



wwPDB X-ray Structure Validation Summary Report ⓘ

May 7, 2026 – 11:17 AM EDT

PDB ID : 7V3X / pdb_00007v3x
Title : Crystal Structure of Cyanobacterial Circadian Clock Protein KaiC
Authors : Furuike, Y.; Akiyama, S.
Deposited on : 2021-08-11
Resolution : 3.10 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

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

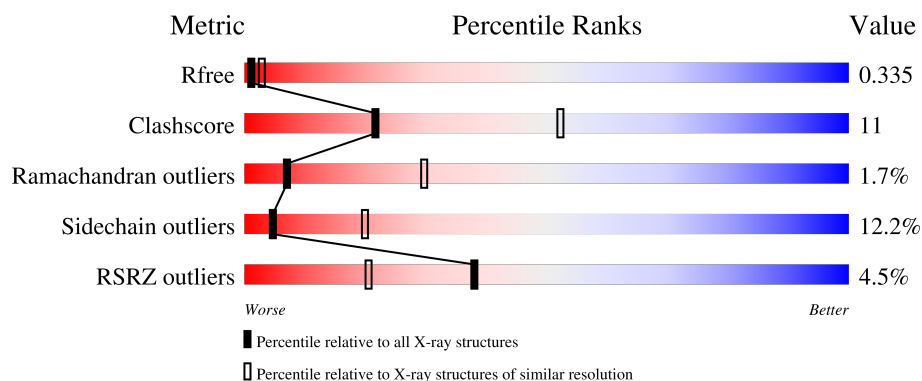
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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.



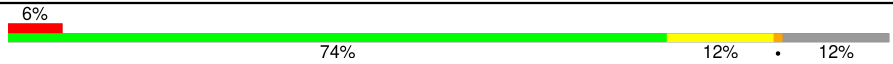
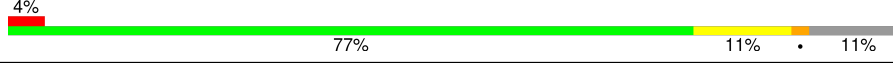
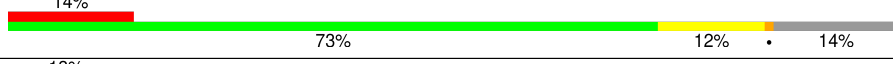
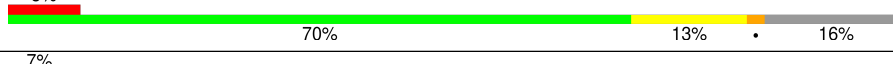
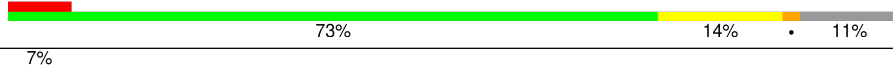
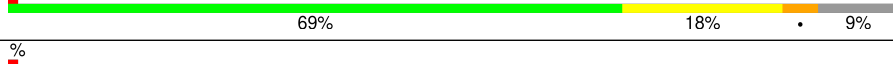
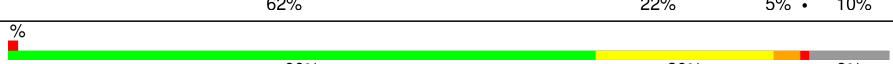
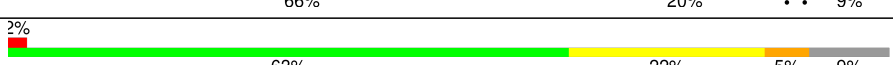
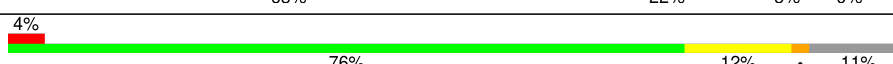
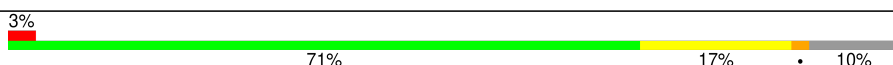
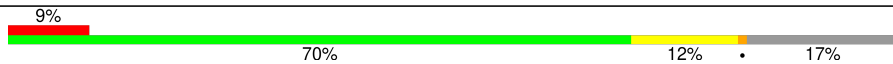
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 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	519	
1	B	519	
1	G	519	
1	H	519	
1	M	519	

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Mol	Chain	Length	Quality of chain
1	N	519	
1	P	519	
1	R	519	
1	S	519	
1	T	519	
1	V	519	
1	W	519	
1	X	519	
2	C	519	
2	D	519	
2	E	519	
2	F	519	
2	I	519	
2	J	519	
2	K	519	
2	L	519	
2	O	519	
2	Q	519	
2	U	519	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ADP	U	702	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 78739 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 Circadian clock protein kinase KaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	P	S	0	0	0
			3506	2208	606	677	1	14			
1	B	469	Total	C	N	O	P	S	0	0	0
			3432	2156	601	662	1	12			
1	G	467	Total	C	N	O	P	S	0	0	0
			3448	2178	590	666	1	13			
1	H	468	Total	C	N	O	P	S	0	0	0
			3476	2183	608	671	1	13			
1	N	455	Total	C	N	O	P	S	0	0	0
			3010	1858	545	594	1	12			
1	R	463	Total	C	N	O	P	S	0	0	0
			3201	1997	572	619	1	12			
1	M	463	Total	C	N	O	P	S	0	0	0
			3123	1935	557	616	1	14			
1	P	456	Total	C	N	O	P	S	0	0	0
			3096	1922	541	620	1	12			
1	T	415	Total	C	N	O	P	S	0	0	0
			2427	1462	473	485	1	6			
1	X	461	Total	C	N	O	P	S	0	0	0
			3074	1907	553	601	1	12			
1	S	444	Total	C	N	O	P	S	0	0	0
			2706	1648	509	541	1	7			
1	V	437	Total	C	N	O	P	S	0	0	0
			2914	1800	522	582	1	9			
1	W	464	Total	C	N	O	P	S	0	0	0
			3126	1926	573	613	1	13			

- Molecule 2 is a protein called Circadian clock protein kinase KaiC.

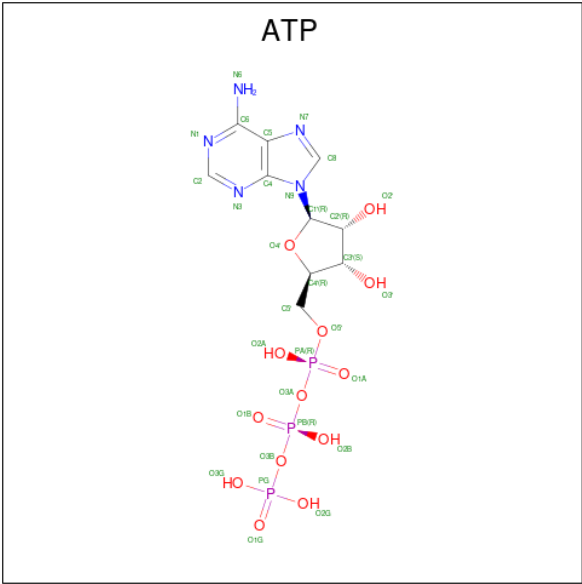
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	470	Total	C	N	O	P	S	0	0	0
			3424	2159	590	661	2	12			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	F	468	Total	C	N	O	P	S	0	0	0
			3436	2156	599	666	2	13			
2	C	472	Total	C	N	O	P	S	0	0	0
			3436	2159	595	666	2	14			
2	D	471	Total	C	N	O	P	S	0	0	0
			3456	2170	594	676	2	14			
2	K	471	Total	C	N	O	P	S	0	0	0
			3444	2171	592	666	2	13			
2	L	470	Total	C	N	O	P	S	0	0	0
			3471	2181	598	676	2	14			
2	I	473	Total	C	N	O	P	S	0	0	0
			3477	2181	603	678	2	13			
2	J	468	Total	C	N	O	P	S	0	0	0
			3442	2161	598	668	2	13			
2	O	461	Total	C	N	O	P	S	0	0	0
			3072	1899	552	607	2	12			
2	Q	466	Total	C	N	O	P	S	0	0	0
			3303	2057	583	646	2	15			
2	U	430	Total	C	N	O	P	S	0	0	0
			2635	1596	500	530	2	7			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	J	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	J	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	N	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	N	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	O	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	O	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	R	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	R	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	M	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	M	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	P	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	P	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	Q	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	T	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	T	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	U	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	X	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	X	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	S	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	S	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	V	1	Total 31	C 10	N 5	O 13	P 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	V	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	W	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

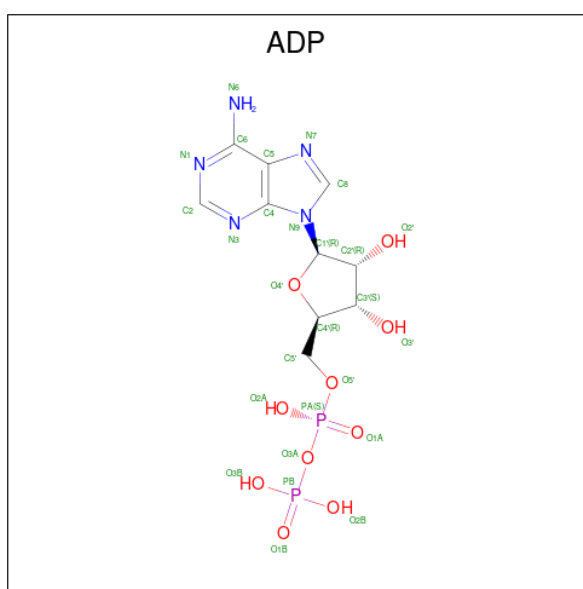
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	B	2	Total	Mg	0	0
			2	2		
4	E	2	Total	Mg	0	0
			2	2		
4	F	2	Total	Mg	0	0
			2	2		
4	C	2	Total	Mg	0	0
			2	2		
4	D	2	Total	Mg	0	0
			2	2		
4	G	2	Total	Mg	0	0
			2	2		
4	H	2	Total	Mg	0	0
			2	2		
4	K	2	Total	Mg	0	0
			2	2		
4	L	2	Total	Mg	0	0
			2	2		
4	I	2	Total	Mg	0	0
			2	2		
4	J	2	Total	Mg	0	0
			2	2		
4	N	2	Total	Mg	0	0
			2	2		
4	O	1	Total	Mg	0	0
			1	1		
4	R	2	Total	Mg	0	0
			2	2		
4	M	1	Total	Mg	0	0
			1	1		
4	P	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Q	1	Total	Mg	0	0
			1	1		
4	T	1	Total	Mg	0	0
			1	1		
4	U	1	Total	Mg	0	0
			1	1		
4	V	1	Total	Mg	0	0
			1	1		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	Q	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	U	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	W	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	6	Total	O	0	0
			6	6		
6	B	9	Total	O	0	0
			9	9		

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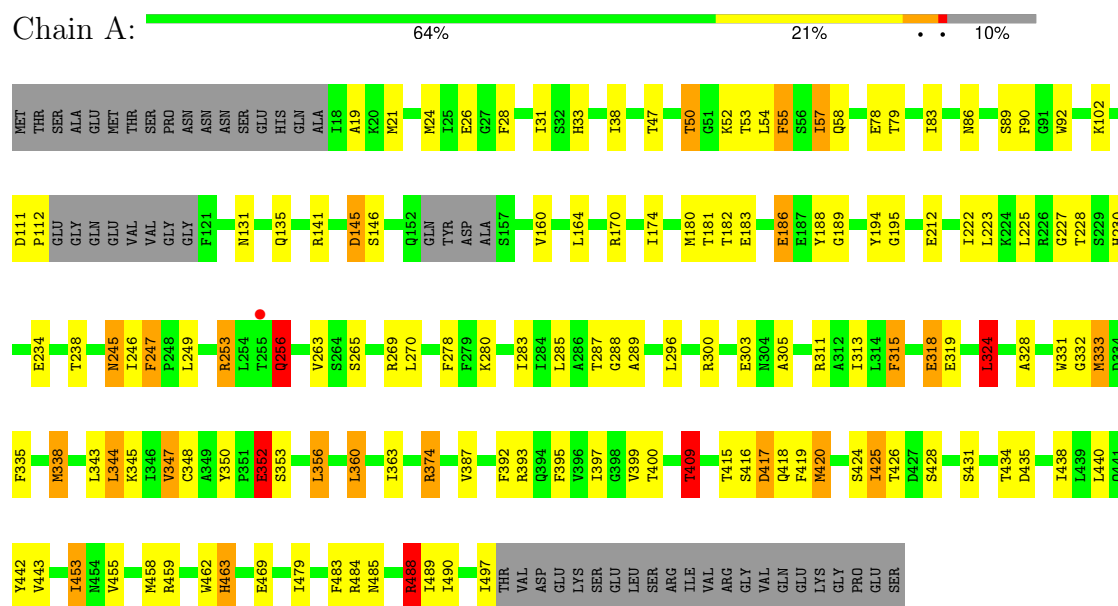
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	4	Total 4	O 4	0	0
6	F	6	Total 6	O 6	0	0
6	C	7	Total 7	O 7	0	0
6	D	4	Total 4	O 4	0	0
6	G	4	Total 4	O 4	0	0
6	H	4	Total 4	O 4	0	0
6	K	3	Total 3	O 3	0	0
6	L	6	Total 6	O 6	0	0
6	I	5	Total 5	O 5	0	0
6	J	4	Total 4	O 4	0	0
6	N	2	Total 2	O 2	0	0
6	O	5	Total 5	O 5	0	0
6	R	2	Total 2	O 2	0	0
6	M	1	Total 1	O 1	0	0
6	P	4	Total 4	O 4	0	0
6	Q	5	Total 5	O 5	0	0
6	U	2	Total 2	O 2	0	0
6	X	2	Total 2	O 2	0	0
6	S	2	Total 2	O 2	0	0
6	V	2	Total 2	O 2	0	0
6	W	3	Total 3	O 3	0	0

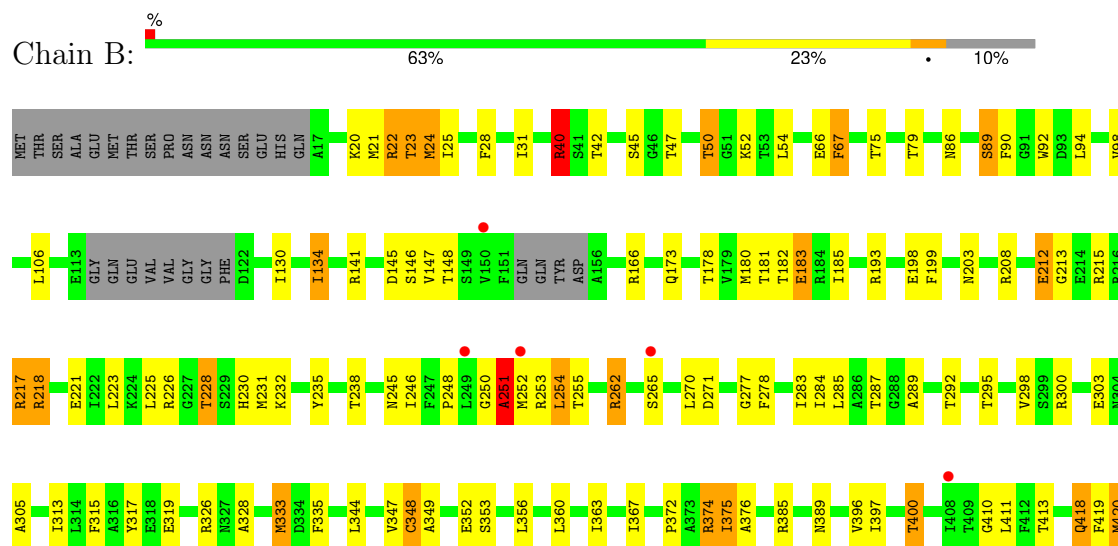
3 Residue-property plots

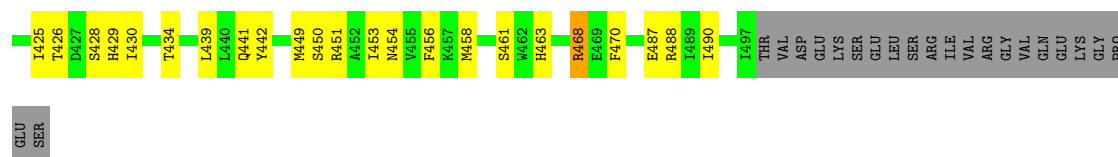
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



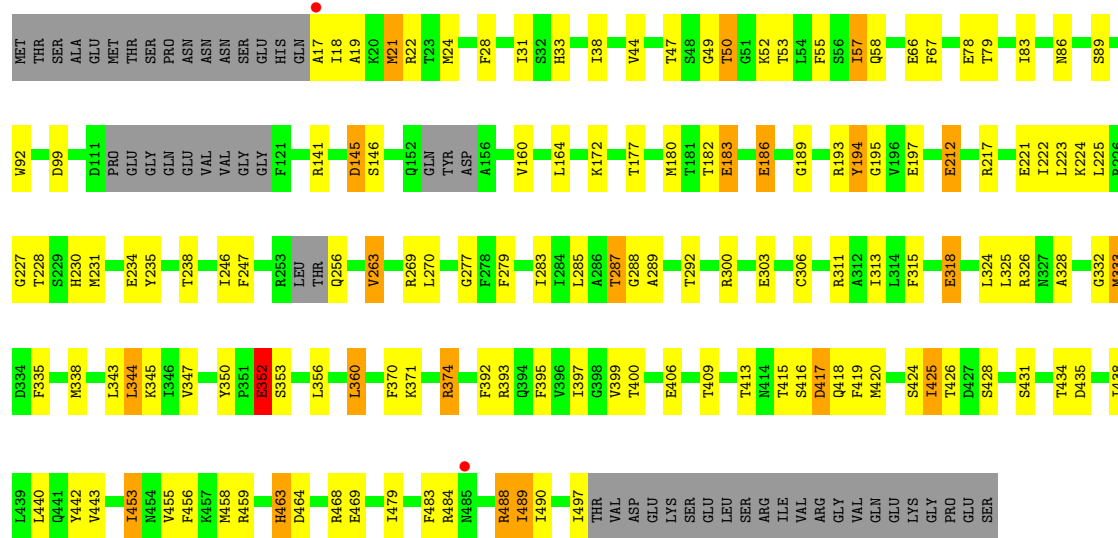
• Molecule 1: Circadian clock protein kinase KaiC





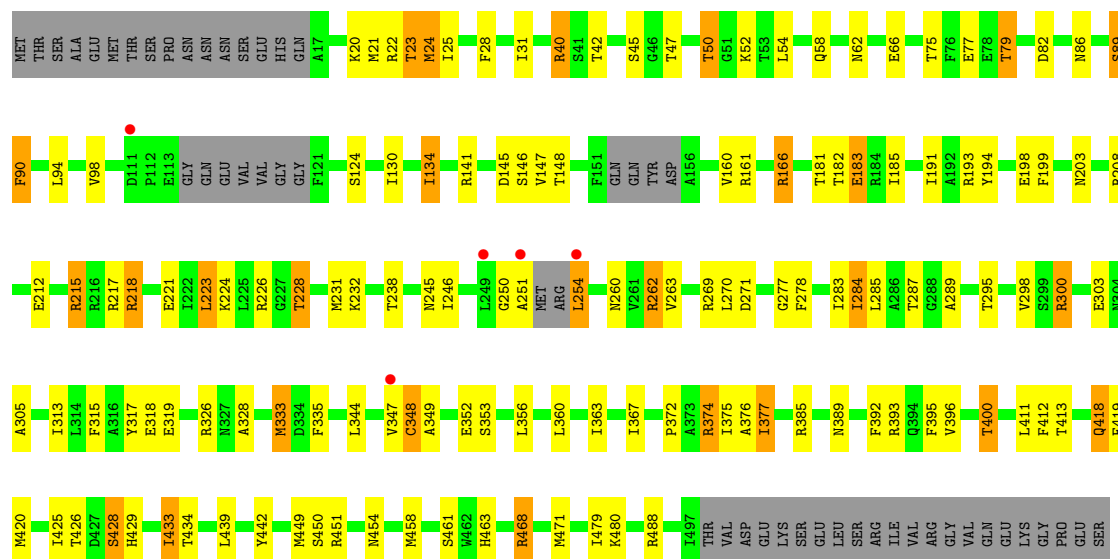
• Molecule 1: Circadian clock protein kinase KaiC

Chain G: 63% 23% 10%



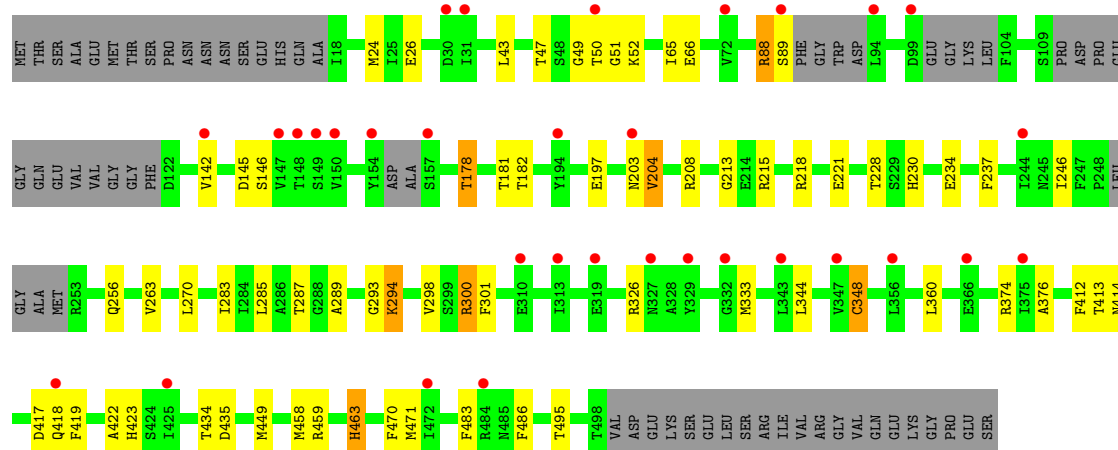
• Molecule 1: Circadian clock protein kinase KaiC

Chain H: 63% 22% 5% 10%

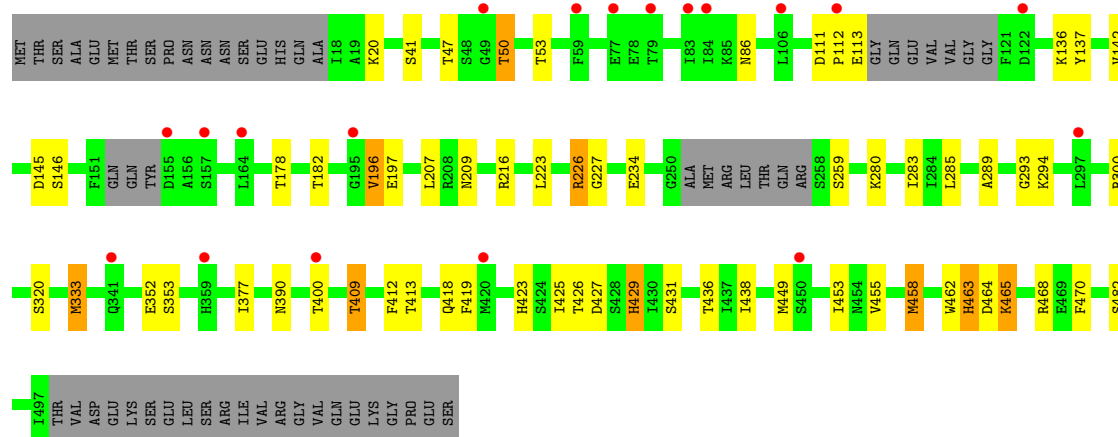
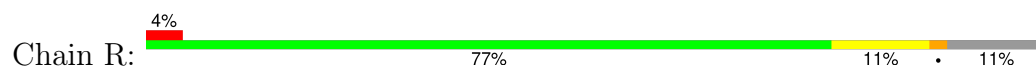


• Molecule 1: Circadian clock protein kinase KaiC

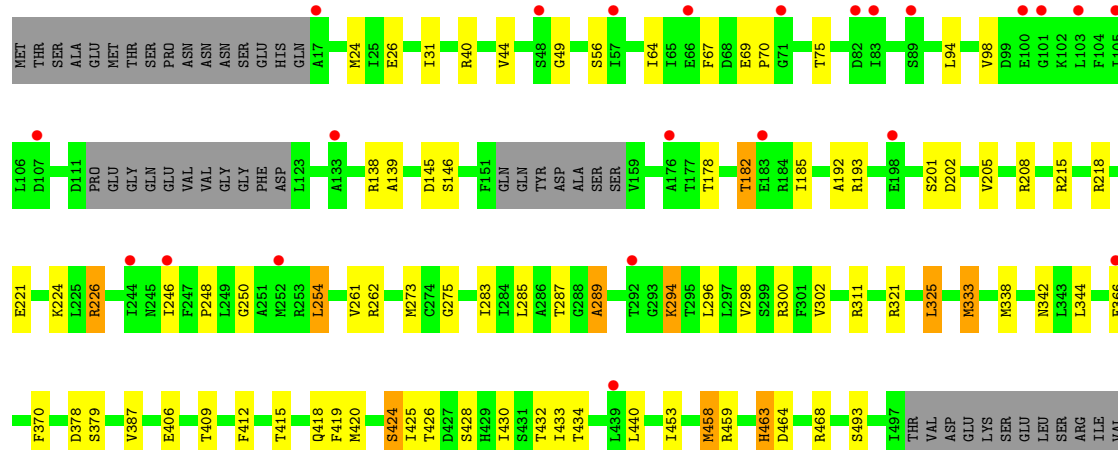
Chain N: 6% 74% 12% 12%



• Molecule 1: Circadian clock protein kinase KaiC



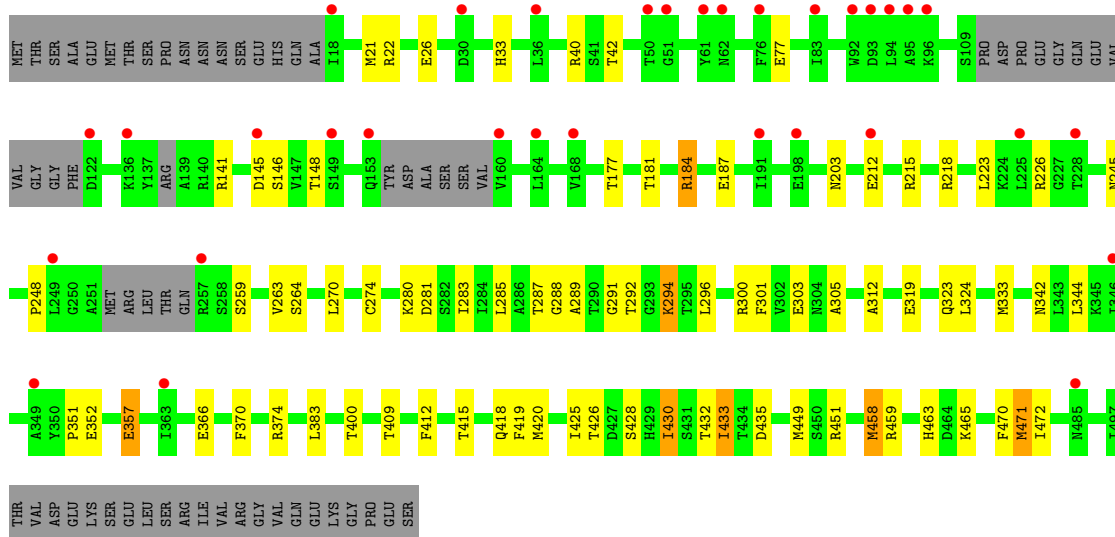
• Molecule 1: Circadian clock protein kinase KaiC



ARG
GLY
VAL
SER
GLN
GLU
LYS
GLY
PRO
GLU
SER

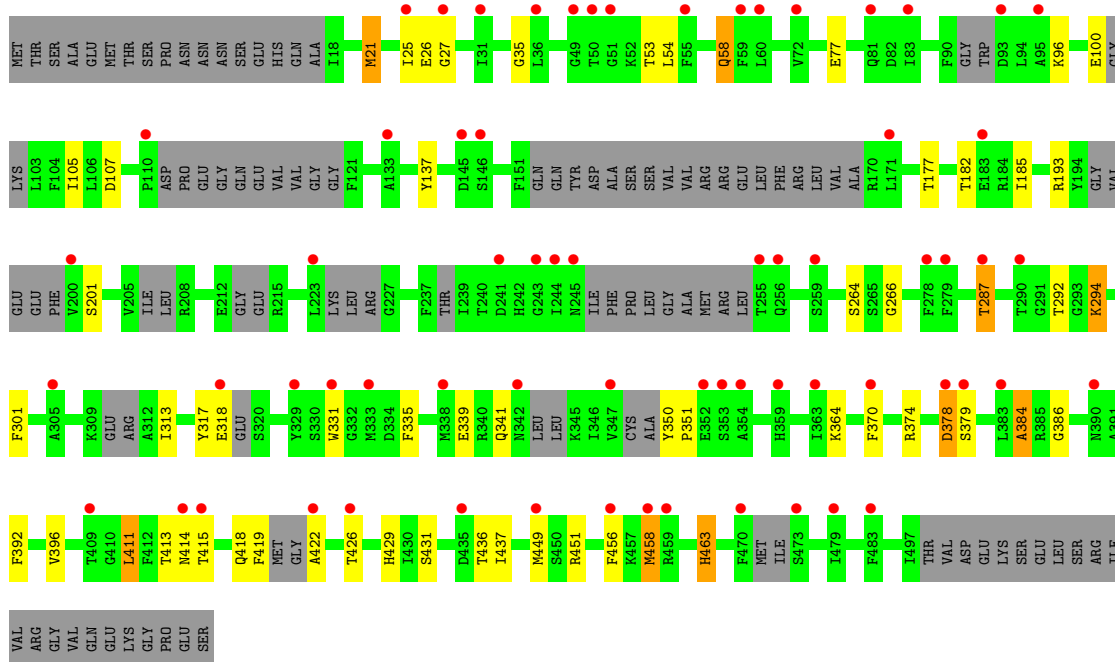
• Molecule 1: Circadian clock protein kinase KaiC

Chain P: 6% 72% 14% 12%



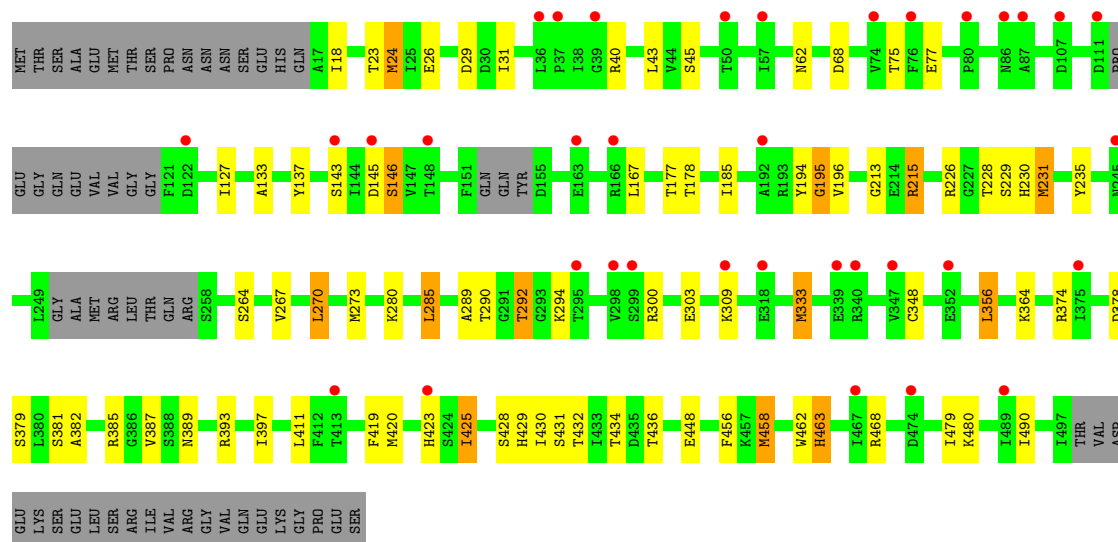
• Molecule 1: Circadian clock protein kinase KaiC

Chain T: 13% 68% 10% 20%

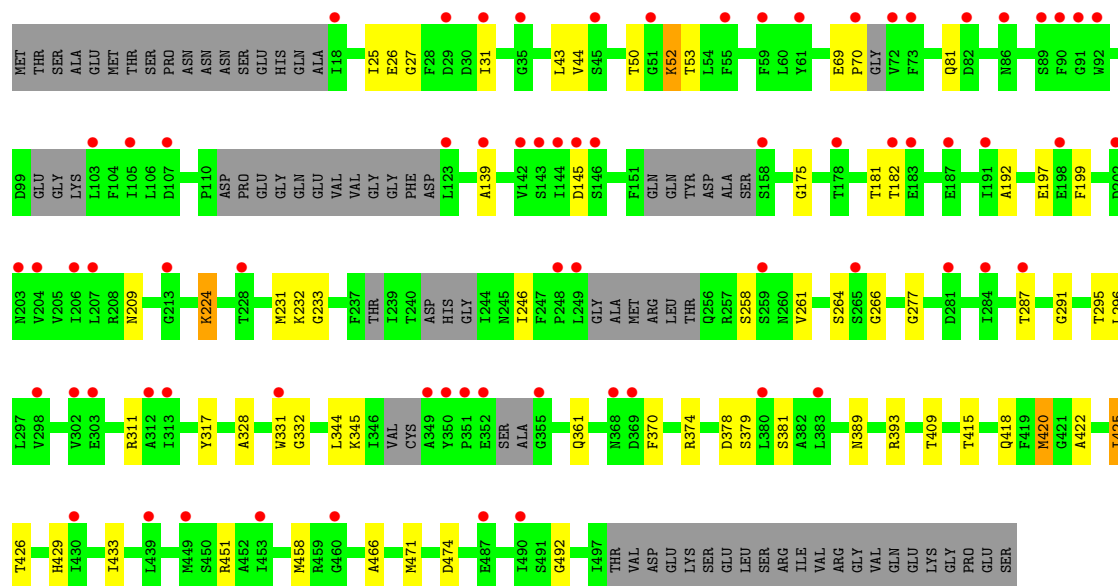


• Molecule 1: Circadian clock protein kinase KaiC

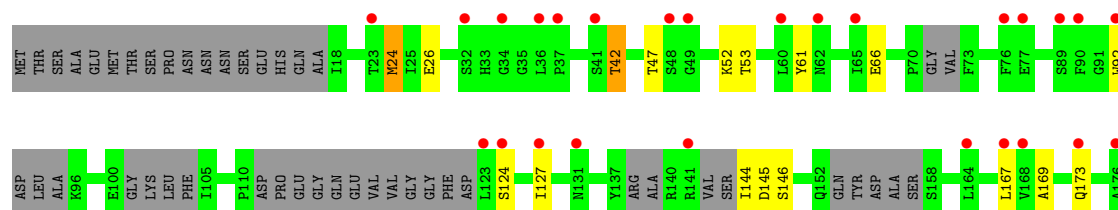
Chain X: 7% 73% 13% 11%

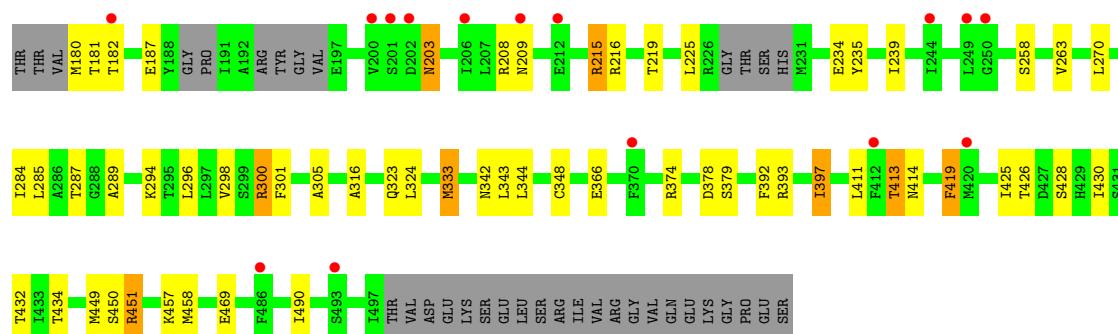


• Molecule 1: Circadian clock protein kinase KaiC

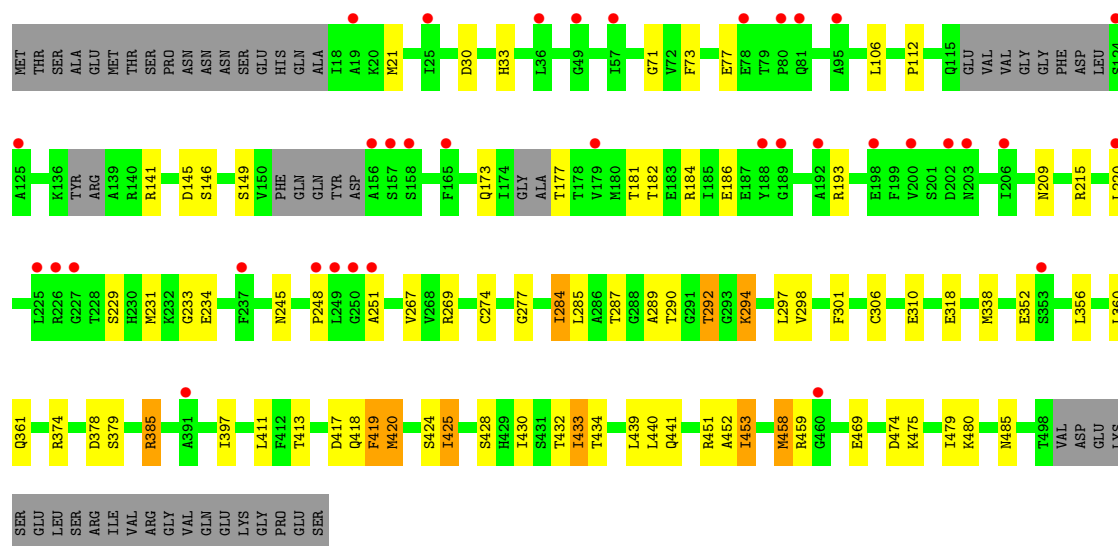
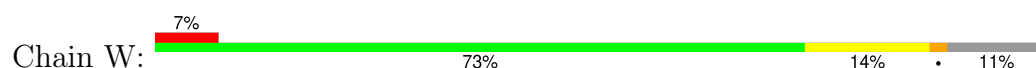


• Molecule 1: Circadian clock protein kinase KaiC

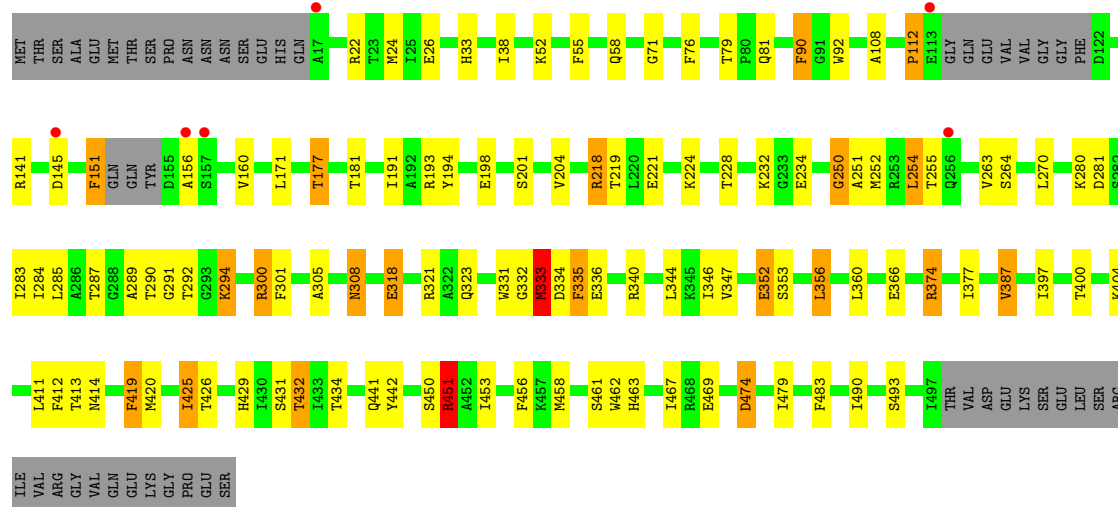




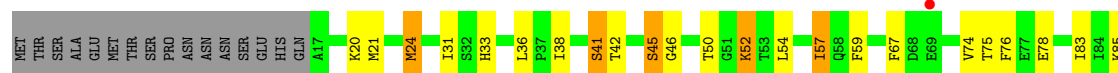
• Molecule 1: Circadian clock protein kinase KaiC

