3234/3276 (99%)	3136 (97%)	98 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	212/216 (98%)	212 (100%)	0	100	100
1	C	212/216 (98%)	212 (100%)	0	100	100
1	E	212/216 (98%)	212 (100%)	0	100	100
1	G	212/216 (98%)	212 (100%)	0	100	100
1	I	212/216 (98%)	212 (100%)	0	100	100
1	K	212/216 (98%)	212 (100%)	0	100	100
2	B	208/206 (101%)	205 (99%)	3 (1%)	69	88
2	D	208/206 (101%)	205 (99%)	3 (1%)	69	88
2	F	208/206 (101%)	205 (99%)	3 (1%)	69	88
2	H	208/206 (101%)	205 (99%)	3 (1%)	69	88
2	J	208/206 (101%)	205 (99%)	3 (1%)	69	88
2	L	208/206 (101%)	205 (99%)	3 (1%)	69	88
All	All	2520/2532 (100%)	2502 (99%)	18 (1%)	86	95

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	153	LYS
2	H	67	ARG
2	J	153	LYS
2	F	67	ARG
2	F	142	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	246	GLN
1	G	86	HIS
1	K	111	GLN
2	F	142	ASN

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Mol	Chain	Res	Type
1	G	10	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 90 ligands modelled in this entry, 6 are monoatomic - leaving 84 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	$\# Z  > 2$
3	ATP	A	301	4	26,33,33	1.33	4 (15%)	27,52,52	1.81	4 (14%)
5	8M0	A	303	-	20,46,48	7.67	8 (40%)	-		
6	J8E	A	304	-	0,14,14	0.00	-	-		
7	MOO	A	305	-	2,4,4	1.33	0	-		
7	MOO	A	306	-	2,4,4	1.35	0	-		
8	OMO	A	307	-	0,3,3	0.00	-	-		
7	MOO	A	308	-	2,4,4	1.32	0	-		
7	MOO	B	801	-	2,4,4	1.34	0	-		
7	MOO	B	802	-	2,4,4	1.34	0	-		
7	MOO	B	803	-	2,4,4	1.35	0	-		
7	MOO	B	804	-	2,4,4	1.33	0	-		
3	ATP	B	805	7	26,33,33	0.69	0	27,52,52	0.92	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	8M0	B	806	-	22,48,48	8.08	12 (54%)	-		
7	MOO	B	807	3	2,4,4	1.34	0	-		
6	J8E	B	808	-	0,14,14	0.00	-	-		
3	ATP	C	301	4	26,33,33	1.33	4 (15%)	27,52,52	1.81	4 (14%)
5	8M0	C	303	-	20,46,48	7.67	8 (40%)	-		
6	J8E	C	304	-	0,14,14	0.00	-	-		
7	MOO	C	305	-	2,4,4	1.33	0	-		
7	MOO	C	306	-	2,4,4	1.34	0	-		
8	OMO	C	307	-	0,3,3	0.00	-	-		
6	J8E	D	901	-	0,14,14	0.00	-	-		
7	MOO	D	902	-	2,4,4	1.34	0	-		
7	MOO	D	903	-	2,4,4	1.33	0	-		
7	MOO	D	904	-	2,4,4	1.33	0	-		
7	MOO	D	905	-	2,4,4	1.33	0	-		
3	ATP	D	906	7	26,33,33	0.69	0	27,52,52	0.92	1 (3%)
5	8M0	D	907	-	22,48,48	8.08	12 (54%)	-		
7	MOO	D	908	3	2,4,4	1.34	0	-		
8	OMO	E	301	-	0,3,3	0.00	-	-		
3	ATP	E	302	4	26,33,33	1.33	4 (15%)	27,52,52	1.81	4 (14%)
5	8M0	E	304	-	20,46,48	7.68	8 (40%)	-		
6	J8E	E	305	-	0,14,14	0.00	-	-		
7	MOO	E	306	-	2,4,4	1.33	0	-		
7	MOO	E	307	-	2,4,4	1.34	0	-		
6	J8E	F	901	-	0,14,14	0.00	-	-		
7	MOO	F	902	-	2,4,4	1.35	0	-		
7	MOO	F	903	-	2,4,4	1.33	0	-		
7	MOO	F	904	-	2,4,4	1.34	0	-		
3	ATP	F	905	7	26,33,33	0.69	0	27,52,52	0.92	1 (3%)
5	8M0	F	906	-	22,48,48	8.07	12 (54%)	-		
7	MOO	F	907	3	2,4,4	1.34	0	-		
3	ATP	G	301	4	26,33,33	1.33	4 (15%)	27,52,52	1.81	4 (14%)
5	8M0	G	303	-	20,46,48	7.67	8 (40%)	-		
6	J8E	G	304	-	0,14,14	0.00	-	-		
7	MOO	G	305	-	2,4,4	1.33	0	-		
7	MOO	G	306	-	2,4,4	1.35	0	-		
7	MOO	G	307	-	2,4,4	1.32	0	-		
8	OMO	G	308	-	0,3,3	0.00	-	-		
7	MOO	H	801	-	2,4,4	1.34	0	-		
7	MOO	H	802	-	2,4,4	1.34	0	-		
7	MOO	H	803	-	2,4,4	1.35	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	MOO	H	804	-	2,4,4	1.33	0	-		
3	ATP	H	805	7	26,33,33	0.69	0	27,52,52	0.92	1 (3%)
5	8M0	H	806	-	22,48,48	8.08	12 (54%)	-		
7	MOO	H	807	3	2,4,4	1.34	0	-		
6	J8E	H	808	-	0,14,14	0.00	-	-		
8	OMO	I	301	-	0,3,3	0.00	-	-		
3	ATP	I	302	4	26,33,33	1.33	4 (15%)	27,52,52	1.81	4 (14%)
5	8M0	I	304	-	20,46,48	7.68	8 (40%)	-		
6	J8E	I	305	-	0,14,14	0.00	-	-		
7	MOO	I	306	-	2,4,4	1.33	0	-		
7	MOO	I	307	-	2,4,4	1.34	0	-		
7	MOO	I	308	-	2,4,4	1.33	0	-		
7	MOO	J	801	-	2,4,4	1.35	0	-		
7	MOO	J	802	-	2,4,4	1.33	0	-		
7	MOO	J	803	-	2,4,4	1.34	0	-		
3	ATP	J	804	7	26,33,33	0.69	0	27,52,52	0.92	1 (3%)
5	8M0	J	805	-	22,48,48	8.07	12 (54%)	-		
7	MOO	J	806	3	2,4,4	1.34	0	-		
6	J8E	J	807	-	0,14,14	0.00	-	-		
8	OMO	K	301	-	0,3,3	0.00	-	-		
3	ATP	K	302	4	26,33,33	1.33	4 (15%)	27,52,52	1.81	4 (14%)
5	8M0	K	304	-	20,46,48	7.67	8 (40%)	-		
6	J8E	K	305	-	0,14,14	0.00	-	-		
7	MOO	K	306	-	2,4,4	1.33	0	-		
7	MOO	K	307	-	2,4,4	1.34	0	-		
6	J8E	L	901	-	0,14,14	0.00	-	-		
7	MOO	L	902	-	2,4,4	1.34	0	-		
7	MOO	L	903	-	2,4,4	1.33	0	-		
7	MOO	L	904	-	2,4,4	1.33	0	-		
3	ATP	L	905	7	26,33,33	0.69	0	27,52,52	0.92	1 (3%)
5	8M0	L	906	-	22,48,48	8.08	12 (54%)	-		
7	MOO	L	907	3	2,4,4	1.34	0	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	301	4	-	1/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	J8E	A	304	-	-	-	0/1/1/1
3	ATP	B	805	7	-	1/18/38/38	0/3/3/3
6	J8E	B	808	-	-	-	0/1/1/1
3	ATP	C	301	4	-	1/18/38/38	0/3/3/3
6	J8E	C	304	-	-	-	0/1/1/1
6	J8E	D	901	-	-	-	0/1/1/1
3	ATP	D	906	7	-	1/18/38/38	0/3/3/3
3	ATP	E	302	4	-	1/18/38/38	0/3/3/3
6	J8E	E	305	-	-	-	0/1/1/1
6	J8E	F	901	-	-	-	0/1/1/1
3	ATP	F	905	7	-	1/18/38/38	0/3/3/3
3	ATP	G	301	4	-	1/18/38/38	0/3/3/3
6	J8E	G	304	-	-	-	0/1/1/1
3	ATP	H	805	7	-	1/18/38/38	0/3/3/3
6	J8E	H	808	-	-	-	0/1/1/1
3	ATP	I	302	4	-	1/18/38/38	0/3/3/3
6	J8E	I	305	-	-	-	0/1/1/1
3	ATP	J	804	7	-	1/18/38/38	0/3/3/3
6	J8E	J	807	-	-	-	0/1/1/1
3	ATP	K	302	4	-	1/18/38/38	0/3/3/3
6	J8E	K	305	-	-	-	0/1/1/1
6	J8E	L	901	-	-	-	0/1/1/1
3	ATP	L	905	7	-	1/18/38/38	0/3/3/3

The worst 5 of 144 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	304	8M0	O20-MO8	22.83	1.96	1.74
5	E	304	8M0	O20-MO8	22.83	1.96	1.74
5	A	303	8M0	O20-MO8	22.79	1.96	1.74
5	G	303	8M0	O20-MO8	22.79	1.96	1.74
5	C	303	8M0	O20-MO8	22.76	1.96	1.74

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	302	ATP	C4'-O4'-C1'	-4.98	104.64	109.83
3	C	301	ATP	C4'-O4'-C1'	-4.98	104.64	109.83
3	E	302	ATP	C4'-O4'-C1'	-4.97	104.64	109.83
3	I	302	ATP	C4'-O4'-C1'	-4.97	104.64	109.83
3	A	301	ATP	C4'-O4'-C1'	-4.95	104.66	109.83

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	906	ATP	C4'-C5'-O5'-PA
3	J	804	ATP	C4'-C5'-O5'-PA
3	B	805	ATP	C4'-C5'-O5'-PA
3	F	905	ATP	C4'-C5'-O5'-PA
3	L	905	ATP	C4'-C5'-O5'-PA

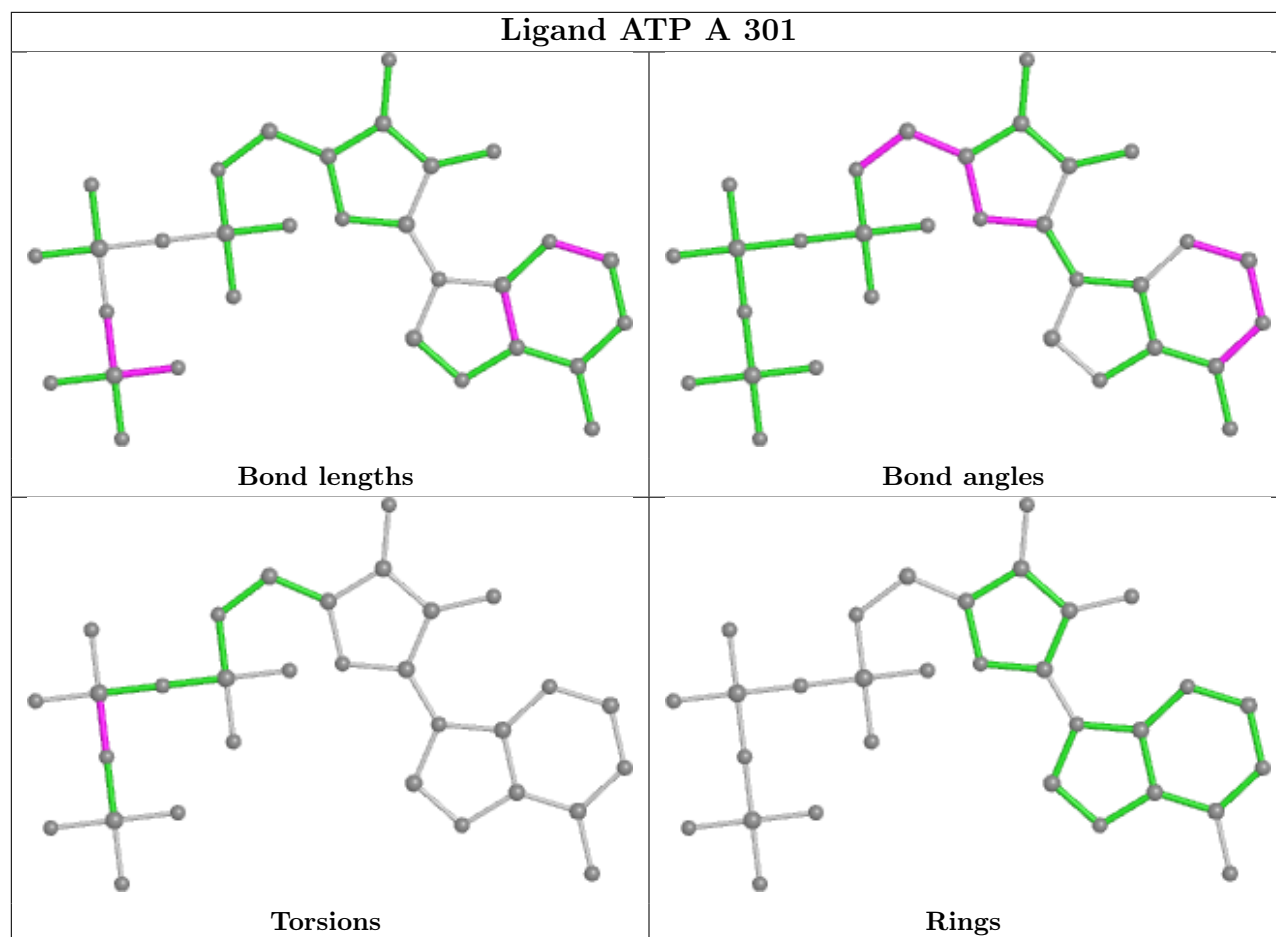
There are no ring outliers.

