



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 11:02 pm BST

PDB ID : 1PK8  
Title : Crystal Structure of Rat Synapsin I C Domain Complexed to Ca.ATP  
Authors : Brautigam, C.A.; Chelliah, Y.; Deisenhofer, J.  
Deposited on : 2003-06-05  
Resolution : 2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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



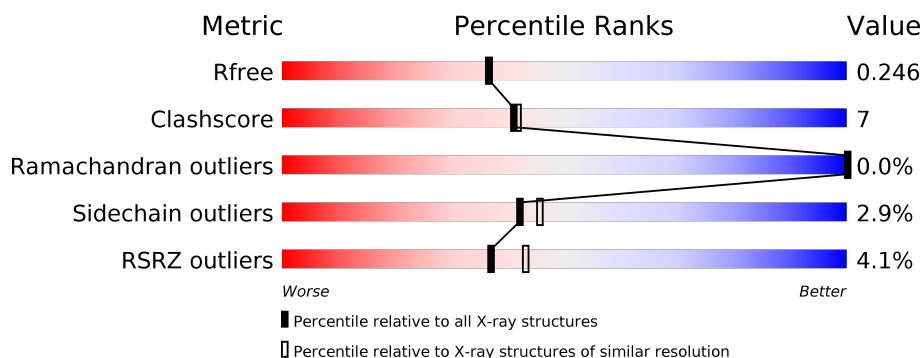
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	422	<div> <div>2%</div> <div> <div></div> <div>61%</div> <div>11%</div> <div>27%</div> </div> </div>
1	B	422	<div> <div>%</div> <div> <div></div> <div>58%</div> <div>11%</div> <div>31%</div> </div> </div>
1	C	422	<div> <div>4%</div> <div> <div></div> <div>54%</div> <div>12%</div> <div>32%</div> </div> </div>
1	D	422	<div> <div>5%</div> <div> <div></div> <div>57%</div> <div>14%</div> <div>29%</div> </div> </div>
1	E	422	<div> <div>2%</div> <div> <div></div> <div>55%</div> <div>12%</div> <div>32%</div> </div> </div>
1	F	422	<div> <div>4%</div> <div> <div></div> <div>55%</div> <div>12%</div> <div>32%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	422	<div><div></div><div>4%</div><div>57%</div><div>12%</div><div>31%</div></div>
1	H	422	<div><div></div><div>%</div><div>54%</div><div>14%</div><div>32%</div></div>



## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19708 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called rat synapsin I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	25	0	0
			2414	1535	417	448	14			
1	B	292	Total	C	N	O	S	8	0	0
			2317	1476	397	430	14			
1	C	285	Total	C	N	O	S	18	0	0
			2272	1451	389	419	13			
1	D	300	Total	C	N	O	S	7	0	0
			2367	1506	406	441	14			
1	E	286	Total	C	N	O	S	40	0	0
			2279	1455	390	421	13			
1	F	286	Total	C	N	O	S	24	0	0
			2279	1455	390	421	13			
1	G	293	Total	C	N	O	S	5	0	0
			2326	1482	399	431	14			
1	H	286	Total	C	N	O	S	25	0	0
			2277	1454	390	420	13			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	CLONING ARTIFACT	UNP P09951
A	1	SER	MET	CLONING ARTIFACT	UNP P09951
B	0	GLY	-	CLONING ARTIFACT	UNP P09951
B	1	SER	MET	CLONING ARTIFACT	UNP P09951
C	0	GLY	-	CLONING ARTIFACT	UNP P09951
C	1	SER	MET	CLONING ARTIFACT	UNP P09951
D	0	GLY	-	CLONING ARTIFACT	UNP P09951
D	1	SER	MET	CLONING ARTIFACT	UNP P09951
E	0	GLY	-	CLONING ARTIFACT	UNP P09951
E	1	SER	MET	CLONING ARTIFACT	UNP P09951
F	0	GLY	-	CLONING ARTIFACT	UNP P09951
F	1	SER	MET	CLONING ARTIFACT	UNP P09951
G	0	GLY	-	CLONING ARTIFACT	UNP P09951

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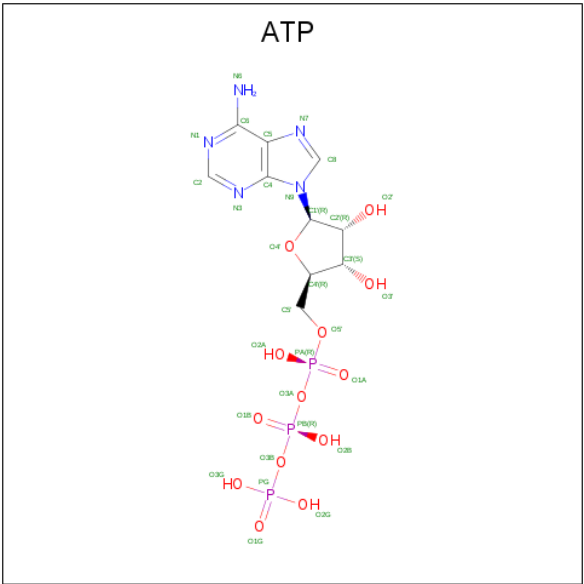
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Chain	Residue	Modelled	Actual	Comment	Reference
G	1	SER	MET	CLONING ARTIFACT	UNP P09951
H	0	GLY	-	CLONING ARTIFACT	UNP P09951
H	1	SER	MET	CLONING ARTIFACT	UNP P09951

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0

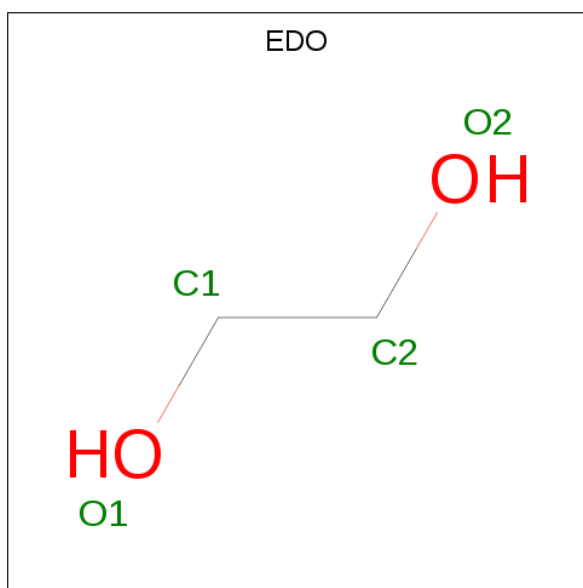
- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			62	20	10	26	6		
3	B	1	Total	C	N	O	P	0	1
			62	20	10	26	6		
3	C	1	Total	C	N	O	P	0	1
			62	20	10	26	6		
3	D	1	Total	C	N	O	P	0	1
			62	20	10	26	6		
3	E	1	Total	C	N	O	P	0	1
			62	20	10	26	6		
3	F	1	Total	C	N	O	P	0	1
			62	20	10	26	6		
3	G	1	Total	C	N	O	P	0	1
			62	20	10	26	6		
3	H	1	Total	C	N	O	P	0	1
			62	20	10	26	6		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.



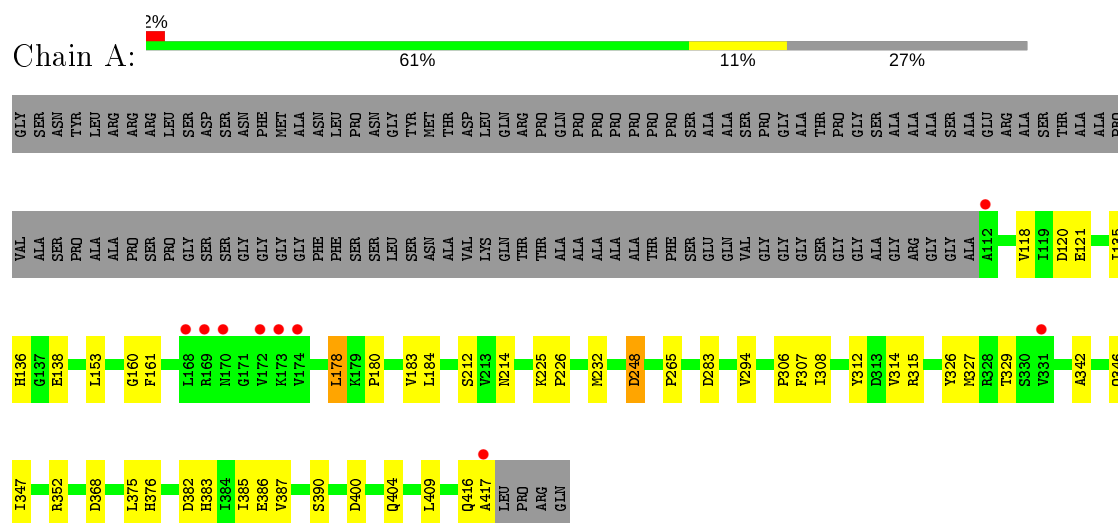
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	117	Total 117	O 117	0	0
5	B	127	Total 127	O 127	0	0
5	C	81	Total 81	O 81	0	0
5	D	77	Total 77	O 77	0	0
5	E	80	Total 80	O 80	0	0
5	F	39	Total 39	O 39	0	0
5	G	68	Total 68	O 68	0	0
5	H	76	Total 76	O 76	0	0



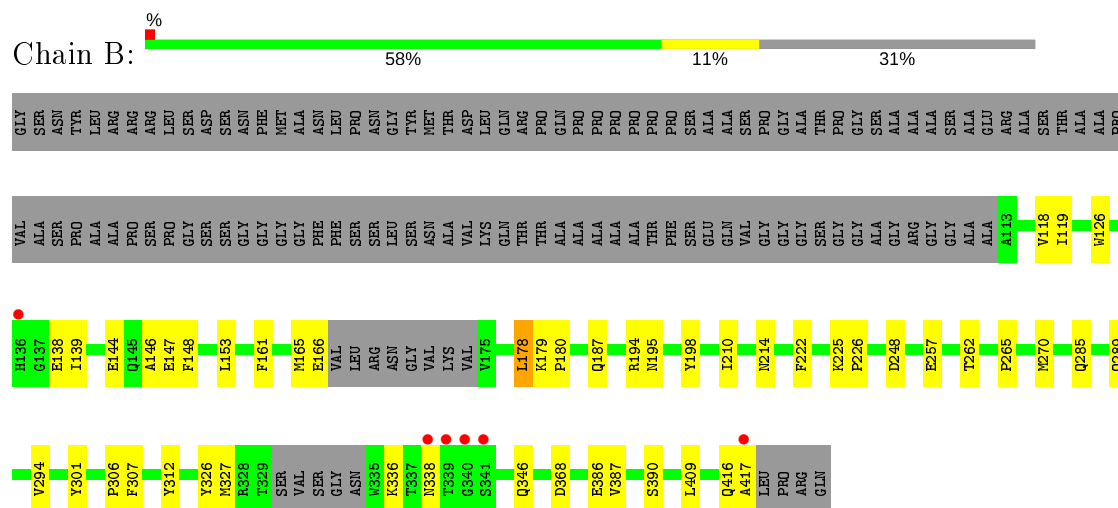
### 3 Residue-property plots

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

#### • Molecule 1: rat synapsin I



#### • Molecule 1: rat synapsin I



#### • Molecule 1: rat synapsin I









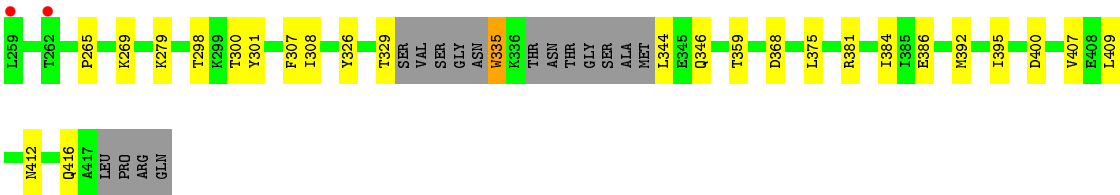
Chain F:

Sequence logo for Chain F. The y-axis represents information content in bits (0.00 to 0.25). The x-axis shows positions 1 to 100. A green bar at the top indicates a 4% overall conservation level. Amino acids are color-coded: yellow for common, green for conserved, orange for highly conserved, and red for critical. Critical residues are marked with red dots above the sequence.

Position	Amino Acid	Information Content (bits)	Conservation Level
1	L405	0.15	Highly Conserved
2	N412	0.10	Conserved
3	Q416	0.15	Highly Conserved
4	A417	0.10	Conserved
5	LEU	0.05	Common
6	PRO	0.05	Common
7	ARG	0.05	Common
8	GLN	0.05	Common
9	V282	0.05	Common
10	Q285	0.05	Common
11	I308	0.05	Common
12	D309	0.05	Common
13	A310	0.05	Common
14	K311	0.05	Common
15	Y312	0.05	Common
16	D313	0.05	Common
17	V314	0.05	Common
18	R315	0.05	Common
19	K318	0.05	Common
20	M327	0.05	Common
21	R328	0.05	Common
22	T329	0.05	Common
23	SER	0.05	Common
24	VAL	0.05	Common
25	SER	0.05	Common
26	GLY	0.05	Common
27	ASN	0.05	Common
28	M335	0.05	Common
29	K336	0.05	Common
30	T337	0.05	Common
31	ASN	0.05	Common
32	THR	0.05	Common
33	GLY	0.05	Common
34	SER	0.05	Common
35	MET	0.05	Common
36	L344	0.05	Common
37	D351	0.05	Common
38	R352	0.05	Common
39	T353	0.05	Common
40	K354	0.05	Common
41	V357	0.05	Common
42	D358	0.05	Common
43	T359	0.05	Common
44	L375	0.05	Common
45	H376	0.05	Common
46	G377	0.05	Common
47	K378	0.05	Common
48	D379	0.05	Common
49	G380	0.05	Common
50	R381	0.05	Common
51	D382	0.05	Common
52	H383	0.05	Common
53	E386	0.05	Common
54	V387	0.05	Common
55	M392	0.05	Common
56	D402	0.05	Common
57	K128	0.10	Conserved
58	Y129	0.05	Common
59	I135	0.05	Common
60	H136	0.05	Common
61	G137	0.05	Common
62	E138	0.05	Common
63	L153	0.05	Common
64	V154	0.05	Common
65	E166	0.05	Common
66	VAL	0.05	Common
67	LEU	0.05	Common
68	ARG	0.05	Common
69	ASN	0.05	Common
70	GLY	0.05	Common
71	VAL	0.05	Common
72	L178	0.05	Common
73	K179	0.05	Common
74	P180	0.05	Common
75	R186	0.05	Common
76	R194	0.05	Common
77	H195	0.05	Common
78	R199	0.05	Common
79	I203	0.05	Common
80	S215	0.05	Common
81	V219	0.05	Common
82	F222	0.05	Common
83	K225	0.05	Common
84	P226	0.05	Common
85	F229	0.05	Common
86	L239	0.05	Common
87	L246	0.05	Common
88	D247	0.05	Common
89	D248	0.05	Common
90	S260	0.05	Common
91	S261	0.05	Common
92	T262	0.05	Common
93	T263	0.05	Common
94	S266	0.05	Common
95	D120	0.05	Common
96	H133	0.10	Conserved
97	R114	0.05	Common
98	V115	0.05	Common
99	H132	0.10	Conserved

[illegible][illegible]







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.60 Å   78.40 Å   135.00 Å 80.60°   76.90°   71.80°	Depositor
Resolution (Å)	20.00 – 2.10 37.16 – 2.09	Depositor EDS
% Data completeness (in resolution range)	91.9 (20.00-2.10) 91.5 (37.16-2.09)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.25 (at 2.10 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.222   ,   0.259 0.210   ,   0.246	Depositor DCC
$R_{free}$ test set	14970 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.7	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 47.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	19708	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.29% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, EDO, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.38	0/2466	0.62	0/3334
1	B	0.39	0/2367	0.64	0/3197
1	C	0.35	0/2321	0.62	0/3133
1	D	0.33	0/2418	0.61	0/3269
1	E	0.34	0/2328	0.60	0/3143
1	F	0.37	0/2328	0.61	0/3143
1	G	0.35	0/2375	0.62	0/3207
1	H	0.35	0/2326	0.60	0/3140
All	All	0.36	0/18929	0.62	0/25566

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2414	0	2397	36	0
1	B	2317	0	2289	33	0
1	C	2272	0	2246	34	0
1	D	2367	0	2341	39	0
1	E	2279	0	2253	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2279	0	2253	29	0
1	G	2326	0	2298	31	0
1	H	2277	0	2251	39	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	62	0	24	1	0
3	B	62	0	24	1	0
3	C	62	0	24	0	0
3	D	62	0	24	2	0
3	E	62	0	24	0	0
3	F	62	0	24	0	0
3	G	62	0	24	0	0
3	H	62	0	24	0	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
5	A	117	0	0	1	0
5	B	127	0	0	2	0
5	C	81	0	0	0	0
5	D	77	0	0	1	0
5	E	80	0	0	2	0
5	F	39	0	0	0	0
5	G	68	0	0	1	0
5	H	76	0	0	1	0
All	All	19708	0	18532	264	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 7.