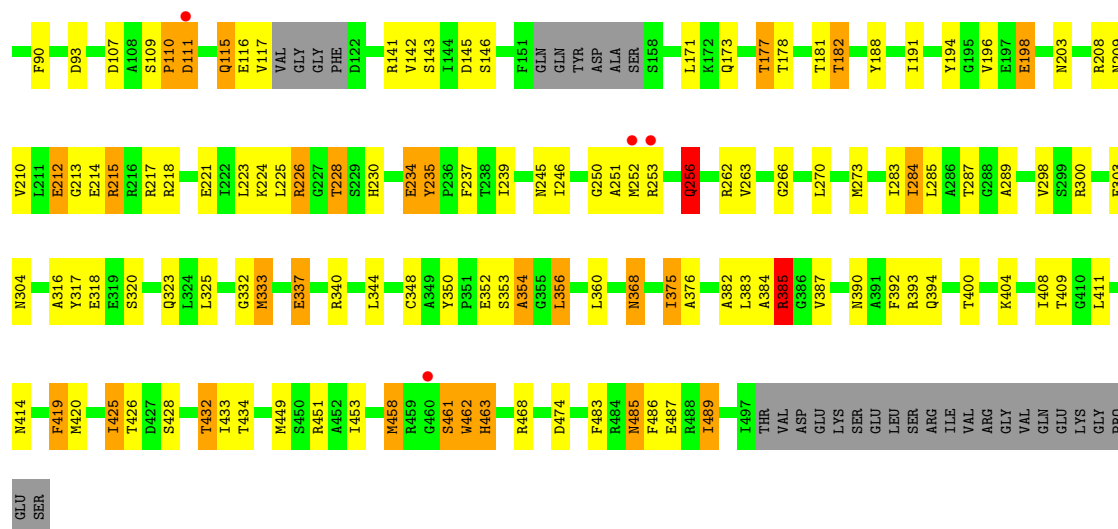


• Molecule 2: Circadian clock protein kinase KaiC

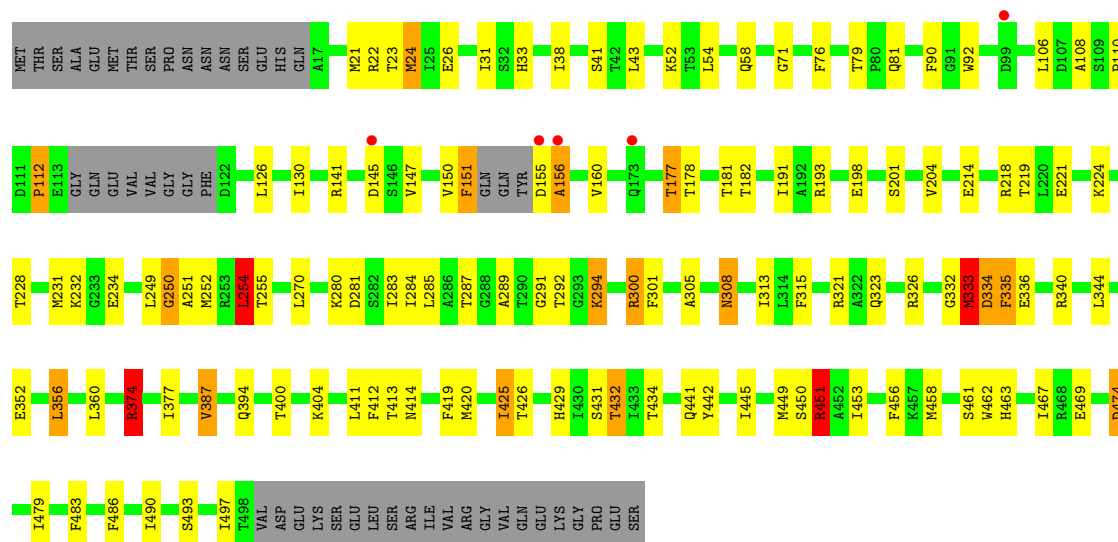


Chain F:

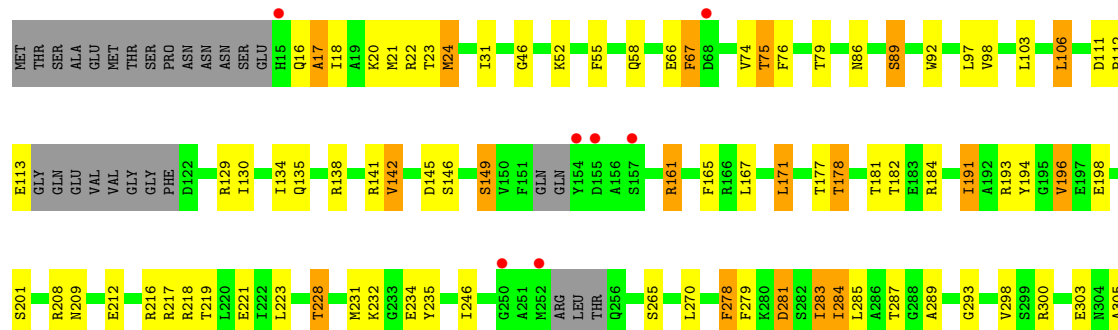


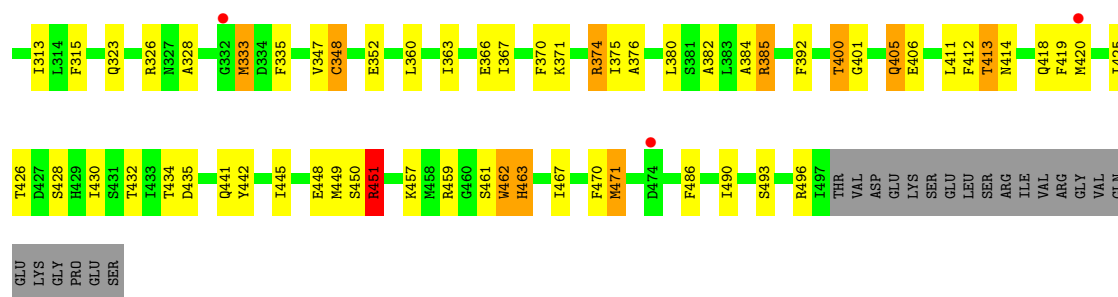


• Molecule 2: Circadian clock protein kinase KaiC

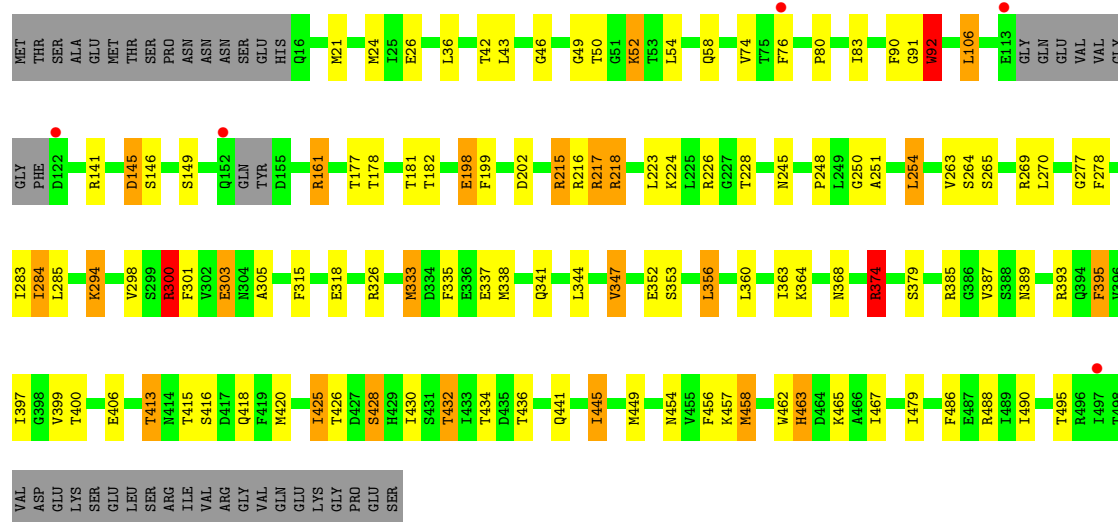


• Molecule 2: Circadian clock protein kinase KaiC

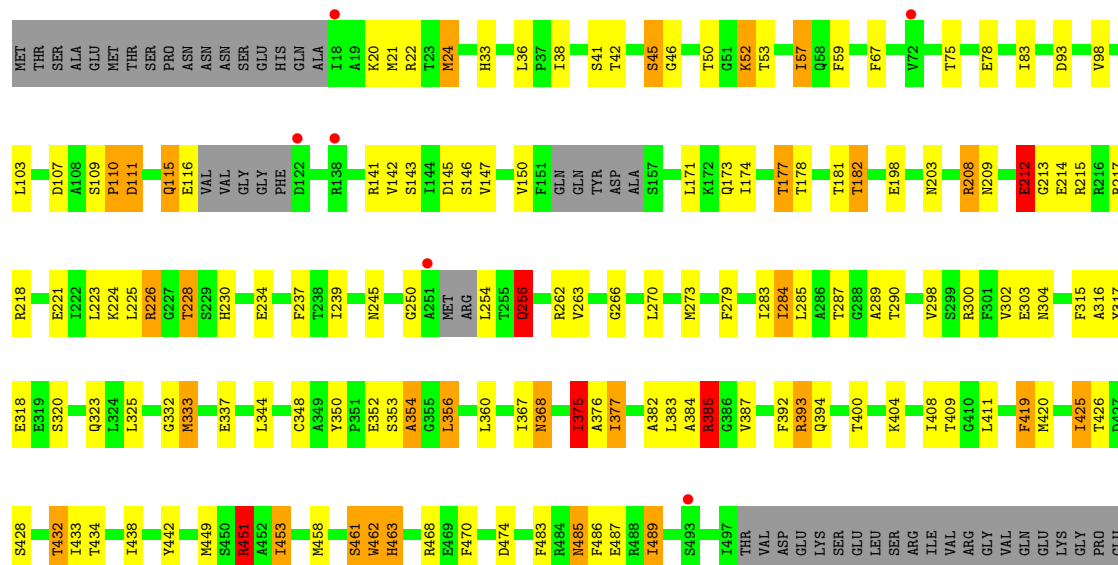




• Molecule 2: Circadian clock protein kinase KaiC

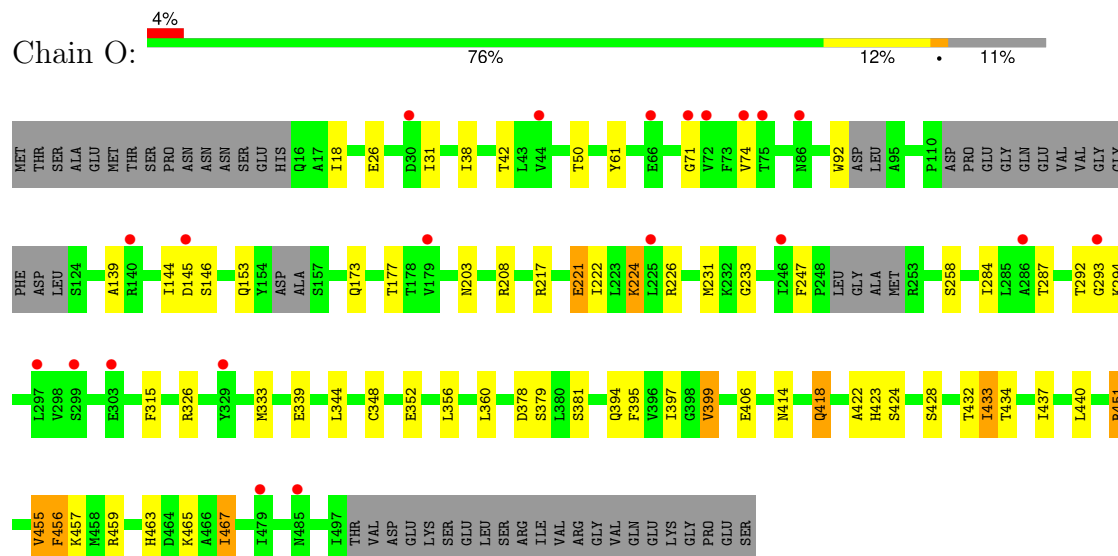


• Molecule 2: Circadian clock protein kinase KaiC

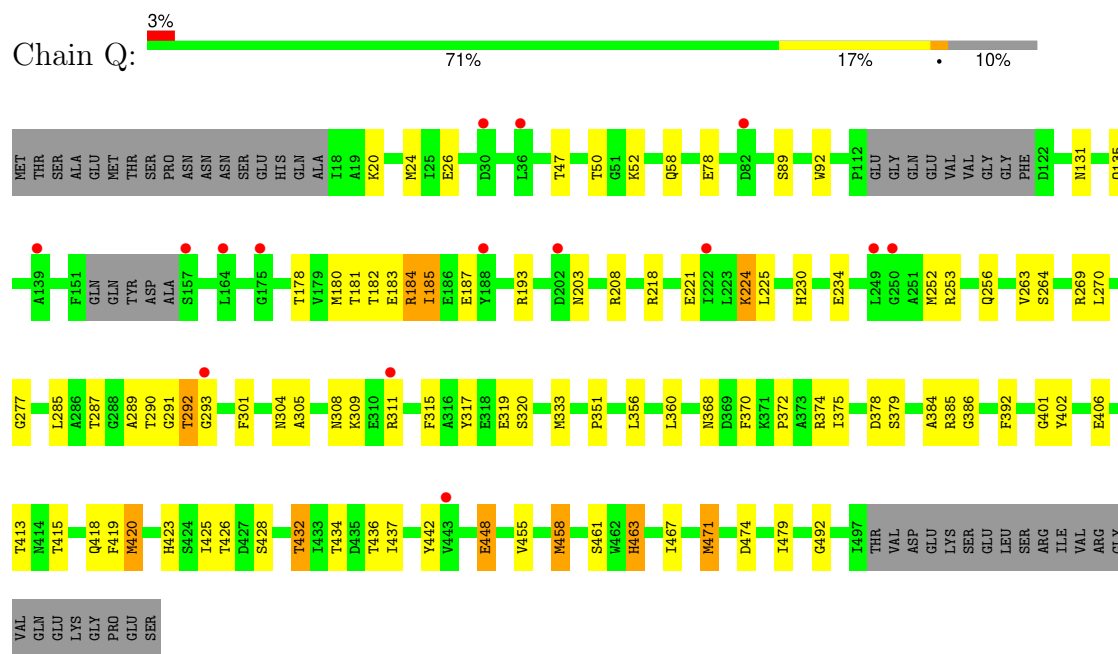


SER

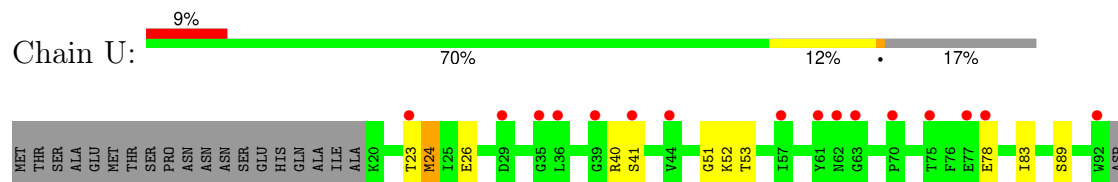
- Molecule 2: Circadian clock protein kinase KaiC



- Molecule 2: Circadian clock protein kinase KaiC



- Molecule 2: Circadian clock protein kinase KaiC





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	185.49Å 205.80Å 186.18Å 90.00° 115.14° 90.00°	Depositor
Resolution (Å)	49.22 – 3.10 49.22 – 3.10	Depositor EDS
% Data completeness (in resolution range)	93.7 (49.22-3.10) 94.0 (49.22-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.275 , 0.340 0.272 , 0.335	Depositor DCC
R_{free} test set	10614 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	59.2	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 65.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	78739	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 74.56 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4924e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, TPO, ADP, 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	1.04	1/3555 (0.0%)	1.53	14/4815 (0.3%)
1	B	1.07	2/3479 (0.1%)	1.68	38/4719 (0.8%)
1	G	1.04	2/3494 (0.1%)	1.53	12/4734 (0.3%)
1	H	1.05	3/3523 (0.1%)	1.65	36/4770 (0.8%)
1	M	1.07	0/3164	1.51	0/4307
1	N	1.10	0/3041	1.52	0/4142
1	P	1.08	0/3132	1.49	0/4259
1	R	1.06	0/3243	1.50	0/4406
1	S	1.15	0/2725	1.57	2/3730 (0.1%)
1	T	1.15	0/2431	1.58	0/3319
1	V	1.08	0/2936	1.48	0/3993
1	W	1.07	0/3160	1.49	1/4293 (0.0%)
1	X	1.09	0/3109	1.52	0/4232
2	C	1.09	5/3473 (0.1%)	1.60	21/4710 (0.4%)
2	D	1.06	2/3491 (0.1%)	1.58	16/4732 (0.3%)
2	E	1.06	3/3460 (0.1%)	1.59	14/4695 (0.3%)
2	F	1.04	1/3471 (0.0%)	1.57	17/4699 (0.4%)
2	I	1.08	3/3513 (0.1%)	1.59	18/4758 (0.4%)
2	J	1.06	2/3476 (0.1%)	1.58	20/4709 (0.4%)
2	K	1.06	3/3479 (0.1%)	1.57	12/4720 (0.3%)
2	L	1.04	0/3507	1.56	15/4752 (0.3%)
2	O	1.09	0/3096	1.53	1/4219 (0.0%)
2	Q	1.03	0/3338	1.46	1/4529 (0.0%)
2	U	1.14	0/2638	1.57	1/3600 (0.0%)
All	All	1.07	27/77934 (0.0%)	1.55	239/105842 (0.2%)

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	B	0	1

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	33	HIS	CE1-NE2	-9.47	1.23	1.32
2	D	33	HIS	CE1-NE2	-9.06	1.23	1.32
2	I	347	VAL	C-O	-8.81	1.14	1.24
2	E	33	HIS	CE1-NE2	-8.35	1.24	1.32
2	C	347	VAL	C-O	-8.29	1.14	1.24

The worst 5 of 239 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	374	ARG	NE-CZ-NH1	13.01	134.51	121.50
2	K	374	ARG	NE-CZ-NH1	12.12	133.62	121.50
1	B	262	ARG	NE-CZ-NH2	11.70	129.73	119.20
2	E	218	ARG	CG-CD-NE	11.21	136.66	112.00
1	B	262	ARG	NE-CZ-NH1	-11.06	110.44	121.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	251	ALA	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	3506	0	3303	125	0
1	B	3432	0	3166	106	0
1	G	3448	0	3229	124	0
1	H	3476	0	3247	115	0
1	M	3123	0	2557	37	0
1	N	3010	0	2393	33	0
1	P	3096	0	2554	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	3201	0	2747	36	0
1	S	2706	0	1911	33	0
1	T	2427	0	1562	33	0
1	V	2914	0	2335	49	0
1	W	3126	0	2564	55	0
1	X	3074	0	2533	44	0
2	C	3436	0	3139	96	0
2	D	3456	0	3185	126	0
2	E	3424	0	3156	93	0
2	F	3436	0	3161	87	0
2	I	3477	0	3211	105	0
2	J	3442	0	3178	123	0
2	K	3444	0	3198	97	0
2	L	3471	0	3211	117	0
2	O	3072	0	2499	24	0
2	Q	3303	0	2875	55	0
2	U	2635	0	1858	43	0
3	A	62	0	24	3	0
3	B	62	0	24	6	0
3	C	62	0	24	6	0
3	D	62	0	24	1	0
3	E	62	0	24	5	0
3	F	62	0	24	3	0
3	G	62	0	24	3	0
3	H	62	0	24	3	0
3	I	62	0	24	5	0
3	J	62	0	24	3	0
3	K	62	0	24	2	0
3	L	62	0	24	5	0
3	M	62	0	24	2	0
3	N	62	0	24	3	0
3	O	62	0	24	1	0
3	P	62	0	24	6	0
3	Q	31	0	12	0	0
3	R	62	0	24	1	0
3	S	62	0	24	2	0
3	T	62	0	24	1	0
3	U	31	0	12	1	0
3	V	62	0	24	3	0
3	W	31	0	12	2	0
3	X	62	0	24	2	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	H	2	0	0	0	0
4	I	2	0	0	0	0
4	J	2	0	0	0	0
4	K	2	0	0	0	0
4	L	2	0	0	0	0
4	M	1	0	0	0	0
4	N	2	0	0	0	0
4	O	1	0	0	0	0
4	P	2	0	0	0	0
4	Q	1	0	0	0	0
4	R	2	0	0	0	0
4	T	1	0	0	0	0
4	U	1	0	0	0	0
4	V	1	0	0	0	0
5	Q	27	0	12	0	0
5	U	27	0	12	9	0
5	W	27	0	12	0	0
6	A	6	0	0	0	0
6	B	9	0	0	0	0
6	C	7	0	0	0	0
6	D	4	0	0	0	0
6	E	4	0	0	0	0
6	F	6	0	0	0	0
6	G	4	0	0	0	0
6	H	4	0	0	0	0
6	I	5	0	0	0	0
6	J	4	0	0	0	0
6	K	3	0	0	0	0
6	L	6	0	0	0	0
6	M	1	0	0	0	0
6	N	2	0	0	0	0
6	O	5	0	0	0	0
6	P	4	0	0	0	0
6	Q	5	0	0	0	0
6	R	2	0	0	0	0
6	S	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	U	2	0	0	0	0
6	V	2	0	0	0	0
6	W	3	0	0	0	0
6	X	2	0	0	0	0
All	All	78739	0	67348	1582	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 11.

The worst 5 of 1582 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:V:419:PHE:CD2	1:W:425:ILE:HD13	1.69	1.26
1:G:47:THR:O	1:G:50:THR:OG1	1.61	1.18
1:H:231:MET:HE1	1:H:251:ALA:CB	1.80	1.11
2:C:419:PHE:CD1	2:D:425:ILE:HD13	1.85	1.10
1:V:419:PHE:CD2	1:W:425:ILE:CD1	2.35	1.09

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	461/519 (89%)	433 (94%)	22 (5%)	6 (1%)	9	35
1	B	462/519 (89%)	431 (93%)	24 (5%)	7 (2%)	8	32
1	G	458/519 (88%)	433 (94%)	23 (5%)	2 (0%)	30	61
1	H	459/519 (88%)	430 (94%)	26 (6%)	3 (1%)	18	49
1	M	456/519 (88%)	410 (90%)	39 (9%)	7 (2%)	8	32
1	N	442/519 (85%)	387 (88%)	43 (10%)	12 (3%)	4	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	445/519 (86%)	400 (90%)	39 (9%)	6 (1%)	9	35
1	R	454/519 (88%)	414 (91%)	35 (8%)	5 (1%)	11	39
1	S	423/519 (82%)	360 (85%)	55 (13%)	8 (2%)	6	27
1	T	380/519 (73%)	299 (79%)	67 (18%)	14 (4%)	2	15
1	V	412/519 (79%)	359 (87%)	50 (12%)	3 (1%)	18	49
1	W	453/519 (87%)	386 (85%)	57 (13%)	10 (2%)	5	24
1	X	452/519 (87%)	408 (90%)	31 (7%)	13 (3%)	3	19
2	C	464/519 (89%)	428 (92%)	31 (7%)	5 (1%)	11	39
2	D	463/519 (89%)	419 (90%)	34 (7%)	10 (2%)	5	24
2	E	462/519 (89%)	427 (92%)	26 (6%)	9 (2%)	6	27
2	F	458/519 (88%)	432 (94%)	19 (4%)	7 (2%)	8	32
2	I	465/519 (90%)	430 (92%)	33 (7%)	2 (0%)	30	61
2	J	458/519 (88%)	414 (90%)	36 (8%)	8 (2%)	7	30
2	K	463/519 (89%)	427 (92%)	26 (6%)	10 (2%)	5	24
2	L	460/519 (89%)	431 (94%)	23 (5%)	6 (1%)	9	35
2	O	449/519 (86%)	399 (89%)	40 (9%)	10 (2%)	5	24
2	Q	458/519 (88%)	416 (91%)	38 (8%)	4 (1%)	14	44
2	U	404/519 (78%)	340 (84%)	53 (13%)	11 (3%)	4	20
All	All	10761/12456 (86%)	9713 (90%)	870 (8%)	178 (2%)	7	30

5 of 178 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	ARG
1	A	256	GLN
1	B	252	MET
1	B	254	LEU
1	B	348	CYS

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	351/443 (79%)	308 (88%)	43 (12%)	4	20
1	B	328/443 (74%)	289 (88%)	39 (12%)	5	21
1	G	338/443 (76%)	295 (87%)	43 (13%)	4	18
1	H	341/443 (77%)	298 (87%)	43 (13%)	4	19
1	M	247/443 (56%)	217 (88%)	30 (12%)	5	20
1	N	222/443 (50%)	201 (90%)	21 (10%)	8	30
1	P	249/443 (56%)	216 (87%)	33 (13%)	4	17
1	R	270/443 (61%)	250 (93%)	20 (7%)	13	40
1	S	155/443 (35%)	141 (91%)	14 (9%)	9	33
1	T	109/443 (25%)	95 (87%)	14 (13%)	4	18
1	V	221/443 (50%)	186 (84%)	35 (16%)	2	12
1	W	242/443 (55%)	208 (86%)	34 (14%)	3	15
1	X	239/443 (54%)	211 (88%)	28 (12%)	5	22
2	C	323/442 (73%)	287 (89%)	36 (11%)	6	24
2	D	332/442 (75%)	287 (86%)	45 (14%)	3	16
2	E	324/442 (73%)	288 (89%)	36 (11%)	6	24
2	F	327/442 (74%)	283 (86%)	44 (14%)	4	16
2	I	334/442 (76%)	292 (87%)	42 (13%)	4	19
2	J	330/442 (75%)	287 (87%)	43 (13%)	4	18
2	K	330/442 (75%)	296 (90%)	34 (10%)	7	27
2	L	336/442 (76%)	289 (86%)	47 (14%)	3	15
2	O	237/442 (54%)	207 (87%)	30 (13%)	4	18
2	Q	289/442 (65%)	256 (89%)	33 (11%)	5	23
2	U	151/442 (34%)	132 (87%)	19 (13%)	4	19
All	All	6625/10621 (62%)	5819 (88%)	806 (12%)	5	20

5 of 806 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	198	GLU
1	M	226	ARG
1	W	430	ILE
2	J	352	GLU

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Mol	Chain	Res	Type
2	J	182	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 126 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	389	ASN
2	U	454	ASN
2	J	441	GLN
2	U	441	GLN
1	S	414	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

35 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	SEP	H	431	1	8,9,10	0.64	0	7,12,14	0.58	0
1	SEP	V	431	1	8,9,10	0.70	0	7,12,14	0.64	0
1	SEP	M	431	1	8,9,10	0.67	0	7,12,14	0.61	0
2	TPO	O	432	2	8,10,11	1.02	1 (12%)	10,14,16	1.05	1 (10%)
2	TPO	U	432	2	8,10,11	1.00	1 (12%)	10,14,16	1.06	1 (10%)
2	TPO	J	432	2	8,10,11	0.89	1 (12%)	10,14,16	0.88	0
2	TPO	K	432	2	8,10,11	1.31	1 (12%)	10,14,16	1.17	0
1	SEP	N	431	1	8,9,10	0.72	0	7,12,14	0.74	0
2	SEP	I	431	2	8,9,10	0.64	0	7,12,14	0.55	0
2	TPO	C	432	2	8,10,11	1.45	2 (25%)	10,14,16	0.80	0
2	SEP	E	431	2	8,9,10	0.60	0	7,12,14	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SEP	R	431	1	8,9,10	0.70	0	7,12,14	0.77	0
1	SEP	G	431	1	8,9,10	1.13	1 (12%)	7,12,14	1.15	1 (14%)
2	SEP	D	431	2	8,9,10	0.70	0	7,12,14	0.55	0
2	TPO	Q	432	2	8,10,11	0.97	1 (12%)	10,14,16	1.11	1 (10%)
1	SEP	T	431	1	8,9,10	0.76	0	7,12,14	0.78	0
2	SEP	Q	431	2	8,9,10	0.70	0	7,12,14	0.61	0
1	SEP	A	431	1	8,9,10	1.15	1 (12%)	7,12,14	1.09	0
2	SEP	F	431	2	8,9,10	0.57	0	7,12,14	0.69	0
1	SEP	B	431	1	8,9,10	0.64	0	7,12,14	0.59	0
2	SEP	L	431	2	8,9,10	0.57	0	7,12,14	0.68	0
2	TPO	L	432	2	8,10,11	1.55	2 (25%)	10,14,16	0.95	0
2	SEP	K	431	2	8,9,10	0.60	0	7,12,14	0.87	0
2	SEP	U	431	2	8,9,10	0.72	0	7,12,14	0.63	0
2	SEP	C	431	2	8,9,10	0.65	0	7,12,14	0.58	0
2	SEP	J	431	2	8,9,10	0.70	0	7,12,14	0.54	0
1	SEP	X	431	1	8,9,10	0.59	0	7,12,14	0.71	0
2	TPO	I	432	2	8,10,11	1.45	2 (25%)	10,14,16	0.83	0
1	SEP	P	431	1	8,9,10	0.64	0	7,12,14	0.61	0
2	TPO	E	432	2	8,10,11	1.35	1 (12%)	10,14,16	1.12	0
1	SEP	S	431	1	8,9,10	0.62	0	7,12,14	0.63	0
2	TPO	D	432	2	8,10,11	0.93	1 (12%)	10,14,16	0.90	0
1	SEP	W	431	1	8,9,10	0.58	0	7,12,14	0.71	0
2	TPO	F	432	2	8,10,11	1.58	2 (25%)	10,14,16	0.95	0
2	SEP	O	431	2	8,9,10	0.72	0	7,12,14	0.79	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	H	431	1	-	1/6/8/10	-
1	SEP	V	431	1	-	2/6/8/10	-
1	SEP	M	431	1	-	1/6/8/10	-
2	TPO	O	432	2	-	1/9/11/13	-
2	TPO	U	432	2	-	1/9/11/13	-
2	TPO	J	432	2	-	2/9/11/13	-
2	TPO	K	432	2	-	3/9/11/13	-
1	SEP	N	431	1	-	2/6/8/10	-
2	SEP	I	431	2	-	1/6/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPO	C	432	2	-	2/9/11/13	-
2	SEP	E	431	2	-	5/6/8/10	-
1	SEP	R	431	1	-	4/6/8/10	-
1	SEP	G	431	1	-	3/6/8/10	-
2	SEP	D	431	2	-	1/6/8/10	-
2	TPO	Q	432	2	-	4/9/11/13	-
1	SEP	T	431	1	-	1/6/8/10	-
2	SEP	Q	431	2	-	1/6/8/10	-
1	SEP	A	431	1	-	1/6/8/10	-
2	SEP	F	431	2	-	1/6/8/10	-
1	SEP	B	431	1	-	1/6/8/10	-
2	SEP	L	431	2	-	1/6/8/10	-
2	TPO	L	432	2	-	6/9/11/13	-
2	SEP	K	431	2	-	5/6/8/10	-
2	SEP	U	431	2	-	2/6/8/10	-
2	SEP	C	431	2	-	1/6/8/10	-
2	SEP	J	431	2	-	2/6/8/10	-
1	SEP	X	431	1	-	0/6/8/10	-
2	TPO	I	432	2	-	3/9/11/13	-
1	SEP	P	431	1	-	3/6/8/10	-
2	TPO	E	432	2	-	1/9/11/13	-
1	SEP	S	431	1	-	1/6/8/10	-
2	TPO	D	432	2	-	2/9/11/13	-
1	SEP	W	431	1	-	0/6/8/10	-
2	TPO	F	432	2	-	4/9/11/13	-
2	SEP	O	431	2	-	1/6/8/10	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	432	TPO	P-O2P	-3.02	1.43	1.54
2	L	432	TPO	P-O2P	-2.98	1.43	1.54
2	E	432	TPO	P-O2P	-2.88	1.44	1.54
2	F	432	TPO	P-OG1	2.72	1.64	1.59
2	L	432	TPO	P-OG1	2.61	1.64	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	432	TPO	O-C-CA	-2.82	117.52	124.77
2	Q	432	TPO	O-C-CA	-2.77	117.65	124.77
2	O	432	TPO	O-C-CA	-2.66	117.93	124.77
1	G	431	SEP	O3P-P-O2P	2.04	115.47	107.80

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	431	SEP	N-CA-CB-OG
2	E	431	SEP	N-CA-CB-OG
2	E	431	SEP	C-CA-CB-OG
2	E	431	SEP	CB-OG-P-O1P
2	E	431	SEP	CB-OG-P-O2P

There are no ring outliers.

13 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	432	TPO	5	0
2	K	432	TPO	1	0
2	C	432	TPO	1	0
2	E	431	SEP	1	0
1	R	431	SEP	2	0
2	Q	432	TPO	1	0
1	T	431	SEP	2	0
2	K	431	SEP	1	0
1	X	431	SEP	1	0
2	I	432	TPO	1	0
2	E	432	TPO	1	0
2	D	432	TPO	5	0
2	F	432	TPO	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 84 ligands modelled in this entry, 36 are monoatomic - leaving 48 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	$\# Z > 2$
5	ADP	W	701	-	28,29,29	0.46	0	43,45,45	0.46	0
3	ATP	D	701	4	32,33,33	0.57	0	48,52,52	0.60	0
3	ATP	H	701	4	32,33,33	0.51	0	48,52,52	0.65	0
3	ATP	V	701	4	32,33,33	0.48	0	48,52,52	0.58	0
3	ATP	M	701	4	32,33,33	0.53	0	48,52,52	0.59	0
3	ATP	F	702	4	32,33,33	0.52	0	48,52,52	0.67	0
3	ATP	C	701	4	32,33,33	0.51	0	48,52,52	0.66	0
3	ATP	A	702	4	32,33,33	0.53	0	48,52,52	0.63	0
3	ATP	I	702	4	32,33,33	0.49	0	48,52,52	0.55	0
3	ATP	X	702	-	32,33,33	0.51	0	48,52,52	0.73	1 (2%)
3	ATP	K	701	4	32,33,33	0.49	0	48,52,52	0.71	1 (2%)
3	ATP	J	702	4	32,33,33	0.53	0	48,52,52	0.71	1 (2%)
3	ATP	V	702	-	32,33,33	0.57	0	48,52,52	0.55	0
3	ATP	G	701	4	32,33,33	0.54	0	48,52,52	0.72	1 (2%)
3	ATP	Q	702	4	32,33,33	0.51	0	48,52,52	0.74	1 (2%)
3	ATP	S	701	-	32,33,33	0.54	0	48,52,52	0.58	0
3	ATP	G	702	4	32,33,33	0.53	0	48,52,52	0.76	1 (2%)
3	ATP	B	702	4	32,33,33	0.50	0	48,52,52	0.70	0
3	ATP	A	701	4	32,33,33	0.59	0	48,52,52	0.71	0
3	ATP	D	702	4	32,33,33	0.49	0	48,52,52	0.66	1 (2%)
3	ATP	S	702	-	32,33,33	0.55	0	48,52,52	0.60	0
3	ATP	N	701	4	32,33,33	0.51	0	48,52,52	0.72	1 (2%)
3	ATP	M	702	-	32,33,33	0.58	0	48,52,52	0.70	1 (2%)
3	ATP	T	702	-	32,33,33	0.51	0	48,52,52	0.58	0
3	ATP	R	701	4	32,33,33	0.61	0	48,52,52	0.59	0
3	ATP	B	701	4	32,33,33	0.51	0	48,52,52	0.62	0
3	ATP	L	701	4	32,33,33	0.48	0	48,52,52	0.72	0
3	ATP	O	701	4	32,33,33	0.58	0	48,52,52	0.70	1 (2%)
5	ADP	Q	701	-	28,29,29	0.43	0	43,45,45	0.48	0
3	ATP	K	702	4	32,33,33	0.53	0	48,52,52	0.61	0
3	ATP	H	702	4	32,33,33	0.50	0	48,52,52	0.64	0
3	ATP	T	701	4	32,33,33	0.54	0	48,52,52	0.70	0
3	ATP	C	702	4	32,33,33	0.51	0	48,52,52	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	U	701	4	32,33,33	0.55	0	48,52,52	0.64	0
3	ATP	P	701	4	32,33,33	0.52	0	48,52,52	0.68	0
3	ATP	P	702	4	32,33,33	0.54	0	48,52,52	0.69	1 (2%)
3	ATP	N	702	4	32,33,33	0.50	0	48,52,52	0.78	0
3	ATP	R	702	4	32,33,33	0.59	0	48,52,52	0.64	0
3	ATP	F	701	4	32,33,33	0.51	0	48,52,52	0.67	0
3	ATP	J	701	4	32,33,33	0.54	0	48,52,52	0.66	0
3	ATP	L	702	4	32,33,33	0.48	0	48,52,52	0.74	1 (2%)
3	ATP	E	702	4	32,33,33	0.49	0	48,52,52	0.61	0
3	ATP	X	701	-	32,33,33	0.55	0	48,52,52	0.60	0
3	ATP	W	702	-	32,33,33	0.58	0	48,52,52	0.70	1 (2%)
5	ADP	U	702	-	28,29,29	0.47	0	43,45,45	0.50	0
3	ATP	E	701	4	32,33,33	0.50	0	48,52,52	0.70	1 (2%)
3	ATP	I	701	4	32,33,33	0.47	0	48,52,52	0.65	0
3	ATP	O	702	-	32,33,33	0.54	0	48,52,52	0.72	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADP	W	701	-	-	6/16/32/32	0/3/3/3
3	ATP	D	701	4	-	8/22/38/38	0/3/3/3
3	ATP	H	701	4	-	2/22/38/38	0/3/3/3
3	ATP	V	701	4	-	2/22/38/38	0/3/3/3
3	ATP	M	701	4	-	4/22/38/38	0/3/3/3
3	ATP	F	702	4	-	7/22/38/38	0/3/3/3
3	ATP	C	701	4	-	2/22/38/38	0/3/3/3
3	ATP	A	702	4	-	4/22/38/38	0/3/3/3
3	ATP	I	702	4	-	7/22/38/38	0/3/3/3
3	ATP	X	702	-	-	6/22/38/38	0/3/3/3
3	ATP	K	701	4	-	1/22/38/38	0/3/3/3
3	ATP	J	702	4	-	1/22/38/38	0/3/3/3
3	ATP	V	702	-	-	6/22/38/38	0/3/3/3
3	ATP	G	701	4	-	1/22/38/38	0/3/3/3
3	ATP	Q	702	4	-	2/22/38/38	0/3/3/3
3	ATP	S	701	-	-	3/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	G	702	4	-	1/22/38/38	0/3/3/3
3	ATP	B	702	4	-	2/22/38/38	0/3/3/3
3	ATP	A	701	4	-	1/22/38/38	0/3/3/3
3	ATP	D	702	4	-	4/22/38/38	0/3/3/3
3	ATP	S	702	-	-	0/22/38/38	0/3/3/3
3	ATP	N	701	4	-	4/22/38/38	0/3/3/3
3	ATP	M	702	-	-	5/22/38/38	0/3/3/3
3	ATP	T	702	-	-	0/22/38/38	0/3/3/3
3	ATP	R	701	4	-	5/22/38/38	0/3/3/3
3	ATP	B	701	4	-	6/22/38/38	0/3/3/3
3	ATP	L	701	4	-	2/22/38/38	0/3/3/3
3	ATP	O	701	4	-	2/22/38/38	0/3/3/3
5	ADP	Q	701	-	-	3/16/32/32	0/3/3/3
3	ATP	K	702	4	-	1/22/38/38	0/3/3/3
3	ATP	H	702	4	-	2/22/38/38	0/3/3/3
3	ATP	T	701	4	-	4/22/38/38	0/3/3/3
3	ATP	C	702	4	-	4/22/38/38	0/3/3/3
3	ATP	U	701	4	-	1/22/38/38	0/3/3/3
3	ATP	P	701	4	-	3/22/38/38	0/3/3/3
3	ATP	P	702	4	-	2/22/38/38	0/3/3/3
3	ATP	N	702	4	-	5/22/38/38	0/3/3/3
3	ATP	R	702	4	-	4/22/38/38	0/3/3/3
3	ATP	F	701	4	-	4/22/38/38	0/3/3/3
3	ATP	J	701	4	-	7/22/38/38	0/3/3/3
3	ATP	L	702	4	-	4/22/38/38	0/3/3/3
3	ATP	E	702	4	-	2/22/38/38	0/3/3/3
3	ATP	X	701	-	-	8/22/38/38	0/3/3/3
3	ATP	W	702	-	-	3/22/38/38	0/3/3/3
5	ADP	U	702	-	-	4/16/32/32	0/3/3/3
3	ATP	E	701	4	-	5/22/38/38	0/3/3/3
3	ATP	I	701	4	-	5/22/38/38	0/3/3/3
3	ATP	O	702	-	-	3/22/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	702	ATP	C3'-C2'-C1'	2.24	105.70	101.46
3	W	702	ATP	C3'-C2'-C1'	2.23	105.68	101.46
3	G	702	ATP	C3'-C2'-C1'	2.16	105.55	101.46
3	N	701	ATP	C3'-C2'-C1'	2.14	105.52	101.46
3	P	702	ATP	C3'-C2'-C1'	2.12	105.48	101.46

There are no chirality outliers.

5 of 168 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	ATP	C5'-O5'-PA-O1A
3	A	702	ATP	C5'-O5'-PA-O2A
3	A	702	ATP	C5'-O5'-PA-O3A
3	B	701	ATP	C5'-O5'-PA-O2A
3	B	701	ATP	C5'-O5'-PA-O3A

There are no ring outliers.