18 monomers are involved in 108 short contacts:

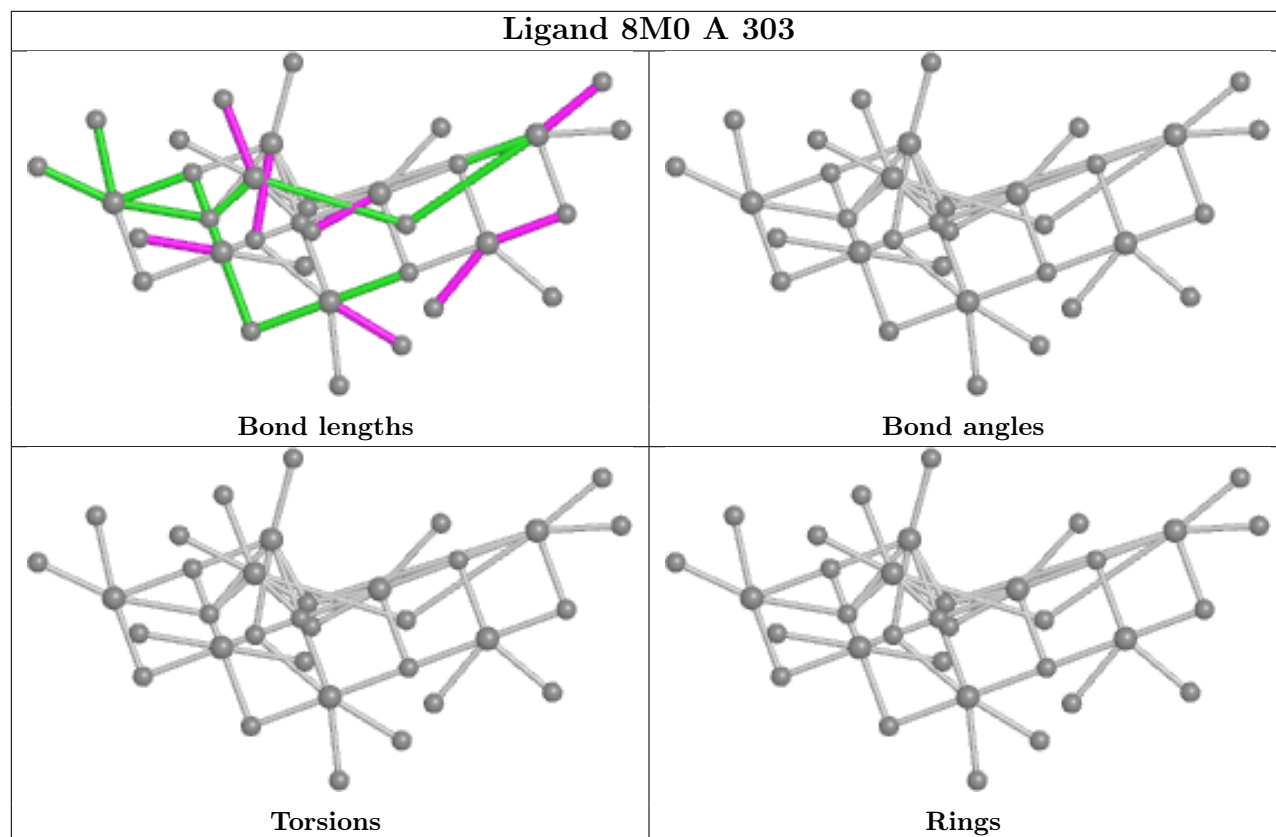
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	ATP	5	0
6	A	304	J8E	3	0
3	B	805	ATP	10	0
3	C	301	ATP	5	0
6	C	304	J8E	3	0
3	D	906	ATP	10	0
3	E	302	ATP	5	0
6	E	305	J8E	3	0
3	F	905	ATP	10	0
3	G	301	ATP	5	0
6	G	304	J8E	3	0
3	H	805	ATP	10	0
3	I	302	ATP	5	0
6	I	305	J8E	3	0
3	J	804	ATP	10	0
3	K	302	ATP	5	0
6	K	305	J8E	3	0
3	L	905	ATP	10	0

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

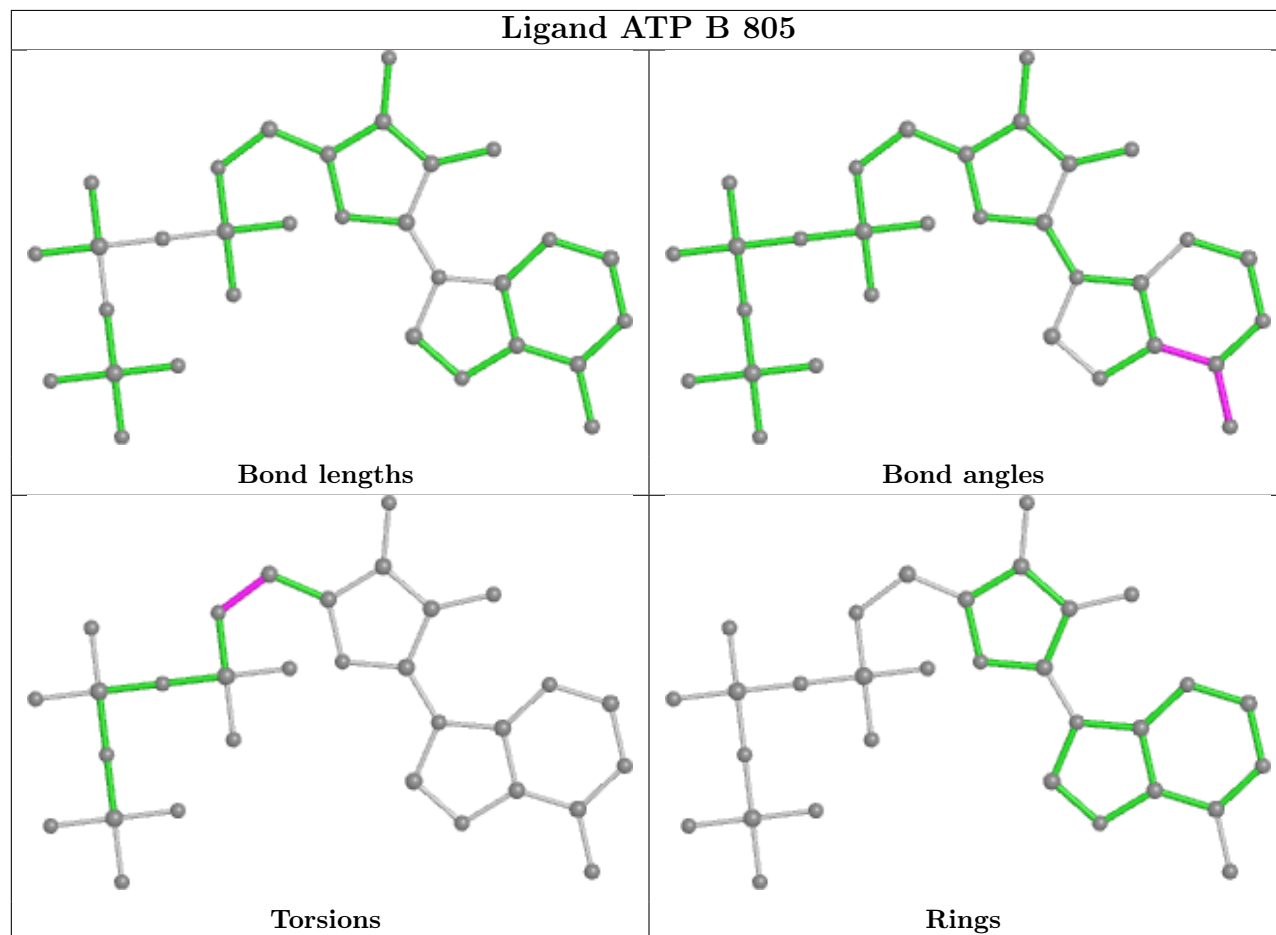
equivalents in the CSD to analyse the geometry.