The worst 5 of 264 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)
1:D:248:ASP:O	1:D:306:PRO:HD3	1.80	0.82
1:E:328:ARG:HD3	1:E:337:THR:HB	1.64	0.78
1:D:407:VAL:O	1:D:411:VAL:HG23	1.94	0.68
1:D:399:GLN:O	1:D:403:LYS:HG3	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:336:LYS:HE2	1:G:290:ASP:OD1	1.94	0.67

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	304/422 (72%)	297 (98%)	7 (2%)	0	100	100
1	B	286/422 (68%)	282 (99%)	4 (1%)	0	100	100
1	C	277/422 (66%)	272 (98%)	5 (2%)	0	100	100
1	D	296/422 (70%)	288 (97%)	7 (2%)	1 (0%)	41	41
1	E	278/422 (66%)	271 (98%)	7 (2%)	0	100	100
1	F	278/422 (66%)	270 (97%)	8 (3%)	0	100	100
1	G	285/422 (68%)	279 (98%)	6 (2%)	0	100	100
1	H	278/422 (66%)	271 (98%)	7 (2%)	0	100	100
All	All	2282/3376 (68%)	2230 (98%)	51 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	337	THR

### 5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was



analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	263/340 (77%)	260 (99%)	3 (1%)	73	79
1	B	252/340 (74%)	248 (98%)	4 (2%)	62	69
1	C	247/340 (73%)	238 (96%)	9 (4%)	35	36
1	D	258/340 (76%)	248 (96%)	10 (4%)	32	33
1	E	248/340 (73%)	241 (97%)	7 (3%)	43	47
1	F	248/340 (73%)	241 (97%)	7 (3%)	43	47
1	G	253/340 (74%)	243 (96%)	10 (4%)	31	32
1	H	247/340 (73%)	239 (97%)	8 (3%)	39	41
All	All	2016/2720 (74%)	1958 (97%)	58 (3%)	42	46

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	114	ARG
1	E	266	VAL
1	H	248	ASP
1	E	123	HIS
1	E	178	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	195	ASN
1	E	195	ASN
1	G	195	ASN
1	C	255	HIS
1	G	334	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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



## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 8 are monoatomic - leaving 18 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	D	803[B]	2	26,33,33	0.80	0	31,52,52	0.98	3 (9%)
3	ATP	F	805[A]	2	26,33,33	0.80	0	31,52,52	0.97	3 (9%)
3	ATP	B	801[A]	2	26,33,33	0.79	0	31,52,52	0.98	3 (9%)
3	ATP	F	805[B]	2	26,33,33	0.82	0	31,52,52	0.99	4 (12%)
3	ATP	C	802[B]	2	26,33,33	0.80	0	31,52,52	0.98	4 (12%)
4	EDO	A	818	-	3,3,3	0.91	0	2,2,2	0.41	0
3	ATP	G	806[A]	2	26,33,33	0.81	0	31,52,52	0.97	3 (9%)
3	ATP	B	801[B]	2	26,33,33	0.79	0	31,52,52	0.99	4 (12%)
3	ATP	H	807[A]	2	26,33,33	0.78	0	31,52,52	0.98	4 (12%)
4	EDO	B	819	-	3,3,3	0.63	0	2,2,2	0.43	0
3	ATP	G	806[B]	2	26,33,33	0.80	0	31,52,52	0.99	3 (9%)
3	ATP	C	802[A]	2	26,33,33	0.77	0	31,52,52	1.00	4 (12%)
3	ATP	A	800[A]	2	26,33,33	0.78	0	31,52,52	0.98	2 (6%)
3	ATP	E	804[B]	2	26,33,33	0.80	0	31,52,52	0.97	3 (9%)
3	ATP	D	803[A]	2	26,33,33	0.77	0	31,52,52	0.98	3 (9%)
3	ATP	H	807[B]	2	26,33,33	0.80	0	31,52,52	0.97	4 (12%)
3	ATP	E	804[A]	2	26,33,33	0.83	0	31,52,52	1.01	4 (12%)
3	ATP	A	800[B]	2	26,33,33	0.84	0	31,52,52	0.98	2 (6%)

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	D	803[B]	2	-	4/18/38/38	0/3/3/3
3	ATP	F	805[A]	2	-	0/18/38/38	0/3/3/3
3	ATP	B	801[A]	2	-	0/18/38/38	0/3/3/3
3	ATP	F	805[B]	2	-	3/18/38/38	0/3/3/3
3	ATP	C	802[B]	2	-	1/18/38/38	0/3/3/3
4	EDO	A	818	-	-	0/1/1/1	-
3	ATP	G	806[A]	2	-	0/18/38/38	0/3/3/3
3	ATP	B	801[B]	2	-	7/18/38/38	0/3/3/3
3	ATP	H	807[A]	2	-	2/18/38/38	0/3/3/3
4	EDO	B	819	-	-	1/1/1/1	-
3	ATP	G	806[B]	2	-	5/18/38/38	0/3/3/3
3	ATP	C	802[A]	2	-	2/18/38/38	0/3/3/3
3	ATP	A	800[A]	2	-	0/18/38/38	0/3/3/3
3	ATP	E	804[B]	2	-	3/18/38/38	0/3/3/3
3	ATP	D	803[A]	2	-	0/18/38/38	0/3/3/3
3	ATP	H	807[B]	2	-	2/18/38/38	0/3/3/3
3	ATP	E	804[A]	2	-	0/18/38/38	0/3/3/3
3	ATP	A	800[B]	2	-	6/18/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	800[A]	ATP	C5-C6-N6	2.55	124.23	120.35
3	E	804[A]	ATP	O3G-PG-O2G	-2.35	98.66	107.64
3	A	800[B]	ATP	C5-C6-N6	2.32	123.88	120.35
3	D	803[A]	ATP	C5-C6-N6	2.31	123.86	120.35
3	E	804[B]	ATP	C5-C6-N6	2.27	123.81	120.35

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	802[A]	ATP	PB-O3B-PG-O2G
3	B	801[B]	ATP	PB-O3B-PG-O3G
3	G	806[B]	ATP	PB-O3B-PG-O3G
3	F	805[B]	ATP	PB-O3B-PG-O3G
3	H	807[A]	ATP	PB-O3B-PG-O2G

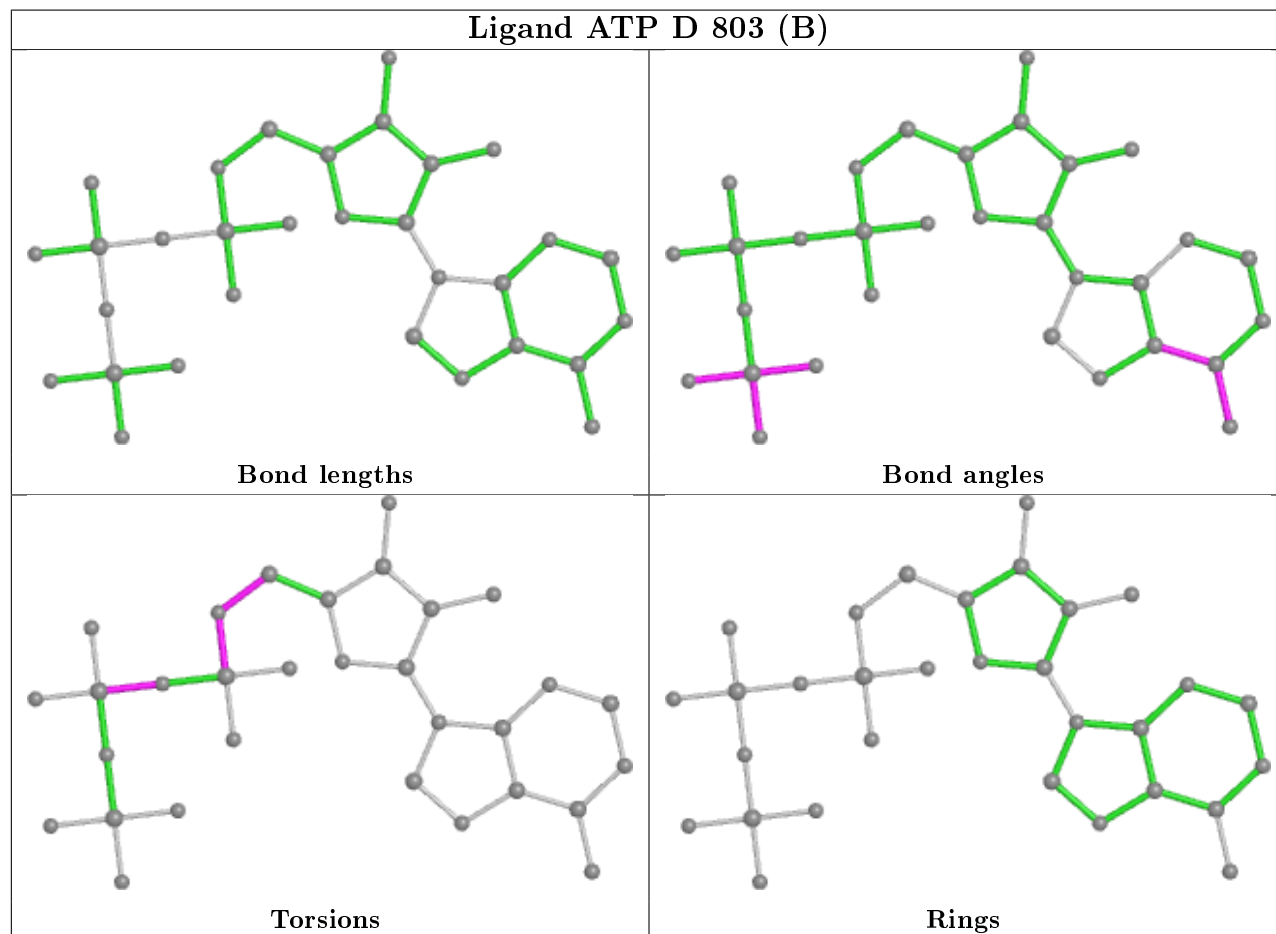
There are no ring outliers.



3 monomers are involved in 4 short contacts:

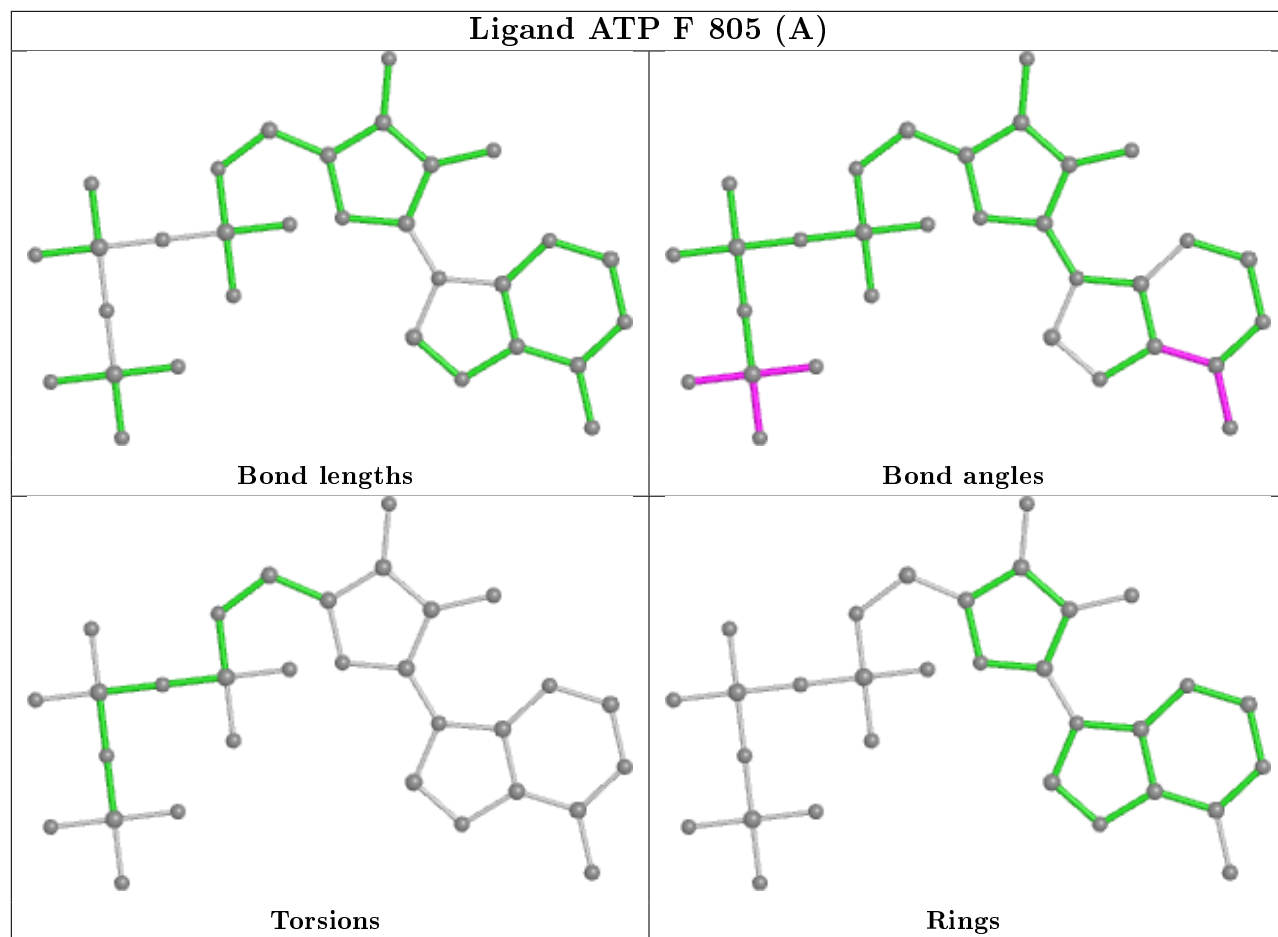
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	803[B]	ATP	2	0
3	B	801[B]	ATP	1	0
3	A	800[B]	ATP	1	0

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.