38 monomers are involved in 78 short contacts:

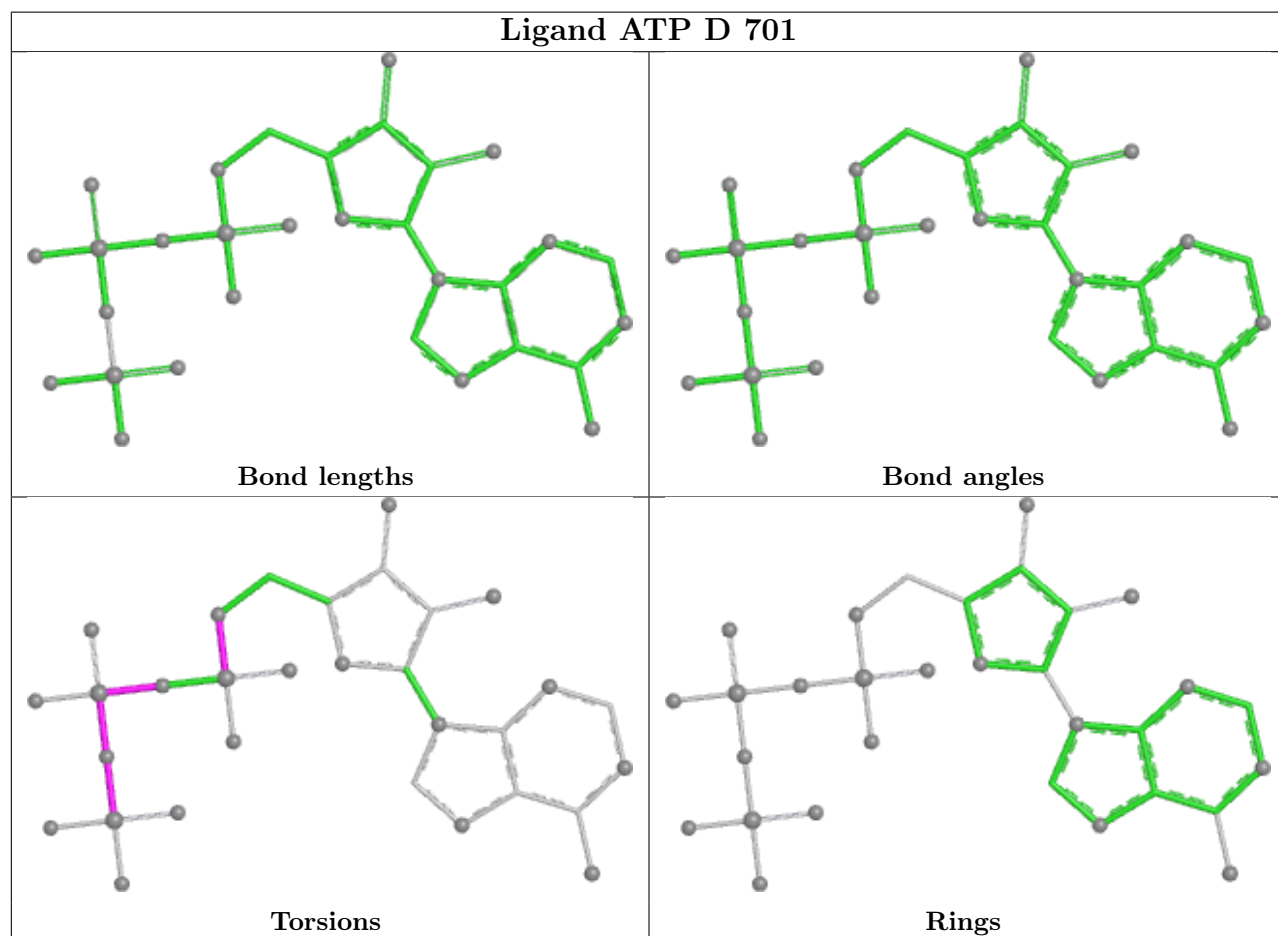
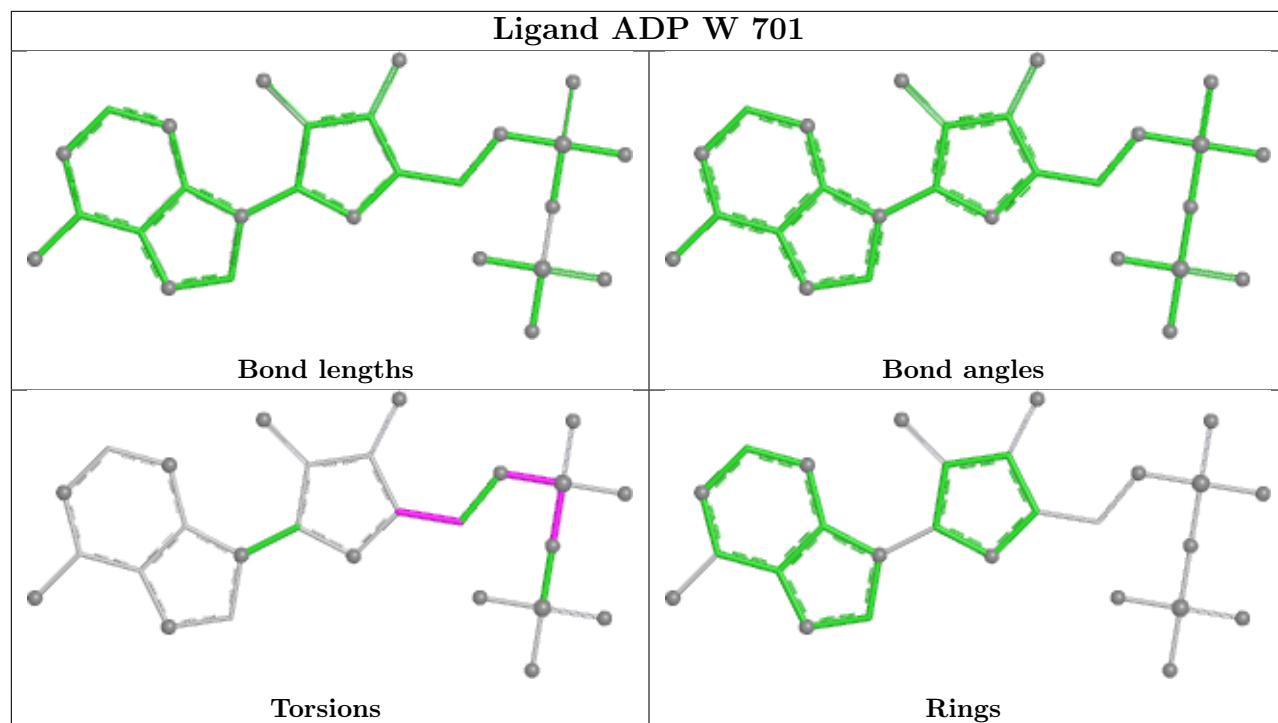
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	701	ATP	2	0
3	V	701	ATP	1	0
3	M	701	ATP	1	0
3	F	702	ATP	1	0
3	C	701	ATP	3	0
3	A	702	ATP	3	0
3	I	702	ATP	4	0
3	X	702	ATP	1	0
3	K	701	ATP	1	0
3	J	702	ATP	2	0
3	V	702	ATP	2	0
3	S	701	ATP	2	0
3	G	702	ATP	3	0
3	B	702	ATP	4	0
3	D	702	ATP	1	0
3	N	701	ATP	1	0
3	M	702	ATP	1	0
3	T	702	ATP	1	0
3	B	701	ATP	2	0
3	L	701	ATP	1	0
3	K	702	ATP	1	0
3	H	702	ATP	1	0

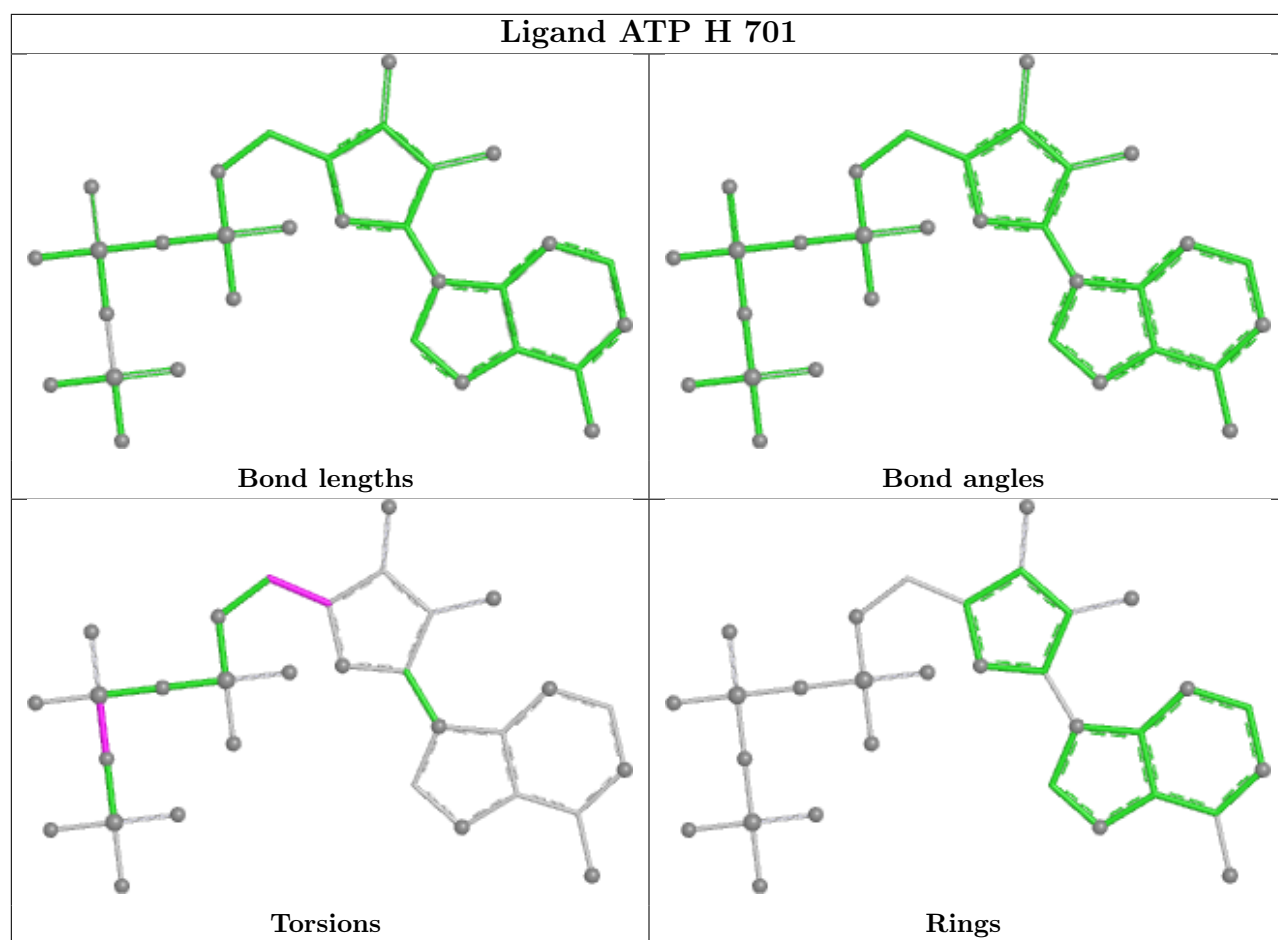
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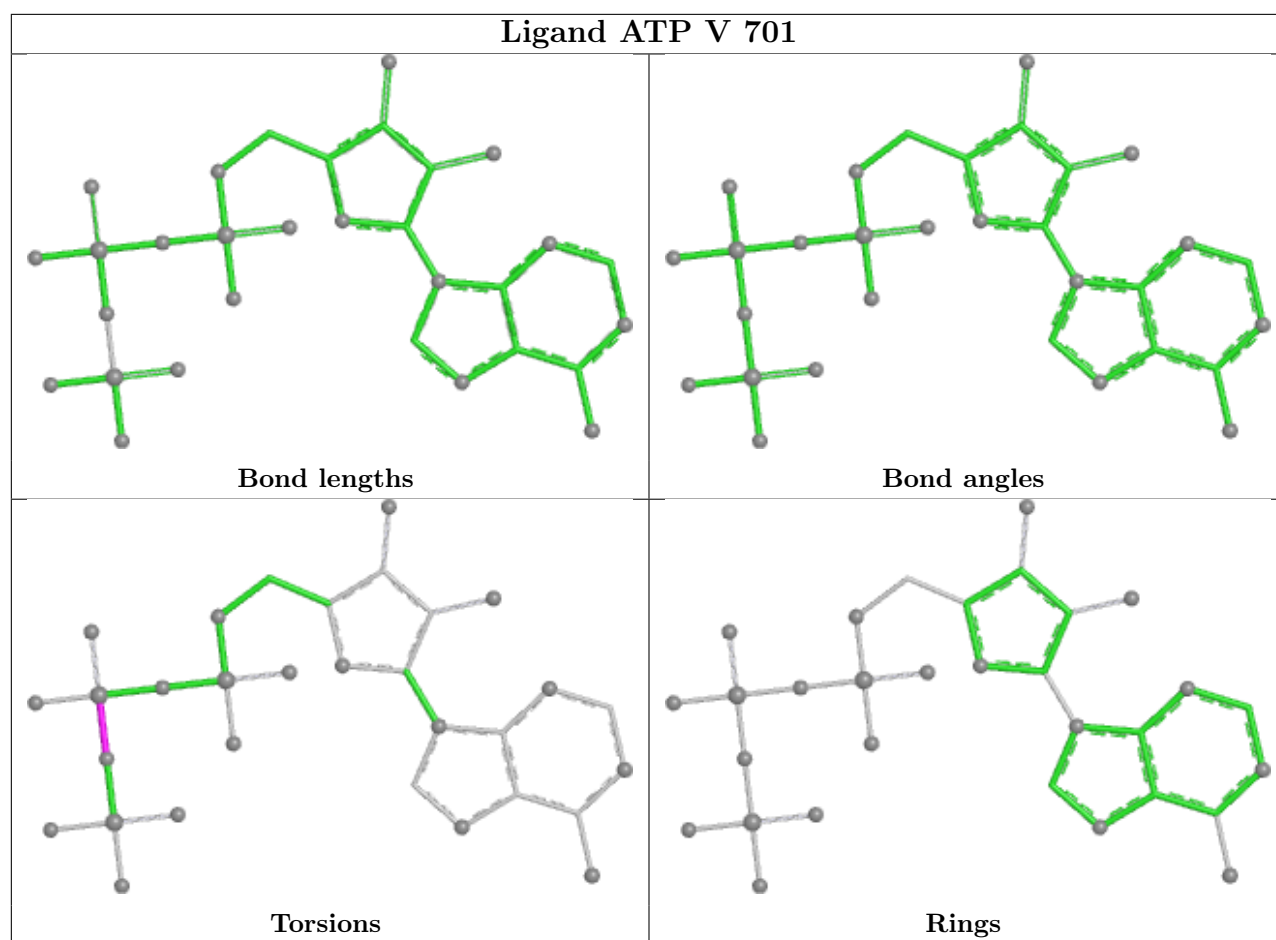
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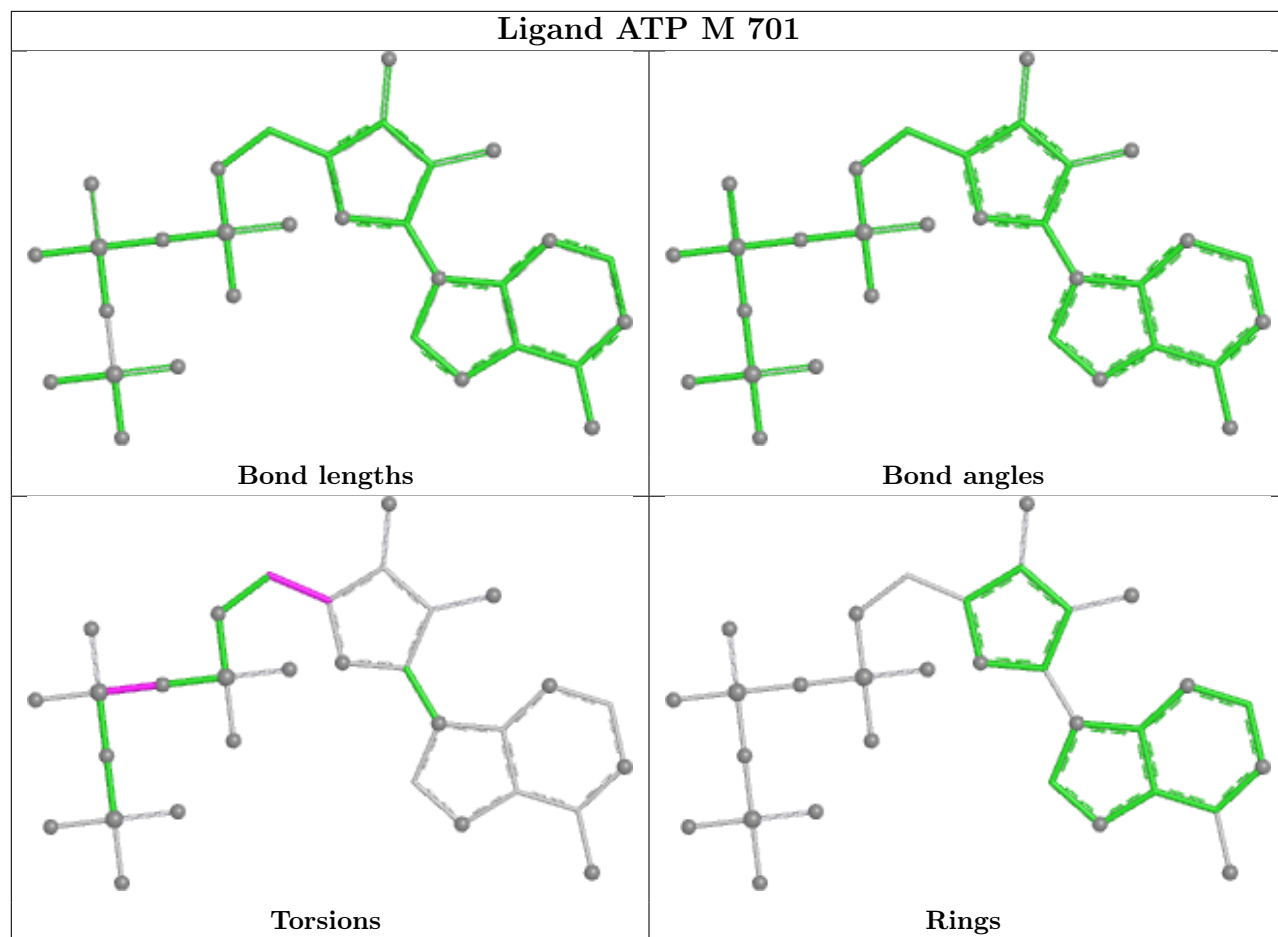
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	702	ATP	3	0
3	U	701	ATP	1	0
3	P	701	ATP	5	0
3	P	702	ATP	1	0
3	N	702	ATP	2	0
3	R	702	ATP	1	0
3	F	701	ATP	2	0
3	J	701	ATP	1	0
3	L	702	ATP	4	0
3	E	702	ATP	1	0
3	X	701	ATP	1	0
3	W	702	ATP	2	0
5	U	702	ADP	9	0
3	E	701	ATP	4	0
3	I	701	ATP	1	0
3	O	702	ATP	1	0

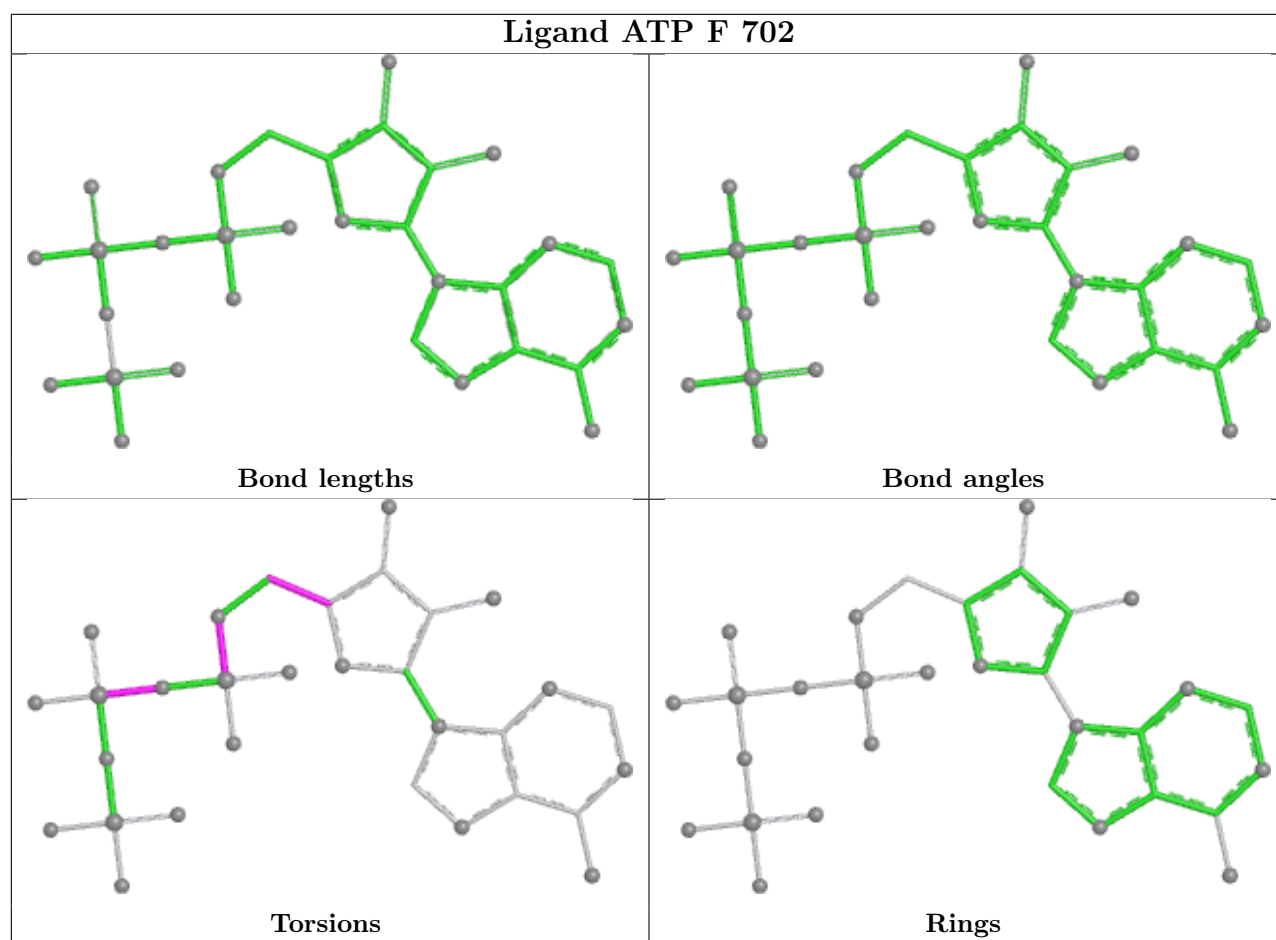
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

