



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 02:05 AM UTC

PDB ID : 9KQD / pdb_00009kqd
Title : YcfA-D19A-ATP-GTP complex
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Deposited on : 2024-11-25
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

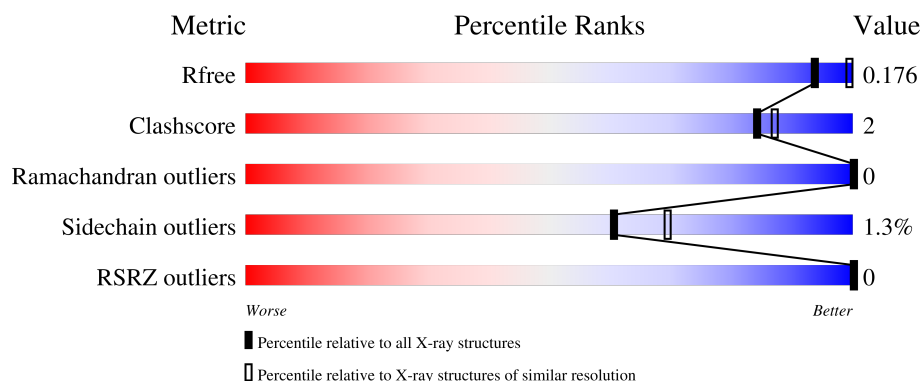
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

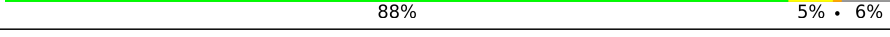
The reported resolution of this entry is 2.10 Å.

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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	234	 89% . . 5%
1	B	234	 87% 7% . 6%
1	C	234	 87% 6% . 6%
1	D	234	 88% 5% . 6%
1	E	234	 84% 9% . 5%

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Mol	Chain	Length	Quality of chain
1	F	234	 85% 7% • 6%
1	G	234	 85% 7% • 6%
1	H	234	 87% 6% • 6%
1	I	234	 88% 5% • 6%
1	J	234	 88% 5% • 5%
1	K	234	 86% 7% • 6%
1	L	234	 82% 9% • 7%
1	M	234	 82% 12% • 5%
1	N	234	 86% 7% • 6%

2 Entry composition

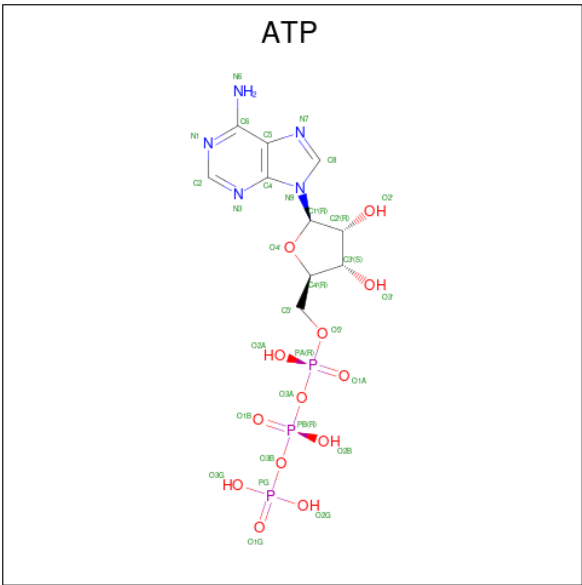
There are 5 unique types of molecules in this entry. The entry contains 27628 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Asparagine synthetase domain-containing protein.

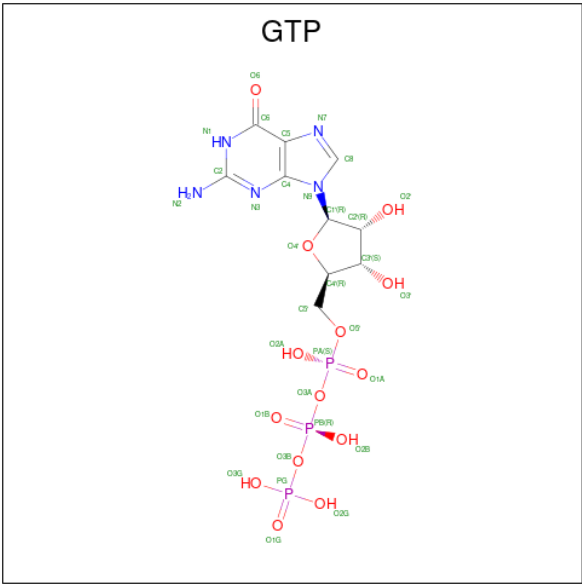
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	221	Total	C	N	O	S	0	0	0
			1735	1105	299	321	10			
1	D	220	Total	C	N	O	S	0	0	0
			1729	1102	298	319	10			
1	G	221	Total	C	N	O	S	0	0	0
			1735	1105	299	321	10			
1	I	221	Total	C	N	O	S	0	0	0
			1735	1105	299	321	10			
1	J	222	Total	C	N	O	S	0	0	0
			1742	1110	300	322	10			
1	K	221	Total	C	N	O	S	0	0	0
			1735	1105	299	321	10			
1	M	222	Total	C	N	O	S	0	0	0
			1742	1110	300	322	10			
1	A	222	Total	C	N	O	S	0	0	0
			1742	1110	300	322	10			
1	C	220	Total	C	N	O	S	0	0	0
			1729	1102	298	319	10			
1	E	222	Total	C	N	O	S	0	0	0
			1747	1114	300	323	10			
1	F	220	Total	C	N	O	S	0	0	0
			1729	1102	298	319	10			
1	H	221	Total	C	N	O	S	0	0	0
			1735	1105	299	321	10			
1	L	218	Total	C	N	O	S	0	0	0
			1711	1091	296	314	10			
1	N	221	Total	C	N	O	S	0	0	0
			1735	1105	299	321	10			

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	G	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	I	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	J	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	K	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	M	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	E	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	F	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	H	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	L	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	N	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	130	Total	O	0	0
			130	130		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	181	Total 181	O 181	0	0
5	G	176	Total 176	O 176	0	0
5	I	174	Total 174	O 174	0	0
5	J	242	Total 242	O 242	0	0
5	K	158	Total 158	O 158	0	0
5	M	154	Total 154	O 154	0	0
5	A	233	Total 233	O 233	0	0
5	C	173	Total 173	O 173	0	0
5	E	167	Total 167	O 167	0	0
5	F	185	Total 185	O 185	0	0
5	H	199	Total 199	O 199	0	0
5	L	140	Total 140	O 140	0	0
5	N	139	Total 139	O 139	0	0

3 Residue-property plots [i](#)

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: Asparagine synthetase domain-containing protein

Chain B:  87% 7% • 6%



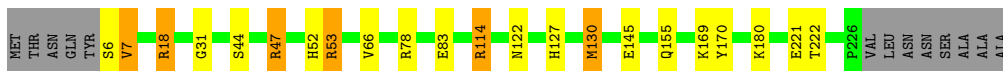
- Molecule 1: Asparagine synthetase domain-containing protein

Chain D:  88% 5% • 6%



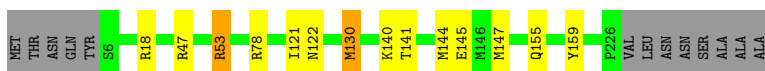
- Molecule 1: Asparagine synthetase domain-containing protein

Chain G:  85% 7% • 6%



- Molecule 1: Asparagine synthetase domain-containing protein

Chain I:  88% 5% • 6%



- Molecule 1: Asparagine synthetase domain-containing protein

Chain J:  88% 5% • 5%



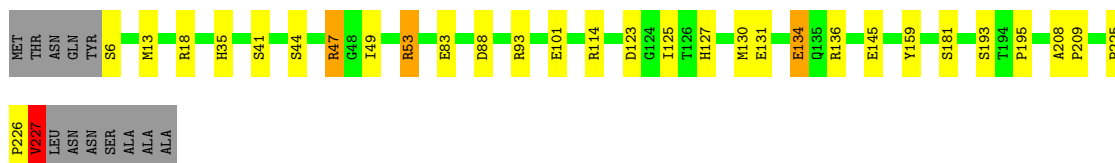
- Molecule 1: Asparagine synthetase domain-containing protein

Chain K:  86% 7% • 6%



- Molecule 1: Asparagine synthetase domain-containing protein

Chain M: 82% 12% 5%



- Molecule 1: Asparagine synthetase domain-containing protein

Chain A: 89% 5% 5%



- Molecule 1: Asparagine synthetase domain-containing protein

Chain C: 87% 6% 6%



- Molecule 1: Asparagine synthetase domain-containing protein

Chain E: 84% 9% 5%



- Molecule 1: Asparagine synthetase domain-containing protein

Chain F: 85% 7% 6%



- Molecule 1: Asparagine synthetase domain-containing protein

Chain H: 87% 6% 6%



- Molecule 1: Asparagine synthetase domain-containing protein

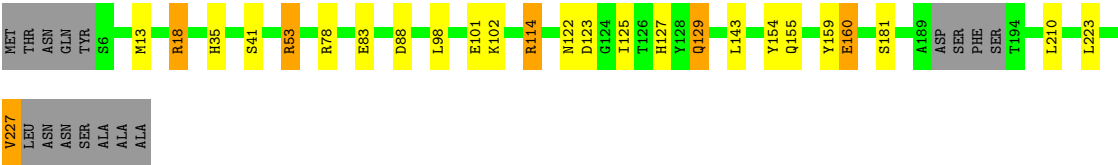
Chain L:

82%

9%

•

7%



● Molecule 1: Asparagine synthetase domain-containing protein

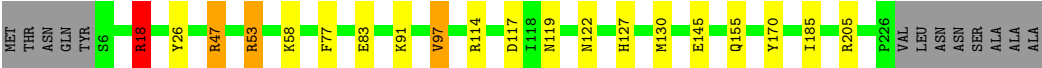
Chain N:

86%

7%

•

6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	74.16Å 135.09Å 234.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.89 – 2.10 48.89 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.89-2.10) 99.4 (48.89-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.166 , 0.192 (Not available) , 0.176	Depositor DCC
R_{free} test set	13266 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 34.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.487 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	27628	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GTP, 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	0.90	1/1777 (0.1%)	1.26	10/2406 (0.4%)
1	B	0.84	0/1770	1.20	10/2396 (0.4%)
1	C	0.81	1/1764 (0.1%)	1.17	12/2388 (0.5%)
1	D	0.87	1/1764 (0.1%)	1.23	12/2388 (0.5%)
1	E	0.85	0/1783	1.23	17/2414 (0.7%)
1	F	0.87	1/1764 (0.1%)	1.24	18/2388 (0.8%)
1	G	0.83	1/1770 (0.1%)	1.18	11/2396 (0.5%)
1	H	0.85	0/1770	1.19	13/2396 (0.5%)
1	I	0.80	0/1770	1.15	8/2396 (0.3%)
1	J	0.92	1/1777 (0.1%)	1.23	11/2406 (0.5%)
1	K	0.86	0/1770	1.26	12/2396 (0.5%)
1	L	0.96	1/1744 (0.1%)	1.37	13/2360 (0.6%)
1	M	0.96	0/1777	1.40	19/2406 (0.8%)
1	N	0.83	0/1770	1.22	9/2396 (0.4%)
All	All	0.87	7/24770 (0.0%)	1.24	175/33532 (0.5%)

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	A	0	2
1	B	0	2
1	C	0	3
1	D	0	4
1	E	0	5
1	F	0	4
1	G	0	5
1	H	0	4
1	I	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	3
1	K	0	2
1	L	0	4
1	M	0	1
1	N	0	4
All	All	0	46

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	46	HIS	CG-CD2	-8.25	1.26	1.35
1	A	41	SER	CB-OG	5.80	1.53	1.42
1	C	47	ARG	NE-CZ	5.67	1.39	1.33
1	J	41	SER	CB-OG	5.46	1.53	1.42
1	D	41	SER	CA-CB	5.16	1.62	1.53
1	L	53	ARG	NE-CZ	-5.08	1.27	1.33
1	G	52	HIS	CE1-NE2	5.04	1.37	1.32

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	53	ARG	CD-NE-CZ	12.97	142.56	124.40
1	K	53	ARG	CD-NE-CZ	12.89	142.44	124.40
1	N	91	LYS	CG-CD-CE	12.57	140.21	111.30
1	F	53	ARG	CD-NE-CZ	12.45	141.82	124.40
1	A	53	ARG	CD-NE-CZ	12.18	141.46	124.40
1	N	53	ARG	CD-NE-CZ	12.01	141.21	124.40
1	L	53	ARG	CD-NE-CZ	11.67	140.74	124.40
1	L	53	ARG	NE-CZ-NH2	-11.19	109.13	119.20
1	M	53	ARG	CD-NE-CZ	11.02	139.83	124.40
1	M	53	ARG	NE-CZ-NH2	-10.60	109.67	119.20
1	A	53	ARG	NE-CZ-NH2	-9.92	110.27	119.20
1	D	114	ARG	NE-CZ-NH1	-9.73	111.77	121.50
1	N	53	ARG	NE-CZ-NH2	-9.70	110.47	119.20
1	L	18	ARG	CB-CG-CD	-9.60	89.22	111.30
1	M	18	ARG	CB-CG-CD	-9.58	89.27	111.30
1	D	53	ARG	NE-CZ-NH2	-9.41	110.73	119.20
1	F	53	ARG	NE-CZ-NH2	-9.18	110.94	119.20
1	K	18	ARG	NH1-CZ-NH2	9.11	131.14	119.30
1	K	18	ARG	NE-CZ-NH1	-9.06	112.44	121.50
1	M	83	GLU	CG-CD-OE2	-8.73	98.33	118.40
1	K	53	ARG	NE-CZ-NH2	-8.53	111.52	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	83	GLU	CG-CD-OE1	8.48	137.90	118.40
1	I	130	MET	CG-SD-CE	8.45	119.50	100.90
1	H	226	PRO	CA-C-O	-8.38	93.86	119.00
1	F	7	VAL	N-CA-CB	8.31	125.63	111.50
1	D	114	ARG	NE-CZ-NH2	8.30	126.67	119.20
1	K	18	ARG	CB-CG-CD	-8.27	92.27	111.30
1	C	114	ARG	NE-CZ-NH2	7.82	126.23	119.20
1	B	83	GLU	CG-CD-OE2	-7.78	100.50	118.40
1	B	53	ARG	CD-NE-CZ	7.78	135.29	124.40
1	A	18	ARG	NE-CZ-NH1	-7.78	113.72	121.50
1	C	114	ARG	NE-CZ-NH1	-7.77	113.73	121.50
1	I	53	ARG	CD-NE-CZ	7.68	135.15	124.40
1	L	13	MET	CG-SD-CE	-7.54	84.31	100.90
1	B	83	GLU	CG-CD-OE1	7.51	135.68	118.40
1	G	130	MET	CA-CB-CG	7.50	129.09	114.10
1	J	53	ARG	CD-NE-CZ	7.46	134.85	124.40
1	J	53	ARG	NE-CZ-NH2	-7.40	112.54	119.20
1	J	18	ARG	NE-CZ-NH1	-7.38	114.12	121.50
1	E	53	ARG	CD-NE-CZ	7.36	134.71	124.40
1	C	53	ARG	CD-NE-CZ	7.31	134.64	124.40
1	H	47	ARG	NE-CZ-NH2	7.30	125.77	119.20
1	B	91	LYS	CG-CD-CE	7.26	128.01	111.30
1	E	18	ARG	CB-CG-CD	-7.25	94.63	111.30
1	E	145	GLU	CB-CG-CD	7.17	124.79	112.60
1	D	145	GLU	CB-CG-CD	7.12	124.70	112.60
1	F	18	ARG	CG-CD-NE	-7.03	96.55	112.00
1	G	53	ARG	CD-NE-CZ	7.01	134.22	124.40
1	K	114	ARG	NE-CZ-NH2	-6.95	112.94	119.20
1	N	47	ARG	CG-CD-NE	-6.94	96.74	112.00
1	E	18	ARG	CG-CD-NE	-6.91	96.79	112.00
1	A	47	ARG	CG-CD-NE	-6.90	96.81	112.00
1	H	53	ARG	CD-NE-CZ	6.90	134.06	124.40
1	N	18	ARG	NE-CZ-NH1	-6.84	114.66	121.50
1	E	47	ARG	NE-CZ-NH1	-6.81	114.69	121.50
1	M	13	MET	CG-SD-CE	-6.80	85.94	100.90
1	F	18	ARG	CB-CG-CD	-6.62	96.08	111.30
1	H	18	ARG	NE-CZ-NH1	-6.55	114.95	121.50
1	M	114	ARG	CB-CG-CD	6.47	126.17	111.30
1	F	83	GLU	CB-CG-CD	-6.43	101.67	112.60
1	D	55	GLU	CA-CB-CG	6.43	126.95	114.10
1	A	114	ARG	NE-CZ-NH2	-6.42	113.42	119.20
1	H	145	GLU	CB-CG-CD	6.42	123.51	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	53	ARG	NE-CZ-NH1	6.39	127.89	121.50
1	H	53	ARG	CG-CD-NE	-6.36	98.00	112.00
1	F	114	ARG	NE-CZ-NH2	-6.36	113.48	119.20
1	J	83	GLU	CB-CG-CD	-6.34	101.82	112.60
1	L	83	GLU	CG-CD-OE2	-6.33	103.84	118.40
1	E	18	ARG	NE-CZ-NH1	-6.30	115.20	121.50
1	A	18	ARG	NH1-CZ-NH2	6.30	127.48	119.30
1	F	52	HIS	CB-CG-CD2	-6.29	123.02	131.20
1	G	83	GLU	CB-CG-CD	-6.28	101.93	112.60
1	I	47	ARG	CD-NE-CZ	6.27	133.18	124.40
1	L	114	ARG	CB-CG-CD	-6.24	96.94	111.30
1	M	130	MET	CG-SD-CE	-6.21	87.23	100.90
1	H	53	ARG	NE-CZ-NH2	-6.18	113.64	119.20
1	G	52	HIS	CB-CG-CD2	-6.13	123.22	131.20
1	G	53	ARG	NE-CZ-NH2	-6.13	113.68	119.20
1	E	5	TYR	CB-CA-C	6.12	121.72	110.10
1	E	18	ARG	NH1-CZ-NH2	6.10	127.23	119.30
1	J	18	ARG	NH1-CZ-NH2	6.10	127.23	119.30
1	M	131	GLU	CG-CD-OE2	-6.08	104.42	118.40
1	E	53	ARG	CG-CD-NE	-6.08	98.64	112.00
1	B	53	ARG	CG-CD-NE	-6.07	98.65	112.00
1	M	193	SER	CA-C-O	6.06	127.97	121.55
1	N	53	ARG	NE-CZ-NH1	6.04	127.54	121.50
1	N	170	TYR	CB-CA-C	6.04	122.62	109.99
1	G	53	ARG	CG-CD-NE	-6.04	98.72	112.00
1	K	145	GLU	CB-CG-CD	6.03	122.86	112.60
1	B	53	ARG	NE-CZ-NH2	-6.01	113.79	119.20
1	C	145	GLU	CB-CG-CD	6.00	122.81	112.60
1	F	145	GLU	CB-CG-CD	6.00	122.80	112.60
1	K	131	GLU	CG-CD-OE1	-5.99	104.61	118.40
1	M	53	ARG	NE-CZ-NH1	5.98	127.48	121.50
1	B	145	GLU	CB-CG-CD	5.95	122.71	112.60
1	E	47	ARG	CG-CD-NE	-5.95	98.91	112.00
1	E	114	ARG	NE-CZ-NH2	-5.93	113.86	119.20
1	I	53	ARG	CG-CD-NE	-5.92	98.98	112.00
1	B	170	TYR	CB-CA-C	5.90	122.32	109.99
1	C	47	ARG	CA-C-N	5.90	126.64	120.03
1	C	47	ARG	C-N-CA	5.90	126.64	120.03
1	F	47	ARG	CG-CD-NE	-5.87	99.08	112.00
1	I	145	GLU	CB-CG-CD	5.87	122.57	112.60
1	H	114	ARG	NE-CZ-NH2	-5.86	113.92	119.20
1	M	47	ARG	NE-CZ-NH1	-5.85	115.65	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	18	ARG	NH1-CZ-NH2	5.85	126.91	119.30
1	C	130	MET	CG-SD-CE	5.83	113.73	100.90
1	G	47	ARG	CG-CD-NE	-5.83	99.17	112.00
1	J	170	TYR	CB-CA-C	5.82	122.15	109.99
1	J	53	ARG	CG-CD-NE	-5.77	99.31	112.00
1	F	170	TYR	CB-CA-C	5.76	122.02	109.99
1	C	170	TYR	CB-CA-C	5.75	122.00	109.99
1	A	149	GLN	CG-CD-NE2	-5.70	107.85	116.40
1	H	18	ARG	CG-CD-NE	-5.69	99.48	112.00
1	H	170	TYR	CB-CA-C	5.67	121.84	109.99
1	E	170	TYR	CB-CA-C	5.66	121.82	109.99
1	G	170	TYR	CB-CA-C	5.65	121.81	109.99
1	C	53	ARG	CG-CD-NE	-5.65	99.56	112.00
1	K	170	TYR	CB-CA-C	5.64	121.77	109.99
1	L	18	ARG	NE-CZ-NH1	-5.64	115.86	121.50
1	A	170	TYR	CB-CA-C	5.61	121.71	109.99
1	K	55	GLU	CB-CG-CD	5.61	122.13	112.60
1	M	145	GLU	CB-CG-CD	5.52	121.98	112.60
1	E	114	ARG	CB-CG-CD	-5.51	98.62	111.30
1	F	18	ARG	NH1-CZ-NH2	5.51	126.47	119.30
1	C	53	ARG	NE-CZ-NH2	-5.50	114.25	119.20
1	L	83	GLU	CG-CD-OE1	5.47	130.98	118.40
1	D	170	TYR	CB-CA-C	5.45	121.38	109.99
1	N	83	GLU	CB-CG-CD	-5.45	103.33	112.60
1	H	88	ASP	CA-CB-CG	5.45	118.05	112.60
1	E	5	TYR	N-CA-CB	-5.44	101.25	110.50
1	F	114	ARG	CB-CG-CD	-5.43	98.81	111.30
1	D	18	ARG	CG-CD-NE	-5.43	100.06	112.00
1	L	18	ARG	NH1-CZ-NH2	5.41	126.33	119.30
1	A	83	GLU	CB-CG-CD	-5.41	103.41	112.60
1	M	88	ASP	CA-CB-CG	5.40	118.00	112.60
1	J	149	GLN	CG-CD-NE2	-5.40	108.31	116.40
1	G	18	ARG	NE-CZ-NH1	-5.39	116.11	121.50
1	L	88	ASP	CA-CB-CG	5.39	117.99	112.60
1	E	53	ARG	NE-CZ-NH2	-5.38	114.36	119.20
1	F	88	ASP	CA-CB-CG	5.38	117.98	112.60
1	M	227	VAL	N-CA-CB	5.37	120.63	111.50
1	A	18	ARG	CG-CD-NE	-5.36	100.21	112.00
1	H	114	ARG	CB-CG-CD	-5.35	98.99	111.30
1	J	155	GLN	OE1-CD-NE2	-5.35	117.25	122.60
1	M	93	ARG	CB-CG-CD	5.32	123.55	111.30
1	F	7	VAL	CA-CB-CG1	5.31	119.43	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	47	ARG	CA-C-N	5.26	125.92	120.03
1	I	47	ARG	C-N-CA	5.26	125.92	120.03
1	K	114	ARG	CB-CG-CD	-5.26	99.19	111.30
1	E	5	TYR	CA-CB-CG	-5.25	104.45	113.90
1	D	167	ASP	CA-CB-CG	5.25	117.85	112.60
1	K	53	ARG	NE-CZ-NH1	5.25	126.75	121.50
1	D	52	HIS	CB-CG-CD2	-5.25	124.38	131.20
1	J	6	SER	CB-CA-C	5.24	120.05	110.10
1	L	129	GLN	CB-CG-CD	5.21	121.45	112.60
1	I	53	ARG	NE-CZ-NH2	-5.21	114.52	119.20
1	L	114	ARG	NE-CZ-NH2	-5.20	114.52	119.20
1	F	53	ARG	NE-CZ-NH1	5.19	126.69	121.50
1	B	114	ARG	CB-CG-CD	-5.17	99.41	111.30
1	M	131	GLU	CB-CA-C	5.13	119.57	110.85
1	F	18	ARG	NE-CZ-NH2	-5.13	114.58	119.20
1	B	18	ARG	NE-CZ-NH1	-5.13	116.37	121.50
1	C	146	MET	CG-SD-CE	-5.12	89.63	100.90
1	D	88	ASP	CA-CB-CG	5.12	117.72	112.60
1	G	114	ARG	CB-CG-CD	-5.11	99.55	111.30
1	C	52	HIS	CB-CG-CD2	-5.10	124.57	131.20
1	D	53	ARG	NE-CZ-NH1	5.08	126.58	121.50
1	N	145	GLU	CB-CG-CD	5.06	121.20	112.60
1	M	134	GLU	CG-CD-OE2	5.05	130.02	118.40
1	J	88	ASP	CA-CB-CG	5.04	117.64	112.60
1	G	18	ARG	CG-CD-NE	-5.04	100.92	112.00
1	E	88	ASP	CA-CB-CG	5.04	117.64	112.60
1	M	131	GLU	CG-CD-OE1	5.04	129.98	118.40
1	F	55	GLU	CB-CG-CD	5.01	121.12	112.60