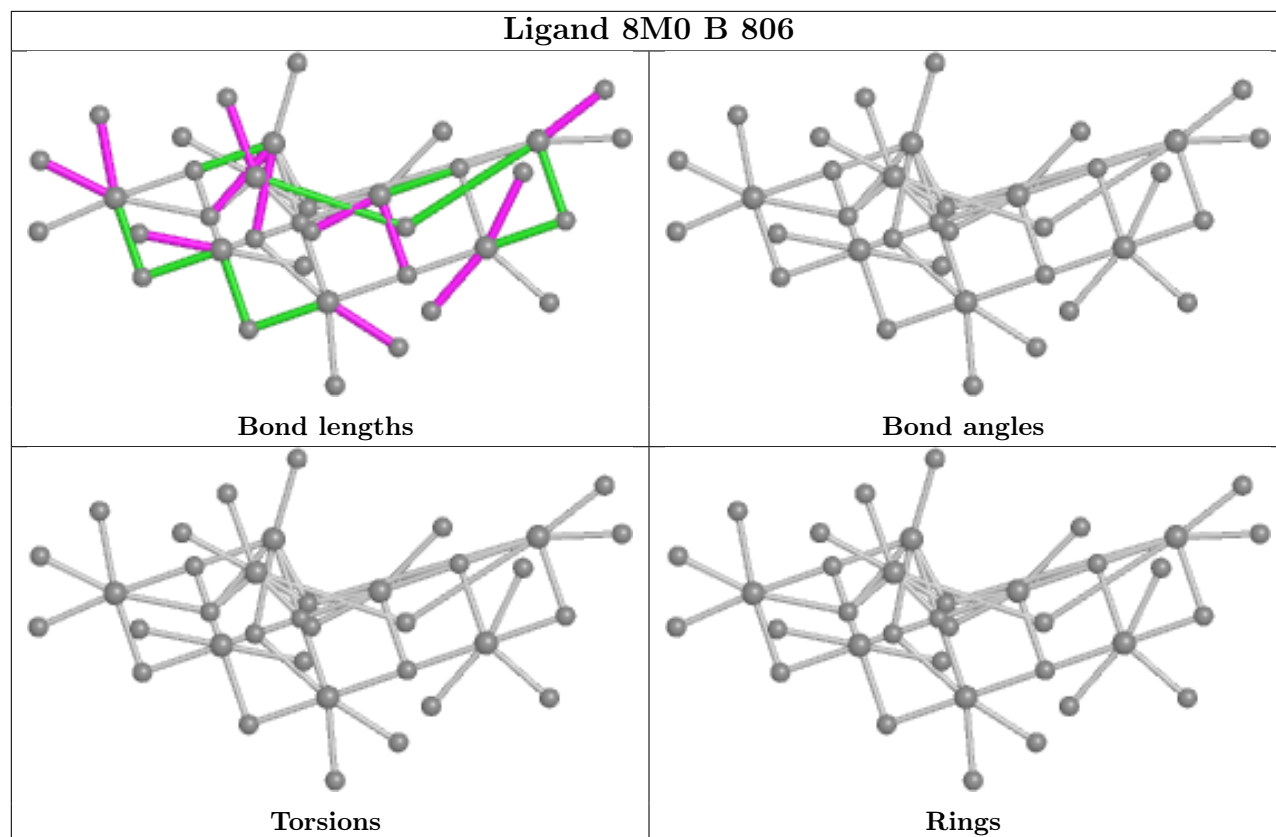
## Ligand 8M0 A 303



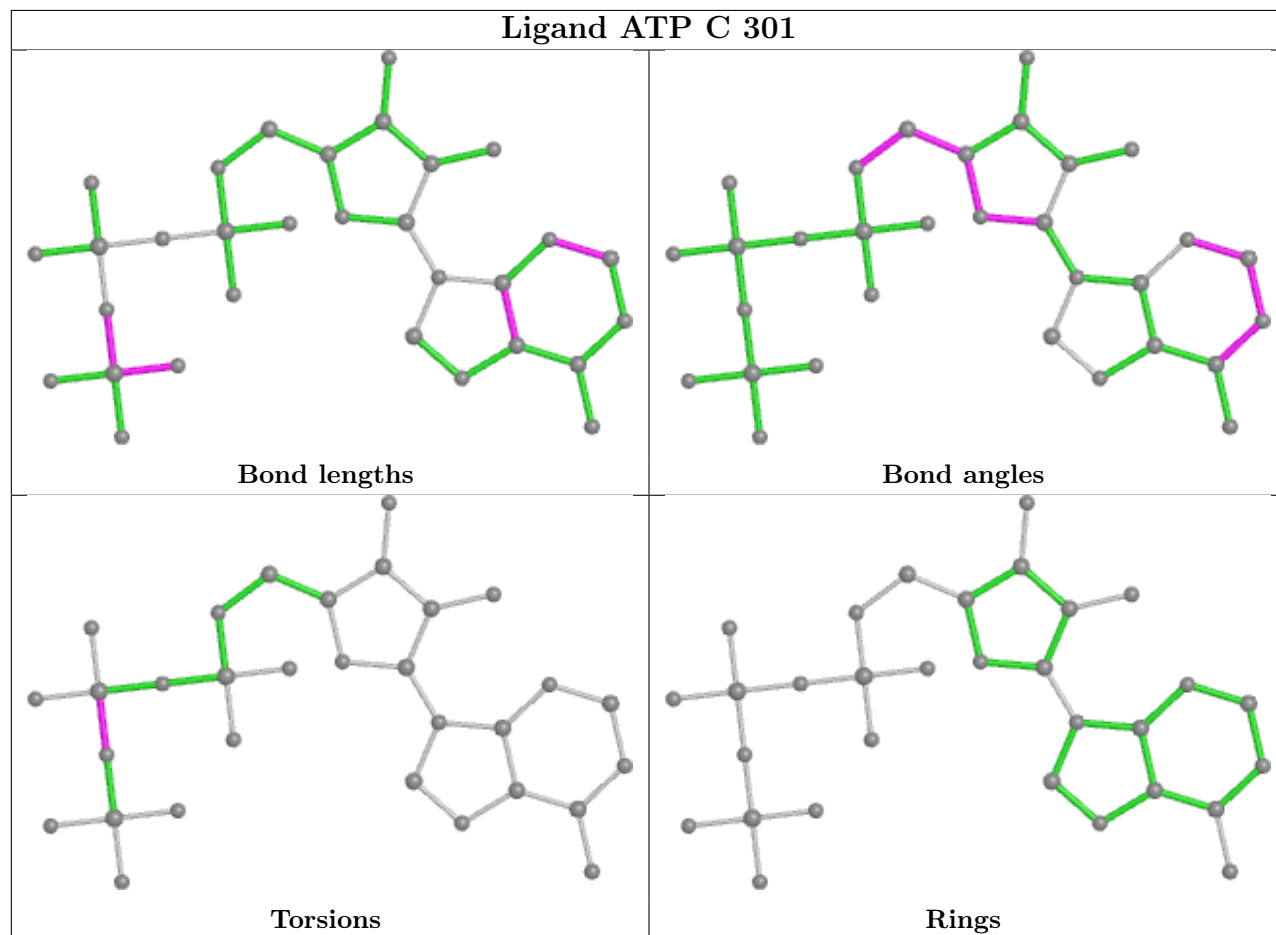
## Ligand ATP B 805



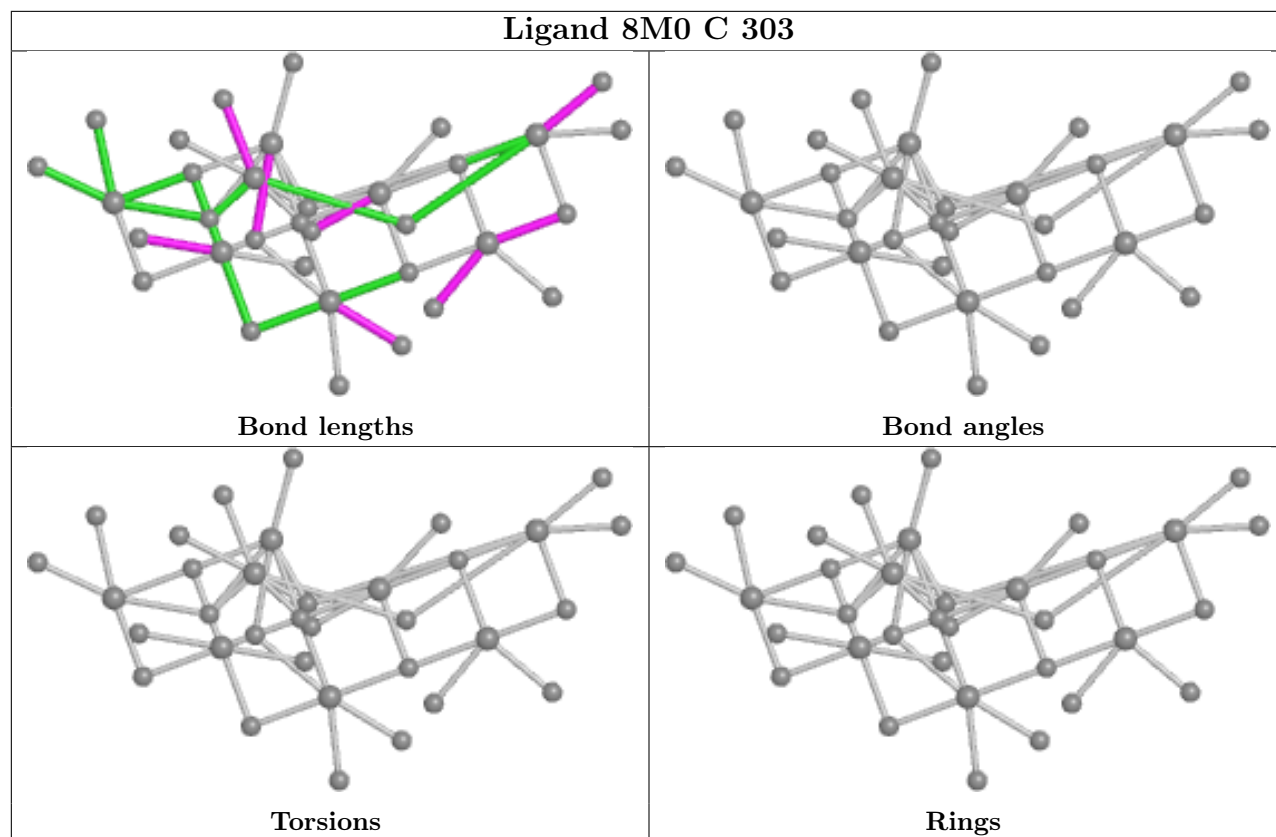
## Ligand 8M0 B 806



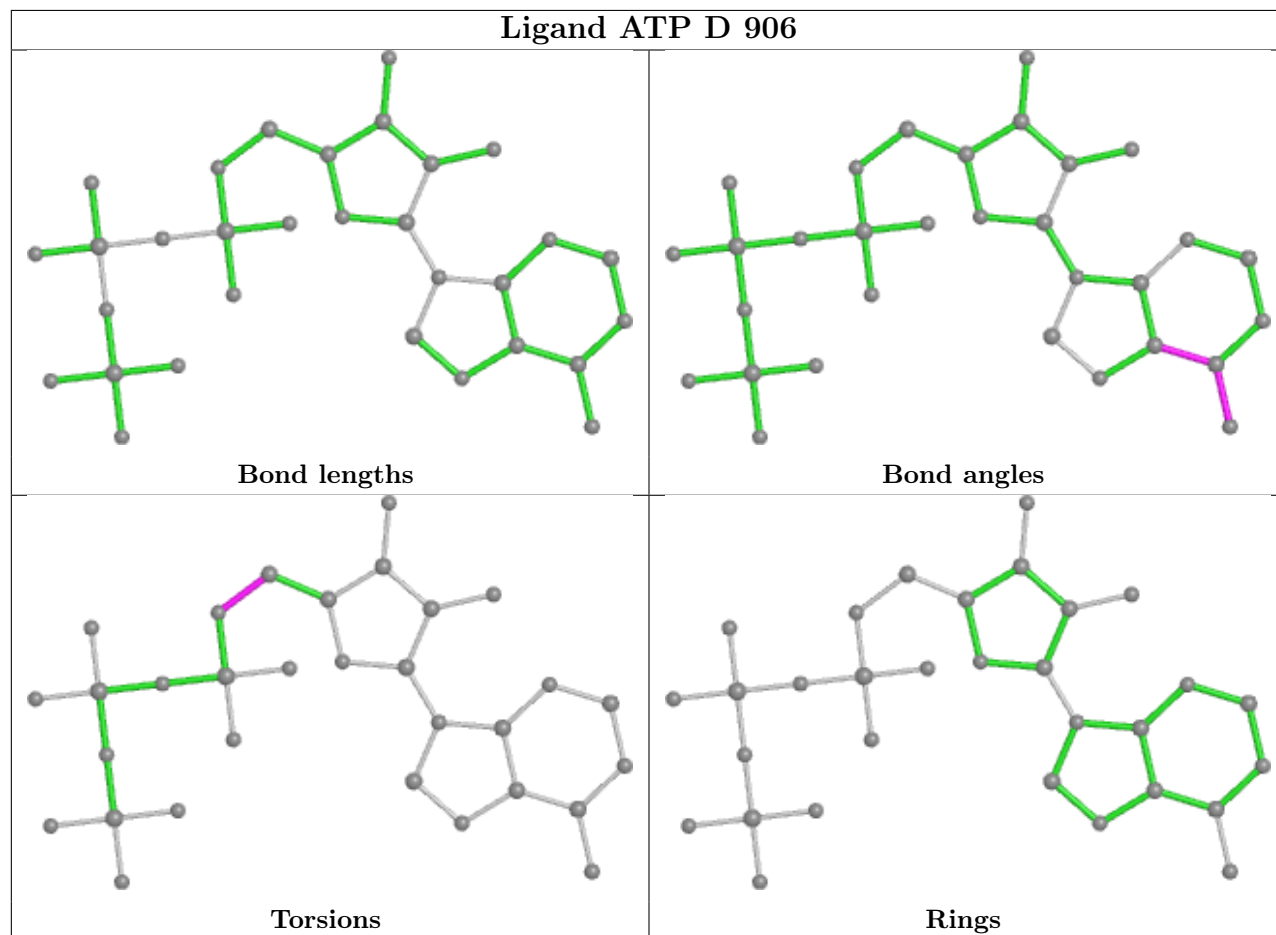