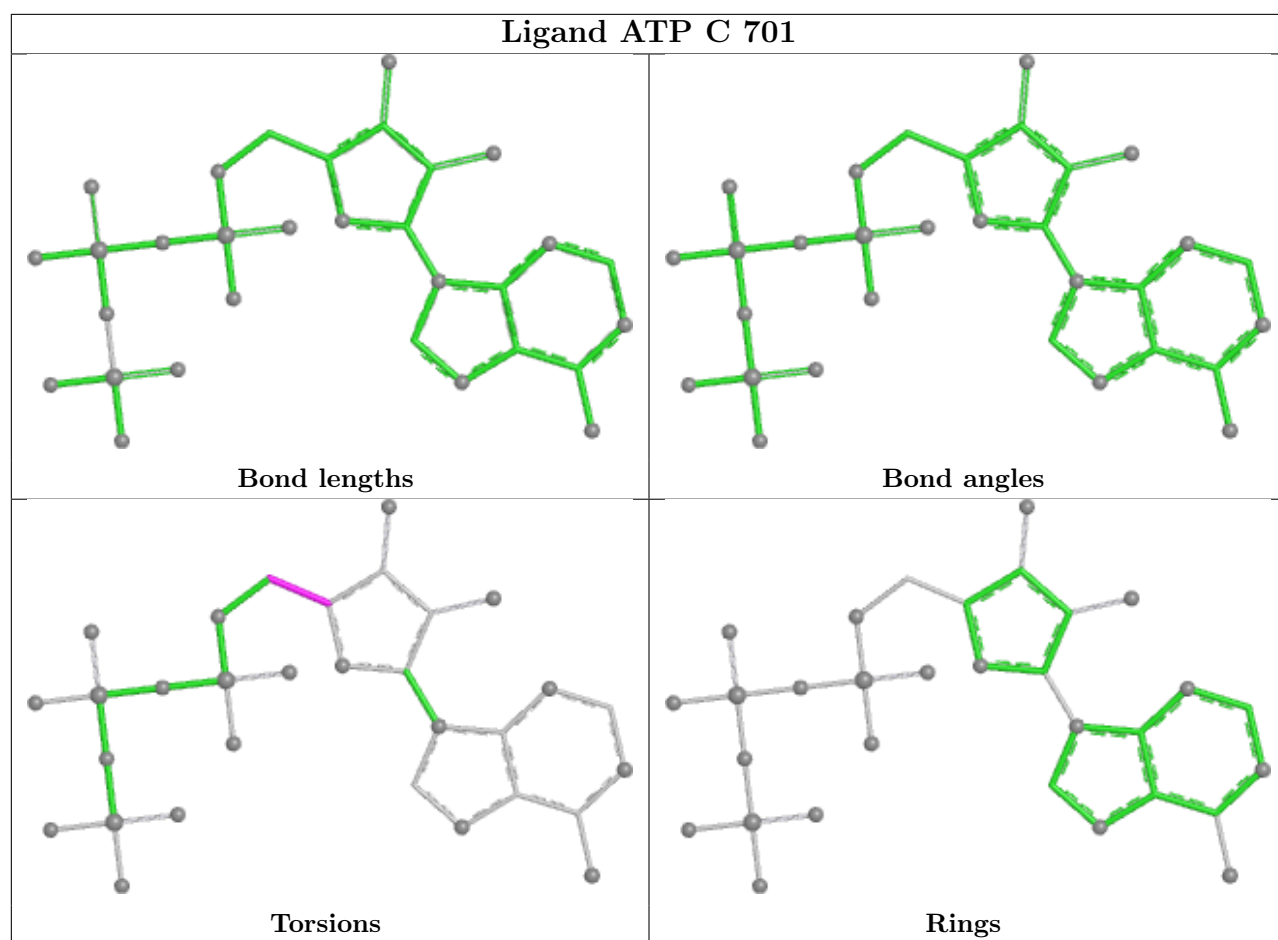


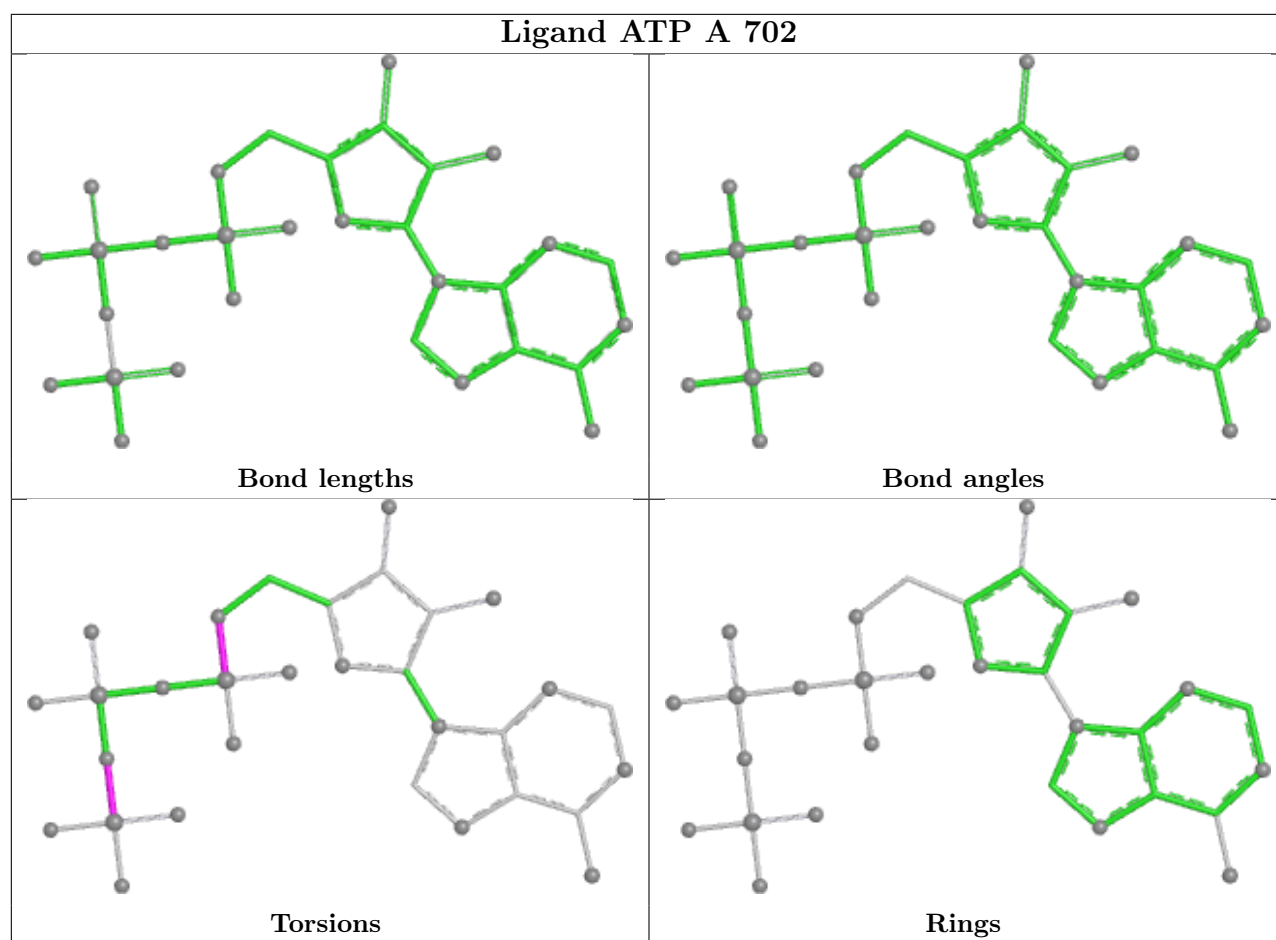




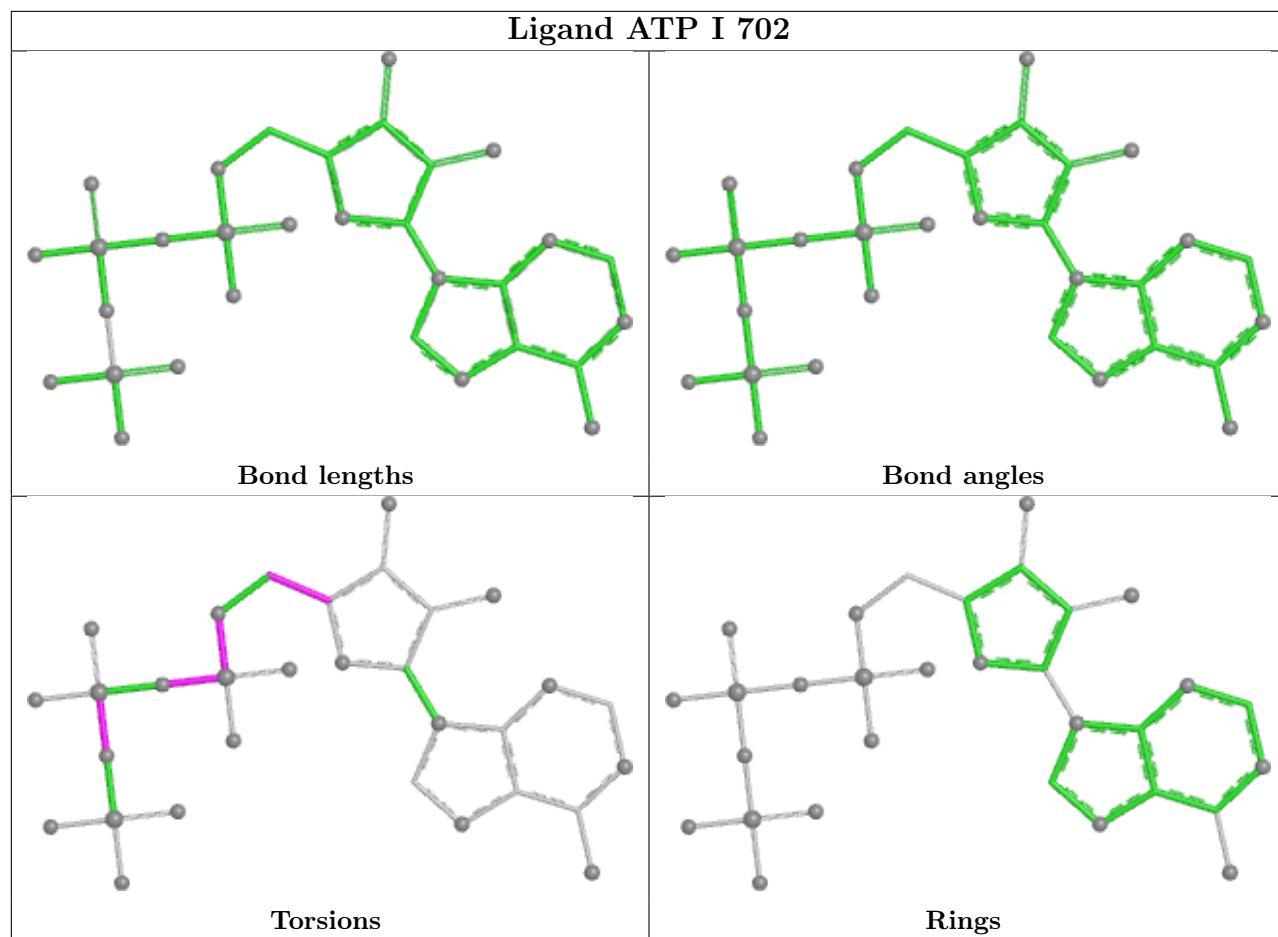


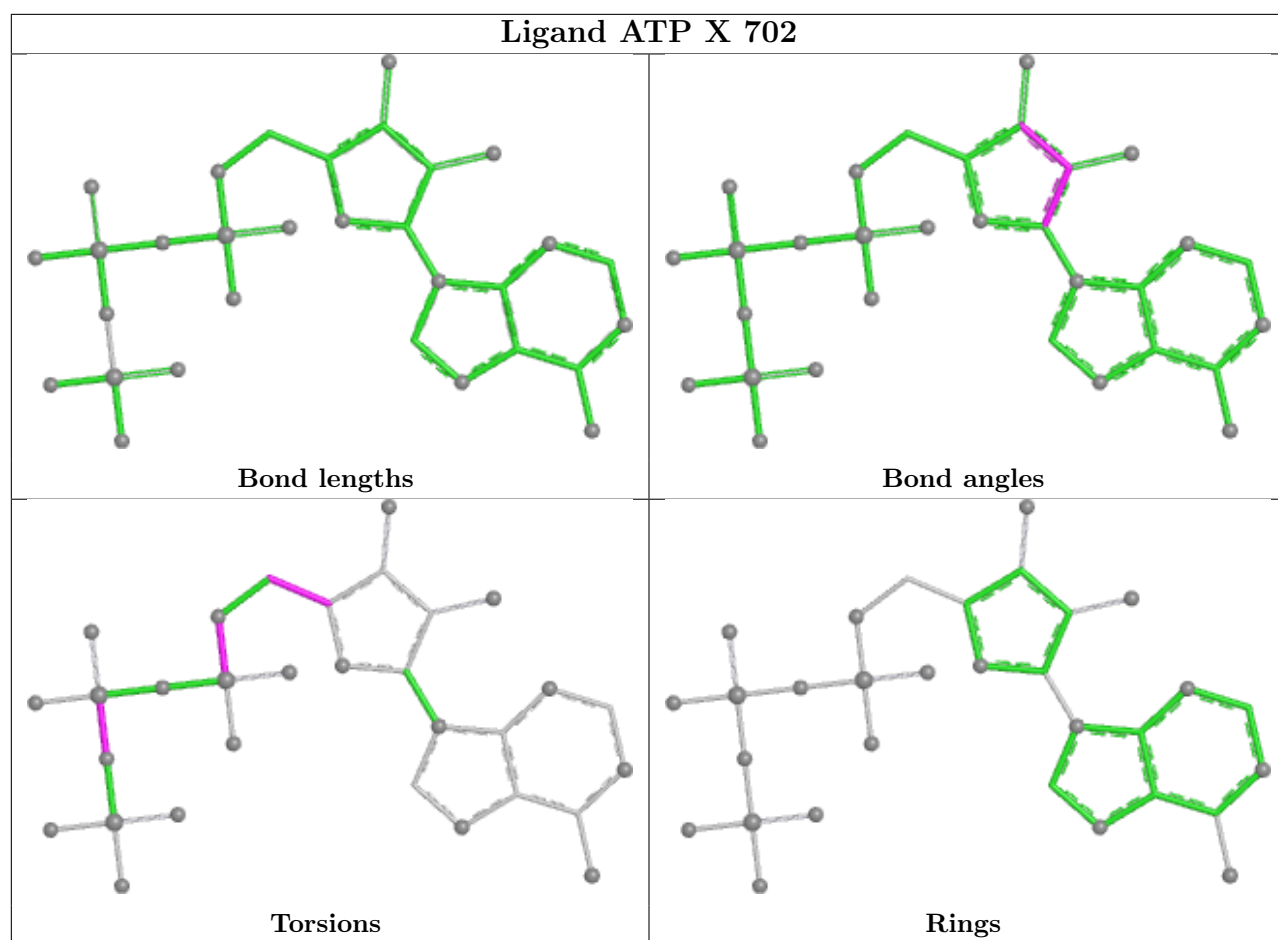


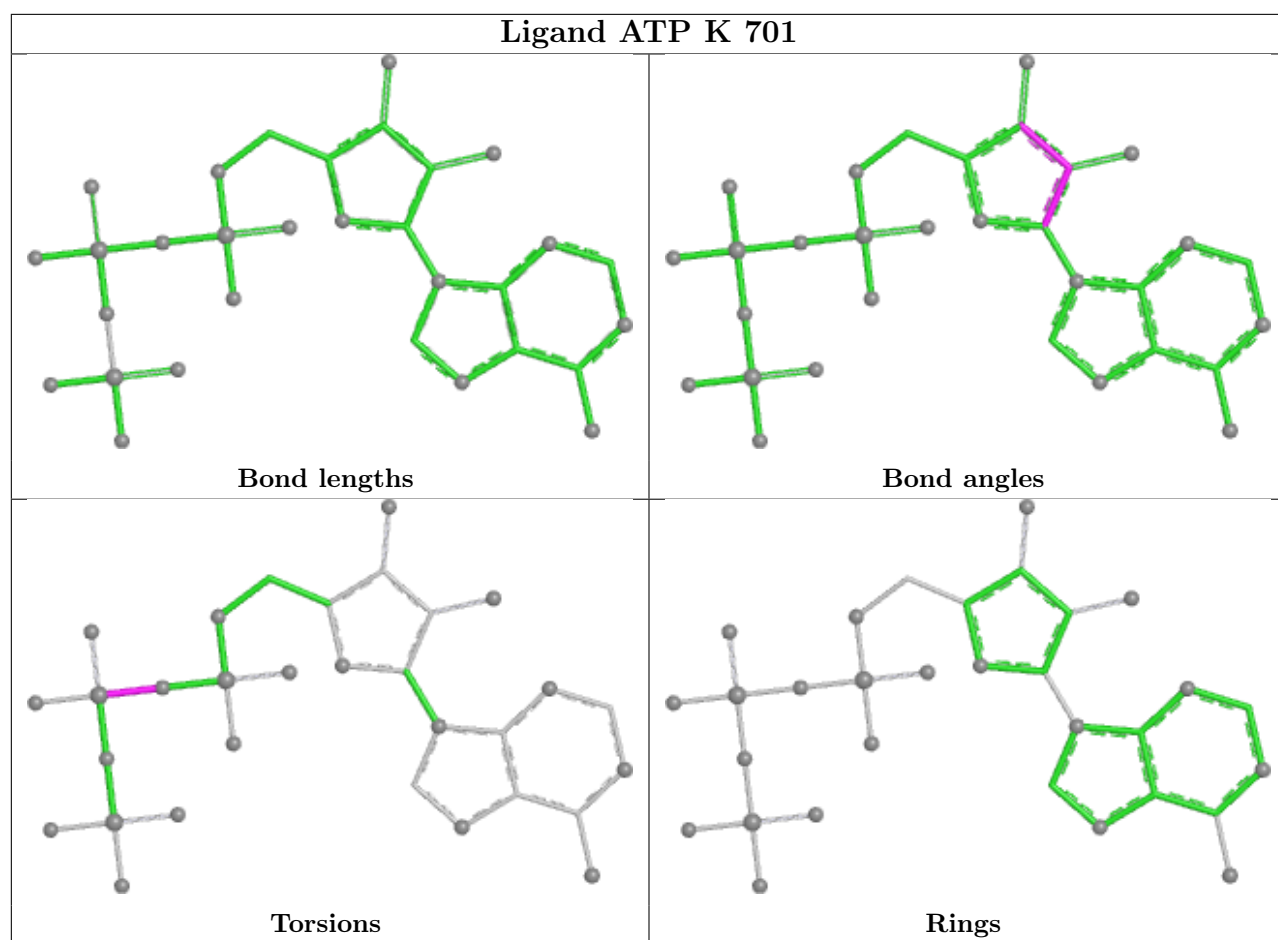


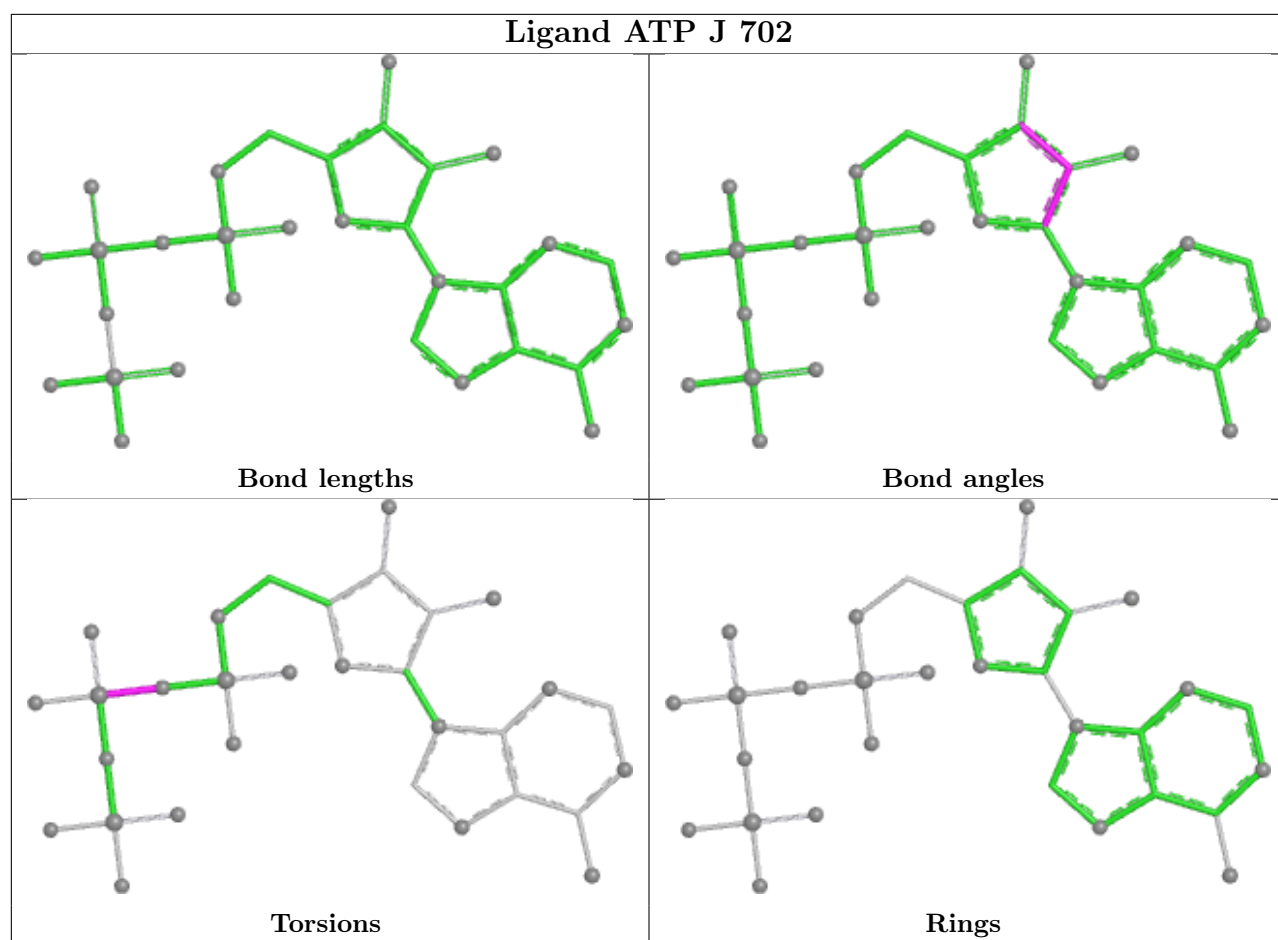


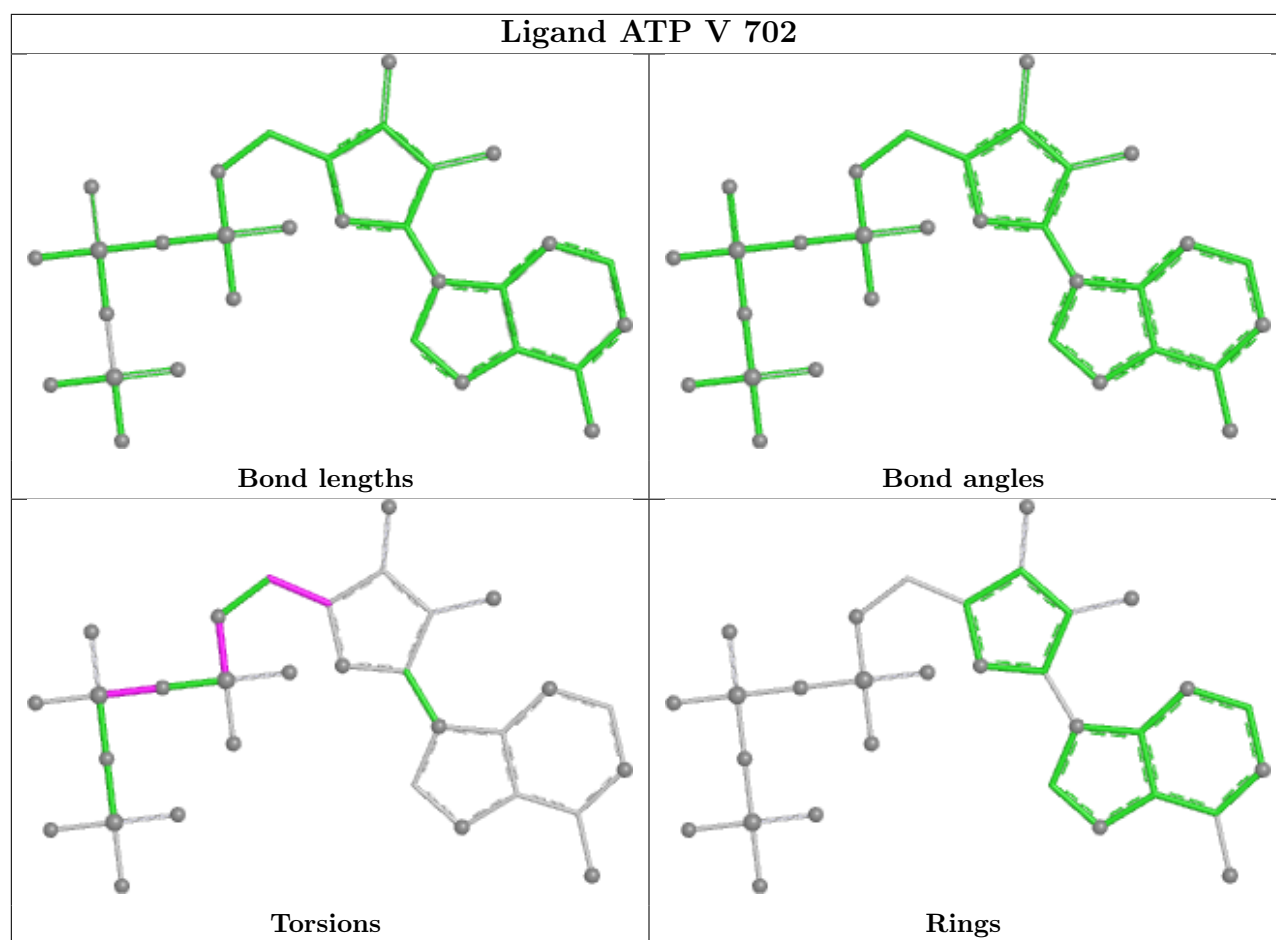
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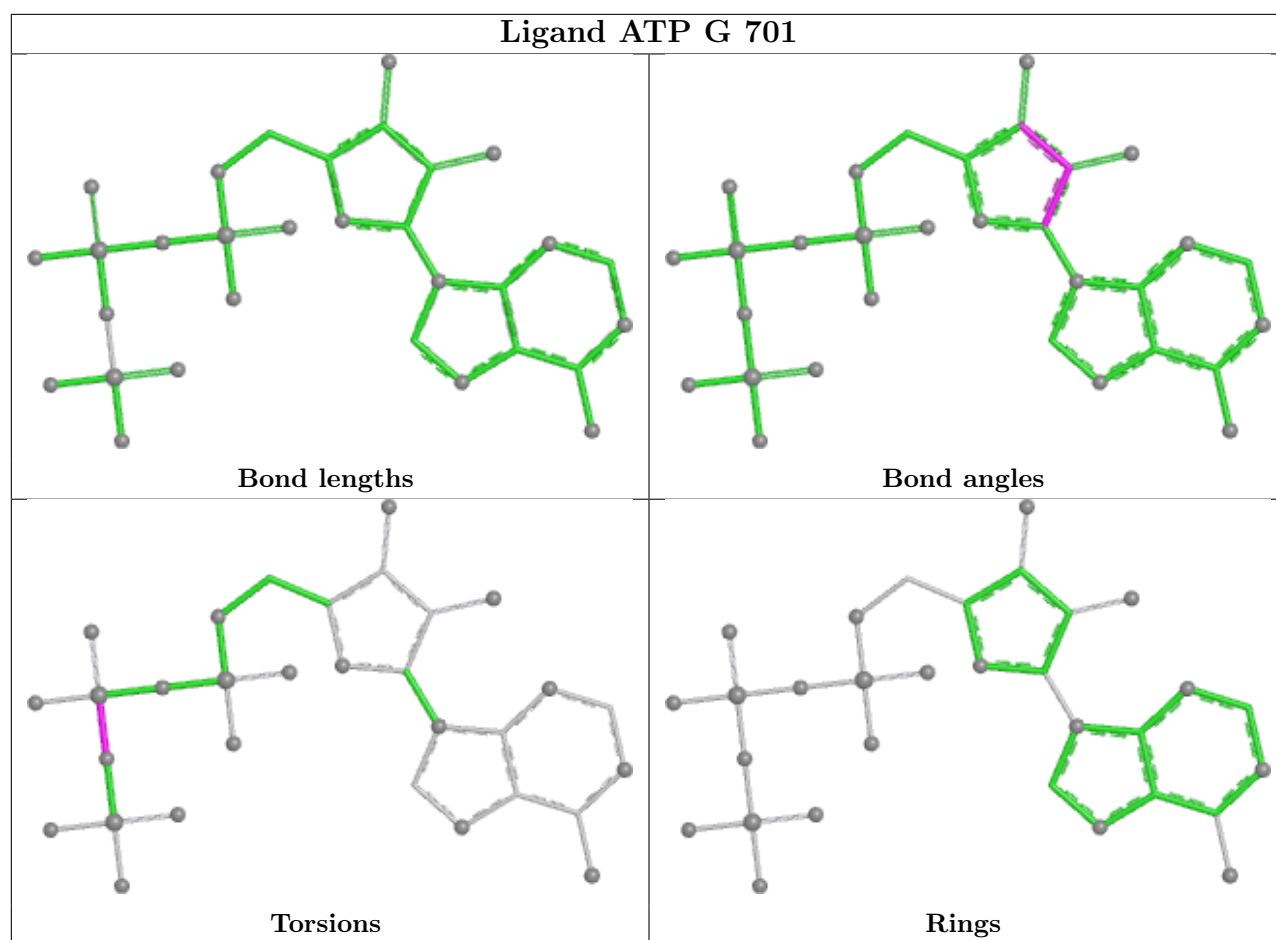