There are no chirality outliers.

All (46) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	18	ARG	Sidechain
1	A	53	ARG	Sidechain
1	B	18	ARG	Sidechain
1	B	53	ARG	Sidechain
1	C	18	ARG	Sidechain
1	C	47	ARG	Sidechain
1	C	53	ARG	Sidechain
1	D	114	ARG	Sidechain
1	D	18	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	D	47	ARG	Sidechain
1	D	53	ARG	Sidechain
1	E	18	ARG	Sidechain
1	E	47	ARG	Sidechain
1	E	53	ARG	Sidechain
1	E	78	ARG	Sidechain
1	E	93	ARG	Sidechain
1	F	18	ARG	Sidechain
1	F	47	ARG	Sidechain
1	F	53	ARG	Sidechain
1	F	93	ARG	Sidechain
1	G	114	ARG	Sidechain
1	G	18	ARG	Sidechain
1	G	47	ARG	Sidechain
1	G	53	ARG	Sidechain
1	G	78	ARG	Sidechain
1	H	114	ARG	Sidechain
1	H	18	ARG	Sidechain
1	H	47	ARG	Sidechain
1	H	53	ARG	Sidechain
1	I	18	ARG	Sidechain
1	I	53	ARG	Sidechain
1	I	78	ARG	Sidechain
1	J	18	ARG	Sidechain
1	J	53	ARG	Sidechain
1	J	78	ARG	Sidechain
1	K	53	ARG	Sidechain
1	K	78	ARG	Sidechain
1	L	154	TYR	Sidechain
1	L	18	ARG	Sidechain
1	L	53	ARG	Sidechain
1	L	78	ARG	Sidechain
1	M	53	ARG	Sidechain
1	N	114	ARG	Sidechain
1	N	18	ARG	Sidechain
1	N	205	ARG	Sidechain
1	N	53	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1742	0	1740	5	0
1	B	1735	0	1731	9	0
1	C	1729	0	1726	7	0
1	D	1729	0	1726	1	0
1	E	1747	0	1740	12	1
1	F	1729	0	1726	6	0
1	G	1735	0	1731	10	3
1	H	1735	0	1731	5	1
1	I	1735	0	1731	8	0
1	J	1742	0	1740	3	0
1	K	1735	0	1731	10	0
1	L	1711	0	1716	16	0
1	M	1742	0	1740	16	0
1	N	1735	0	1731	10	0
2	A	31	0	12	0	0
2	B	31	0	12	0	0
2	C	31	0	12	0	0
2	D	31	0	12	0	0
2	E	31	0	12	0	0
2	F	31	0	12	0	0
2	G	31	0	12	0	0
2	H	31	0	12	0	0
2	I	31	0	12	0	0
2	J	31	0	12	0	0
2	K	31	0	12	0	0
2	L	31	0	12	1	0
2	M	31	0	12	1	0
2	N	31	0	12	0	0
3	A	32	0	12	0	0
3	B	32	0	12	1	0
3	C	32	0	12	0	1
3	D	32	0	12	0	0
3	E	32	0	12	0	0
3	F	32	0	12	0	0
3	G	32	0	12	0	0
3	H	32	0	12	0	0
3	I	32	0	12	1	0
3	J	32	0	12	0	3
3	K	32	0	12	0	0
3	L	32	0	12	1	0
3	M	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	32	0	12	0	1
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
5	A	233	0	0	3	0
5	B	130	0	0	3	0
5	C	173	0	0	1	0
5	D	181	0	0	0	0
5	E	167	0	0	1	0
5	F	185	0	0	4	0
5	G	176	0	0	3	0
5	H	199	0	0	3	0
5	I	174	0	0	2	0
5	J	242	0	0	2	0
5	K	158	0	0	1	0
5	L	140	0	0	6	0
5	M	154	0	0	7	0
5	N	139	0	0	6	0
All	All	27628	0	24576	116	5

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 2.

All (116) 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:M:47:ARG:HD3	5:M:515:HOH:O	1.27	1.31
1:J:63:ASP:HB2	5:J:581:HOH:O	1.40	1.17
1:K:141:THR:HA	1:K:144:MET:HE3	1.38	1.05
1:E:141:THR:HA	1:E:144:MET:HE3	1.37	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:141:THR:HA	1:I:144:MET:HE3	1.41	1.01
1:E:140:LYS:HG2	1:E:144:MET:HE2	1.51	0.90
1:K:140:LYS:HG2	1:K:144:MET:HE2	1.53	0.88
1:I:140:LYS:HG2	1:I:144:MET:HE2	1.55	0.87
1:H:226:PRO:HA	5:H:404:HOH:O	1.75	0.86
1:F:226:PRO:C	5:F:442:HOH:O	2.22	0.81
1:G:145:GLU:OE1	5:G:401:HOH:O	2.05	0.75
1:M:225:PRO:O	5:M:401:HOH:O	2.04	0.74
1:E:144:MET:HE1	5:E:452:HOH:O	1.89	0.72
1:F:87:GLN:HG3	5:F:505:HOH:O	1.89	0.71
1:M:125:ILE:HG22	1:M:159:TYR:CD1	2.26	0.70
1:L:181:SER:OG	2:L:301:ATP:O1G	2.10	0.69
1:M:6:SER:N	5:M:402:HOH:O	2.26	0.68
1:L:125:ILE:HG22	1:L:159:TYR:CD1	2.29	0.67
1:N:47:ARG:HD3	5:N:511:HOH:O	1.96	0.65
1:B:47:ARG:NH1	5:B:402:HOH:O	2.27	0.63
1:K:144:MET:HE1	5:K:418:HOH:O	1.97	0.62
1:G:127:HIS:O	1:G:130:MET:HG2	1.99	0.62
1:G:6:SER:HB2	5:G:533:HOH:O	1.99	0.62
1:I:141:THR:HA	1:I:144:MET:CE	2.26	0.61
1:F:129:GLN:NE2	5:F:403:HOH:O	2.32	0.59
1:H:149:GLN:NE2	5:H:403:HOH:O	2.35	0.59
1:I:144:MET:HE1	5:I:484:HOH:O	2.03	0.58
1:M:181:SER:OG	2:M:301:ATP:O2G	2.12	0.58
1:K:141:THR:HA	1:K:144:MET:CE	2.24	0.57
1:M:35:HIS:HB2	5:M:502:HOH:O	2.06	0.56
1:G:127:HIS:HA	1:G:130:MET:HE3	1.89	0.55
1:L:125:ILE:HG22	1:L:159:TYR:HD1	1.70	0.54
1:N:119:ASN:HB3	5:N:416:HOH:O	2.06	0.54
3:B:302:GTP:O2A	5:B:401:HOH:O	2.18	0.54
1:M:125:ILE:HG22	1:M:159:TYR:HD1	1.72	0.54
1:C:121:ILE:HD13	1:C:147:MET:HE2	1.89	0.54
1:C:103:LEU:HD11	1:C:146:MET:HE1	1.88	0.53
1:E:141:THR:HA	1:E:144:MET:CE	2.24	0.53
1:B:26:TYR:CE1	1:K:223:LEU:HD13	2.45	0.52
1:L:35:HIS:HB2	5:L:479:HOH:O	2.08	0.52
1:A:49:ILE:HG23	5:A:536:HOH:O	2.09	0.52
1:C:130:MET:HE2	1:C:159:TYR:OH	2.10	0.52
1:I:121:ILE:HD13	1:I:147:MET:HE2	1.91	0.51
1:B:47:ARG:NH2	5:B:402:HOH:O	2.44	0.51
1:K:141:THR:CA	1:K:144:MET:HE3	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:141:THR:CA	1:E:144:MET:HE3	2.26	0.50
1:L:129:GLN:HB2	5:L:448:HOH:O	2.10	0.50
1:M:134:GLU:OE1	3:M:302:GTP:N2	2.30	0.50
1:L:114:ARG:O	5:L:401:HOH:O	2.19	0.49
1:A:129:GLN:HE21	1:A:129:GLN:HA	1.77	0.49
1:L:129:GLN:HE21	1:L:129:GLN:HA	1.76	0.49
1:N:58:LYS:NZ	5:N:406:HOH:O	2.33	0.49
1:J:49:ILE:HG23	5:J:553:HOH:O	2.13	0.49
1:L:41:SER:HB3	1:L:101:GLU:OE2	2.14	0.48
1:L:123:ASP:OD2	1:L:125:ILE:CD1	2.62	0.48
1:E:102:LYS:HE3	1:E:106:HIS:NE2	2.29	0.47
1:G:6:SER:CB	5:G:533:HOH:O	2.59	0.47
1:L:125:ILE:HA	5:L:448:HOH:O	2.14	0.47
1:E:223:LEU:HD13	1:N:26:TYR:CD1	2.49	0.47
1:N:77:PHE:CZ	1:N:97:VAL:HG13	2.49	0.46
1:B:26:TYR:CD1	1:K:223:LEU:HD13	2.49	0.46
1:H:83:GLU:OE2	5:H:401:HOH:O	2.20	0.46
1:M:136:ARG:NH2	1:M:195:PRO:HD2	2.31	0.46
1:E:223:LEU:HD13	1:N:26:TYR:CE1	2.52	0.45
1:L:160:GLU:HG3	5:L:492:HOH:O	2.15	0.45
1:B:35:HIS:HE1	1:B:69:THR:OG1	1.99	0.45
1:M:41:SER:HB3	1:M:101:GLU:OE1	2.17	0.45
1:A:47:ARG:HD3	5:A:551:HOH:O	2.16	0.45
1:N:18:ARG:HD3	5:N:413:HOH:O	2.16	0.44
1:K:102:LYS:HE3	1:K:106:HIS:NE2	2.32	0.44
1:I:130:MET:HE3	1:I:159:TYR:CZ	2.53	0.44
1:M:47:ARG:NH1	5:M:404:HOH:O	2.36	0.43
1:B:35:HIS:CE1	1:B:69:THR:OG1	2.70	0.43
1:B:41:SER:HB3	1:B:101:GLU:OE2	2.19	0.43
1:B:129:GLN:HE21	1:B:129:GLN:HA	1.83	0.43
1:C:103:LEU:CD1	1:C:146:MET:HE1	2.48	0.43
1:M:49:ILE:HG23	5:M:514:HOH:O	2.18	0.43
3:I:302:GTP:O1A	5:I:401:HOH:O	2.21	0.42
1:N:122:ASN:HA	1:N:155:GLN:O	2.18	0.42
1:B:122:ASN:HA	1:B:155:GLN:O	2.18	0.42
1:I:122:ASN:HA	1:I:155:GLN:O	2.20	0.42
1:M:226:PRO:O	1:M:227:VAL:HB	2.20	0.42
1:C:83:GLU:OE1	5:C:401:HOH:O	2.22	0.42
1:G:7:VAL:HG11	1:G:31:GLY:O	2.20	0.42
1:J:122:ASN:HA	1:J:155:GLN:O	2.20	0.42
1:A:122:ASN:HA	1:A:155:GLN:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:ILE:CD1	1:C:147:MET:HE2	2.48	0.42
1:G:221:GLU:O	1:G:222:THR:HG23	2.20	0.42
1:A:47:ARG:HD2	5:A:452:HOH:O	2.19	0.42
1:E:41:SER:HB3	1:E:101:GLU:OE1	2.20	0.42
1:N:119:ASN:ND2	5:N:416:HOH:O	2.53	0.42
1:E:122:ASN:HA	1:E:155:GLN:O	2.19	0.41
1:F:52:HIS:HE1	5:F:449:HOH:O	2.02	0.41
1:L:227:VAL:C	5:L:408:HOH:O	2.62	0.41
1:N:117:ASP:N	5:N:415:HOH:O	2.52	0.41
1:K:122:ASN:HA	1:K:155:GLN:O	2.19	0.41
1:H:122:ASN:HA	1:H:155:GLN:O	2.20	0.41
1:L:129:GLN:HA	1:L:129:GLN:NE2	2.35	0.41
1:D:122:ASN:HA	1:D:155:GLN:O	2.20	0.41
1:G:122:ASN:HA	1:G:155:GLN:O	2.20	0.41
1:C:122:ASN:HA	1:C:155:GLN:O	2.20	0.41
1:M:208:ALA:HB3	1:M:209:PRO:HD3	2.02	0.41
1:L:122:ASN:HA	1:L:155:GLN:O	2.20	0.41
1:F:122:ASN:HA	1:F:155:GLN:O	2.21	0.41
1:M:136:ARG:HD3	5:M:492:HOH:O	2.21	0.41
1:F:41:SER:HB3	1:F:101:GLU:OE1	2.20	0.41
1:L:102:LYS:HD2	1:L:143:LEU:HD13	2.02	0.41
1:I:141:THR:CA	1:I:144:MET:HE3	2.30	0.41
1:M:123:ASP:OD2	1:M:125:ILE:HG12	2.21	0.41
1:G:221:GLU:O	1:G:222:THR:CG2	2.69	0.40
1:E:77:PHE:CZ	1:E:97:VAL:HG13	2.56	0.40
1:G:130:MET:HE2	1:G:130:MET:HB3	1.82	0.40
1:L:98:LEU:HD12	3:L:302:GTP:N2	2.36	0.40
1:K:208:ALA:HB3	1:K:209:PRO:HD3	2.03	0.40
1:E:208:ALA:HB3	1:E:209:PRO:HD3	2.03	0.40
1:H:208:ALA:HB3	1:H:209:PRO:HD3	2.03	0.40

All (5) 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)
1:G:180:LYS:NZ	3:J:302:GTP:O1G[2_657]	1.00	1.20
1:H:180:LYS:NZ	3:C:302:GTP:O2G[2_358]	1.67	0.53
1:E:180:LYS:NZ	3:N:302:GTP:O1G[2_358]	1.70	0.50
1:G:169:LYS:NZ	3:J:302:GTP:O2B[2_657]	2.08	0.12
1:G:180:LYS:CE	3:J:302:GTP:O1G[2_657]	2.13	0.07

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	220/234 (94%)	219 (100%)	1 (0%)	0	100	100
1	B	219/234 (94%)	218 (100%)	1 (0%)	0	100	100
1	C	218/234 (93%)	217 (100%)	1 (0%)	0	100	100
1	D	218/234 (93%)	217 (100%)	1 (0%)	0	100	100
1	E	220/234 (94%)	219 (100%)	1 (0%)	0	100	100
1	F	218/234 (93%)	217 (100%)	1 (0%)	0	100	100
1	G	219/234 (94%)	218 (100%)	1 (0%)	0	100	100
1	H	219/234 (94%)	218 (100%)	1 (0%)	0	100	100
1	I	219/234 (94%)	218 (100%)	1 (0%)	0	100	100
1	J	220/234 (94%)	219 (100%)	1 (0%)	0	100	100
1	K	219/234 (94%)	218 (100%)	1 (0%)	0	100	100
1	L	214/234 (92%)	213 (100%)	1 (0%)	0	100	100
1	M	220/234 (94%)	218 (99%)	2 (1%)	0	100	100
1	N	219/234 (94%)	218 (100%)	1 (0%)	0	100	100
All	All	3062/3276 (94%)	3047 (100%)	15 (0%)	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	190/200 (95%)	189 (100%)	1 (0%)	81	88
1	B	189/200 (94%)	187 (99%)	2 (1%)	65	74
1	C	188/200 (94%)	187 (100%)	1 (0%)	81	88
1	D	188/200 (94%)	187 (100%)	1 (0%)	81	88
1	E	190/200 (95%)	188 (99%)	2 (1%)	65	74
1	F	188/200 (94%)	184 (98%)	4 (2%)	47	54
1	G	189/200 (94%)	186 (98%)	3 (2%)	55	64
1	H	189/200 (94%)	186 (98%)	3 (2%)	55	64
1	I	189/200 (94%)	189 (100%)	0	100	100
1	J	190/200 (95%)	188 (99%)	2 (1%)	65	74
1	K	189/200 (94%)	185 (98%)	4 (2%)	47	54
1	L	186/200 (93%)	181 (97%)	5 (3%)	39	45
1	M	190/200 (95%)	187 (98%)	3 (2%)	55	64
1	N	189/200 (94%)	185 (98%)	4 (2%)	47	54
All	All	2644/2800 (94%)	2609 (99%)	35 (1%)	61	69

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	127	HIS
1	B	130	MET
1	D	160	GLU
1	G	7	VAL
1	G	44	SER
1	G	66	VAL
1	J	93	ARG
1	J	131	GLU
1	K	55	GLU
1	K	127	HIS
1	K	130	MET
1	K	223	LEU
1	M	44	SER
1	M	127	HIS
1	M	227	VAL
1	A	93	ARG
1	C	93	ARG
1	E	130	MET
1	E	223	LEU

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Mol	Chain	Res	Type
1	F	7	VAL
1	F	44	SER
1	F	55	GLU
1	F	130	MET
1	H	130	MET
1	H	160	GLU
1	H	210	LEU
1	L	127	HIS
1	L	160	GLU
1	L	210	LEU
1	L	223	LEU
1	L	227	VAL
1	N	97	VAL
1	N	127	HIS
1	N	130	MET
1	N	185	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	35	HIS
1	B	59	ASN
1	B	129	GLN
1	D	10	GLN
1	D	30	GLN
1	D	52	HIS
1	D	122	ASN
1	D	127	HIS
1	D	163	GLN
1	G	52	HIS
1	G	127	HIS
1	J	10	GLN
1	J	122	ASN
1	K	10	GLN
1	K	122	ASN
1	K	129	GLN
1	K	163	GLN
1	A	10	GLN
1	A	122	ASN
1	A	129	GLN
1	A	155	GLN
1	C	52	HIS

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Mol	Chain	Res	Type
1	C	127	HIS
1	E	10	GLN
1	E	122	ASN
1	F	52	HIS
1	F	87	GLN
1	F	127	HIS
1	H	10	GLN
1	H	122	ASN
1	H	127	HIS
1	H	149	GLN
1	L	10	GLN
1	L	52	HIS
1	L	122	ASN
1	L	127	HIS
1	L	129	GLN
1	N	127	HIS
1	N	163	GLN

