



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 12:16 PM UTC

PDB ID : 5MCP / pdb_00005mcp
Title : Structure of IMP dehydrogenase from Ashbya gossypii bound to ATP
Authors : Winter, G.; Fernandez-Justel, D.; de Pereda, J.M.; Revuelta, J.L.; Buey, R.M.
Deposited on : 2016-11-10
Resolution : 2.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

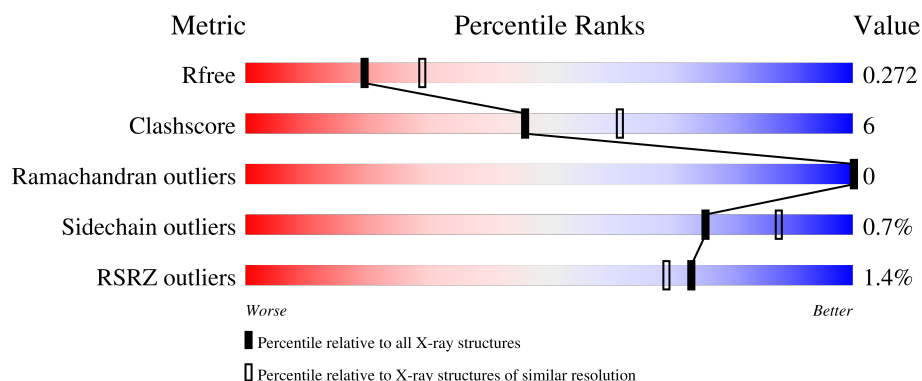
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	523	
1	B	523	
1	C	523	
1	D	523	
1	E	523	

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Mol	Chain	Length	Quality of chain
1	F	523	2% 59% 7% 35%
1	G	523	2% 63% 9% 27%
1	H	523	3% 56% 5% 39%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 45606 atoms, of which 21090 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 Inosine-5'-monophosphate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	440	Total	C	H	N	O	S	0	0	0
			6568	2057	3293	563	632	23			
1	B	444	Total	C	H	N	O	S	0	0	0
			6442	2039	3187	564	631	21			
1	C	446	Total	C	H	N	O	S	0	1	0
			6556	2068	3260	567	637	24			
1	D	443	Total	C	H	N	O	S	0	1	0
			6541	2060	3267	566	625	23			
1	E	387	Total	C	H	N	O	S	0	0	0
			5039	1659	2384	464	517	15			
1	F	342	Total	C	H	N	O	S	0	1	0
			4054	1379	1832	407	423	13			
1	G	382	Total	C	H	N	O	S	0	0	0
			4580	1561	2066	455	484	14			
1	H	321	Total	C	H	N	O	S	0	0	0
			3526	1225	1529	374	387	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP Q756Z6
B	0	HIS	-	expression tag	UNP Q756Z6
C	0	HIS	-	expression tag	UNP Q756Z6
D	0	HIS	-	expression tag	UNP Q756Z6
E	0	HIS	-	expression tag	UNP Q756Z6
F	0	HIS	-	expression tag	UNP Q756Z6
G	0	HIS	-	expression tag	UNP Q756Z6
H	0	HIS	-	expression tag	UNP Q756Z6

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	A	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	A	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		
2	B	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	B	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	B	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		
2	B	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	B	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	C	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	C	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	C	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		
2	D	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	D	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	D	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	H	N	O	P	
			42	10	11	5	13	3	0
2	E	1	Total	C	H	N	O	P	
			42	10	11	5	13	3	0
2	E	1	Total	C	H	N	O	P	
			43	10	12	5	13	3	0
2	F	1	Total	C	H	N	O	P	
			43	10	12	5	13	3	0
2	G	1	Total	C	H	N	O	P	
			42	10	11	5	13	3	0
2	G	1	Total	C	H	N	O	P	
			42	10	11	5	13	3	0
2	G	1	Total	C	H	N	O	P	
			43	10	12	5	13	3	0
2	H	1	Total	C	H	N	O	P	
			42	10	11	5	13	3	0
2	H	1	Total	C	H	N	O	P	
			42	10	11	5	13	3	0
2	H	1	Total	C	H	N	O	P	
			43	10	12	5	13	3	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg		
			1	1	0	0
3	C	2	Total	Mg		
			2	2	0	0
3	D	1	Total	Mg		
			1	1	0	0
3	E	2	Total	Mg		
			2	2	0	0
3	F	1	Total	Mg		
			1	1	0	0
3	G	1	Total	Mg		
			1	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	277	Total	O		
			277	277	0	0

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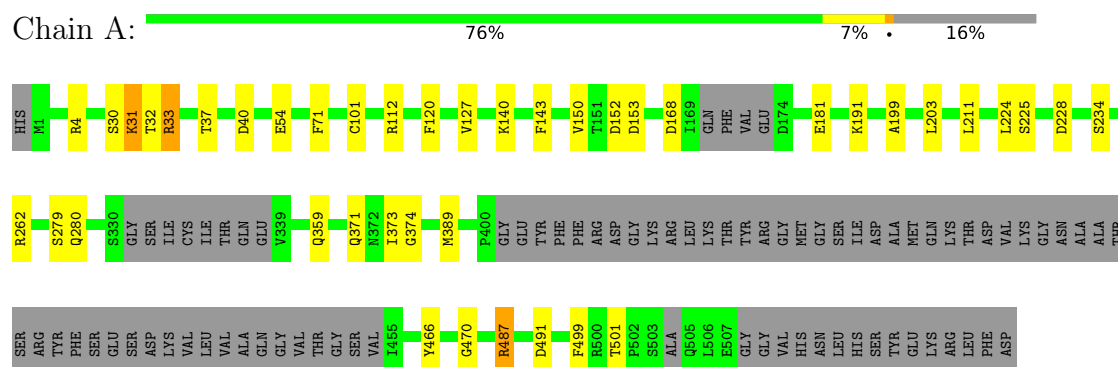
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	283	Total 283	O 283	0	0
4	C	301	Total 301	O 301	0	0
4	D	285	Total 285	O 285	0	0
4	E	51	Total 51	O 51	0	0
4	F	38	Total 38	O 38	0	0
4	G	24	Total 24	O 24	0	0
4	H	17	Total 17	O 17	0	0

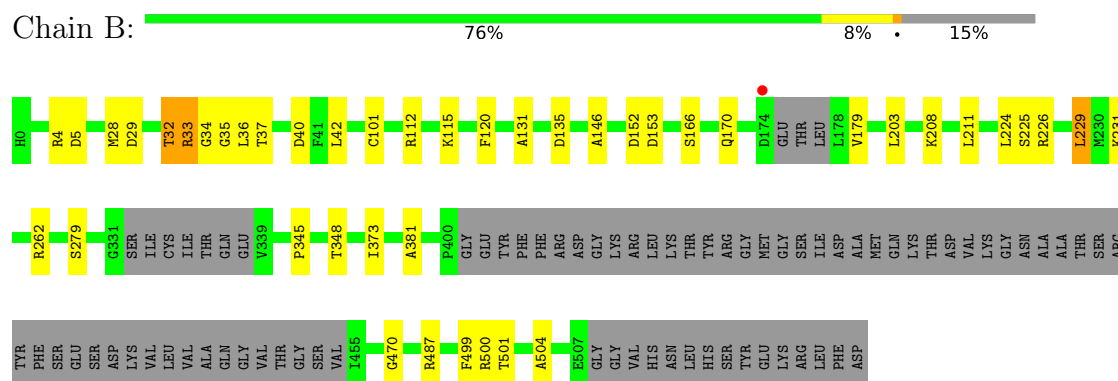
3 Residue-property plots

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

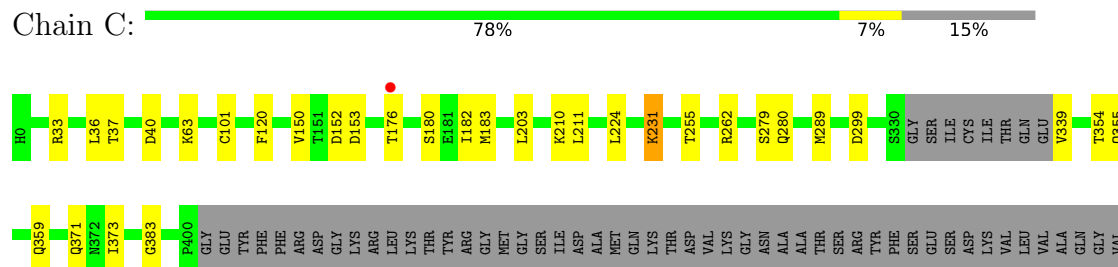
- Molecule 1: Inosine-5'-monophosphate dehydrogenase

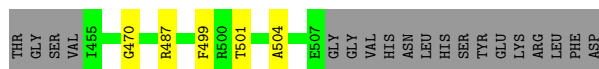


- Molecule 1: Inosine-5'-monophosphate dehydrogenase



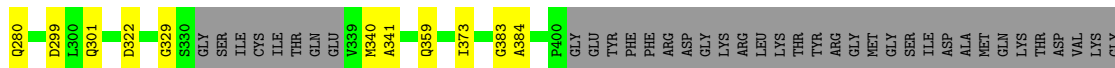
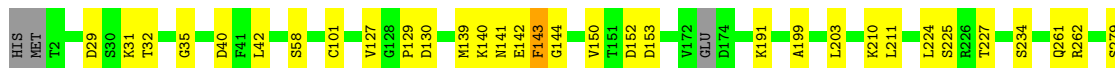
- Molecule 1: Inosine-5'-monophosphate dehydrogenase





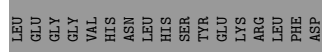
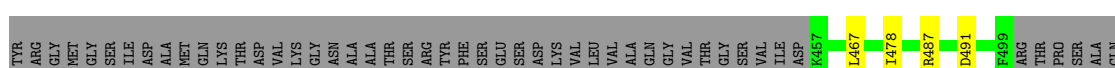
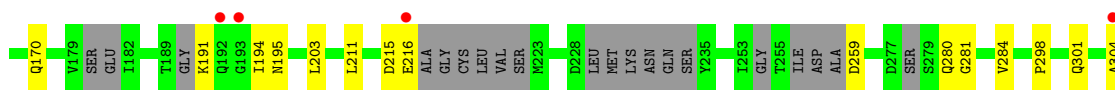
• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain D: 75% 9% 15%



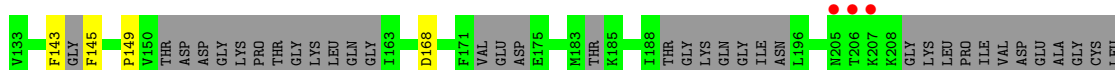
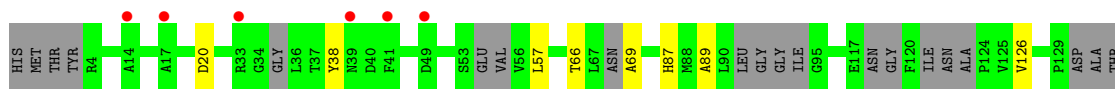
• Molecule 1: Inosine-5'-monophosphate dehydrogenase

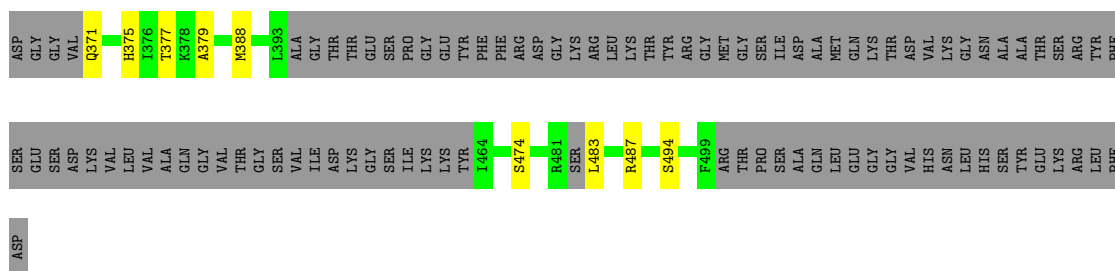
Chain E: 65% 8% 26%



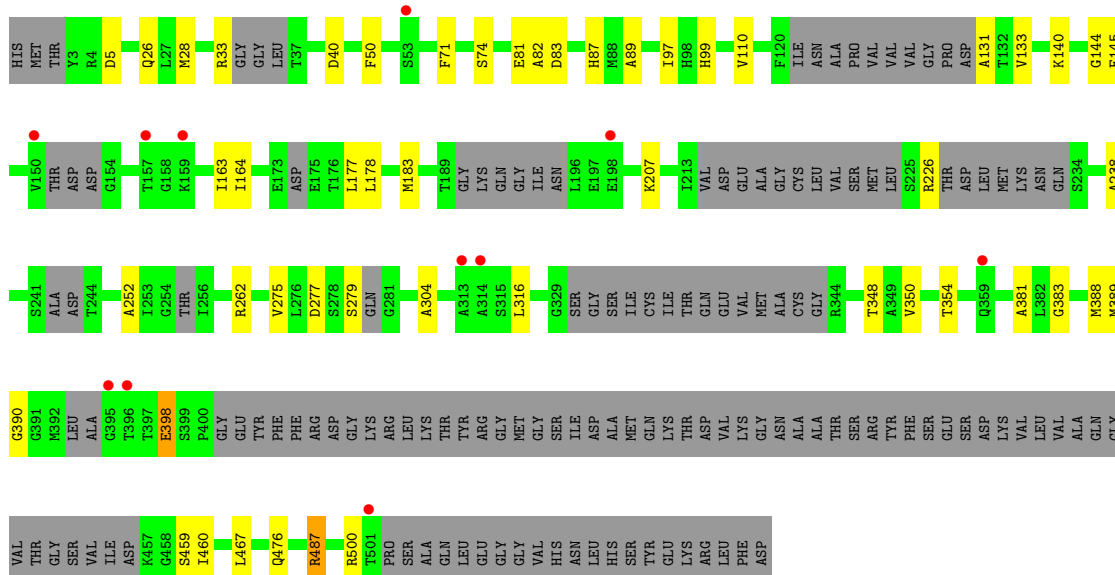
• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain F: 59% 7% 35%

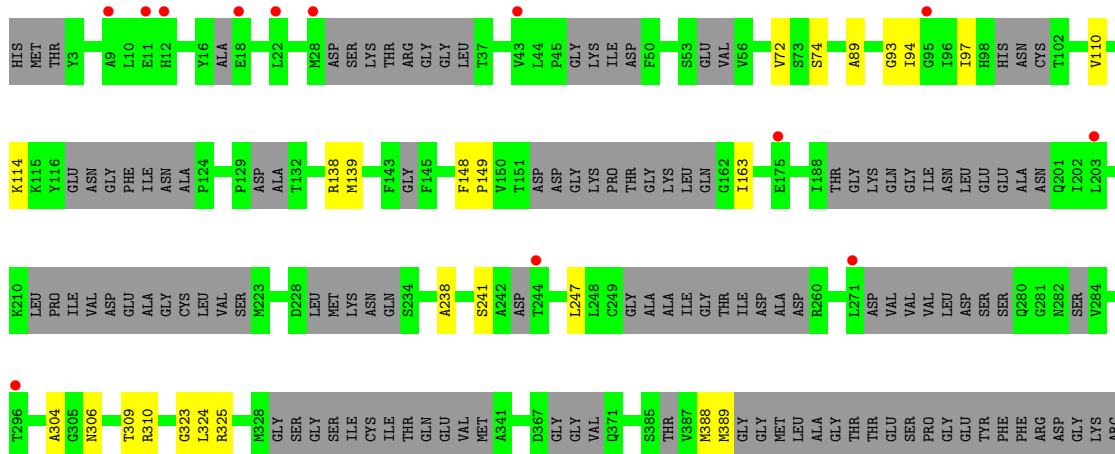


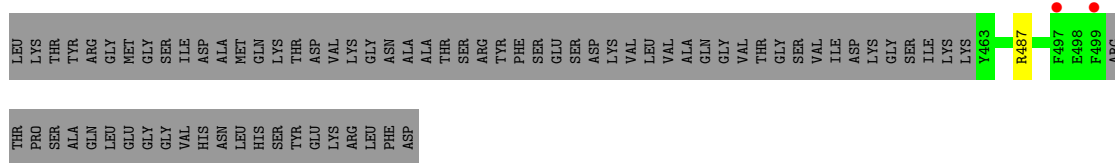


• Molecule 1: Inosine-5'-monophosphate dehydrogenase



• Molecule 1: Inosine-5'-monophosphate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	127.89Å 152.09Å 152.25Å 90.00° 93.03° 90.00°	Depositor
Resolution (Å)	152.04 – 2.40 152.04 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (152.04-2.40) 92.3 (152.04-2.40)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.40Å)	Xtriage
Refinement program	PHENIX (1.11_2567: ???)	Depositor
R, R_{free}	0.249 , 0.271 0.250 , 0.272	Depositor DCC
R_{free} test set	11359 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.651	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	45606	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.37	7/3318 (0.2%)	0.38	0/4484
1	B	0.36	2/3300 (0.1%)	0.43	1/4469 (0.0%)
1	C	0.46	4/3345 (0.1%)	0.47	0/4526
1	D	0.30	2/3322 (0.1%)	0.39	0/4493
1	E	0.52	0/2678	0.51	0/3629
1	F	0.21	0/2241	0.33	0/3038
1	G	0.44	1/2544 (0.0%)	0.47	0/3459
1	H	0.40	1/2004 (0.0%)	0.42	0/2716
All	All	0.39	17/22752 (0.1%)	0.43	1/30814 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	THR	CA-C	7.06	1.59	1.53
1	A	33	ARG	CZ-NH2	6.87	1.42	1.33
1	A	33	ARG	CZ-NH1	6.46	1.41	1.32
1	C	359	GLN	CA-C	6.15	1.61	1.52
1	B	32	THR	CA-C	5.68	1.59	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	231	LYS	N-CA-C	-5.33	102.16	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	305	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3275	3293	3286	39	0
1	B	3255	3187	3194	40	0
1	C	3296	3260	3260	26	0
1	D	3274	3267	3262	40	0
1	E	2655	2384	2365	47	0
1	F	2222	1832	1816	22	0
1	G	2514	2066	2057	42	0
1	H	1997	1529	1508	15	0
2	A	93	34	36	6	0
2	B	155	56	60	4	0
2	C	93	34	36	3	0
2	D	93	34	36	4	0
2	E	93	34	36	1	0
2	F	31	12	12	1	0
2	G	93	34	36	4	0
2	H	93	34	36	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
3	E	2	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
4	A	277	0	0	11	0
4	B	283	0	0	8	0
4	C	301	0	0	8	2
4	D	285	0	0	8	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	51	0	0	5	0
4	F	38	0	0	4	0
4	G	24	0	0	3	0
4	H	17	0	0	0	0
All	All	24516	21090	21036	257	2

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 6.