## Ligand ATP C 301



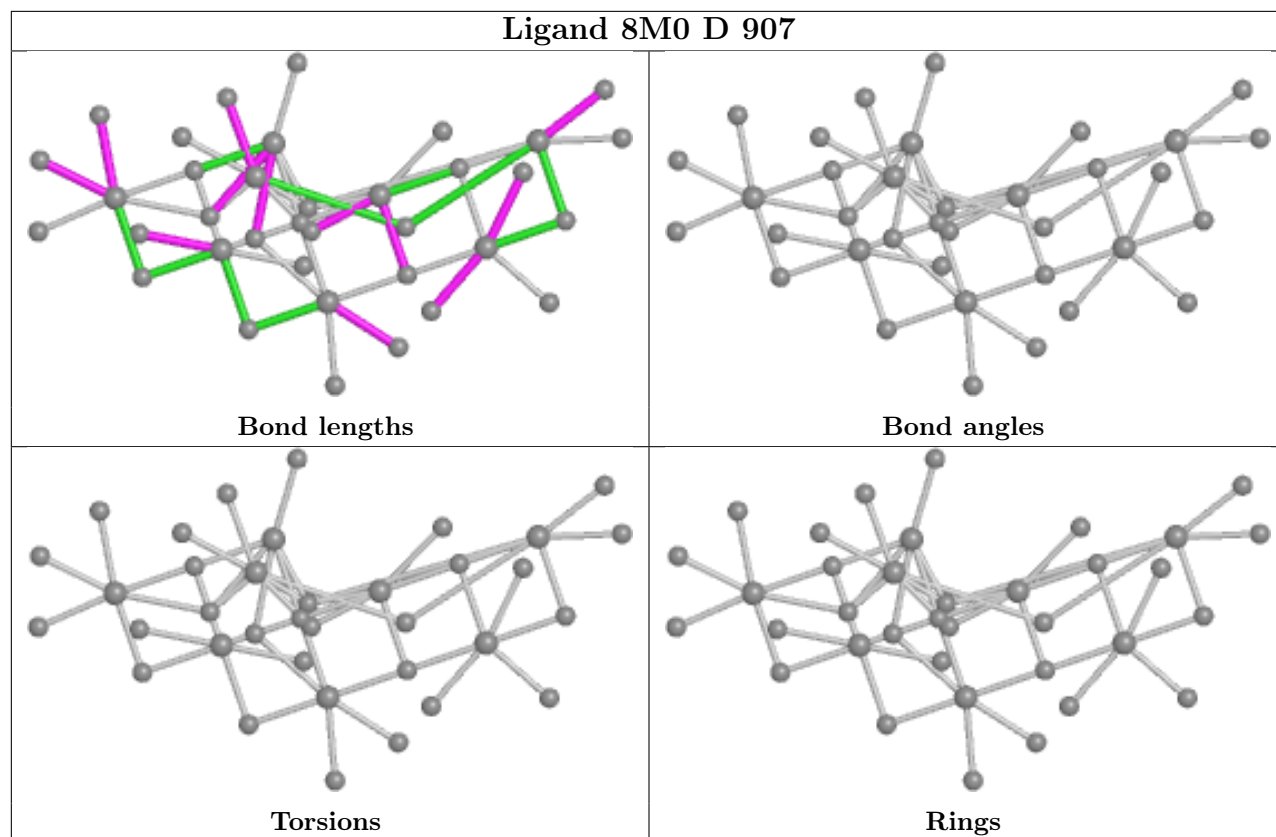
## Ligand 8M0 C 303



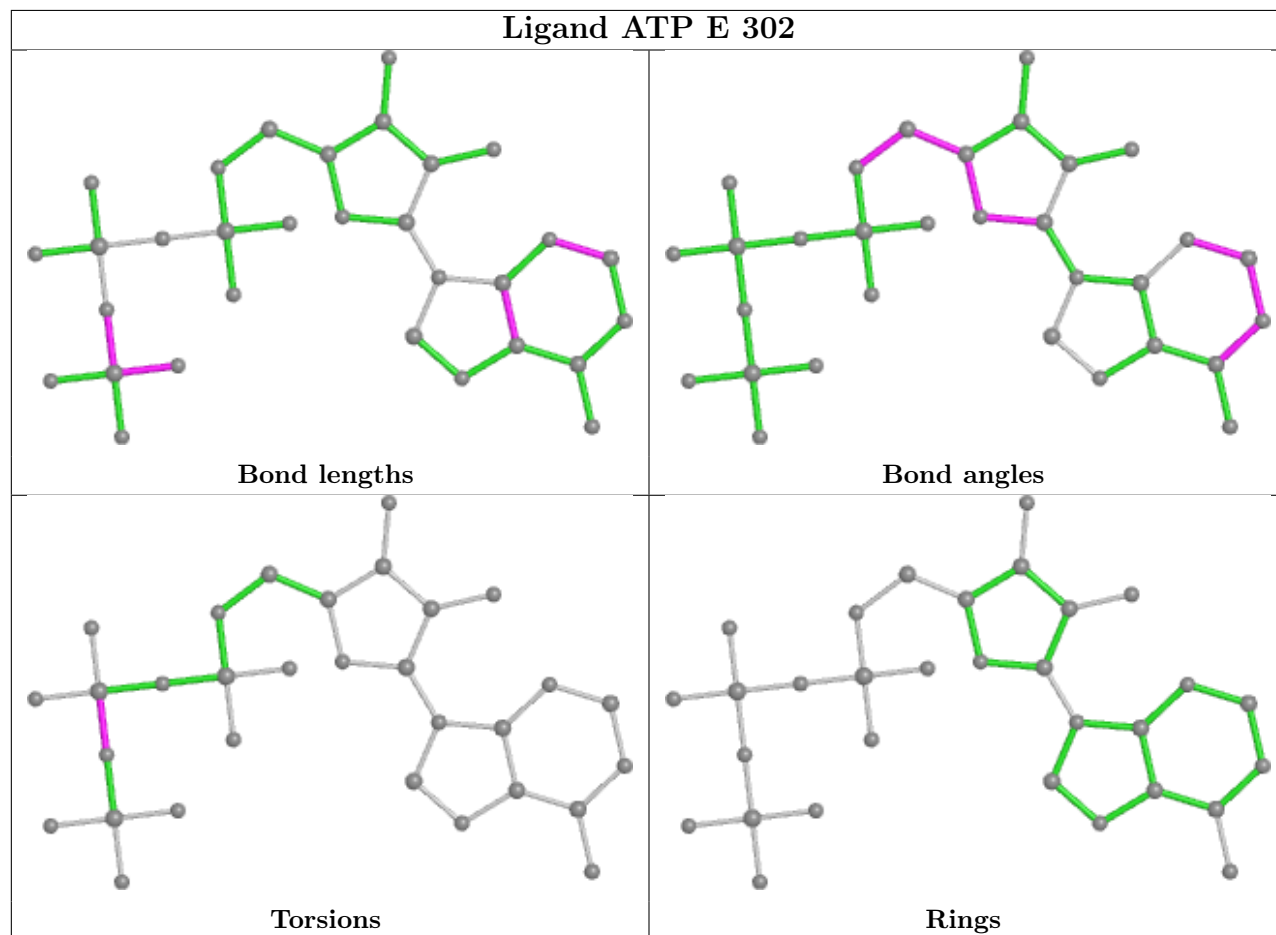
## Ligand ATP D 906



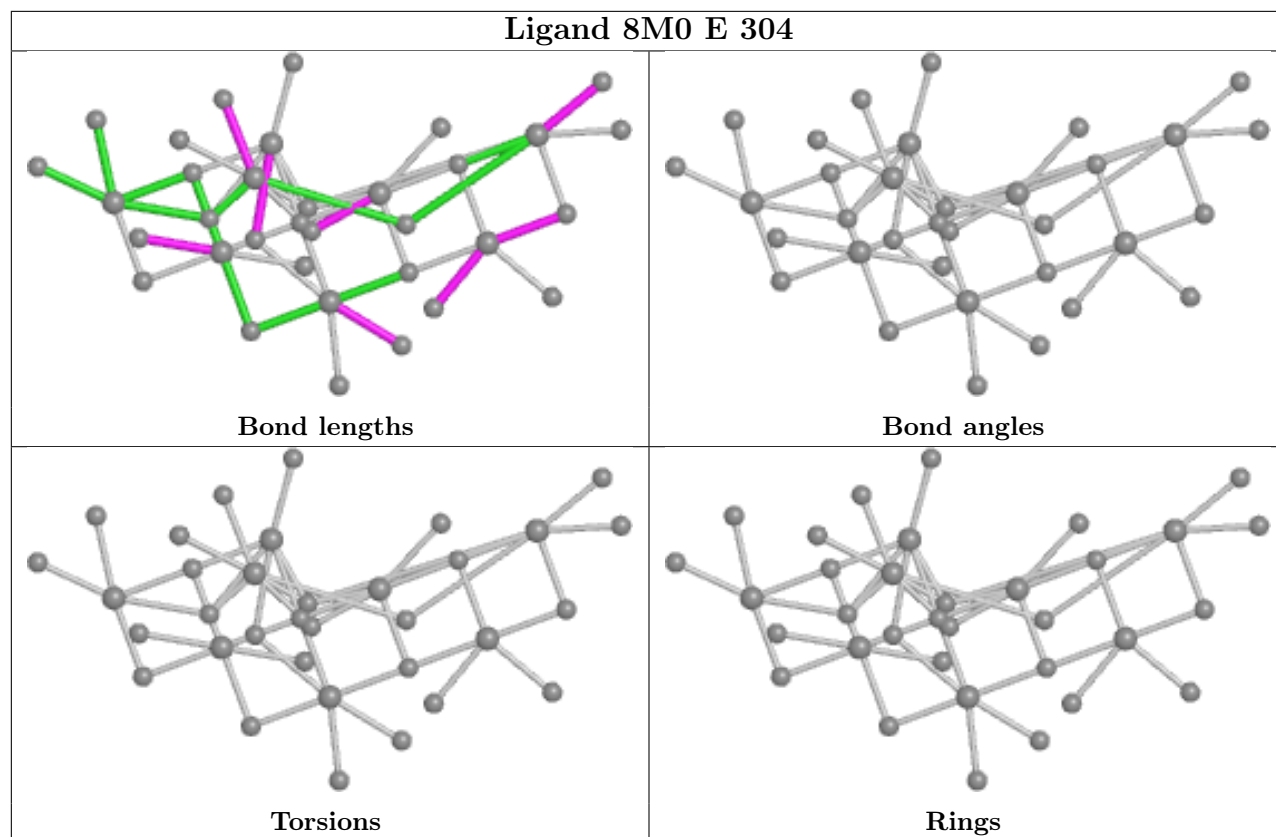
## Ligand 8M0 D 907



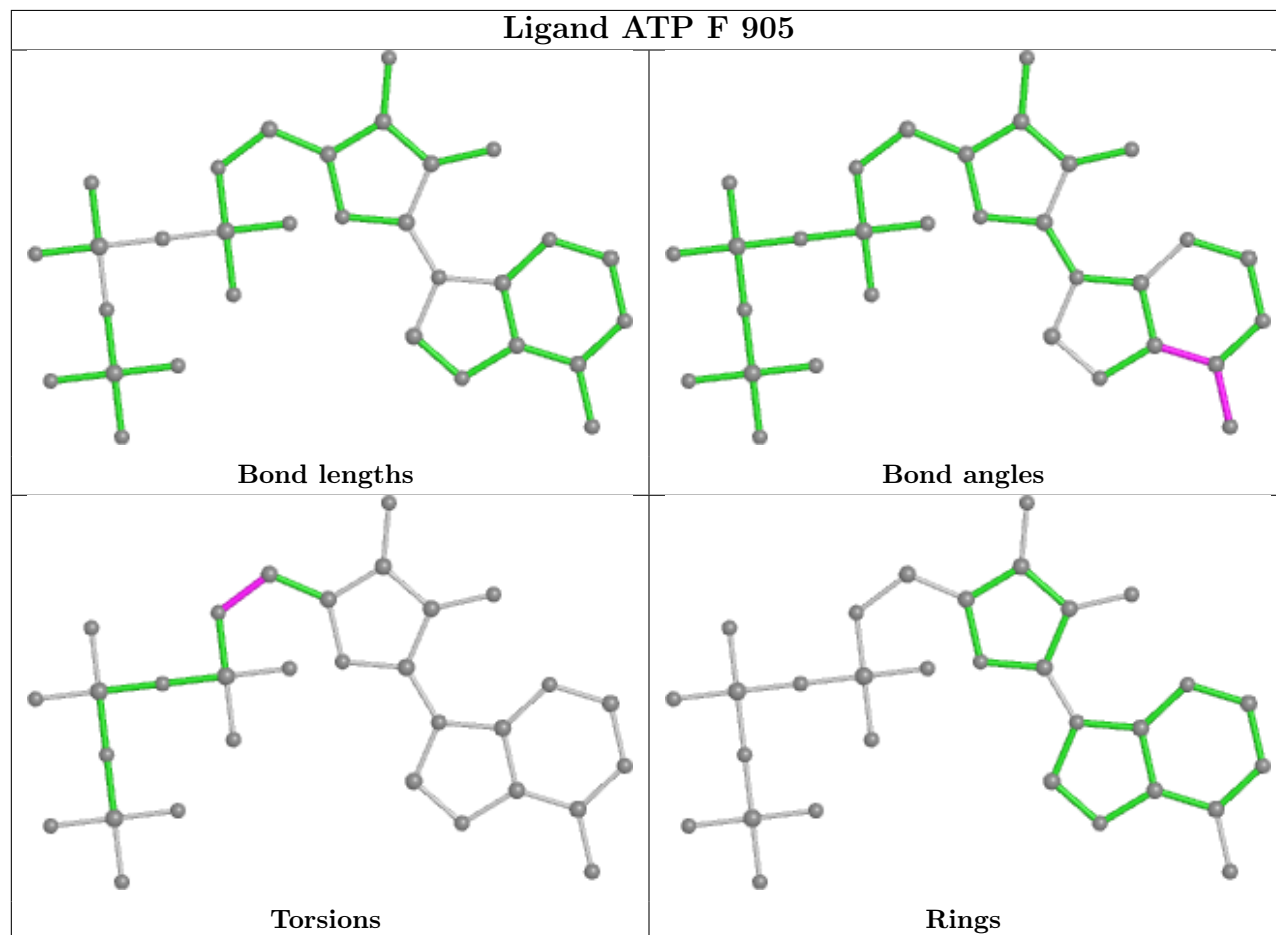