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 42 ligands modelled in this entry, 14 are monoatomic - leaving 28 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	M	301	4	32,33,33	0.66	1 (3%)	48,52,52	0.63	0
3	GTP	H	302	-	33,34,34	0.59	0	50,54,54	0.53	0
3	GTP	L	302	-	33,34,34	1.24	4 (12%)	50,54,54	1.32	7 (14%)
3	GTP	J	302	-	33,34,34	0.59	0	50,54,54	0.58	0
2	ATP	B	301	4	32,33,33	0.60	0	48,52,52	0.58	0
3	GTP	N	302	-	33,34,34	0.57	0	50,54,54	0.56	0
3	GTP	M	302	-	33,34,34	0.93	1 (3%)	50,54,54	1.41	7 (14%)
2	ATP	A	301	4	32,33,33	0.61	0	48,52,52	0.57	0
3	GTP	B	302	-	33,34,34	0.94	1 (3%)	50,54,54	1.17	5 (10%)
2	ATP	D	301	4	32,33,33	0.62	0	48,52,52	0.54	0
2	ATP	K	301	4	32,33,33	0.61	0	48,52,52	0.62	0
3	GTP	K	302	-	33,34,34	0.59	0	50,54,54	0.59	0
2	ATP	G	301	4	32,33,33	0.60	0	48,52,52	0.56	0
2	ATP	J	301	4	32,33,33	0.61	0	48,52,52	0.60	0
2	ATP	I	301	4	32,33,33	0.63	0	48,52,52	0.55	0
3	GTP	F	302	-	33,34,34	0.58	0	50,54,54	0.57	0
2	ATP	C	301	4	32,33,33	0.61	0	48,52,52	0.62	0
2	ATP	L	301	4	32,33,33	0.61	0	48,52,52	0.69	0
3	GTP	D	302	-	33,34,34	0.57	0	50,54,54	0.58	0
3	GTP	G	302	-	33,34,34	0.56	0	50,54,54	0.57	0
3	GTP	I	302	-	33,34,34	0.54	0	50,54,54	0.55	0
2	ATP	N	301	4	32,33,33	0.60	0	48,52,52	0.59	0
3	GTP	A	302	-	33,34,34	0.56	0	50,54,54	0.60	0
2	ATP	E	301	4	32,33,33	0.60	0	48,52,52	0.62	0
2	ATP	H	301	4	32,33,33	0.63	0	48,52,52	0.54	0
3	GTP	E	302	-	33,34,34	0.58	0	50,54,54	0.55	0
2	ATP	F	301	4	32,33,33	0.60	0	48,52,52	0.58	0
3	GTP	C	302	-	33,34,34	0.56	0	50,54,54	0.52	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
2	ATP	M	301	4	-	4/22/38/38	0/3/3/3
3	GTP	H	302	-	-	2/22/38/38	0/3/3/3
3	GTP	L	302	-	-	5/22/38/38	0/3/3/3
3	GTP	J	302	-	-	2/22/38/38	0/3/3/3
2	ATP	B	301	4	-	4/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GTP	N	302	-	-	2/22/38/38	0/3/3/3
3	GTP	M	302	-	-	2/22/38/38	0/3/3/3
2	ATP	A	301	4	-	4/22/38/38	0/3/3/3
3	GTP	B	302	-	-	4/22/38/38	0/3/3/3
2	ATP	D	301	4	-	2/22/38/38	0/3/3/3
2	ATP	K	301	4	-	6/22/38/38	0/3/3/3
3	GTP	K	302	-	-	1/22/38/38	0/3/3/3
2	ATP	G	301	4	-	6/22/38/38	0/3/3/3
2	ATP	J	301	4	-	7/22/38/38	0/3/3/3
2	ATP	I	301	4	-	4/22/38/38	0/3/3/3
3	GTP	F	302	-	-	1/22/38/38	0/3/3/3
2	ATP	C	301	4	-	5/22/38/38	0/3/3/3
2	ATP	L	301	4	-	6/22/38/38	0/3/3/3
3	GTP	D	302	-	-	0/22/38/38	0/3/3/3
3	GTP	G	302	-	-	2/22/38/38	0/3/3/3
3	GTP	I	302	-	-	1/22/38/38	0/3/3/3
2	ATP	N	301	4	-	7/22/38/38	0/3/3/3
3	GTP	A	302	-	-	0/22/38/38	0/3/3/3
2	ATP	E	301	4	-	6/22/38/38	0/3/3/3
2	ATP	H	301	4	-	2/22/38/38	0/3/3/3
3	GTP	E	302	-	-	1/22/38/38	0/3/3/3
2	ATP	F	301	4	-	5/22/38/38	0/3/3/3
3	GTP	C	302	-	-	1/22/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	302	GTP	PA-O3A	4.25	1.64	1.59
3	B	302	GTP	PA-O3A	3.31	1.63	1.59
3	L	302	GTP	PB-O3A	2.75	1.62	1.59
3	L	302	GTP	PG-O1G	2.48	1.58	1.50
3	M	302	GTP	PA-O3A	2.45	1.62	1.59
3	L	302	GTP	PB-O3B	2.25	1.61	1.59
2	M	301	ATP	PG-O2G	-2.15	1.46	1.54

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	302	GTP	O2B-PB-O3A	3.88	117.75	107.27
3	M	302	GTP	O2A-PA-O3A	-3.58	97.60	107.27
3	L	302	GTP	O3A-PB-O1B	-3.54	100.06	110.70
3	M	302	GTP	C3'-C2'-C1'	3.06	107.25	101.46
3	B	302	GTP	O3'-C3'-C4'	-2.93	102.66	111.08
3	M	302	GTP	C2'-C1'-N9	2.79	121.03	113.25
3	L	302	GTP	O3B-PB-O1B	-2.69	102.60	110.70
3	M	302	GTP	C4'-O4'-C1'	2.61	115.24	109.47
3	M	302	GTP	O2A-PA-O1A	2.57	124.42	112.44
3	L	302	GTP	O3A-PA-O1A	-2.55	103.04	110.70
3	B	302	GTP	O2A-PA-O1A	2.54	124.27	112.44
3	M	302	GTP	O3B-PG-O1G	-2.47	98.07	111.04
3	M	302	GTP	O3'-C3'-C2'	2.45	119.68	111.82
3	B	302	GTP	O3A-PB-O1B	-2.41	103.46	110.70
3	L	302	GTP	O3G-PG-O2G	2.29	116.40	107.80
3	B	302	GTP	C1'-N9-C8	2.29	133.22	126.73
3	L	302	GTP	C3'-C2'-C1'	2.28	105.78	101.46
3	B	302	GTP	O2B-PB-O3A	2.25	113.35	107.27
3	L	302	GTP	O2A-PA-O1A	2.22	122.78	112.44

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	ATP	PB-O3B-PG-O3G
2	D	301	ATP	PB-O3B-PG-O2G
2	G	301	ATP	PB-O3B-PG-O3G
2	J	301	ATP	PB-O3B-PG-O3G
2	K	301	ATP	PB-O3B-PG-O2G
2	A	301	ATP	PB-O3B-PG-O3G
2	C	301	ATP	PB-O3B-PG-O3G
2	E	301	ATP	PB-O3B-PG-O3G
2	F	301	ATP	PB-O3B-PG-O3G
2	H	301	ATP	PB-O3B-PG-O3G
2	L	301	ATP	PB-O3B-PG-O2G
2	L	301	ATP	PB-O3B-PG-O3G
2	N	301	ATP	PB-O3B-PG-O2G
3	L	302	GTP	PB-O3B-PG-O3G
3	B	302	GTP	O4'-C4'-C5'-O5'
3	M	302	GTP	O4'-C4'-C5'-O5'
2	M	301	ATP	C3'-C4'-C5'-O5'
2	F	301	ATP	O4'-C4'-C5'-O5'
2	L	301	ATP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	J	301	ATP	O4'-C4'-C5'-O5'
2	J	301	ATP	C3'-C4'-C5'-O5'
2	M	301	ATP	O4'-C4'-C5'-O5'
2	F	301	ATP	C3'-C4'-C5'-O5'
2	L	301	ATP	O4'-C4'-C5'-O5'
2	N	301	ATP	O4'-C4'-C5'-O5'
2	N	301	ATP	C3'-C4'-C5'-O5'
3	M	302	GTP	C3'-C4'-C5'-O5'
2	B	301	ATP	O4'-C4'-C5'-O5'
2	B	301	ATP	C3'-C4'-C5'-O5'
2	K	301	ATP	O4'-C4'-C5'-O5'
2	E	301	ATP	C3'-C4'-C5'-O5'
3	B	302	GTP	C3'-C4'-C5'-O5'
2	K	301	ATP	C3'-C4'-C5'-O5'
2	E	301	ATP	O4'-C4'-C5'-O5'
3	J	302	GTP	PB-O3B-PG-O1G
2	C	301	ATP	O4'-C4'-C5'-O5'
3	J	302	GTP	PA-O3A-PB-O1B
3	N	302	GTP	O4'-C4'-C5'-O5'
2	M	301	ATP	PB-O3B-PG-O3G
3	L	302	GTP	PB-O3B-PG-O2G
3	B	302	GTP	PG-O3B-PB-O1B
3	E	302	GTP	PA-O3A-PB-O1B
2	C	301	ATP	C3'-C4'-C5'-O5'
2	M	301	ATP	C4'-C5'-O5'-PA
2	L	301	ATP	C4'-C5'-O5'-PA
2	G	301	ATP	PA-O3A-PB-O1B
3	B	302	GTP	PA-O3A-PB-O1B
3	G	302	GTP	PG-O3B-PB-O2B
3	L	302	GTP	PG-O3B-PB-O2B
2	E	301	ATP	C4'-C5'-O5'-PA
2	I	301	ATP	PB-O3B-PG-O1G
2	F	301	ATP	C4'-C5'-O5'-PA
2	G	301	ATP	PA-O3A-PB-O2B
2	A	301	ATP	PA-O3A-PB-O1B
2	C	301	ATP	C4'-C5'-O5'-PA
2	N	301	ATP	C4'-C5'-O5'-PA
2	L	301	ATP	PB-O3B-PG-O1G
2	N	301	ATP	PB-O3B-PG-O1G
3	L	302	GTP	PB-O3B-PG-O1G
2	D	301	ATP	PB-O3B-PG-O3G
2	G	301	ATP	PB-O3B-PG-O2G

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Mol	Chain	Res	Type	Atoms
2	I	301	ATP	PB-O3B-PG-O2G
2	I	301	ATP	PB-O3B-PG-O3G
2	J	301	ATP	PB-O3B-PG-O2G
2	K	301	ATP	PB-O3B-PG-O3G
2	A	301	ATP	PB-O3B-PG-O2G
2	C	301	ATP	PB-O3B-PG-O2G
2	E	301	ATP	PB-O3B-PG-O2G
2	F	301	ATP	PB-O3B-PG-O2G
2	H	301	ATP	PB-O3B-PG-O2G
2	B	301	ATP	C4'-C5'-O5'-PA
2	K	301	ATP	C4'-C5'-O5'-PA
3	I	302	GTP	O4'-C4'-C5'-O5'
3	H	302	GTP	PA-O3A-PB-O3B
2	A	301	ATP	PA-O3A-PB-O2B
2	N	301	ATP	PB-O3A-PA-O1A
2	N	301	ATP	PB-O3A-PA-O2A
3	G	302	GTP	PG-O3B-PB-O1B
3	K	302	GTP	PB-O3A-PA-O1A
3	H	302	GTP	PA-O3A-PB-O1B
3	N	302	GTP	PG-O3B-PB-O2B
2	J	301	ATP	C4'-C5'-O5'-PA
2	G	301	ATP	PB-O3B-PG-O1G
2	K	301	ATP	PB-O3B-PG-O1G
2	E	301	ATP	PB-O3B-PG-O1G
2	G	301	ATP	PB-O3A-PA-O2A
2	I	301	ATP	PB-O3A-PA-O2A
2	J	301	ATP	PB-O3A-PA-O1A
2	J	301	ATP	PB-O3A-PA-O2A
3	C	302	GTP	PG-O3B-PB-O2B
3	F	302	GTP	PB-O3A-PA-O2A
3	L	302	GTP	PG-O3B-PB-O1B

There are no ring outliers.

9 monomers are involved in 11 short contacts:

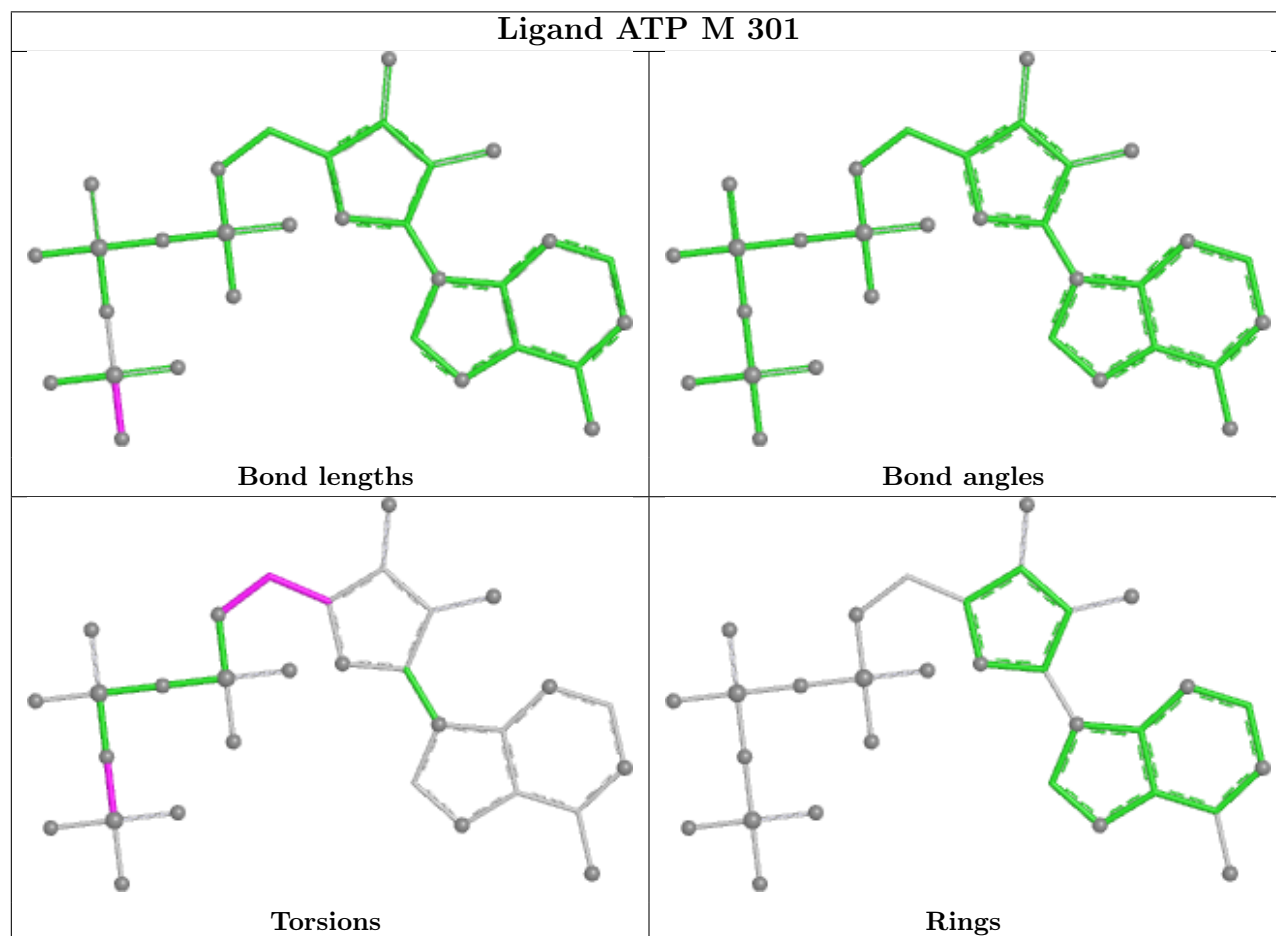
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	301	ATP	1	0
3	L	302	GTP	1	0
3	J	302	GTP	0	3
3	N	302	GTP	0	1
3	M	302	GTP	1	0
3	B	302	GTP	1	0

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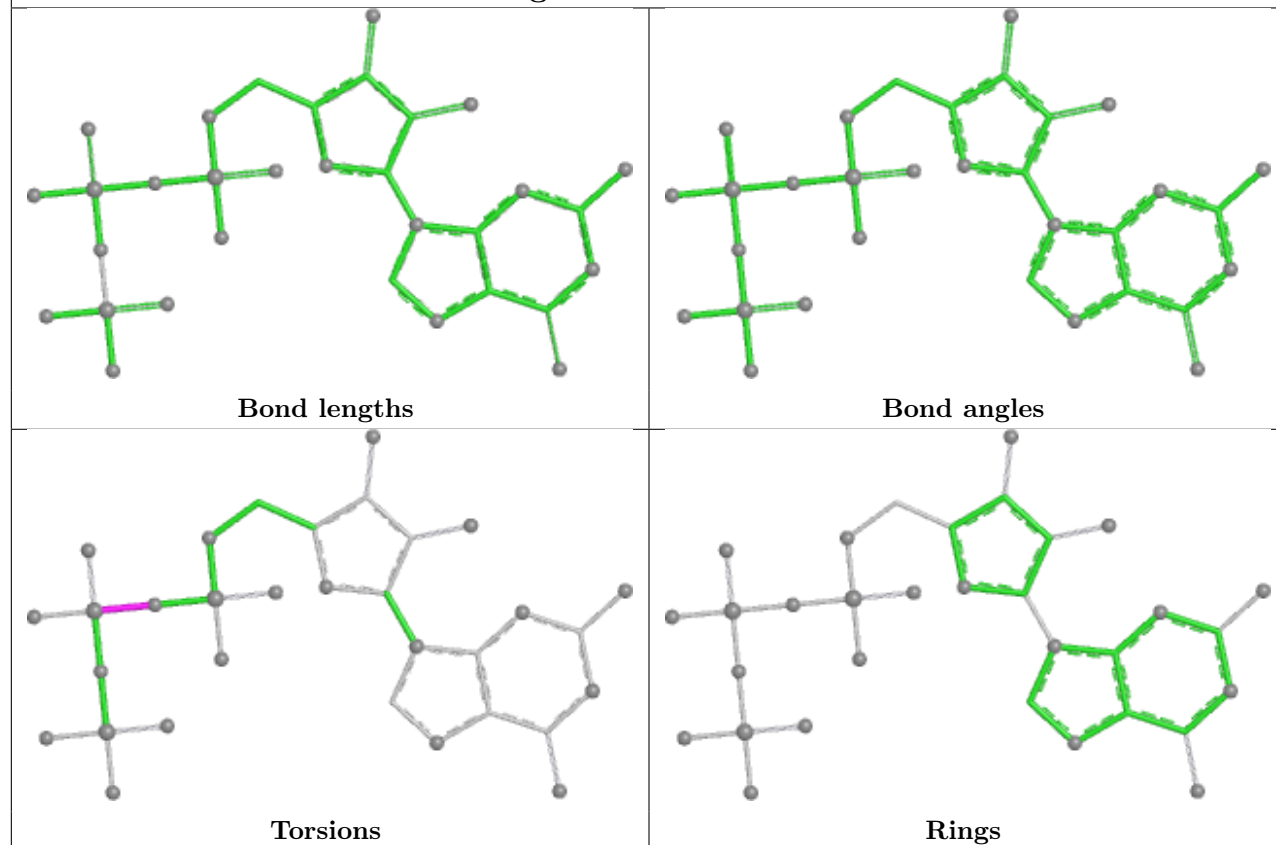
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	301	ATP	1	0
3	I	302	GTP	1	0
3	C	302	GTP	0	1

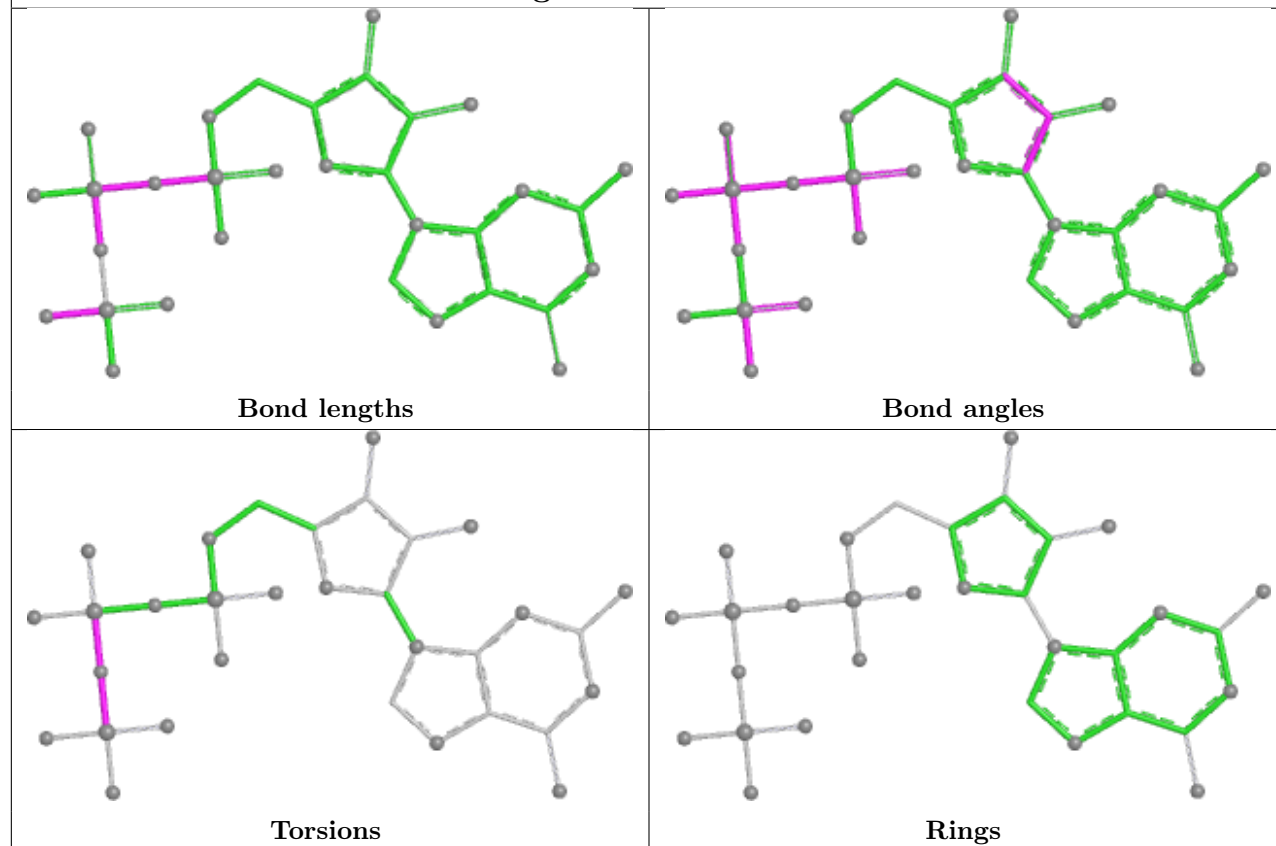
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