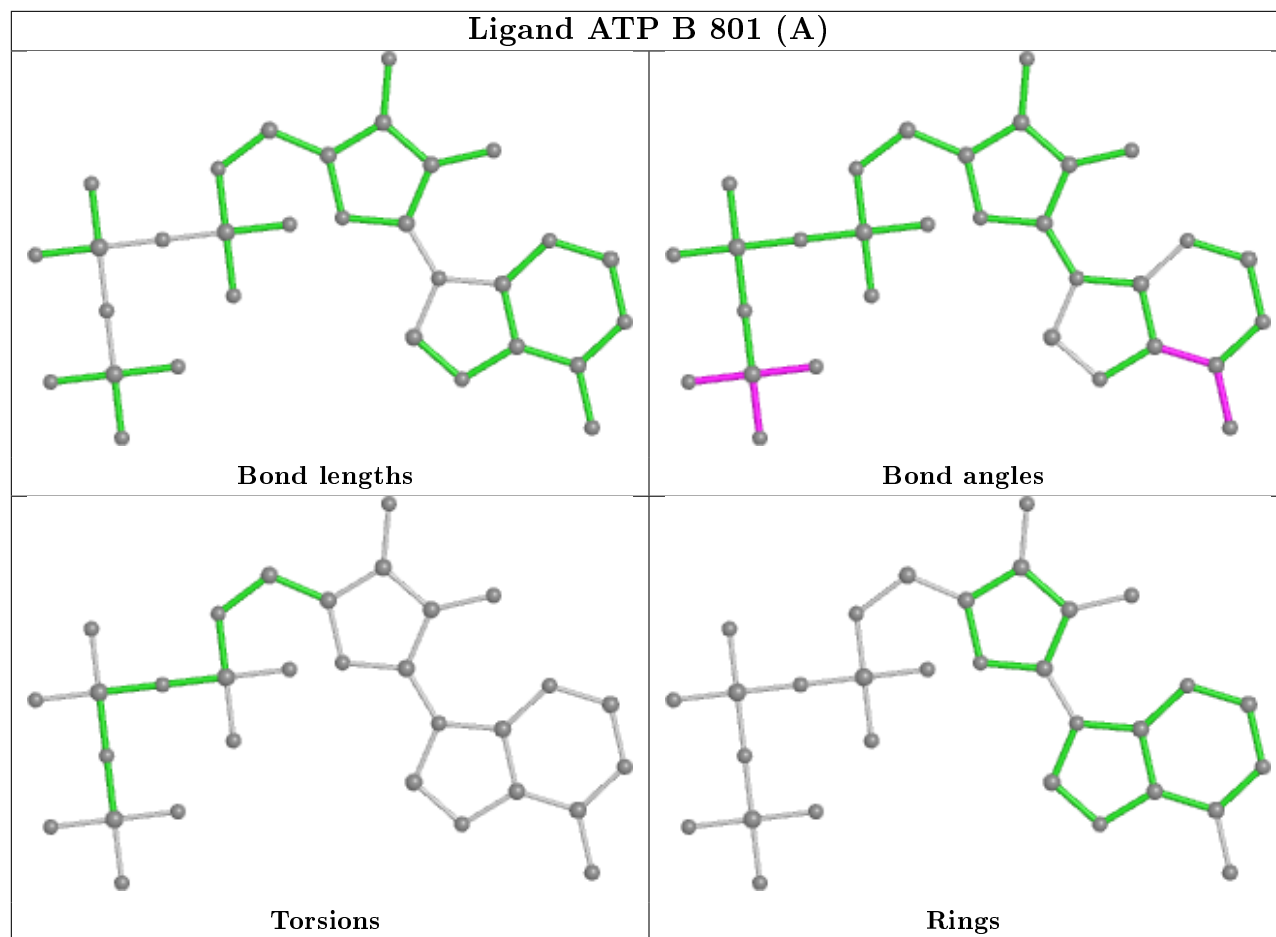




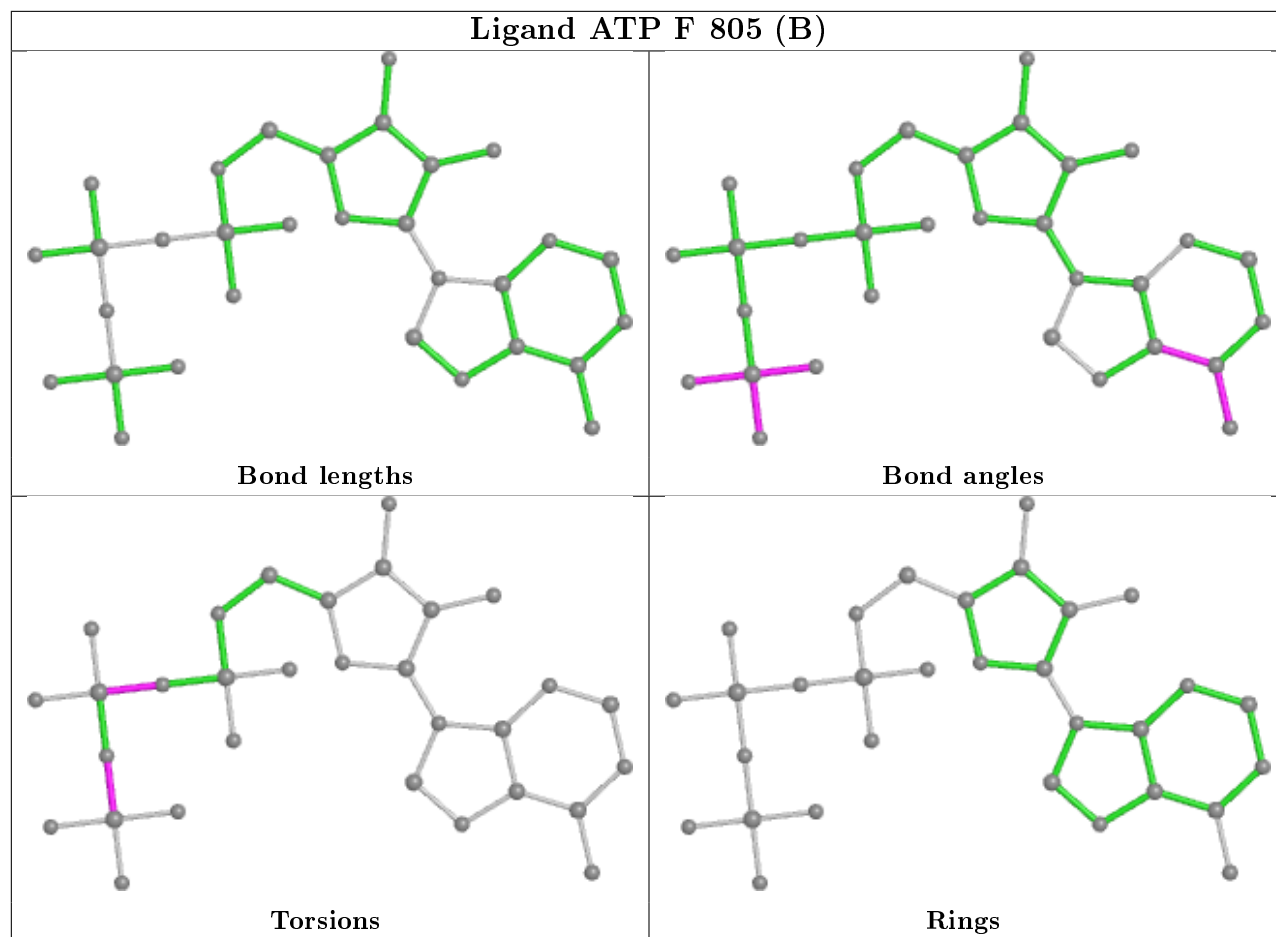
## Ligand ATP F 805 (A)