## Ligand ATP E 302



## Ligand 8M0 E 304

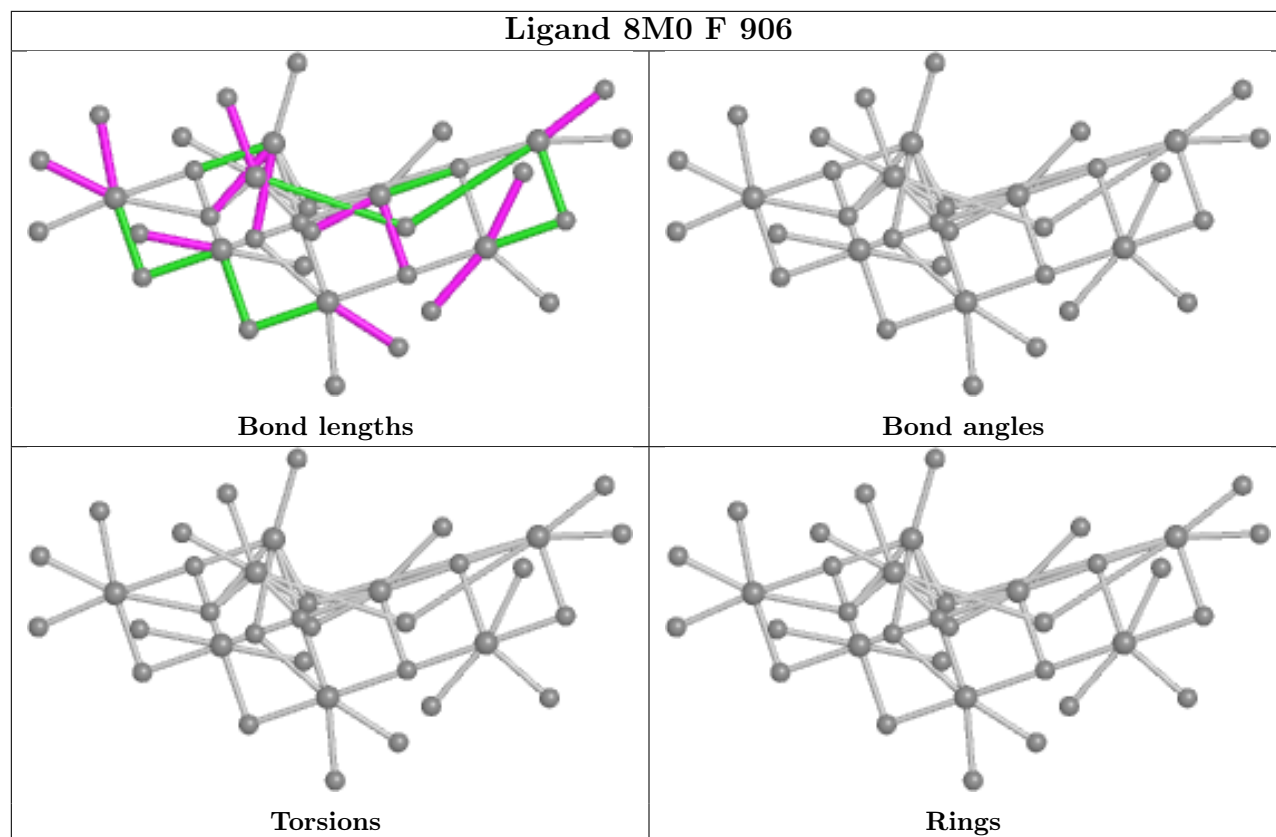


## Ligand ATP F 905

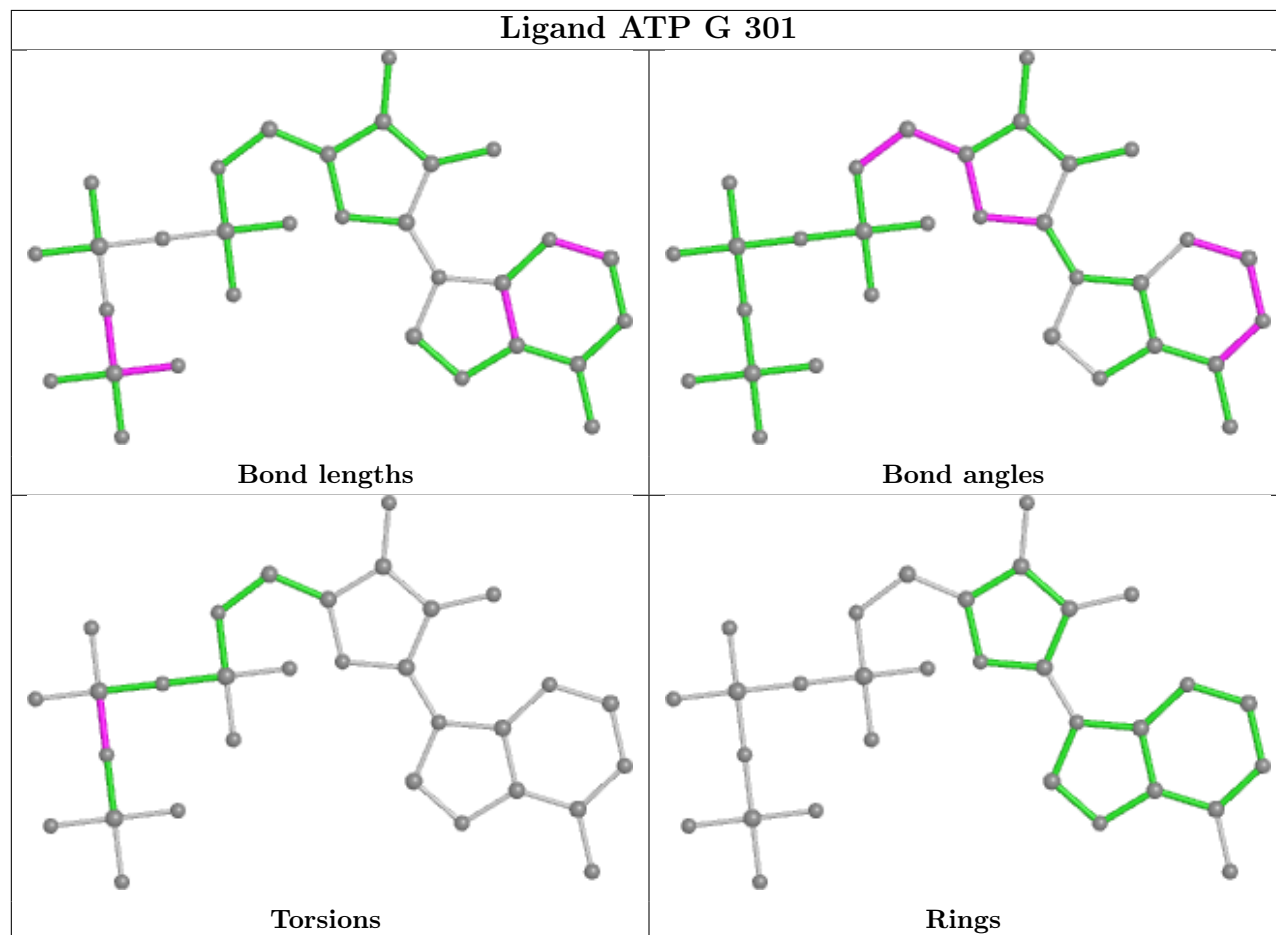




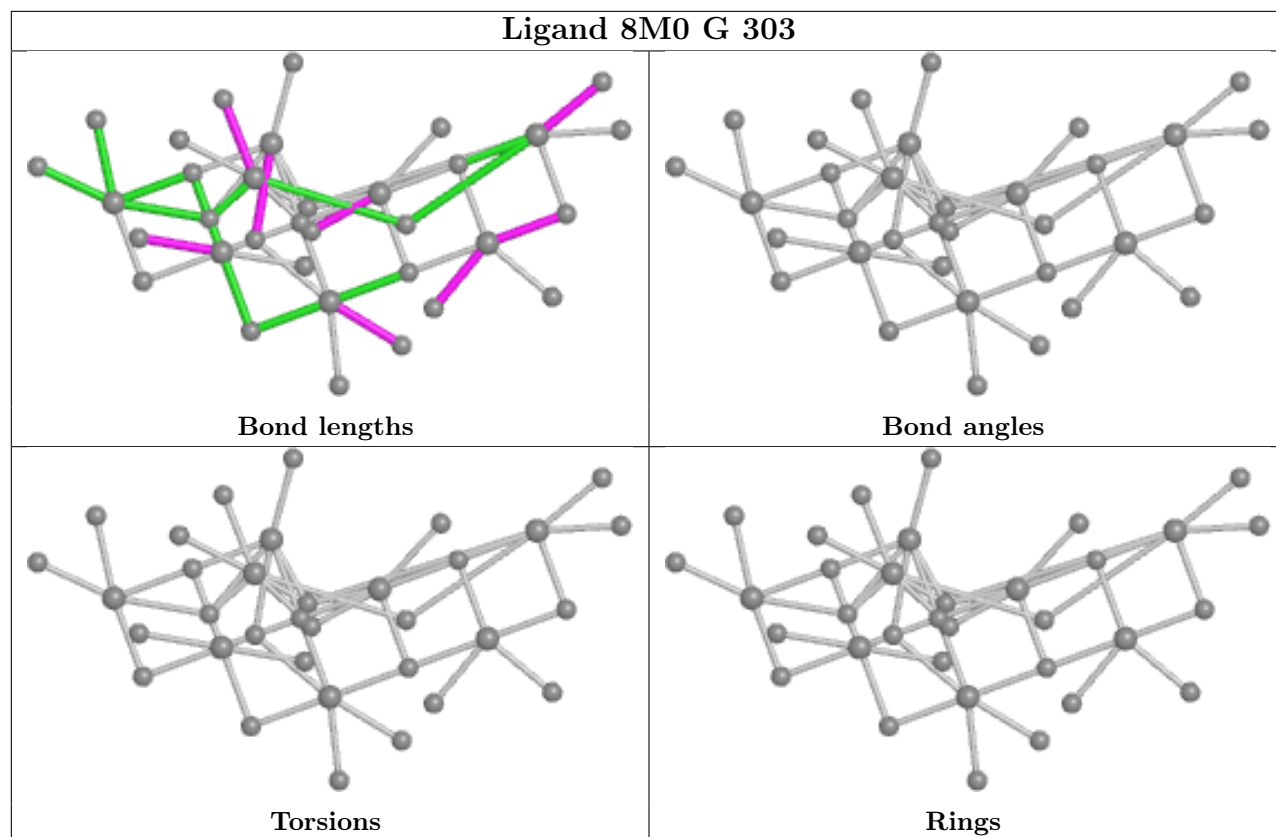