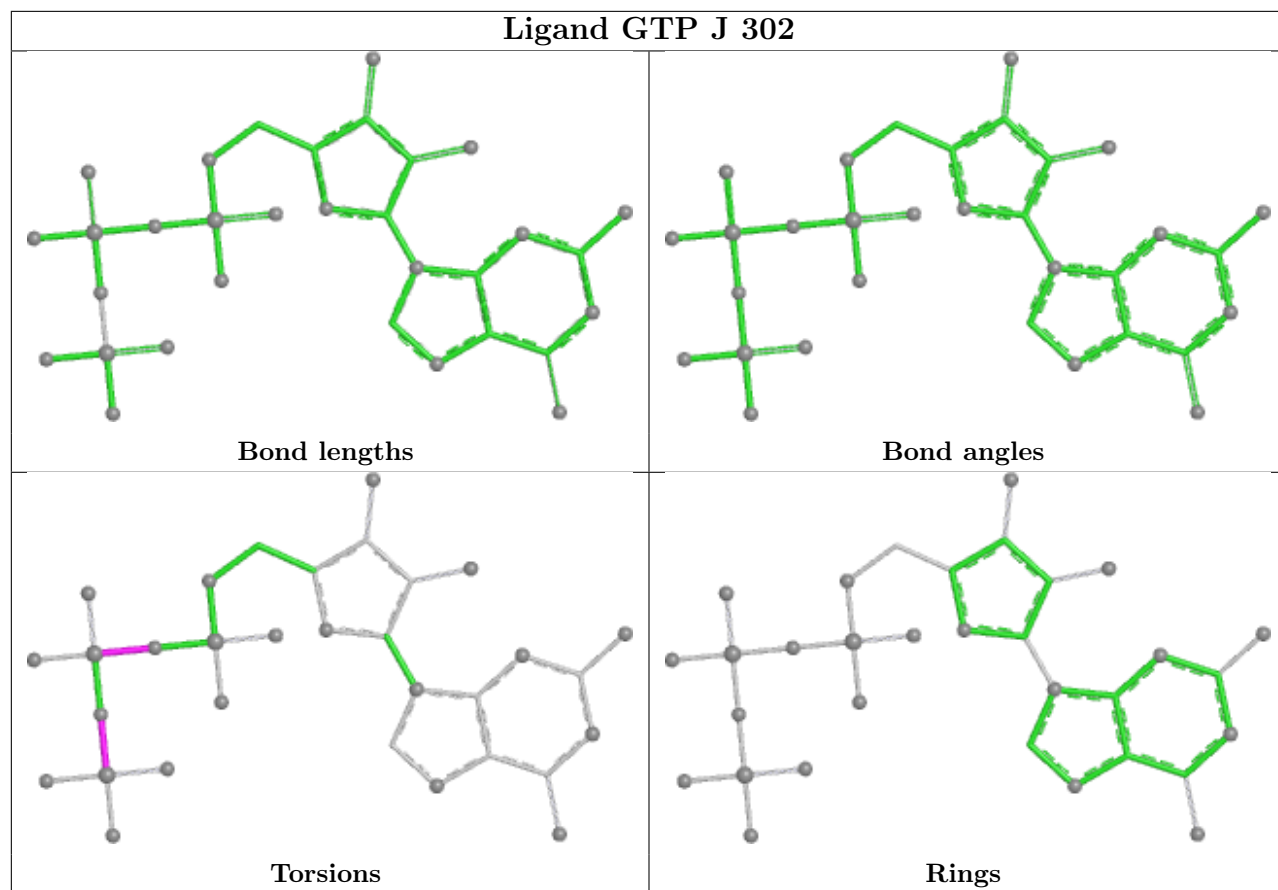


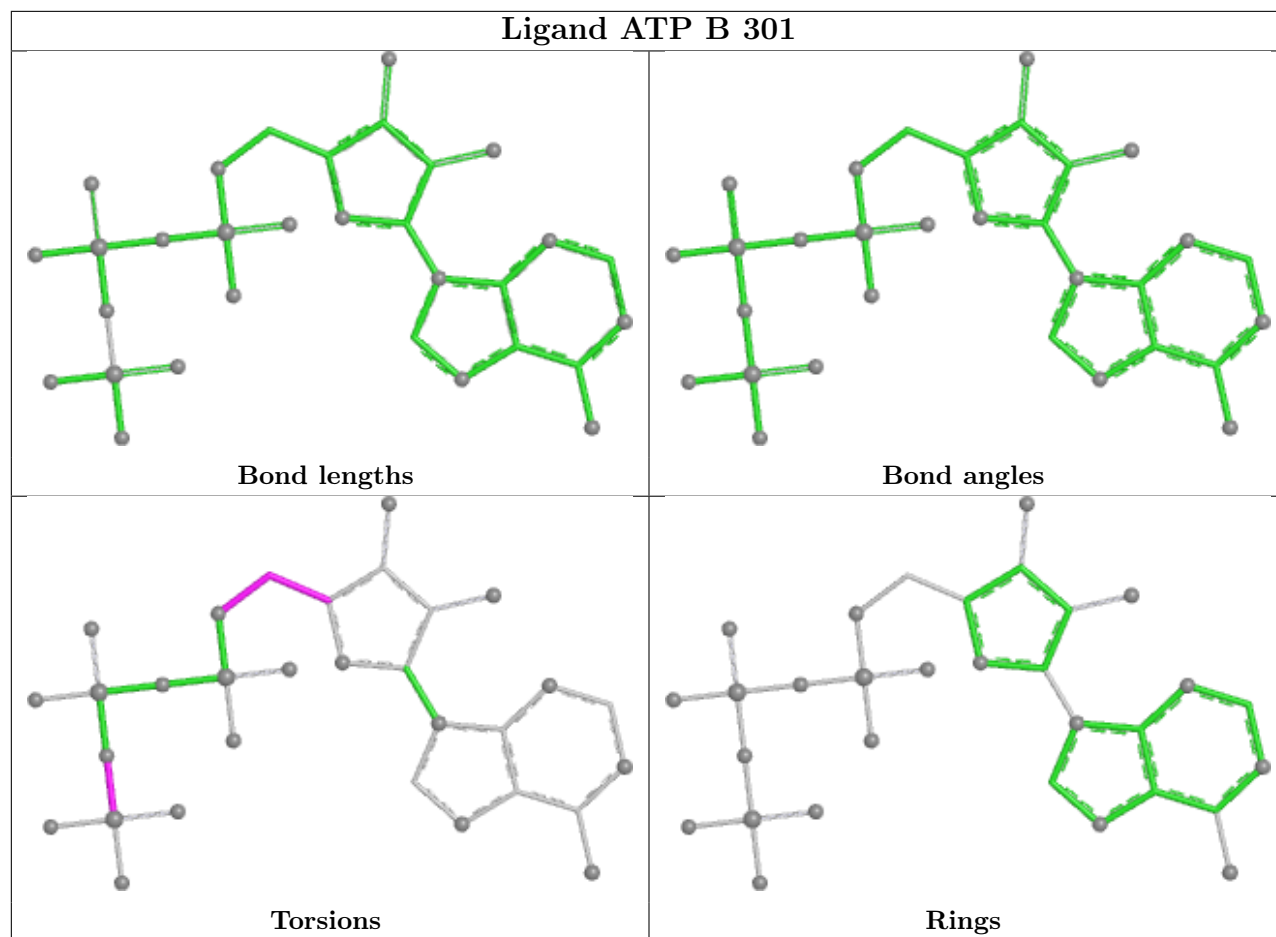
Ligand GTP H 302



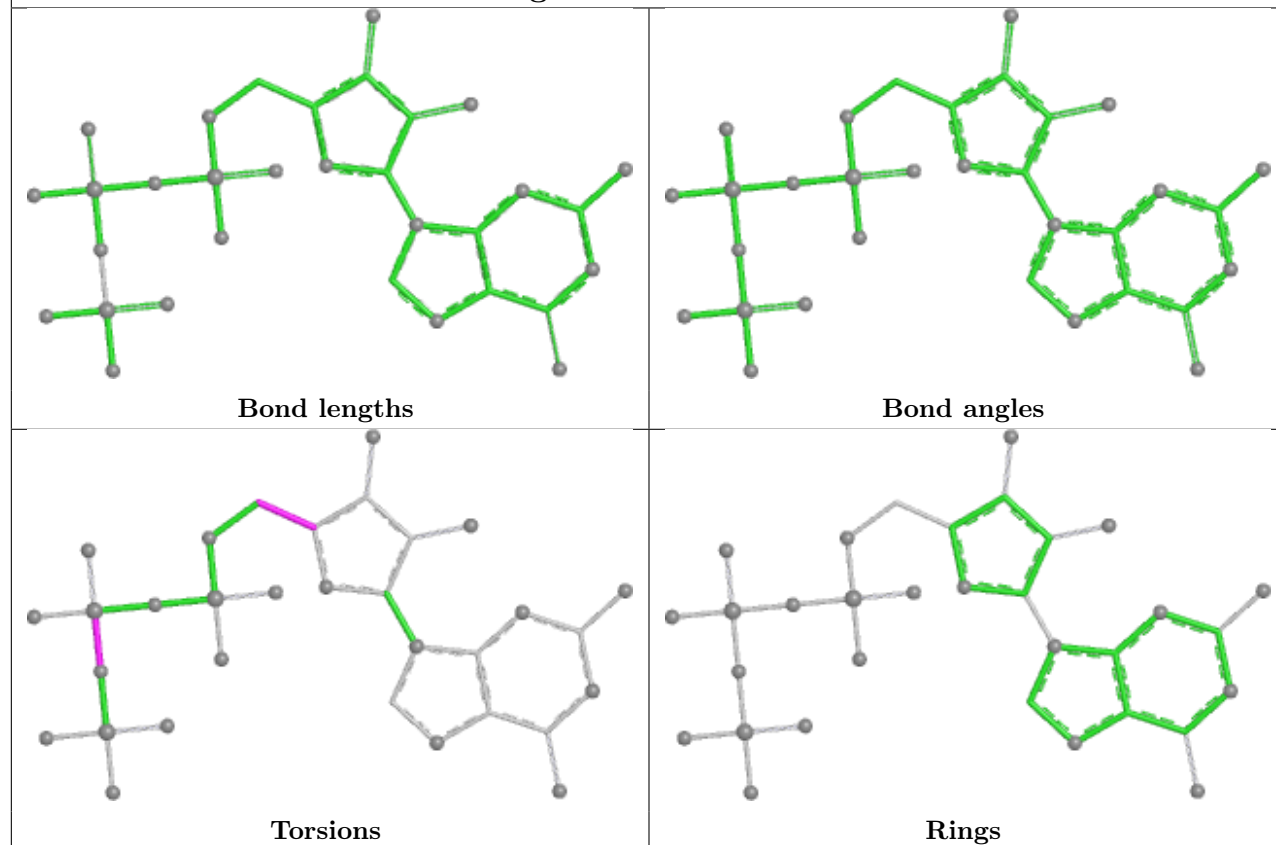
Ligand GTP L 302



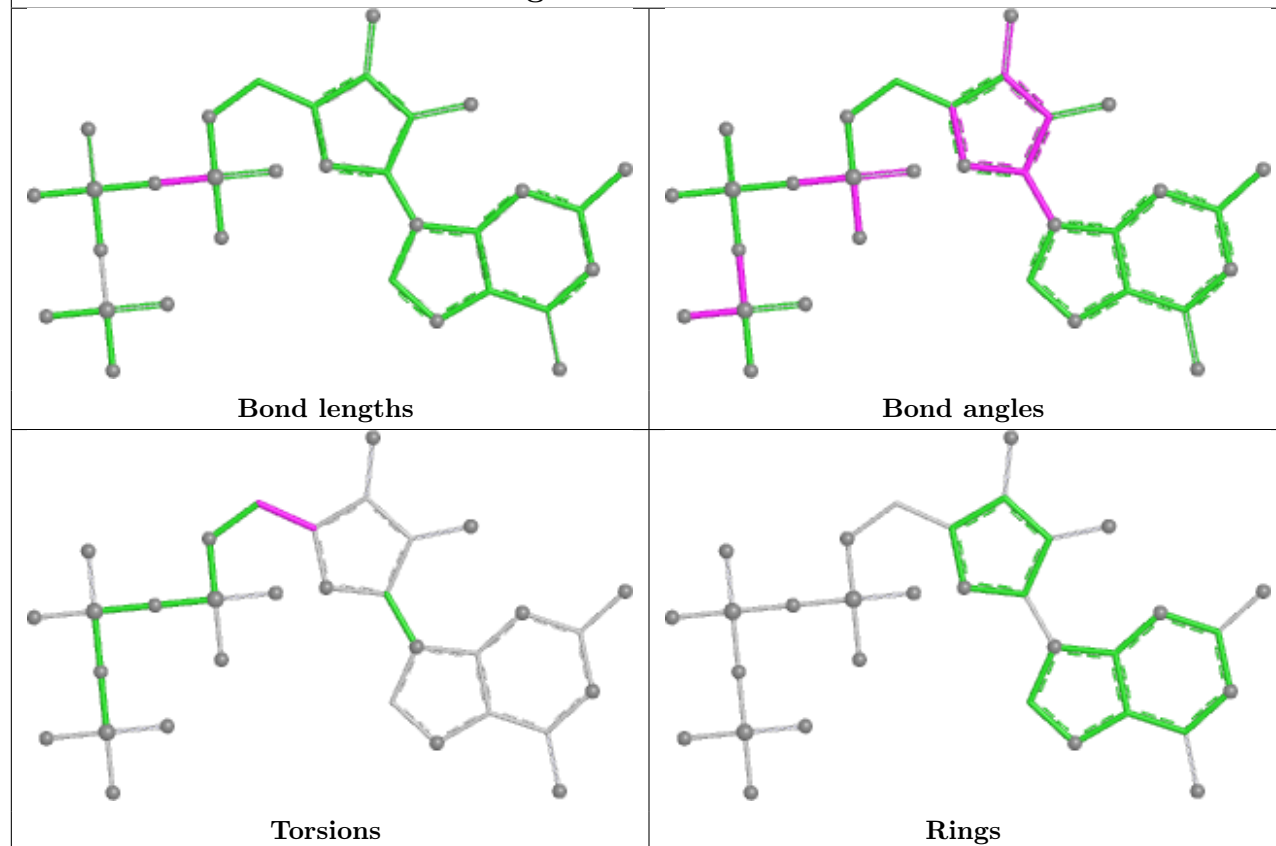


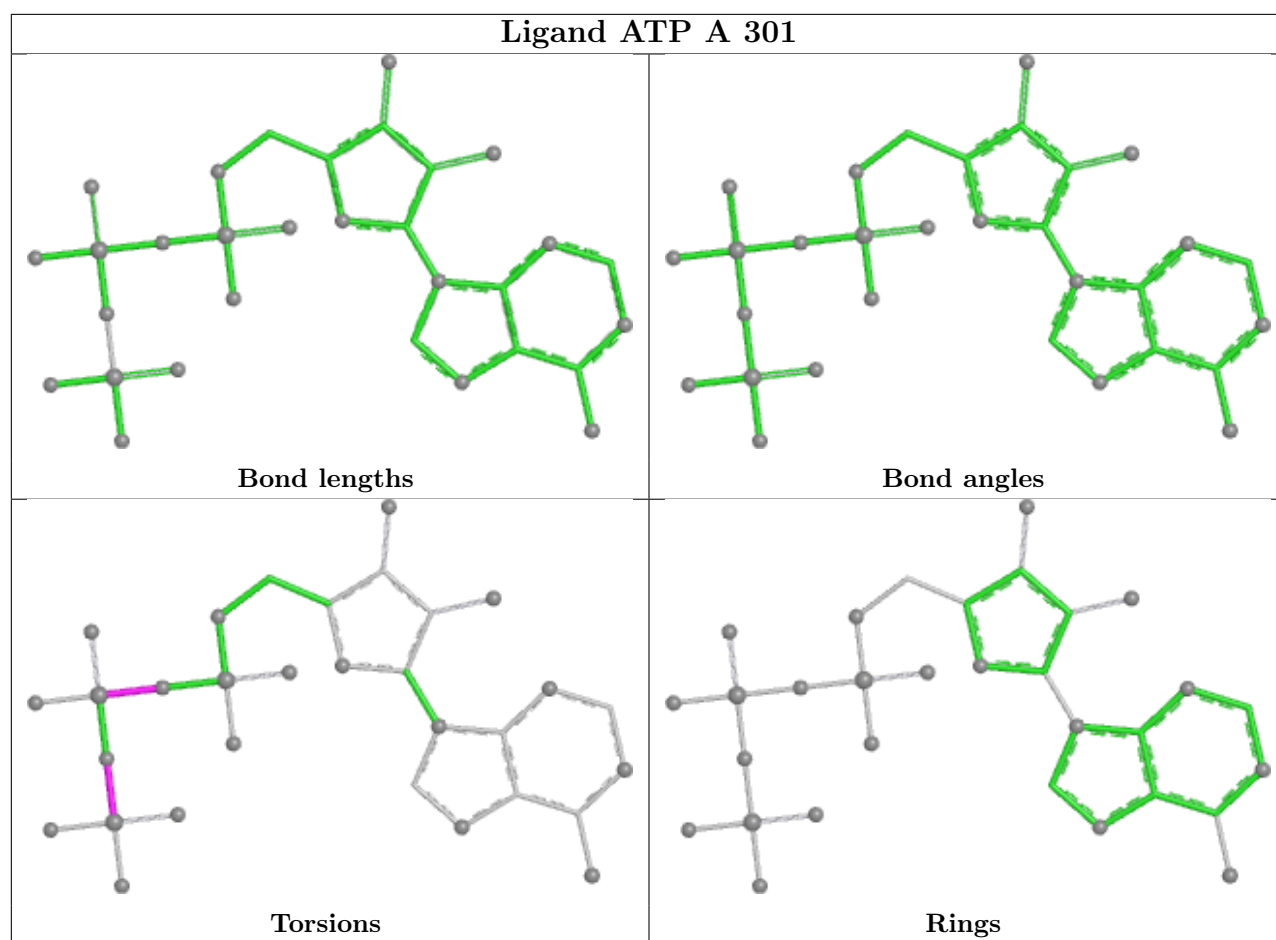


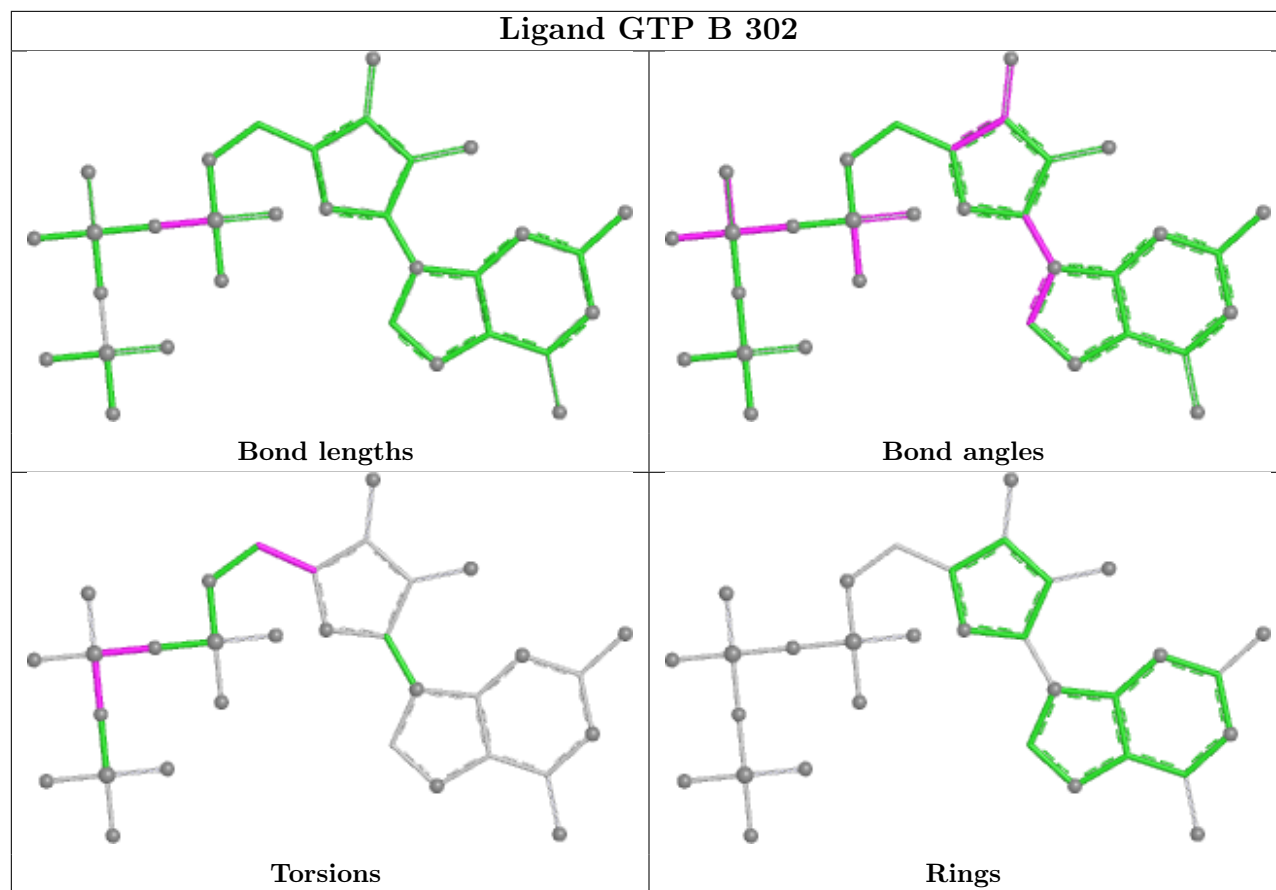
Ligand GTP N 302

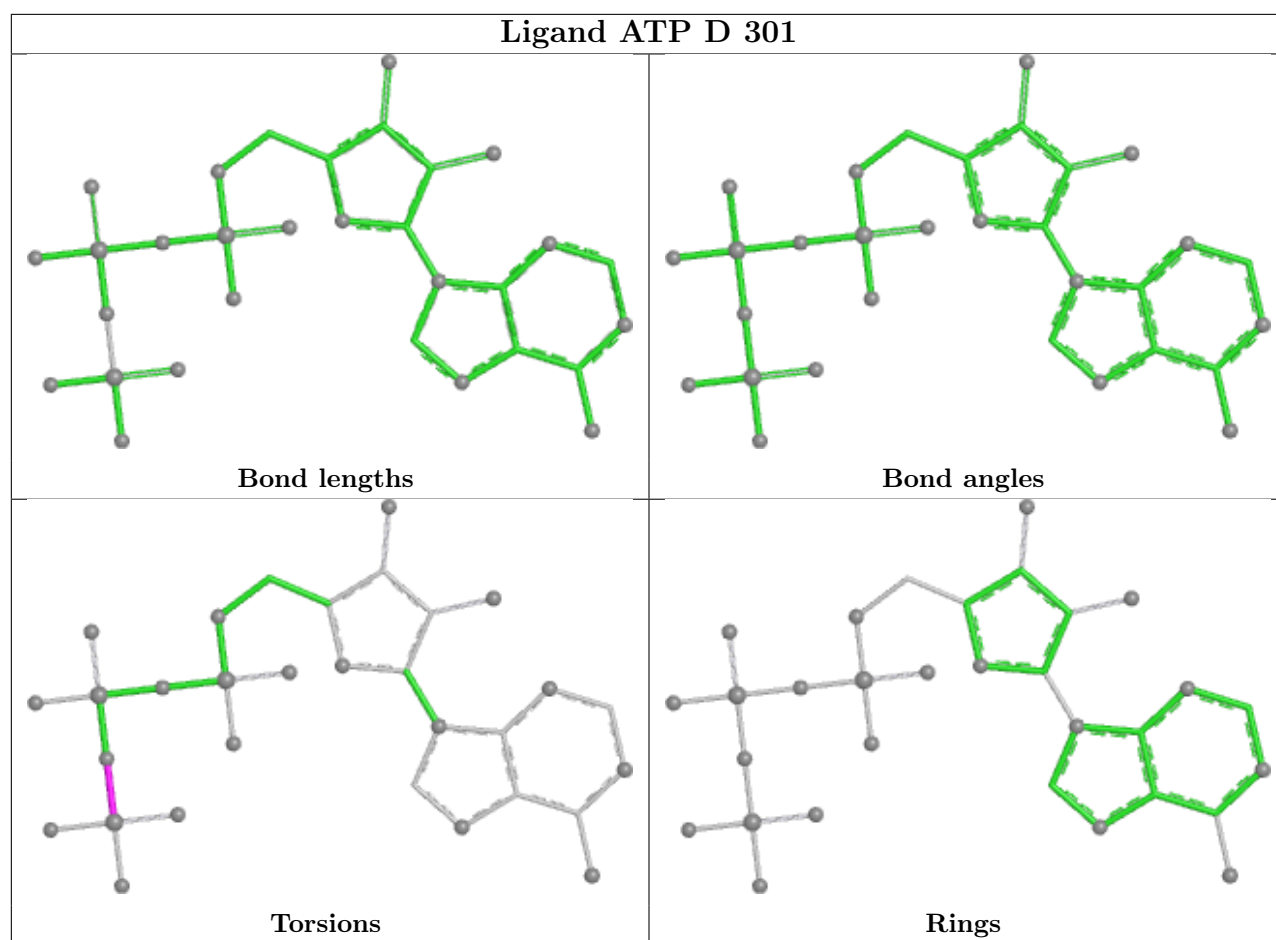


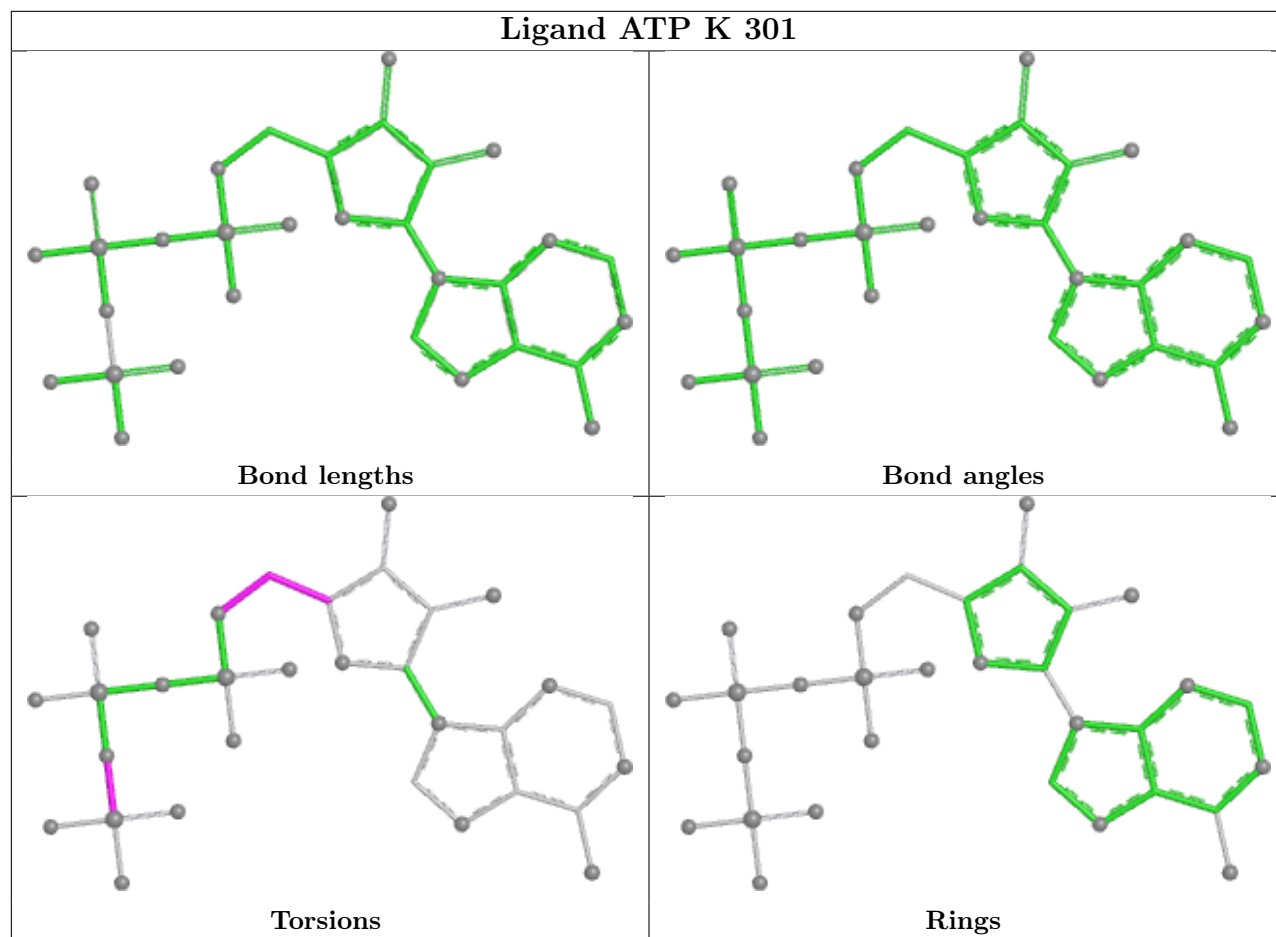
Ligand GTP M 302

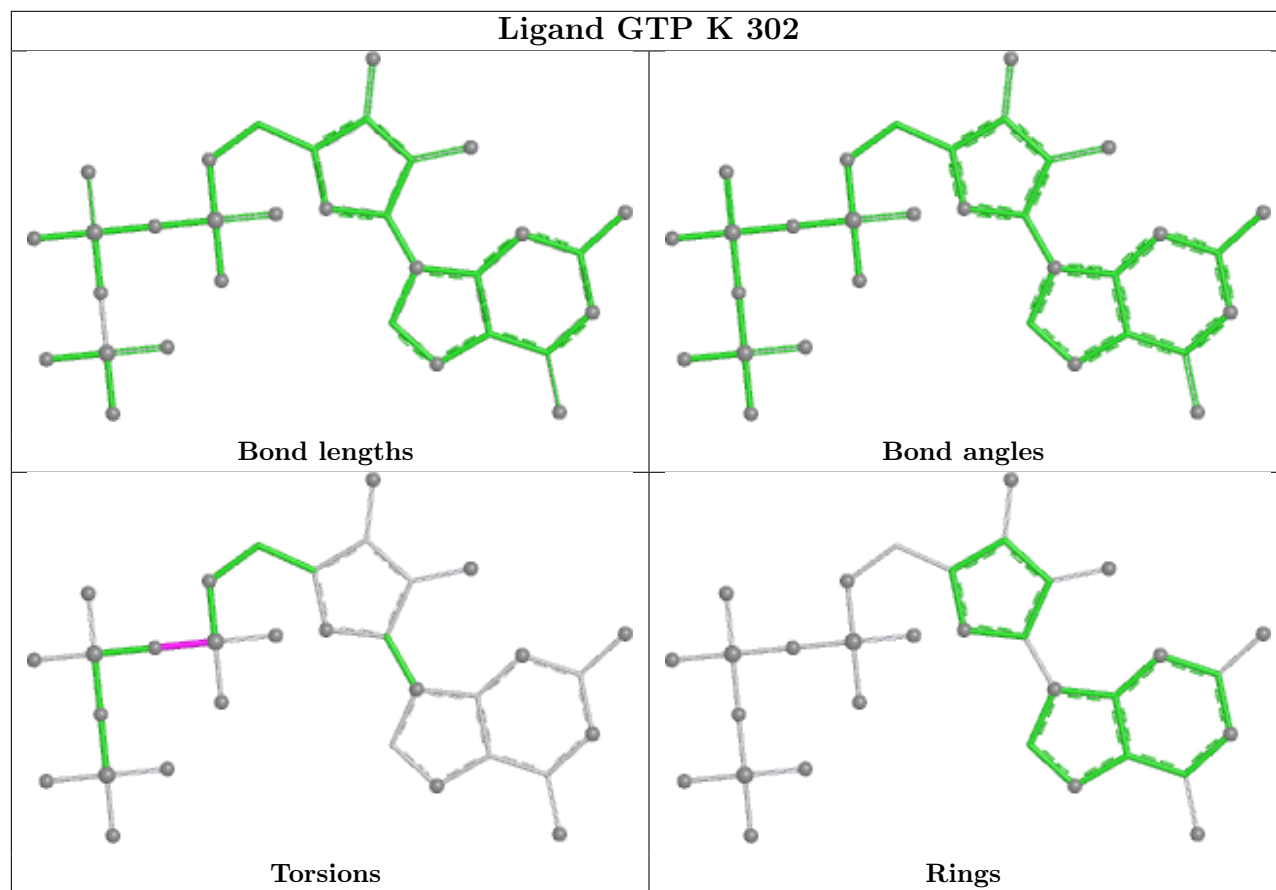


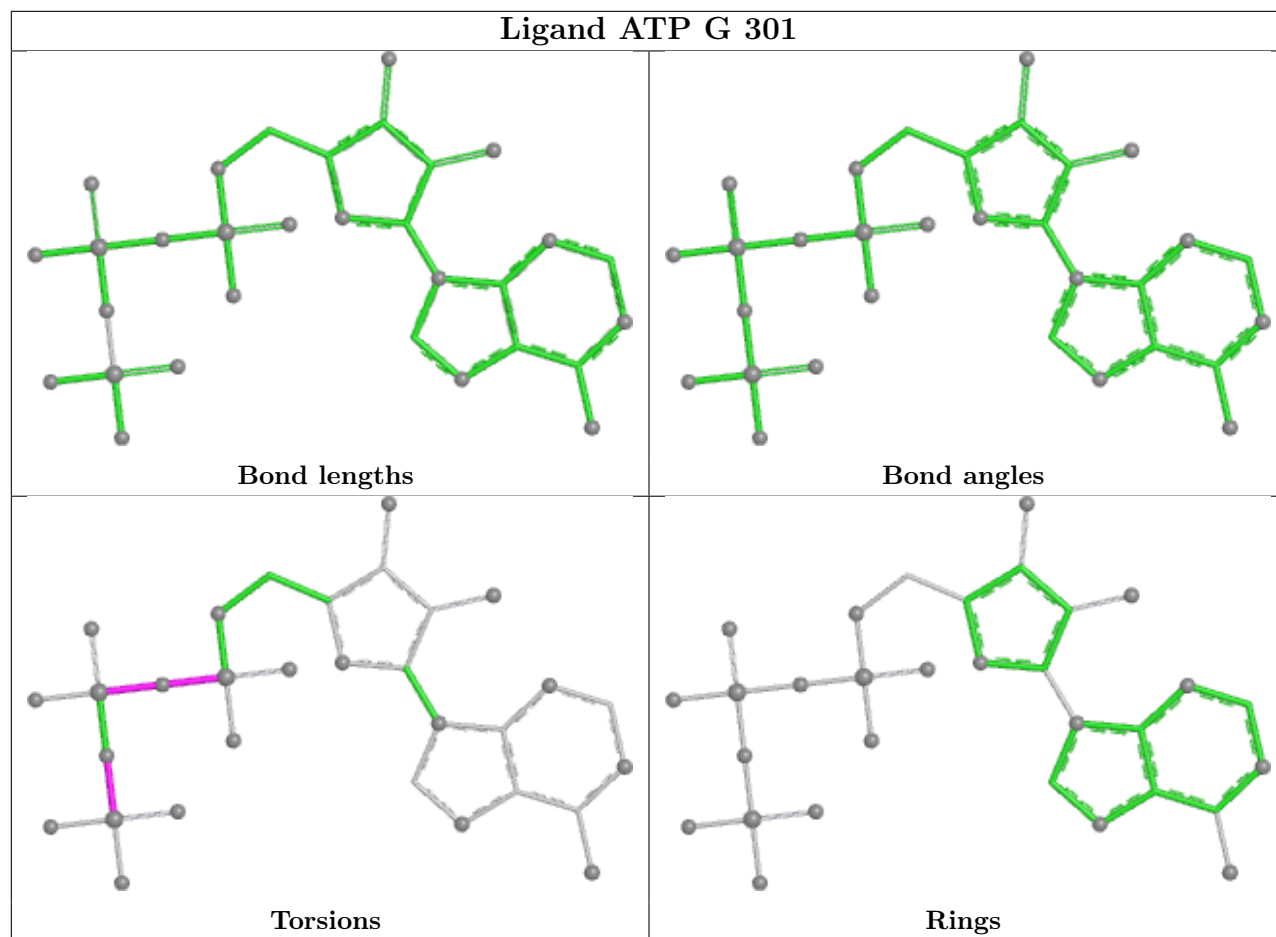




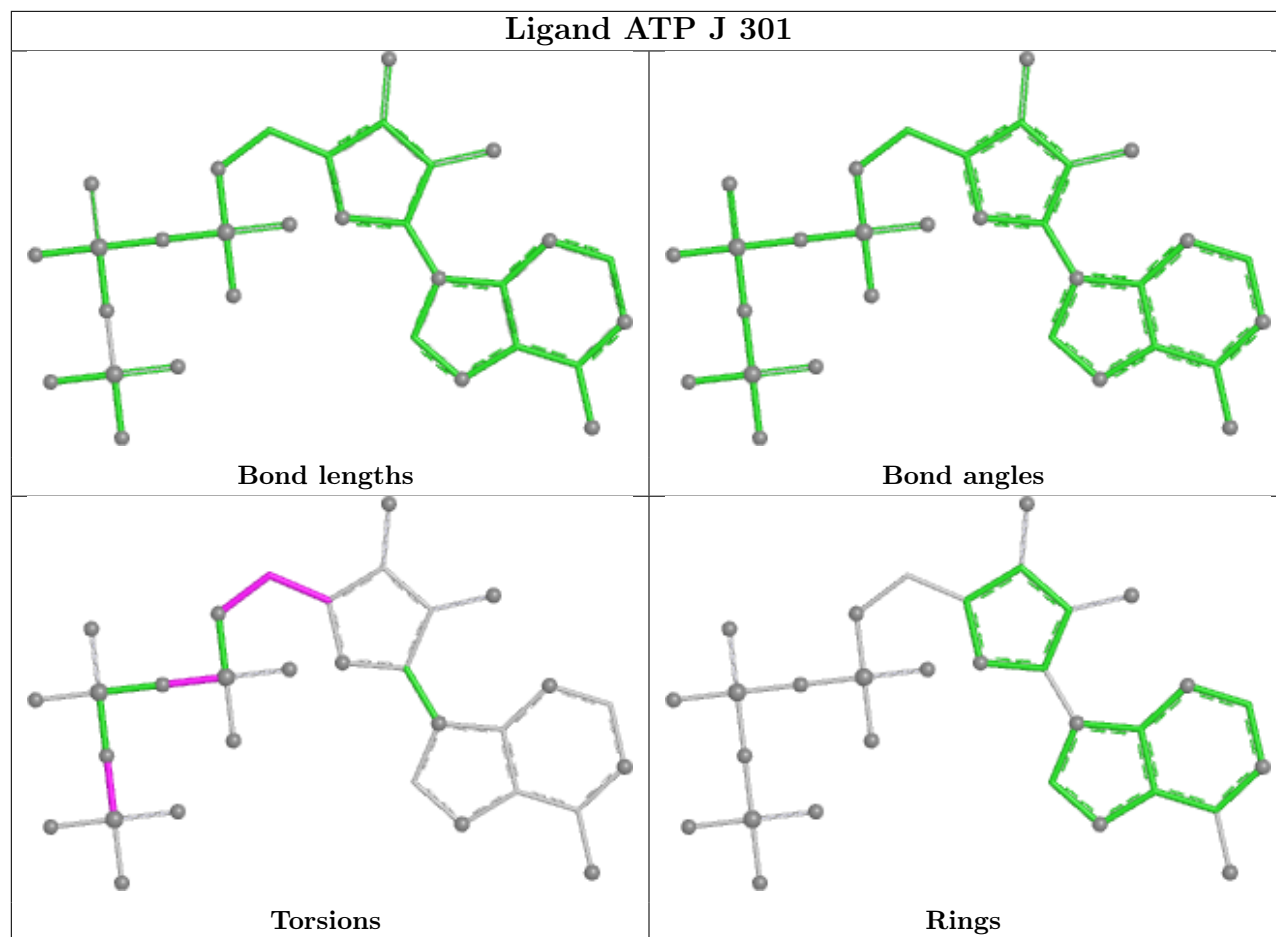


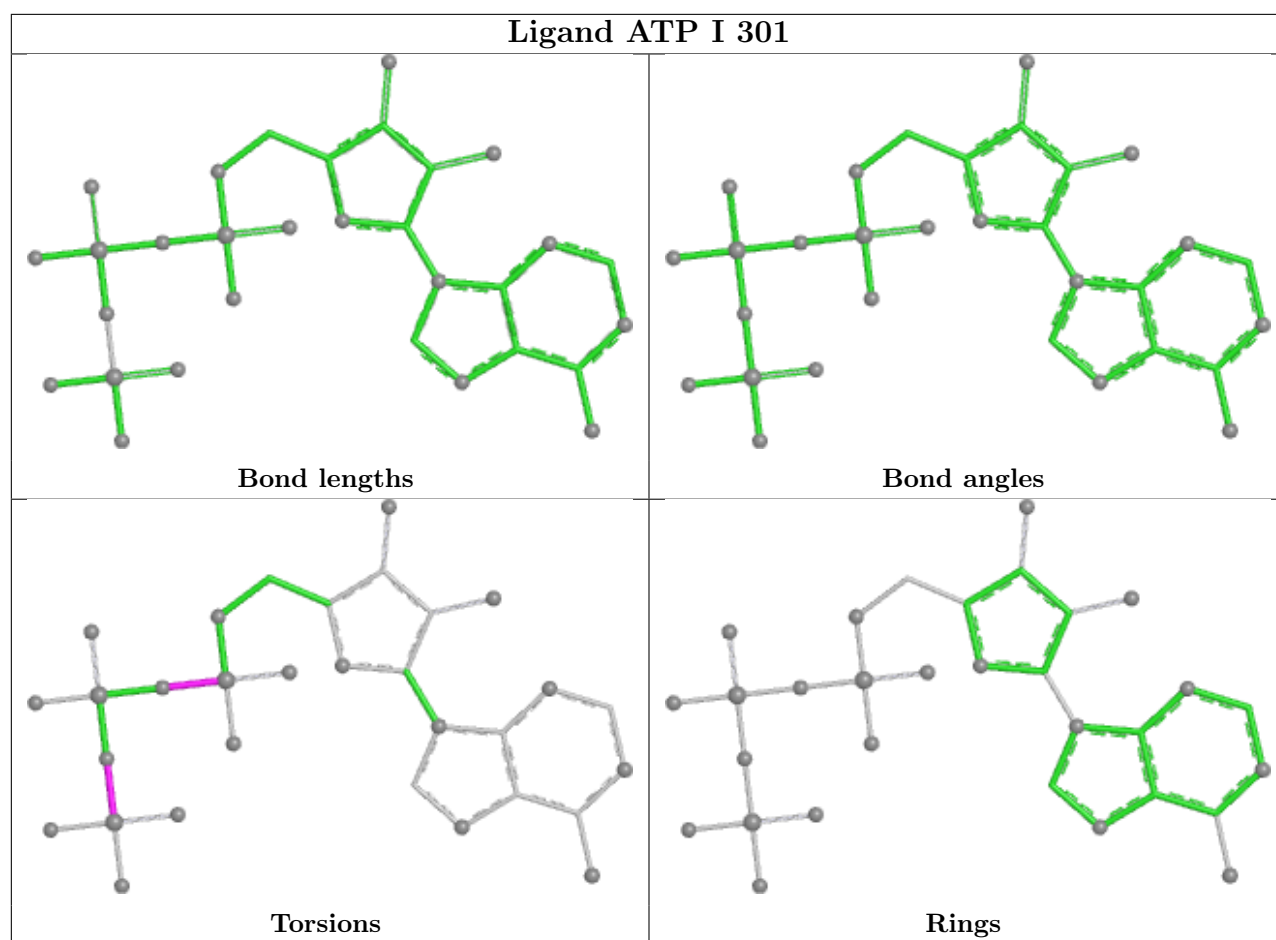


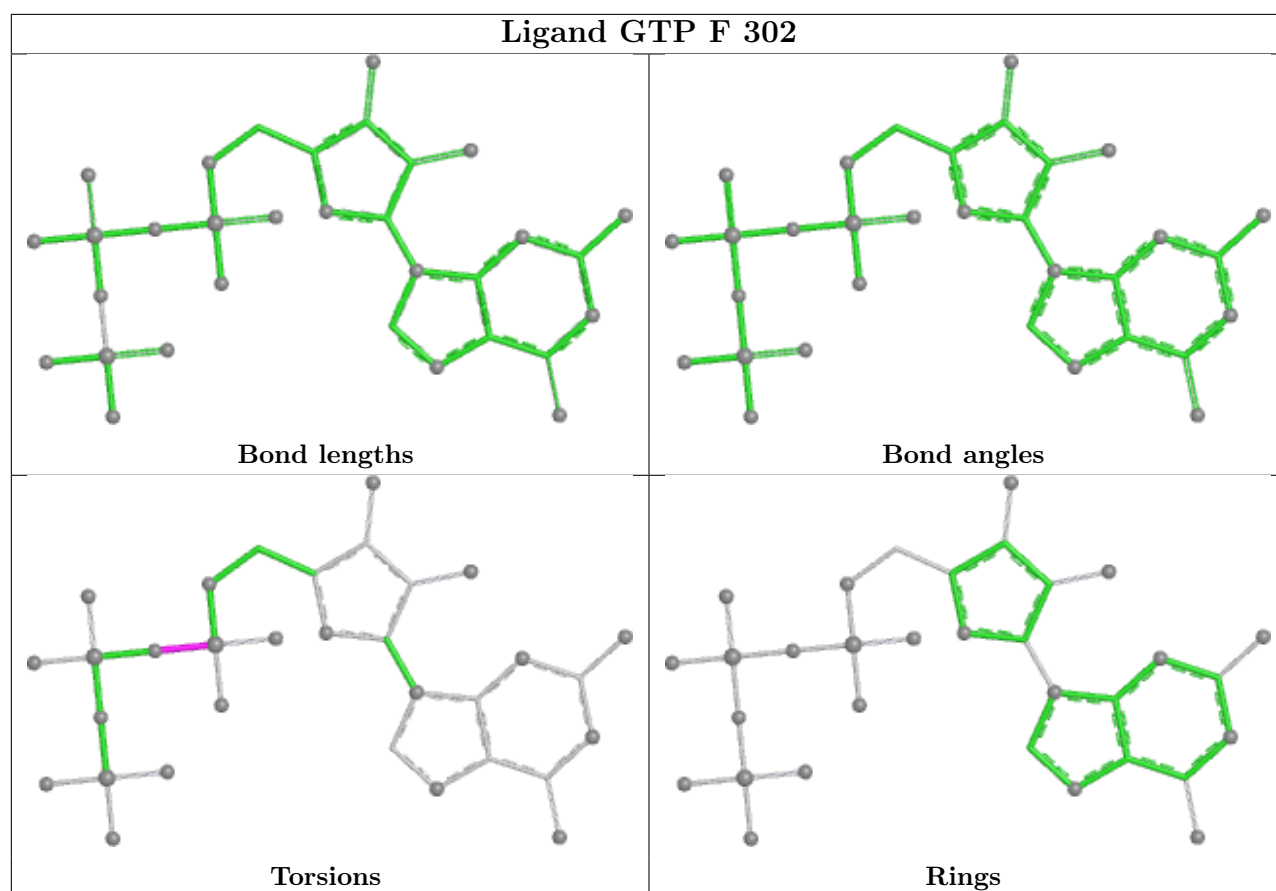


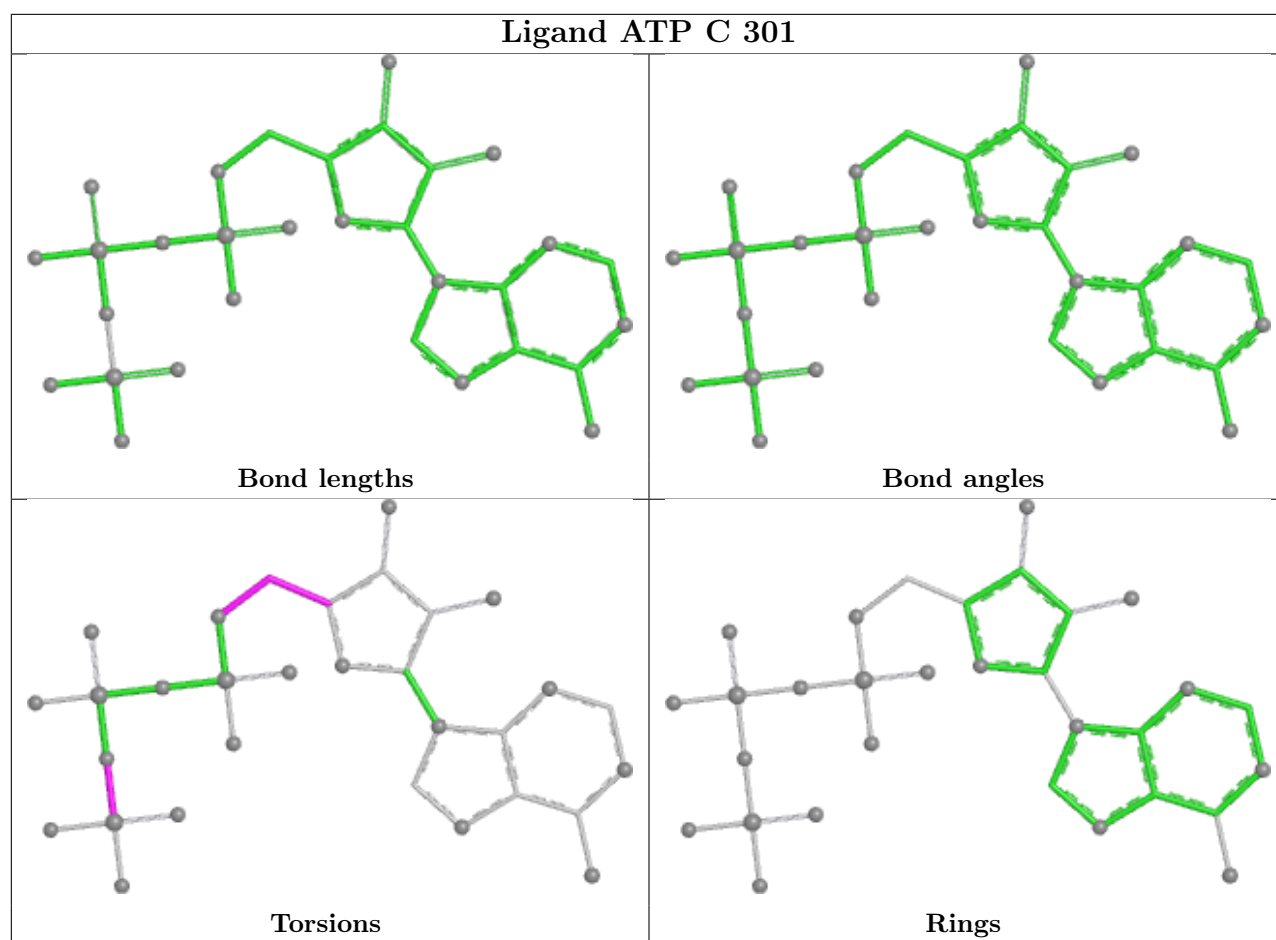


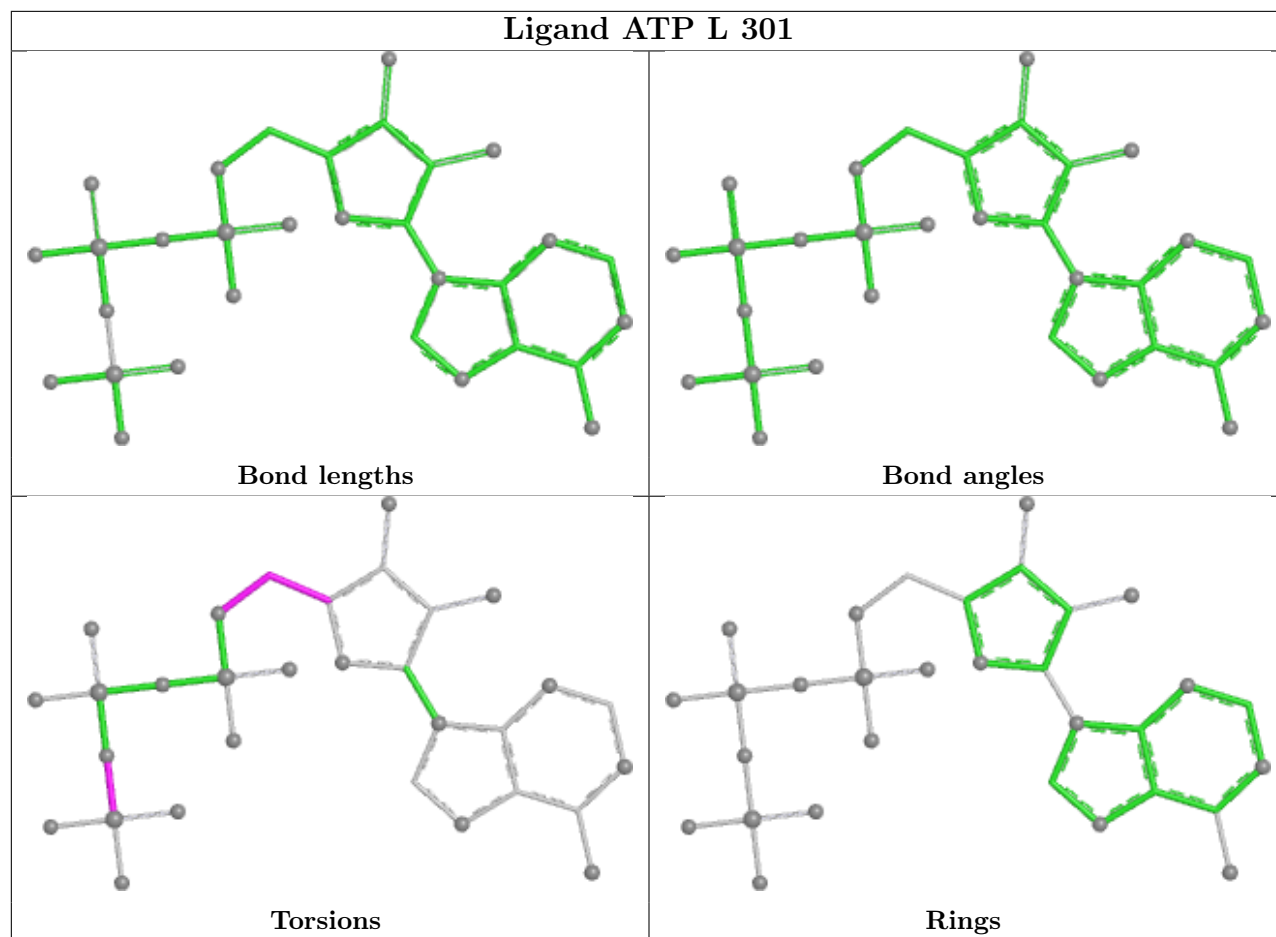
Ligand ATP J 301



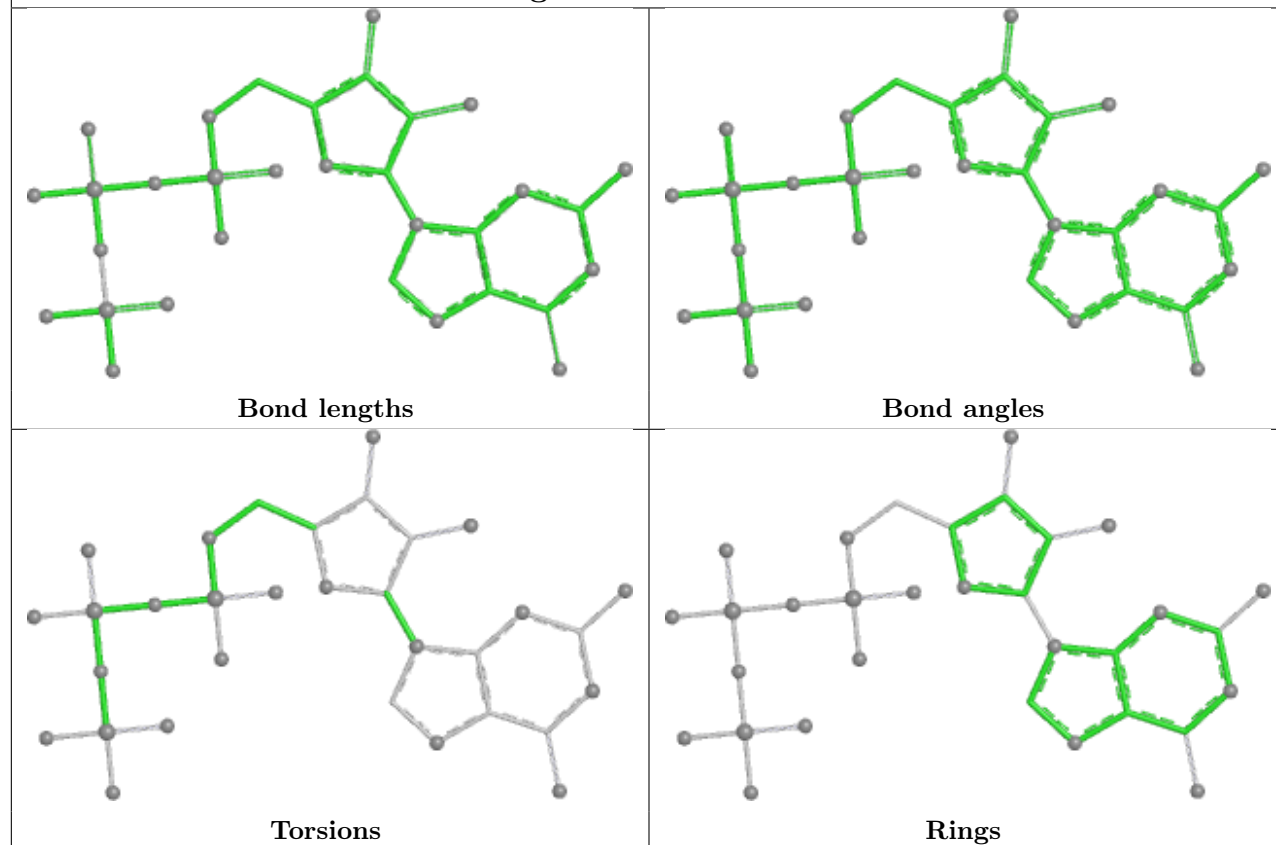




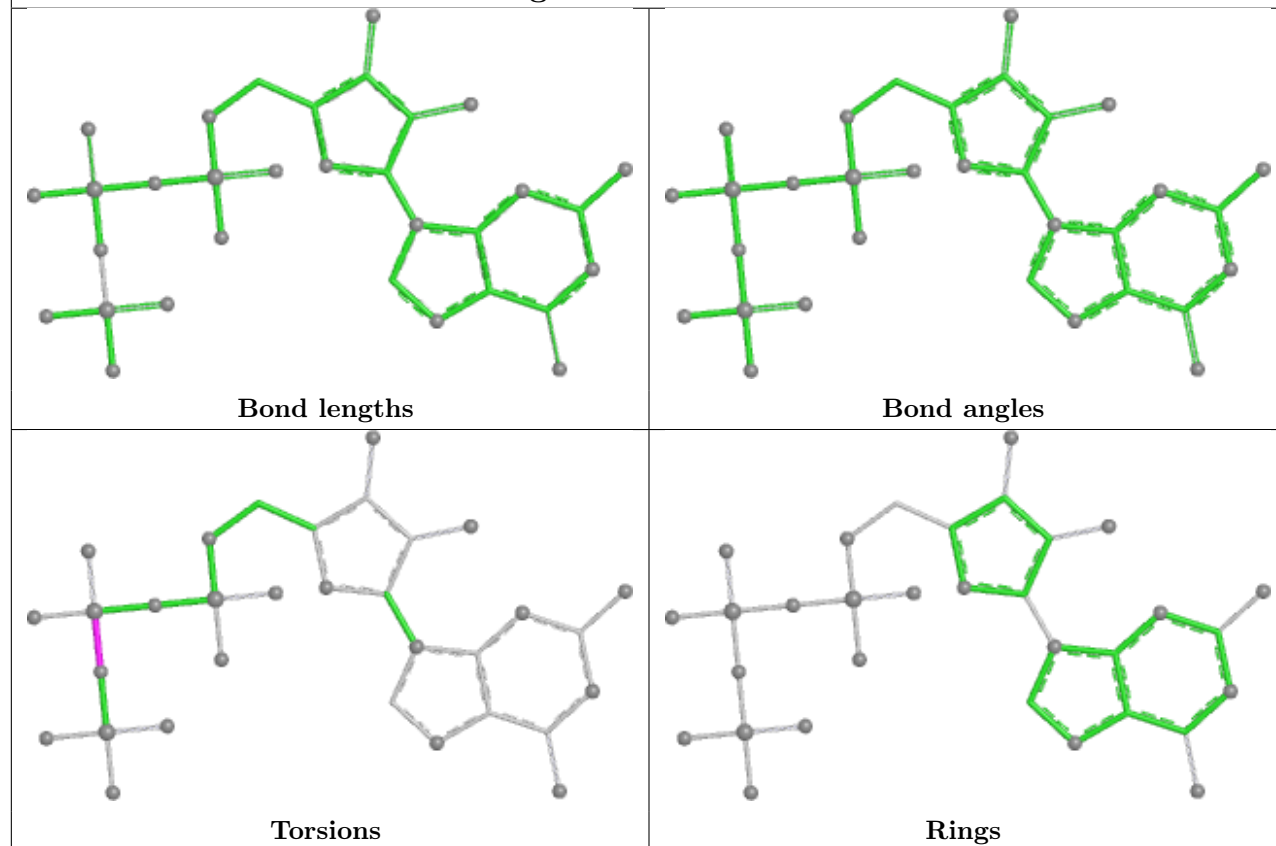


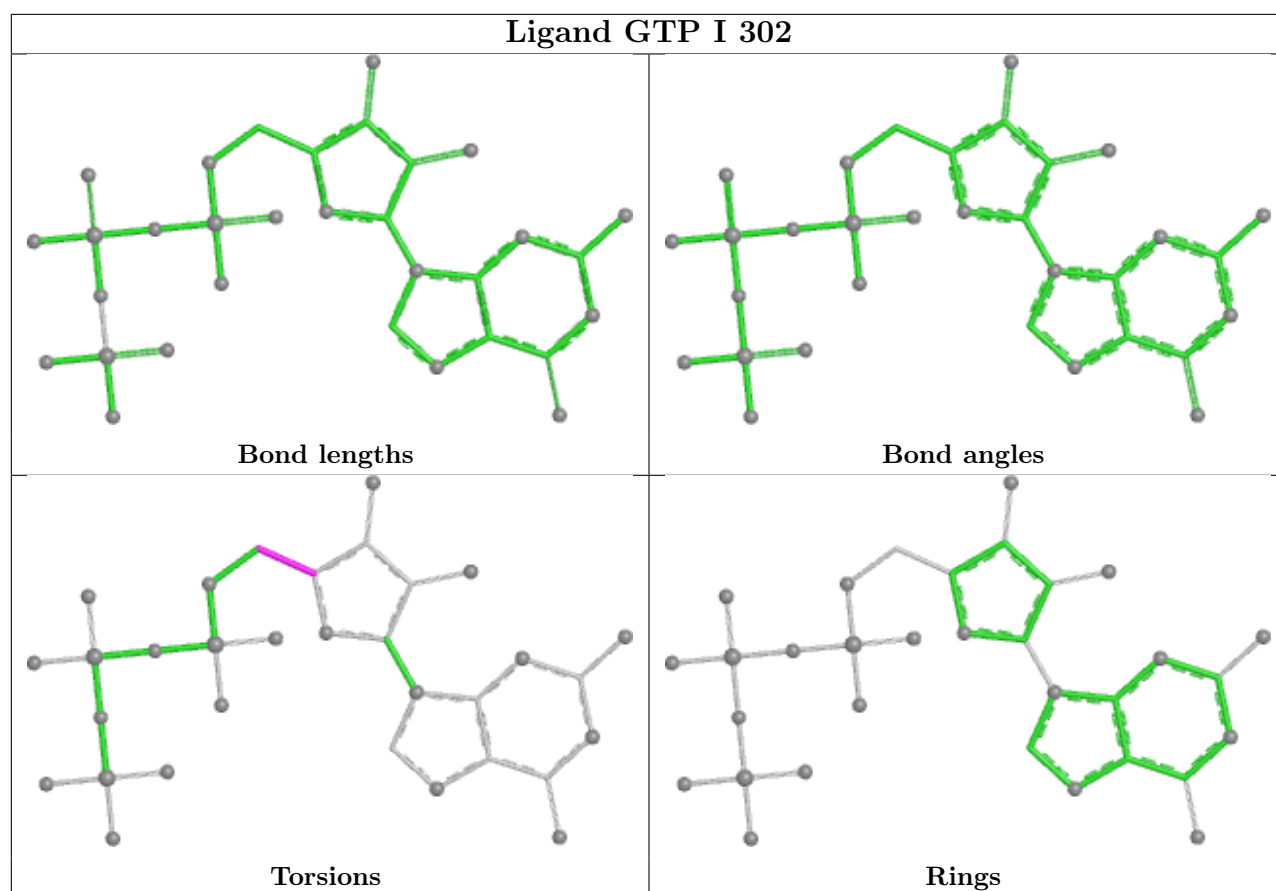


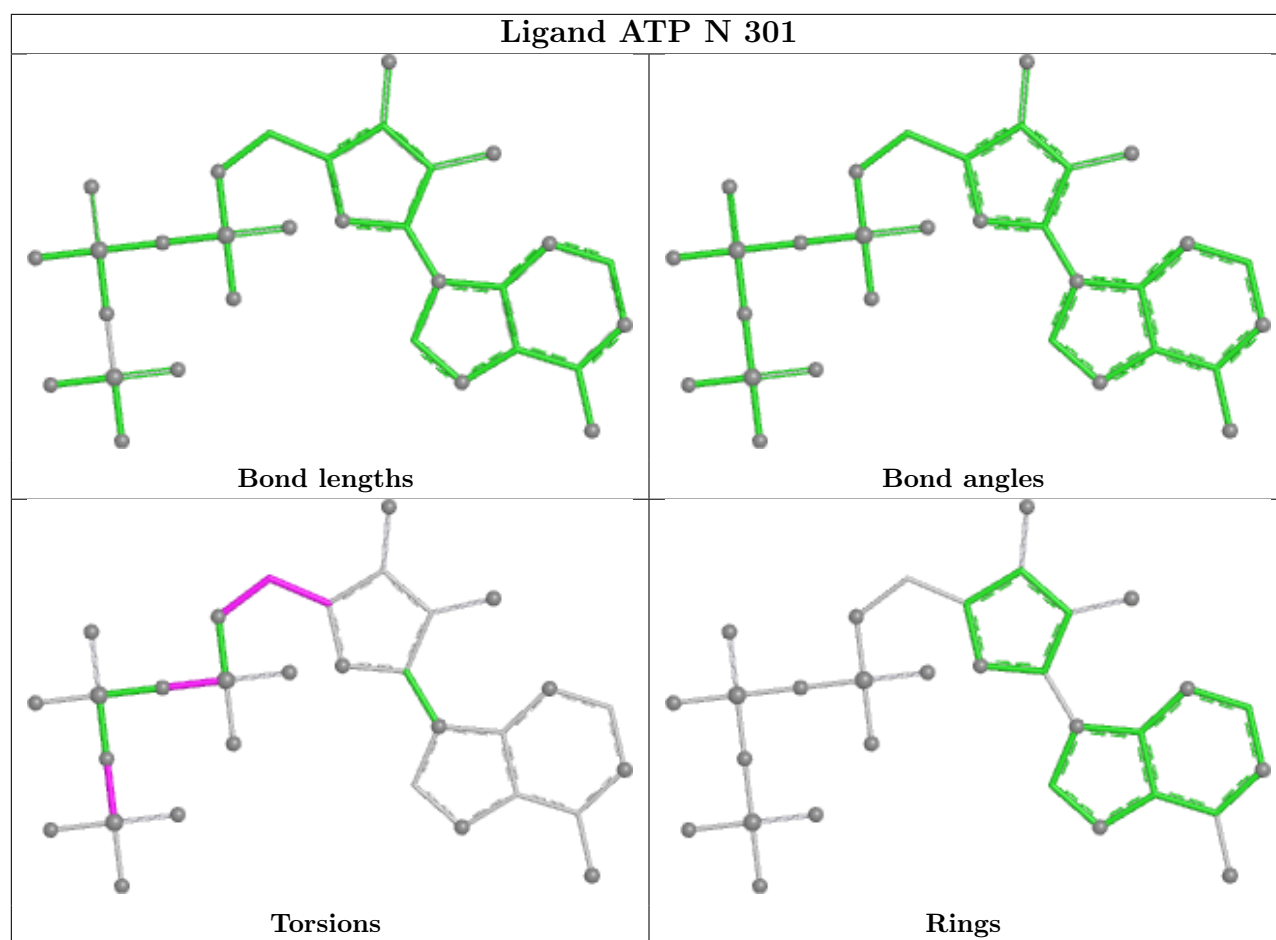
Ligand GTP D 302

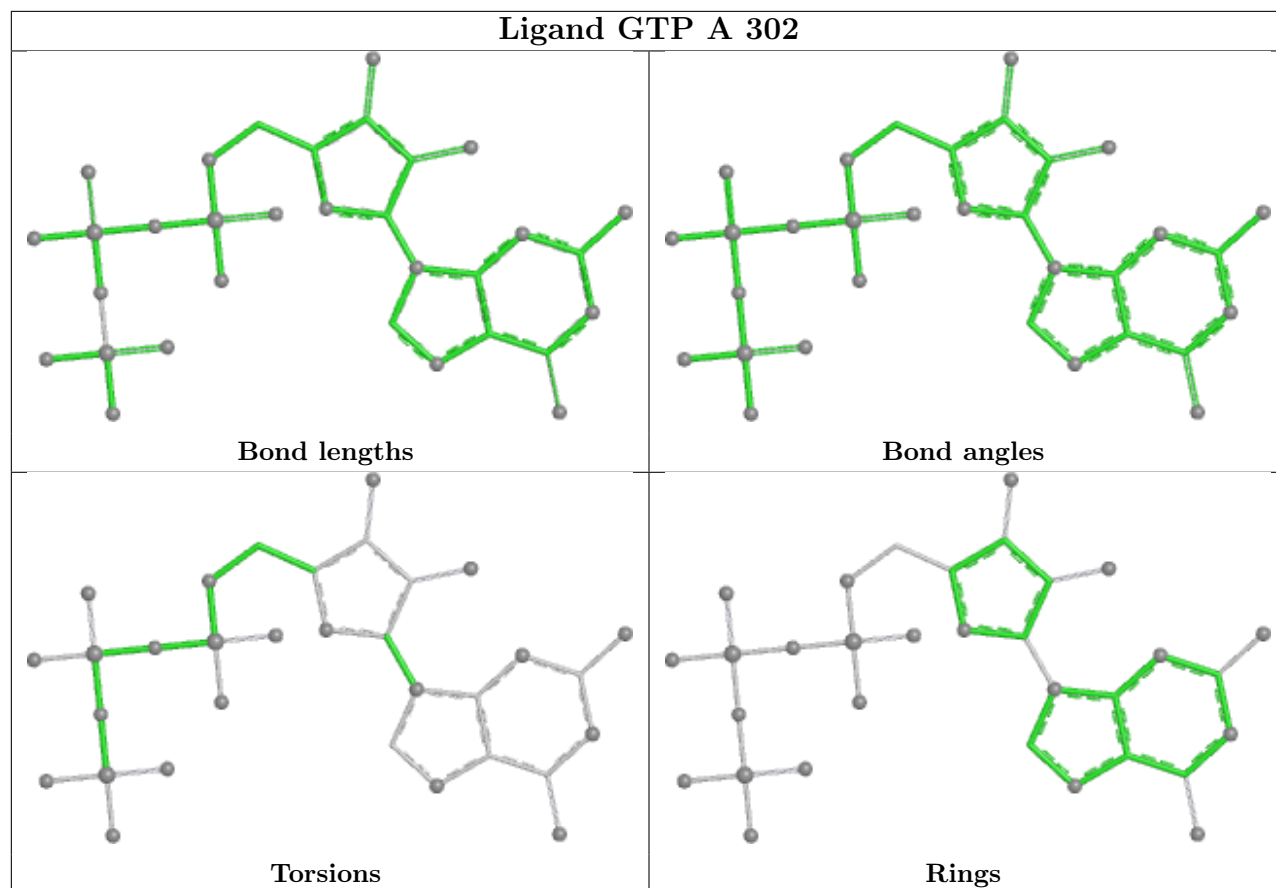


Ligand GTP G 302

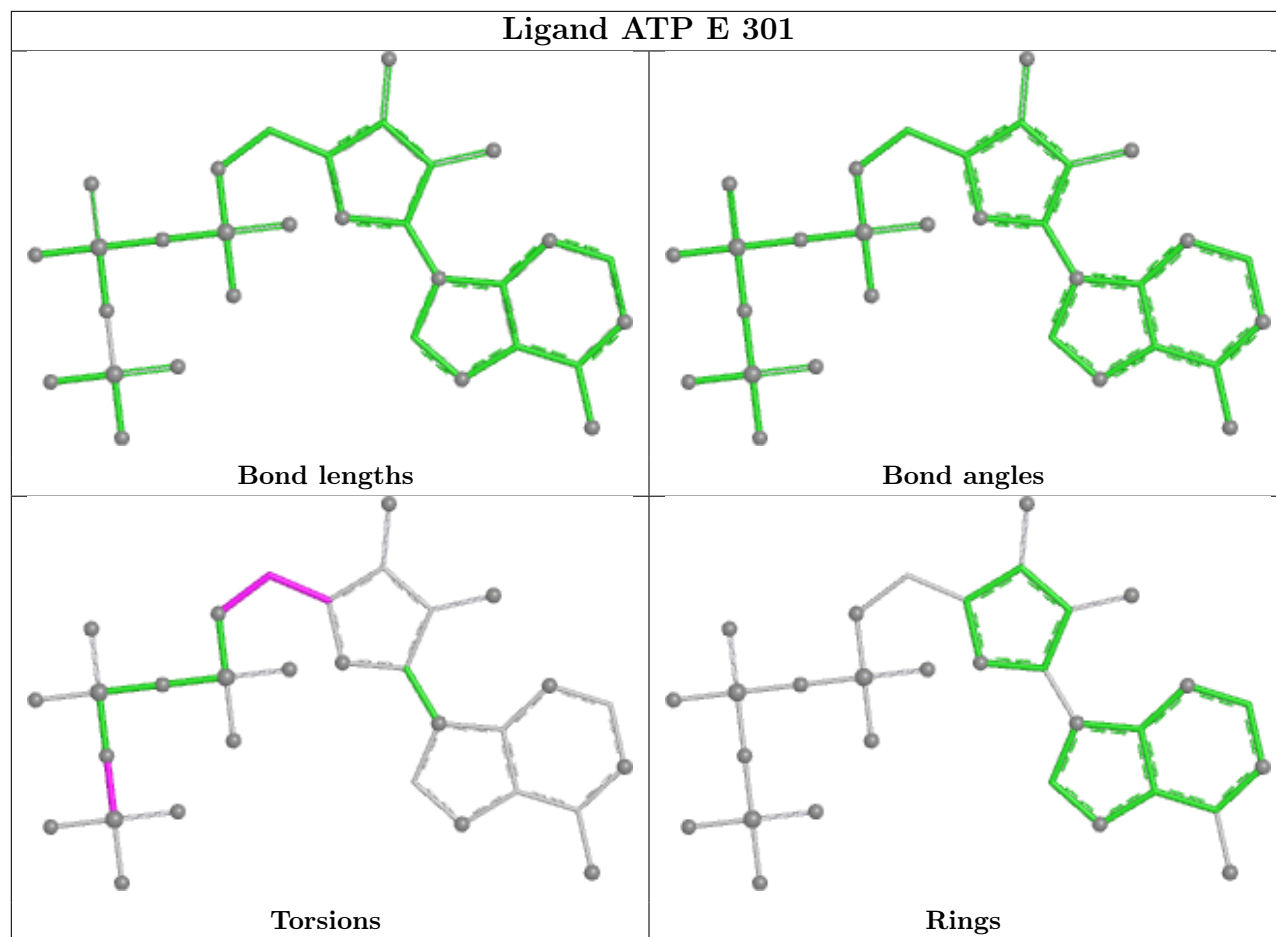


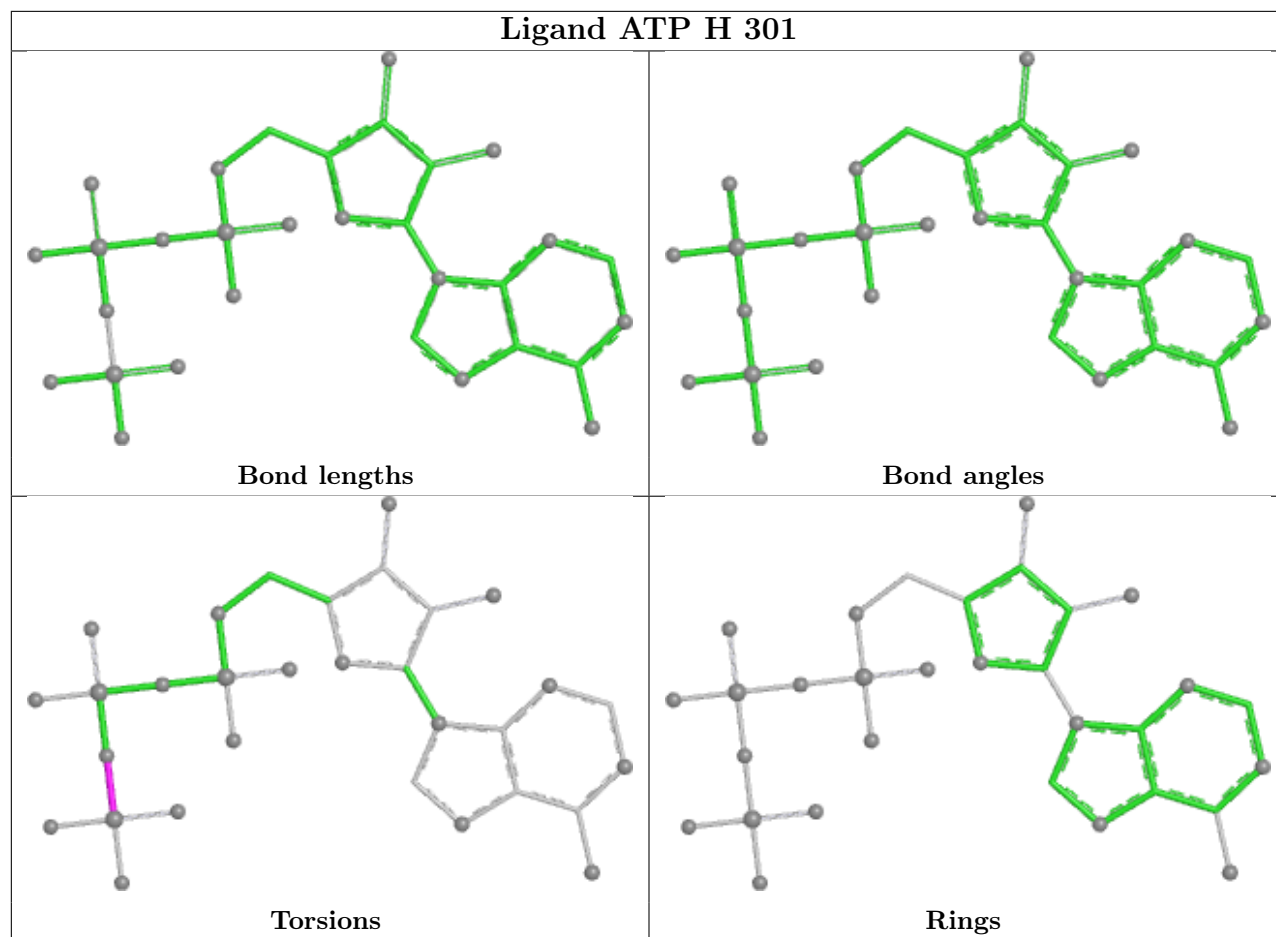