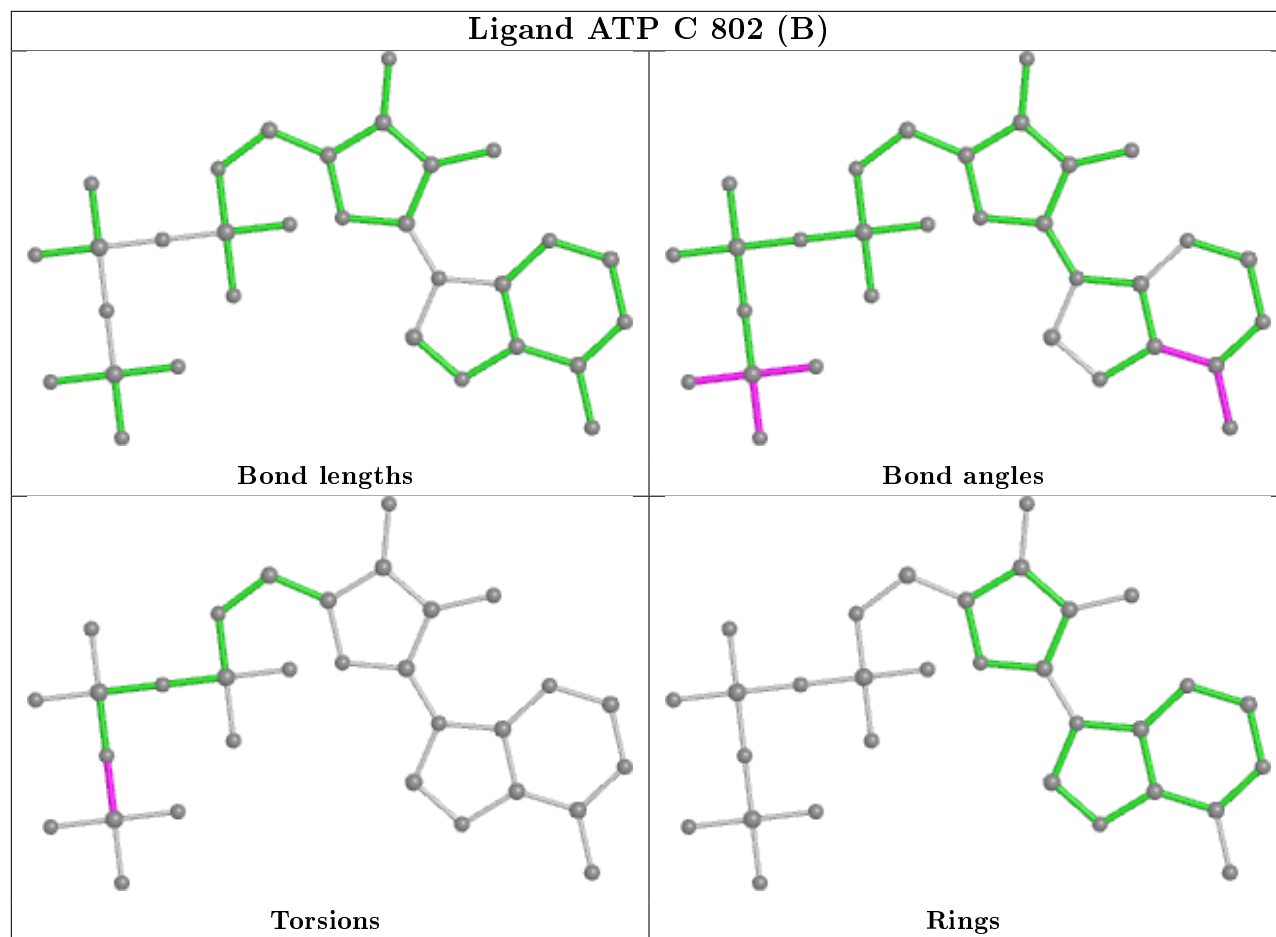




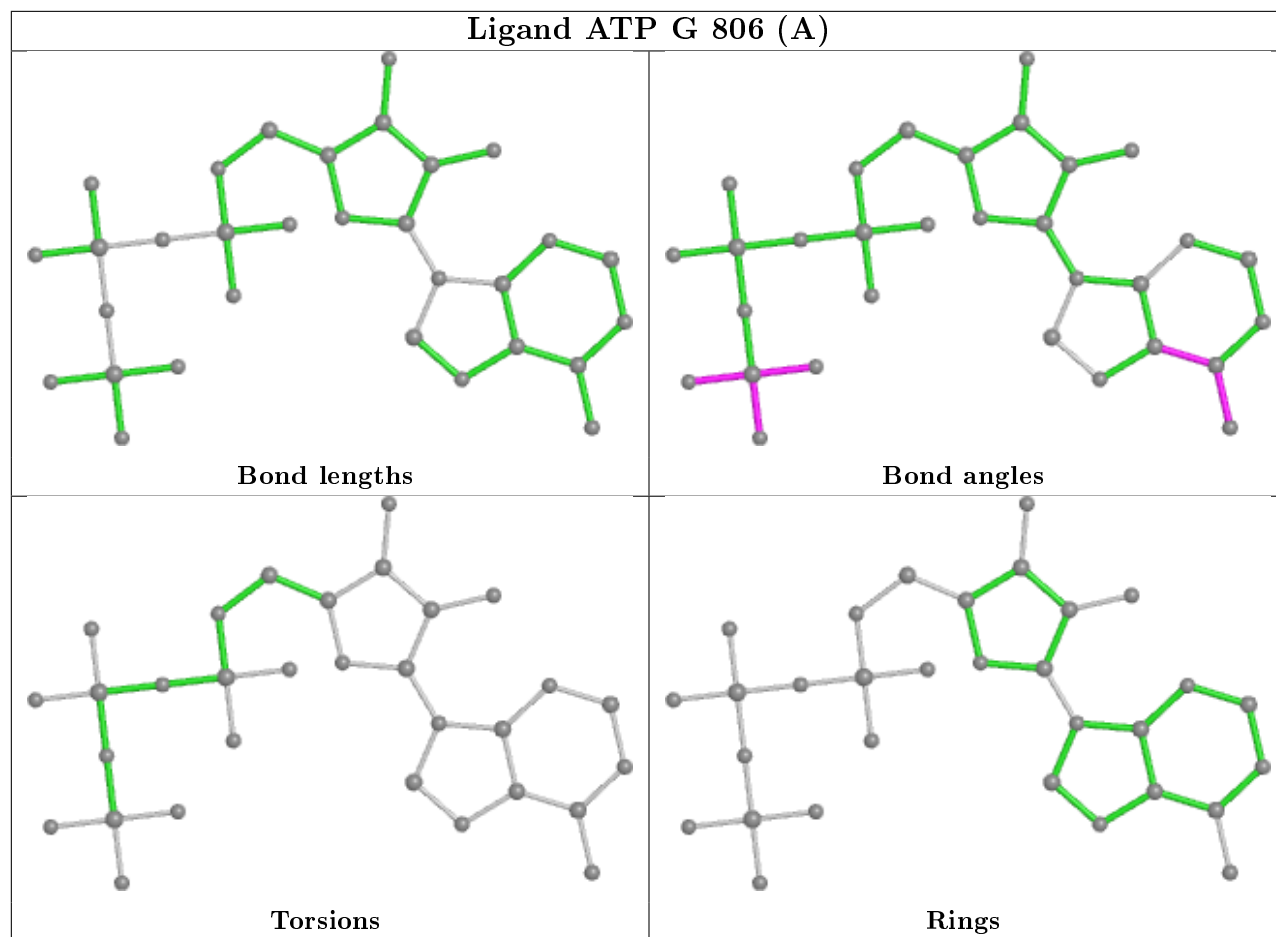




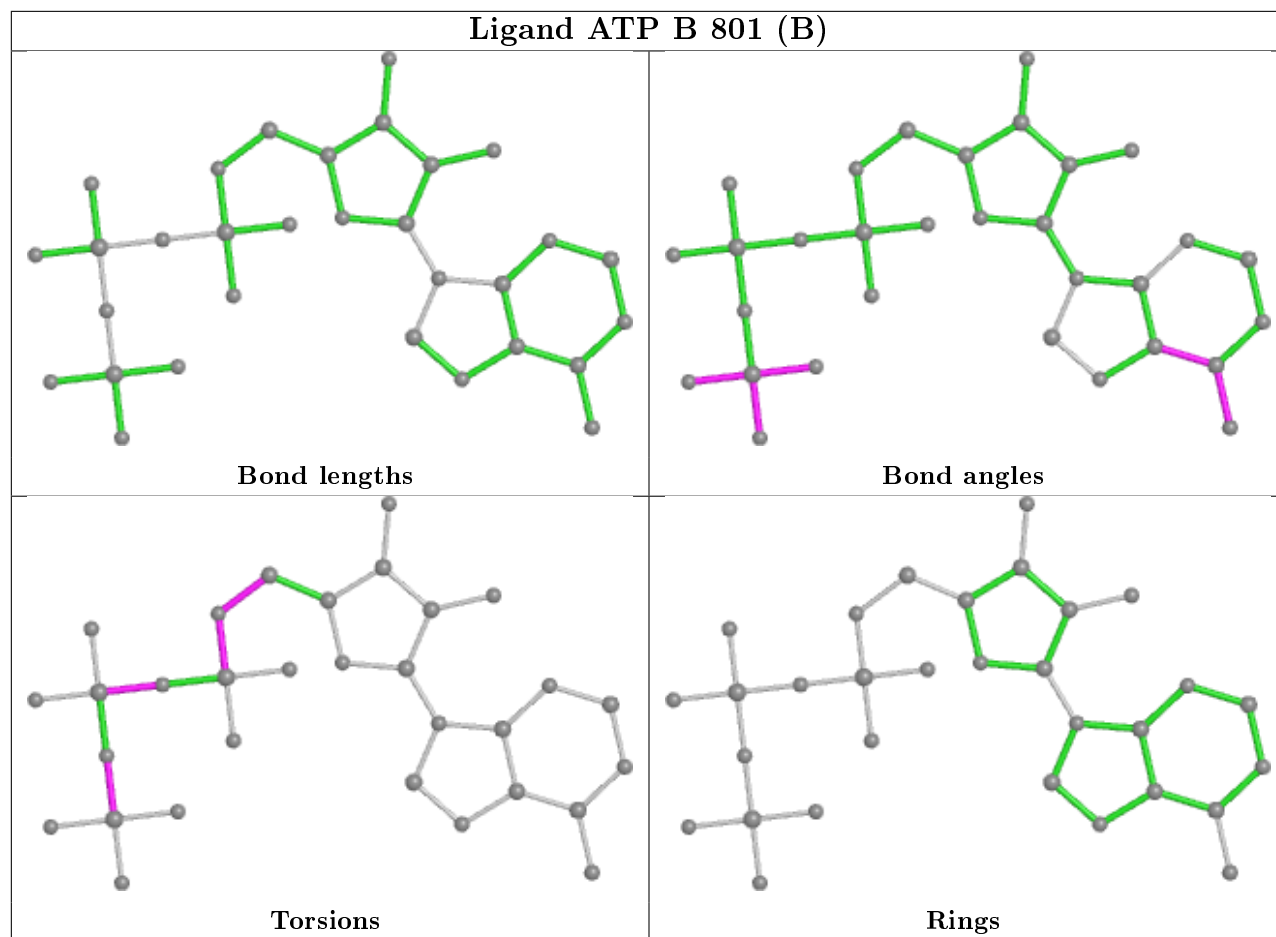




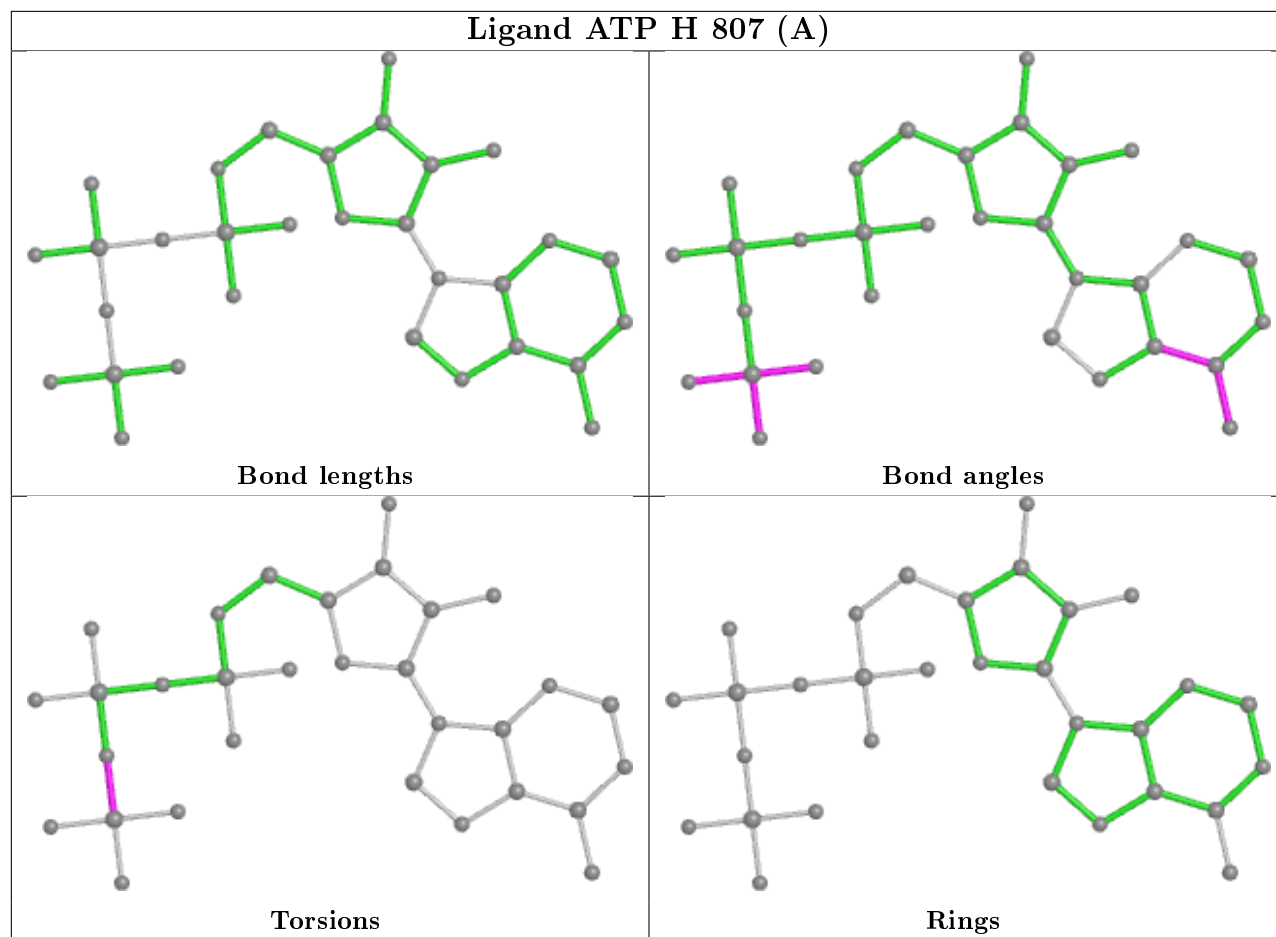






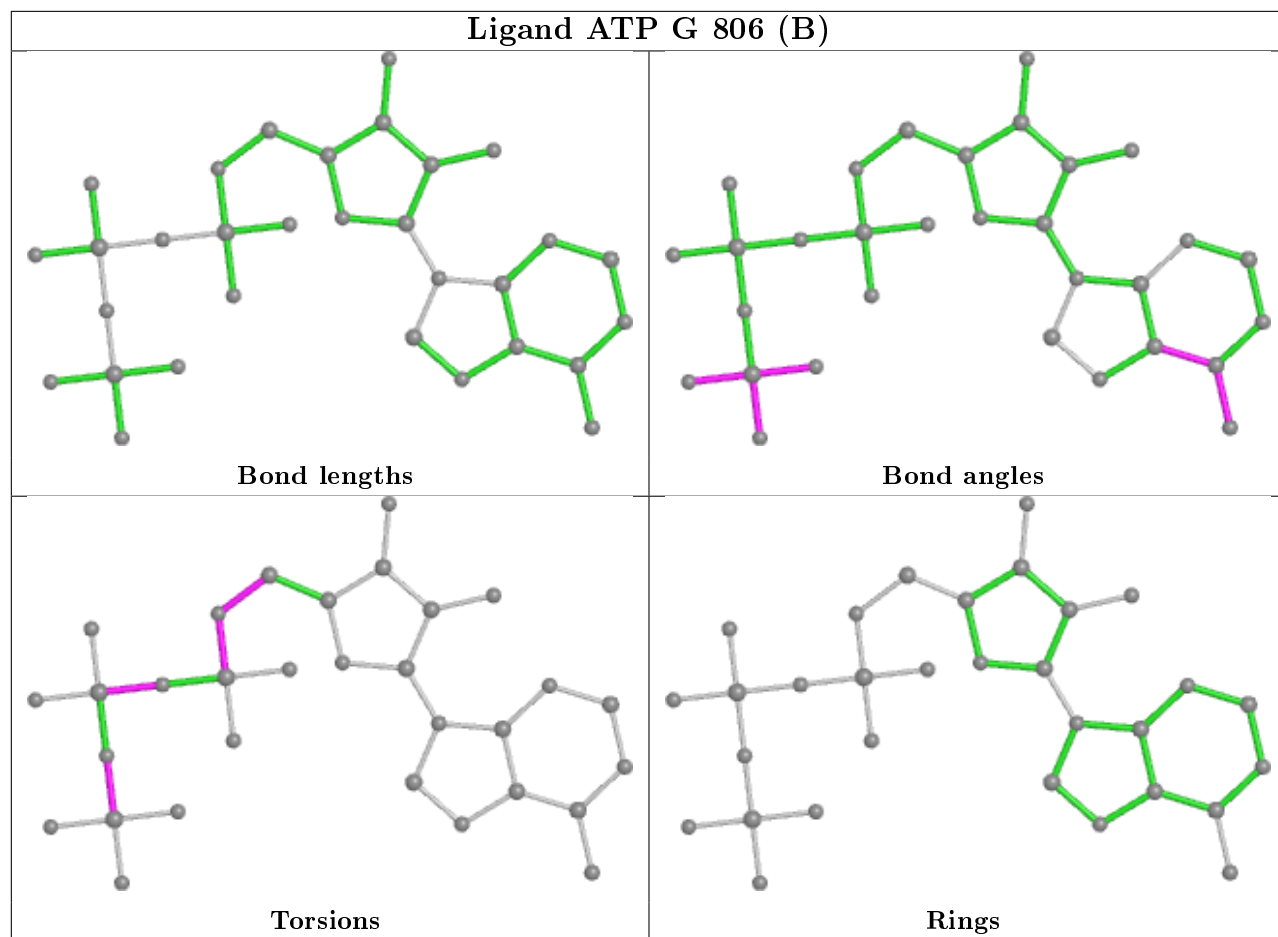




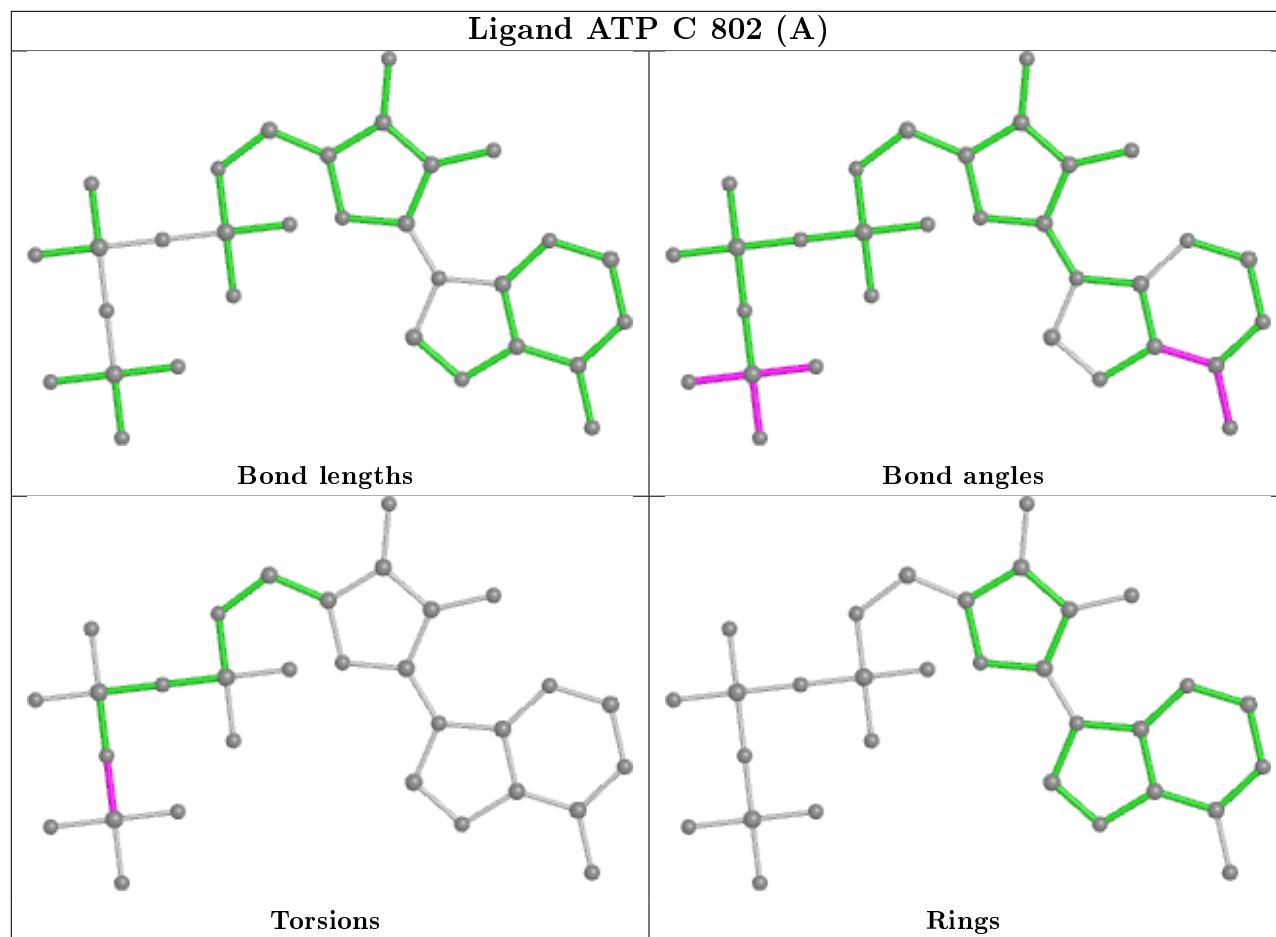