The worst 5 of 257 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:G:133:VAL:HG23	1:G:177:LEU:O	1.38	1.22
1:E:64:LYS:HB2	1:E:301:GLN:NE2	1.54	1.20
1:E:71:PHE:CD1	1:E:389:MET:CE	2.26	1.18
1:E:71:PHE:CD1	1:E:389:MET:HE1	1.81	1.15
1:E:71:PHE:HD1	1:E:389:MET:CE	1.57	1.14

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:705:HOH:O	4:D:802:HOH:O[2_554]	2.09	0.11
4:C:975:HOH:O	4:D:873:HOH:O[2_554]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	430/523 (82%)	421 (98%)	9 (2%)	0	100	100
1	B	436/523 (83%)	430 (99%)	6 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	441/523 (84%)	432 (98%)	9 (2%)	0	100	100
1	D	436/523 (83%)	426 (98%)	10 (2%)	0	100	100
1	E	356/523 (68%)	343 (96%)	13 (4%)	0	100	100
1	F	306/523 (58%)	295 (96%)	11 (4%)	0	100	100
1	G	354/523 (68%)	346 (98%)	8 (2%)	0	100	100
1	H	279/523 (53%)	272 (98%)	7 (2%)	0	100	100
All	All	3038/4184 (73%)	2965 (98%)	73 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	350/430 (81%)	347 (99%)	3 (1%)	70	85
1	B	337/430 (78%)	336 (100%)	1 (0%)	86	93
1	C	345/430 (80%)	343 (99%)	2 (1%)	78	89
1	D	343/430 (80%)	339 (99%)	4 (1%)	63	81
1	E	234/430 (54%)	233 (100%)	1 (0%)	84	92
1	F	165/430 (38%)	164 (99%)	1 (1%)	78	89
1	G	191/430 (44%)	189 (99%)	2 (1%)	68	84
1	H	128/430 (30%)	127 (99%)	1 (1%)	73	86
All	All	2093/3440 (61%)	2078 (99%)	15 (1%)	76	88

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	191	LYS
1	G	487	ARG
1	D	280	GLN
1	H	487	ARG

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Mol	Chain	Res	Type
1	F	487	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	359	GLN
1	H	12	HIS
1	H	359	GLN
1	C	359	GLN
1	D	12	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

Of 32 ligands modelled in this entry, 8 are monoatomic - leaving 24 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	$\# Z > 2$
2	ATP	G	601	3	32,33,33	4.47	10 (31%)	48,52,52	2.33	12 (25%)
2	ATP	B	601	3	32,33,33	4.37	8 (25%)	48,52,52	2.32	13 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	C	601	3	32,33,33	4.45	9 (28%)	48,52,52	2.36	14 (29%)
2	ATP	A	603	-	32,33,33	4.56	10 (31%)	48,52,52	2.29	13 (27%)
2	ATP	H	603	-	32,33,33	4.54	10 (31%)	48,52,52	2.31	13 (27%)
2	ATP	D	602	3	32,33,33	4.05	8 (25%)	48,52,52	2.26	13 (27%)
2	ATP	F	601	-	32,33,33	4.58	10 (31%)	48,52,52	2.27	13 (27%)
2	ATP	B	606	3	32,33,33	4.37	10 (31%)	48,52,52	2.31	13 (27%)
2	ATP	G	602	3	32,33,33	4.53	10 (31%)	48,52,52	2.30	12 (25%)
2	ATP	H	601	3	32,33,33	4.45	8 (25%)	48,52,52	2.31	13 (27%)
2	ATP	E	601	3	32,33,33	4.81	9 (28%)	48,52,52	2.20	13 (27%)
2	ATP	B	605	3	32,33,33	4.47	9 (28%)	48,52,52	2.31	12 (25%)
2	ATP	B	602	3	32,33,33	4.42	7 (21%)	48,52,52	2.32	12 (25%)
2	ATP	E	602	3	32,33,33	4.37	10 (31%)	48,52,52	2.33	13 (27%)
2	ATP	C	603	-	32,33,33	4.52	10 (31%)	48,52,52	2.27	11 (22%)
2	ATP	E	603	-	32,33,33	4.69	10 (31%)	48,52,52	2.22	11 (22%)
2	ATP	G	603	-	32,33,33	4.77	10 (31%)	48,52,52	2.31	13 (27%)
2	ATP	A	602	3	32,33,33	4.38	9 (28%)	48,52,52	2.30	13 (27%)
2	ATP	A	601	3	32,33,33	4.29	9 (28%)	48,52,52	2.31	12 (25%)
2	ATP	B	603	-	32,33,33	4.60	10 (31%)	48,52,52	2.32	13 (27%)
2	ATP	C	602	3	32,33,33	4.37	9 (28%)	48,52,52	2.36	14 (29%)
2	ATP	H	602	3	32,33,33	4.43	10 (31%)	48,52,52	2.27	12 (25%)
2	ATP	D	603	-	32,33,33	4.47	9 (28%)	48,52,52	2.30	13 (27%)
2	ATP	D	601	3	32,33,33	4.40	10 (31%)	48,52,52	2.34	13 (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
2	ATP	G	601	3	-	4/22/38/38	0/3/3/3
2	ATP	B	601	3	-	4/22/38/38	0/3/3/3
2	ATP	C	601	3	-	7/22/38/38	0/3/3/3
2	ATP	A	603	-	-	2/22/38/38	0/3/3/3
2	ATP	H	603	-	-	2/22/38/38	0/3/3/3
2	ATP	D	602	3	-	6/22/38/38	0/3/3/3
2	ATP	F	601	-	-	5/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	B	606	3	-	3/22/38/38	0/3/3/3
2	ATP	G	602	3	-	1/22/38/38	0/3/3/3
2	ATP	H	601	3	-	4/22/38/38	0/3/3/3
2	ATP	E	601	3	-	2/22/38/38	0/3/3/3
2	ATP	B	605	3	-	5/22/38/38	0/3/3/3
2	ATP	B	602	3	-	0/22/38/38	0/3/3/3
2	ATP	E	602	3	-	2/22/38/38	0/3/3/3
2	ATP	C	603	-	-	1/22/38/38	0/3/3/3
2	ATP	E	603	-	-	2/22/38/38	0/3/3/3
2	ATP	G	603	-	-	4/22/38/38	0/3/3/3
2	ATP	A	602	3	-	4/22/38/38	0/3/3/3
2	ATP	A	601	3	-	2/22/38/38	0/3/3/3
2	ATP	B	603	-	-	3/22/38/38	0/3/3/3
2	ATP	C	602	3	-	5/22/38/38	0/3/3/3
2	ATP	H	602	3	-	6/22/38/38	0/3/3/3
2	ATP	D	603	-	-	2/22/38/38	0/3/3/3
2	ATP	D	601	3	-	3/22/38/38	0/3/3/3

The worst 5 of 224 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	ATP	PB-O3A	24.37	1.85	1.59
2	G	603	ATP	PB-O3A	24.31	1.85	1.59
2	E	603	ATP	PB-O3A	23.55	1.84	1.59
2	B	603	ATP	PB-O3A	23.38	1.84	1.59
2	F	601	ATP	PB-O3A	22.87	1.84	1.59

The worst 5 of 304 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	602	ATP	O3A-PB-O1B	-7.66	87.66	110.70
2	B	603	ATP	O3A-PB-O1B	-7.43	88.36	110.70
2	C	602	ATP	O3A-PB-O1B	-7.38	88.50	110.70
2	A	603	ATP	O3A-PB-O1B	-7.26	88.85	110.70
2	F	601	ATP	O3A-PB-O1B	-7.25	88.89	110.70

There are no chirality outliers.

5 of 79 torsion outliers are listed below:

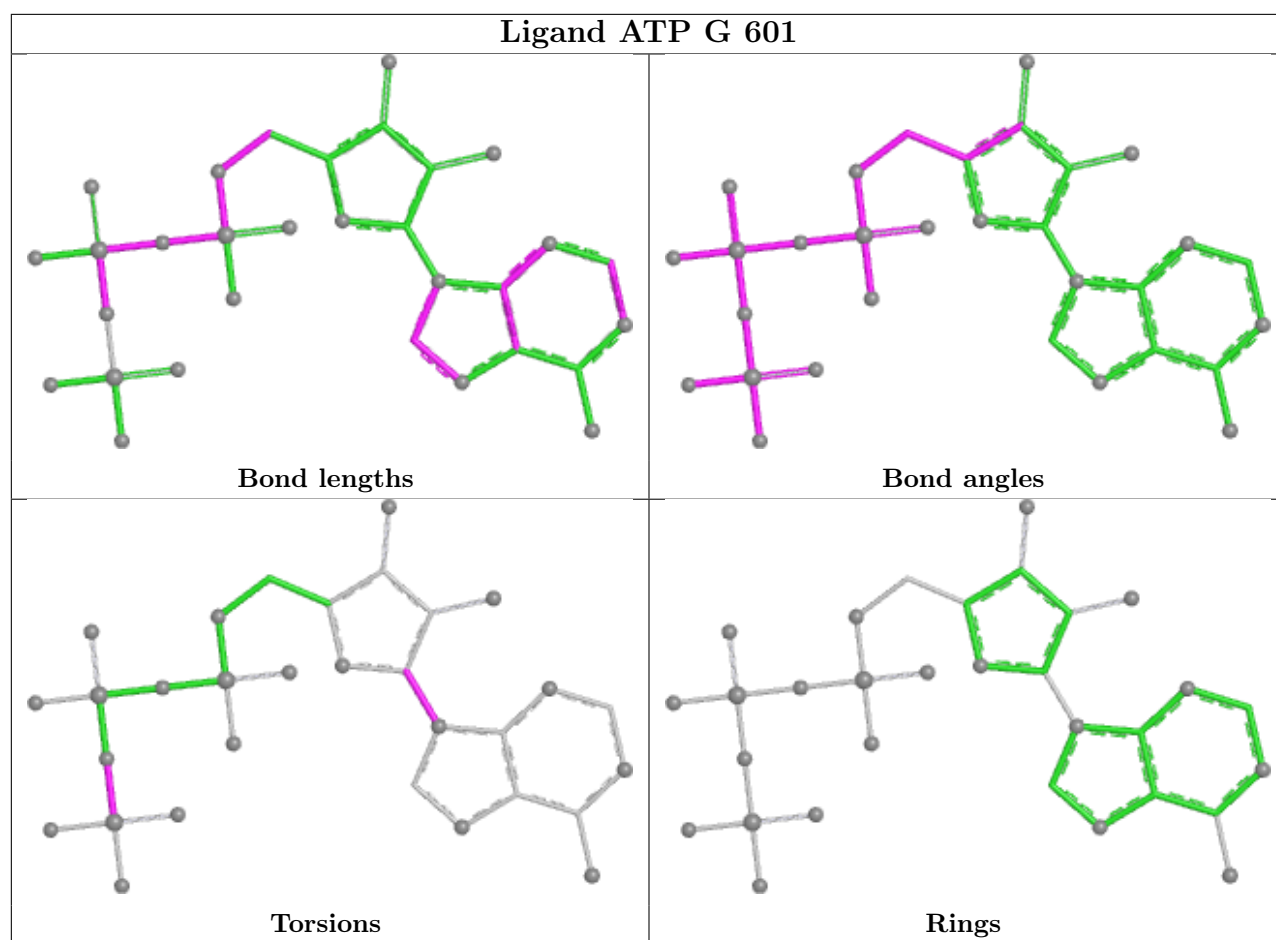
Mol	Chain	Res	Type	Atoms
2	A	602	ATP	C5'-O5'-PA-O1A
2	A	602	ATP	C5'-O5'-PA-O2A
2	A	602	ATP	C5'-O5'-PA-O3A
2	B	601	ATP	PB-O3B-PG-O3G
2	B	605	ATP	C5'-O5'-PA-O2A

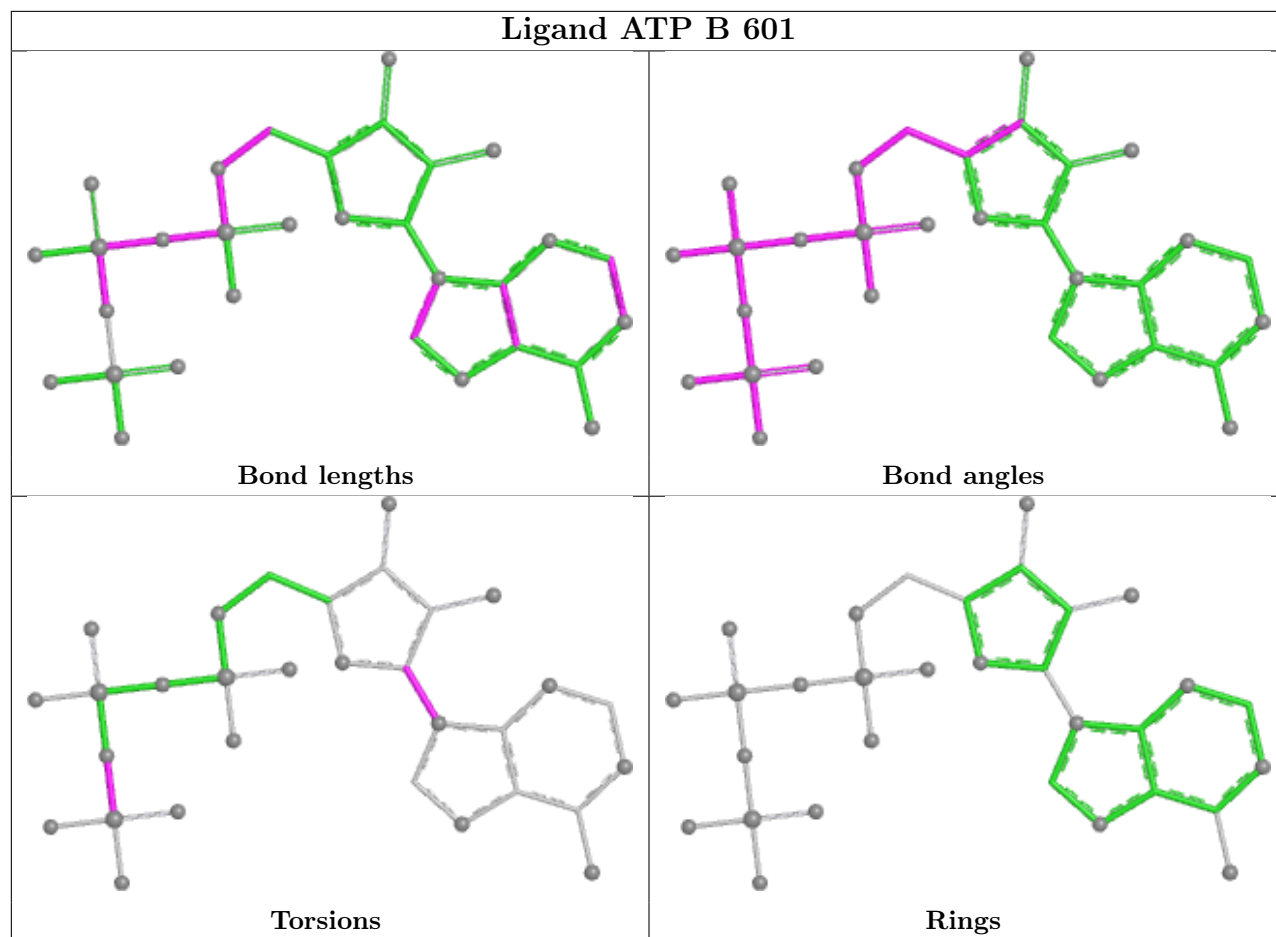
There are no ring outliers.

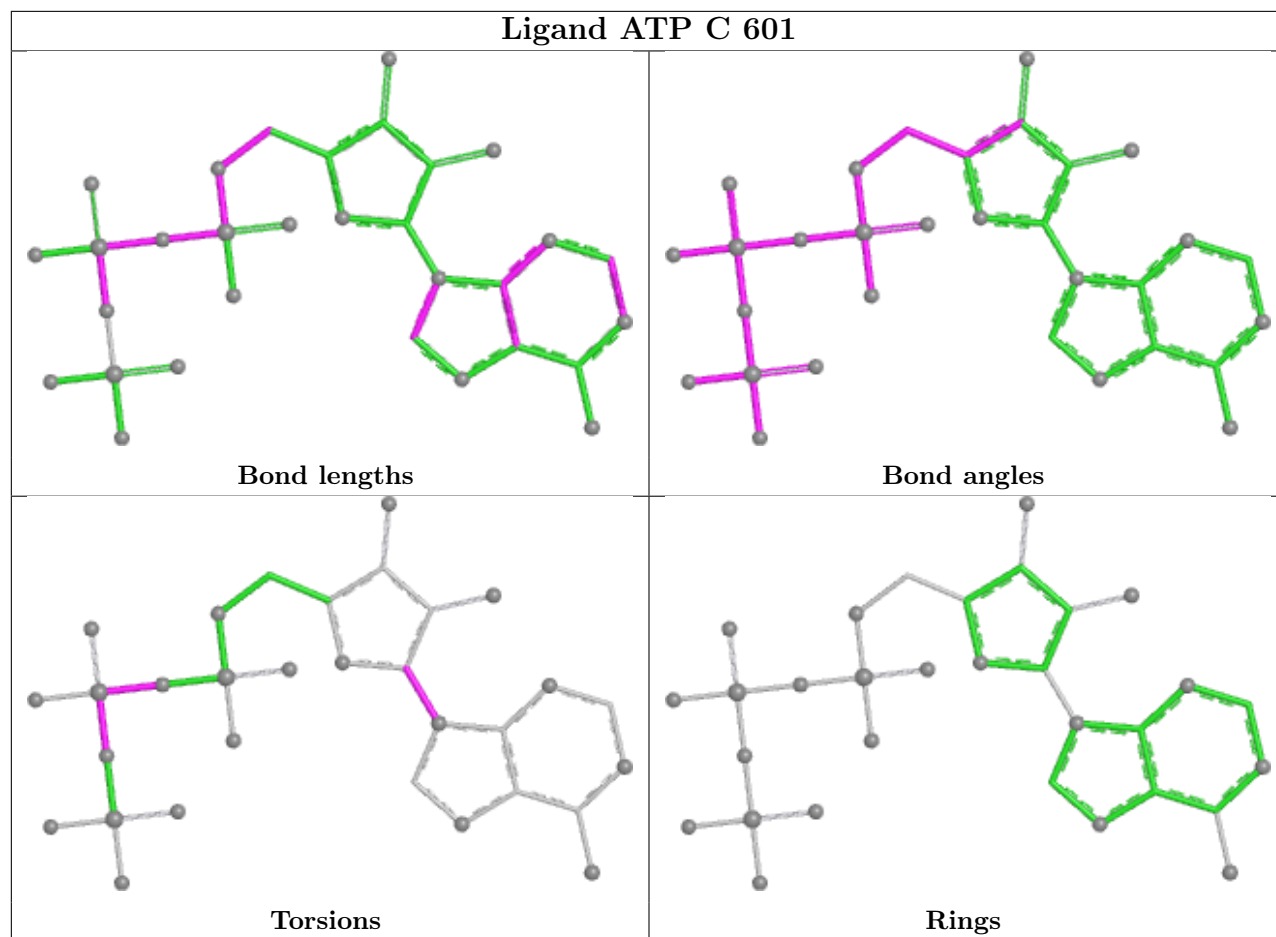
15 monomers are involved in 23 short contacts:

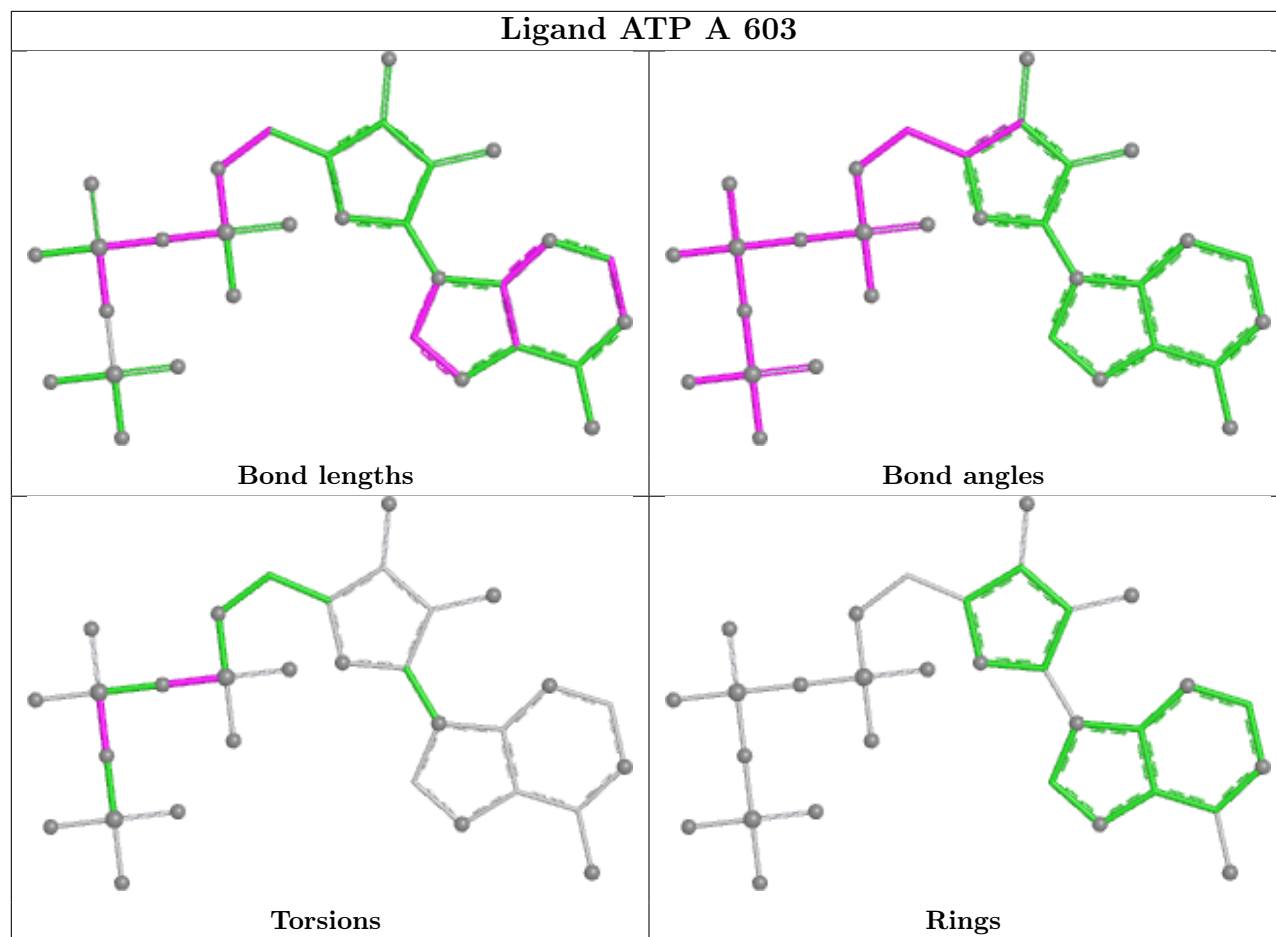
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	ATP	2	0
2	A	603	ATP	2	0
2	D	602	ATP	3	0
2	F	601	ATP	1	0
2	G	602	ATP	1	0
2	E	601	ATP	1	0
2	B	605	ATP	2	0
2	B	602	ATP	1	0
2	C	603	ATP	1	0
2	G	603	ATP	3	0
2	A	602	ATP	2	0
2	A	601	ATP	2	0
2	B	603	ATP	1	0
2	C	602	ATP	1	0
2	D	603	ATP	1	0