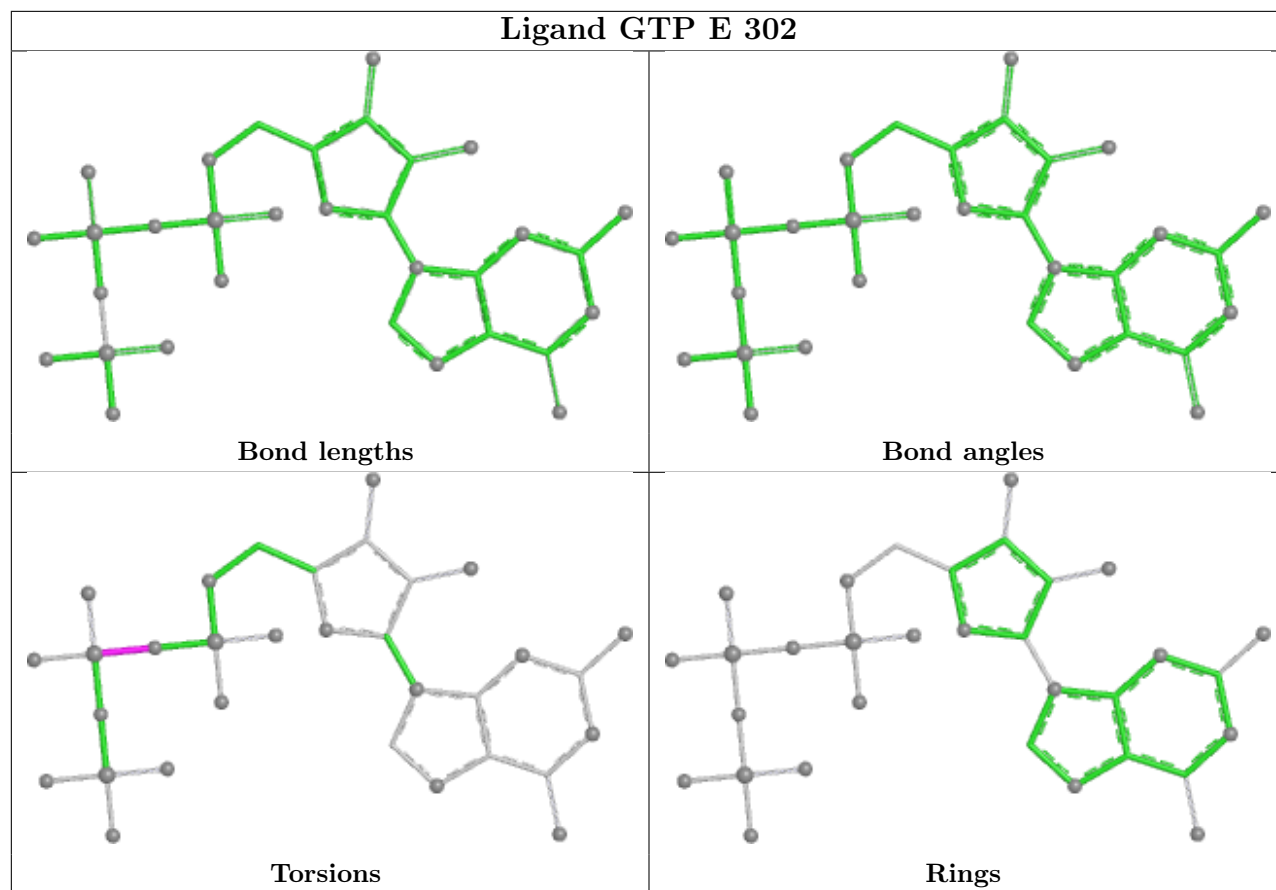




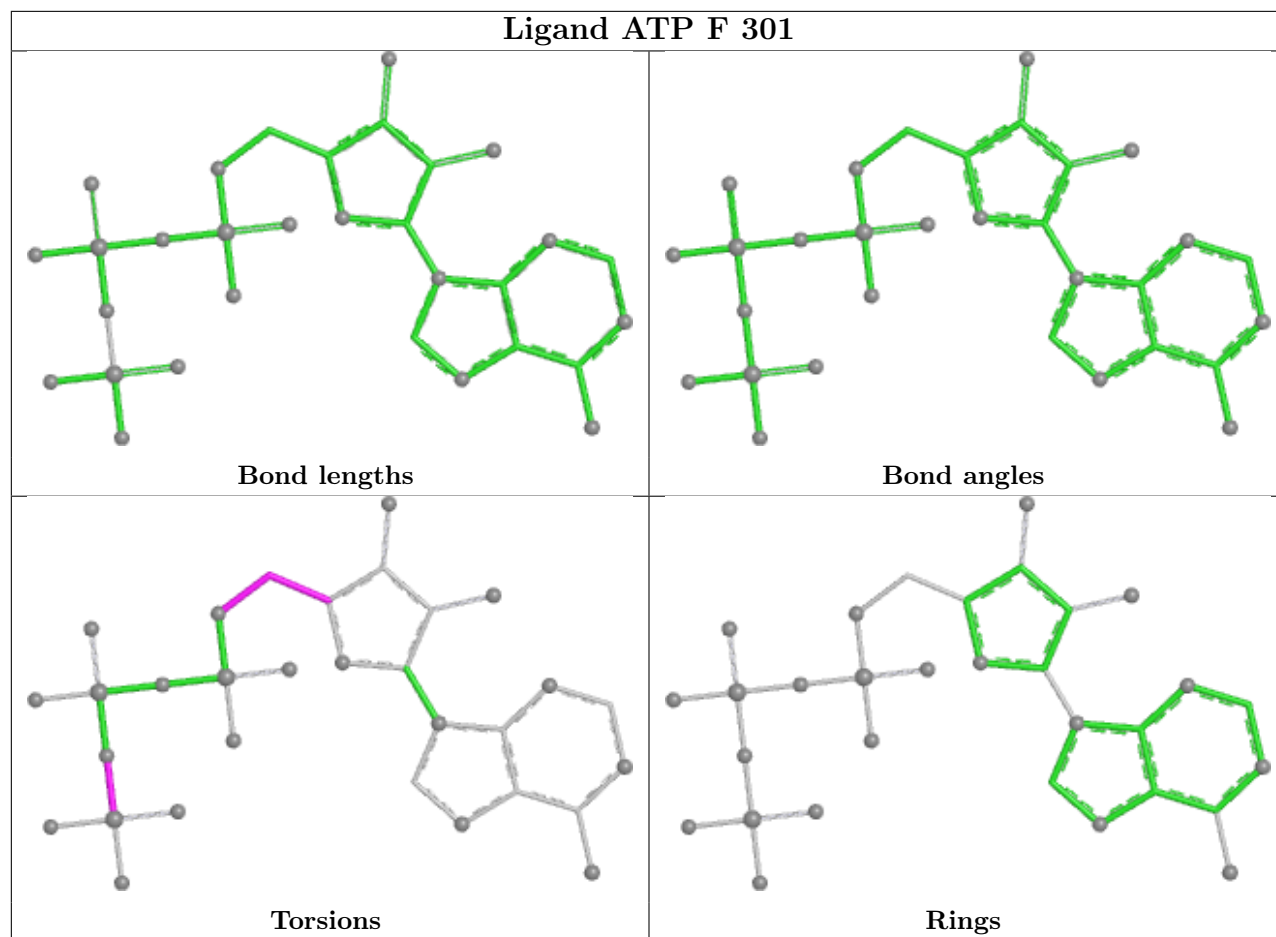
Ligand ATP E 301

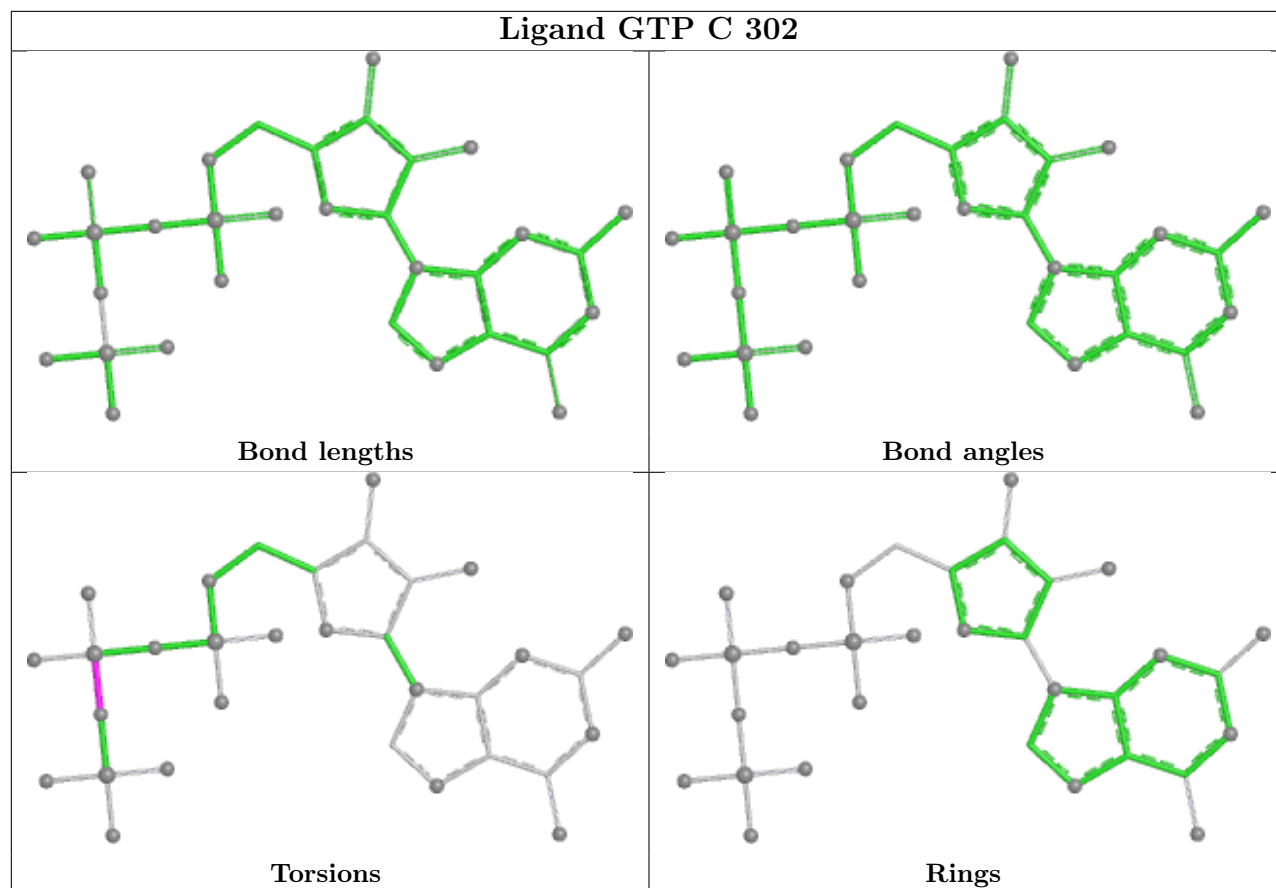






Ligand ATP F 301





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	222/234 (94%)	-1.46	0 100 100	21, 28, 44, 83	0
1	B	221/234 (94%)	-1.28	0 100 100	30, 43, 60, 72	0
1	C	220/234 (94%)	-1.37	0 100 100	25, 37, 55, 66	0
1	D	220/234 (94%)	-1.41	0 100 100	21, 33, 46, 61	0
1	E	222/234 (94%)	-1.35	0 100 100	28, 36, 51, 102	0
1	F	220/234 (94%)	-1.39	0 100 100	28, 36, 50, 63	0
1	G	221/234 (94%)	-1.38	0 100 100	27, 36, 51, 79	0
1	H	221/234 (94%)	-1.45	0 100 100	21, 33, 48, 71	0
1	I	221/234 (94%)	-1.38	0 100 100	26, 37, 55, 75	0
1	J	222/234 (94%)	-1.43	0 100 100	21, 28, 43, 83	0
1	K	221/234 (94%)	-1.37	0 100 100	27, 36, 50, 91	0
1	L	218/234 (93%)	-1.26	0 100 100	26, 39, 65, 82	0
1	M	222/234 (94%)	-1.27	0 100 100	27, 39, 68, 83	0
1	N	221/234 (94%)	-1.26	0 100 100	30, 43, 62, 72	0
All	All	3092/3276 (94%)	-1.36	0 100 100	21, 36, 55, 102	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