## Ligand 8M0 F 906



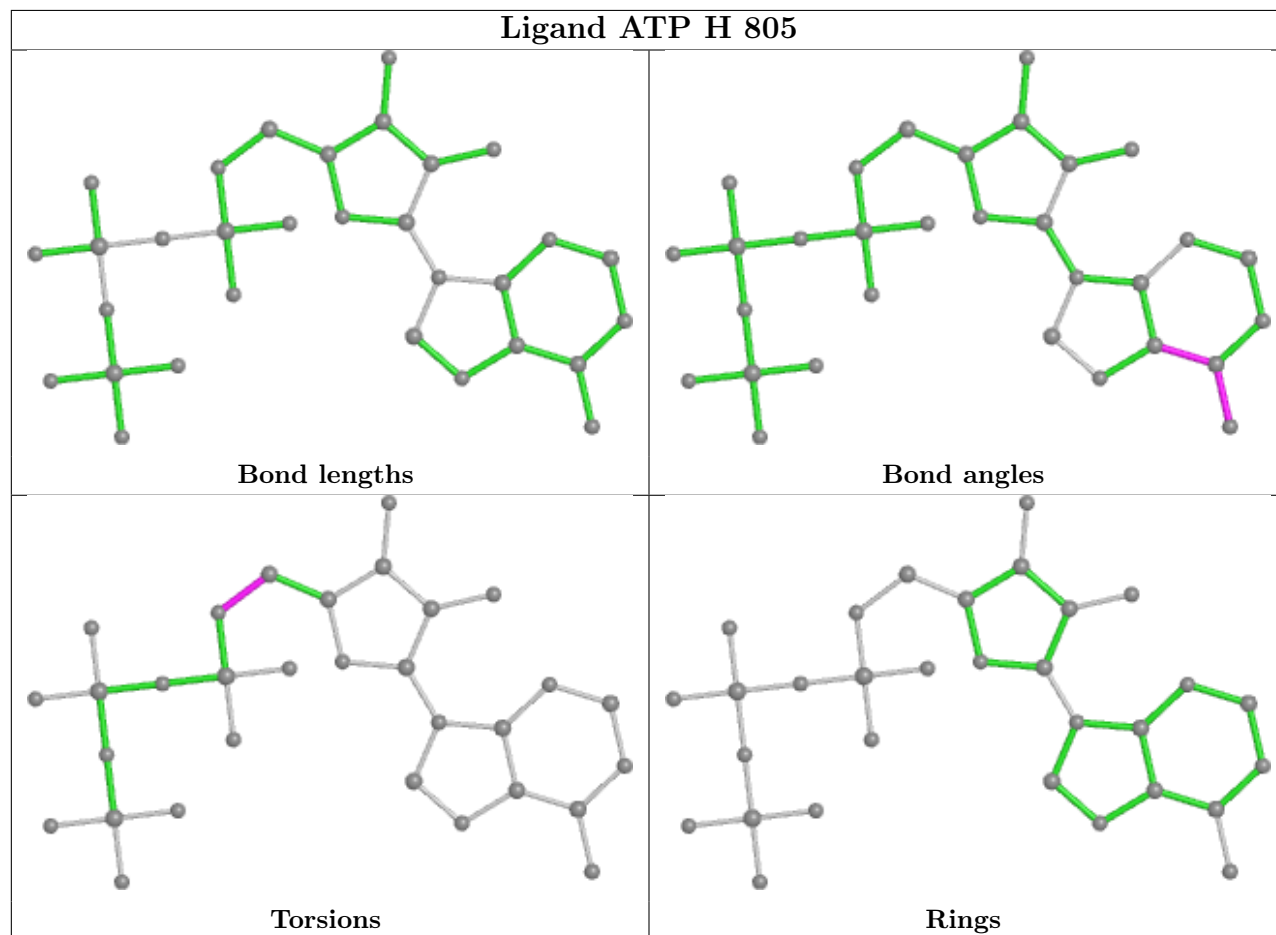
## Ligand ATP G 301



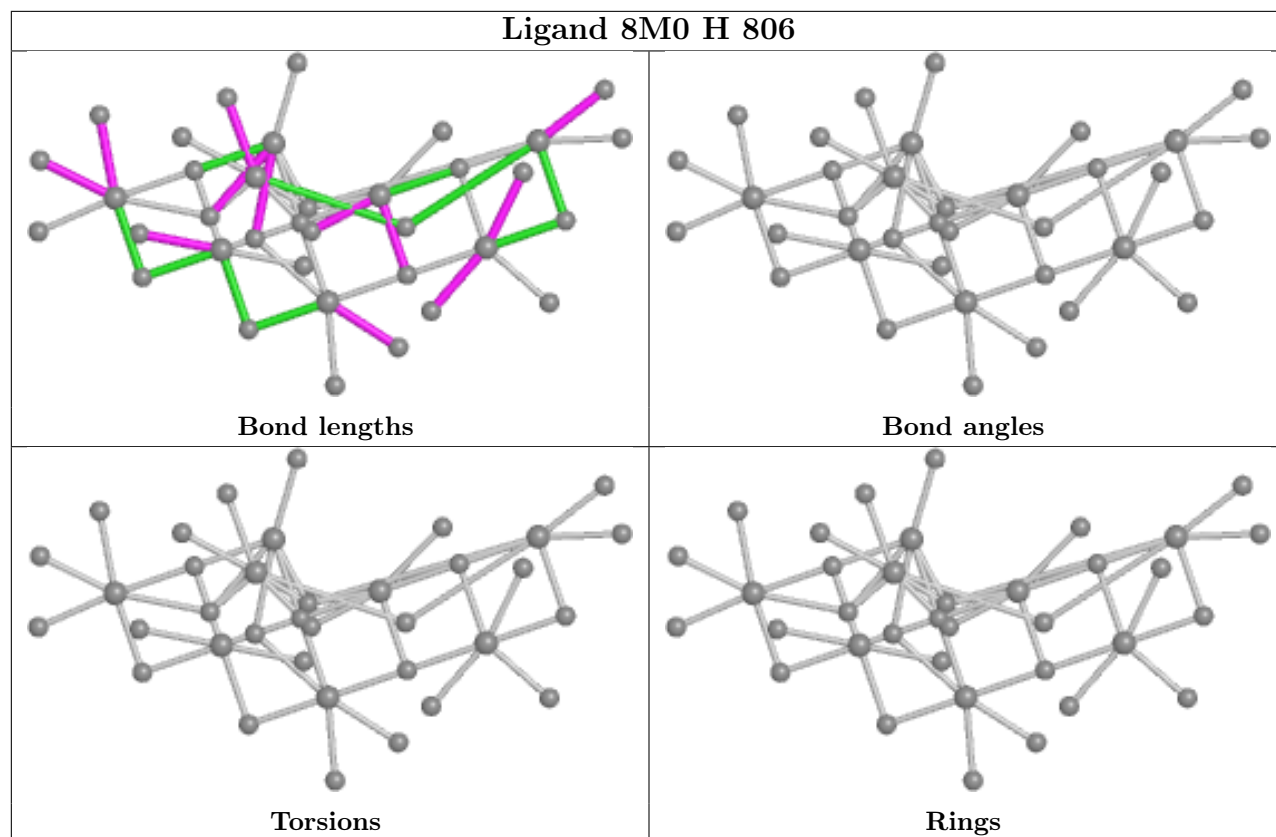
## Ligand 8M0 G 303



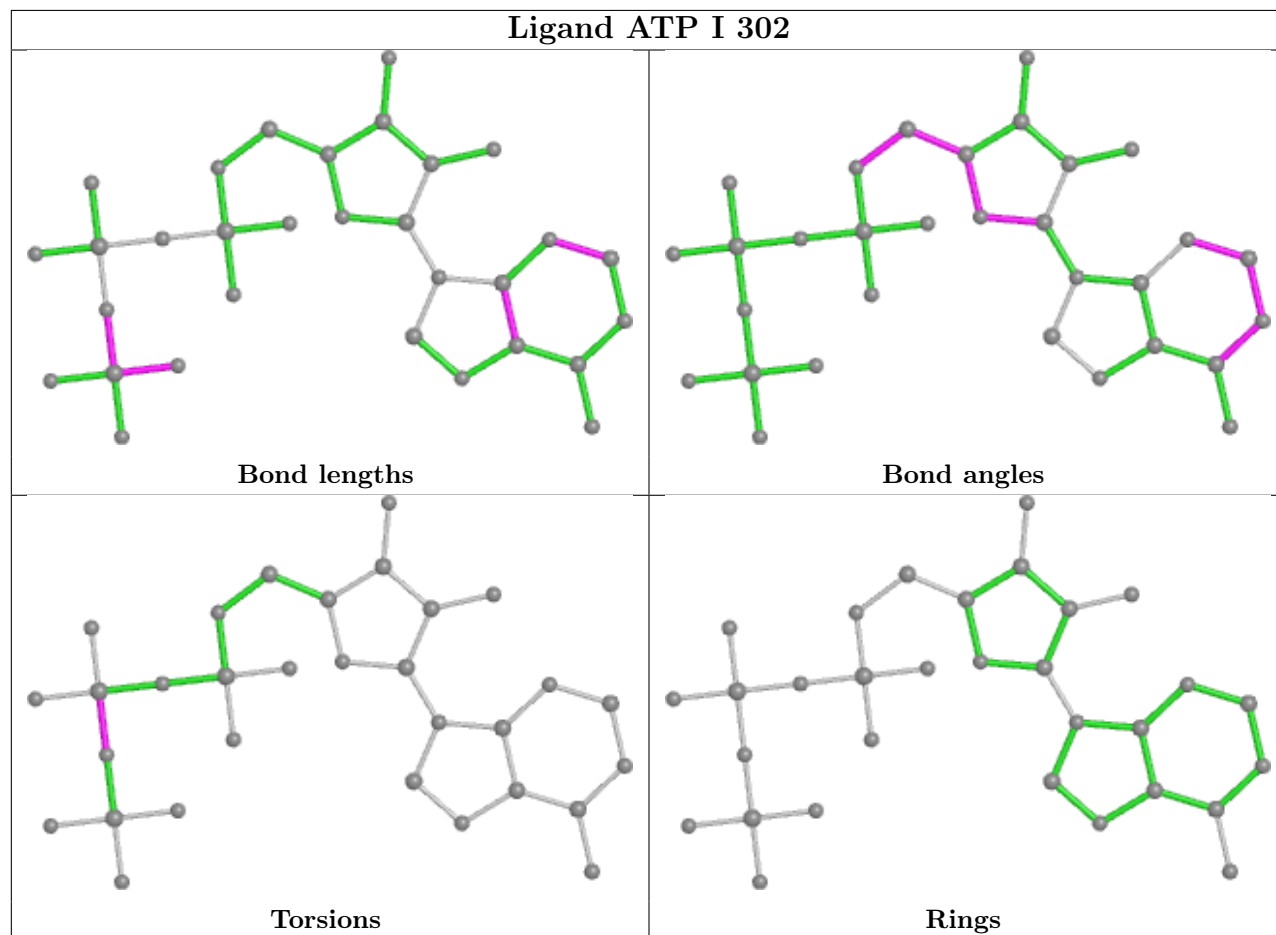
## Ligand ATP H 805



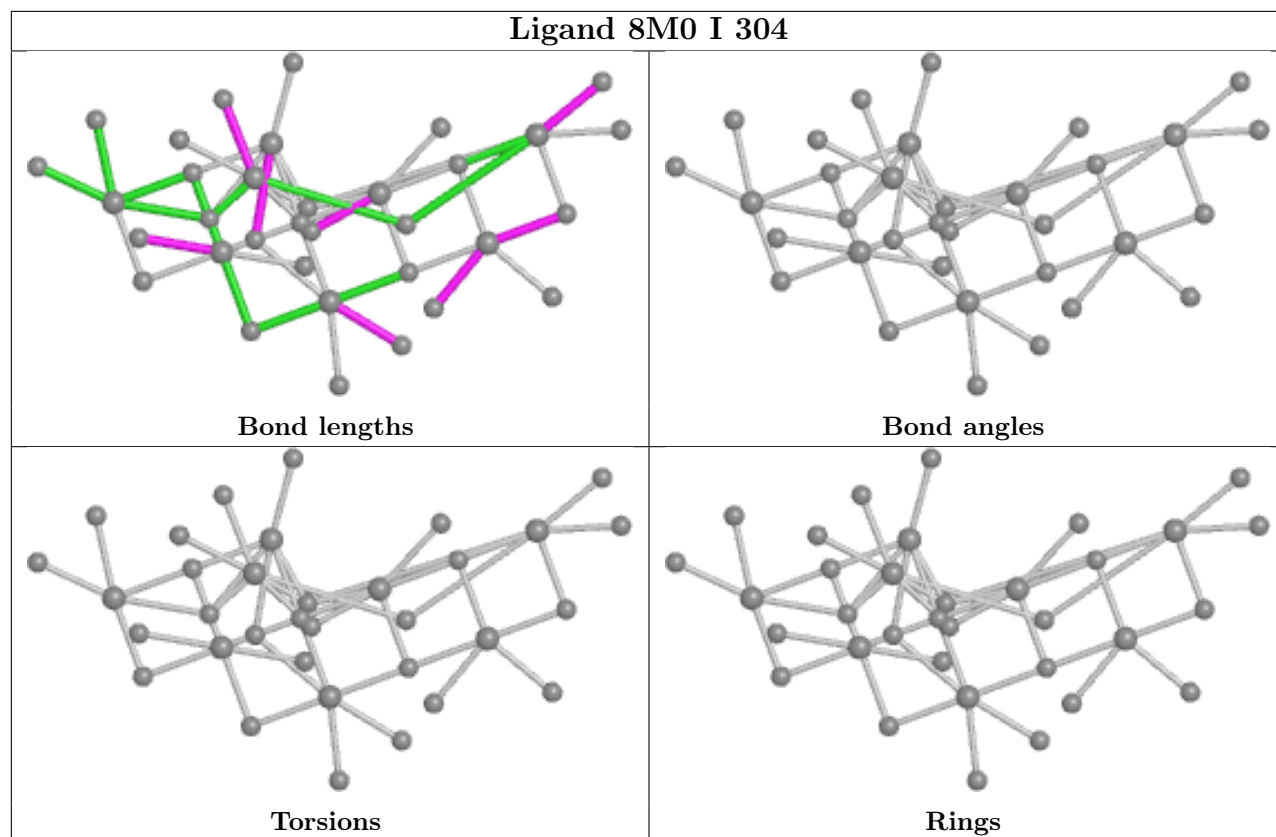