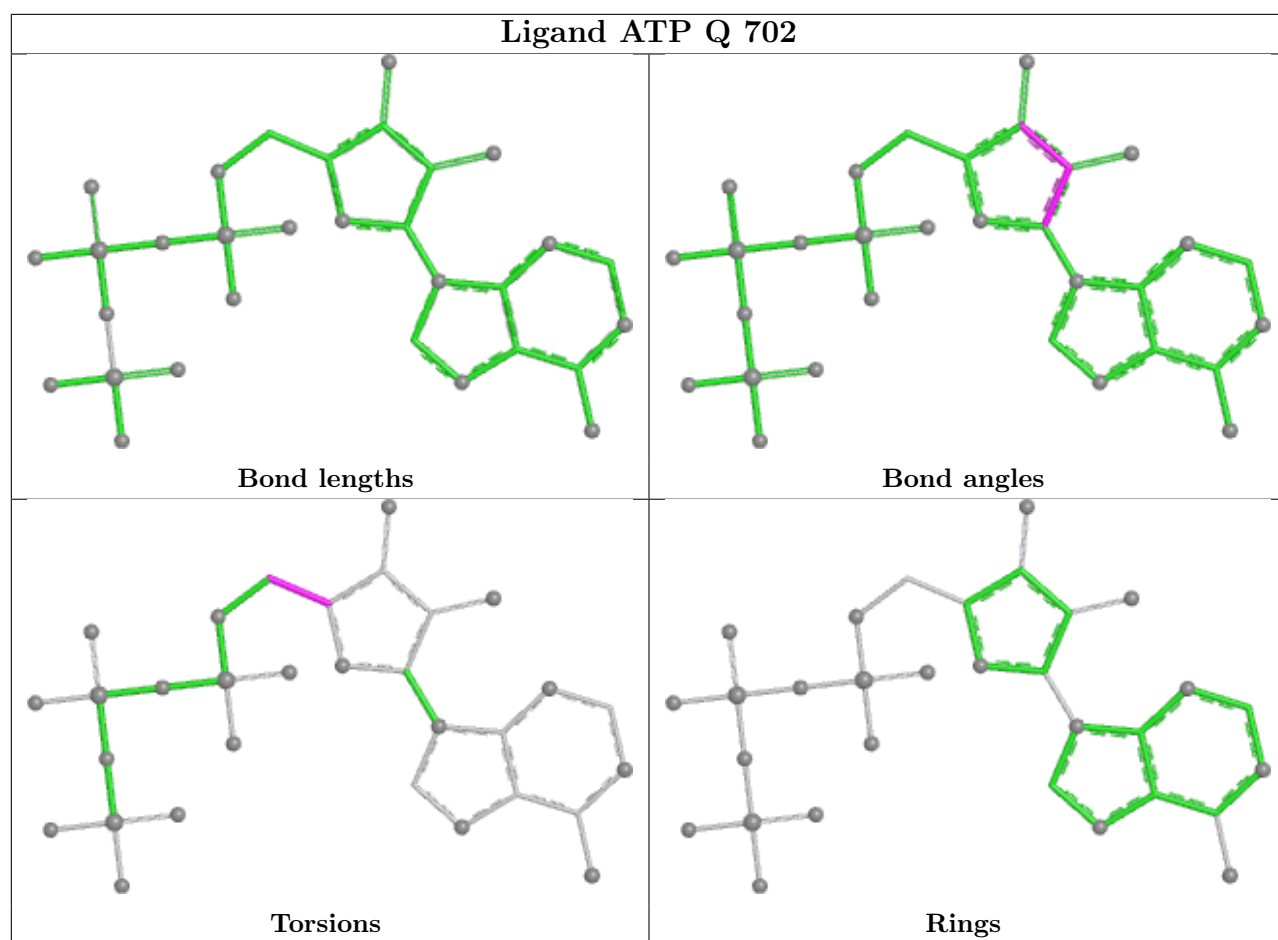


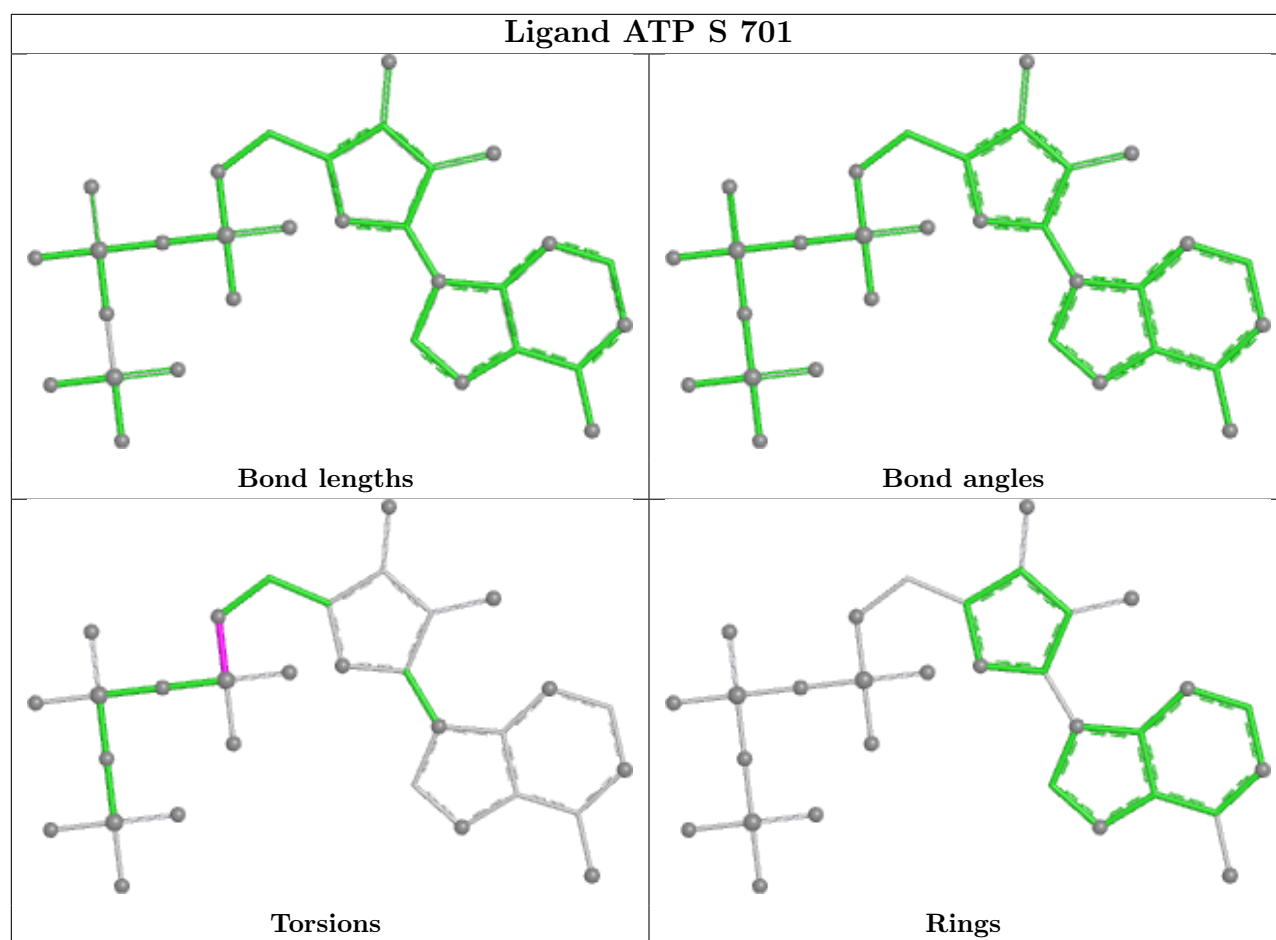


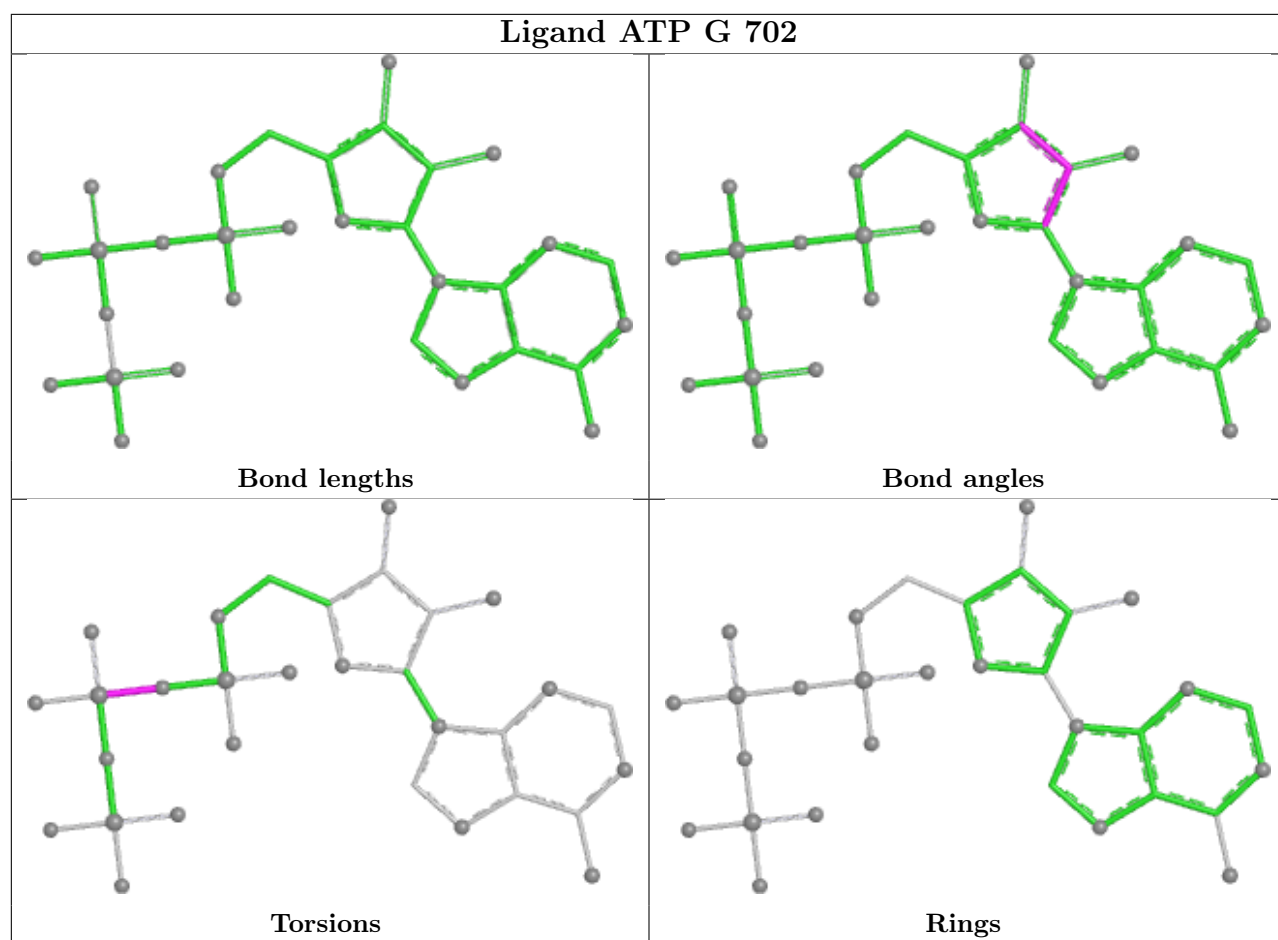


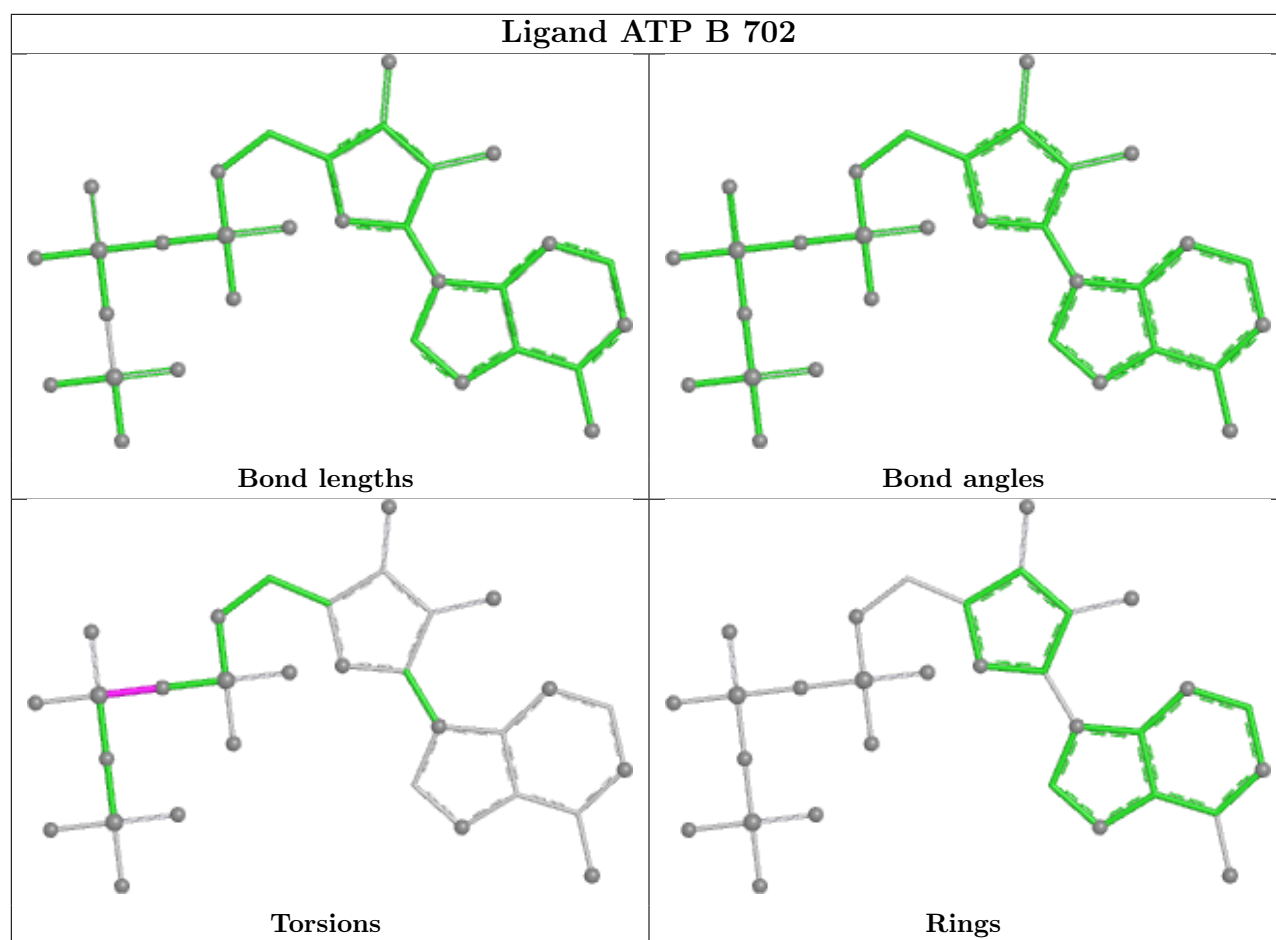


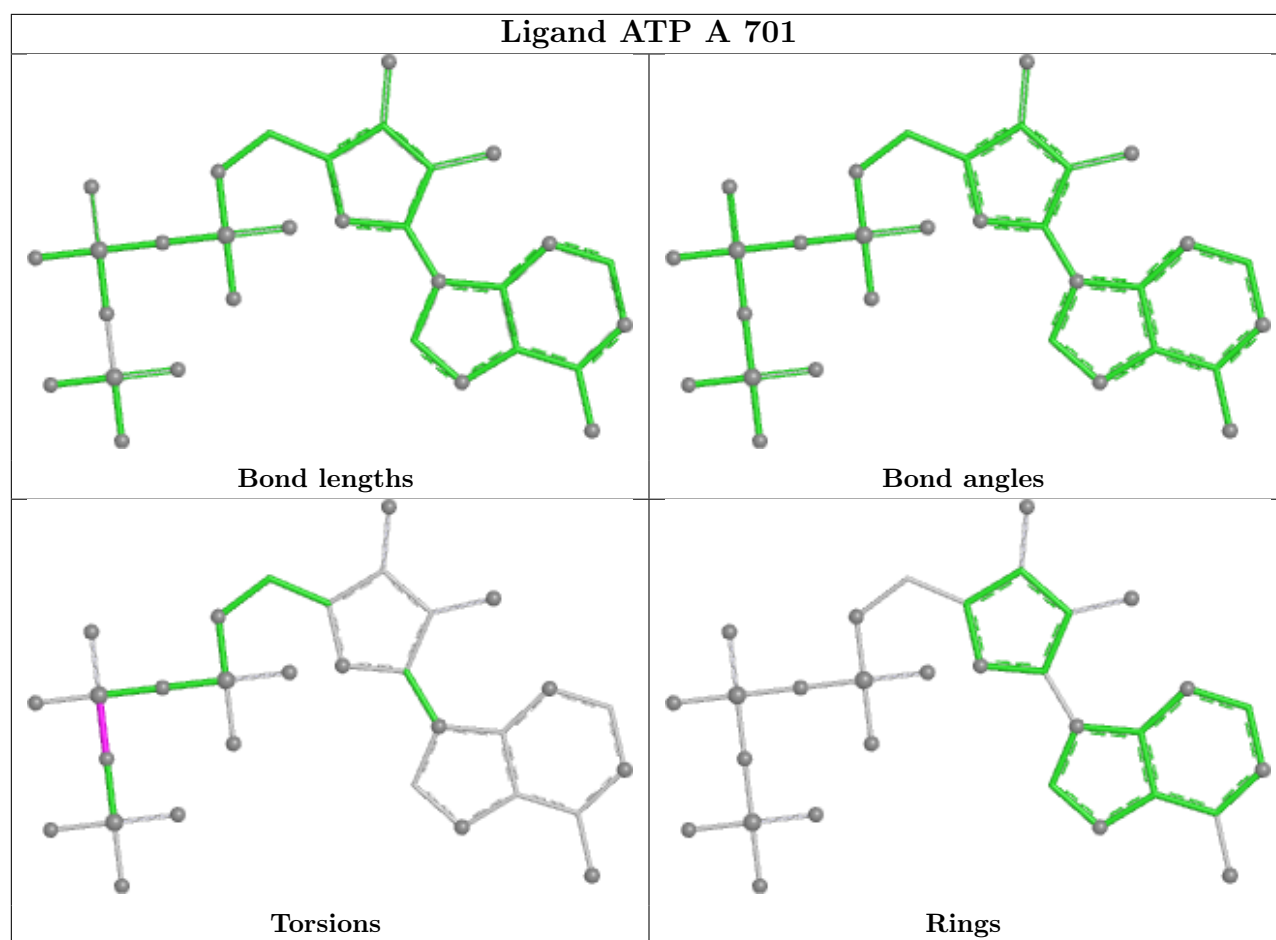


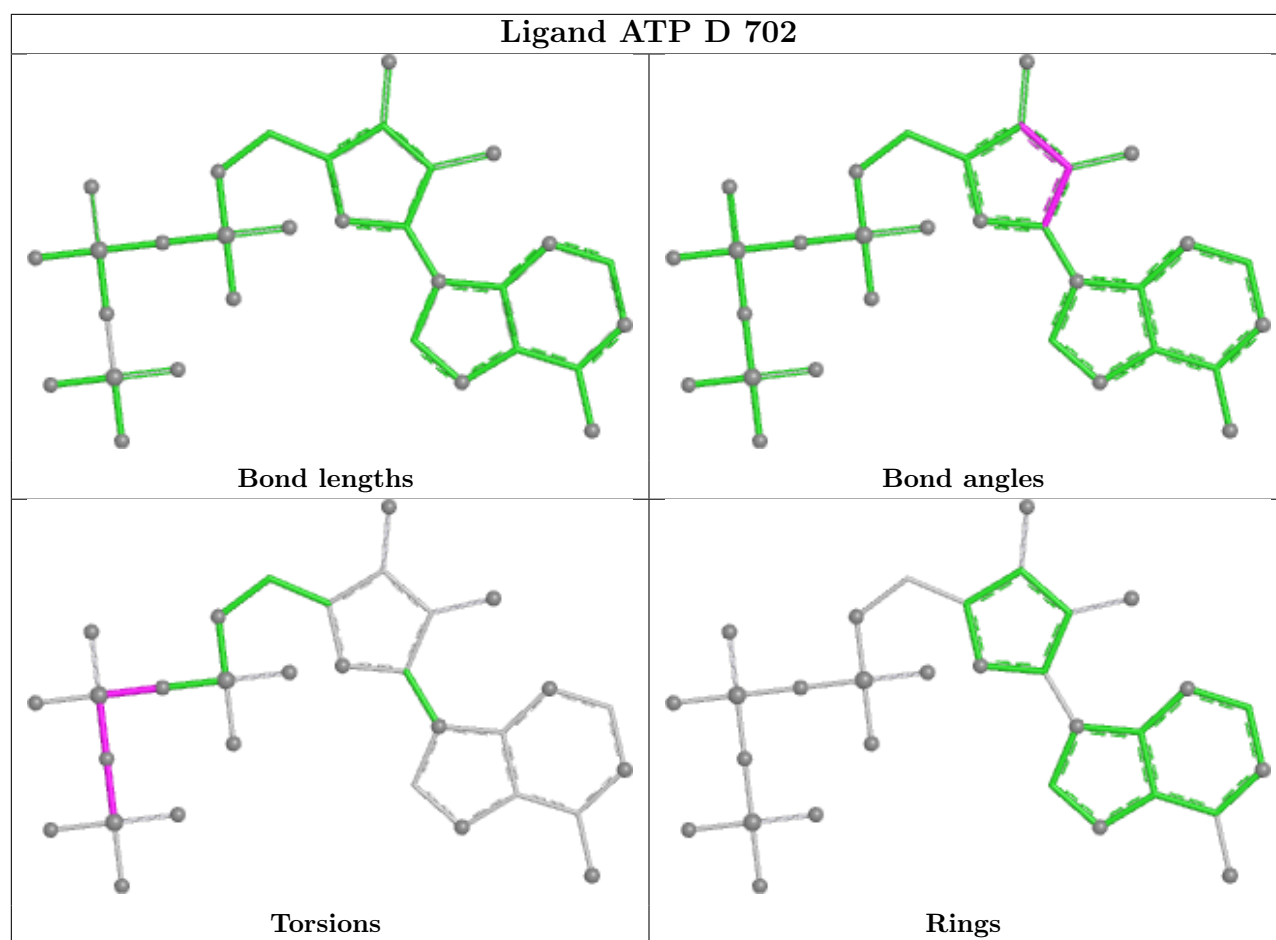


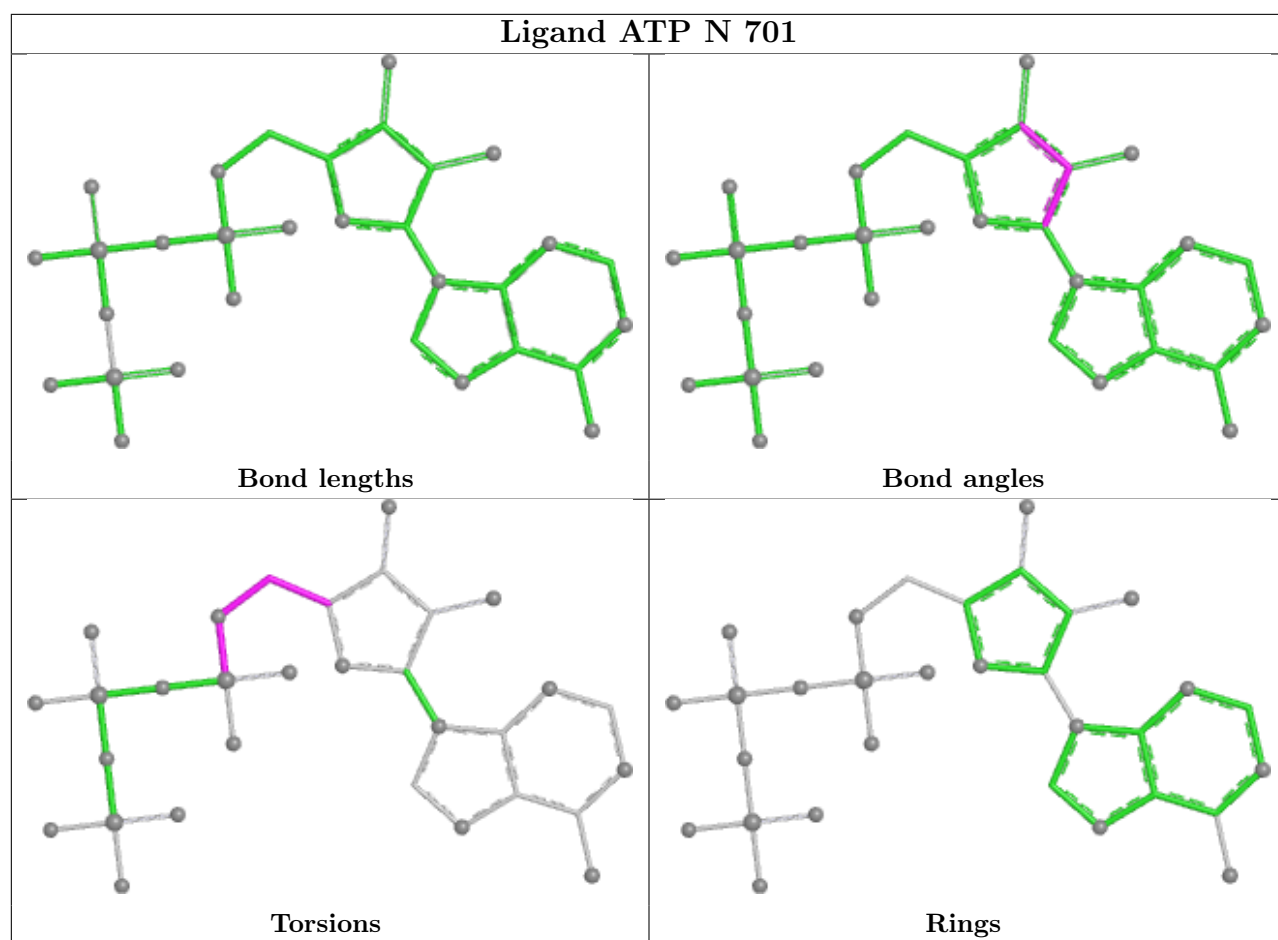


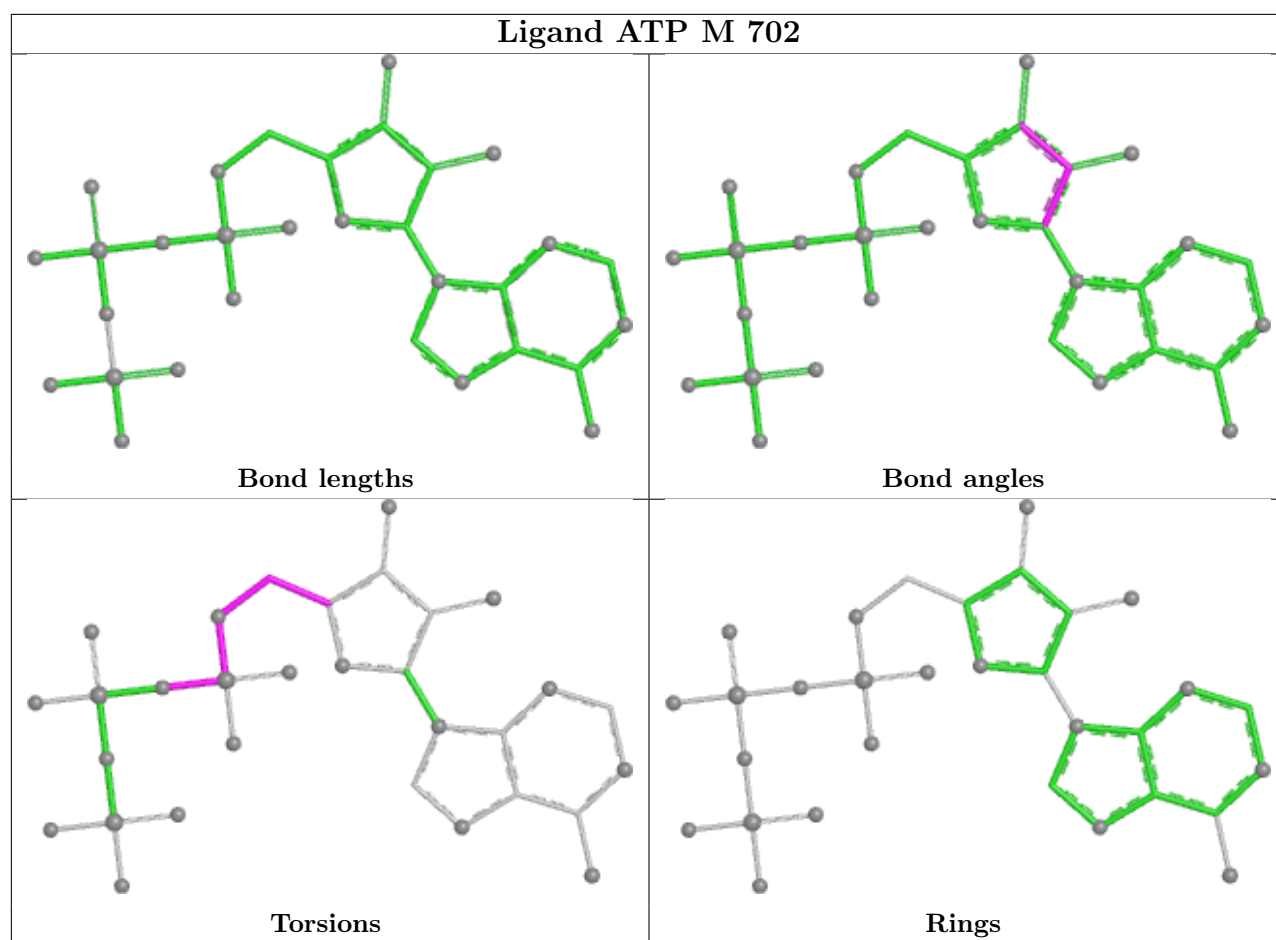


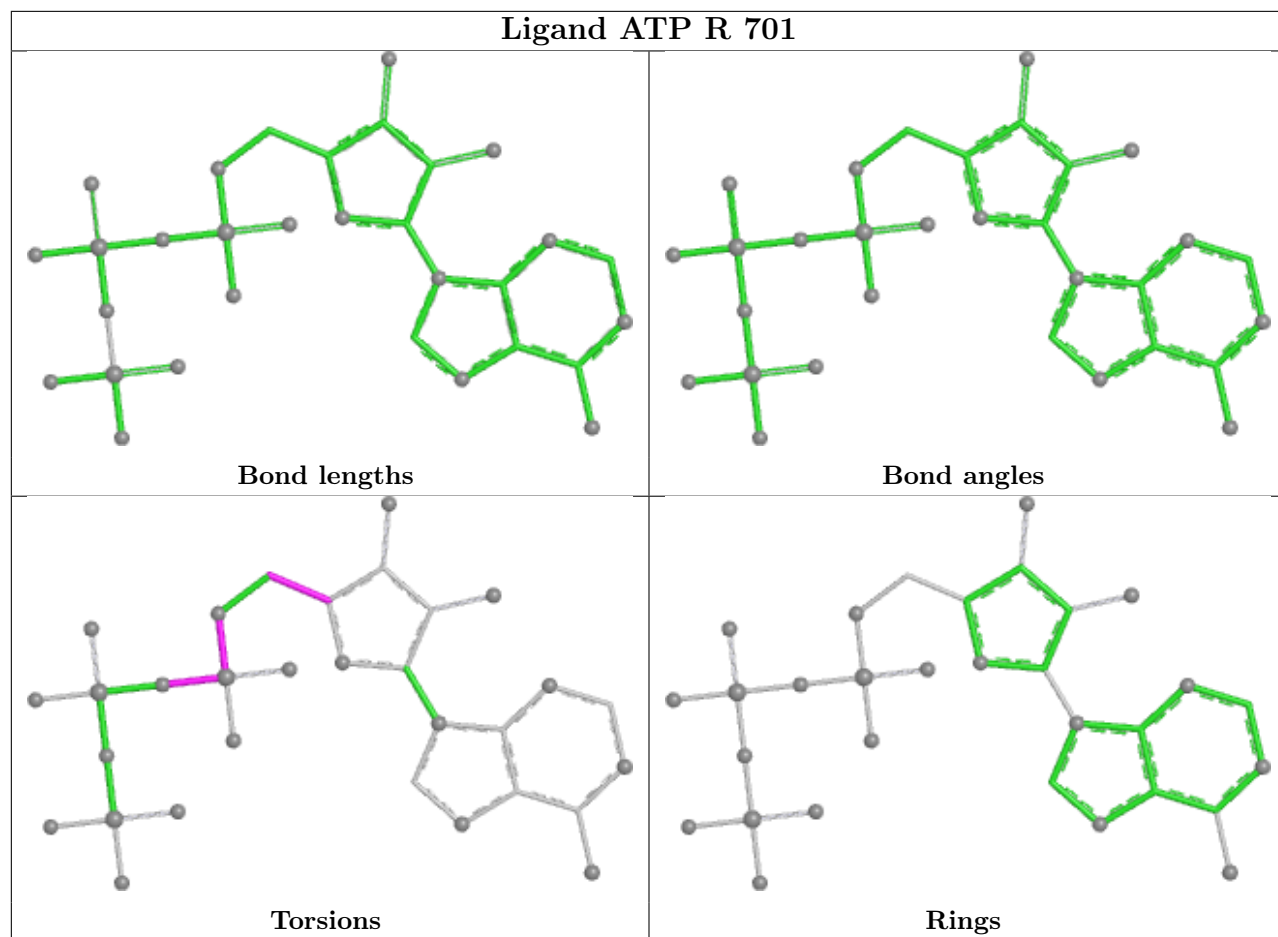


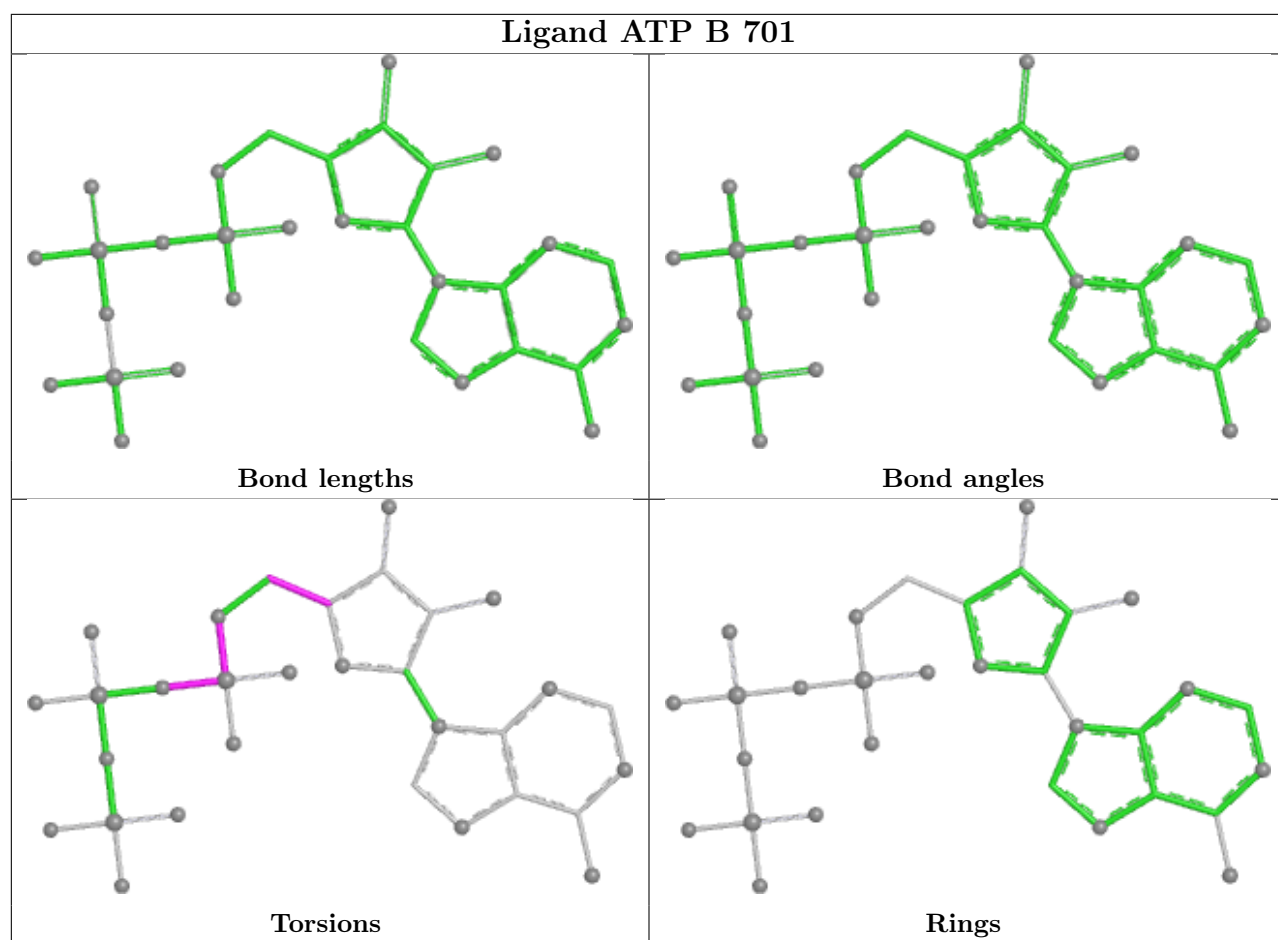


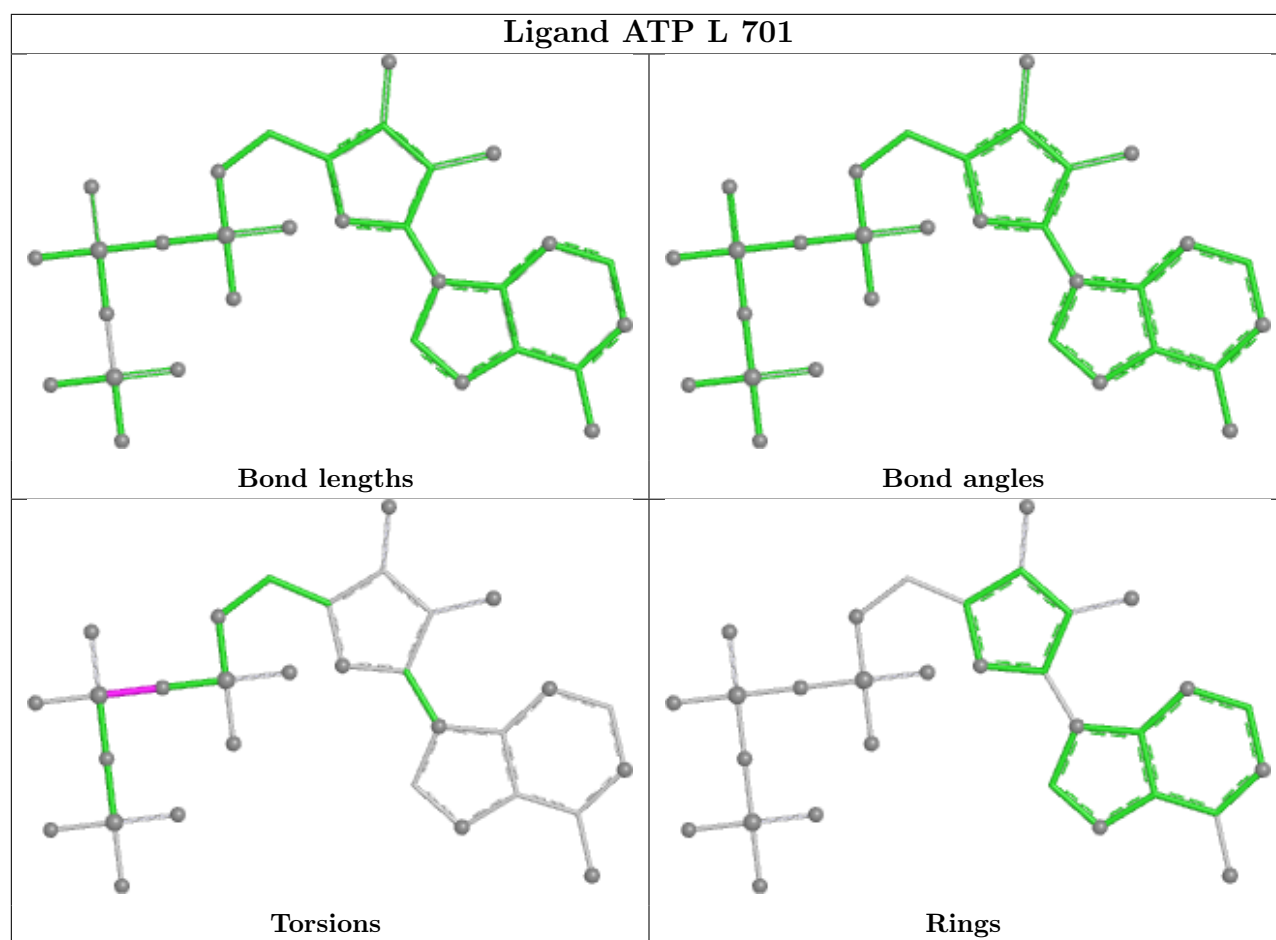




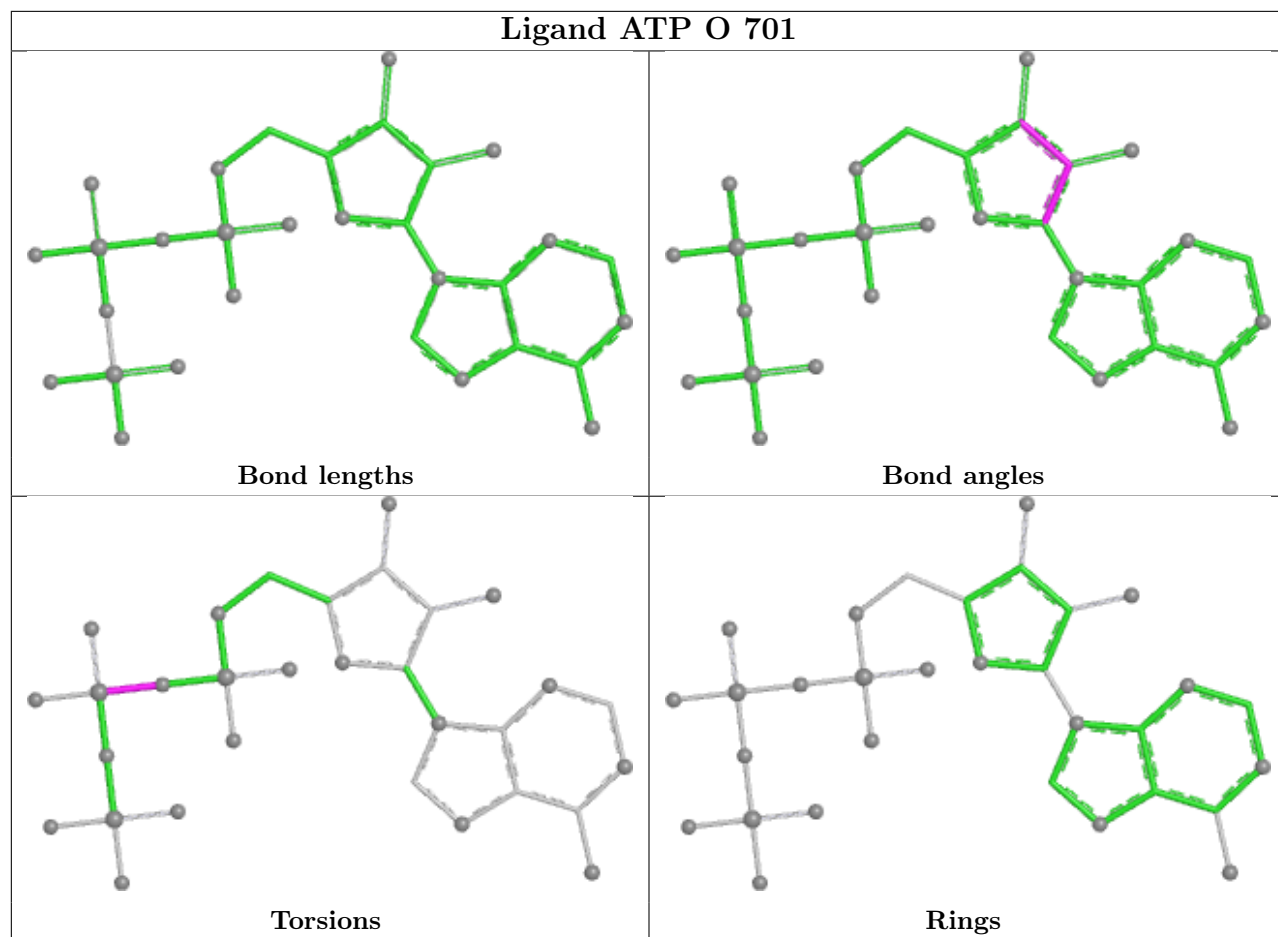




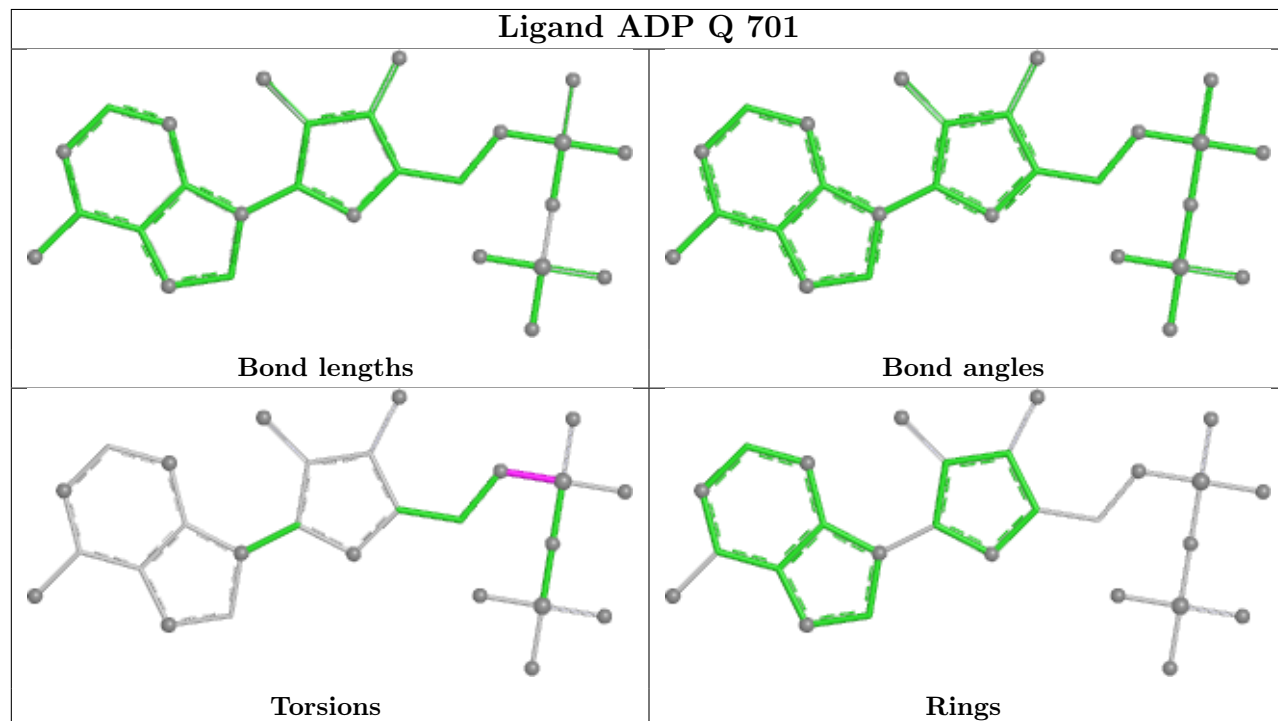


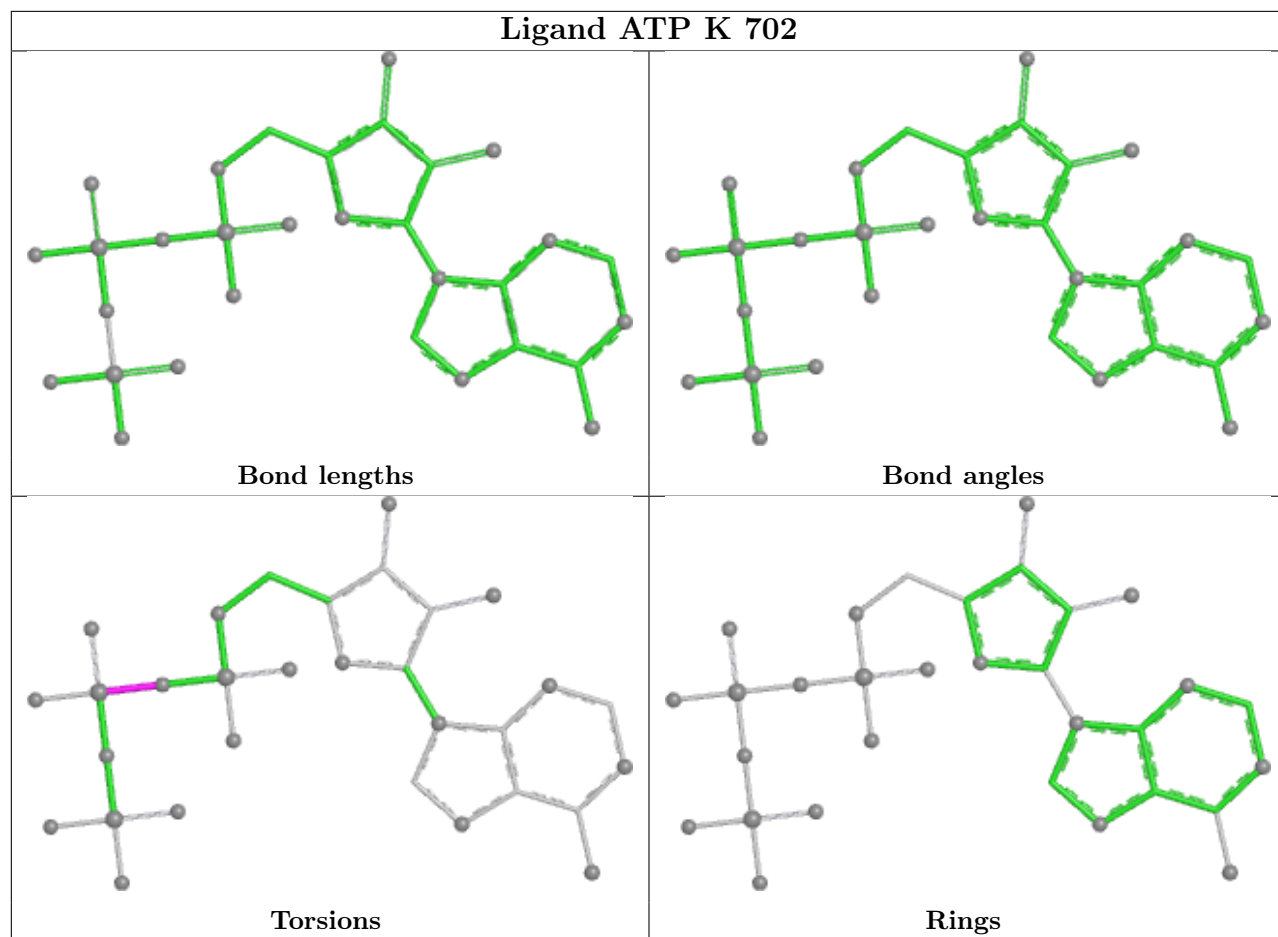


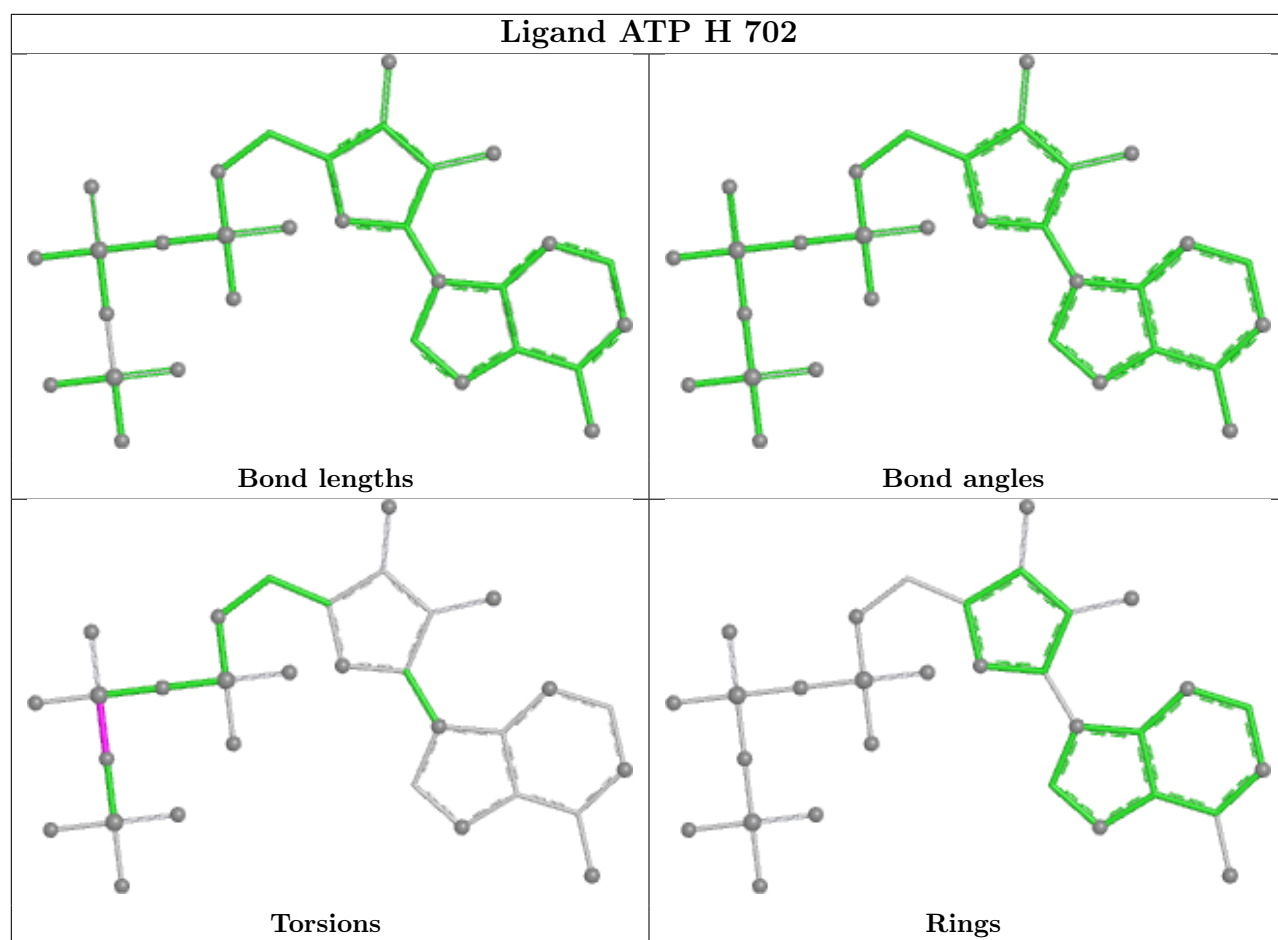
Ligand ATP O 701

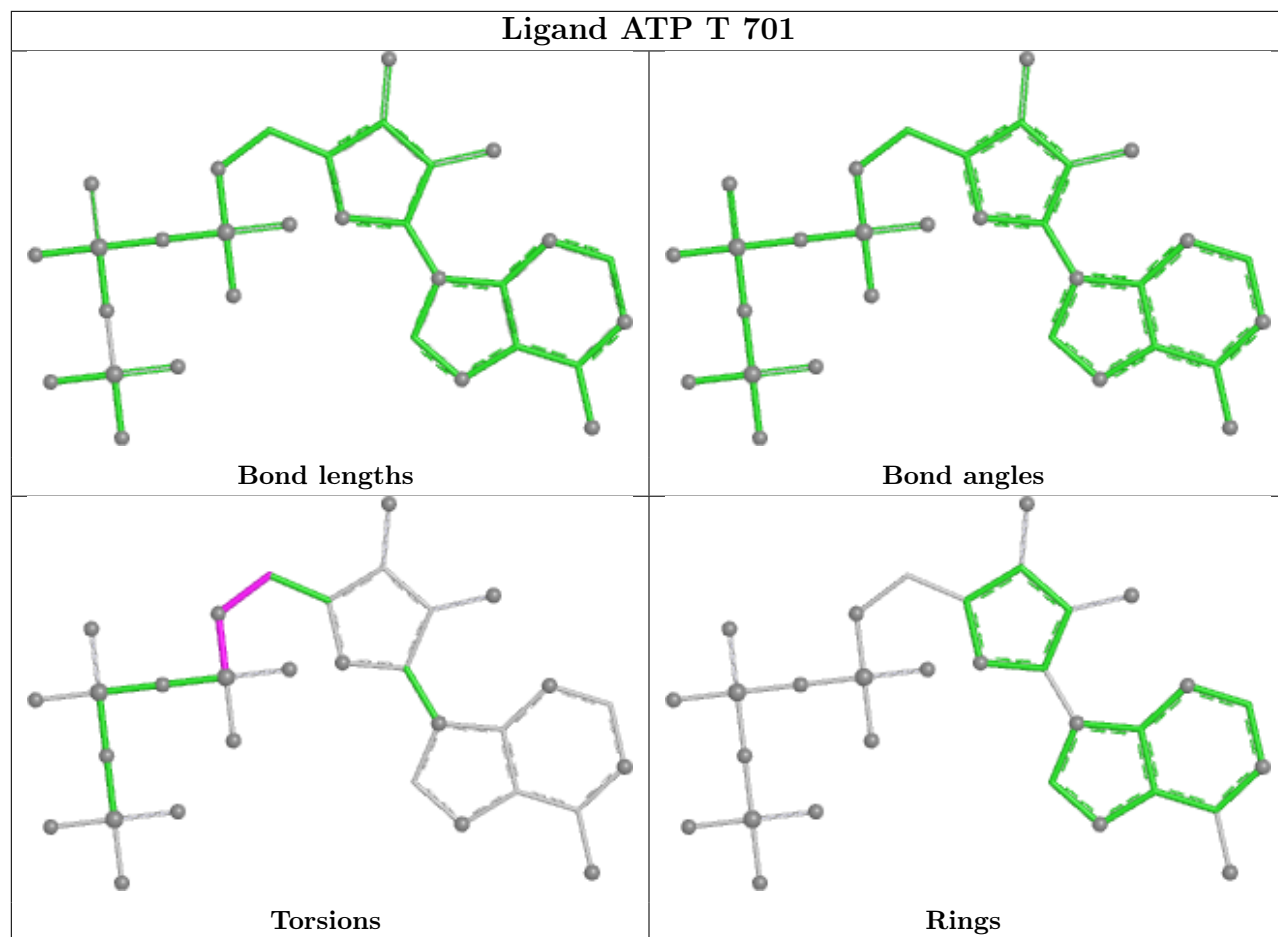


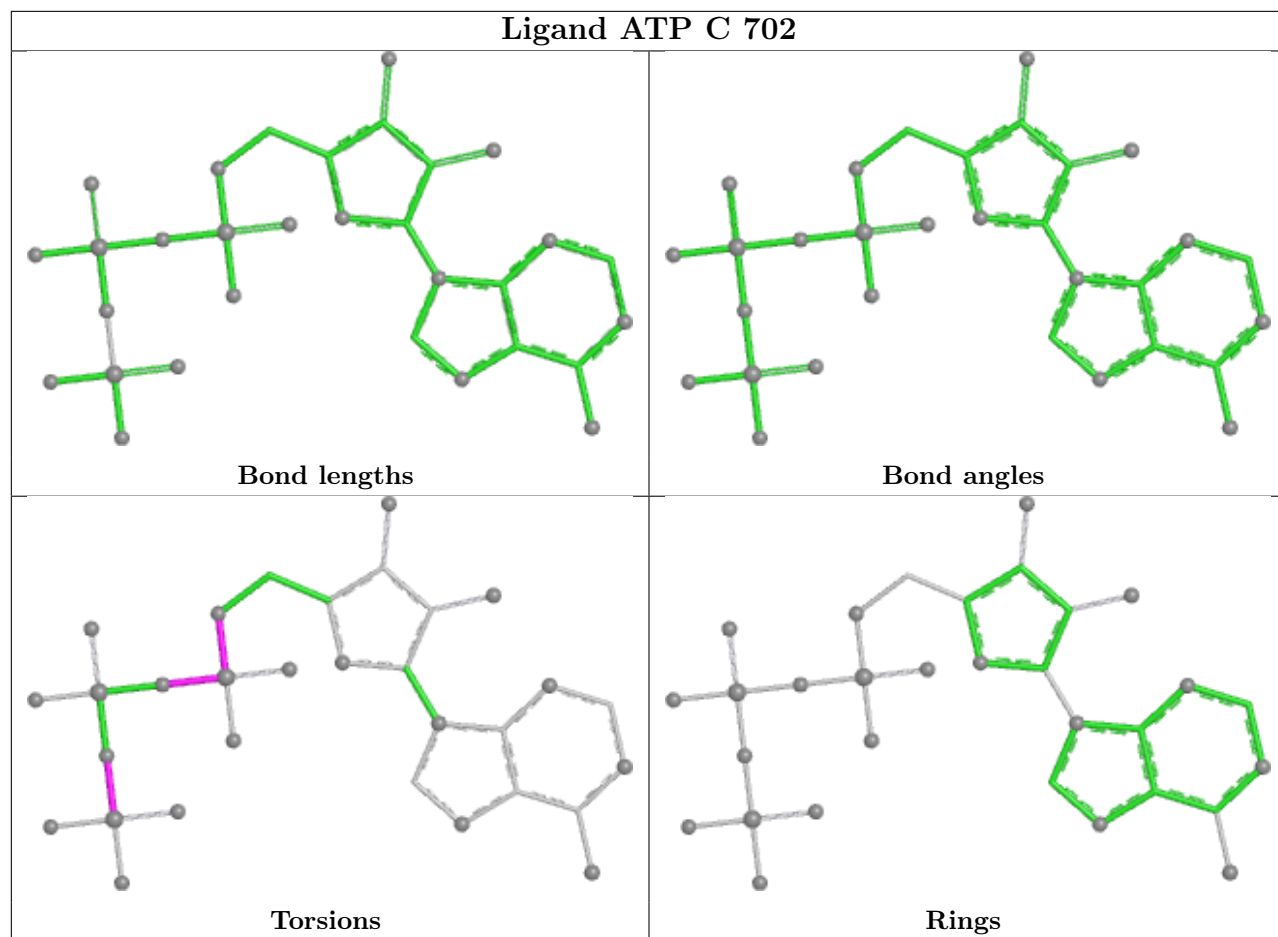
Ligand ADP Q 701

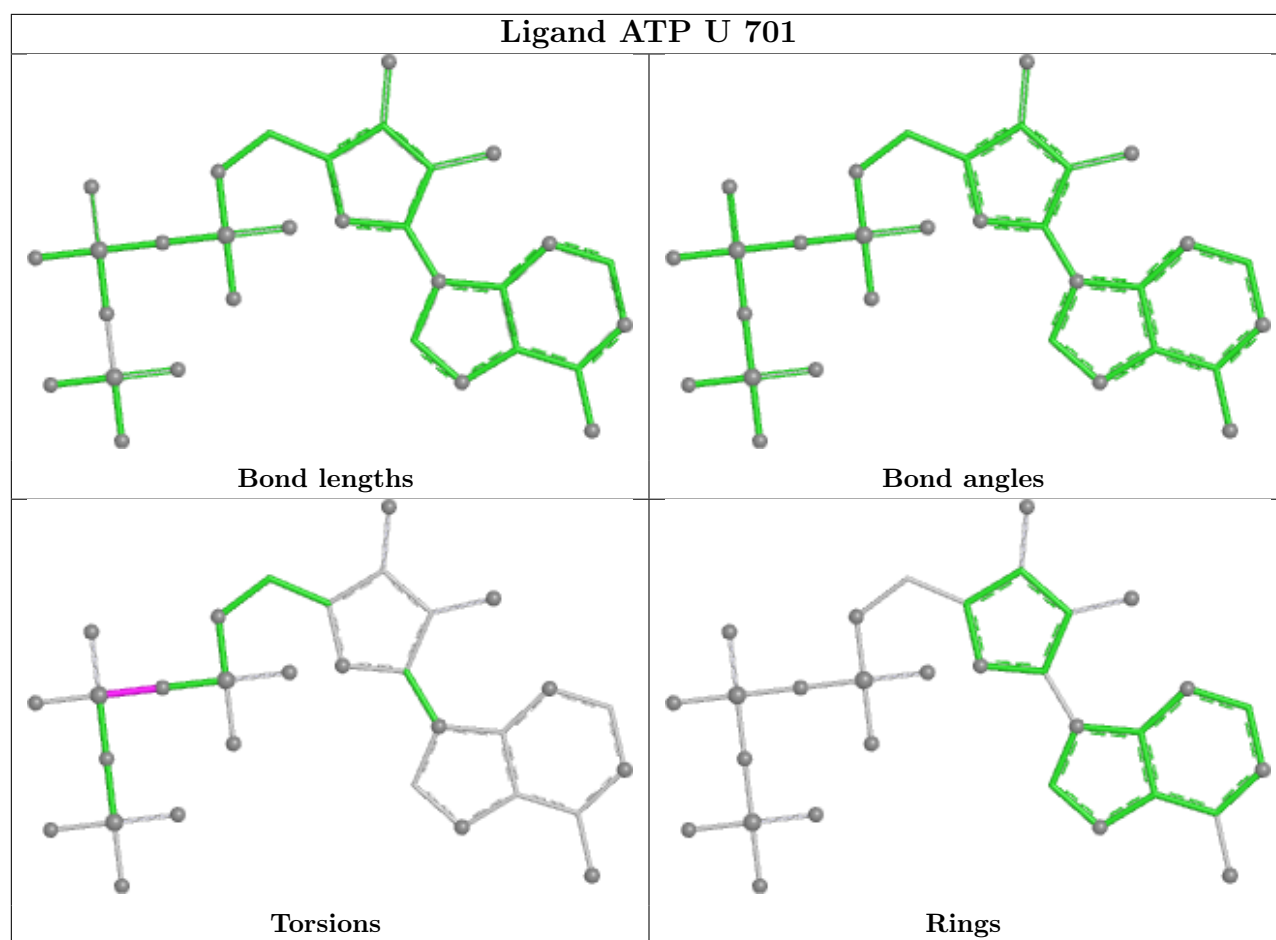


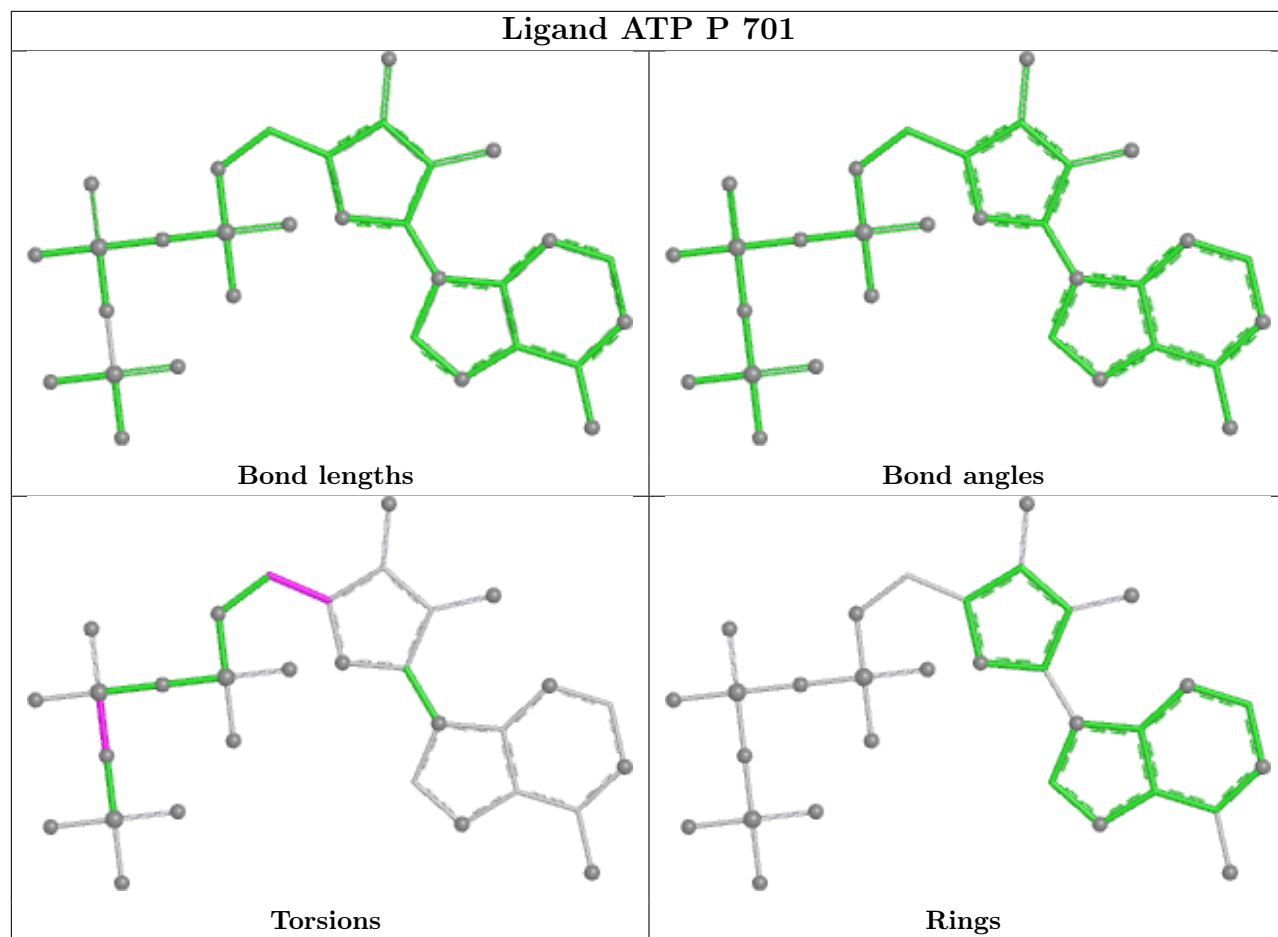


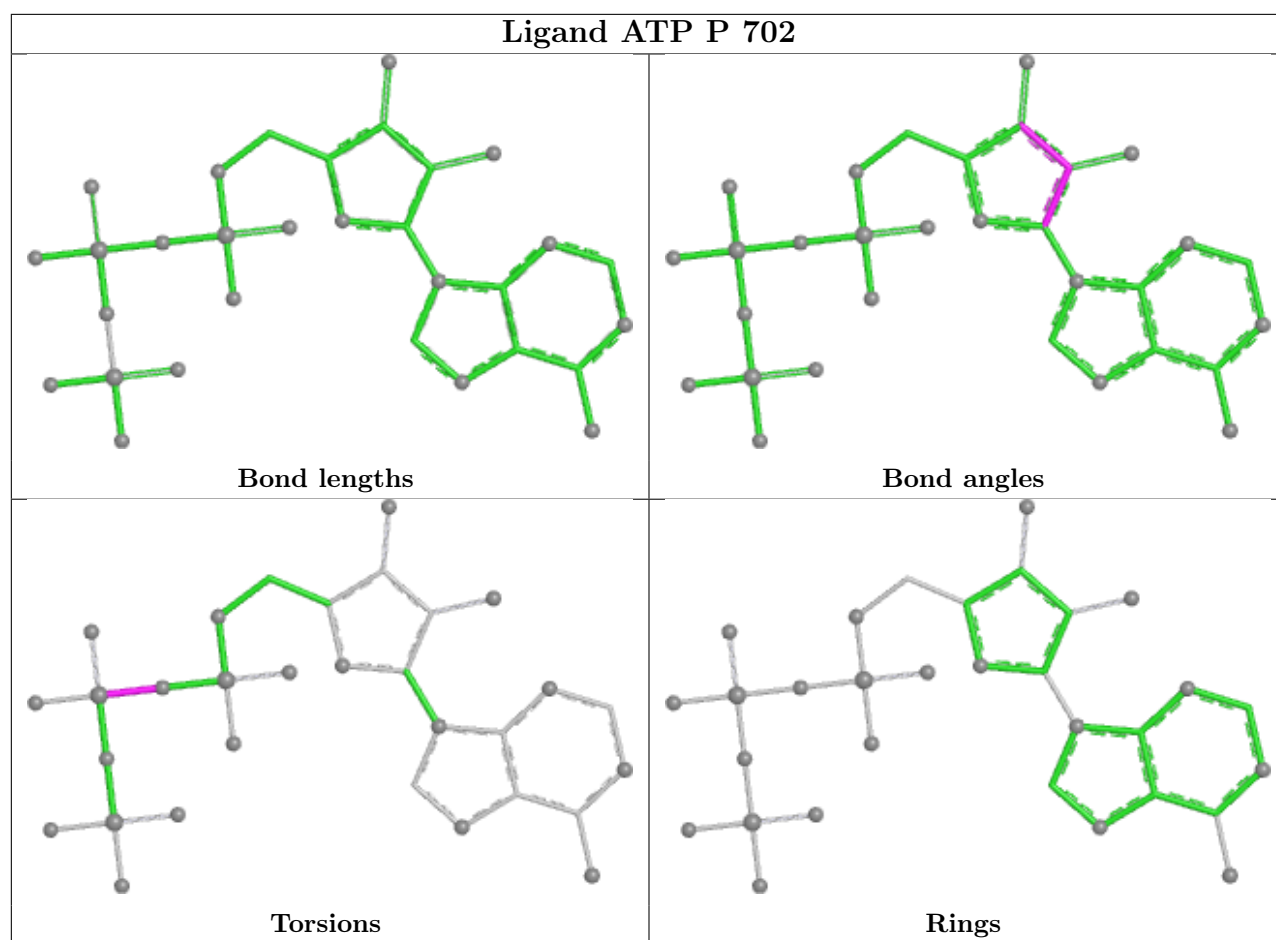


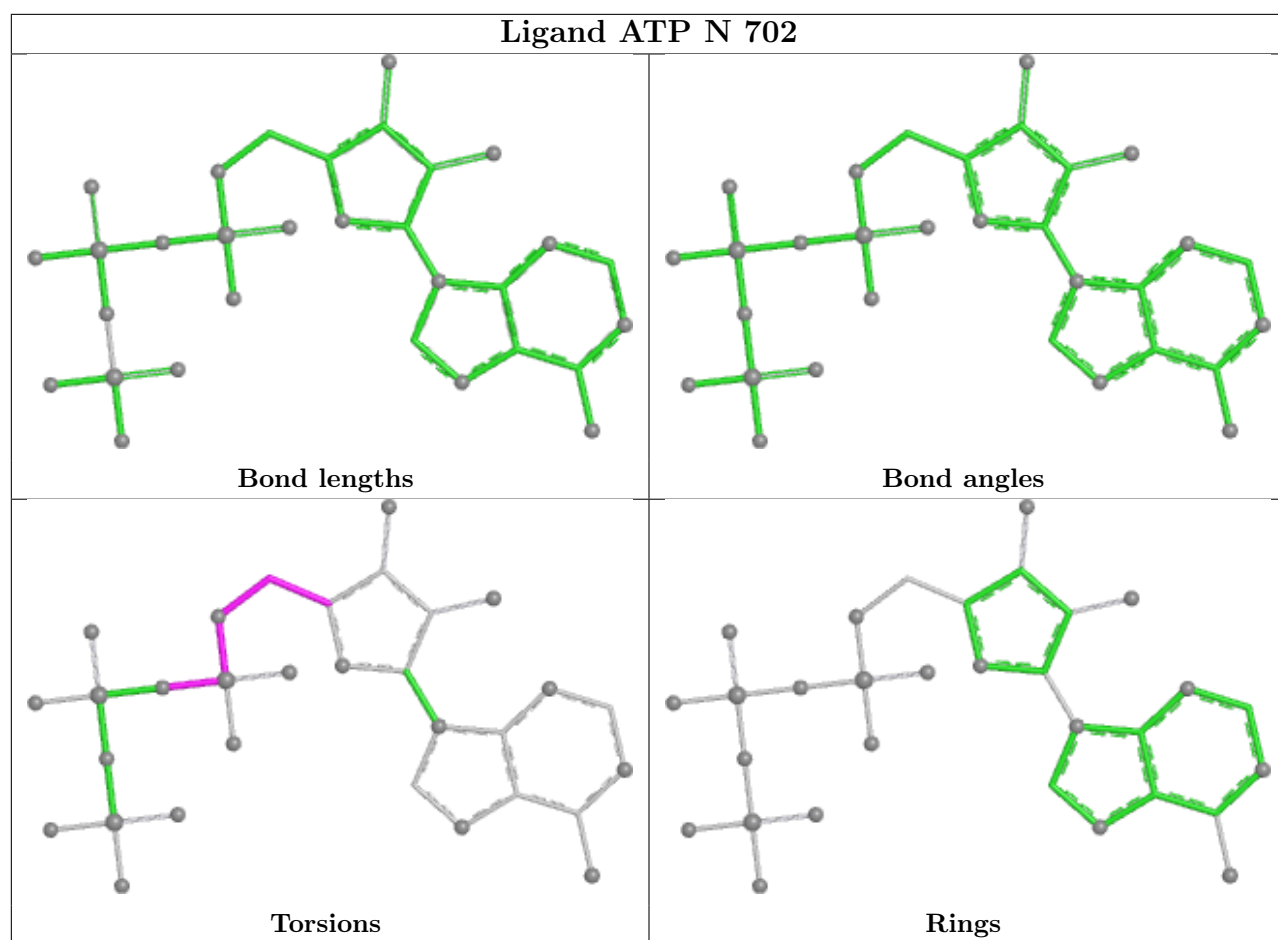


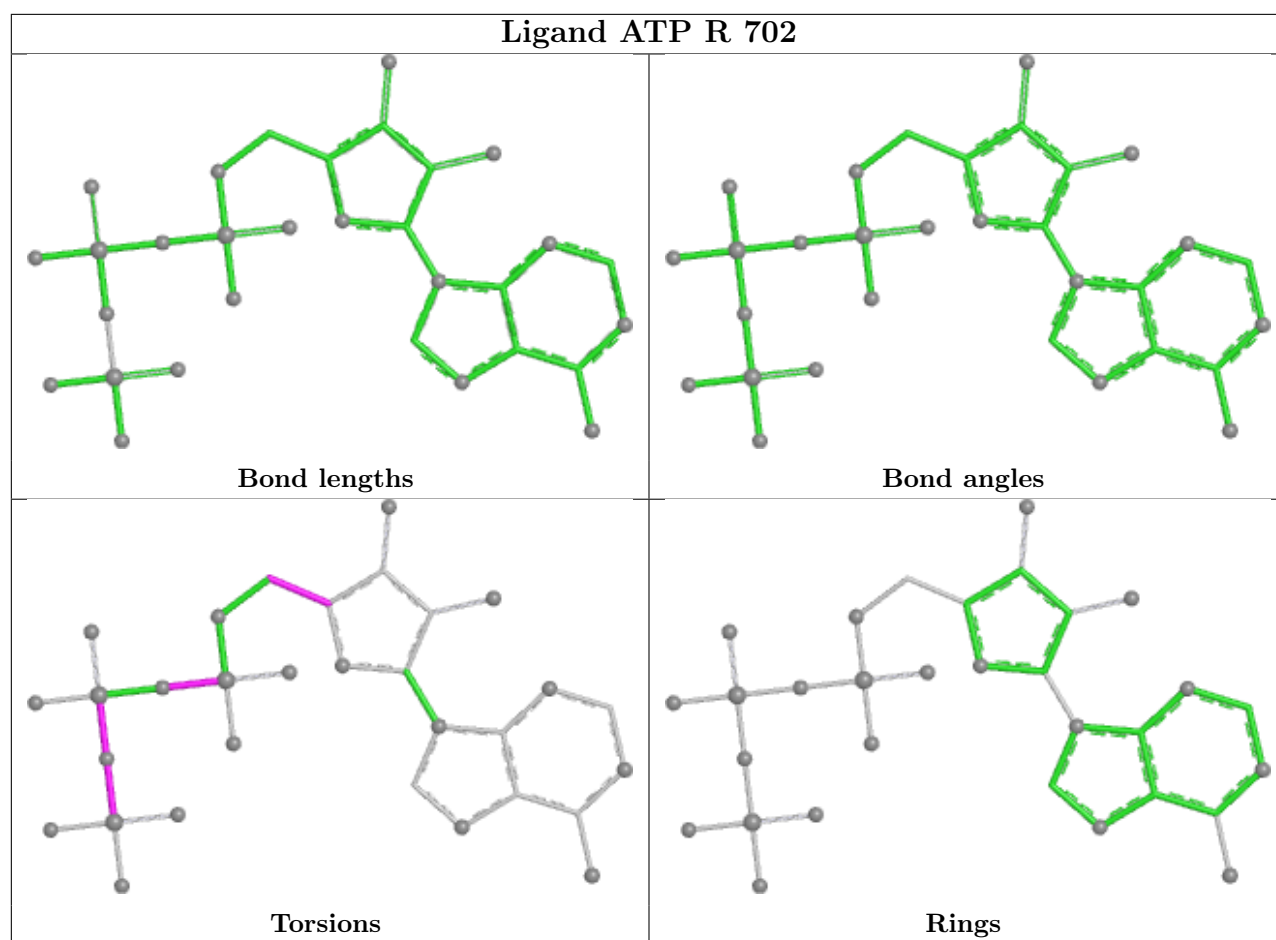


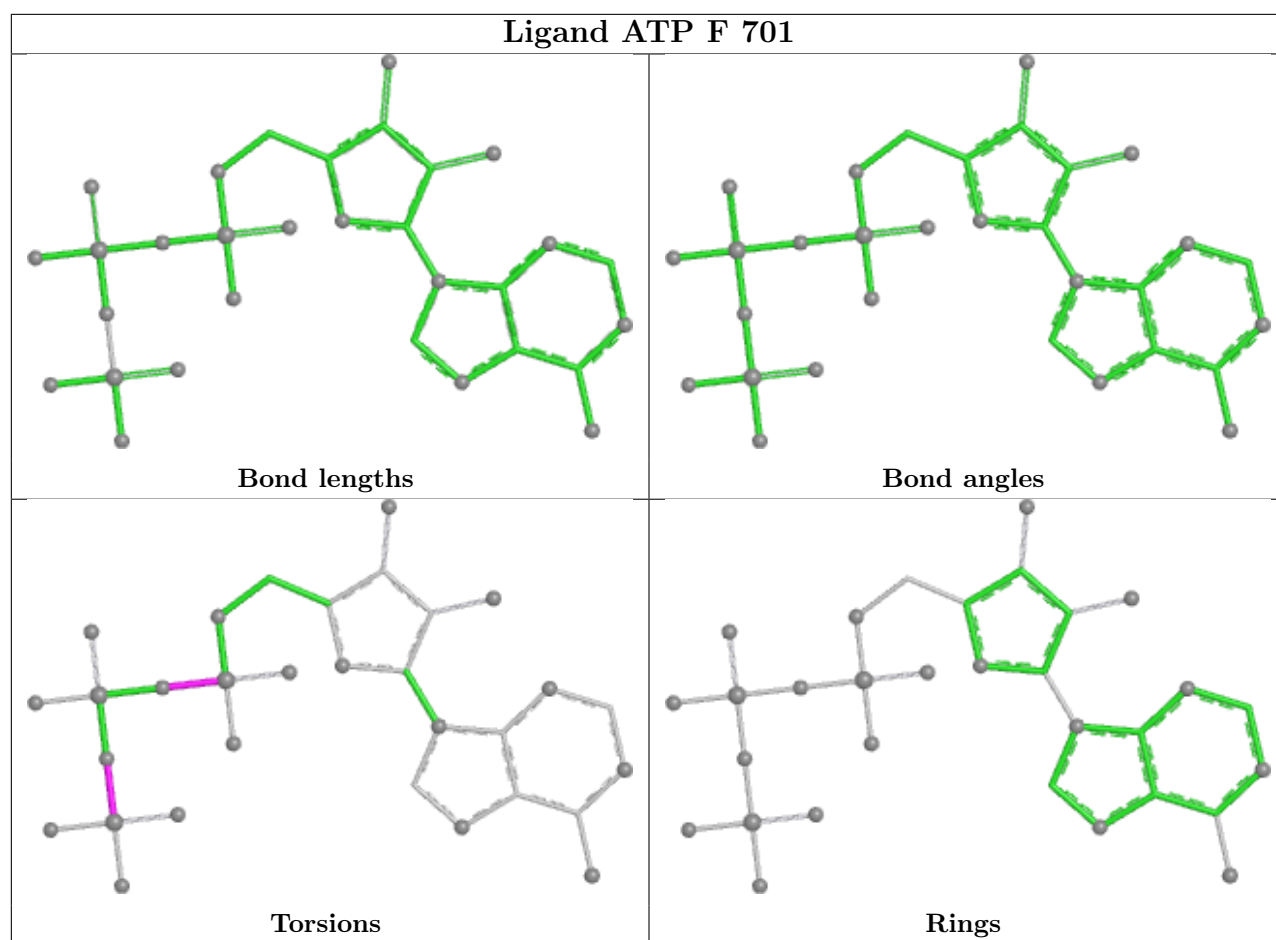




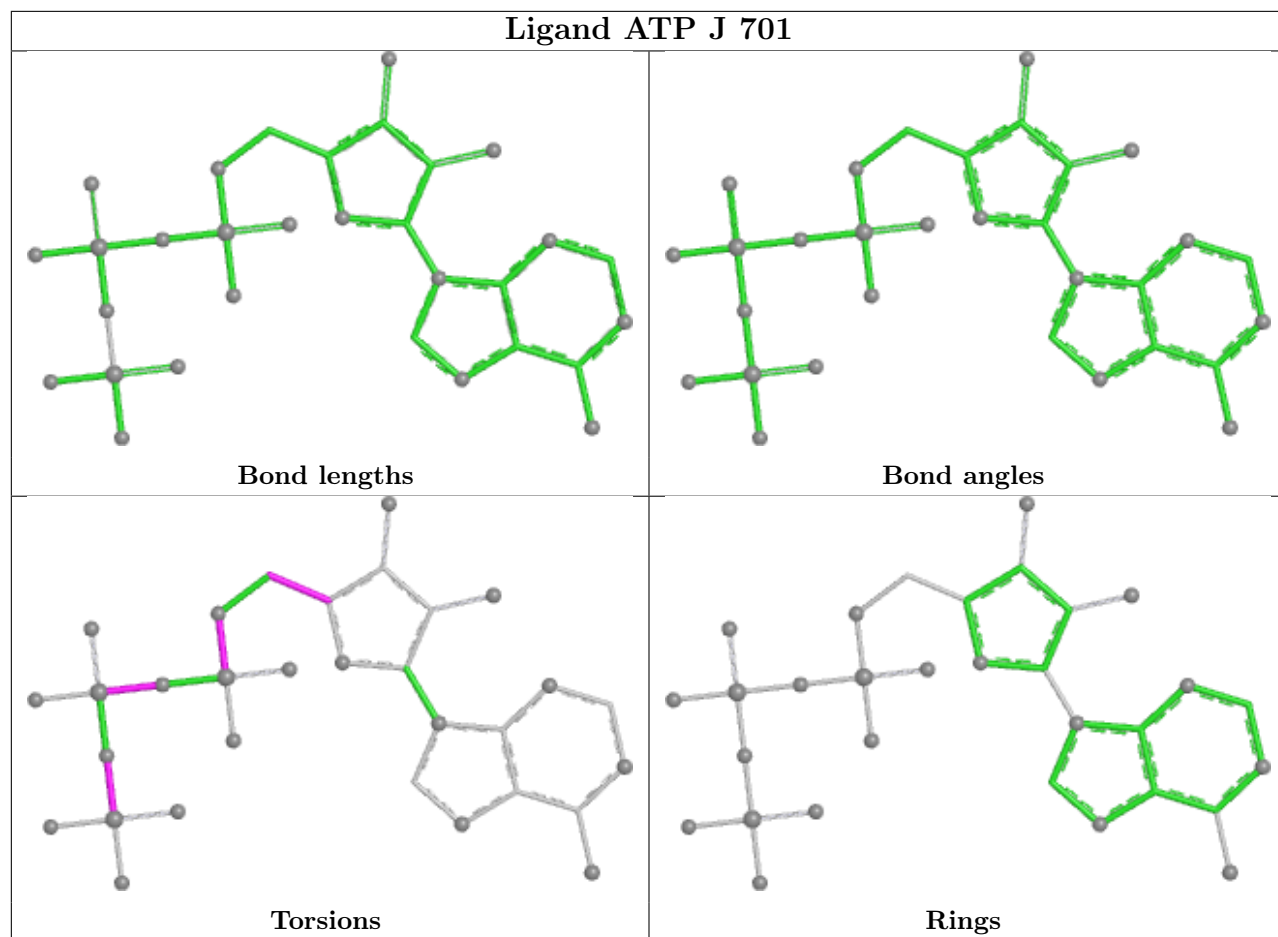




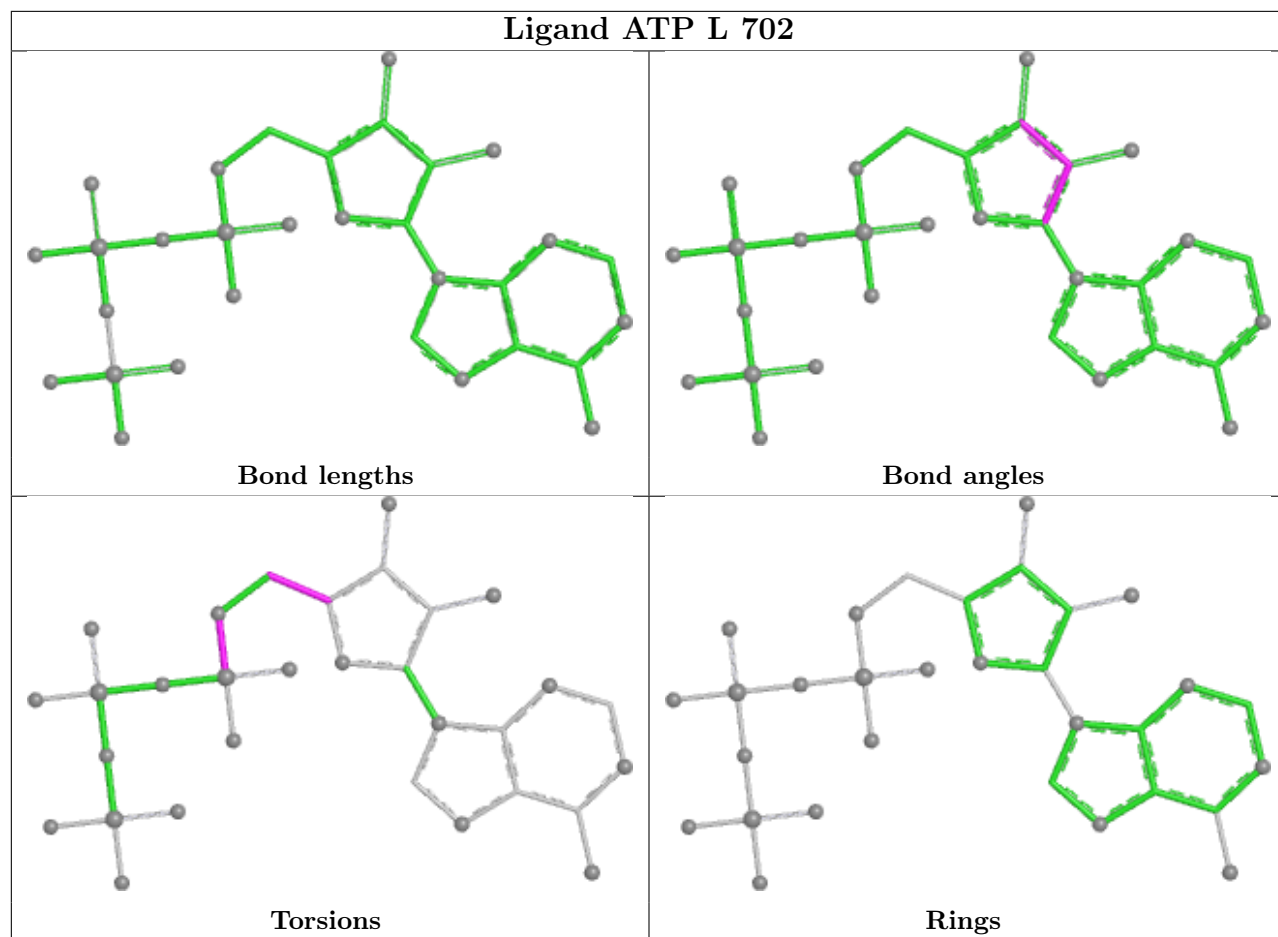


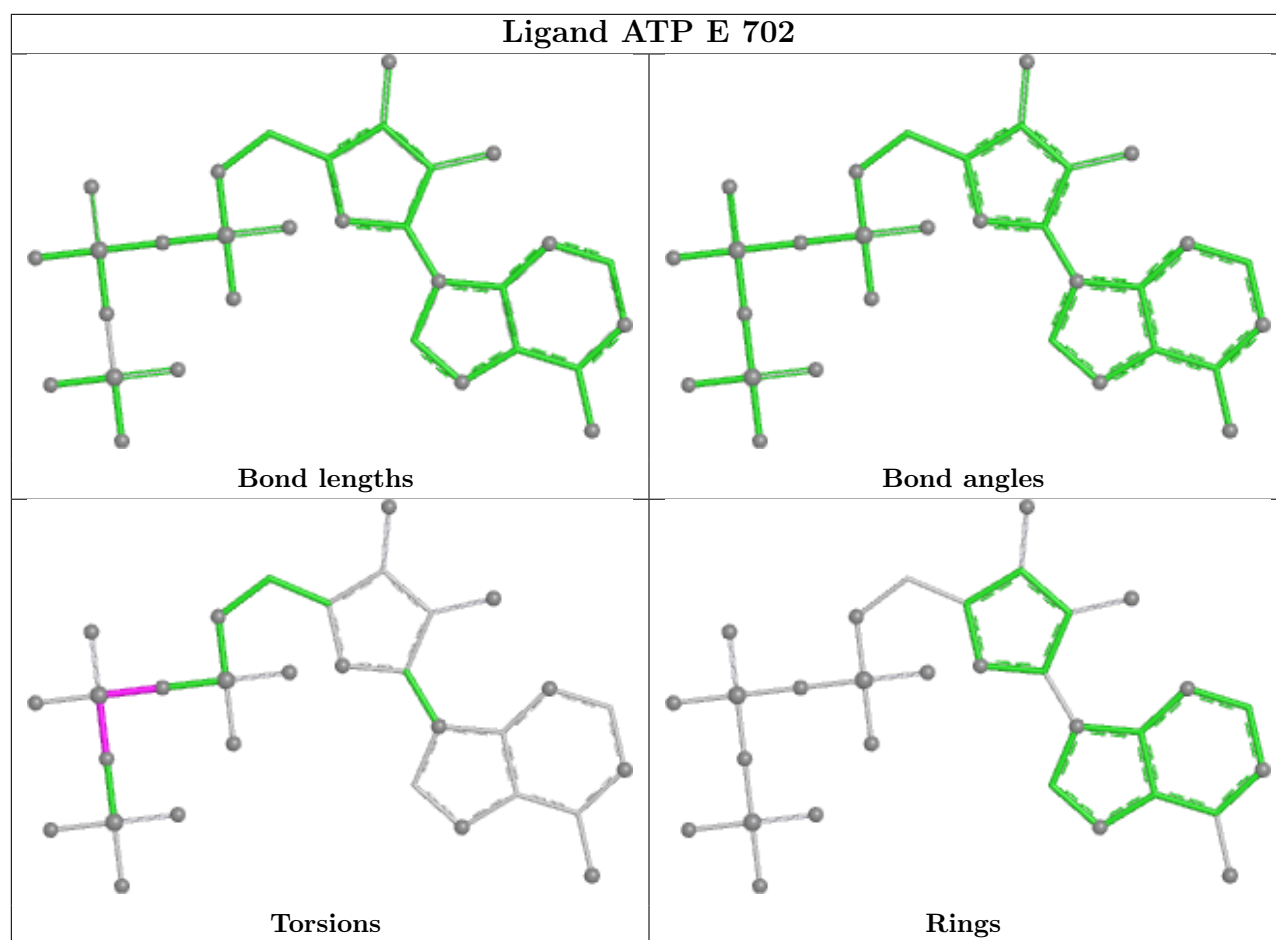


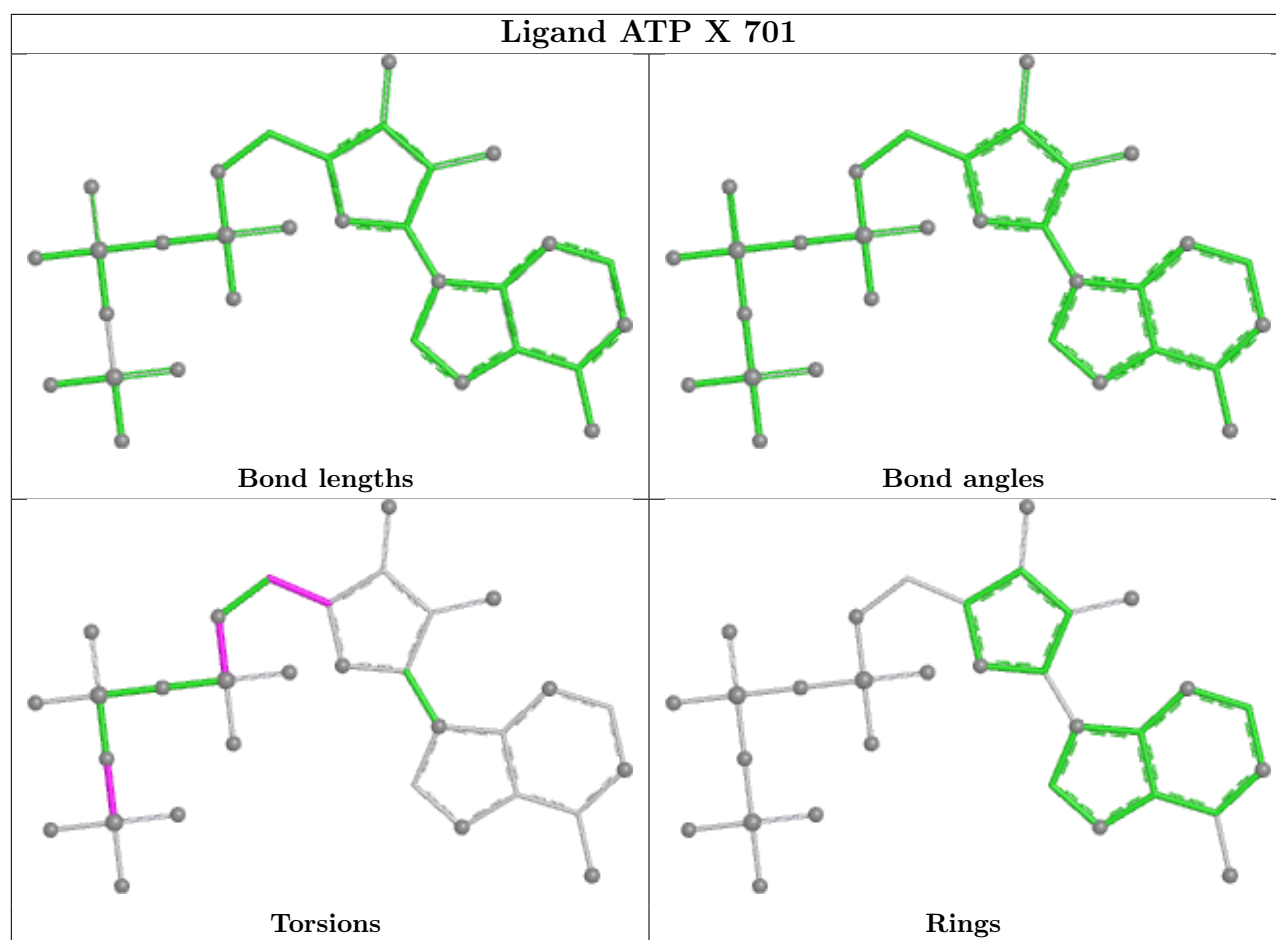
Ligand ATP J 701

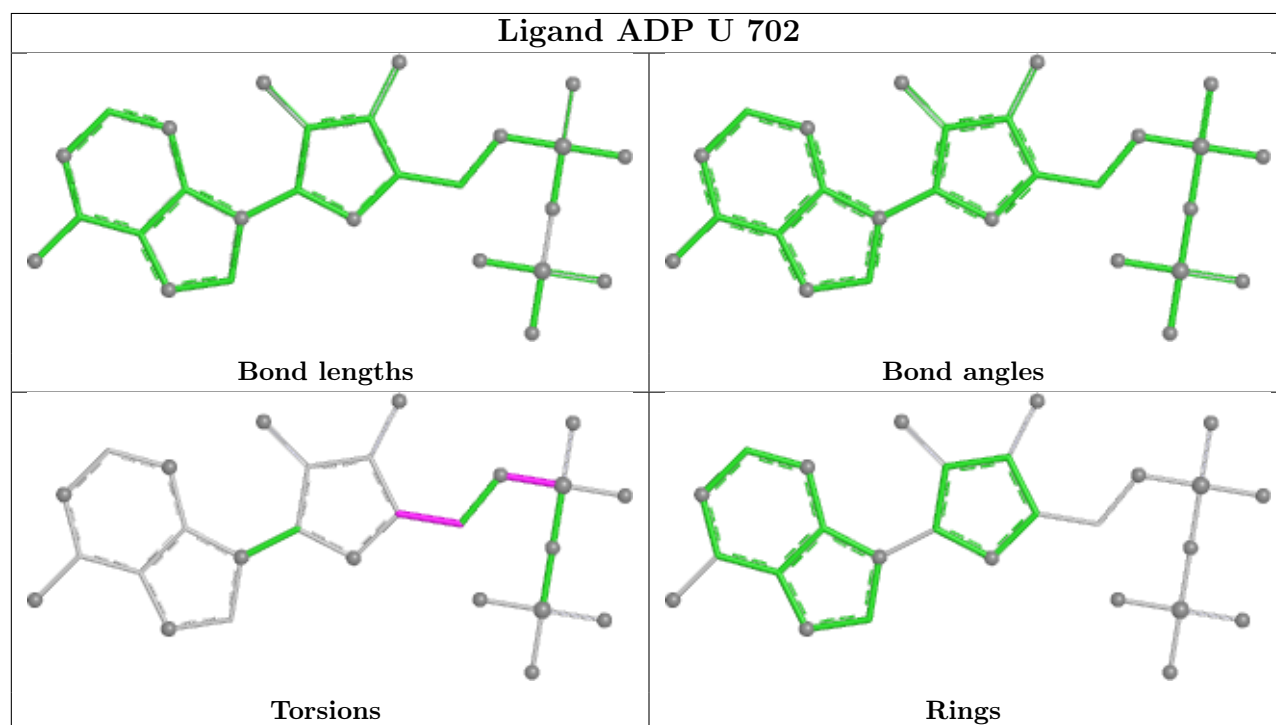
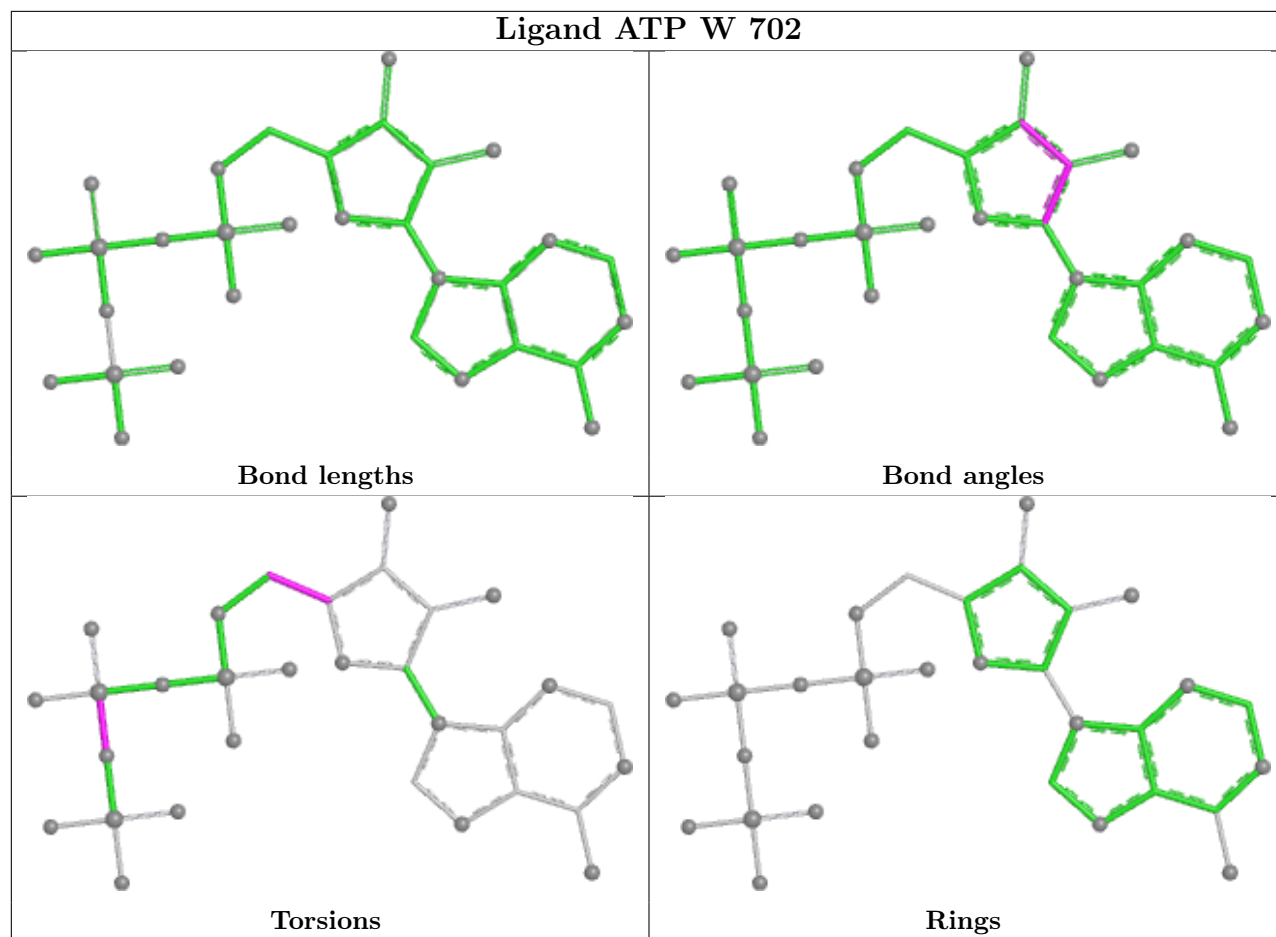


Ligand ATP L 702

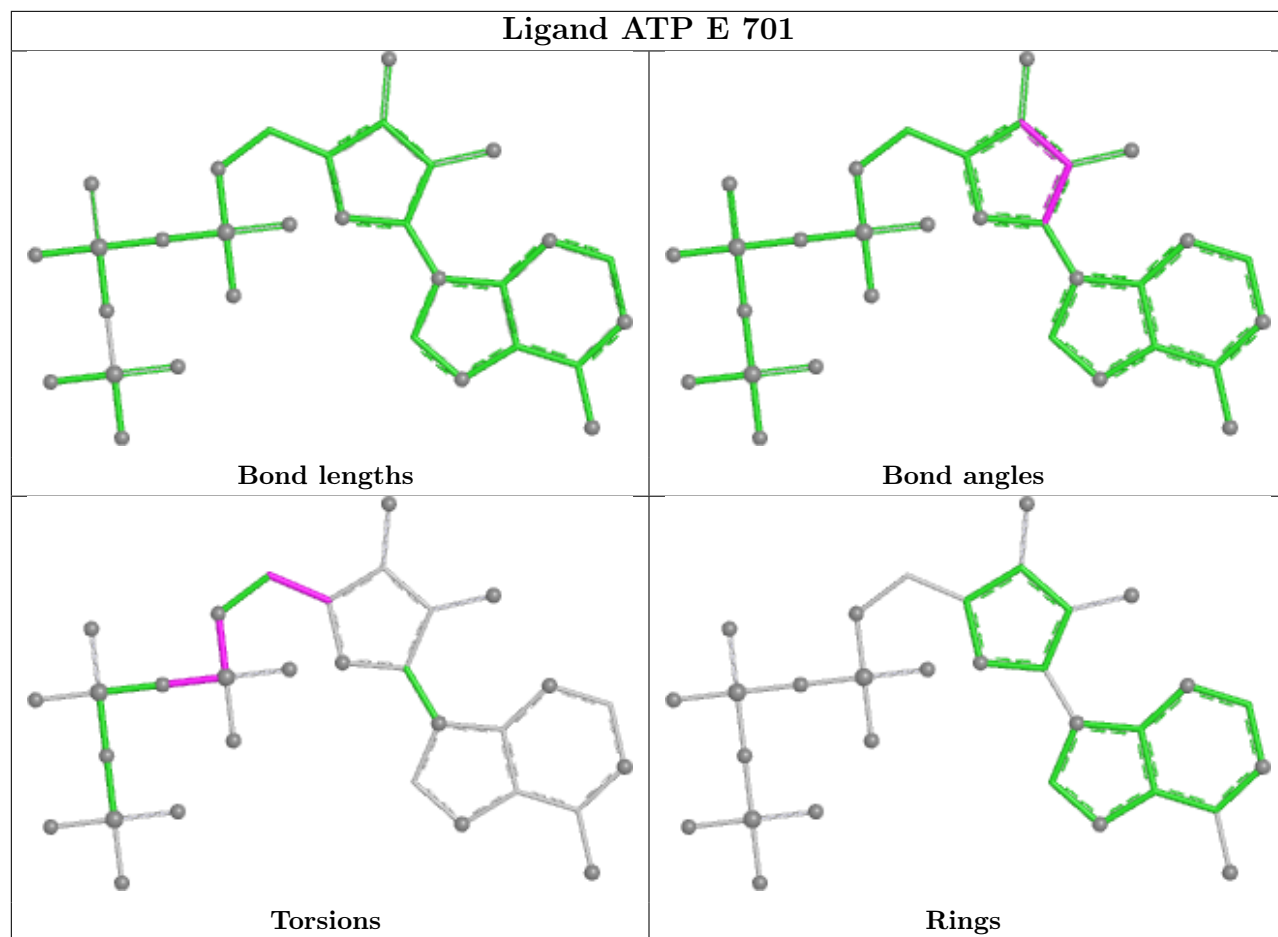




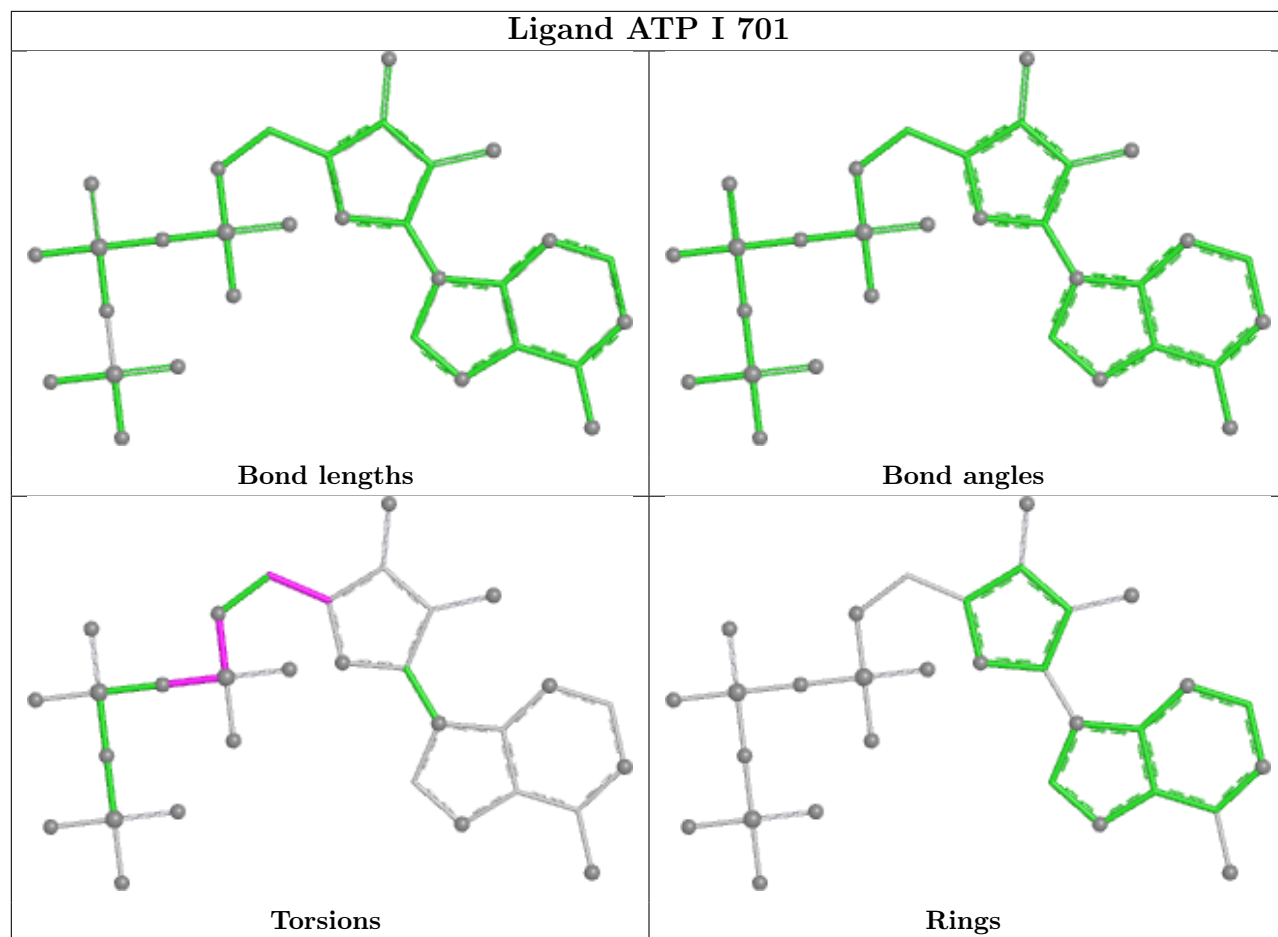


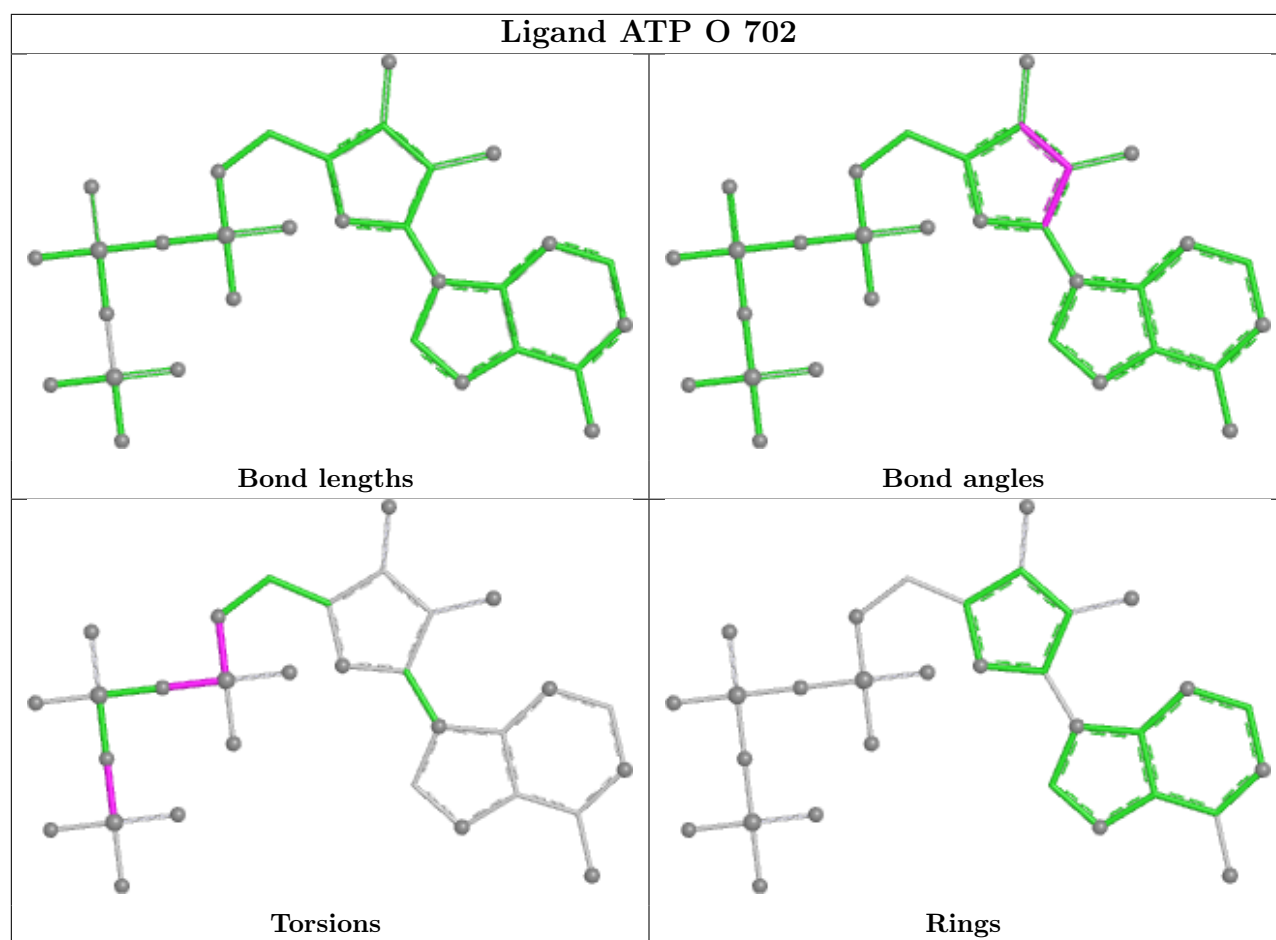


Ligand ATP E 701