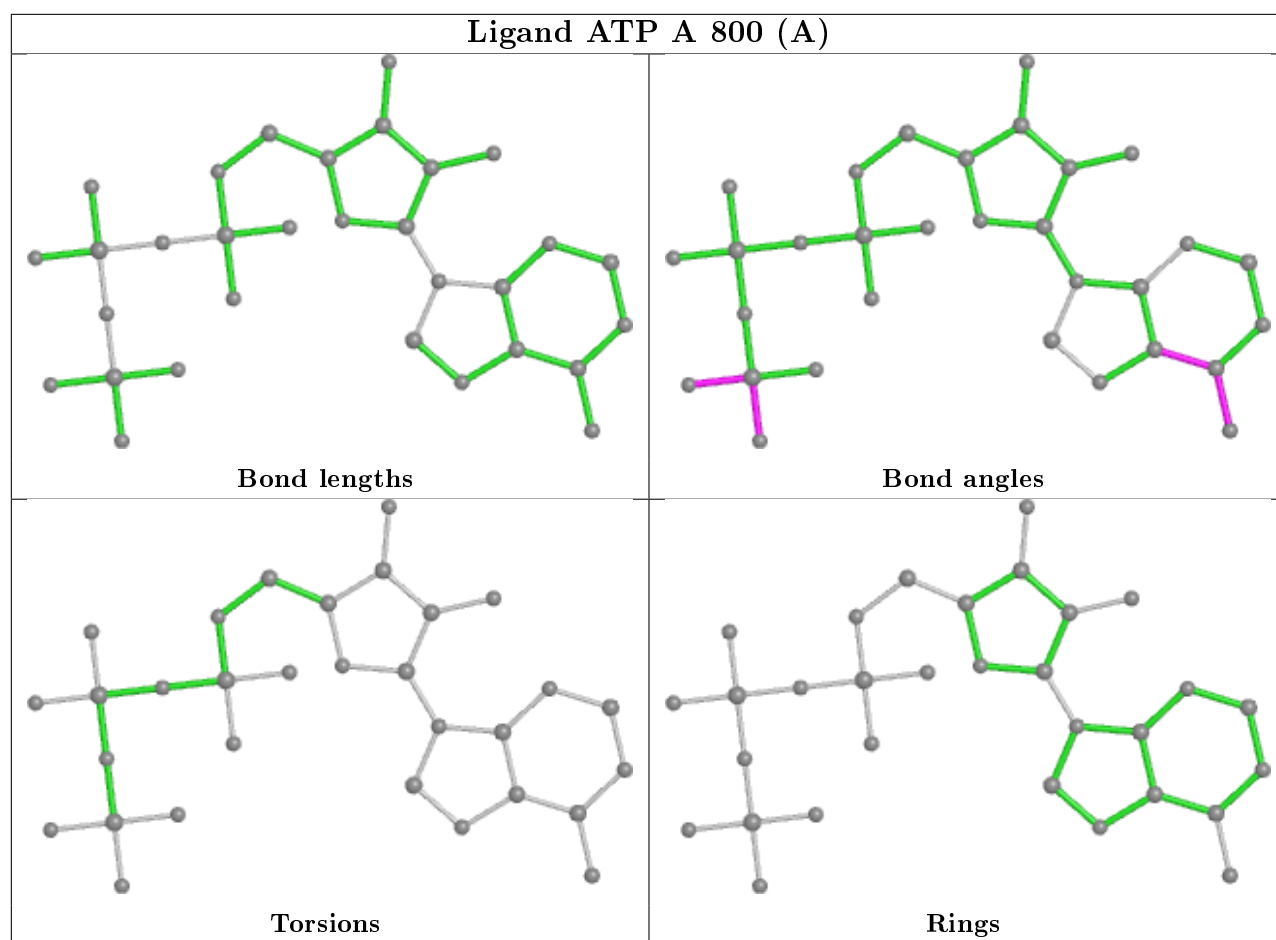
## Ligand ATP G 806 (B)





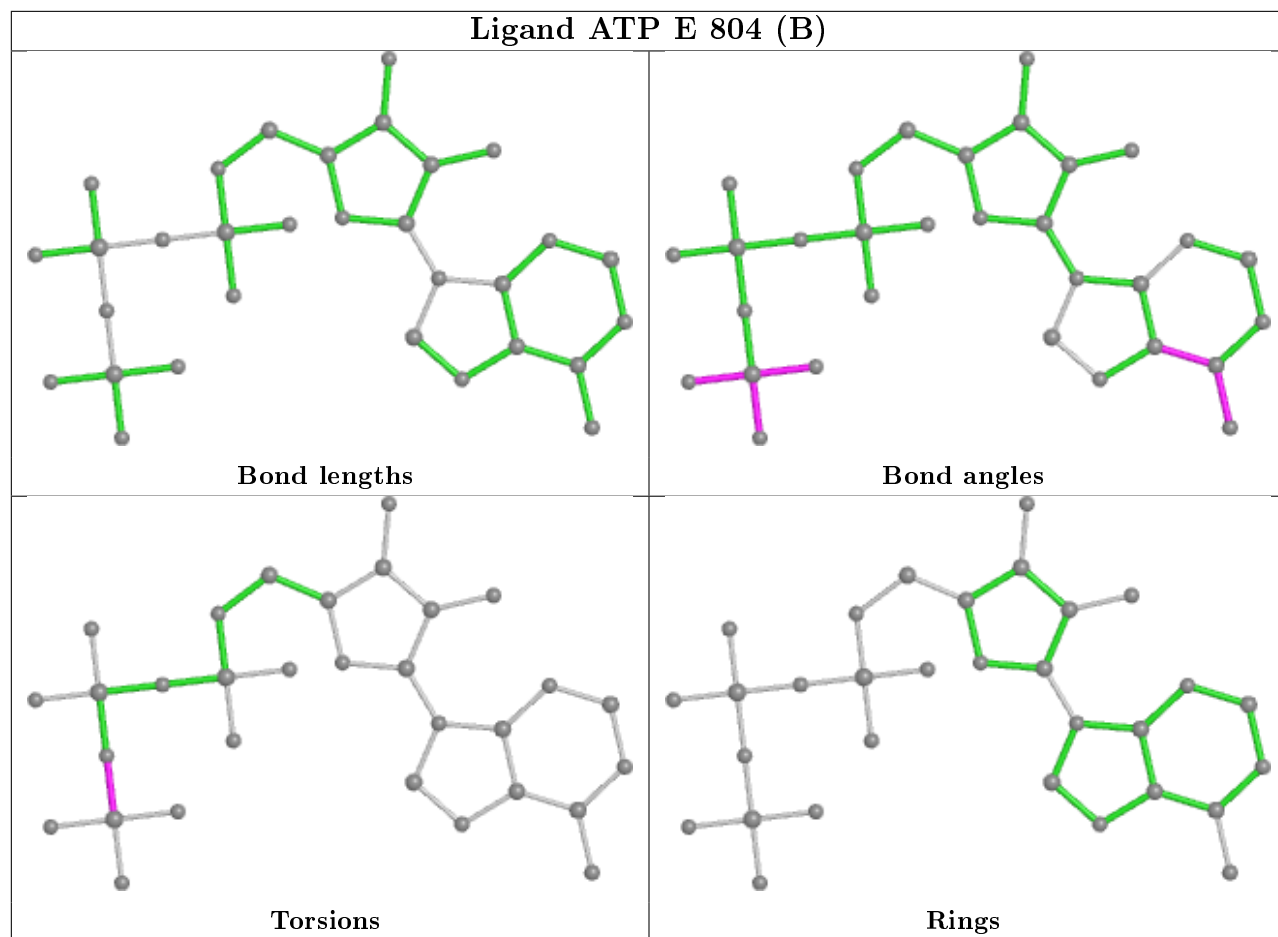




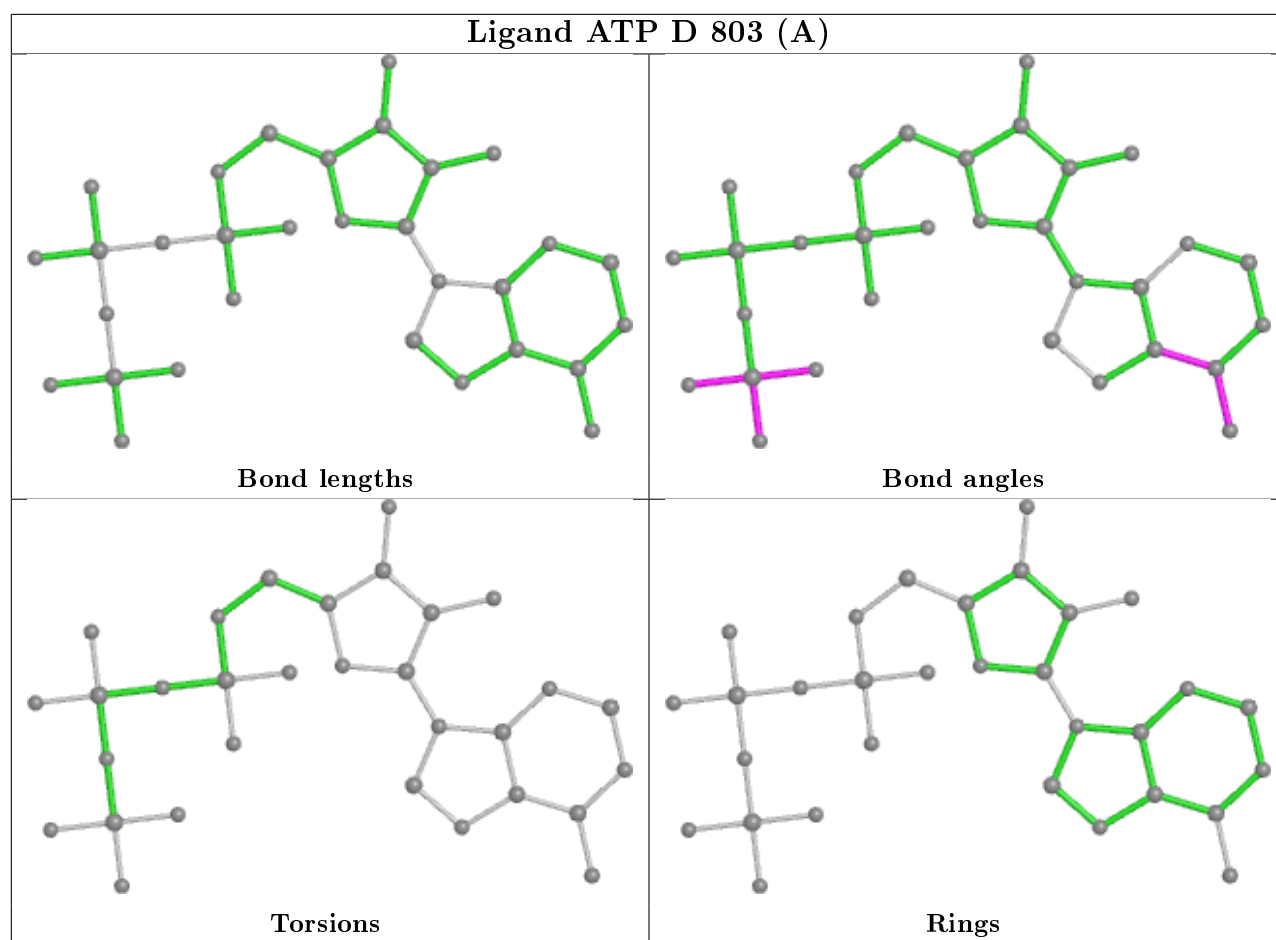




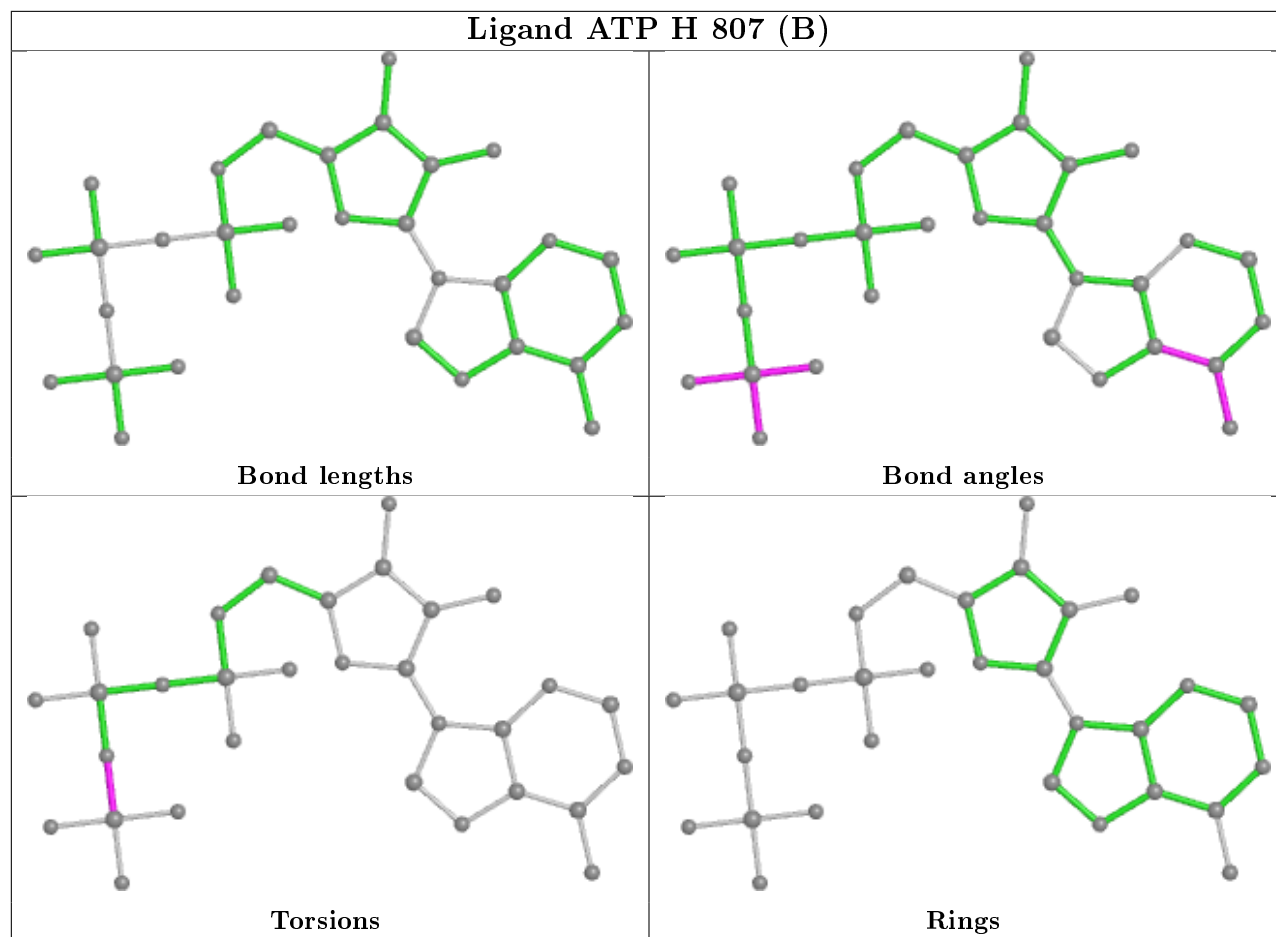
## Ligand ATP E 804 (B)