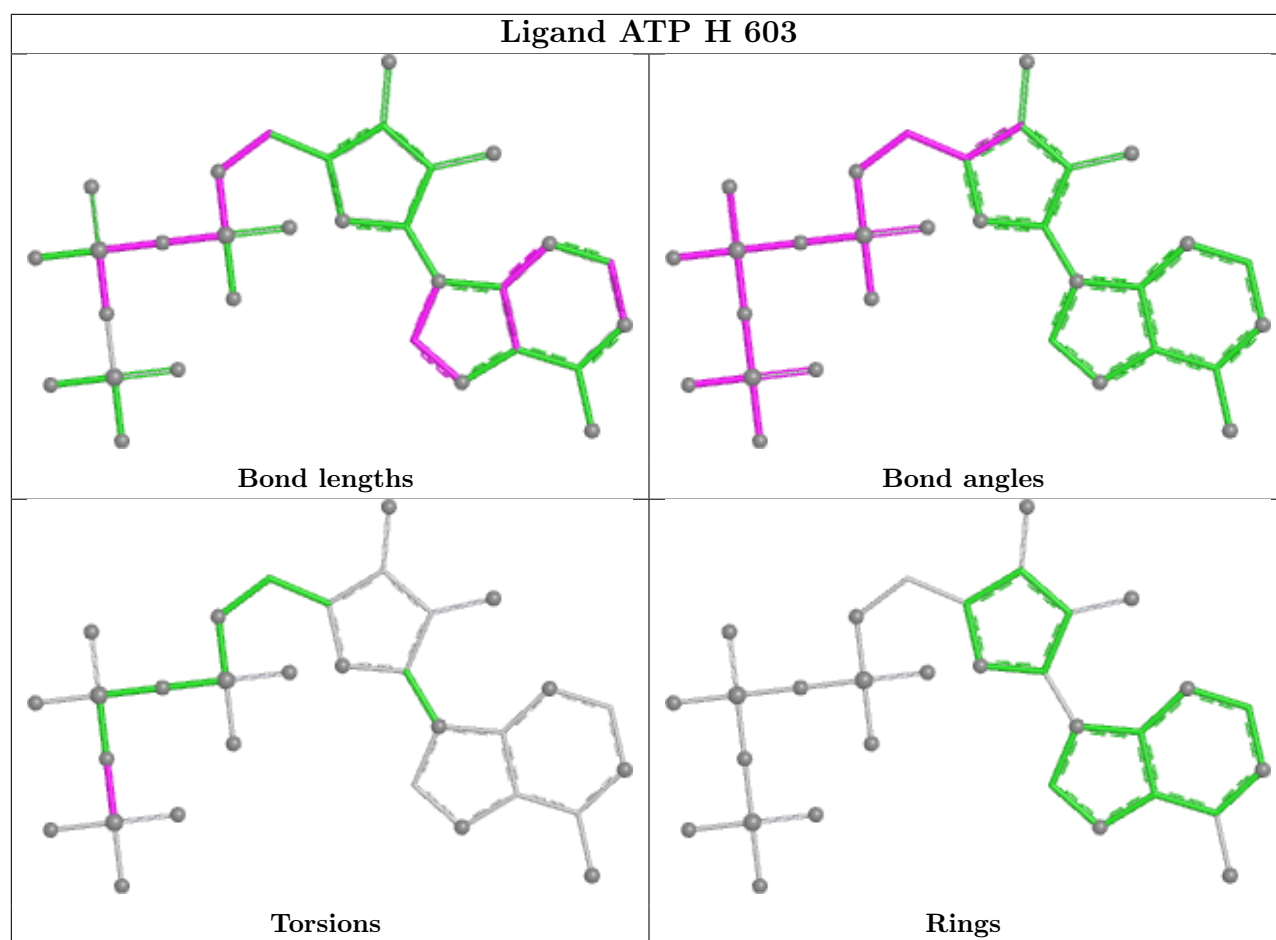
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