Ligand ATP I 701





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	467/519 (89%)	0.17	1 (0%) 91 83	23, 46, 74, 115	0
1	B	468/519 (90%)	0.17	5 (1%) 78 59	25, 48, 69, 106	0
1	G	466/519 (89%)	0.09	2 (0%) 88 76	23, 43, 63, 98	0
1	H	467/519 (89%)	0.15	5 (1%) 78 59	26, 45, 69, 105	0
1	M	462/519 (89%)	0.71	23 (4%) 34 18	43, 68, 102, 130	0
1	N	454/519 (87%)	0.72	32 (7%) 22 12	48, 70, 99, 120	0
1	P	455/519 (87%)	0.64	33 (7%) 21 11	39, 62, 96, 129	0
1	R	462/519 (89%)	0.54	19 (4%) 41 23	37, 61, 84, 142	0
1	S	443/519 (85%)	1.14	71 (16%) 5 2	56, 89, 118, 132	0
1	T	414/519 (79%)	1.20	66 (15%) 5 2	57, 96, 121, 131	0
1	V	436/519 (84%)	0.79	41 (9%) 14 8	41, 68, 119, 132	0
1	W	463/519 (89%)	0.64	36 (7%) 19 10	37, 63, 99, 137	0
1	X	460/519 (88%)	0.73	35 (7%) 20 11	42, 68, 94, 118	0
2	C	470/519 (90%)	0.15	7 (1%) 72 52	26, 46, 75, 122	0
2	D	469/519 (90%)	0.15	5 (1%) 78 59	22, 47, 77, 124	0
2	E	468/519 (90%)	0.04	6 (1%) 75 56	20, 40, 71, 113	0
2	F	466/519 (89%)	0.13	6 (1%) 75 56	21, 45, 72, 88	0
2	I	471/519 (90%)	0.16	5 (1%) 78 59	22, 43, 78, 121	0
2	J	466/519 (89%)	0.16	6 (1%) 75 56	20, 45, 75, 108	0
2	K	469/519 (90%)	0.06	5 (1%) 78 59	20, 40, 72, 119	0
2	L	468/519 (90%)	0.11	10 (2%) 63 42	23, 44, 72, 105	0
2	O	459/519 (88%)	0.70	21 (4%) 37 20	47, 70, 101, 125	0
2	Q	464/519 (89%)	0.43	15 (3%) 50 30	36, 56, 83, 125	0
2	U	428/519 (82%)	0.98	46 (10%) 11 6	51, 82, 120, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	11015/12456 (88%)	0.44	501 (4%) 38 20	20, 56, 104, 142	0