## Ligand 8M0 H 806



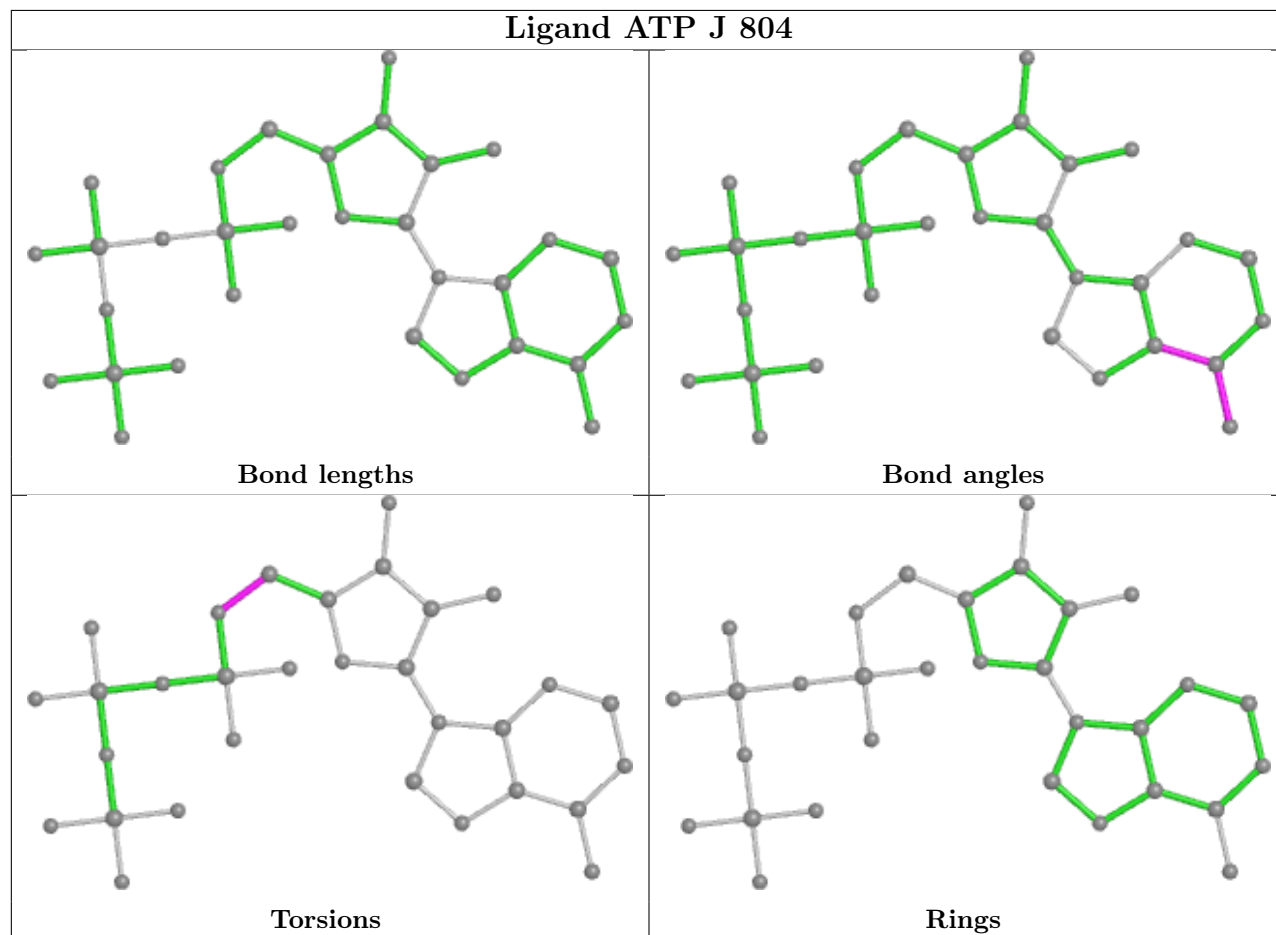
## Ligand ATP I 302



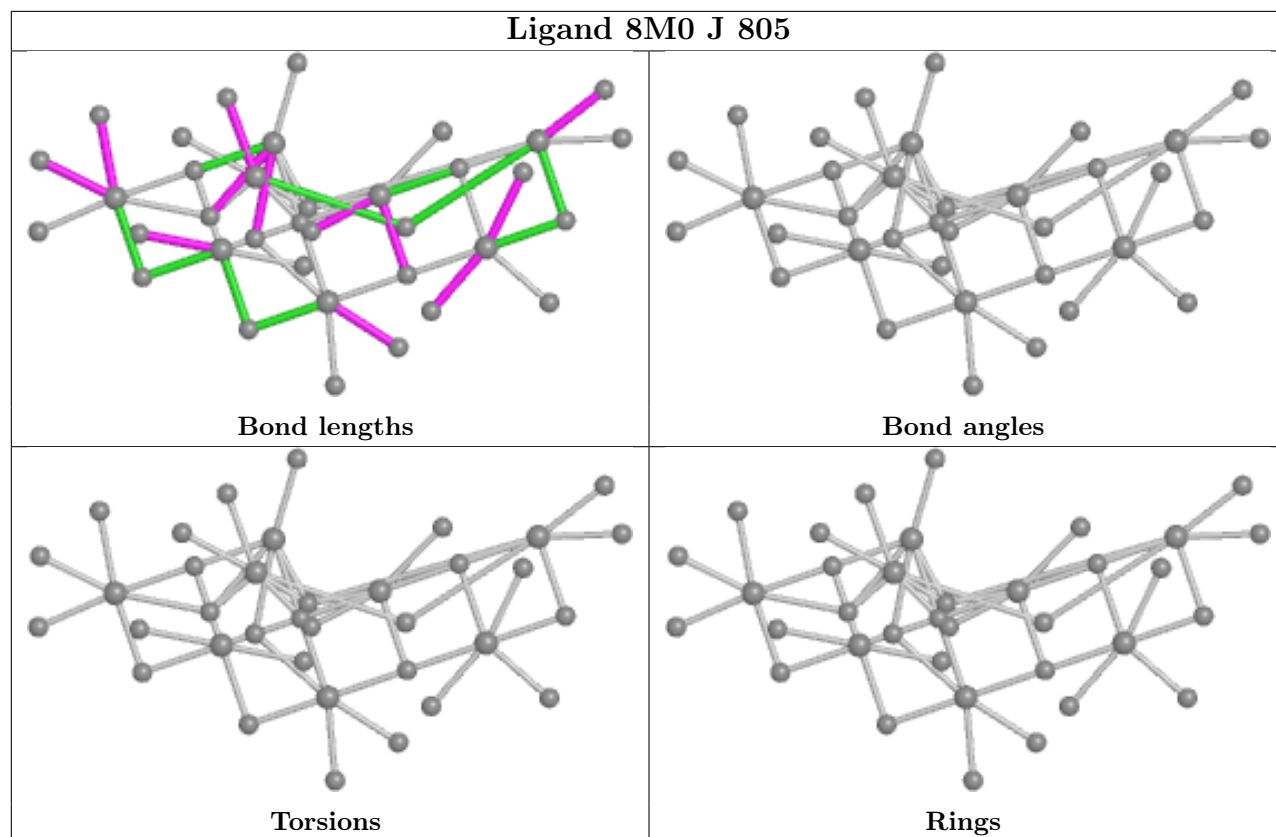
## Ligand 8M0 I 304



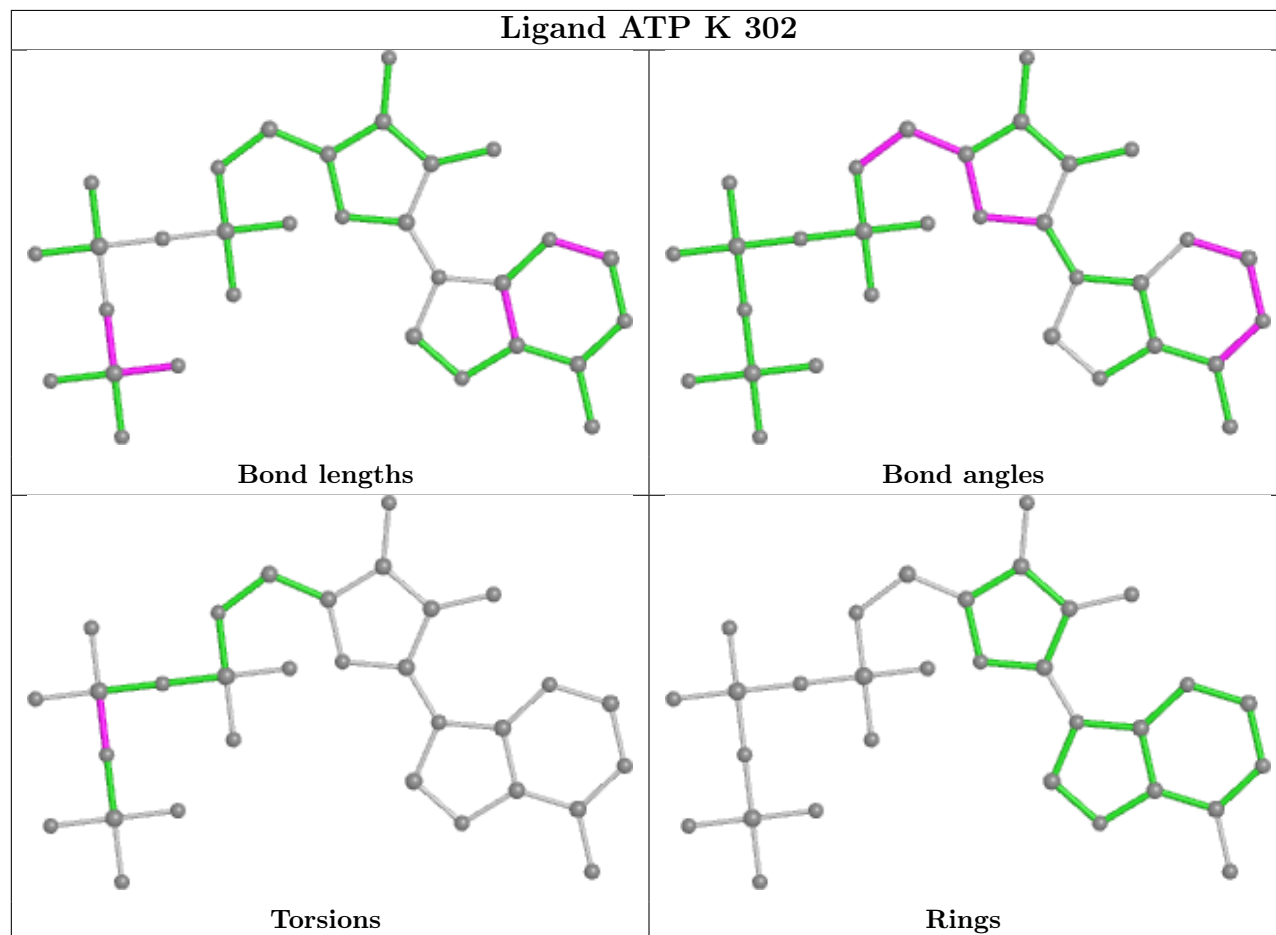
## Ligand ATP J 804



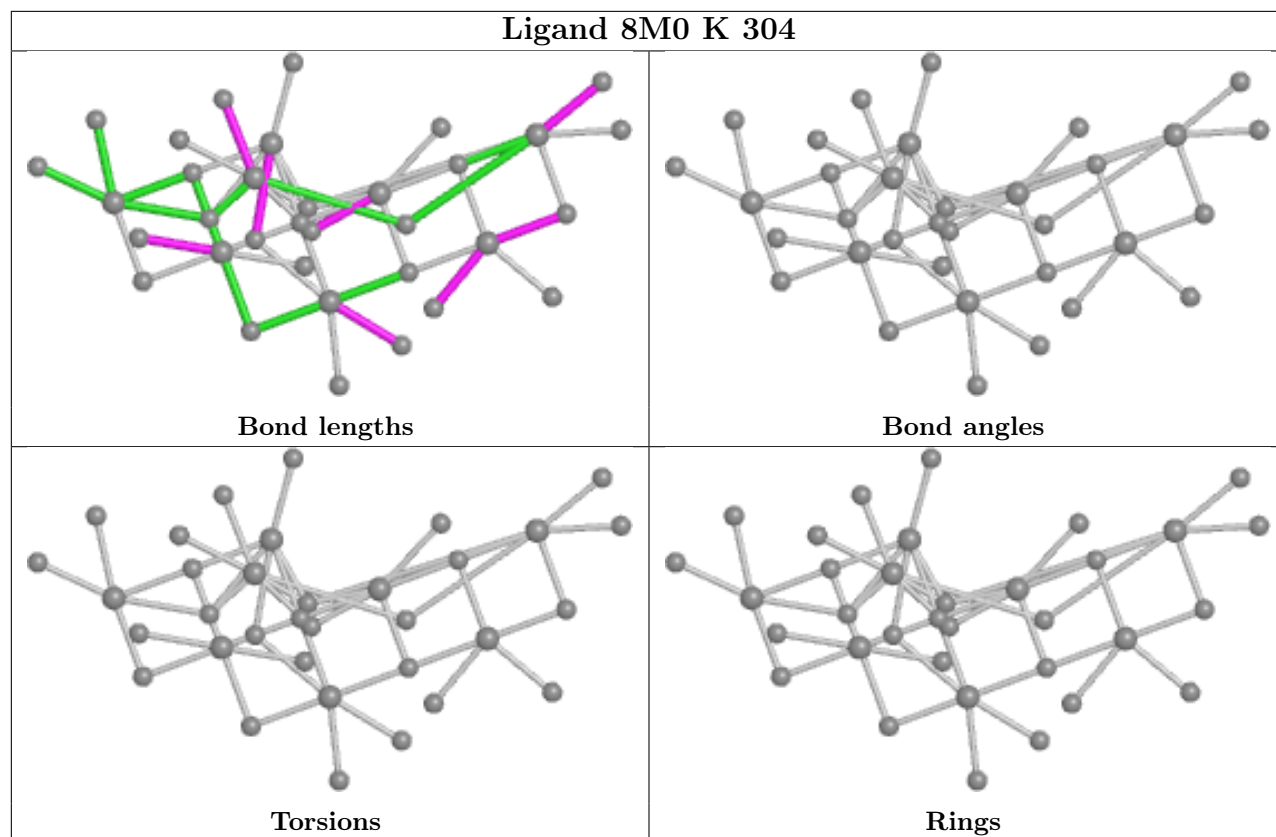