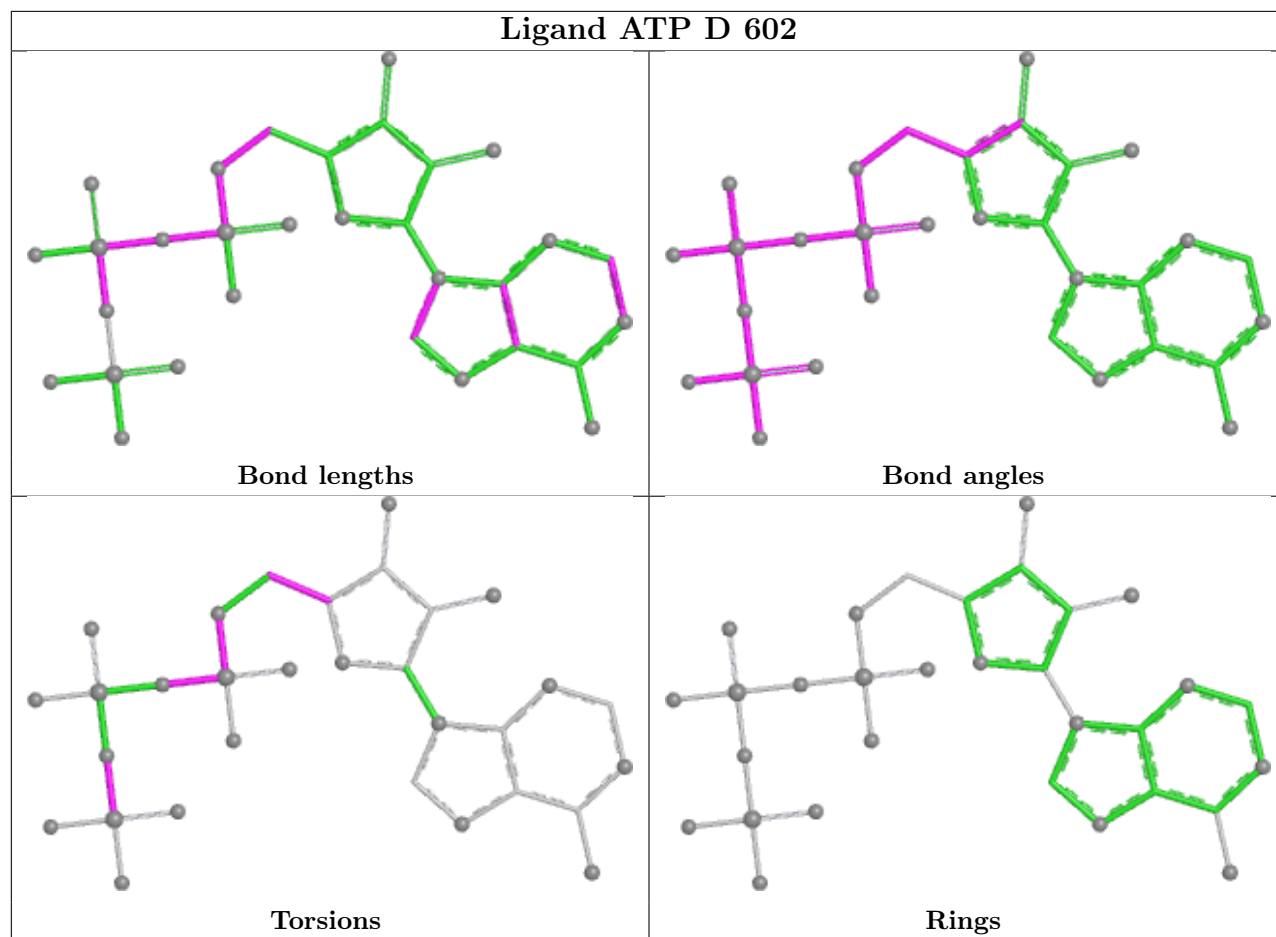




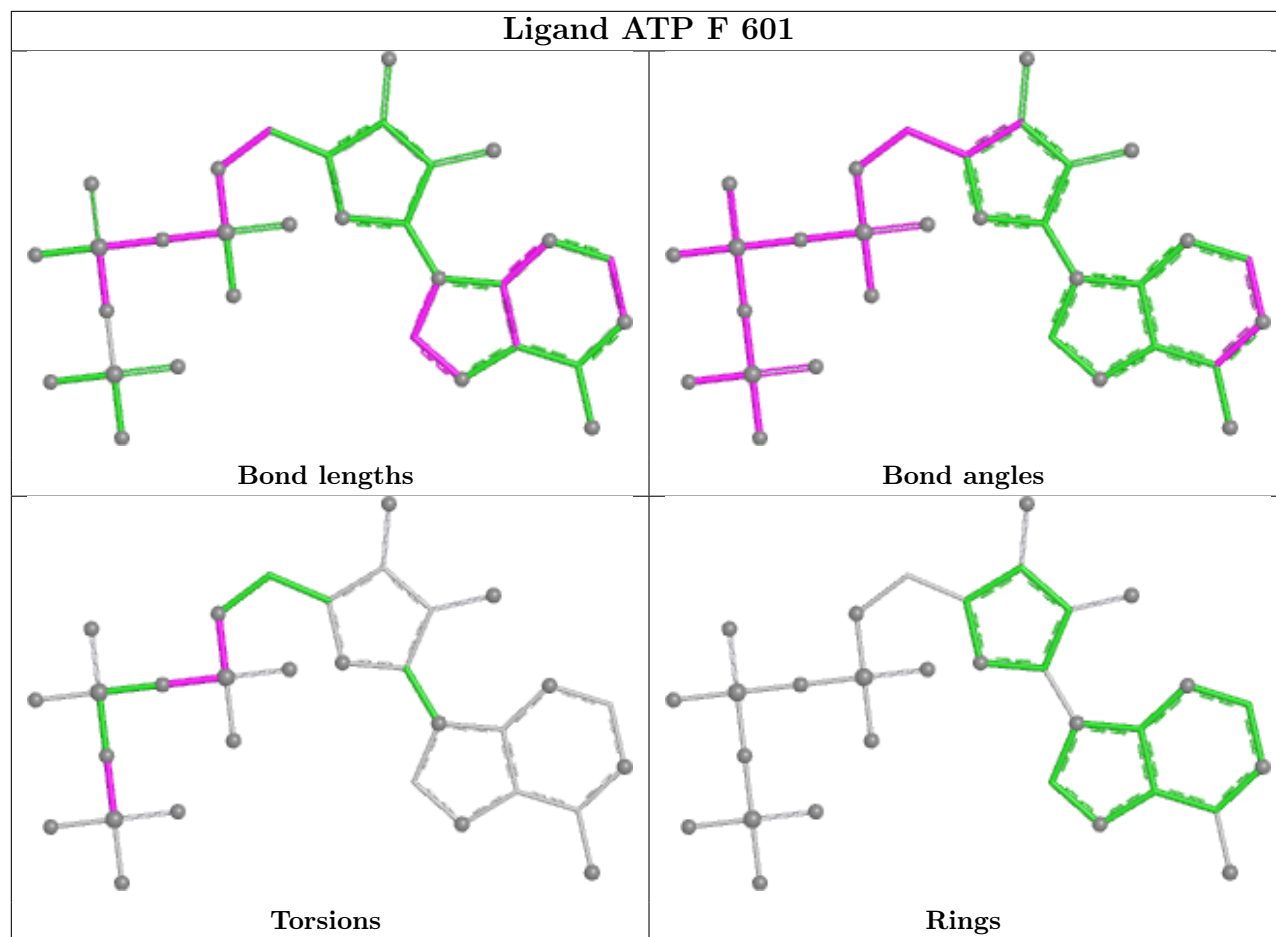


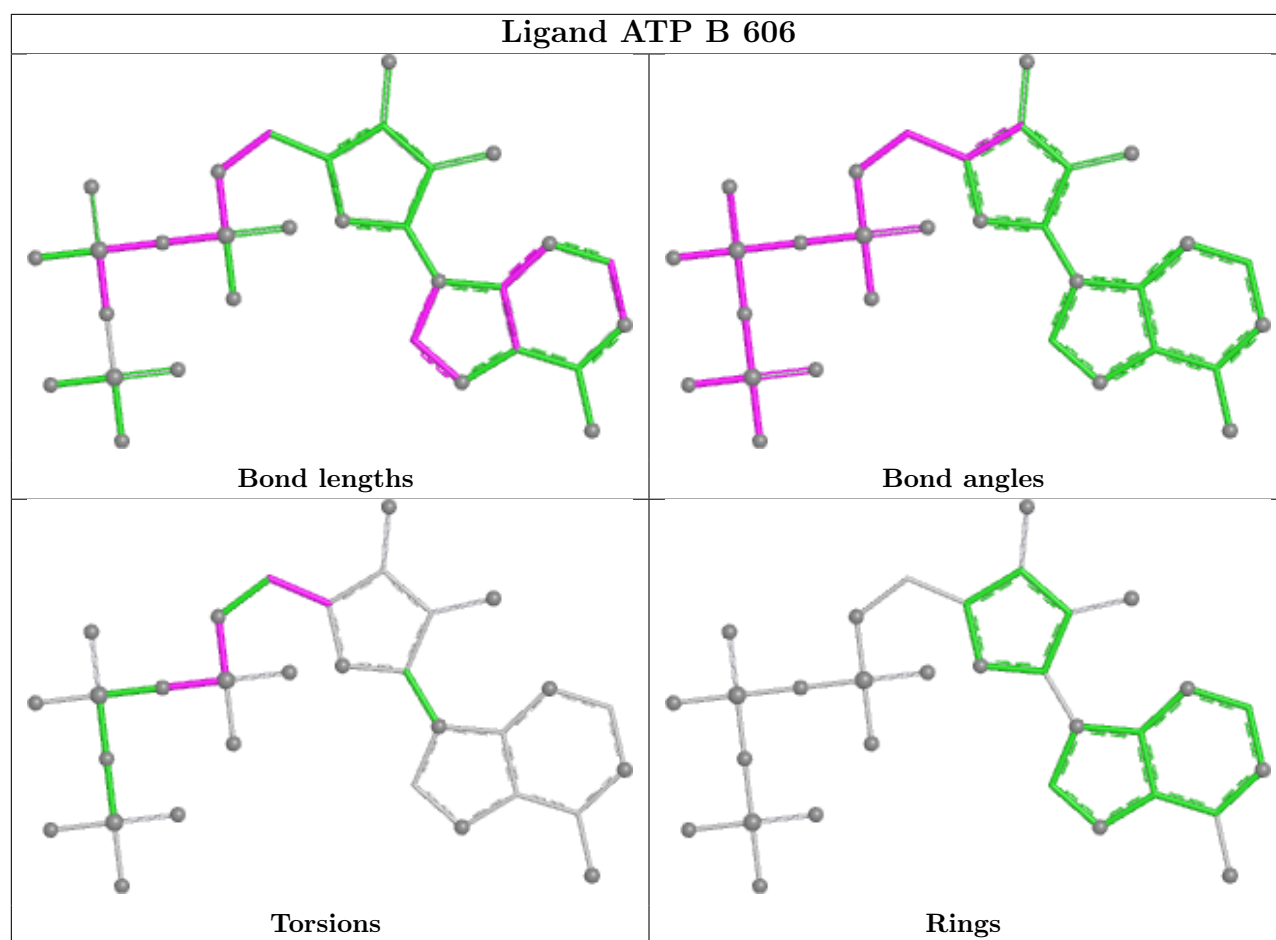


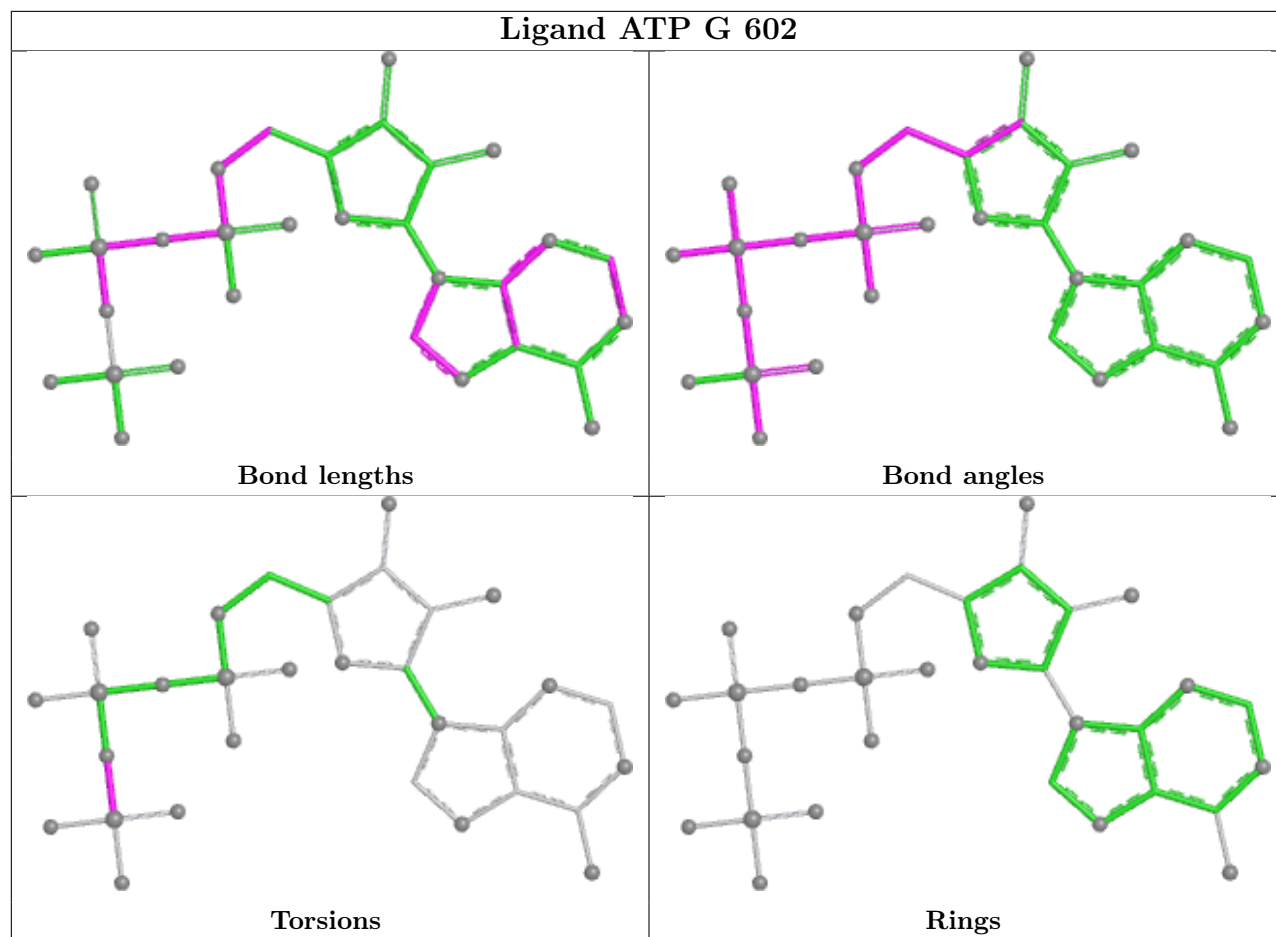


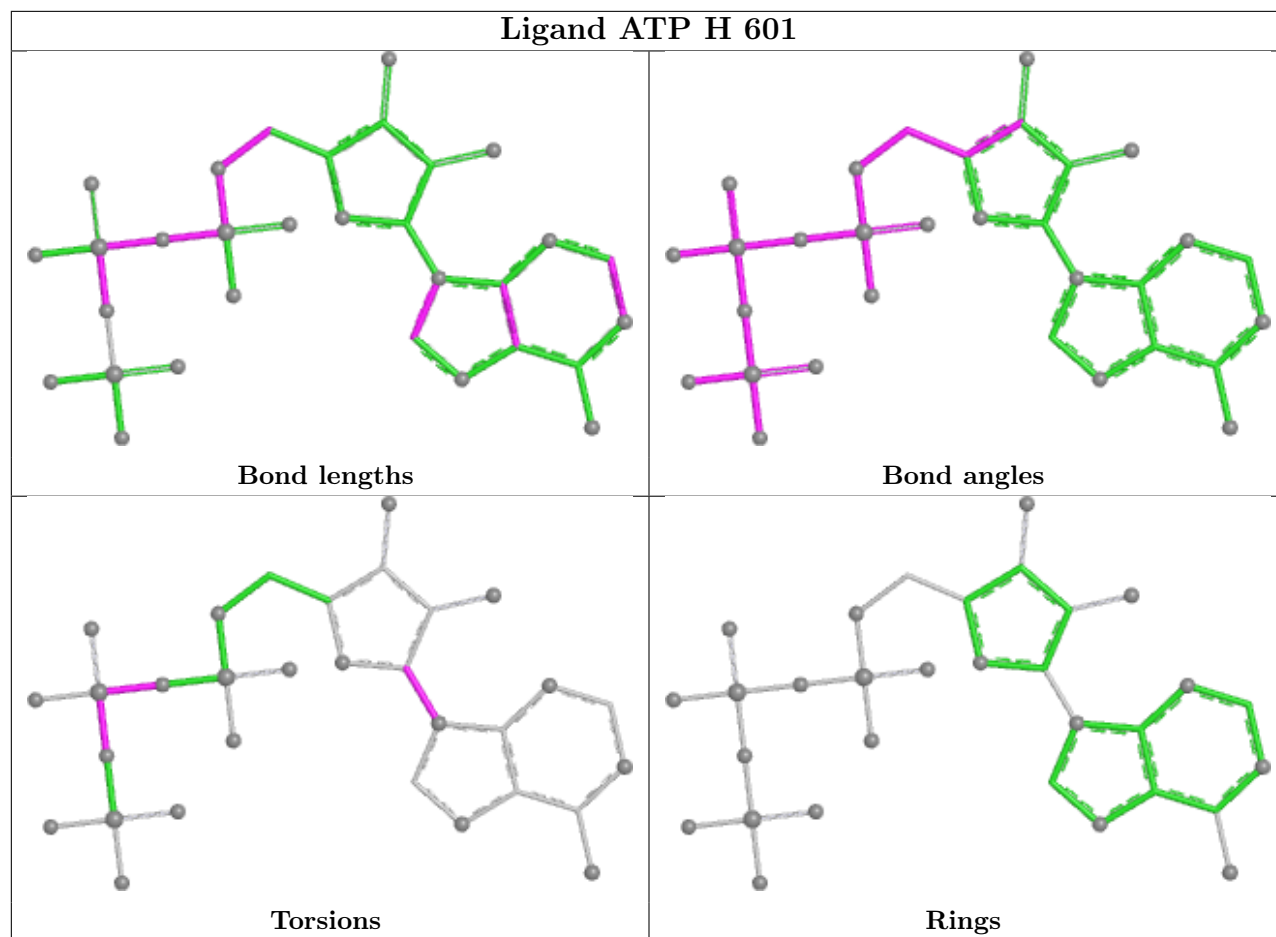


Ligand ATP F 601

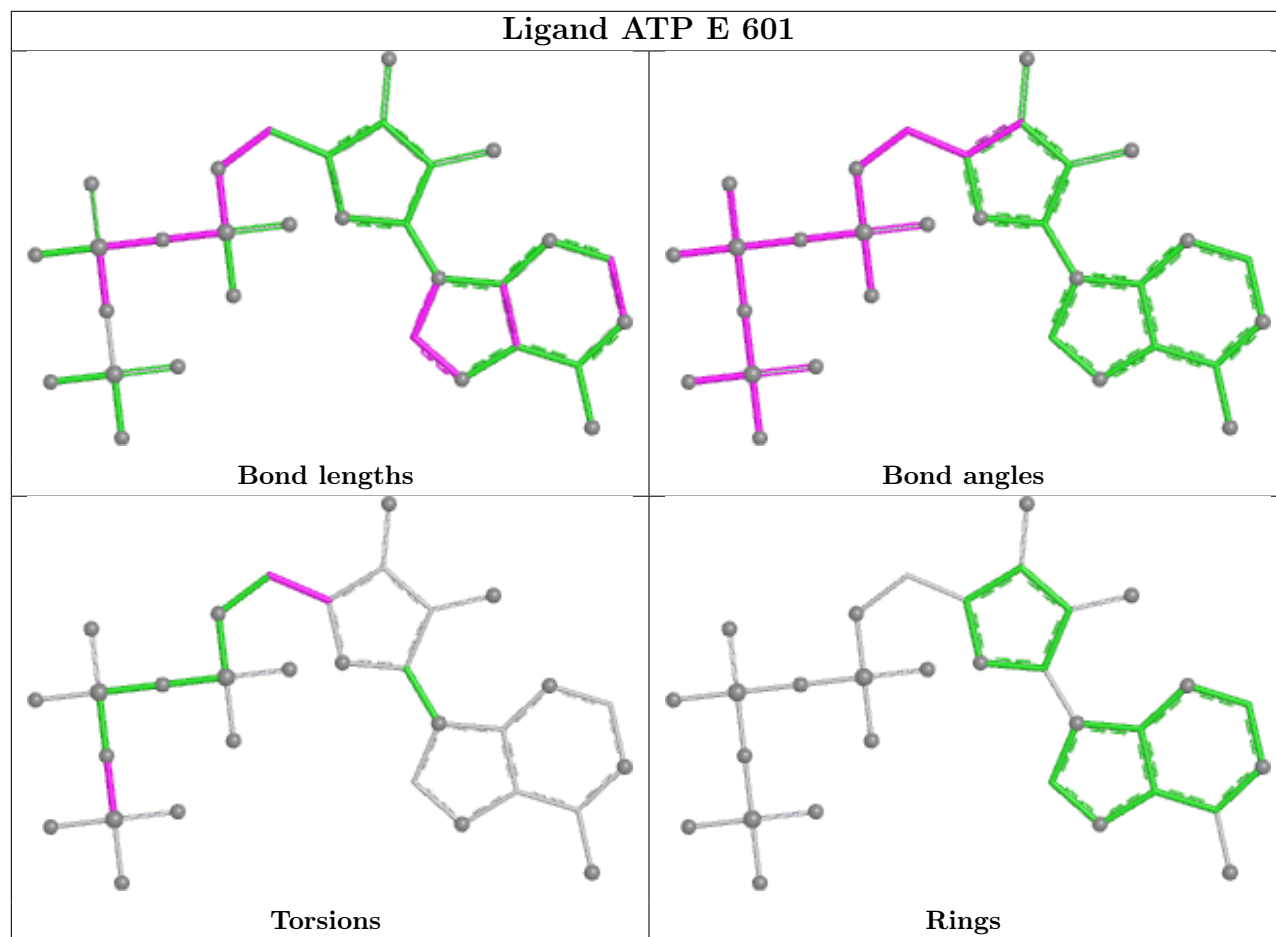


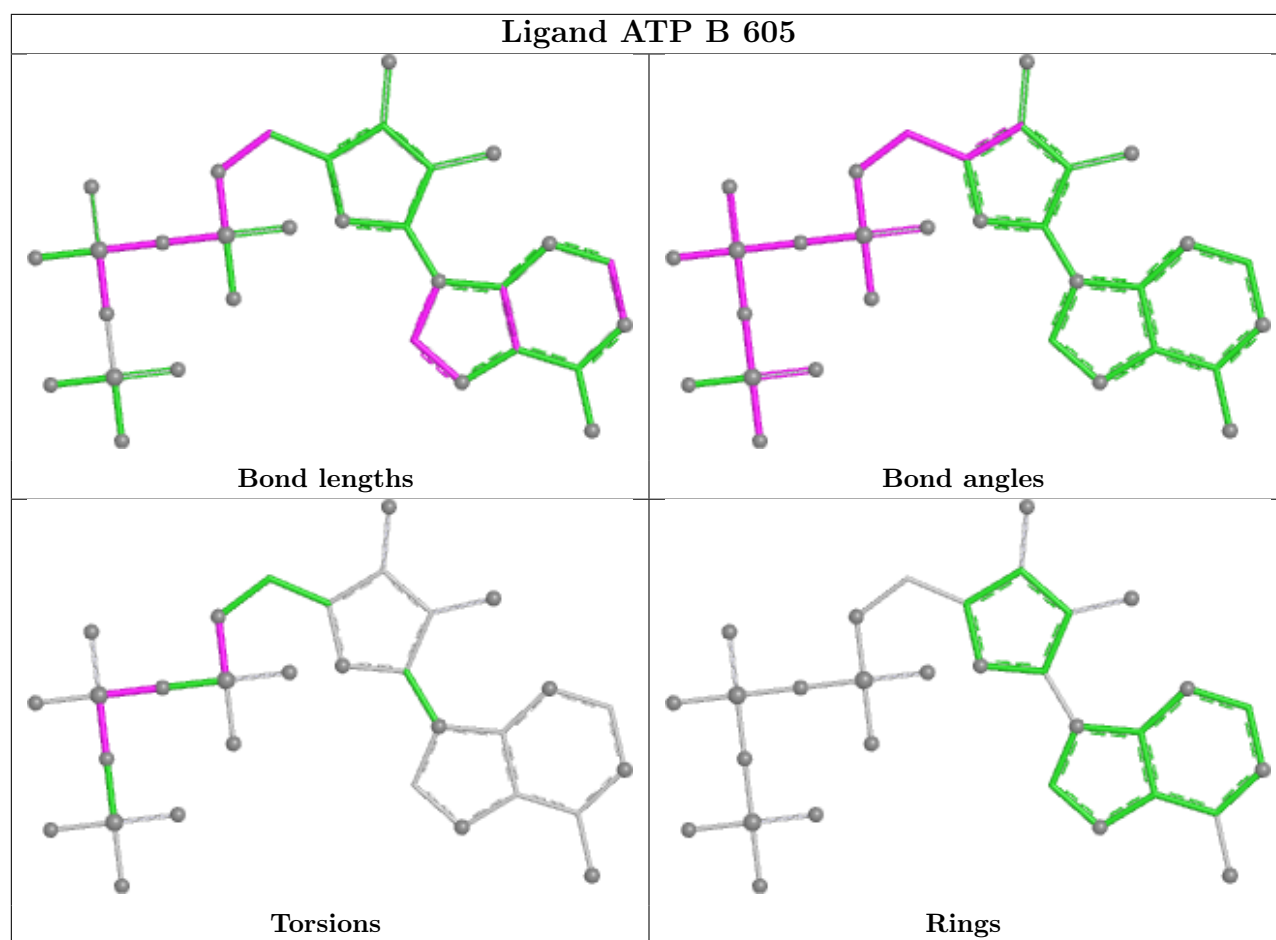


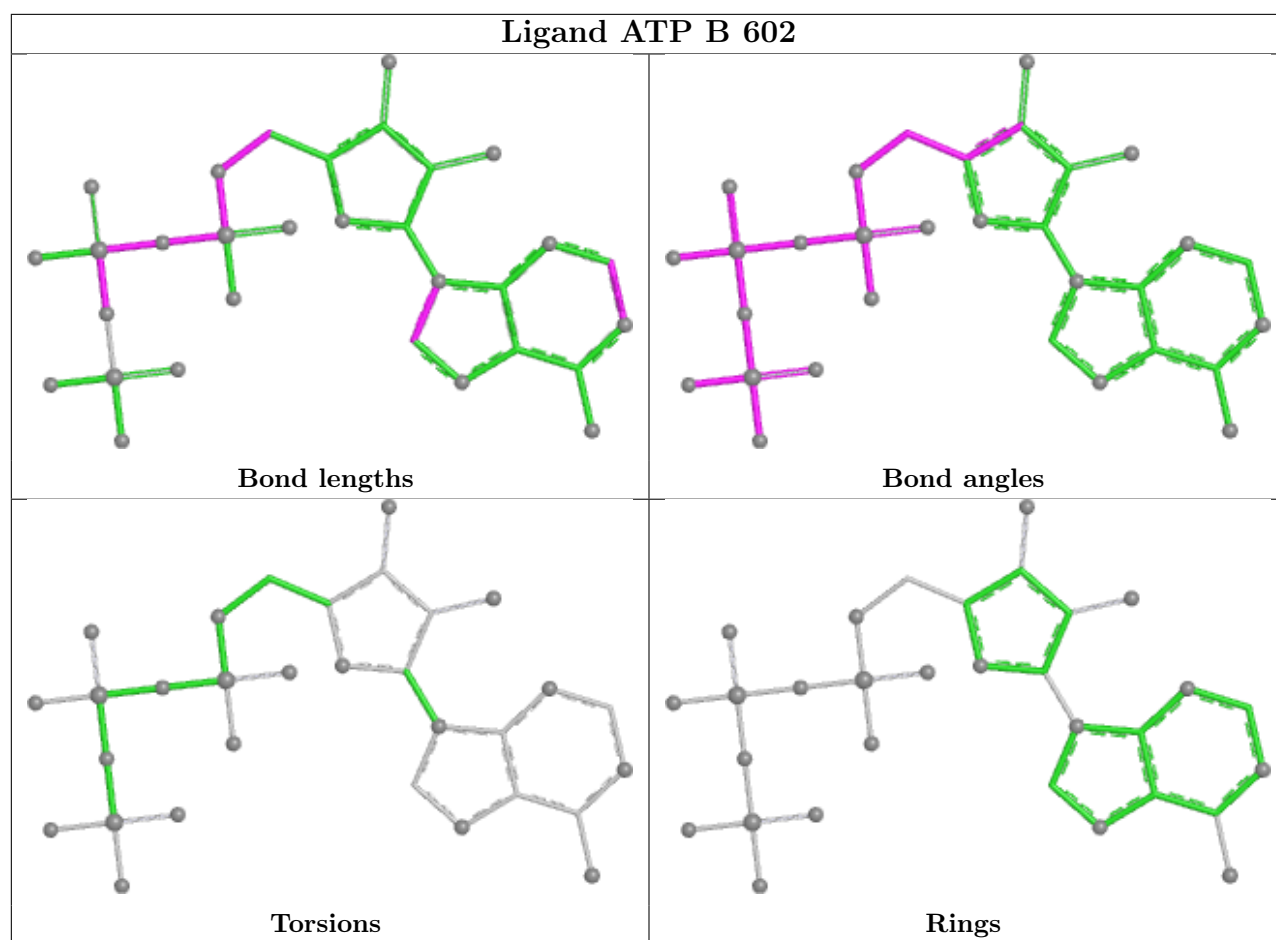


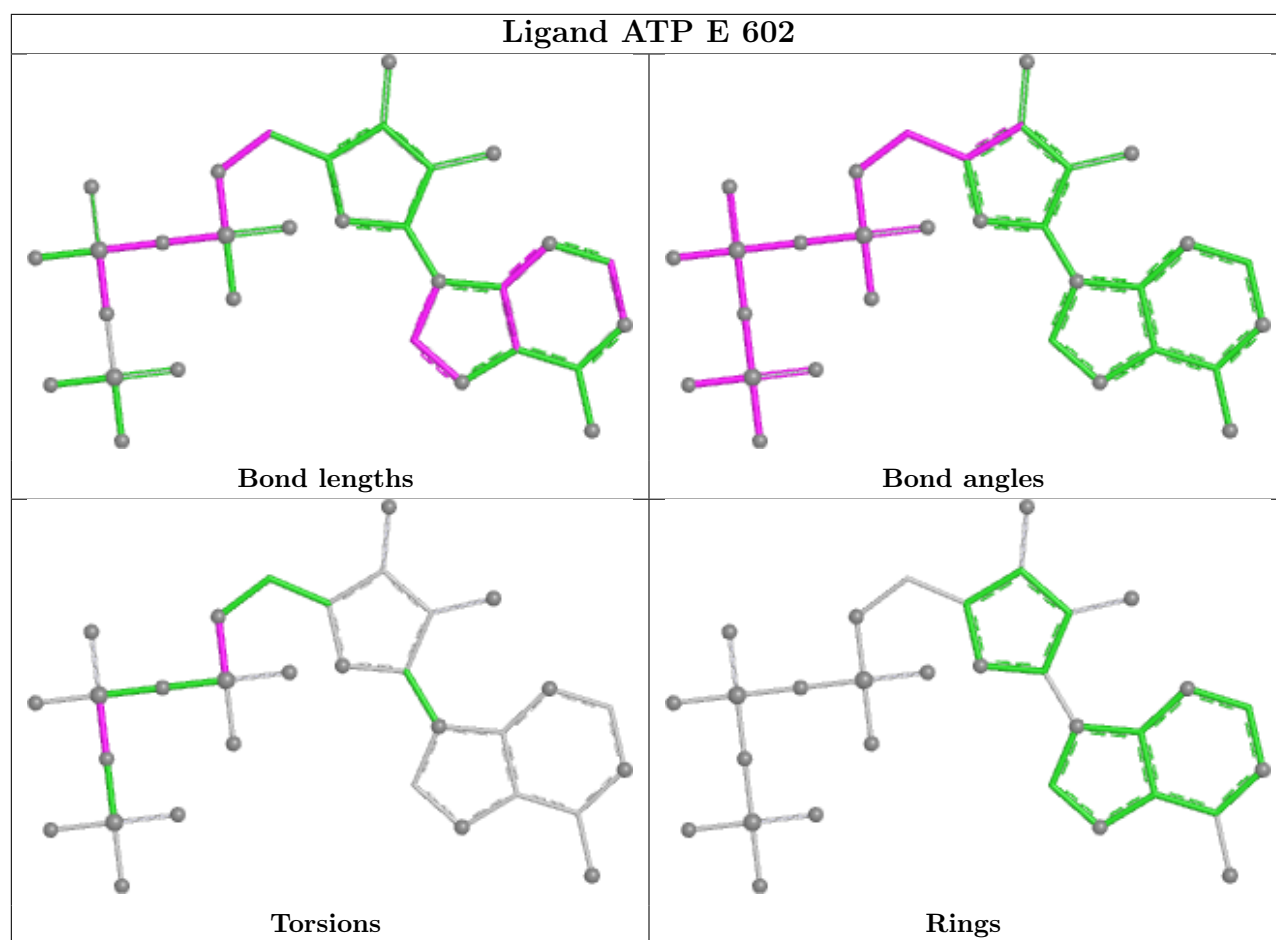


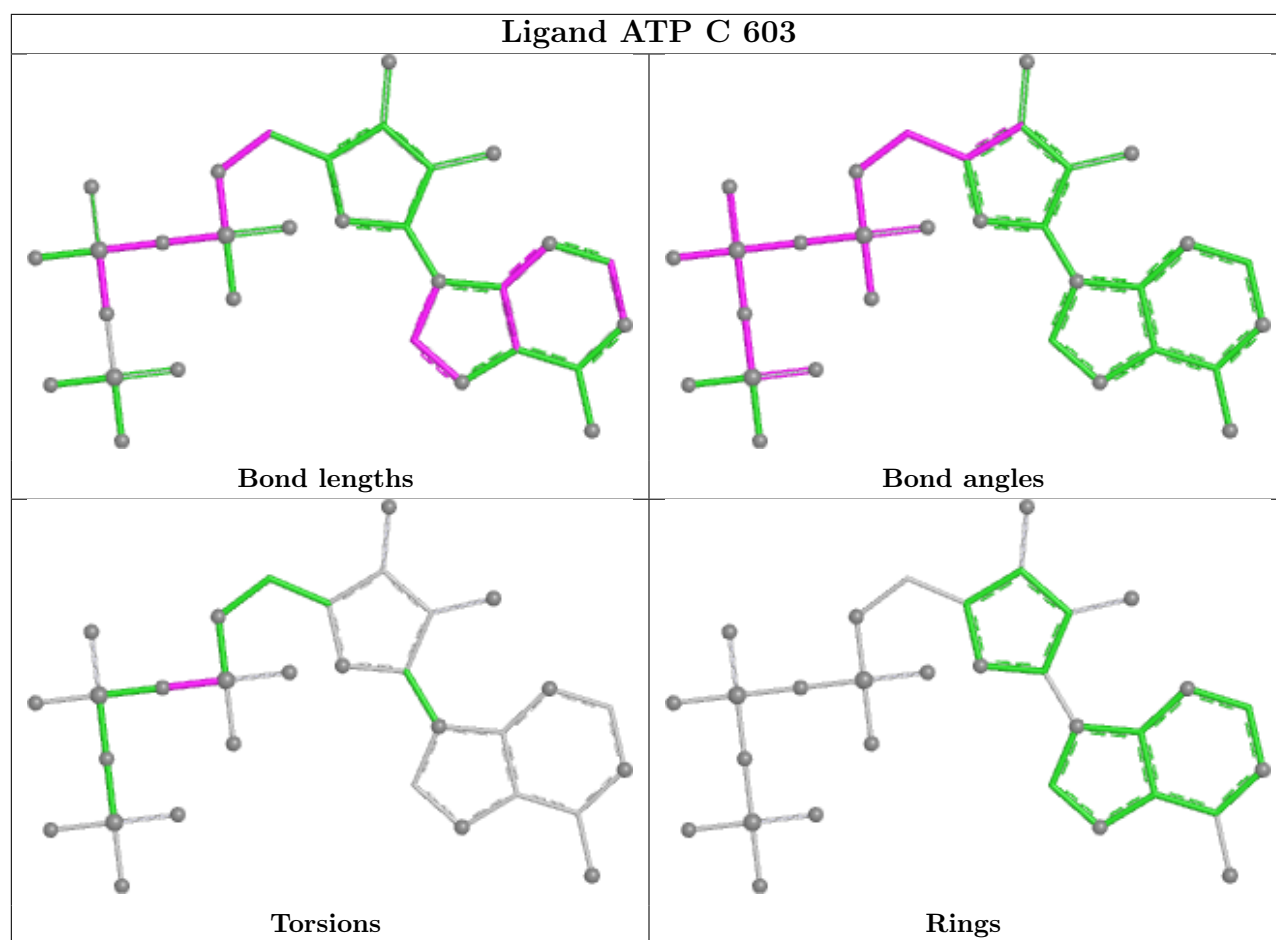
Ligand ATP E 601



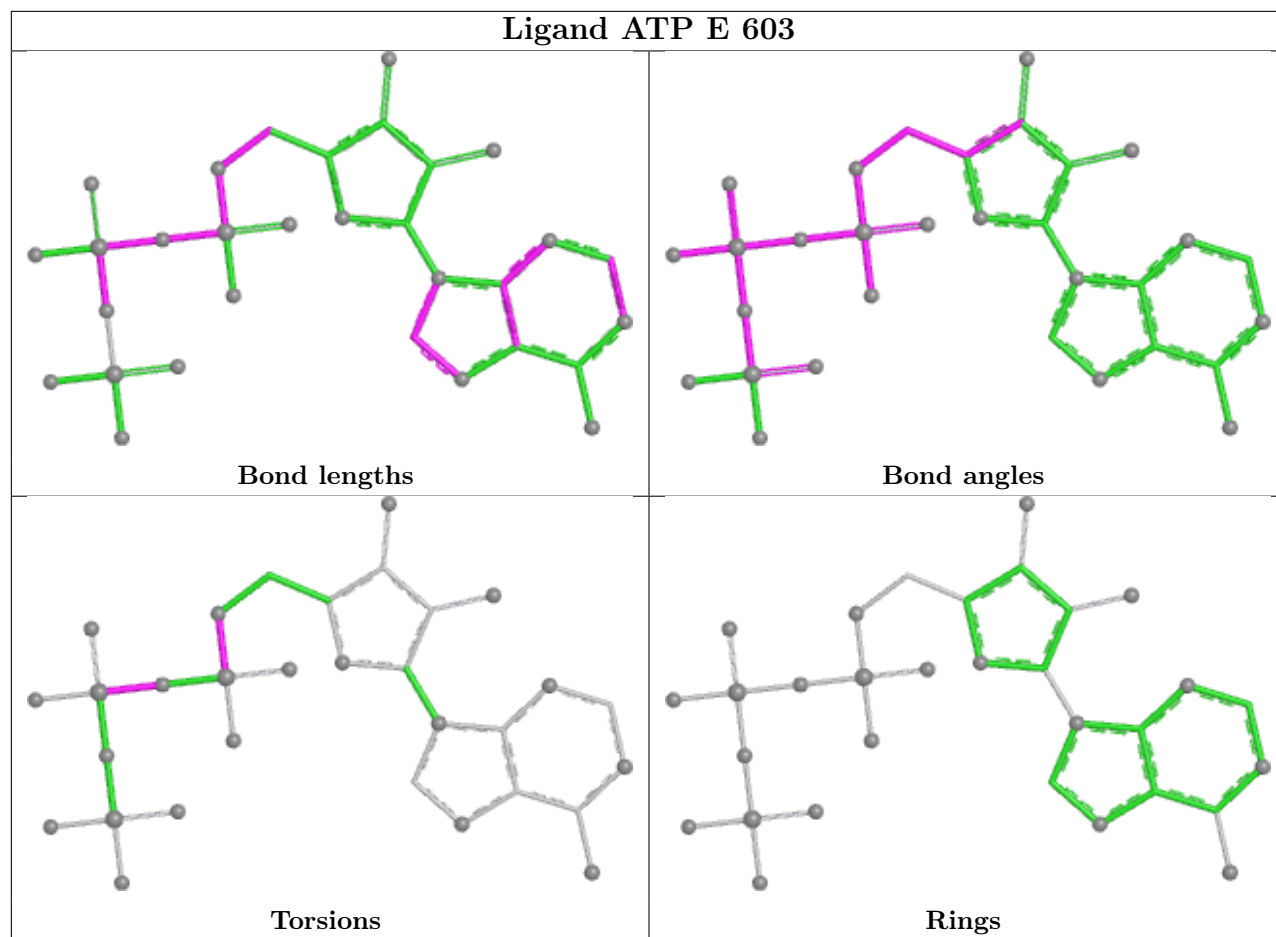


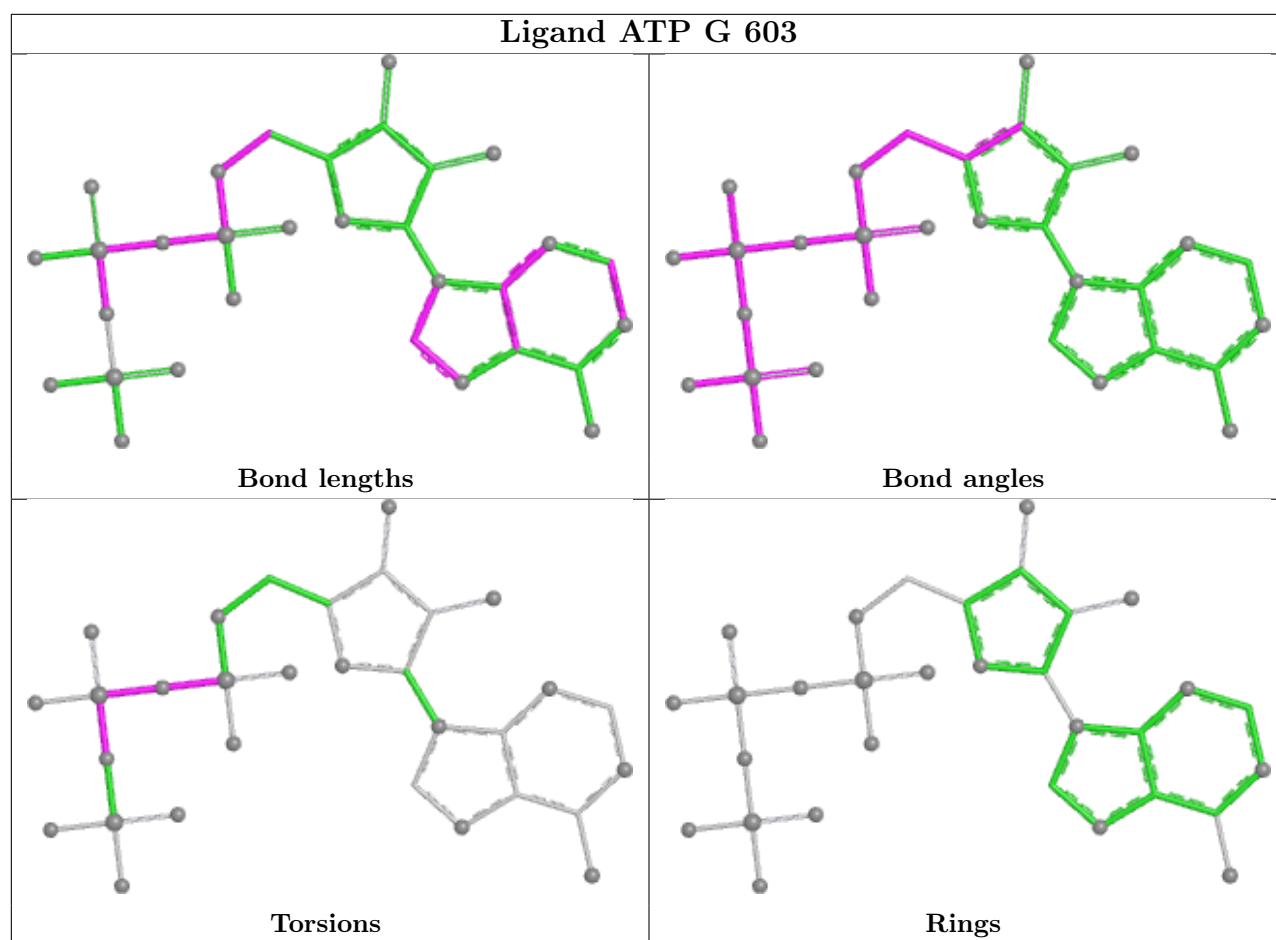


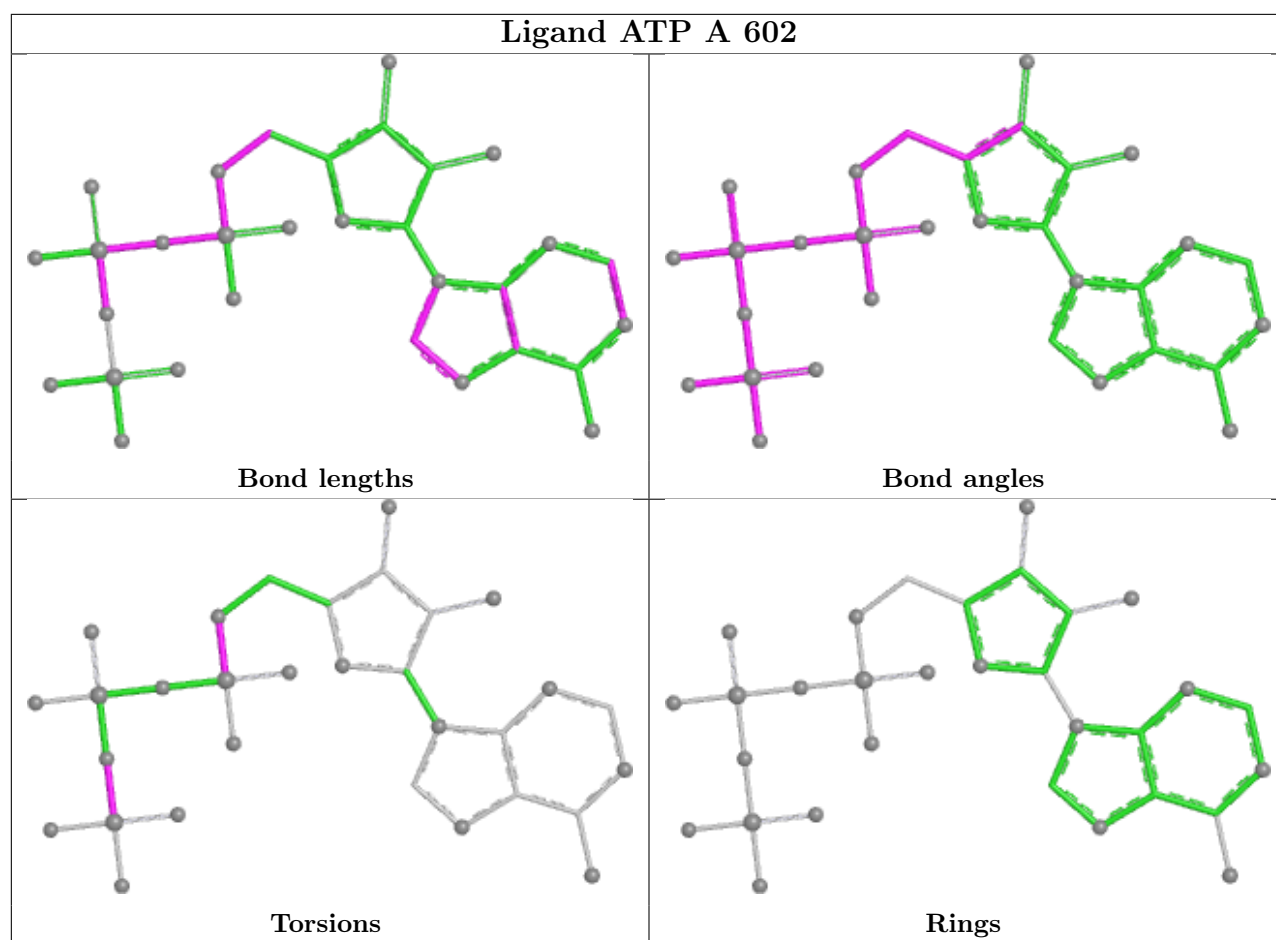


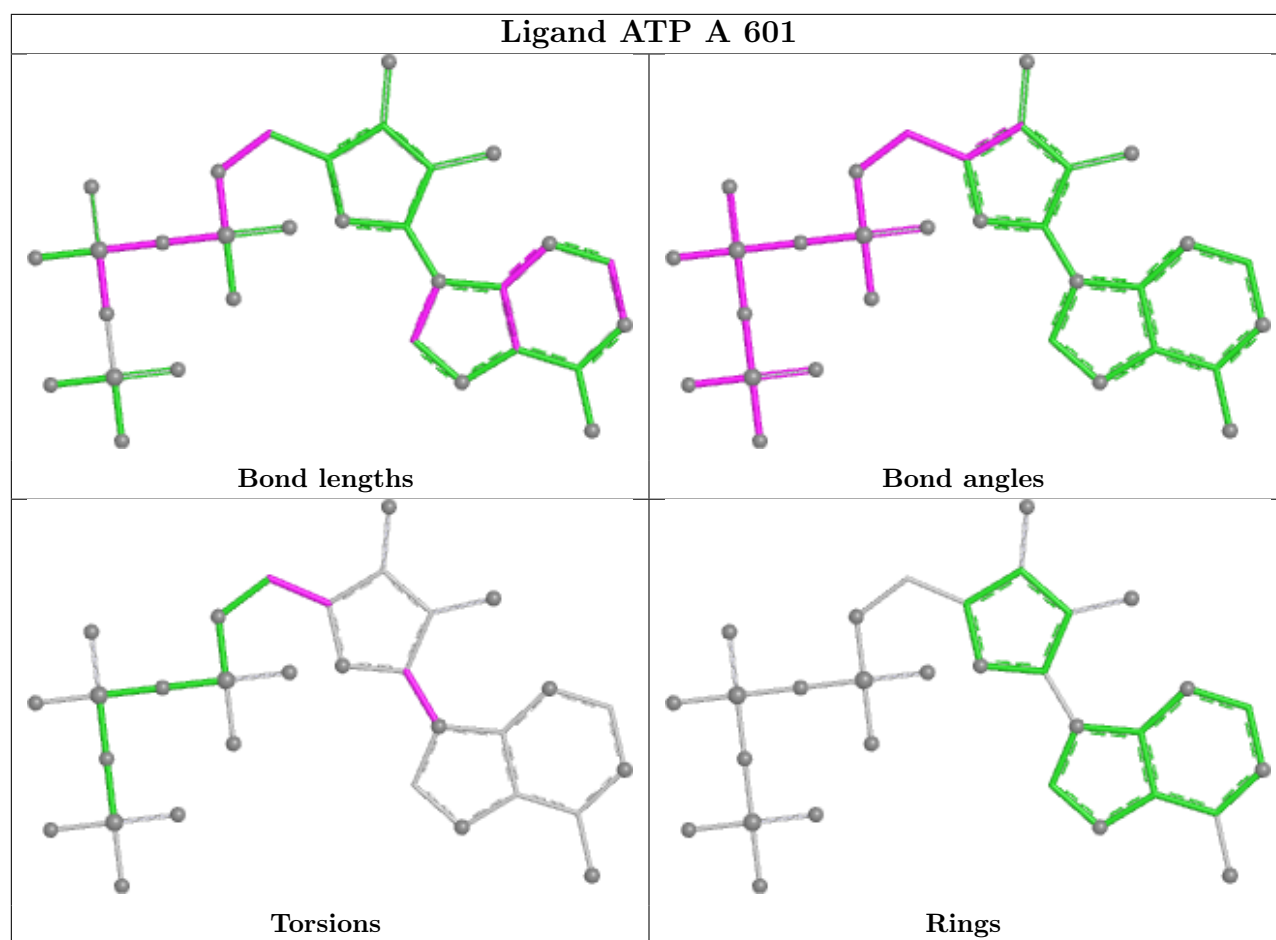


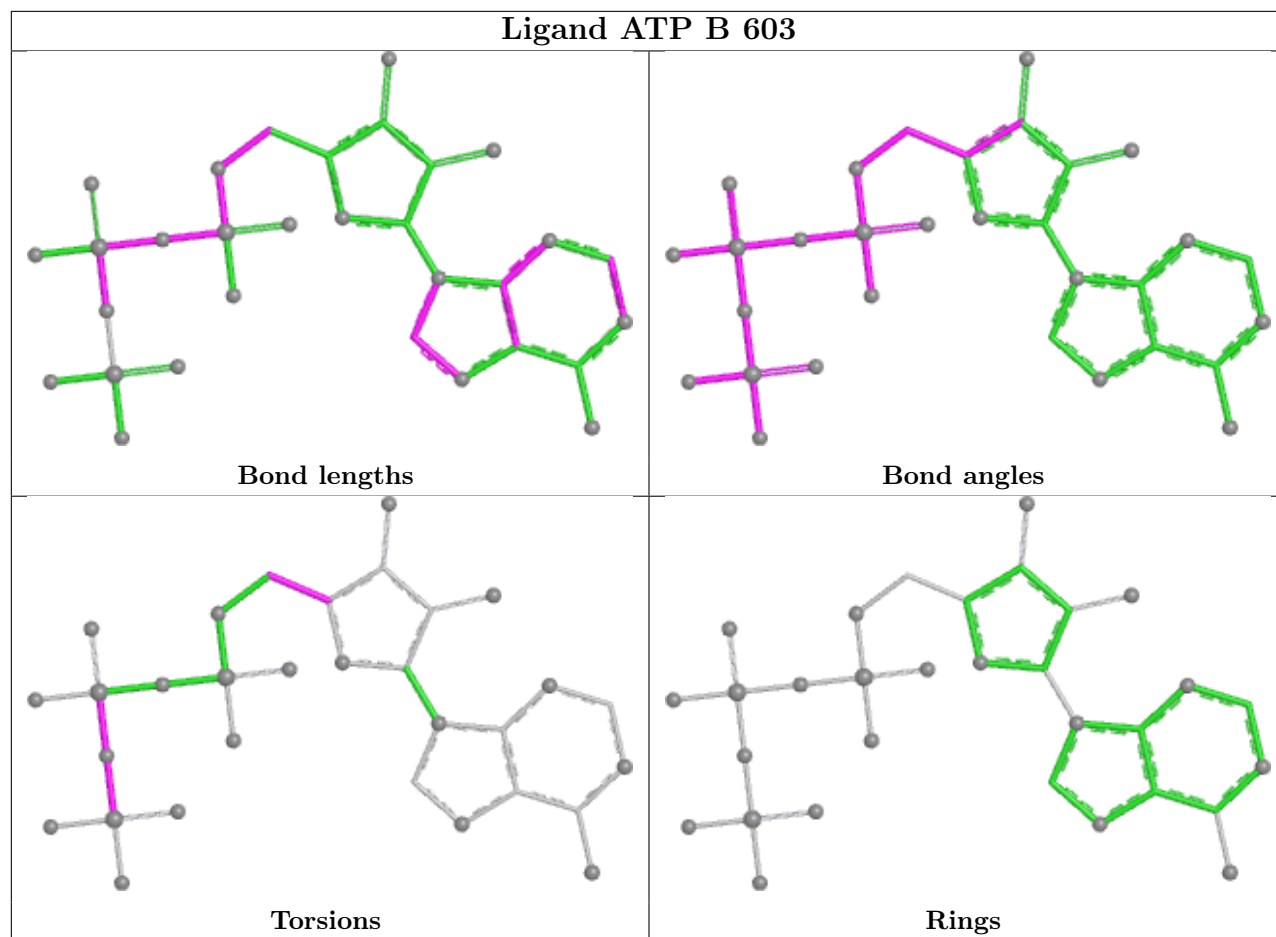
Ligand ATP E 603

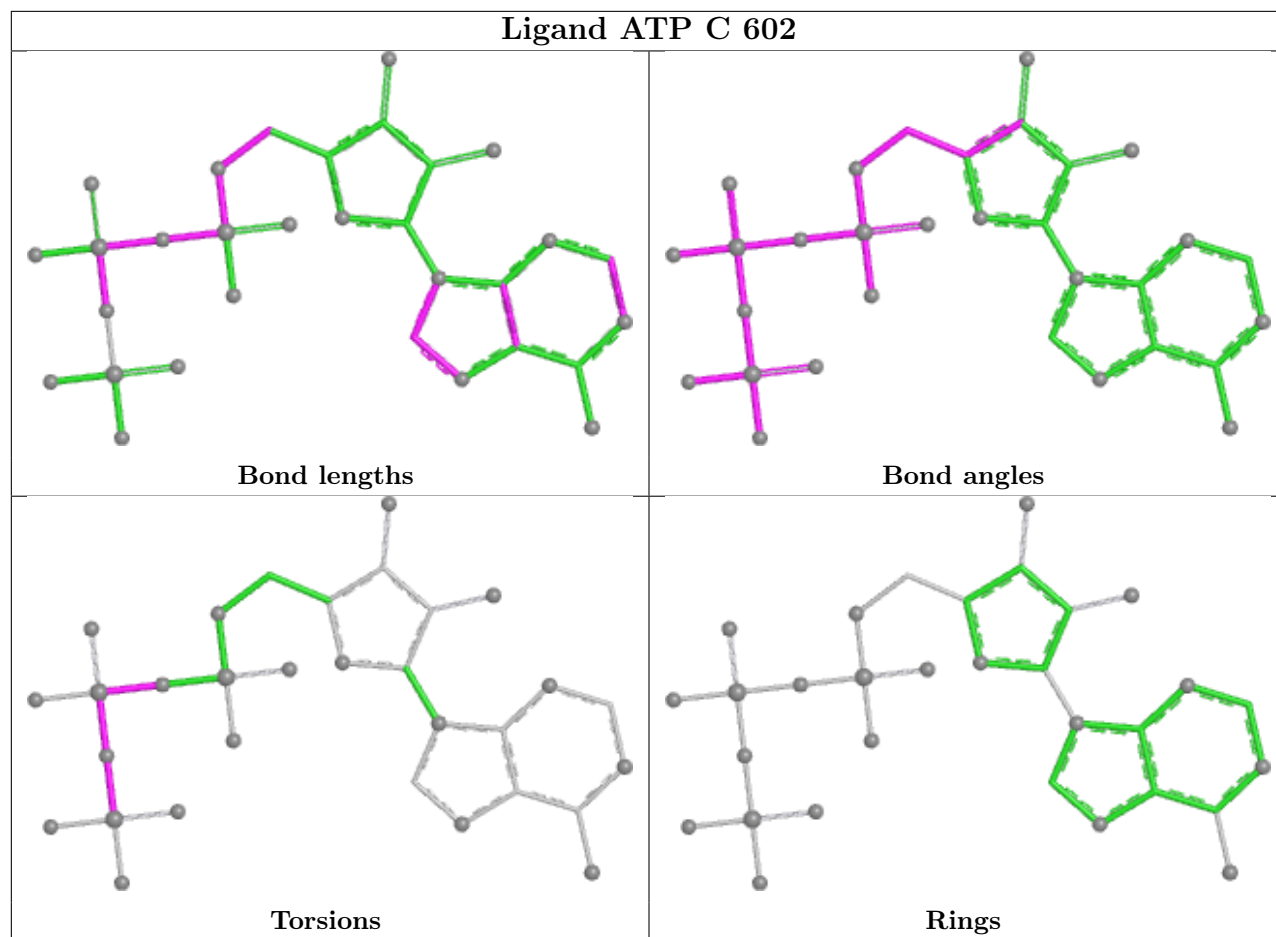


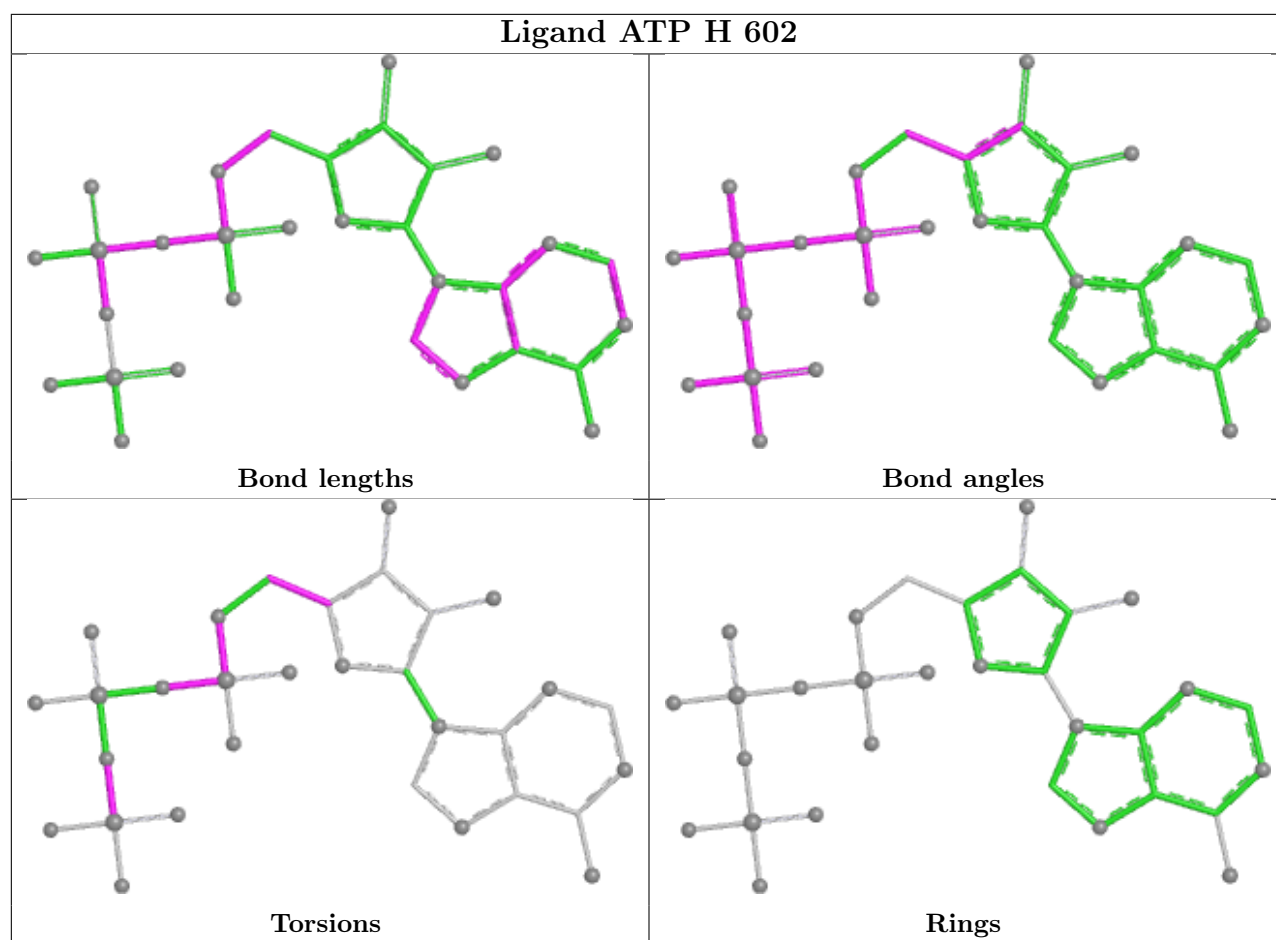


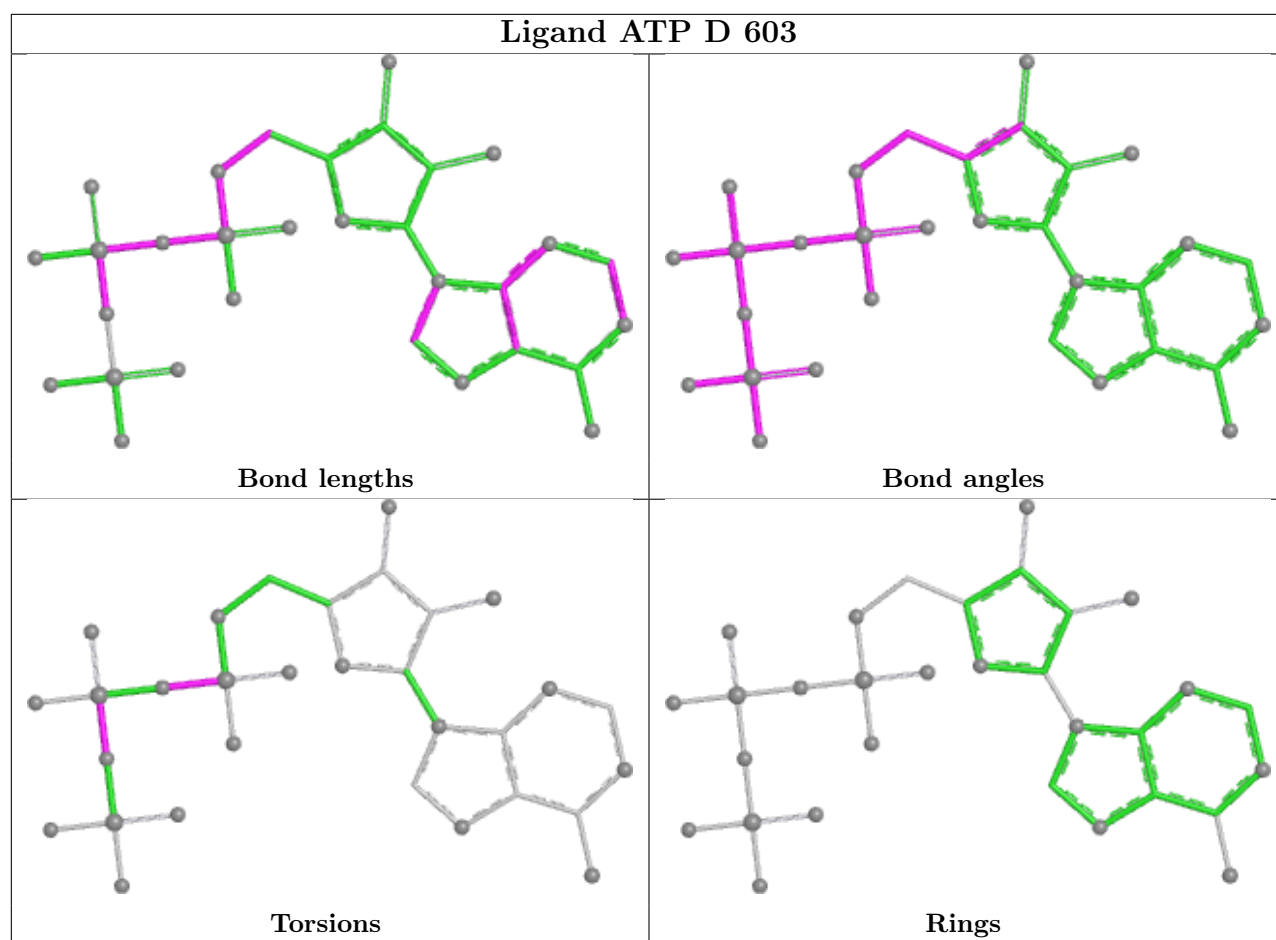


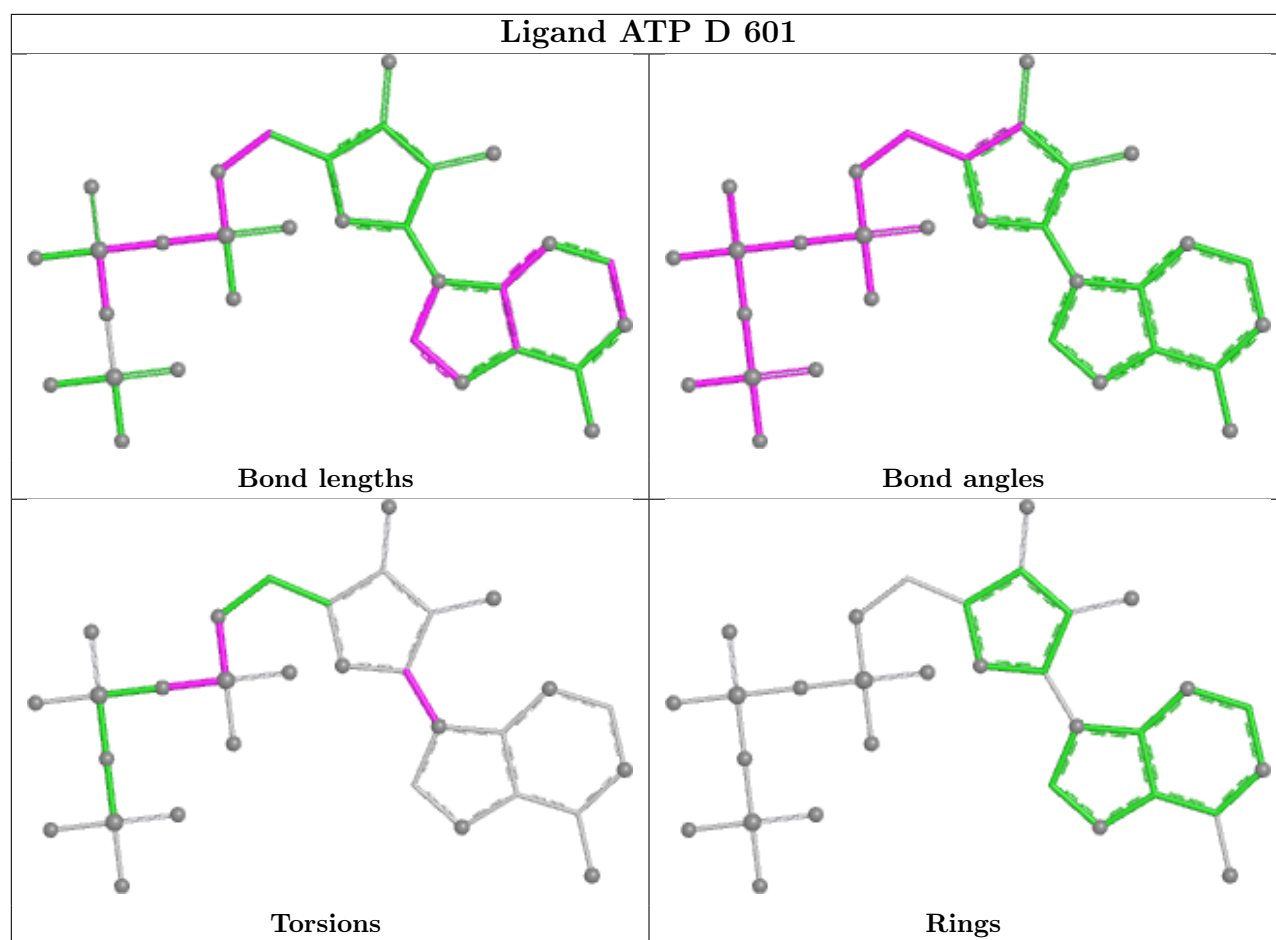












5.7 Other polymers [i](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	440/523 (84%)	-1.03	0 100 100	21, 39, 99, 181	0
1	B	444/523 (84%)	-1.01	1 (0%) 91 89	24, 41, 106, 155	0