The worst 5 of 501 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	51	GLY	6.0
1	T	456	PHE	5.8
1	P	51	GLY	5.7
2	Q	250	GLY	4.8
1	R	195	GLY	4.7

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

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	TPO	U	432	11/12	0.72	0.16	72,76,79,79	4
1	SEP	S	431	10/11	0.76	0.17	71,75,82,82	0
2	TPO	Q	432	11/12	0.78	0.19	58,61,63,64	4
2	TPO	L	432	11/12	0.80	0.17	46,51,56,56	4
2	SEP	U	431	10/11	0.80	0.17	75,78,82,83	0
2	TPO	O	432	11/12	0.80	0.14	71,74,80,80	0
1	SEP	M	431	10/11	0.80	0.15	65,68,72,72	0
1	SEP	T	431	10/11	0.81	0.18	82,84,87,87	0
2	TPO	C	432	11/12	0.81	0.16	52,56,61,61	4
2	TPO	F	432	11/12	0.81	0.15	41,45,50,50	4
2	TPO	I	432	11/12	0.81	0.17	46,50,54,54	4
1	SEP	V	431	10/11	0.81	0.16	55,58,61,62	4
2	SEP	C	431	10/11	0.86	0.16	55,57,62,62	0
1	SEP	R	431	10/11	0.86	0.13	58,60,61,61	0
1	SEP	N	431	10/11	0.86	0.15	65,66,69,70	0
1	SEP	W	431	10/11	0.86	0.11	51,52,53,53	4
1	SEP	H	431	10/11	0.87	0.14	41,43,46,46	4
2	SEP	Q	431	10/11	0.88	0.13	53,55,57,58	0
2	TPO	J	432	11/12	0.88	0.14	41,44,48,48	4
1	SEP	X	431	10/11	0.89	0.10	52,56,60,60	0
2	SEP	O	431	10/11	0.89	0.15	70,71,71,71	4
2	TPO	D	432	11/12	0.89	0.13	40,43,45,45	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SEP	K	431	10/11	0.89	0.14	42,43,45,46	0
1	SEP	A	431	10/11	0.90	0.12	46,46,47,47	4
2	SEP	I	431	10/11	0.91	0.12	48,50,54,54	0
2	TPO	K	432	11/12	0.91	0.10	40,43,45,45	4
1	SEP	P	431	10/11	0.91	0.12	52,53,53,54	4
1	SEP	B	431	10/11	0.91	0.10	42,43,44,44	4
1	SEP	G	431	10/11	0.92	0.11	48,49,50,51	0
2	SEP	J	431	10/11	0.92	0.10	42,43,44,44	4
2	SEP	D	431	10/11	0.92	0.10	42,43,44,44	4
2	SEP	L	431	10/11	0.93	0.11	46,46,46,47	4
2	TPO	E	432	11/12	0.93	0.09	39,42,44,44	4
2	SEP	E	431	10/11	0.93	0.12	38,39,41,41	0
2	SEP	F	431	10/11	0.94	0.10	41,42,42,42	4

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
3	ATP	S	701	31/31	0.81	0.13	77,78,83,83	0
5	ADP	U	702	27/27	0.82	0.12	92,104,112,112	0
3	ATP	S	702	31/31	0.83	0.11	94,95,99,99	0
3	ATP	M	702	31/31	0.83	0.13	76,79,81,81	0
3	ATP	T	702	31/31	0.85	0.11	85,88,90,91	0
4	MG	B	704	1/1	0.86	0.07	58,58,58,58	0
4	MG	C	704	1/1	0.86	0.09	48,48,48,48	0
3	ATP	X	701	31/31	0.86	0.13	59,63,70,70	0
4	MG	U	703	1/1	0.87	0.09	51,51,51,51	0
3	ATP	R	701	31/31	0.88	0.12	48,55,59,59	0
3	ATP	O	701	31/31	0.88	0.12	60,62,64,65	0
4	MG	R	704	1/1	0.88	0.12	44,44,44,44	0
4	MG	P	704	1/1	0.88	0.06	44,44,44,44	0
3	ATP	V	702	31/31	0.88	0.10	83,85,89,90	0
3	ATP	W	702	31/31	0.88	0.10	71,74,76,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ATP	P	702	31/31	0.89	0.10	55,56,60,62	0
4	MG	H	704	1/1	0.89	0.06	46,46,46,46	0
3	ATP	O	702	31/31	0.89	0.10	84,98,105,105	0
3	ATP	X	702	31/31	0.90	0.10	66,70,74,75	0
3	ATP	N	701	31/31	0.90	0.10	56,60,64,64	0
3	ATP	Q	702	31/31	0.90	0.10	59,62,73,73	0
3	ATP	R	702	31/31	0.91	0.09	58,59,63,63	0
3	ATP	T	701	31/31	0.91	0.11	69,71,74,75	0
4	MG	G	703	1/1	0.91	0.08	43,43,43,43	0
3	ATP	M	701	31/31	0.91	0.09	54,56,58,58	0
5	ADP	W	701	27/27	0.91	0.09	45,49,52,52	0
3	ATP	U	701	31/31	0.92	0.09	60,62,62,62	0
4	MG	Q	703	1/1	0.92	0.06	51,51,51,51	0
4	MG	I	704	1/1	0.92	0.10	47,47,47,47	0
5	ADP	Q	701	27/27	0.92	0.09	45,49,51,51	0
3	ATP	N	702	31/31	0.92	0.10	61,64,69,70	0
4	MG	M	703	1/1	0.92	0.18	27,27,27,27	0
3	ATP	B	701	31/31	0.93	0.09	39,39,40,40	0
3	ATP	F	702	31/31	0.93	0.10	40,41,44,44	0
4	MG	E	704	1/1	0.93	0.08	22,22,22,22	0
4	MG	F	704	1/1	0.93	0.07	39,39,39,39	0
3	ATP	F	701	31/31	0.94	0.08	39,40,44,44	0
4	MG	R	703	1/1	0.94	0.16	33,33,33,33	0
3	ATP	L	702	31/31	0.95	0.08	38,39,43,43	0
4	MG	D	704	1/1	0.95	0.08	41,41,41,41	0
3	ATP	I	702	31/31	0.95	0.07	41,42,45,45	0
4	MG	H	703	1/1	0.95	0.13	25,25,25,25	0
3	ATP	J	702	31/31	0.95	0.08	42,45,46,47	0
4	MG	K	704	1/1	0.95	0.04	20,20,20,20	0
3	ATP	E	702	31/31	0.95	0.08	43,44,47,48	0
3	ATP	A	702	31/31	0.95	0.09	40,41,45,45	0
3	ATP	B	702	31/31	0.95	0.09	44,46,49,50	0
3	ATP	C	702	31/31	0.95	0.08	41,42,46,47	0
4	MG	P	703	1/1	0.95	0.06	43,43,43,43	0
3	ATP	D	702	31/31	0.95	0.08	43,46,47,48	0
3	ATP	G	701	31/31	0.95	0.08	37,40,44,45	0
3	ATP	H	702	31/31	0.95	0.08	44,46,49,50	0
3	ATP	K	702	31/31	0.95	0.08	39,42,46,47	0
3	ATP	P	701	31/31	0.95	0.10	52,56,65,66	0
3	ATP	L	701	31/31	0.95	0.07	37,38,42,42	0
3	ATP	I	701	31/31	0.96	0.07	29,30,31,31	0
3	ATP	H	701	31/31	0.96	0.07	36,37,38,38	0

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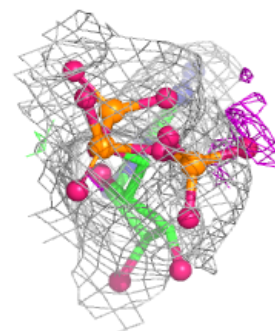
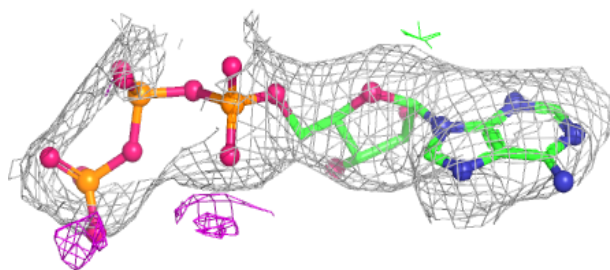
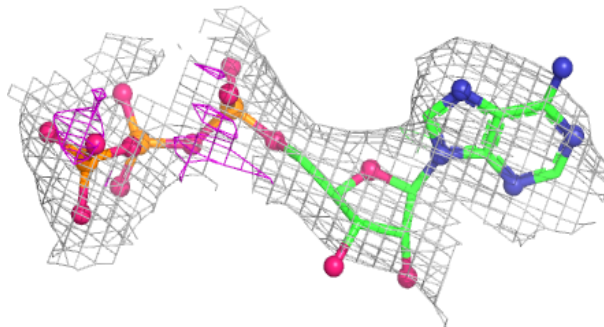
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ATP	J	701	31/31	0.96	0.07	27,29,31,32	0
3	ATP	E	701	31/31	0.96	0.07	30,32,35,35	0
3	ATP	K	701	31/31	0.96	0.07	29,31,33,33	0
3	ATP	A	701	31/31	0.96	0.07	41,45,50,50	0
3	ATP	V	701	31/31	0.96	0.09	44,49,54,55	0
3	ATP	C	701	31/31	0.96	0.07	33,34,34,35	0
3	ATP	G	702	31/31	0.96	0.07	37,40,42,42	0
4	MG	A	703	1/1	0.96	0.07	34,34,34,34	0
4	MG	C	703	1/1	0.97	0.05	43,43,43,43	0
4	MG	A	704	1/1	0.97	0.04	27,27,27,27	0
4	MG	K	703	1/1	0.97	0.04	23,23,23,23	0
4	MG	F	703	1/1	0.97	0.05	40,40,40,40	0
4	MG	L	703	1/1	0.97	0.04	35,35,35,35	0
3	ATP	D	701	31/31	0.97	0.07	28,29,30,30	0
4	MG	V	703	1/1	0.97	0.04	36,36,36,36	0
4	MG	J	703	1/1	0.97	0.10	18,18,18,18	0
4	MG	J	704	1/1	0.97	0.04	23,23,23,23	0
4	MG	G	704	1/1	0.97	0.04	48,48,48,48	0
4	MG	T	703	1/1	0.98	0.07	50,50,50,50	0
4	MG	D	703	1/1	0.98	0.04	26,26,26,26	0
4	MG	L	704	1/1	0.98	0.04	36,36,36,36	0
4	MG	N	704	1/1	0.98	0.03	47,47,47,47	0
4	MG	O	703	1/1	0.98	0.05	38,38,38,38	0
4	MG	E	703	1/1	0.98	0.04	21,21,21,21	0
4	MG	I	703	1/1	0.99	0.02	36,36,36,36	0
4	MG	B	703	1/1	0.99	0.03	31,31,31,31	0
4	MG	N	703	1/1	1.00	0.02	37,37,37,37	0

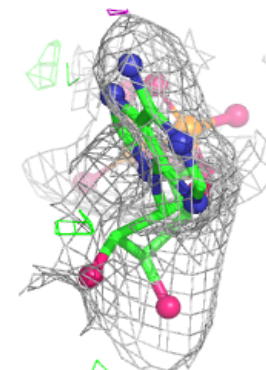
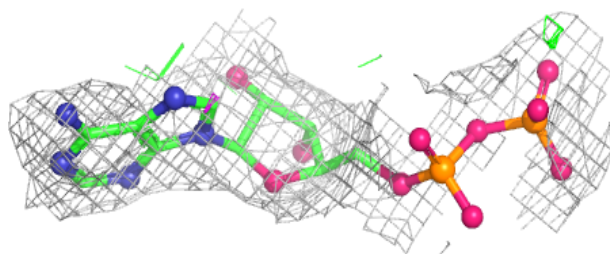
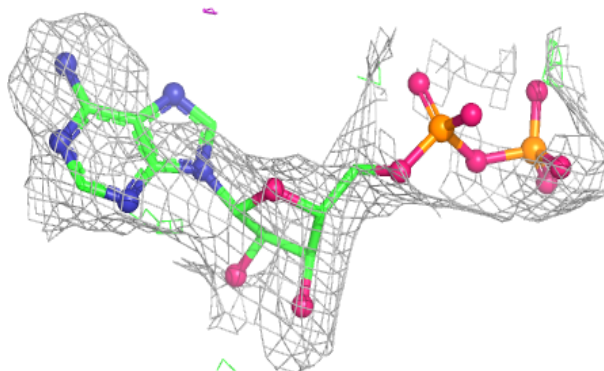
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP S 701:

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

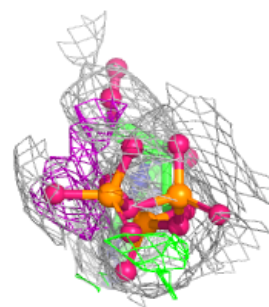
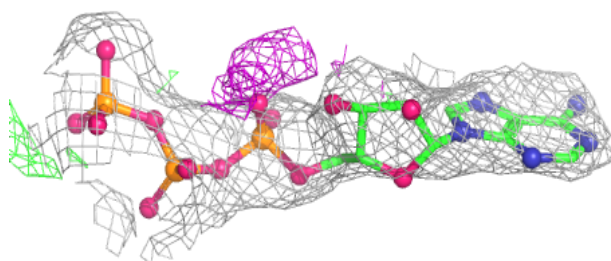
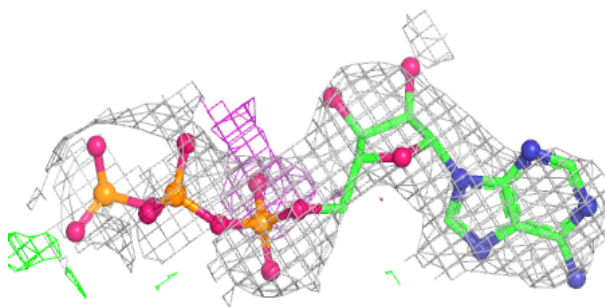
**Electron density around ADP U 702:**

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

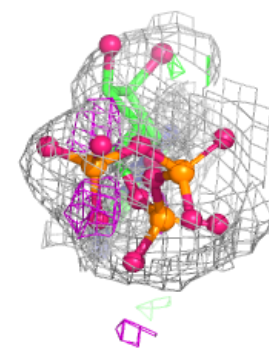
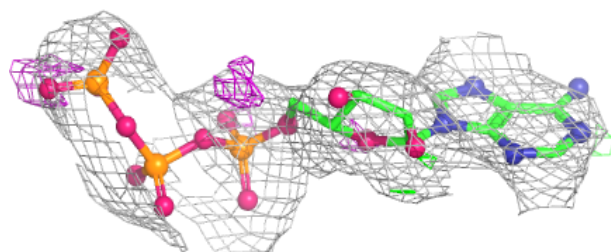
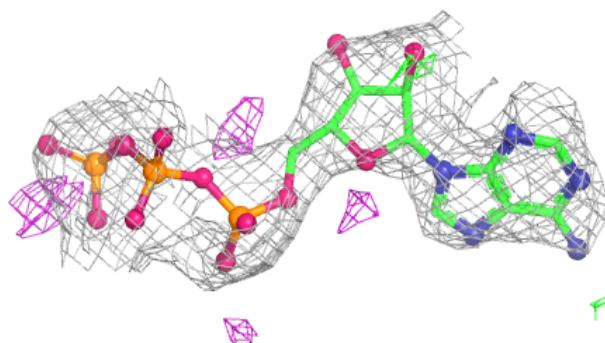


Electron density around ATP M 702:

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

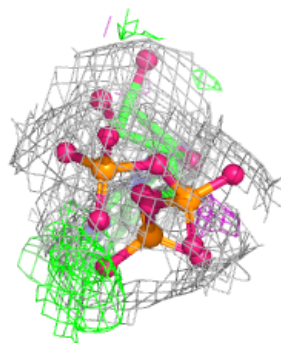
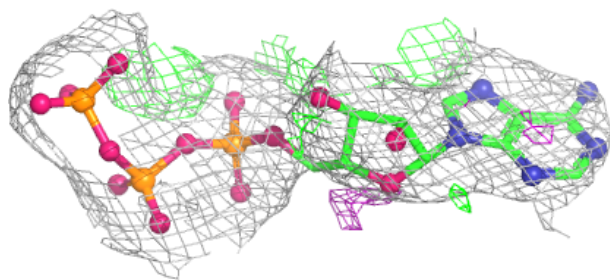
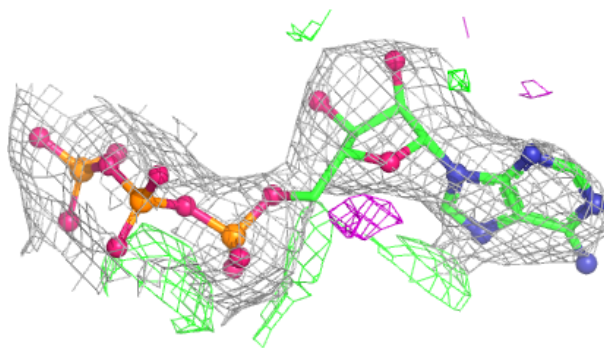
**Electron density around ATP X 701:**

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

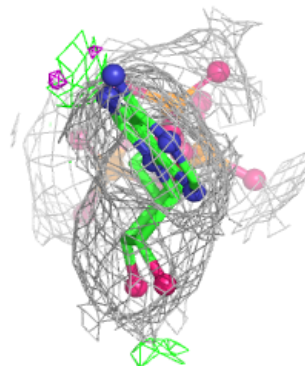
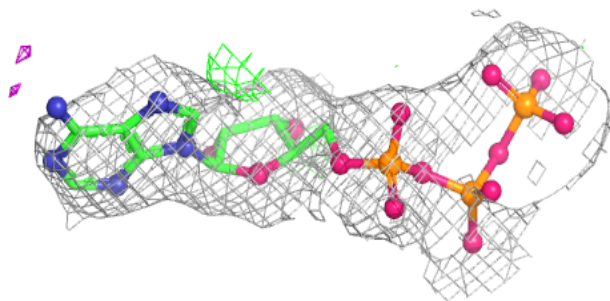
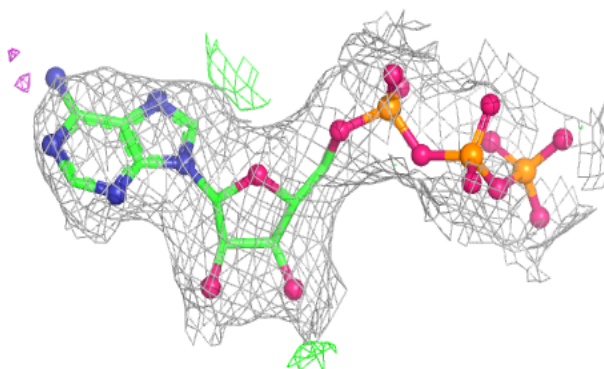


Electron density around ATP R 701:

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

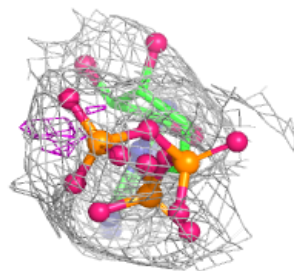
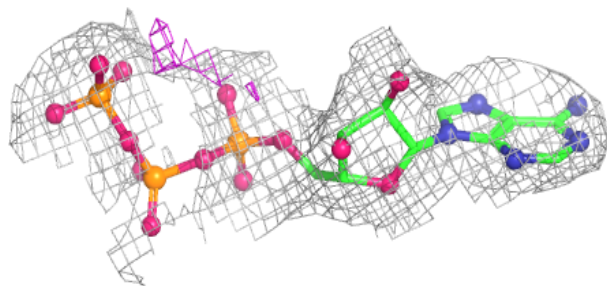
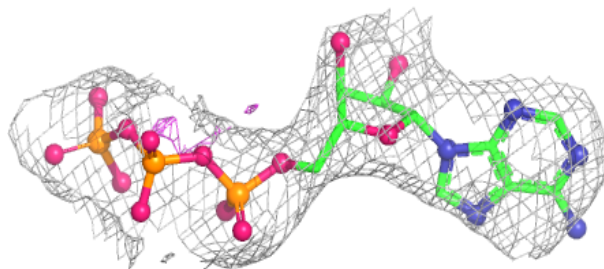
**Electron density around ATP O 701:**

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

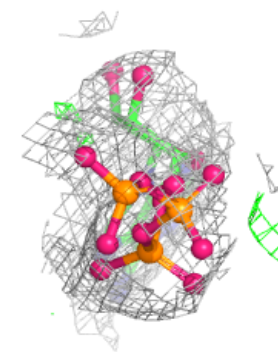
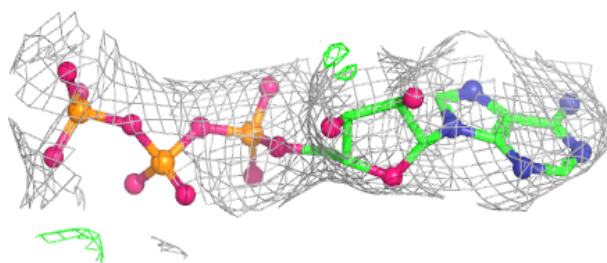
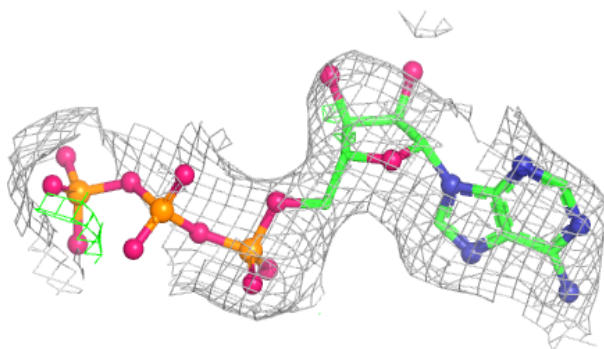


Electron density around ATP V 702:

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

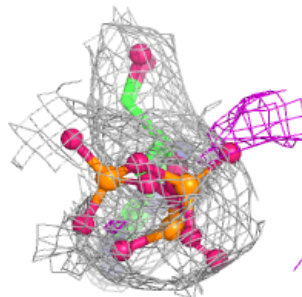
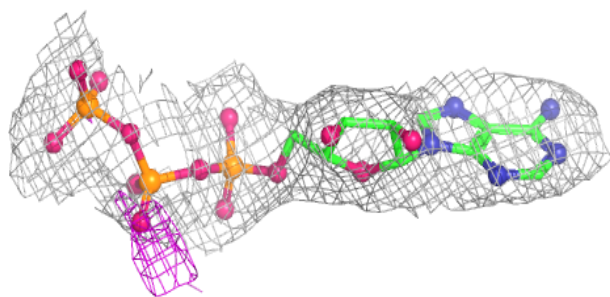
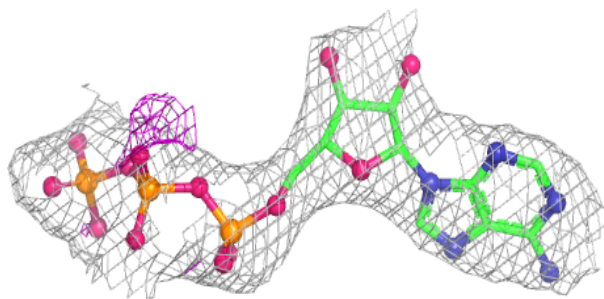
**Electron density around ATP W 702:**

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

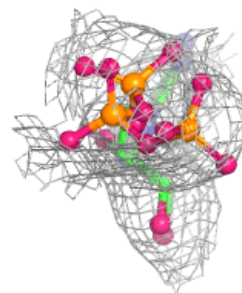
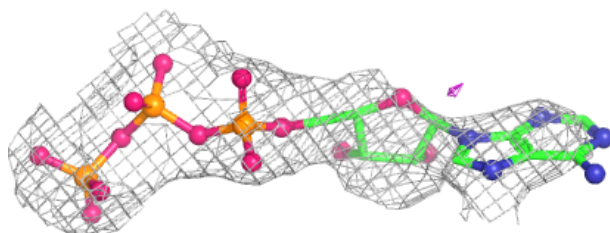
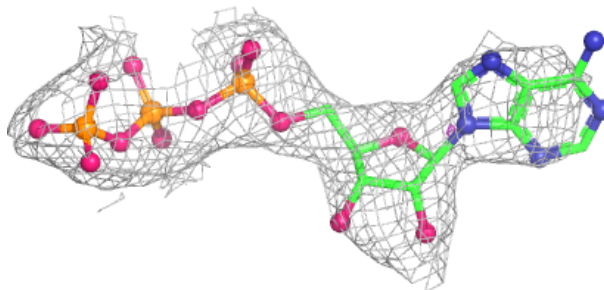


Electron density around ATP P 702:

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

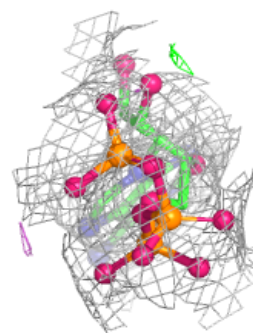
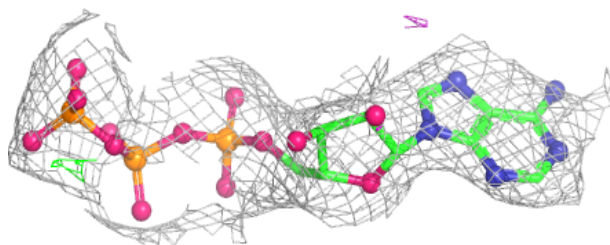
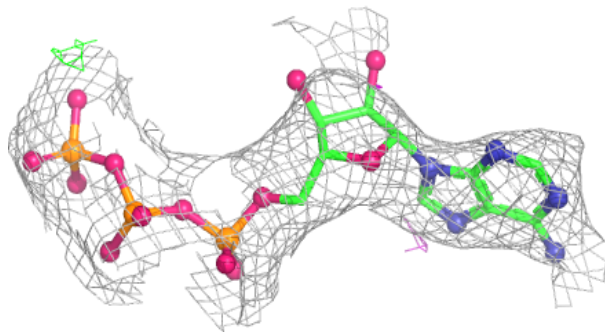
**Electron density around ATP O 702:**

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

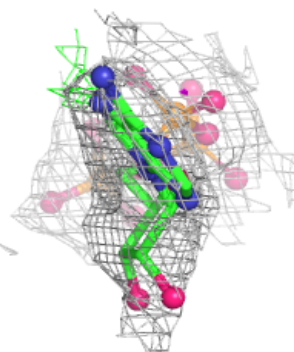
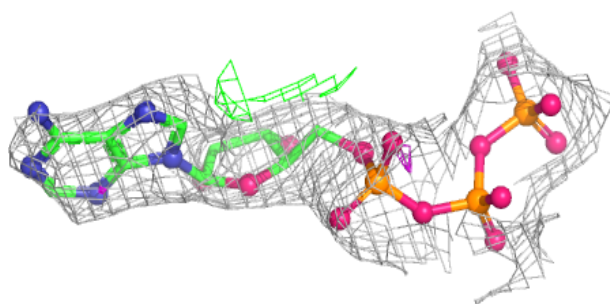
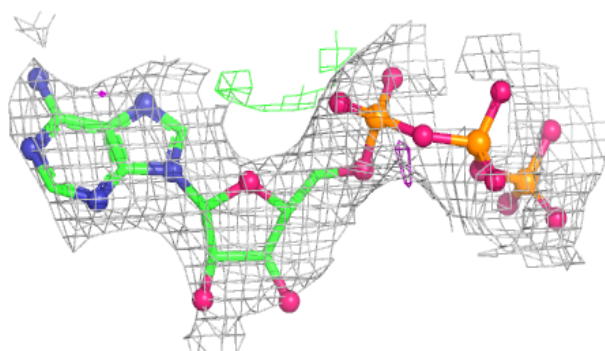


Electron density around ATP X 702:

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

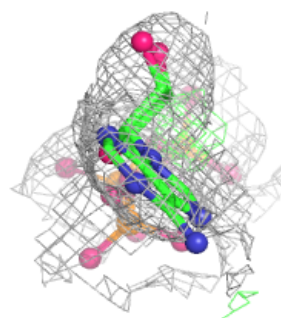
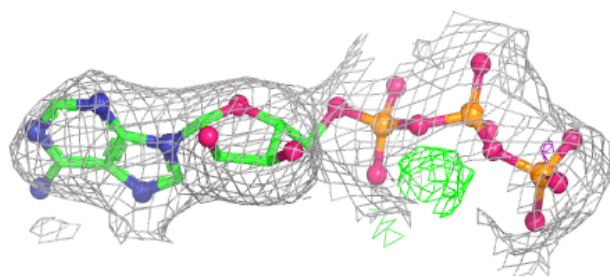
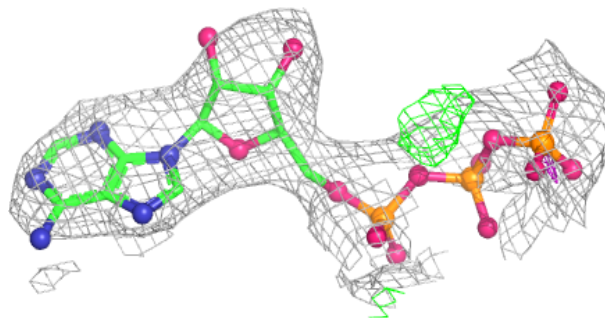
**Electron density around ATP N 701:**

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

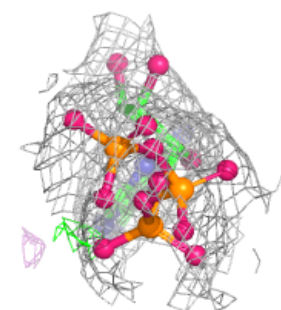
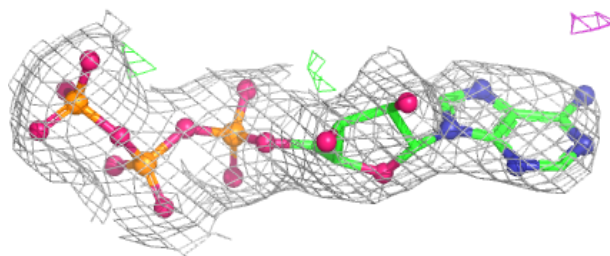
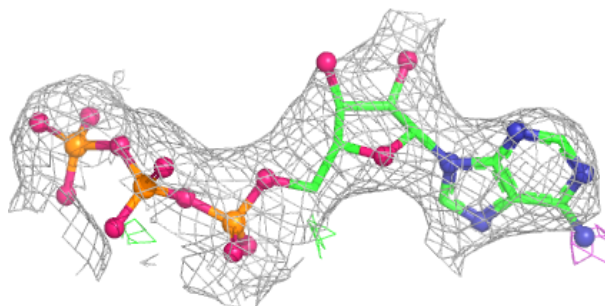


Electron density around ATP Q 702:

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

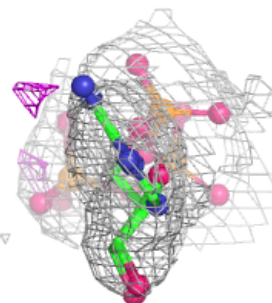
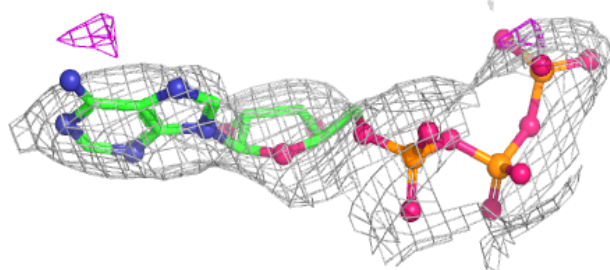
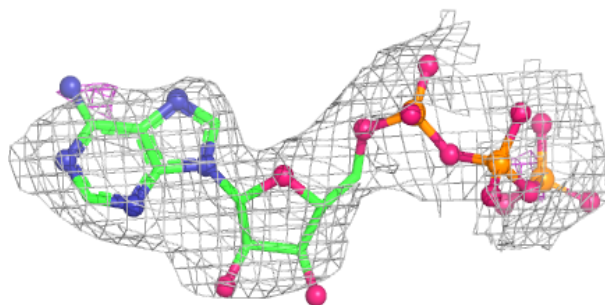
**Electron density around ATP R 702:**

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

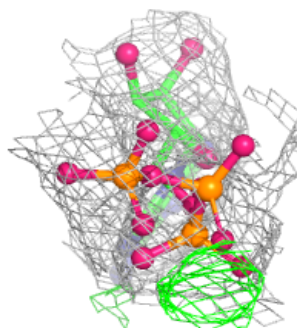
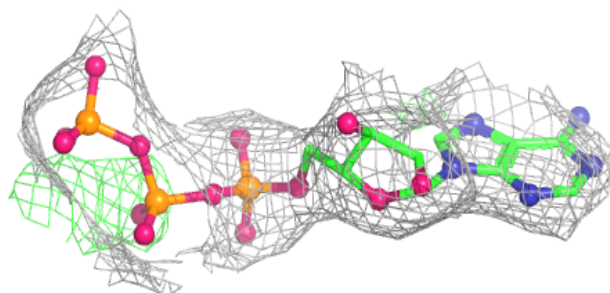
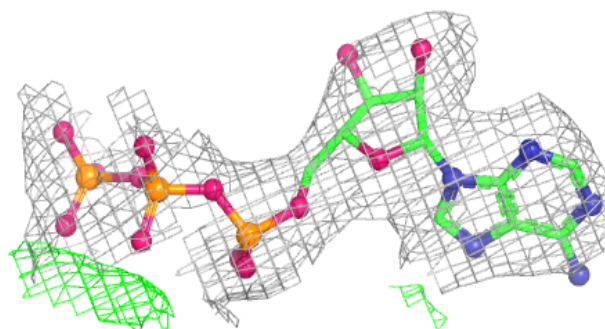


Electron density around ATP T 701:

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

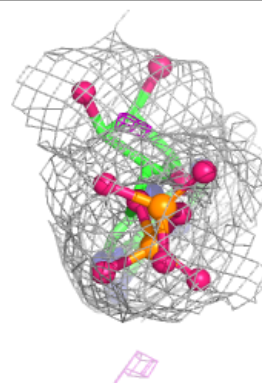
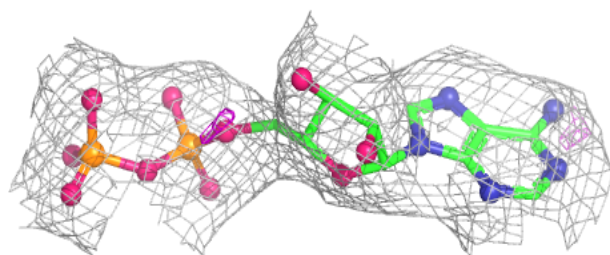
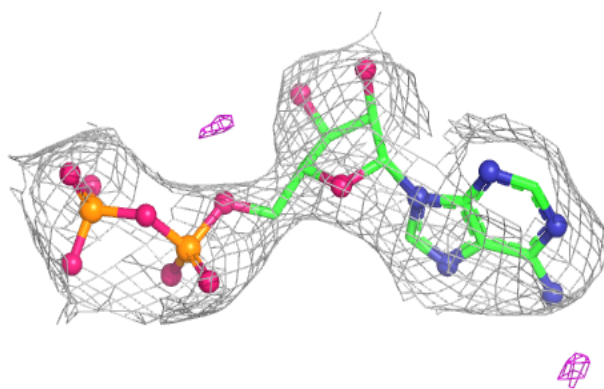
**Electron density around ATP M 701:**

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

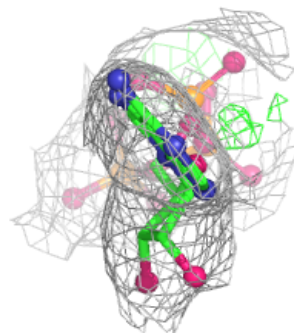
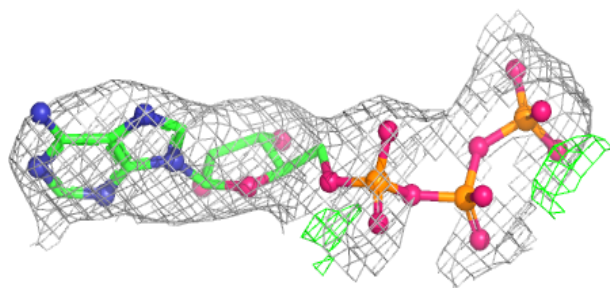
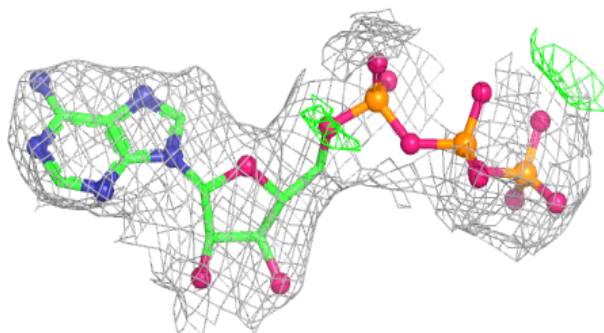


Electron density around ADP W 701:

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and green (positive)

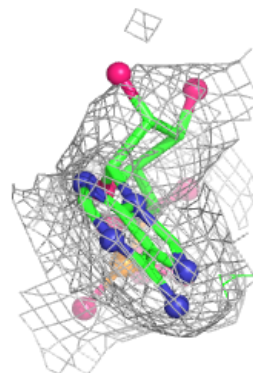
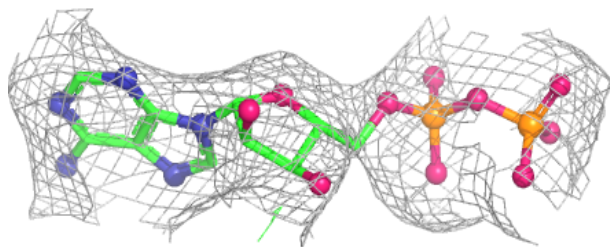
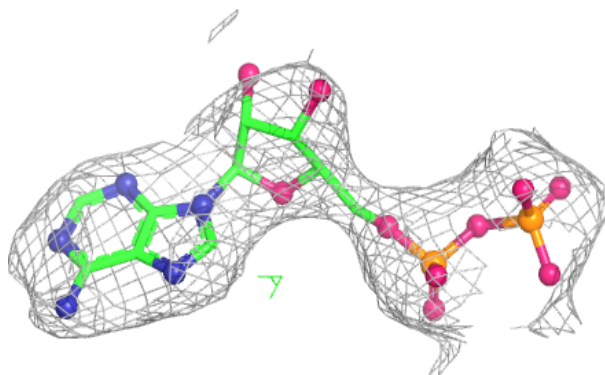
**Electron density around ATP U 701:**