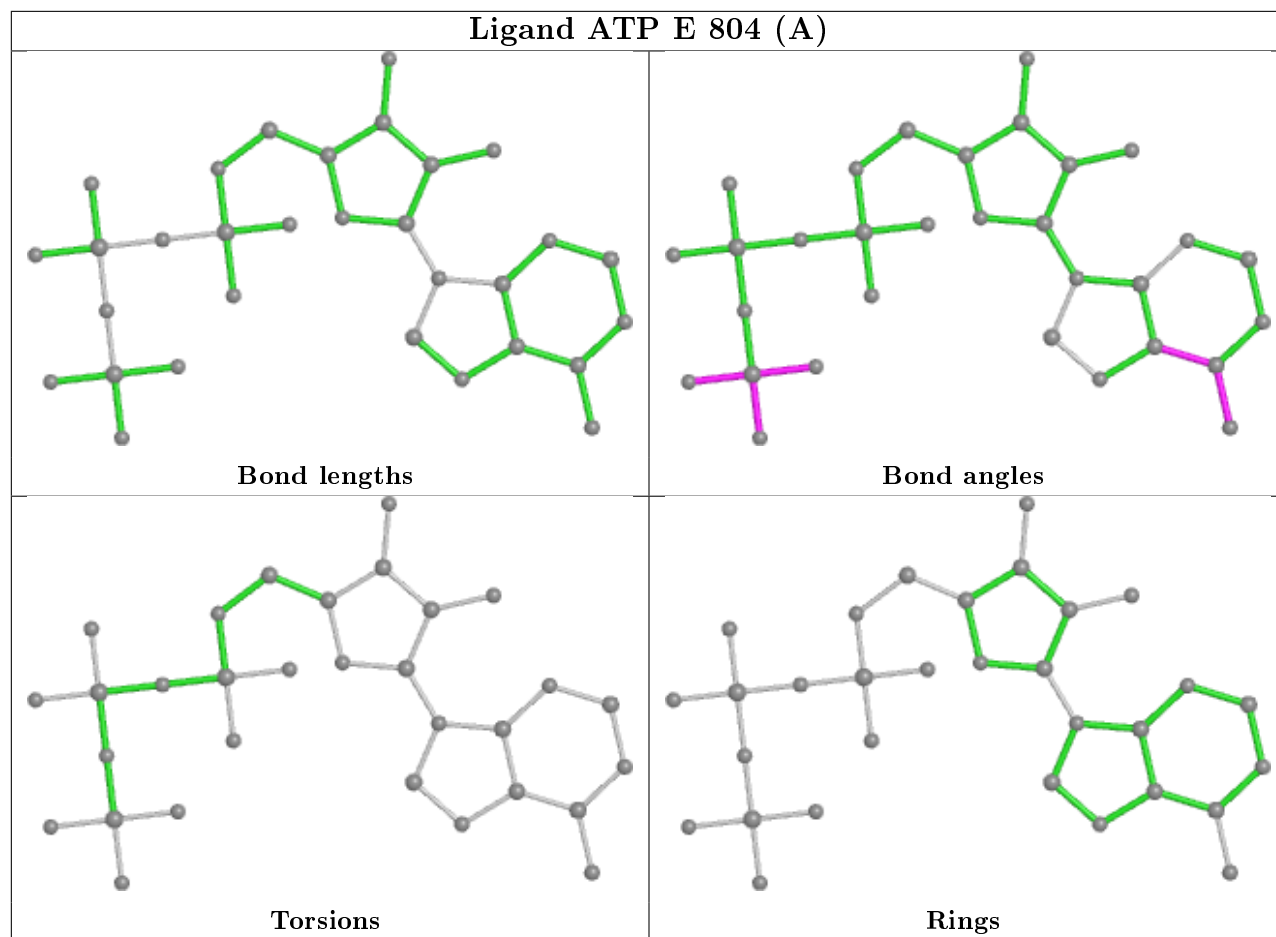




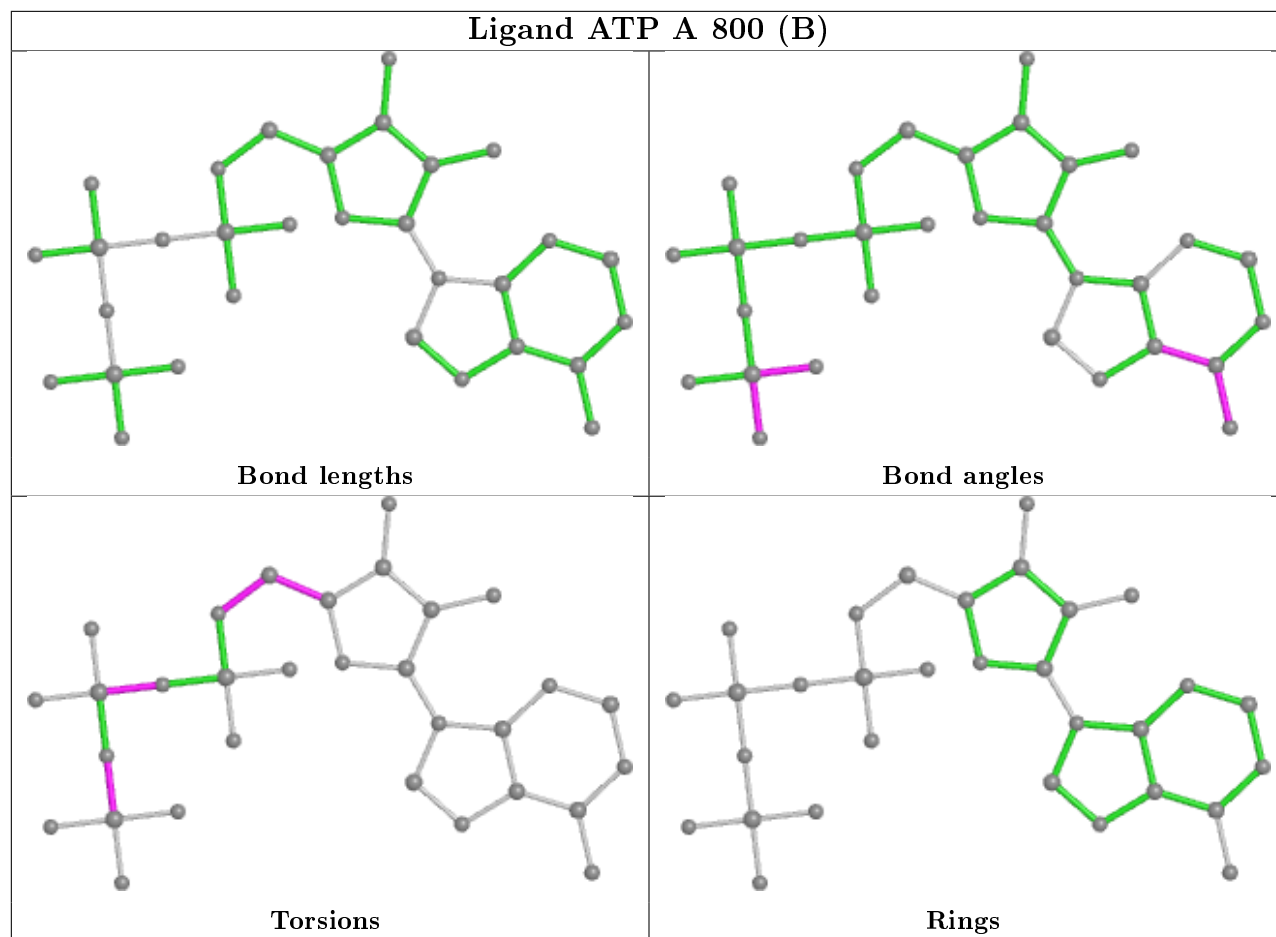












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	306/422 (72%)	0.16	9 (2%) 51 57	11, 24, 47, 69	6 (1%)
1	B	292/422 (69%)	0.03	6 (2%) 63 68	12, 22, 43, 60	2 (0%)
1	C	285/422 (67%)	0.29	15 (5%) 26 32	17, 31, 56, 82	5 (1%)
1	D	300/422 (71%)	0.53	20 (6%) 17 22	19, 35, 59, 72	2 (0%)
1	E	286/422 (67%)	0.22	7 (2%) 59 64	20, 33, 56, 72	10 (3%)
1	F	286/422 (67%)	0.48	16 (5%) 24 29	19, 38, 66, 83	7 (2%)
1	G	293/422 (69%)	0.31	17 (5%) 23 28	15, 33, 59, 73	1 (0%)
1	H	286/422 (67%)	0.16	5 (1%) 70 74	15, 30, 50, 61	6 (2%)
All	All	2334/3376 (69%)	0.27	95 (4%) 37 43	11, 31, 58, 83	39 (1%)

The worst 5 of 95 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	174	VAL	7.3
1	A	168	LEU	7.0
1	D	167	VAL	6.6
1	A	172	VAL	6.3
1	C	139	ILE	5.9

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

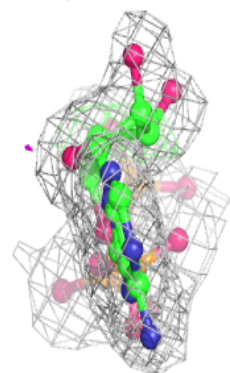
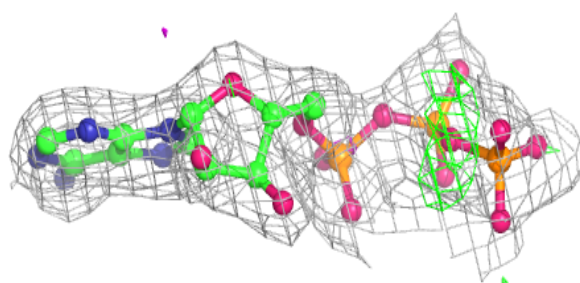
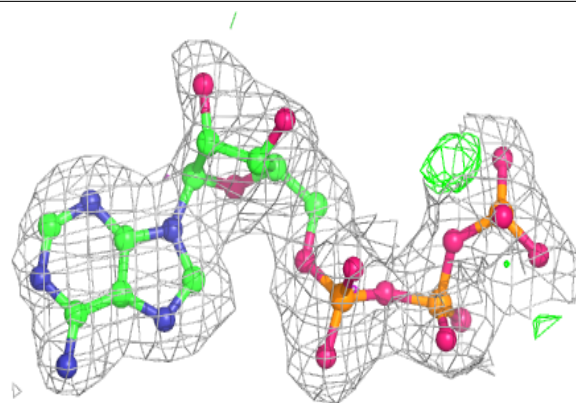
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	EDO	A	818	4/4	0.79	0.18	20,22,26,26	0
2	CA	E	817	1/1	0.83	0.12	56,56,56,56	0
2	CA	F	817	1/1	0.84	0.15	48,48,48,48	0
3	ATP	C	802[A]	31/31	0.92	0.15	21,27,36,37	31
3	ATP	C	802[B]	31/31	0.92	0.15	30,33,36,37	31
3	ATP	F	805[A]	31/31	0.94	0.14	26,35,39,41	31
3	ATP	F	805[B]	31/31	0.94	0.14	33,35,37,37	31
3	ATP	H	807[A]	31/31	0.94	0.14	28,33,43,43	31
3	ATP	H	807[B]	31/31	0.94	0.14	28,31,34,36	31
3	ATP	E	804[B]	31/31	0.94	0.15	33,35,38,40	31
3	ATP	E	804[A]	31/31	0.94	0.15	28,32,37,39	31
2	CA	D	817	1/1	0.94	0.11	39,39,39,39	0
3	ATP	D	803[B]	31/31	0.95	0.16	27,29,33,33	31
2	CA	H	817	1/1	0.95	0.10	38,38,38,38	0
3	ATP	D	803[A]	31/31	0.95	0.16	23,27,30,31	31
4	EDO	B	819	4/4	0.95	0.13	26,28,30,32	0
2	CA	G	817	1/1	0.95	0.10	39,39,39,39	0
3	ATP	B	801[A]	31/31	0.96	0.13	15,20,23,23	31
3	ATP	G	806[B]	31/31	0.96	0.12	24,26,28,28	31
3	ATP	G	806[A]	31/31	0.96	0.12	23,26,30,31	31
3	ATP	B	801[B]	31/31	0.96	0.13	28,31,32,32	31
3	ATP	A	800[A]	31/31	0.97	0.15	11,19,21,22	31
3	ATP	A	800[B]	31/31	0.97	0.15	21,30,33,33	31
2	CA	A	817	1/1	0.98	0.14	29,29,29,29	0
2	CA	B	817	1/1	0.98	0.11	28,28,28,28	0
2	CA	C	817	1/1	0.98	0.09	44,44,44,44	0

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

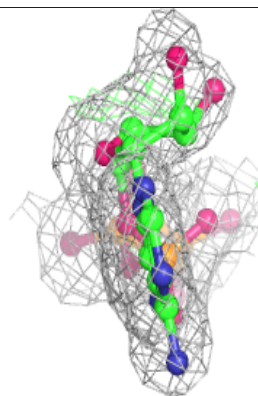
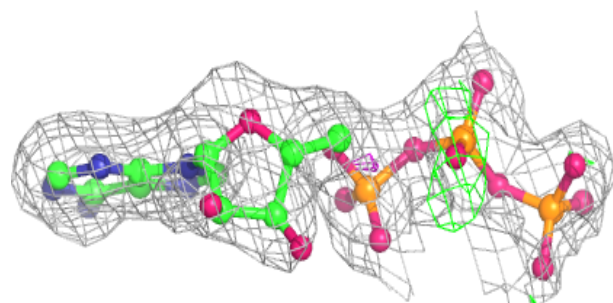
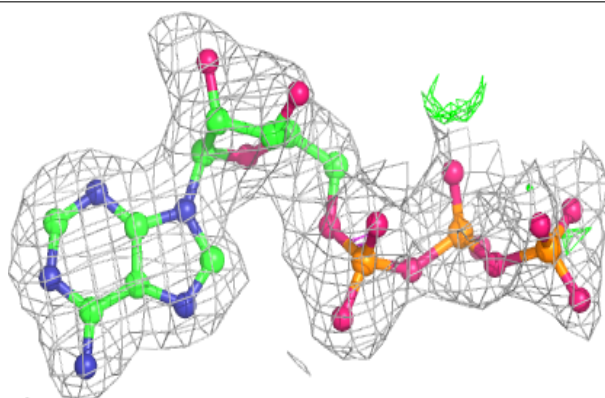