1	C	446/523 (85%)	-1.02	1 (0%) 91 89	22, 40, 104, 168	1 (0%)
1	D	443/523 (84%)	-1.03	0 100 100	22, 39, 100, 132	1 (0%)
1	E	387/523 (73%)	-0.16	5 (1%) 75 71	26, 108, 151, 195	0
1	F	342/523 (65%)	0.16	11 (3%) 50 46	53, 119, 158, 196	1 (0%)
1	G	382/523 (73%)	0.08	11 (2%) 53 50	30, 115, 162, 197	0
1	H	321/523 (61%)	0.38	15 (4%) 36 32	85, 124, 165, 202	0
All	All	3205/4184 (76%)	-0.52	44 (1%) 73 69	21, 84, 147, 202	3 (0%)

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	14	ALA	3.5
1	E	304	ALA	3.5
1	F	33	ARG	3.4
1	H	9	ALA	3.4
1	B	174	ASP	3.3

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 oligosaccharides in this entry.

6.4 Ligands ⓘ

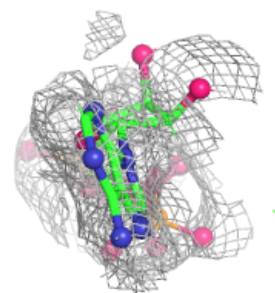
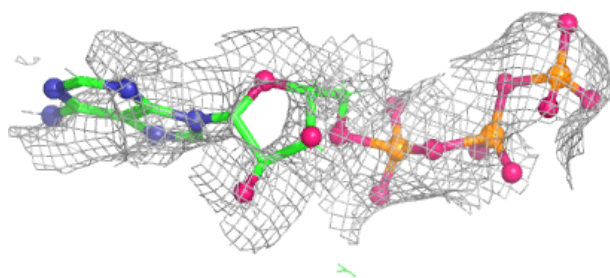
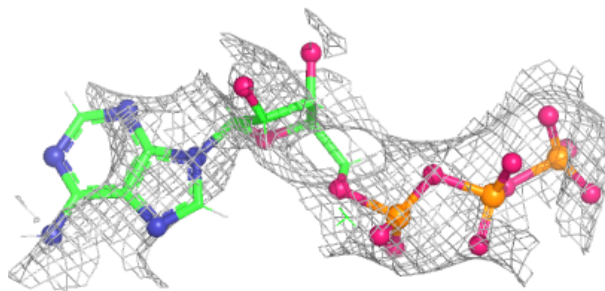
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ATP	E	603	31/31	0.95	0.10	133,141,164,166	0
2	ATP	H	603	31/31	0.95	0.10	101,111,126,129	43
2	ATP	F	601	31/31	0.96	0.07	118,133,146,153	0
2	ATP	G	603	31/31	0.97	0.09	100,106,122,125	43
3	MG	C	604	1/1	0.97	0.13	89,89,89,89	0
2	ATP	A	603	31/31	0.98	0.05	47,57,71,71	0