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
3	GTP	M	302	32/32	0.95	0.12	75,118,141,155	0
3	GTP	L	302	32/32	0.95	0.11	78,109,130,145	0
3	GTP	I	302	32/32	0.98	0.05	46,58,104,153	0
4	MG	L	303	1/1	0.98	0.03	49,49,49,49	0
2	ATP	E	301	31/31	0.99	0.03	29,34,39,40	0
2	ATP	F	301	31/31	0.99	0.03	25,32,36,46	0
2	ATP	L	301	31/31	0.99	0.04	34,42,51,63	0
2	ATP	N	301	31/31	0.99	0.04	36,40,48,53	0
3	GTP	B	302	32/32	0.99	0.04	46,60,136,147	0
3	GTP	D	302	32/32	0.99	0.04	34,48,88,118	0
3	GTP	G	302	32/32	0.99	0.04	38,54,95,126	0
2	ATP	B	301	31/31	0.99	0.03	35,39,45,52	0
3	GTP	J	302	32/32	0.99	0.04	30,46,99,152	0
3	GTP	K	302	32/32	0.99	0.04	35,49,95,115	0
2	ATP	K	301	31/31	0.99	0.03	30,33,38,41	0
3	GTP	A	302	32/32	0.99	0.05	32,46,96,135	0
3	GTP	C	302	32/32	0.99	0.05	46,58,126,140	0
3	GTP	E	302	32/32	0.99	0.04	35,49,108,119	0
3	GTP	F	302	32/32	0.99	0.04	38,55,128,136	0
3	GTP	H	302	32/32	0.99	0.05	36,49,126,139	0
2	ATP	M	301	31/31	0.99	0.04	33,40,52,66	0
3	GTP	N	302	32/32	0.99	0.04	48,58,130,138	0
4	MG	M	303	1/1	0.99	0.03	51,51,51,51	0