**Electron density around ATP C 802 (A):**

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

**Electron density around ATP C 802 (B):**

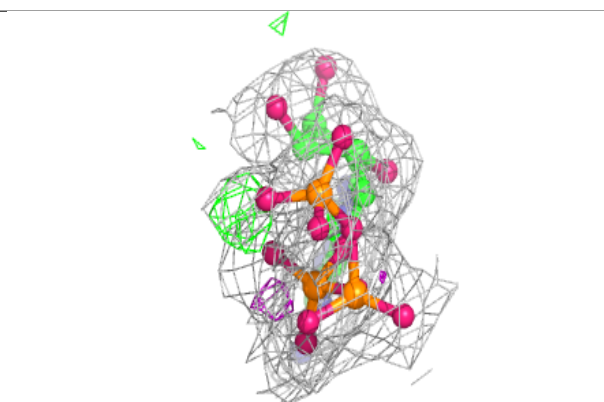
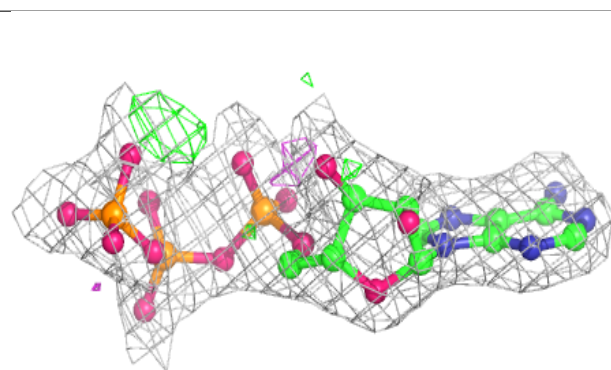
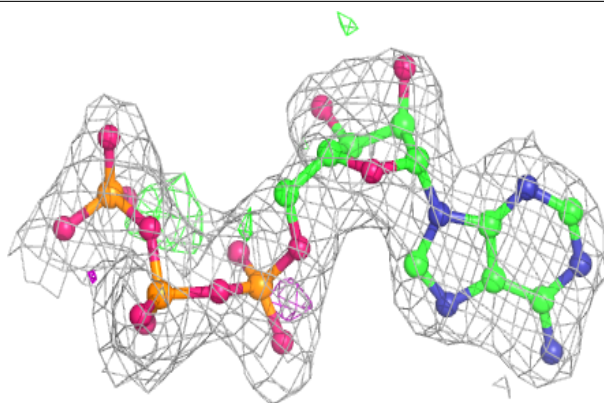
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



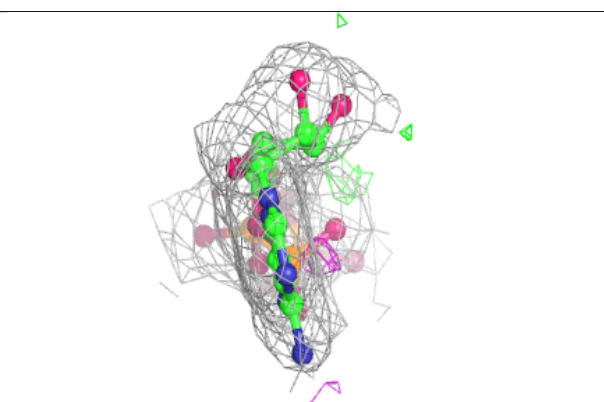
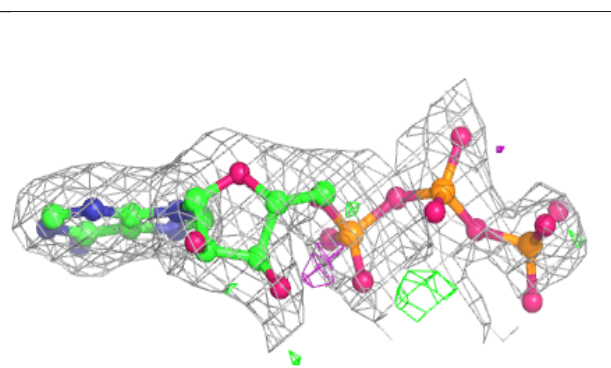
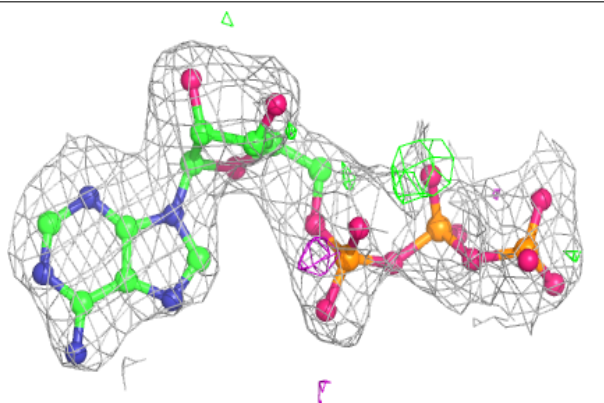


**Electron density around ATP F 805 (A):**

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

**Electron density around ATP F 805 (B):**

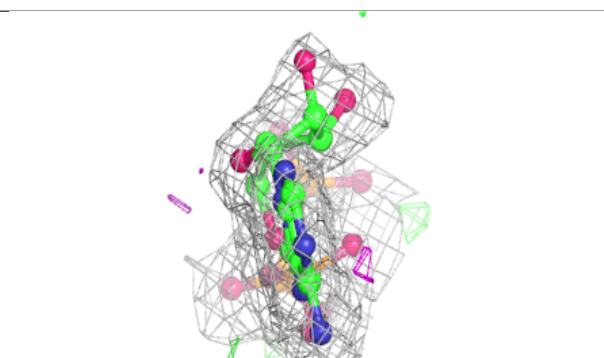
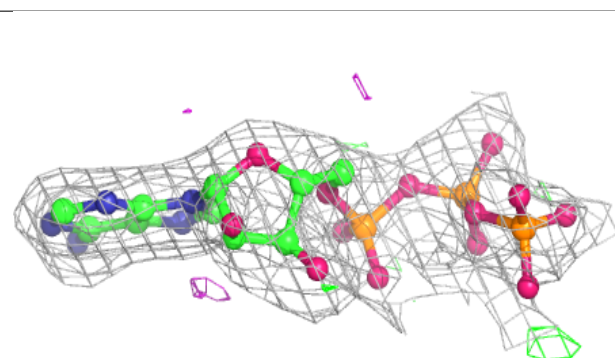
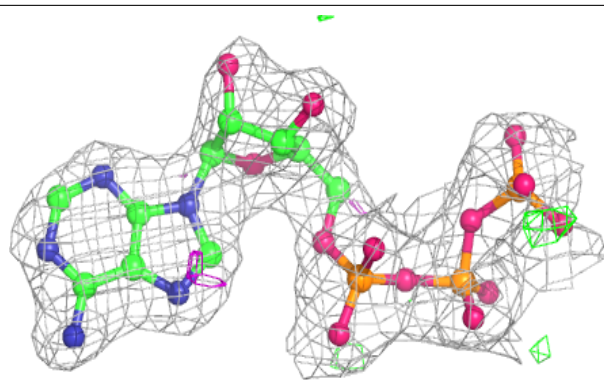
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



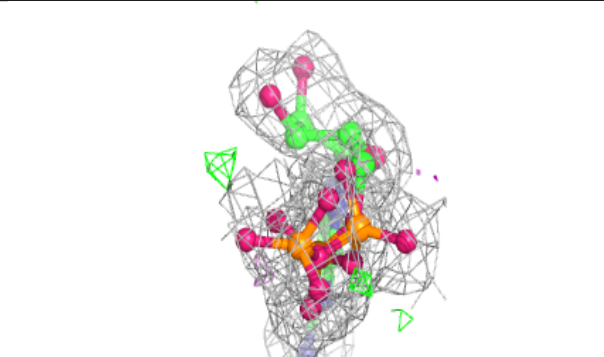
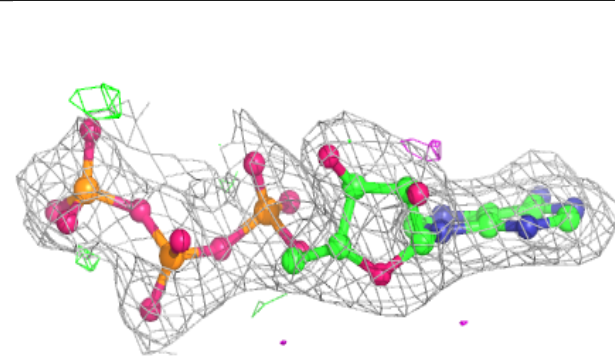
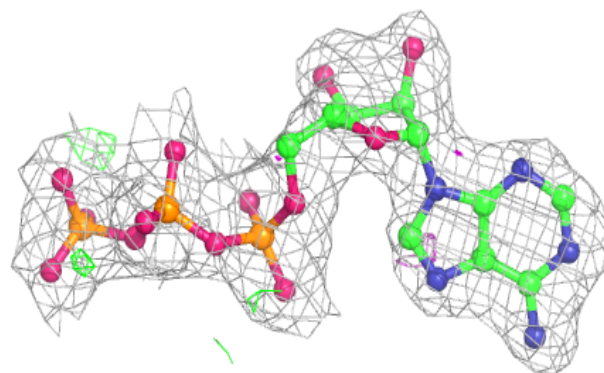


**Electron density around ATP H 807 (A):**

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and green (positive)

**Electron density around ATP H 807 (B):**

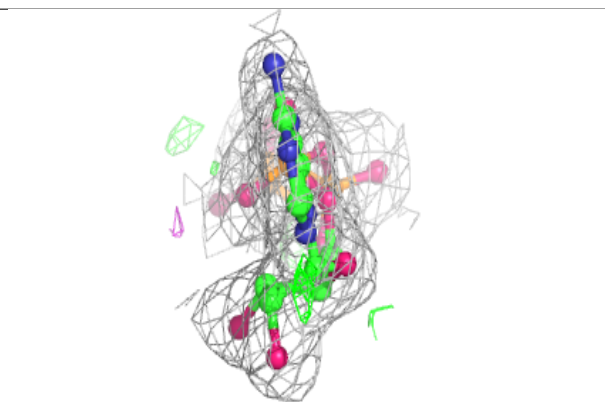
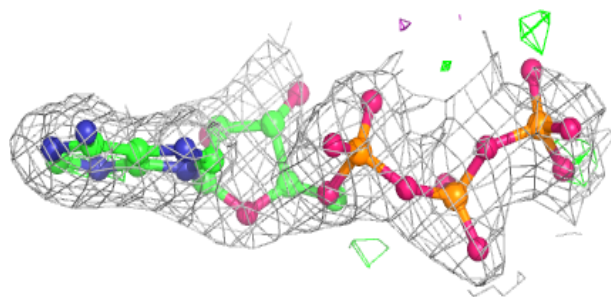
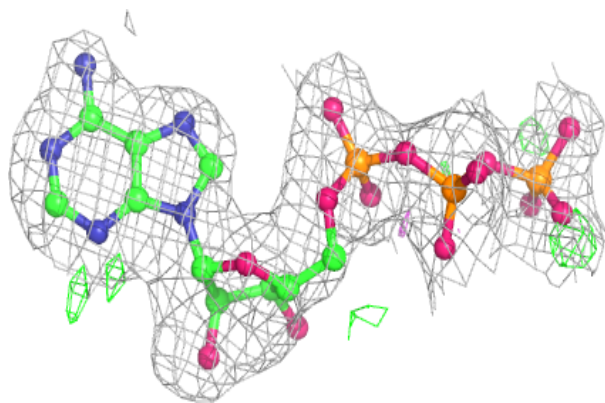
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



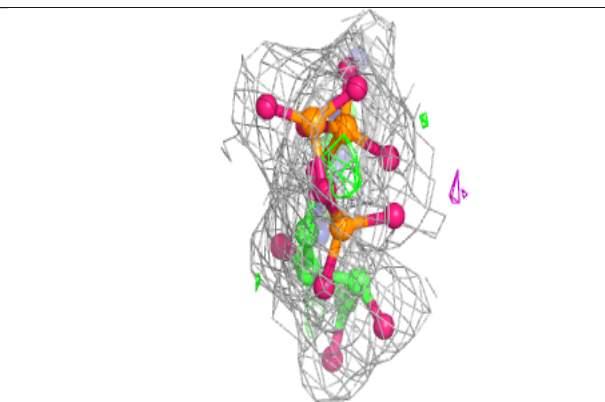
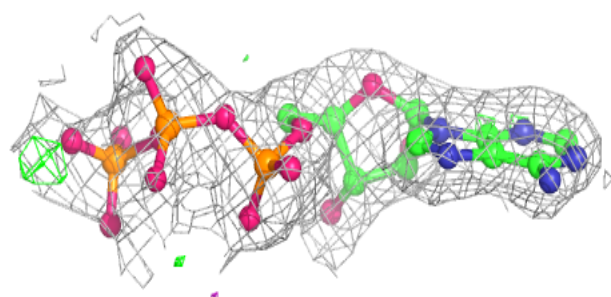
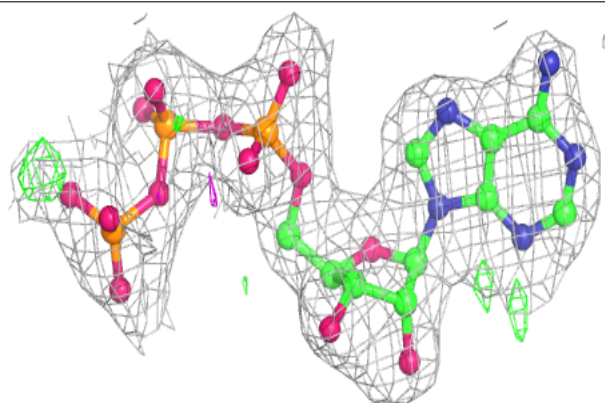


**Electron density around ATP E 804 (B):**

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

**Electron density around ATP E 804 (A):**

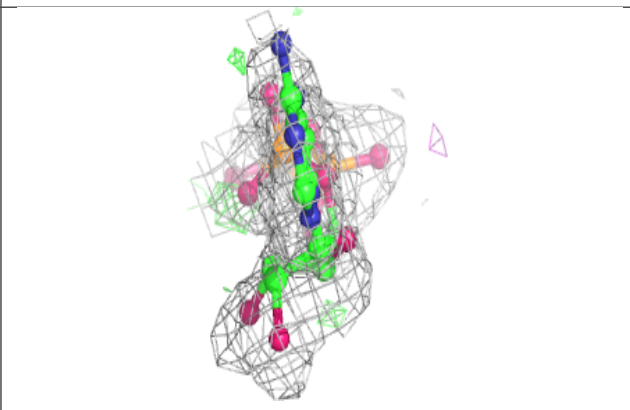
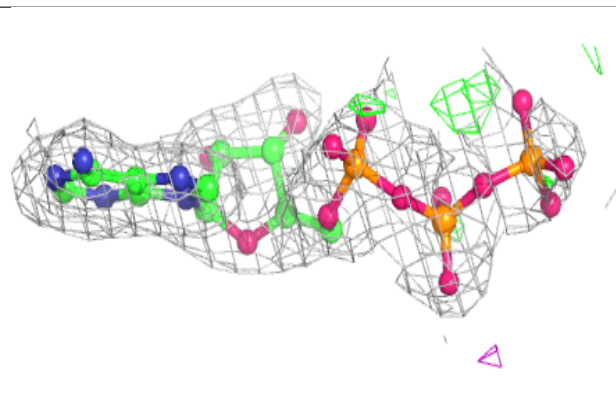
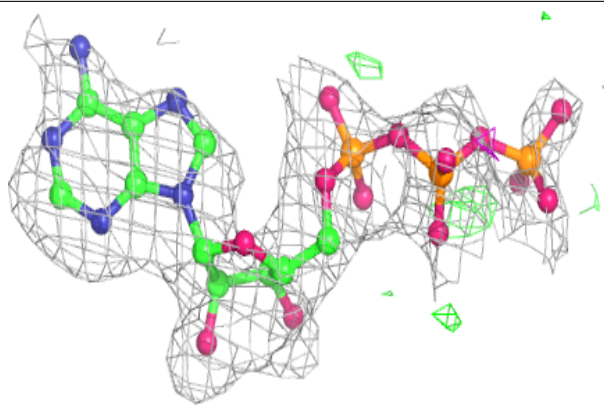
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