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

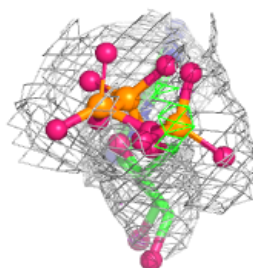
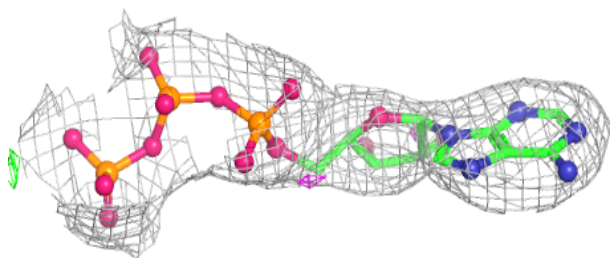
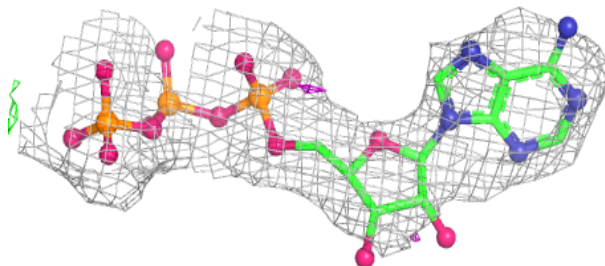


Electron density around ADP Q 701:

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

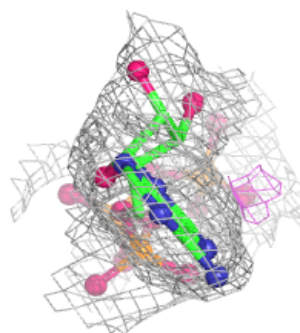
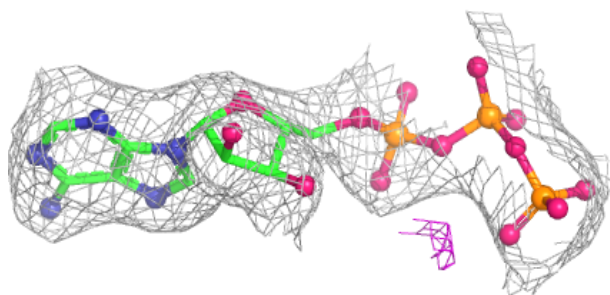
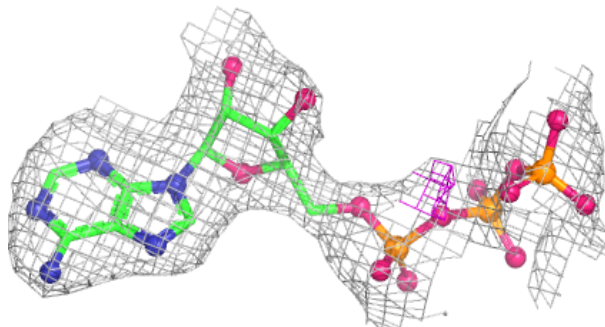
**Electron density around ATP N 702:**

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

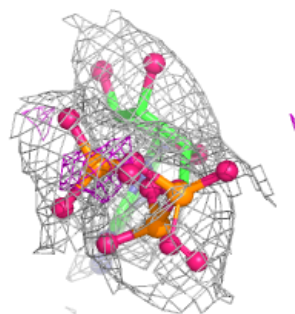
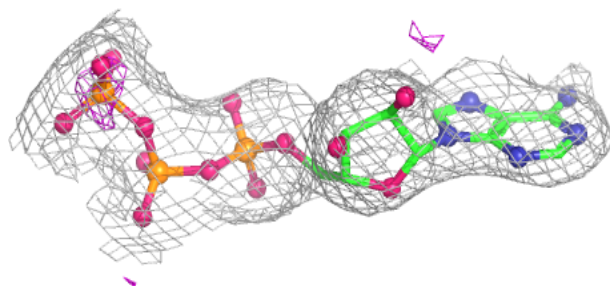
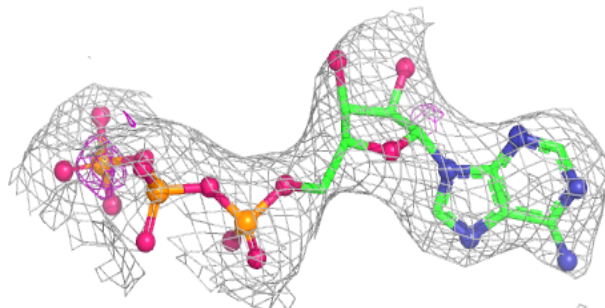


Electron density around ATP B 701:

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

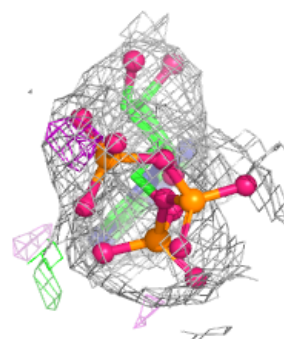
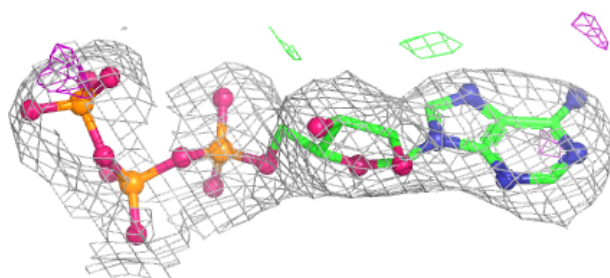
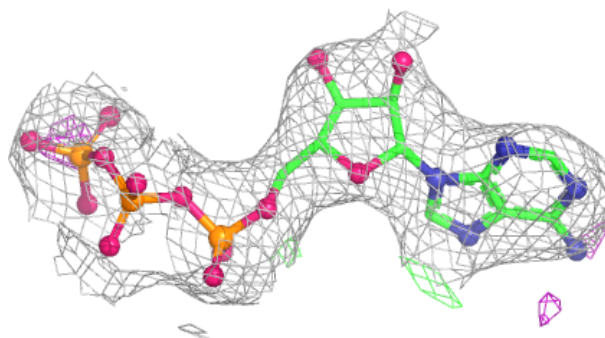
**Electron density around ATP F 702:**

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

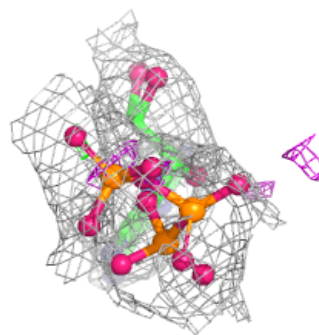
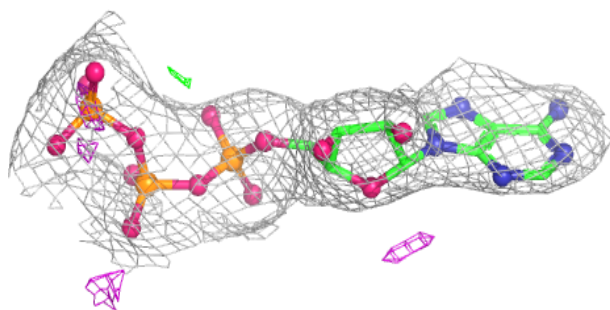
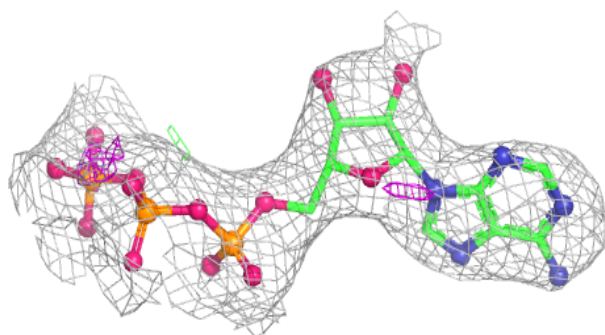


Electron density around ATP F 701:

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

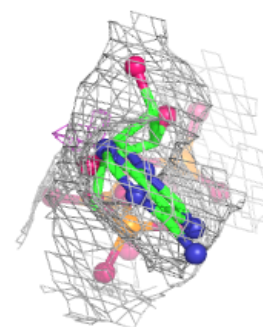
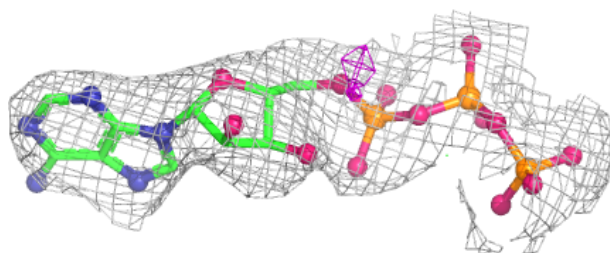
**Electron density around ATP L 702:**

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

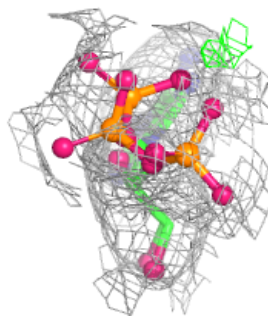
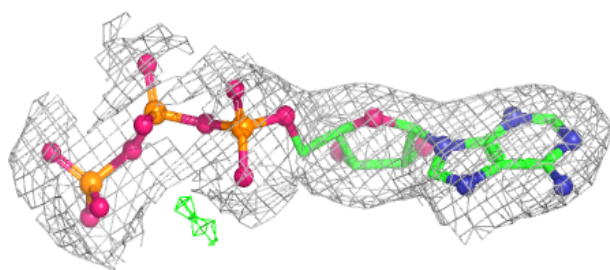
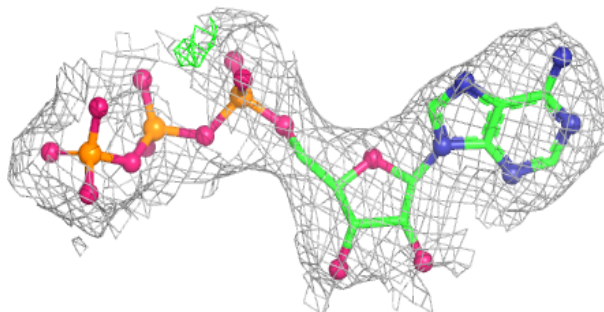


Electron density around ATP I 702:

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

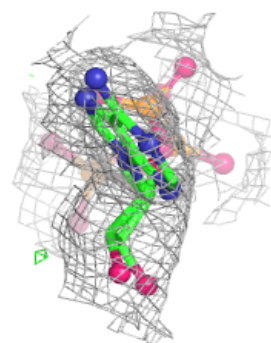
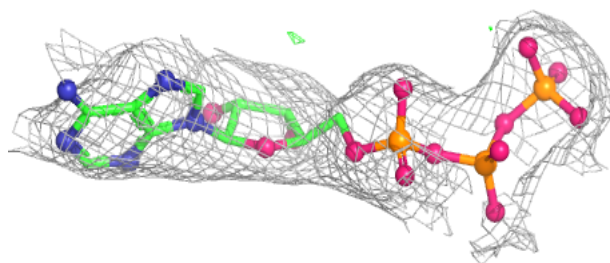
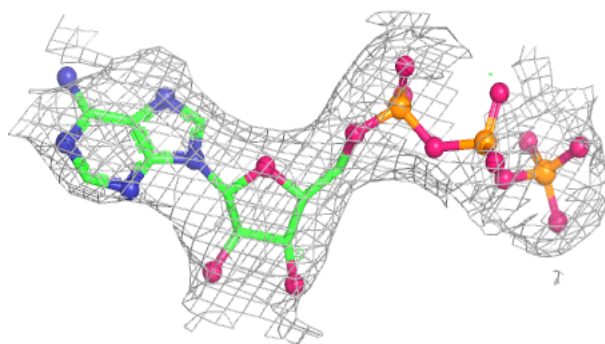
**Electron density around ATP J 702:**

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

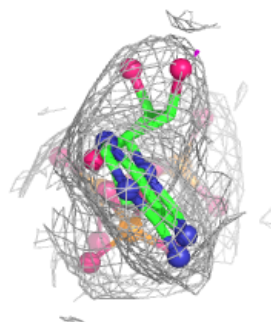
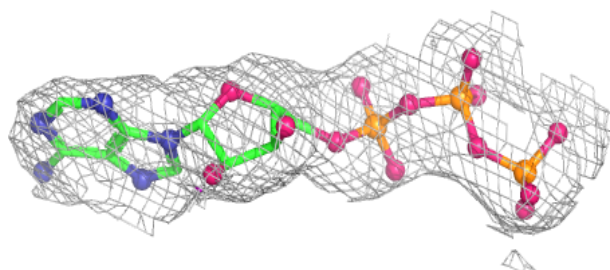
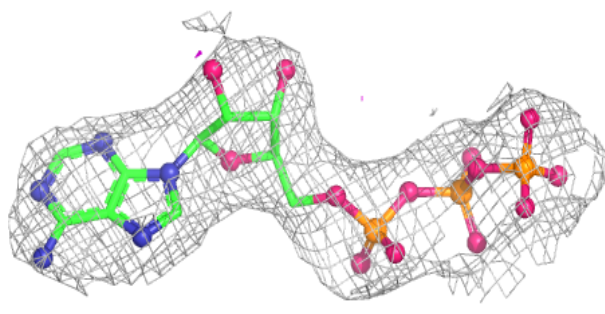


Electron density around ATP E 702:

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

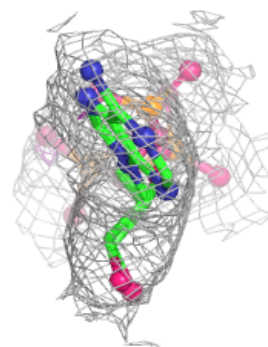
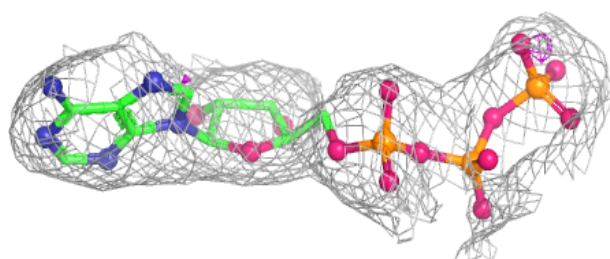
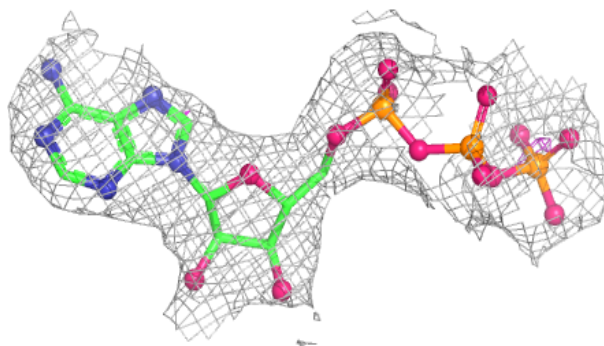
**Electron density around ATP A 702:**

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

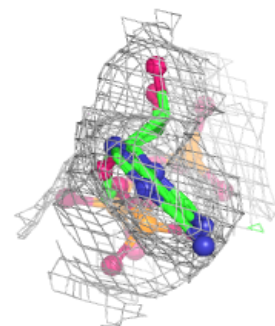
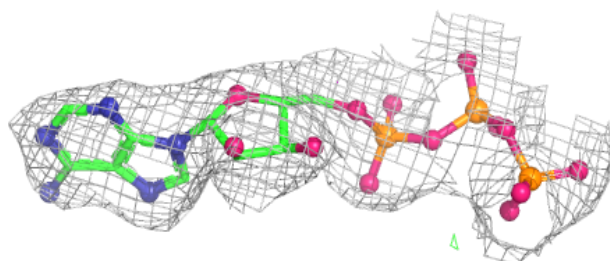
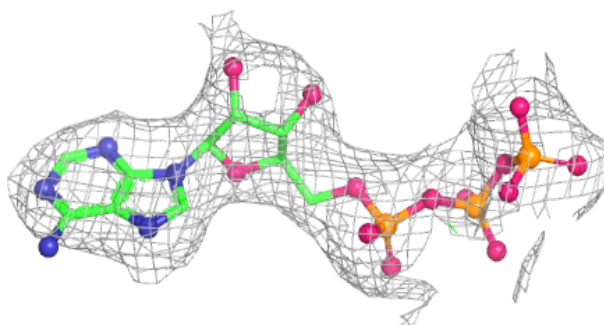


Electron density around ATP B 702:

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

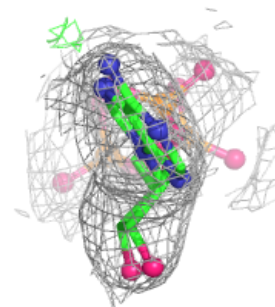
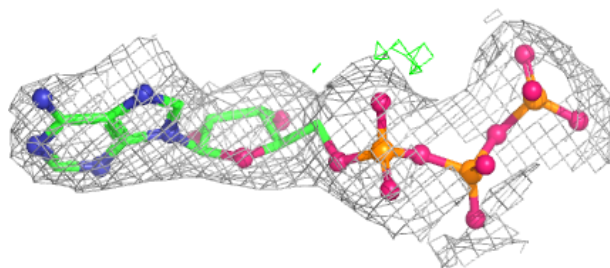
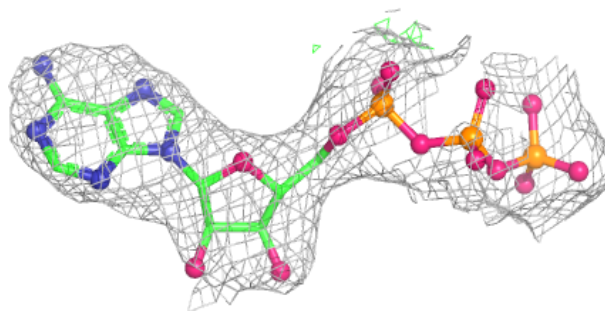
**Electron density around ATP C 702:**

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

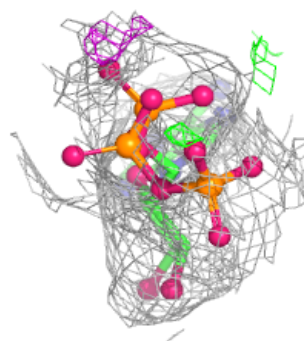
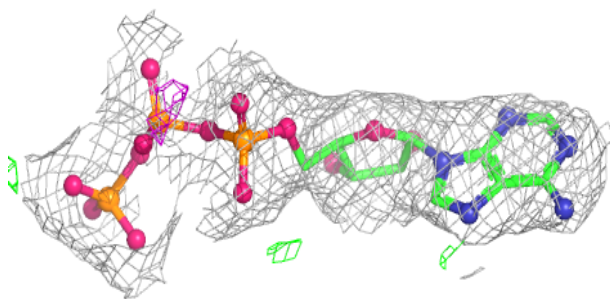
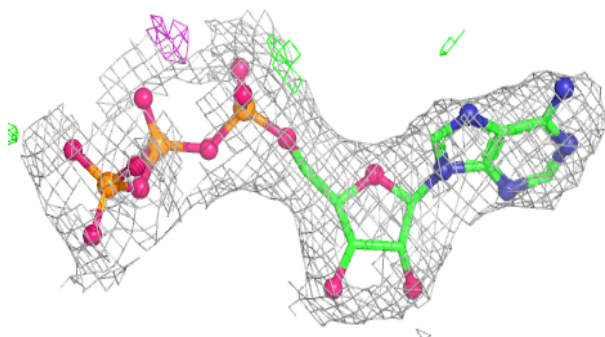


Electron density around ATP D 702:

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

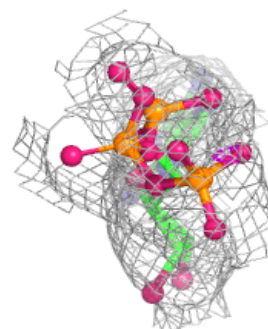
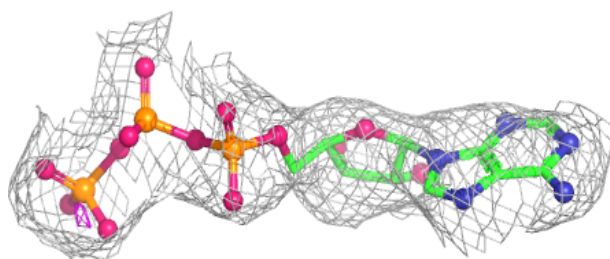
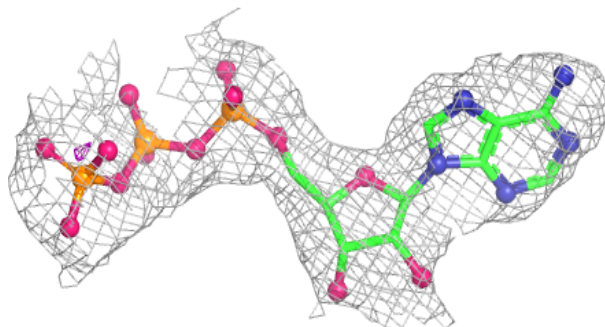
**Electron density around ATP G 701:**

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

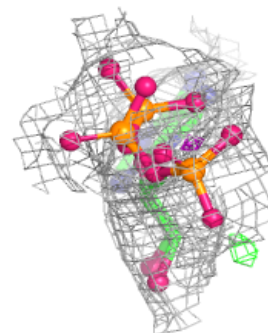
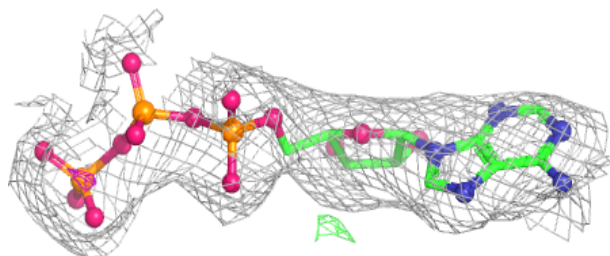
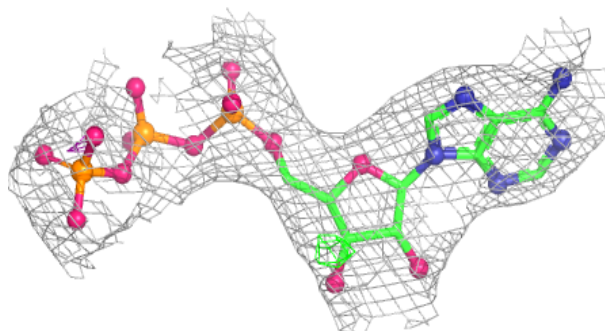


Electron density around ATP H 702:

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

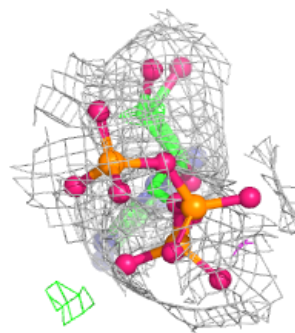
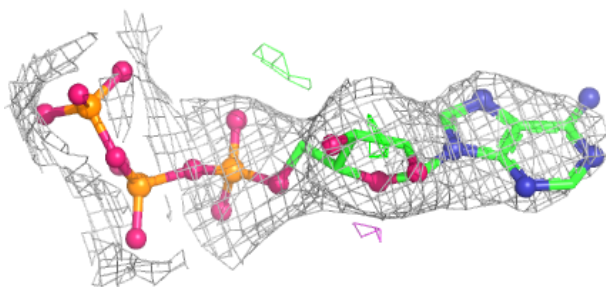
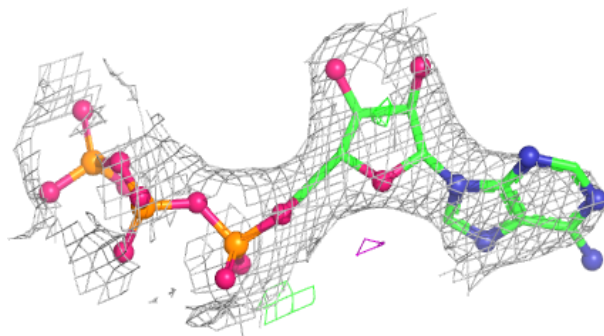
**Electron density around ATP K 702:**

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

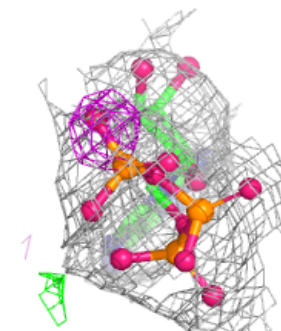
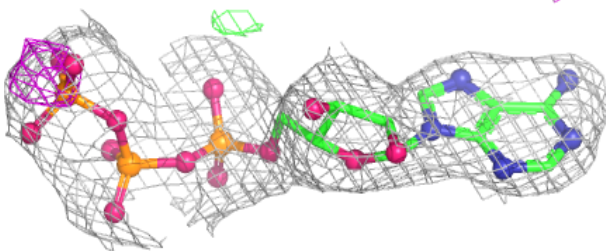
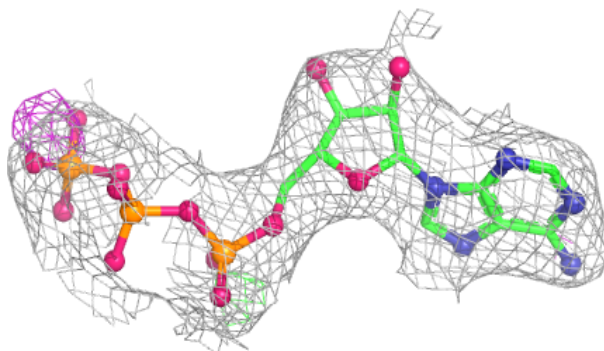


Electron density around ATP P 701:

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

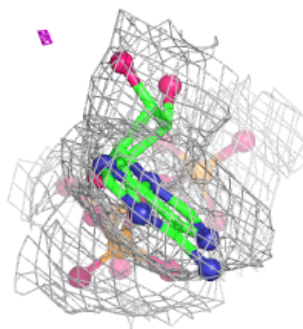
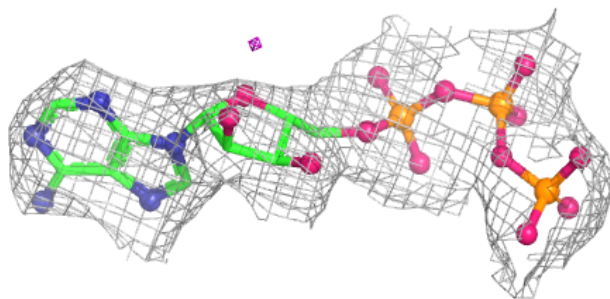
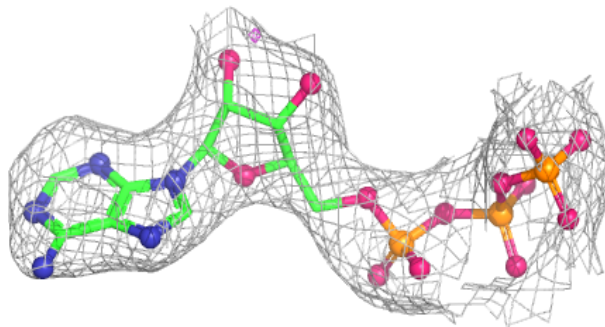
**Electron density around ATP L 701:**

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

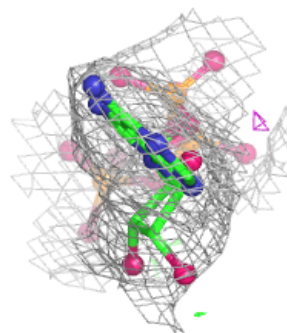
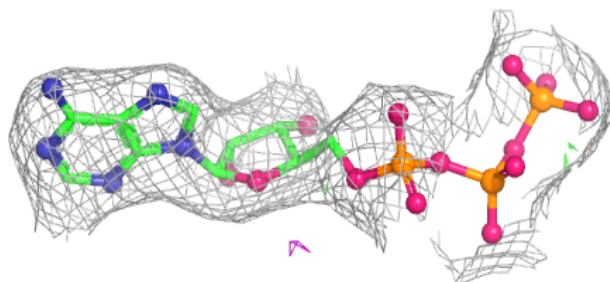
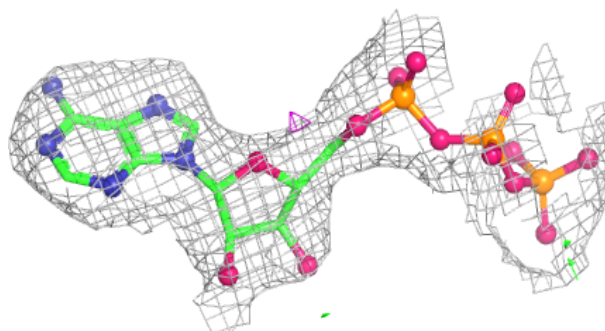


Electron density around ATP I 701:

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

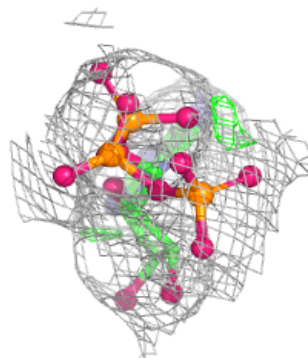
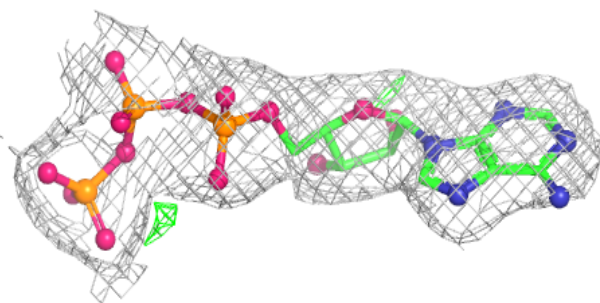
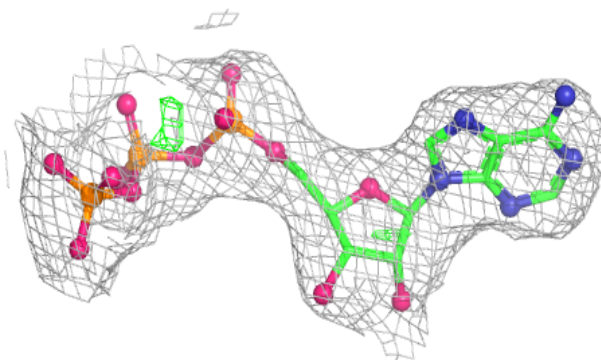
**Electron density around ATP H 701:**

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

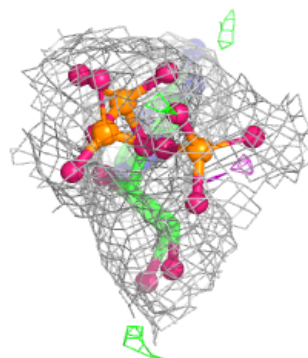
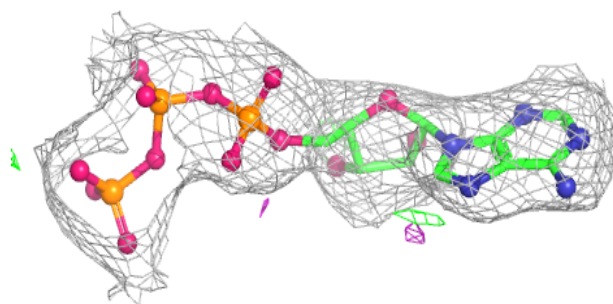
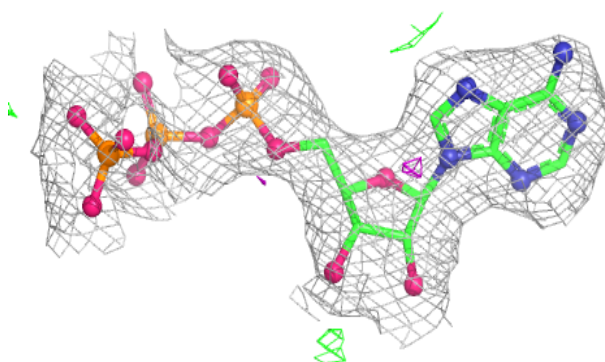


Electron density around ATP J 701:

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

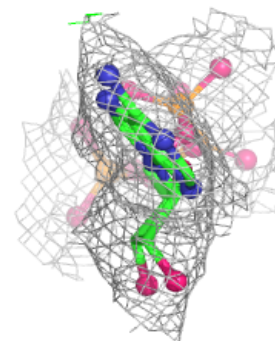
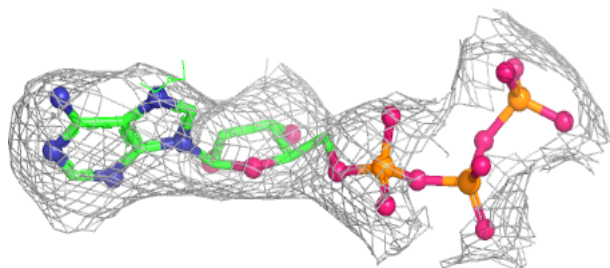
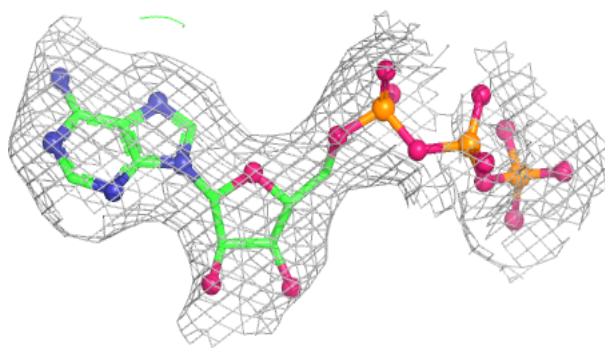
**Electron density around ATP E 701:**

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

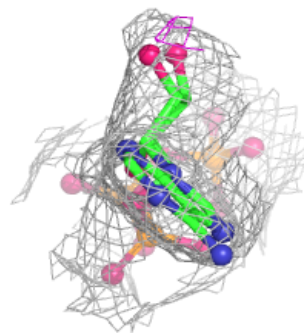
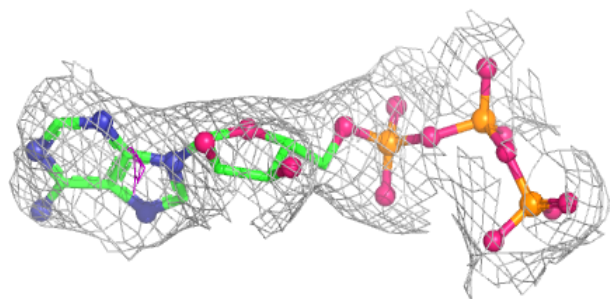
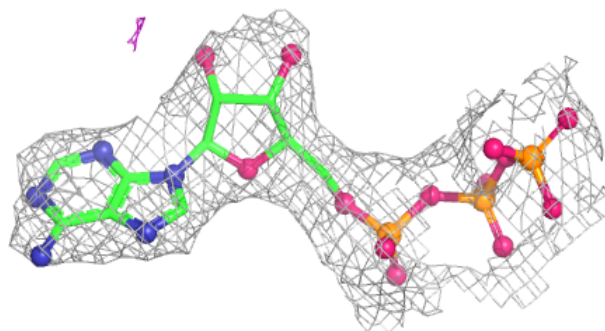


Electron density around ATP K 701:

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

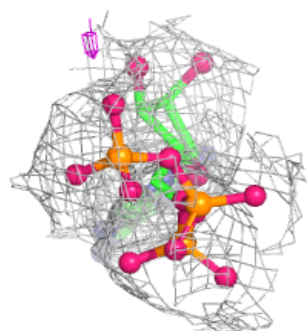
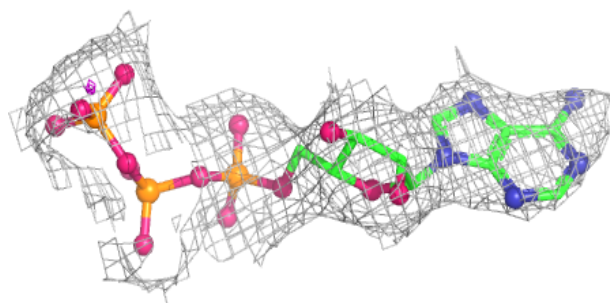
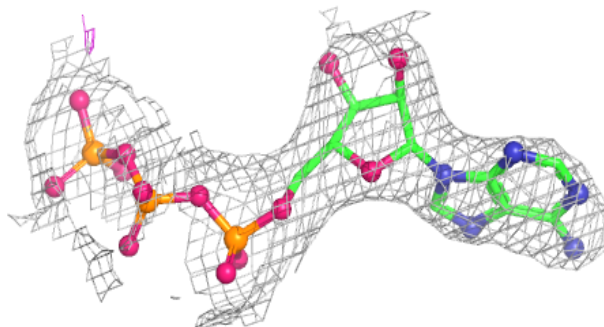
**Electron density around ATP A 701:**

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

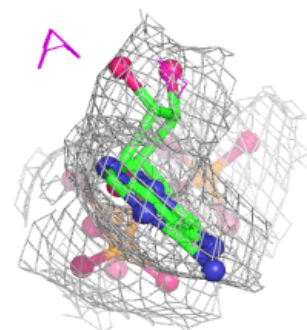
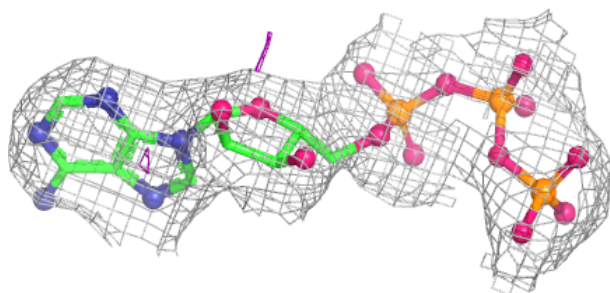
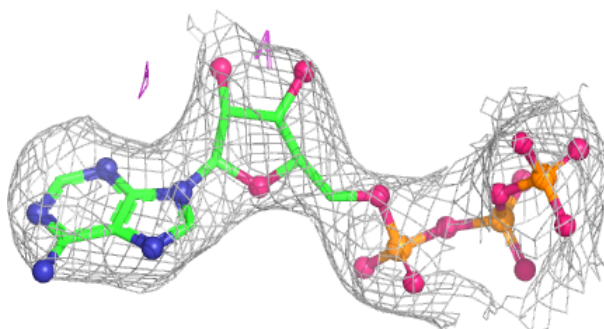


Electron density around ATP V 701:

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

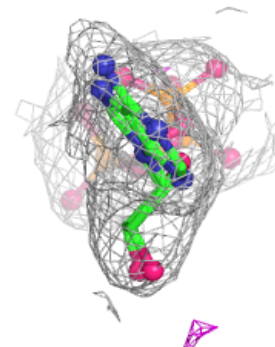
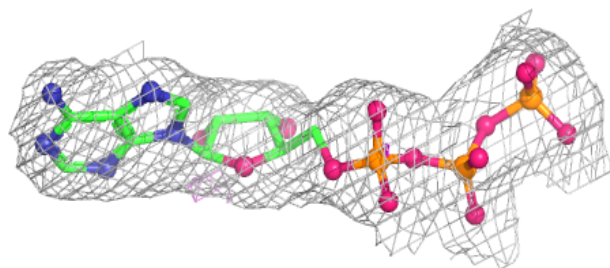
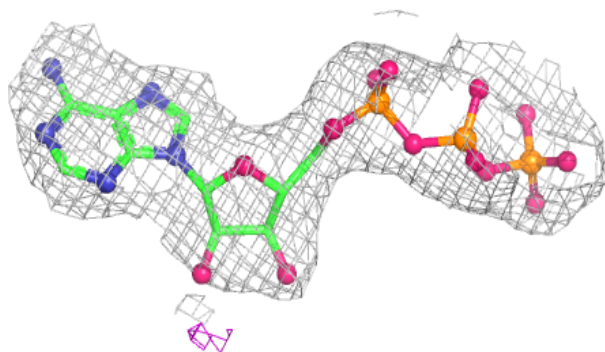
**Electron density around ATP C 701:**

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

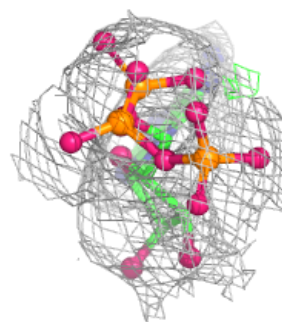
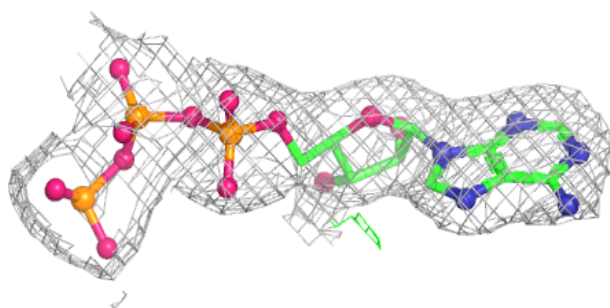
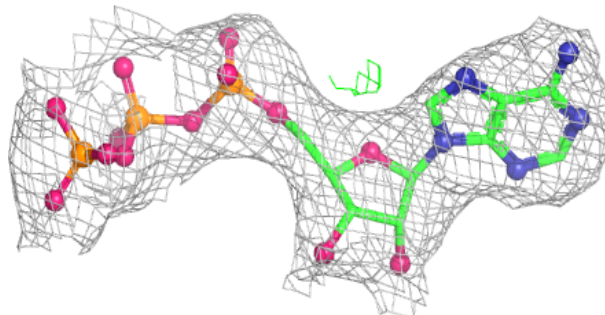


Electron density around ATP G 702:

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

**Electron density around ATP D 701:**

$2mF_o-DF_c$ (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.