2	ATP	C	301	31/31	0.99	0.03	27,32,37,43	0
2	ATP	G	301	31/31	1.00	0.02	28,31,34,36	0
2	ATP	A	301	31/31	1.00	0.02	21,24,30,33	0
2	ATP	I	301	31/31	1.00	0.03	27,30,33,34	0
2	ATP	J	301	31/31	1.00	0.02	22,24,30,36	0
4	MG	B	303	1/1	1.00	0.03	36,36,36,36	0
4	MG	D	303	1/1	1.00	0.01	30,30,30,30	0
4	MG	G	303	1/1	1.00	0.01	31,31,31,31	0
4	MG	I	303	1/1	1.00	0.02	33,33,33,33	0
4	MG	J	303	1/1	1.00	0.01	26,26,26,26	0
4	MG	K	303	1/1	1.00	0.01	33,33,33,33	0
2	ATP	D	301	31/31	1.00	0.03	26,28,32,33	0
4	MG	A	303	1/1	1.00	0.01	26,26,26,26	0
4	MG	C	303	1/1	1.00	0.02	32,32,32,32	0

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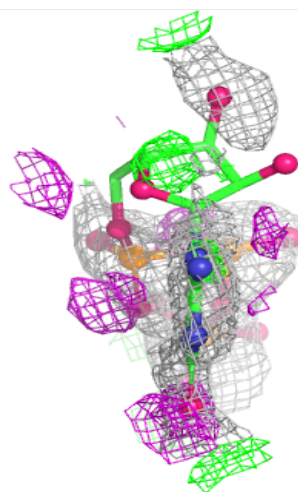
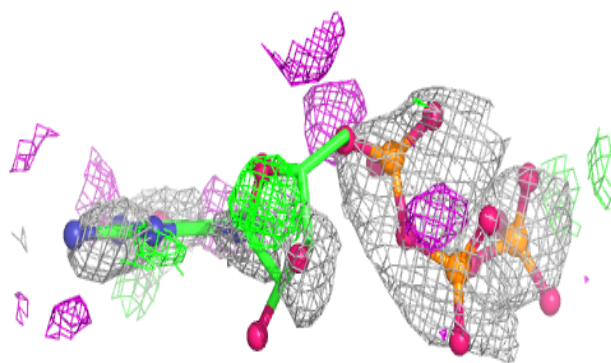
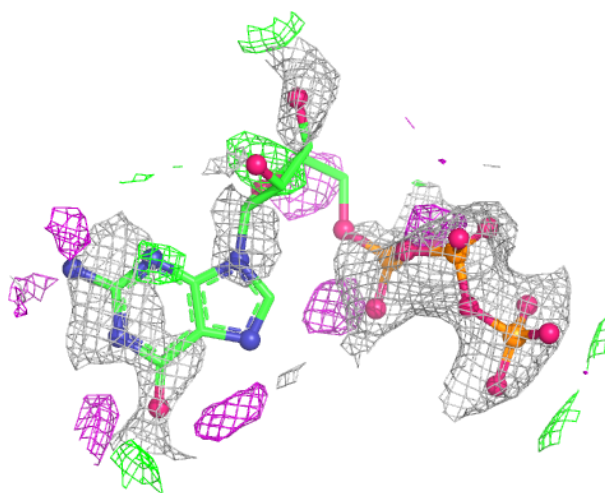
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	E	303	1/1	1.00	0.01	33,33,33,33	0
4	MG	F	303	1/1	1.00	0.01	31,31,31,31	0
4	MG	H	303	1/1	1.00	0.02	29,29,29,29	0
2	ATP	H	301	31/31	1.00	0.02	25,28,31,34	0
4	MG	N	303	1/1	1.00	0.02	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.

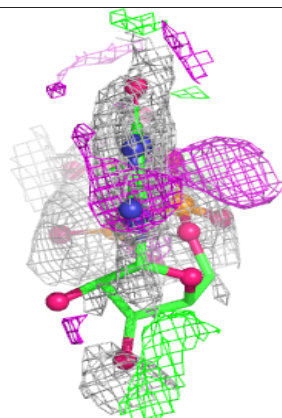