2	ATP	B	603	31/31	0.98	0.06	54,62,72,72	0
2	ATP	G	602	31/31	0.98	0.06	98,105,122,123	0
2	ATP	B	605	31/31	0.98	0.05	92,100,118,127	0
2	ATP	H	602	31/31	0.98	0.06	92,97,112,117	0
2	ATP	B	606	31/31	0.98	0.06	97,103,121,123	0
2	ATP	E	602	31/31	0.98	0.05	100,102,121,124	0
3	MG	E	604	1/1	0.98	0.10	86,86,86,86	0
2	ATP	D	603	31/31	0.99	0.05	53,59,73,74	0
2	ATP	E	601	31/31	0.99	0.05	83,90,105,109	0
2	ATP	B	602	31/31	0.99	0.03	49,59,67,68	0
2	ATP	A	602	31/31	0.99	0.05	49,55,64,68	0
2	ATP	A	601	31/31	0.99	0.04	50,58,67,70	0
2	ATP	G	601	31/31	0.99	0.04	81,89,103,108	0
2	ATP	B	601	31/31	0.99	0.04	63,67,80,84	0
2	ATP	C	601	31/31	0.99	0.04	64,69,81,82	0
2	ATP	H	601	31/31	0.99	0.04	89,97,114,119	0
2	ATP	C	602	31/31	0.99	0.05	46,54,70,93	0
2	ATP	C	603	31/31	0.99	0.05	50,59,70,73	0
3	MG	B	604	1/1	0.99	0.05	79,79,79,79	0
2	ATP	D	601	31/31	0.99	0.04	49,51,61,75	0
3	MG	C	605	1/1	0.99	0.05	113,113,113,113	0
3	MG	D	604	1/1	0.99	0.04	87,87,87,87	0
2	ATP	D	602	31/31	0.99	0.04	45,49,63,68	0
3	MG	E	605	1/1	0.99	0.04	93,93,93,93	0
3	MG	F	602	1/1	0.99	0.06	95,95,95,95	0
3	MG	G	604	1/1	0.99	0.09	64,64,64,64	0