## Ligand 8M0 J 805



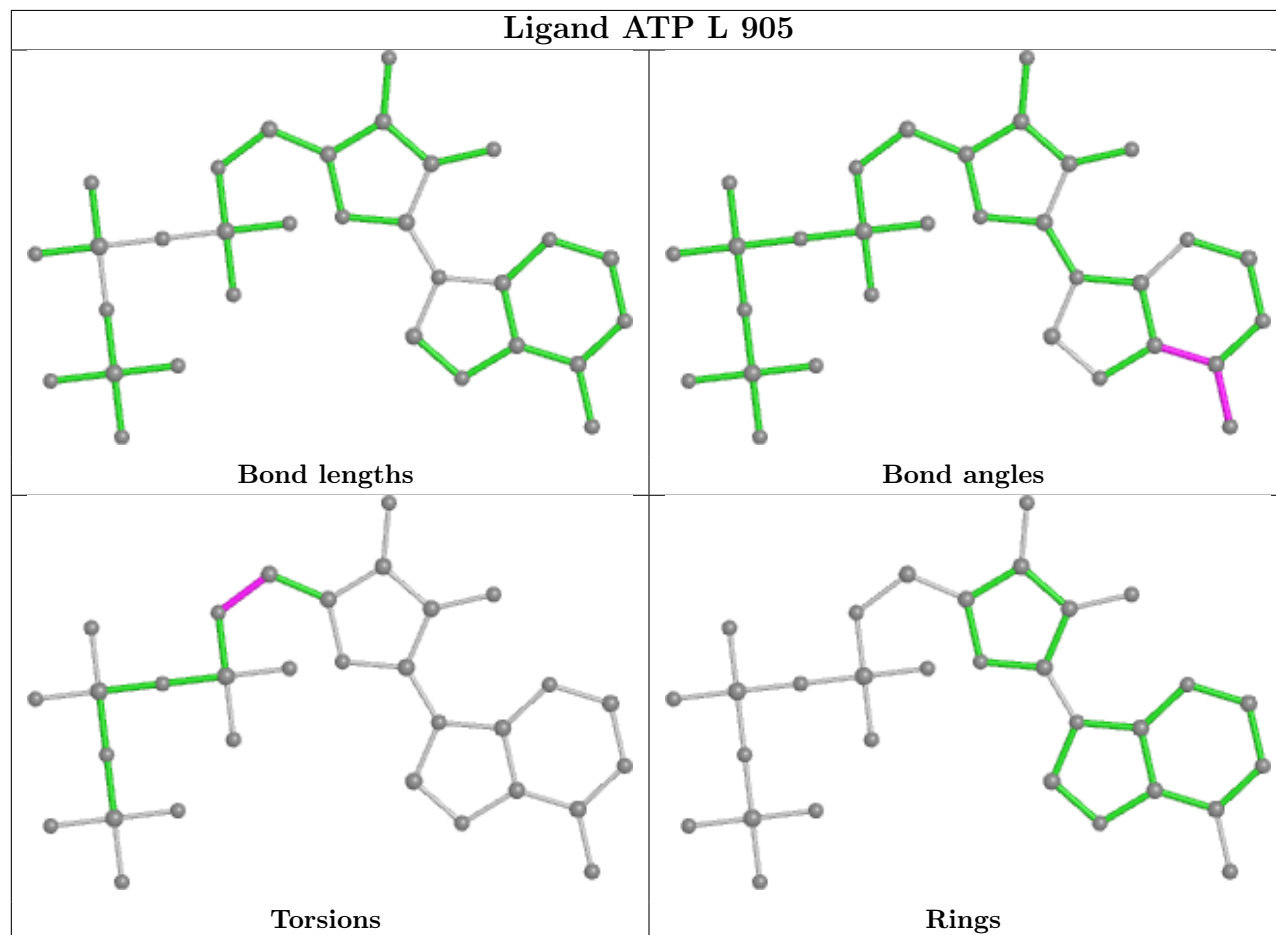
## Ligand ATP K 302

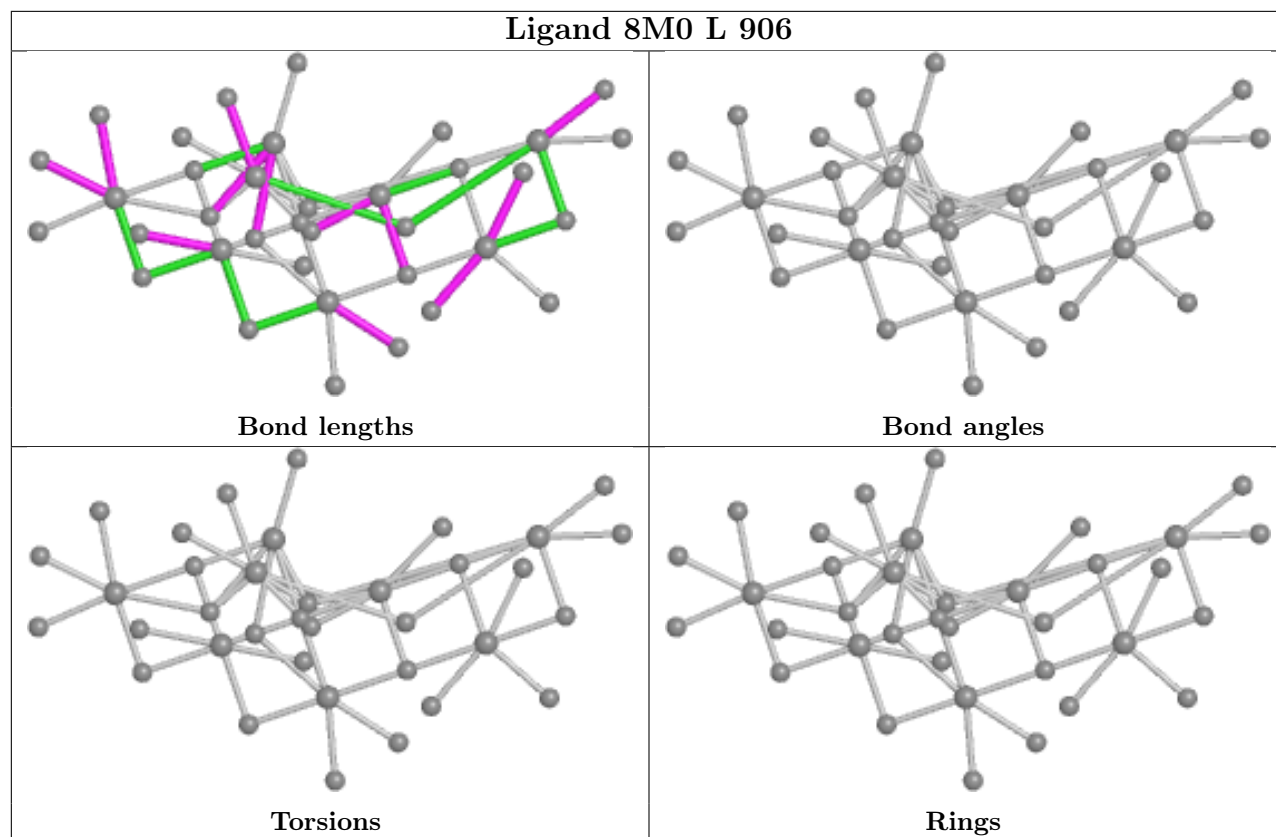


## Ligand 8M0 K 304



## Ligand ATP L 905





## 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.