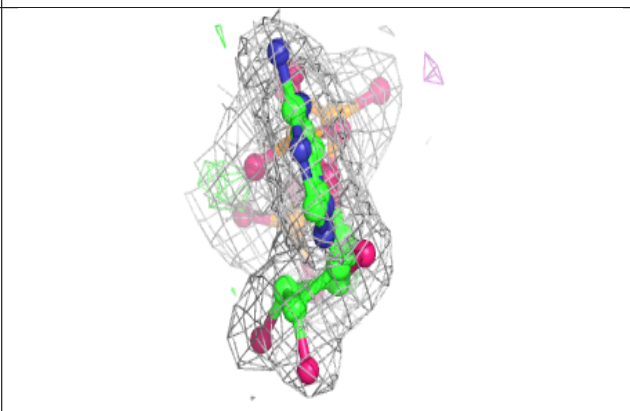
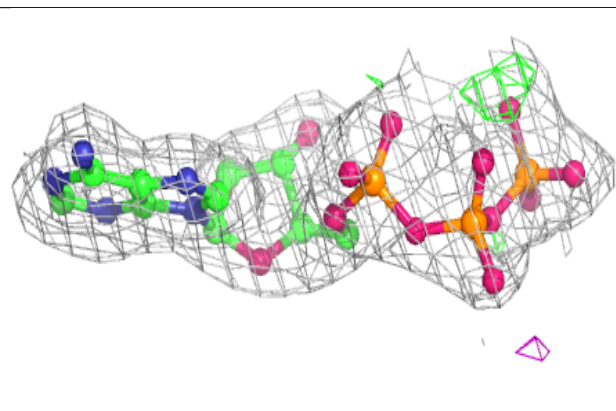
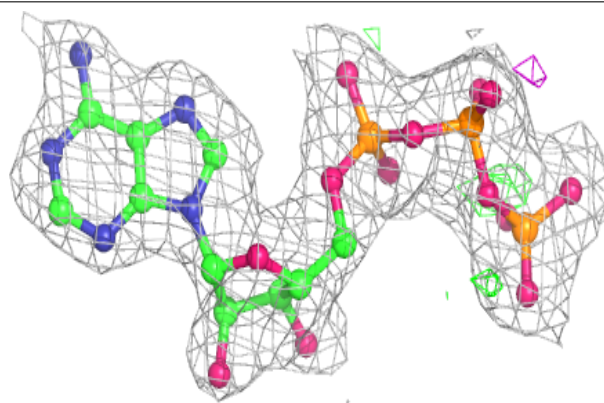


**Electron density around ATP D 803 (B):**

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

**Electron density around ATP D 803 (A):**

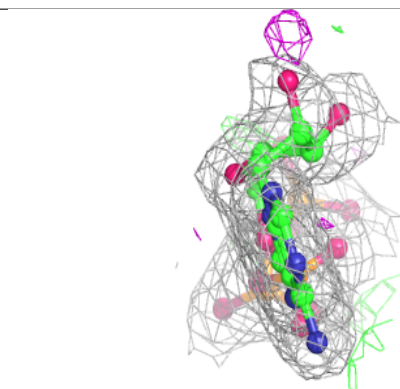
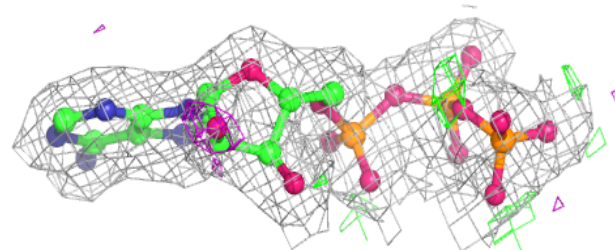
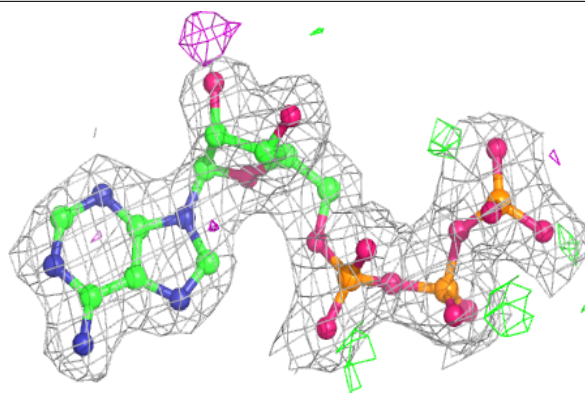
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



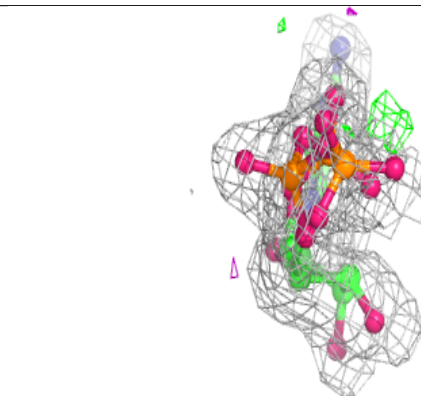
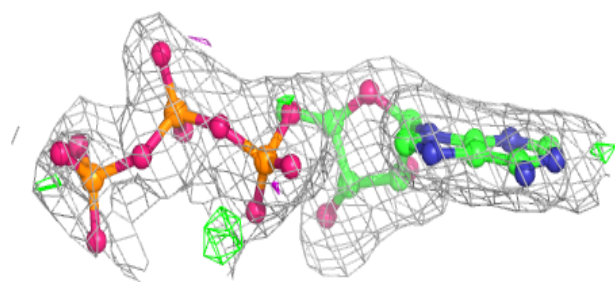
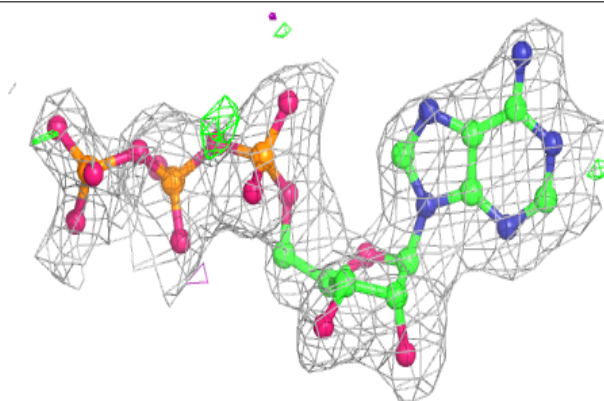


**Electron density around ATP B 801 (A):**

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

**Electron density around ATP G 806 (B):**

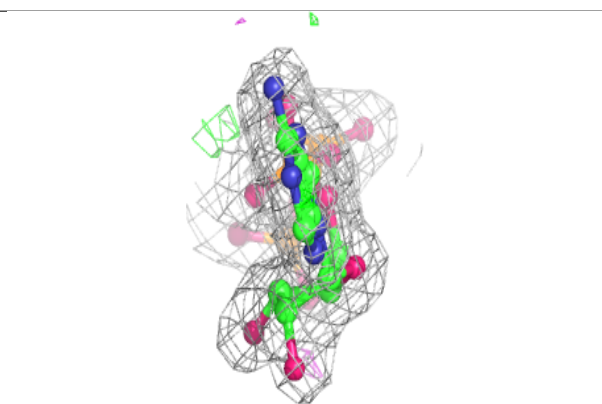
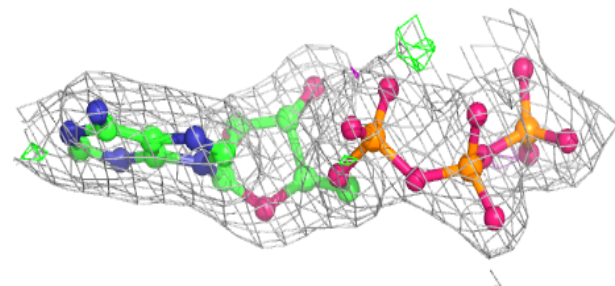
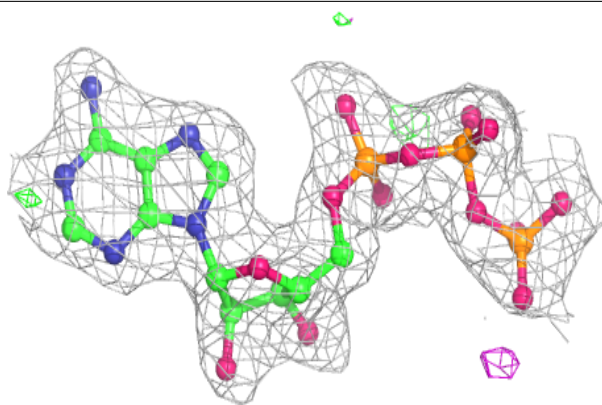
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



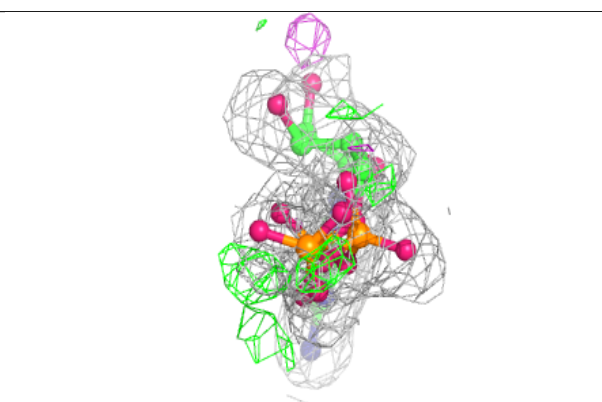
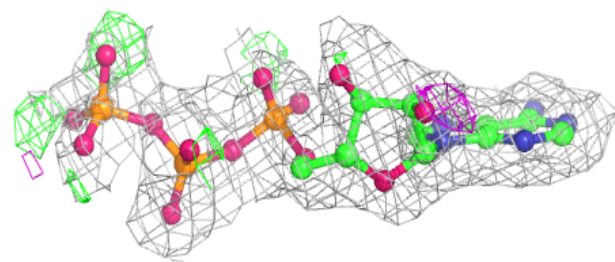
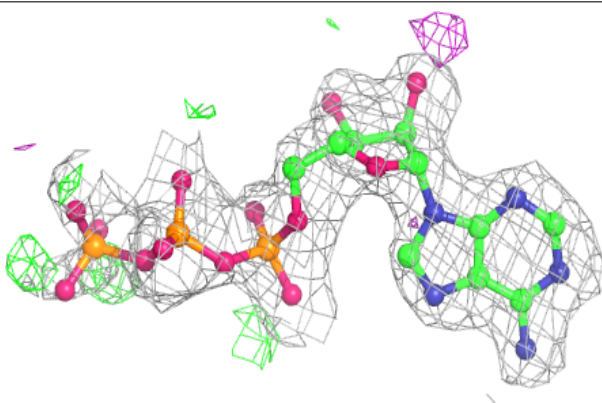


**Electron density around ATP G 806 (A):**

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

**Electron density around ATP B 801 (B):**

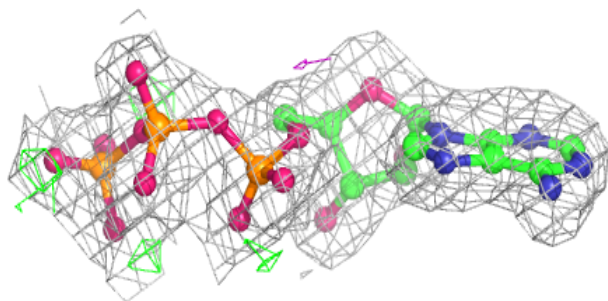
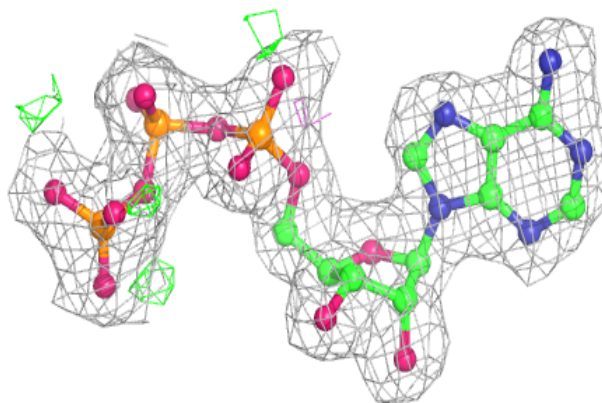
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



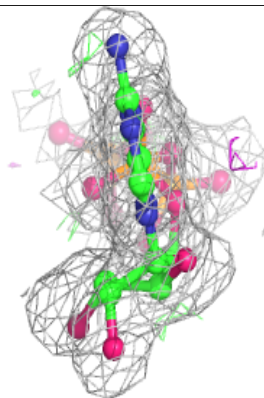
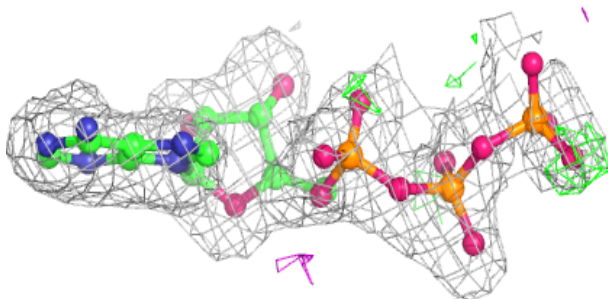
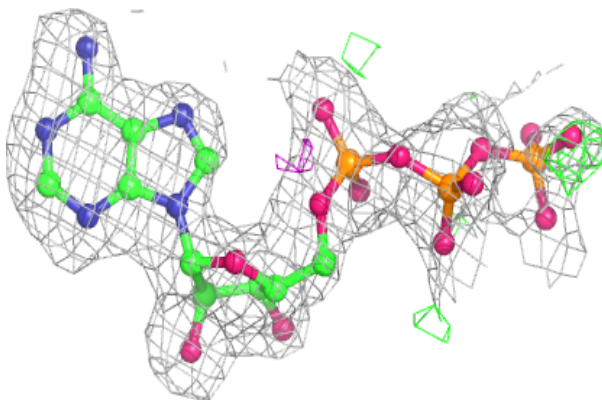


**Electron density around ATP A 800 (A):**

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

**Electron density around ATP A 800 (B):**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.