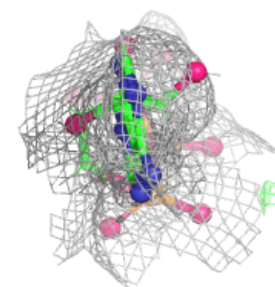
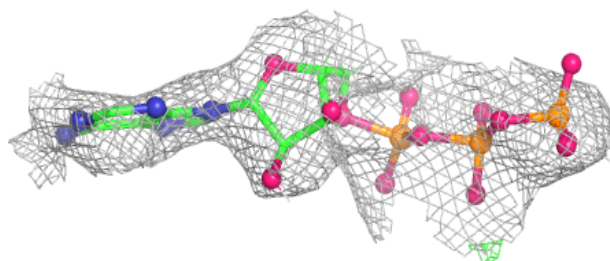
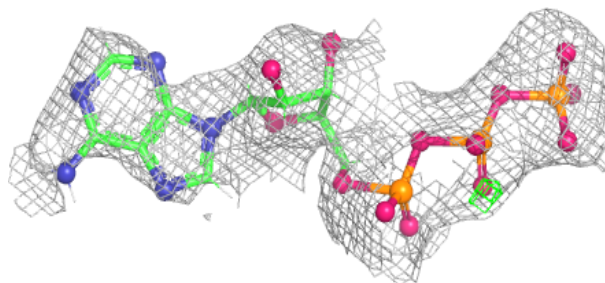
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP E 603:

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

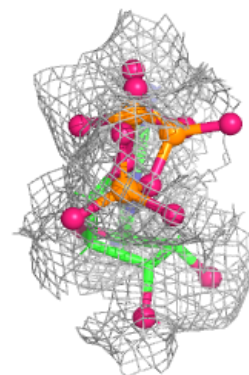
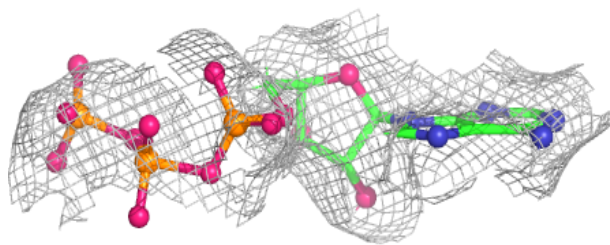
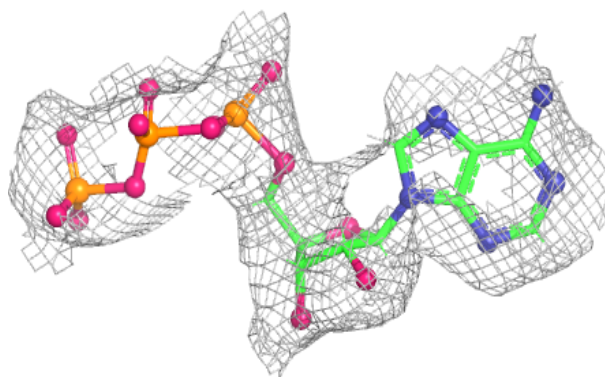
**Electron density around ATP H 603:**

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

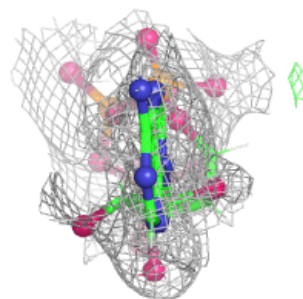
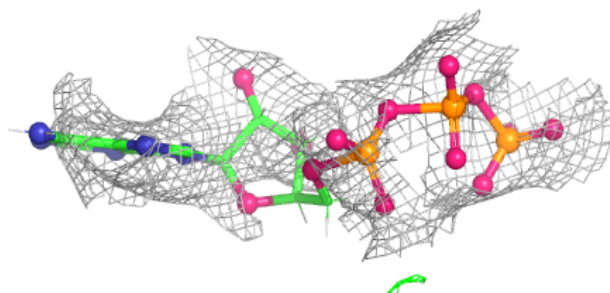
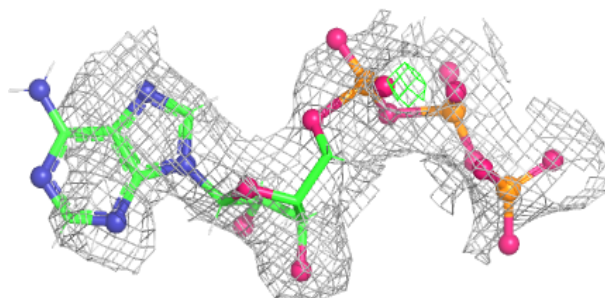


Electron density around ATP F 601:

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

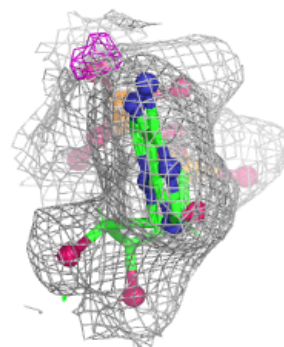
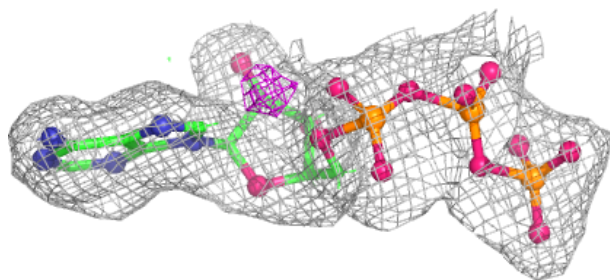
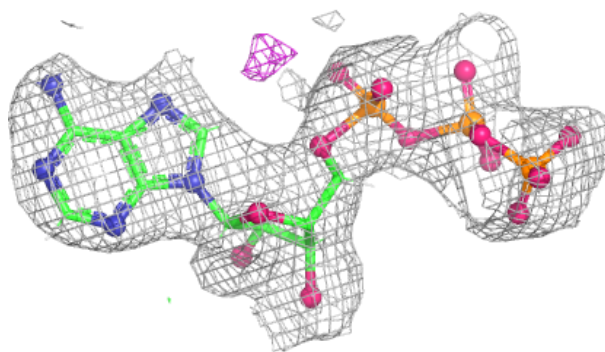
**Electron density around ATP G 603:**

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

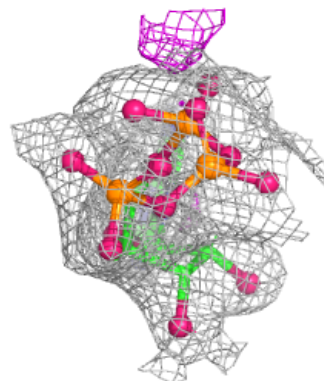
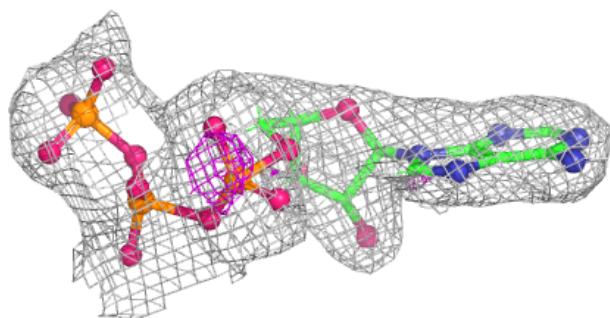
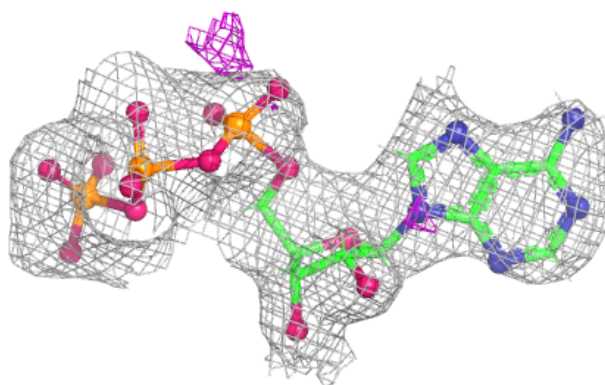


Electron density around ATP A 603:

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

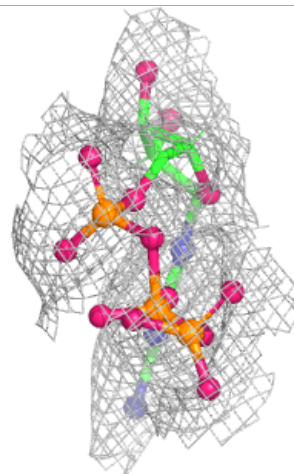
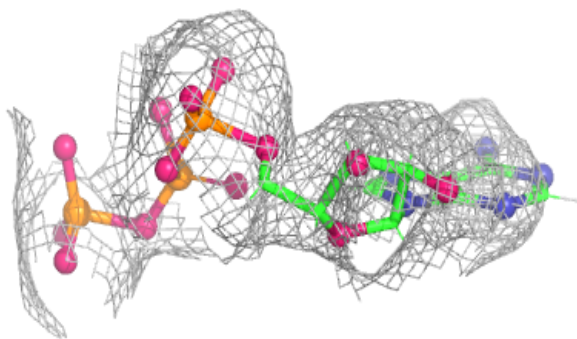
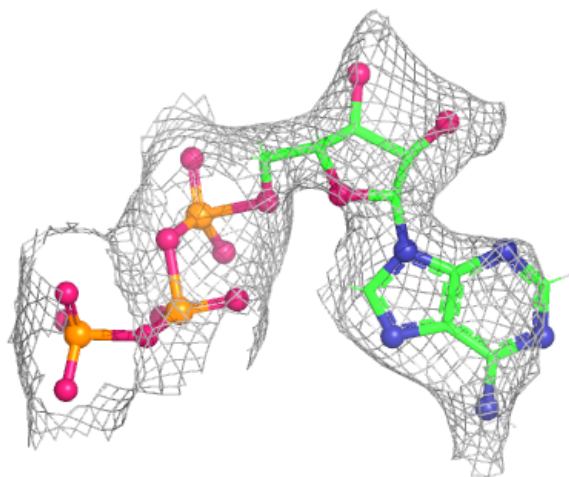
**Electron density around ATP B 603:**

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



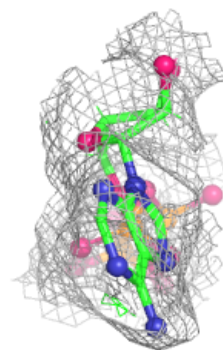
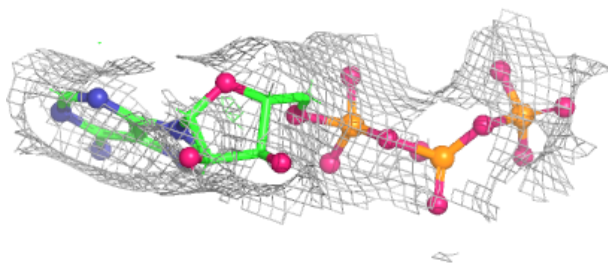
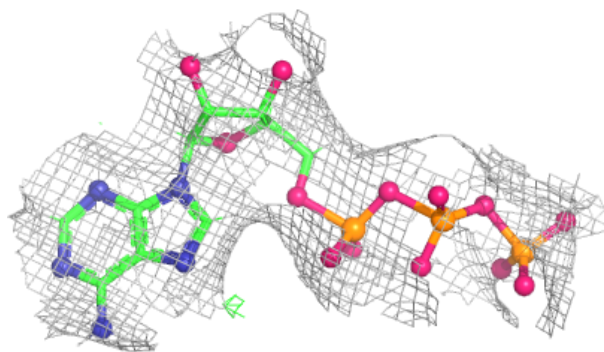
Electron density around ATP G 602:

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



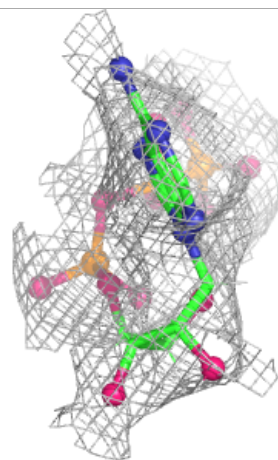
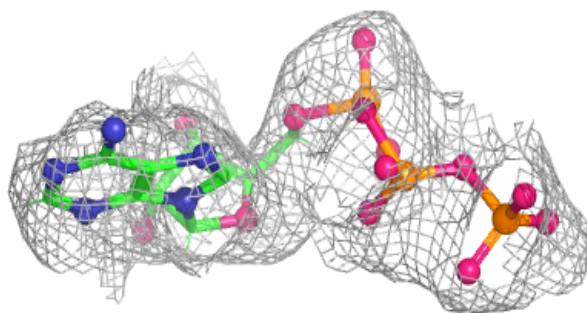
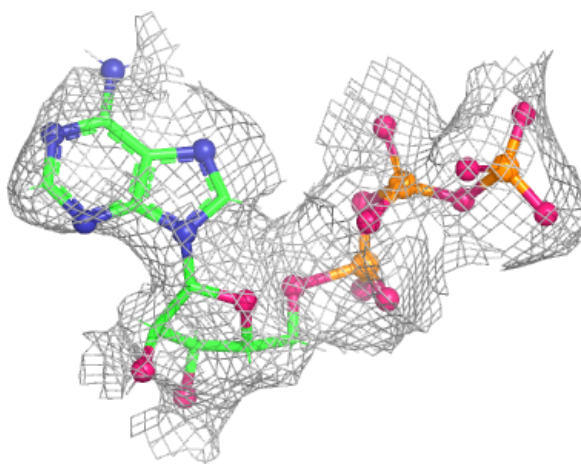
Electron density around ATP B 605:

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



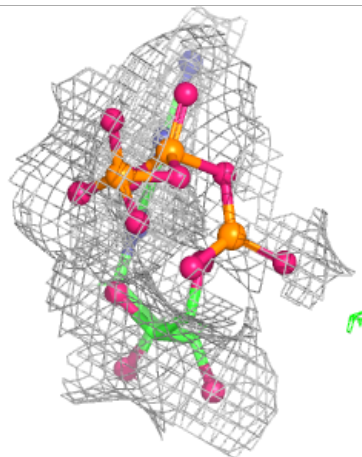
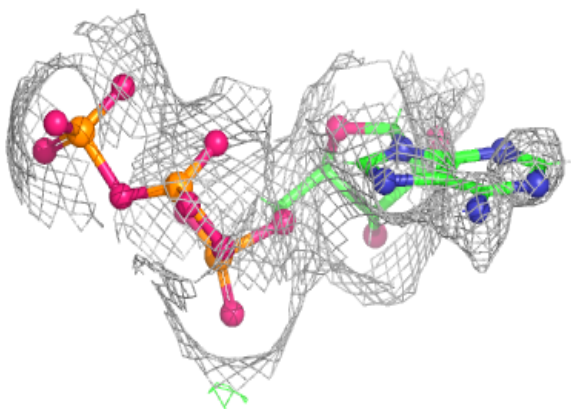
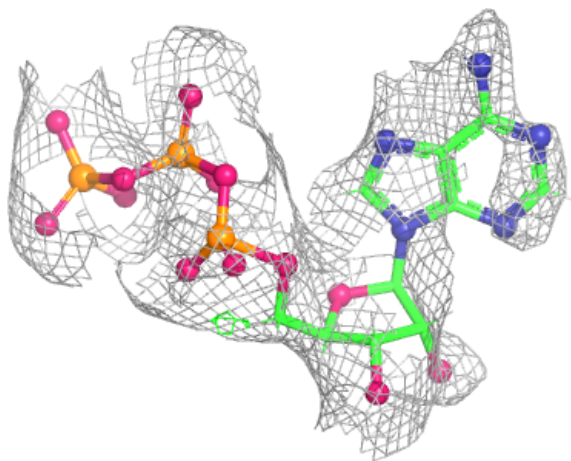
Electron density around ATP H 602:

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



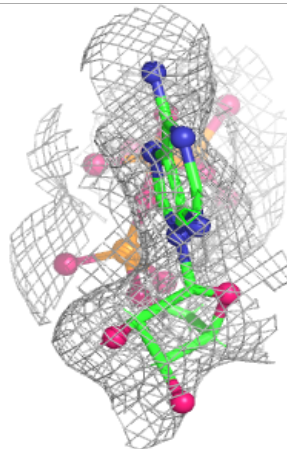
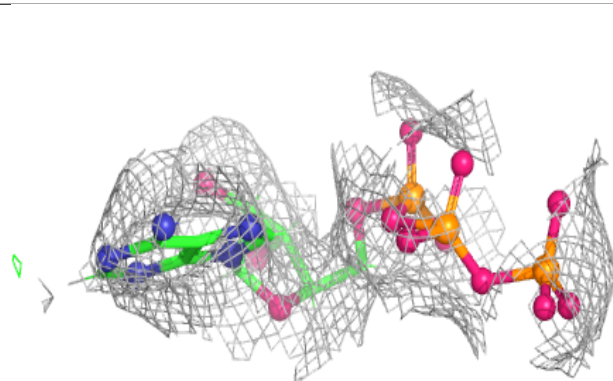
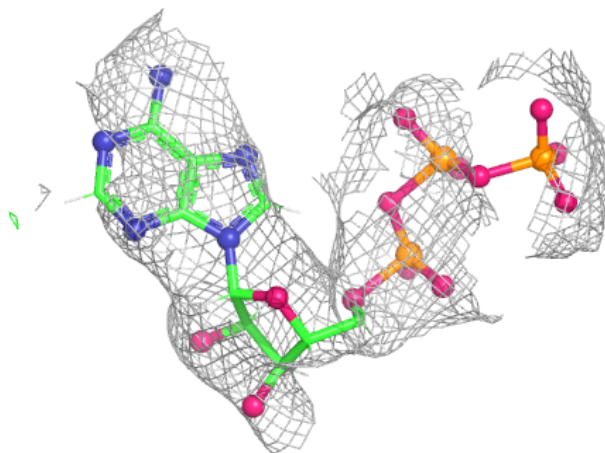
Electron density around ATP B 606:

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



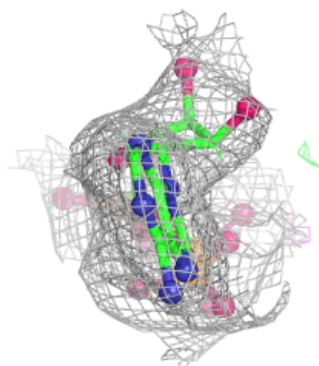
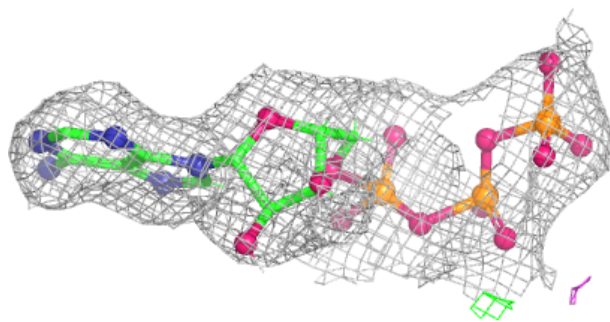
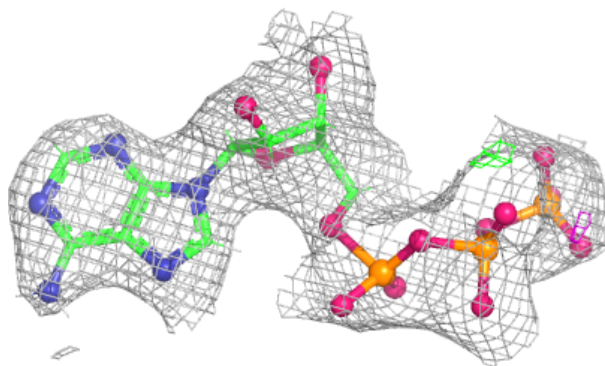
Electron density around ATP E 602:

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

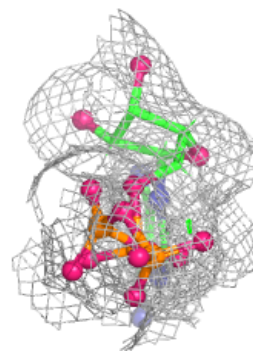
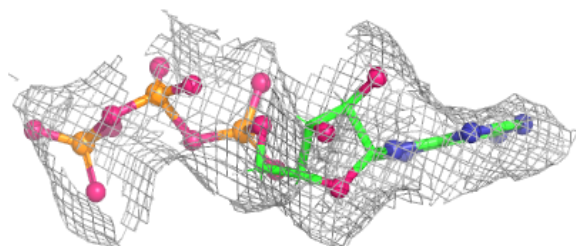
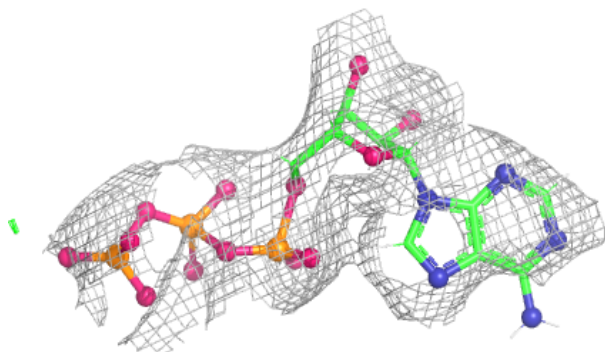


Electron density around ATP D 603:

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

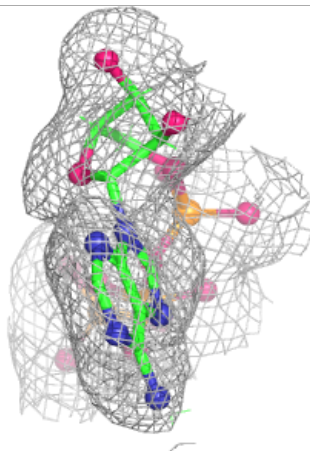
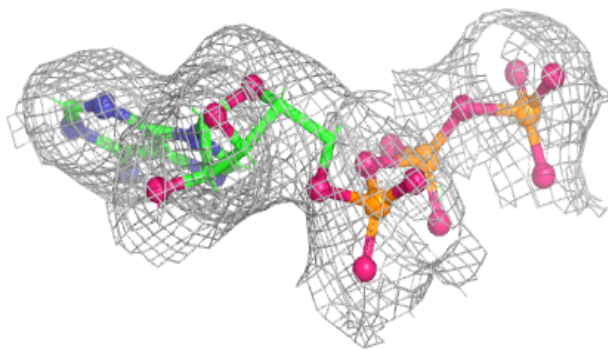
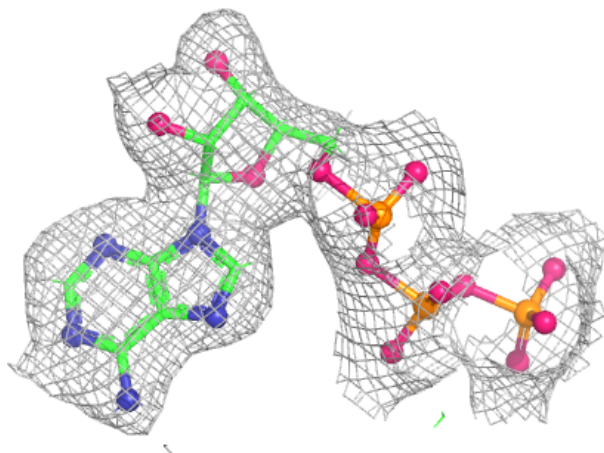
**Electron density around ATP E 601:**

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



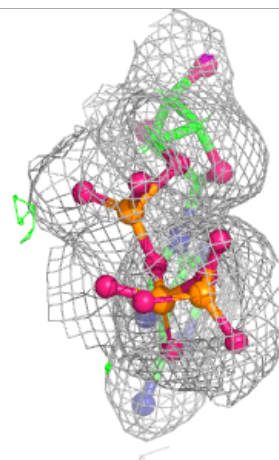
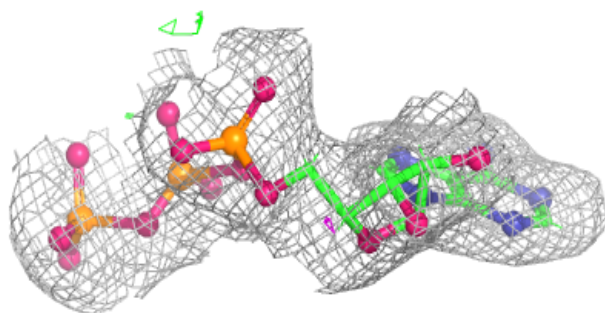
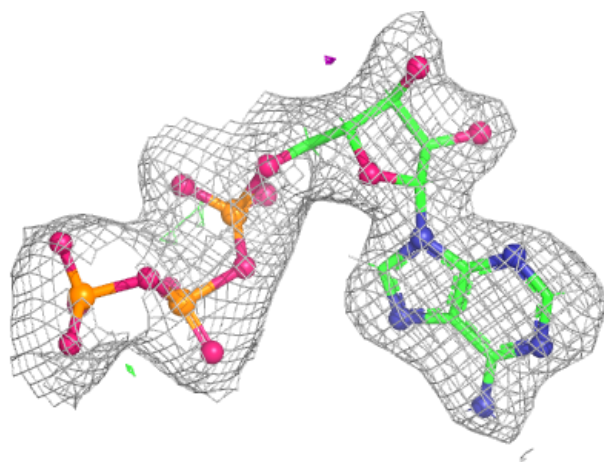
Electron density around ATP B 602:

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



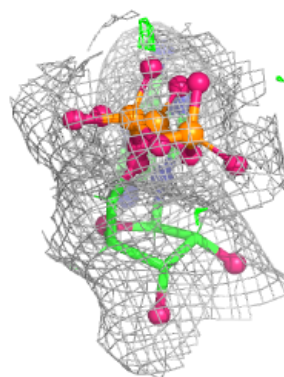
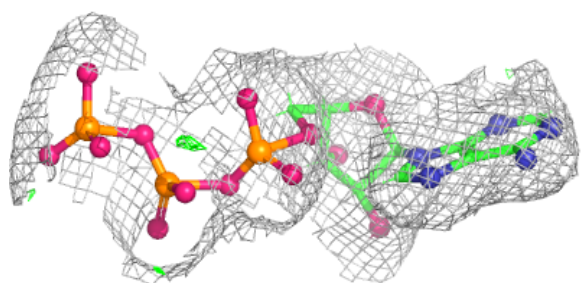
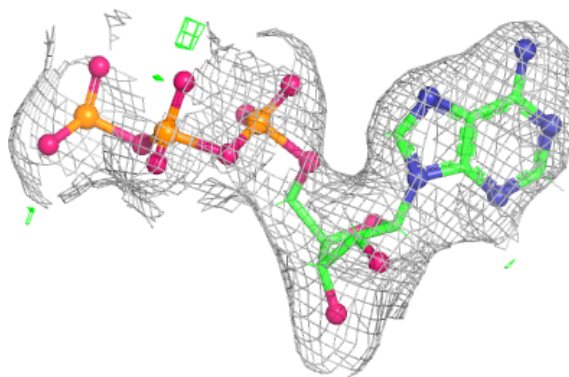
Electron density around ATP A 602:

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

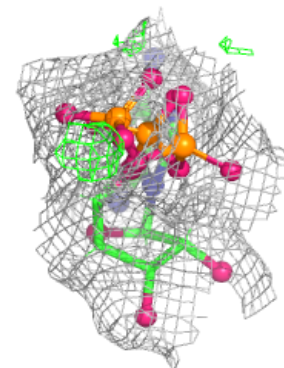
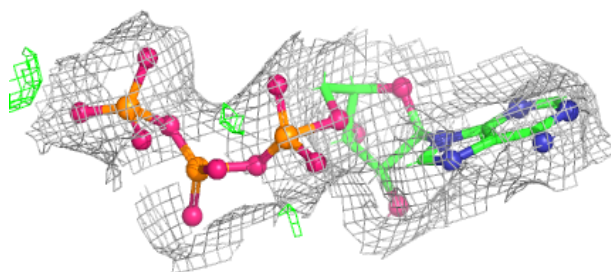
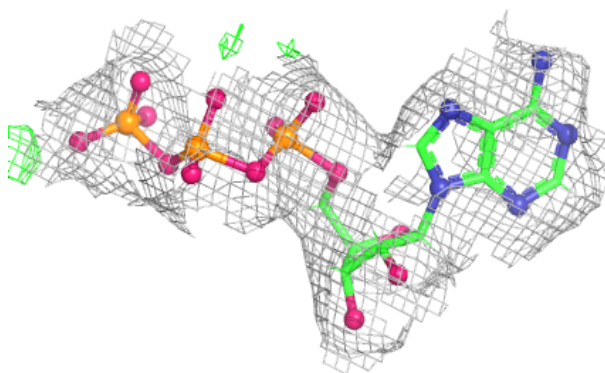


Electron density around ATP A 601:

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

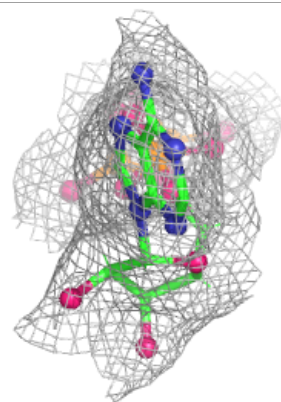
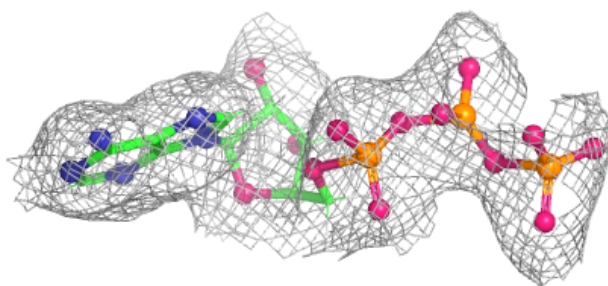
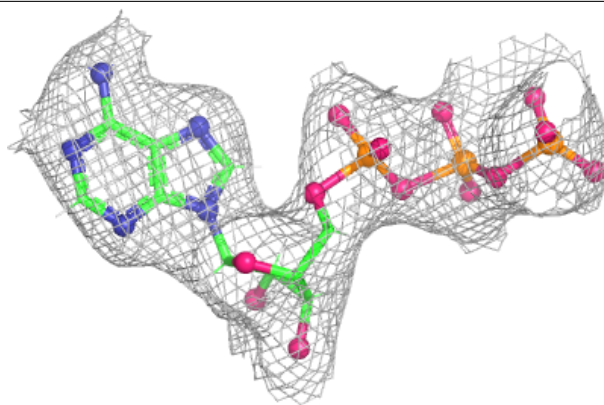
**Electron density around ATP G 601:**

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

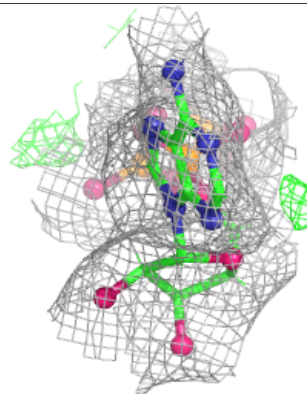
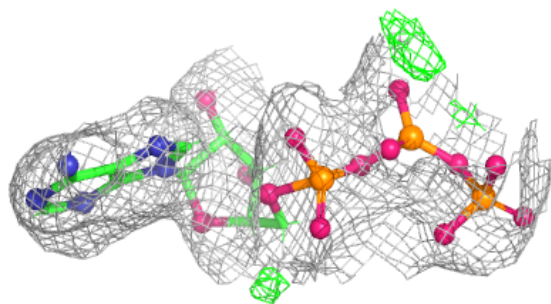
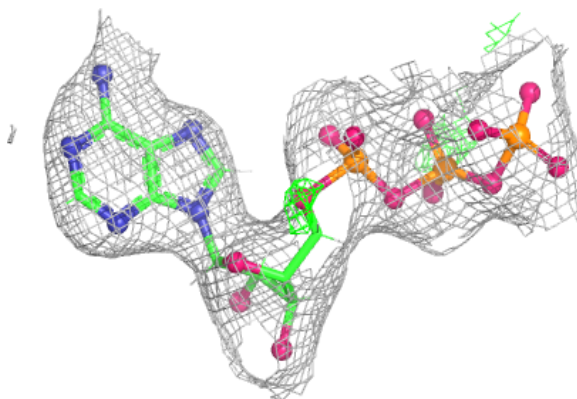


Electron density around ATP B 601:

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

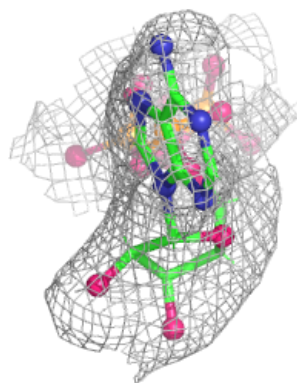
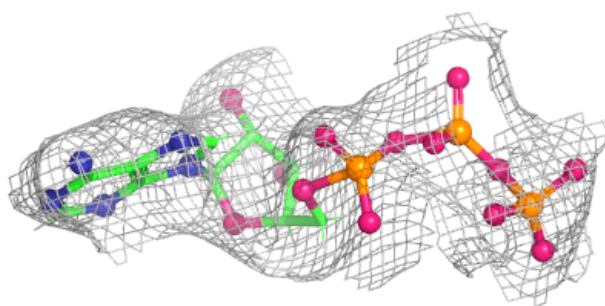
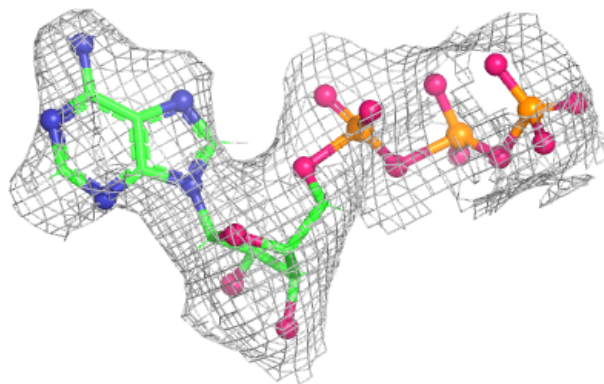
**Electron density around ATP C 601:**

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



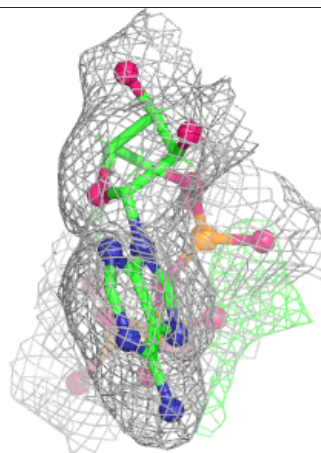
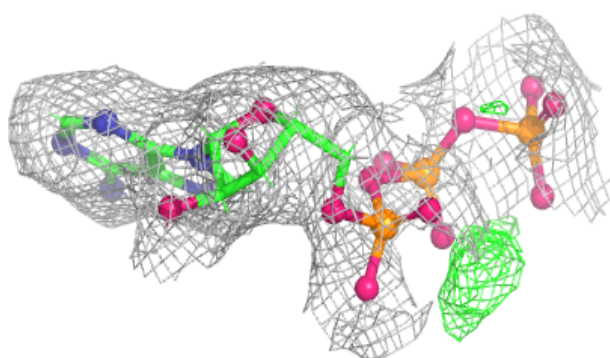
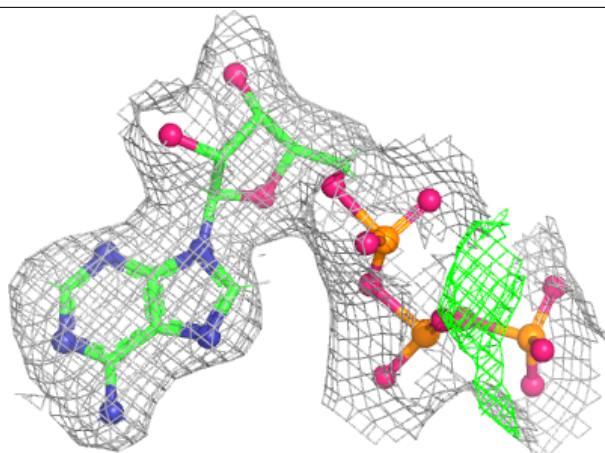
Electron density around ATP H 601:

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

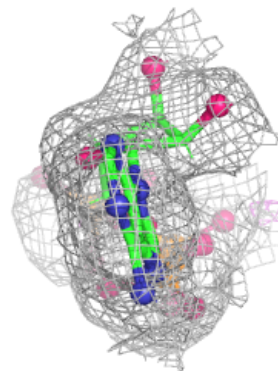
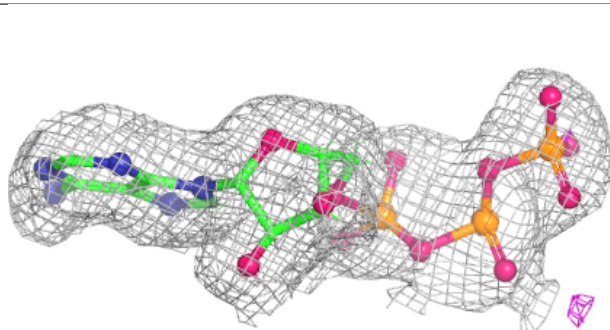
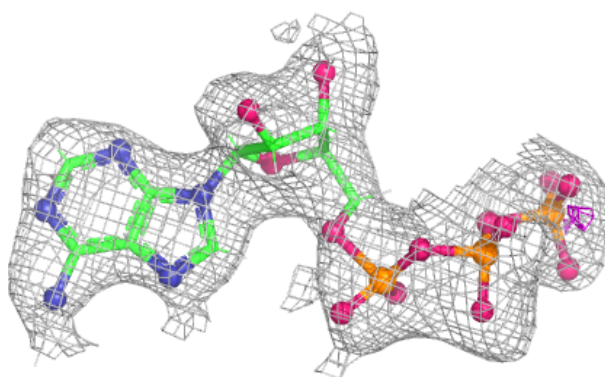


Electron density around ATP C 602:

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

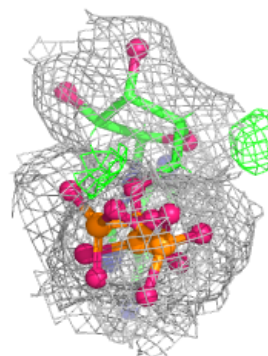
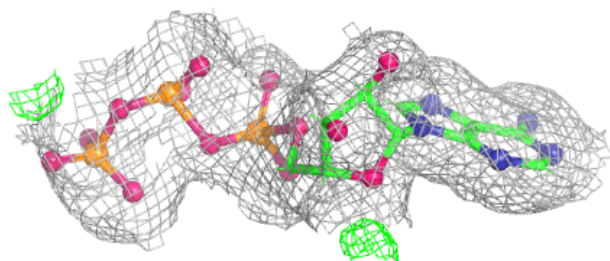
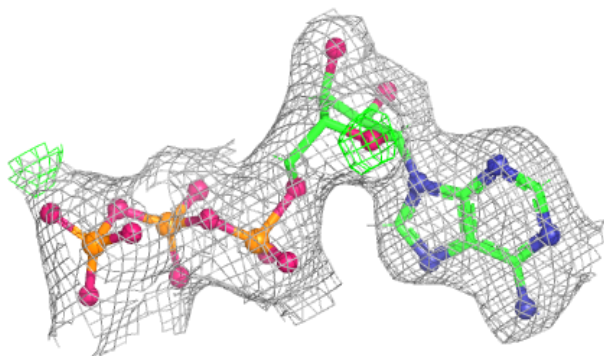
**Electron density around ATP C 603:**

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

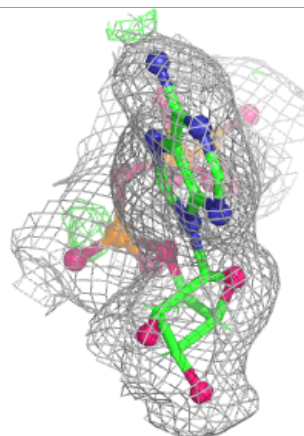
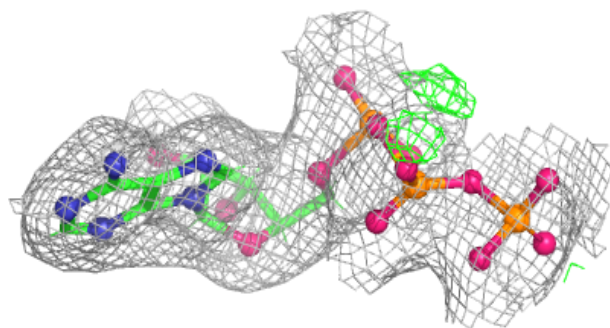
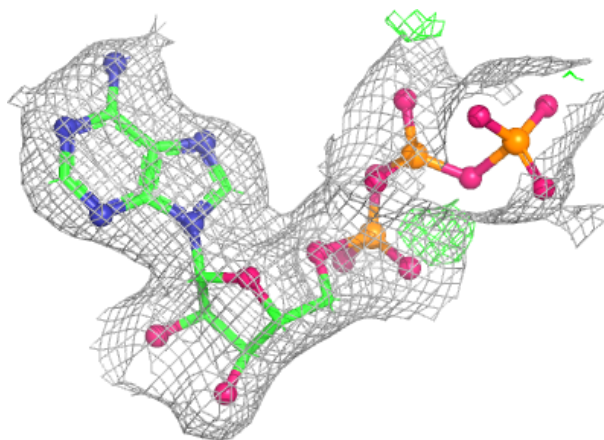


Electron density around ATP D 601:

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

**Electron density around ATP D 602:**

$2mF_o-DF_c$ (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.