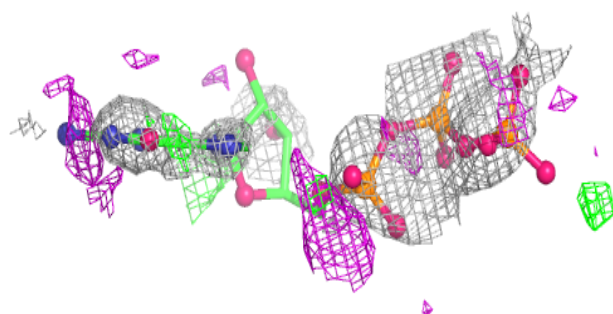
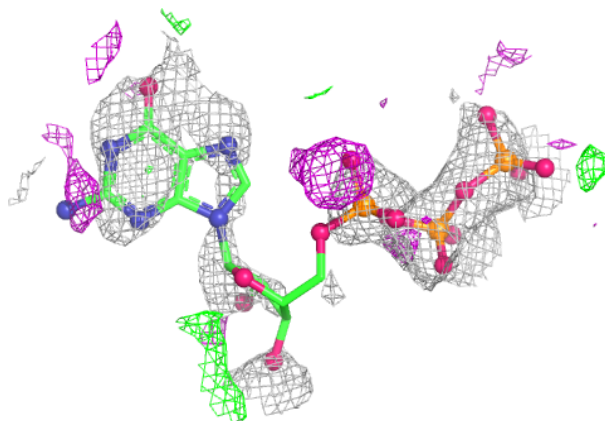
Electron density around GTP M 302:

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

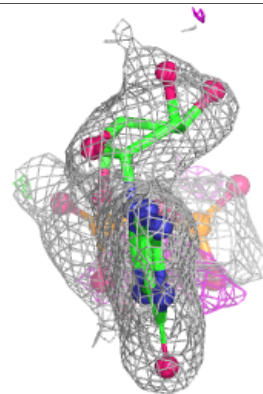
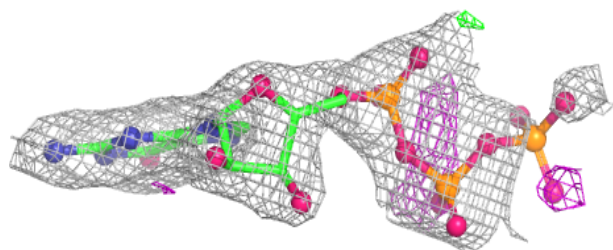
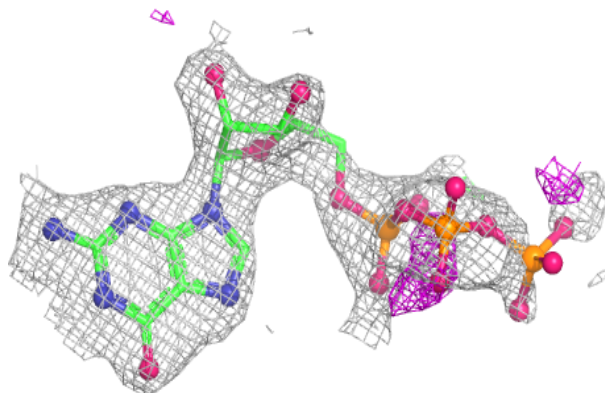


Electron density around GTP L 302:

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

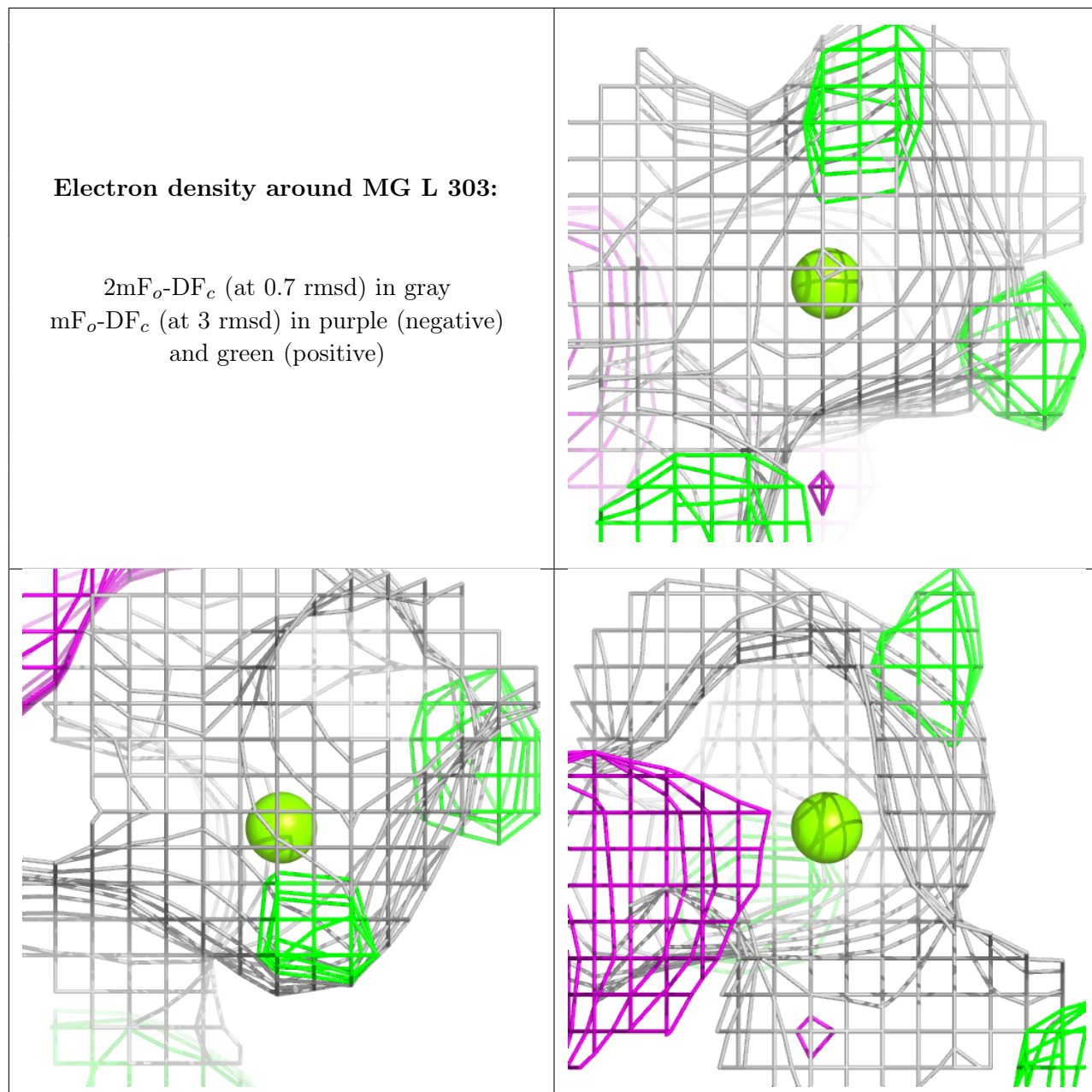
**Electron density around GTP I 302:**

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



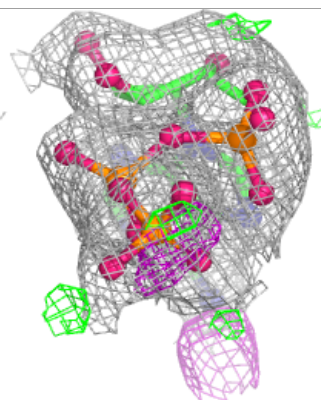
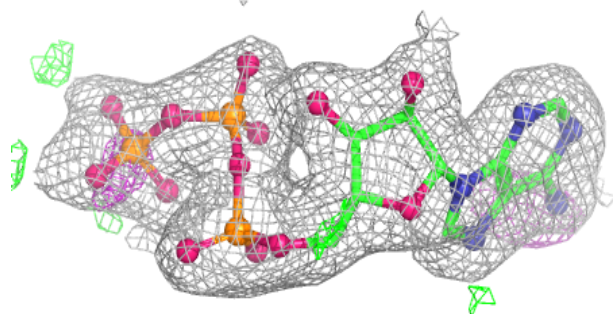
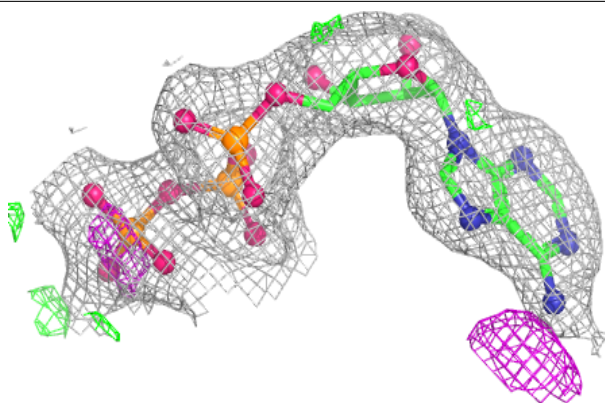
Electron density around MG L 303:

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and green (positive)

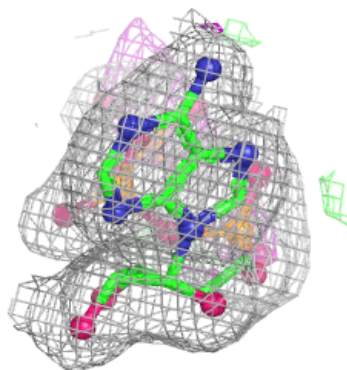
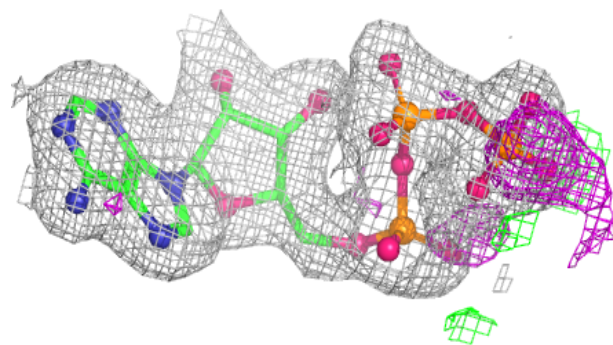
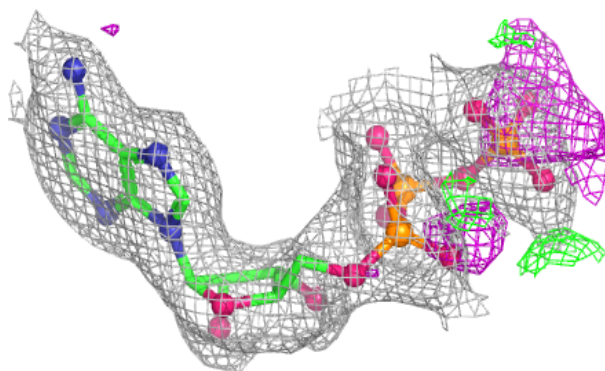


Electron density around ATP E 301:

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and green (positive)

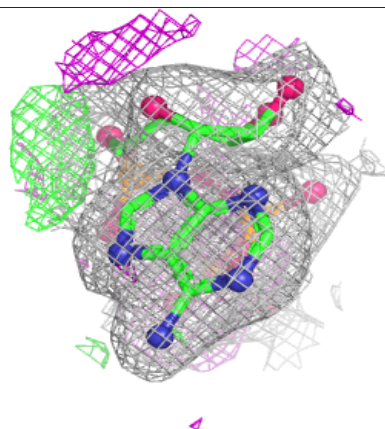
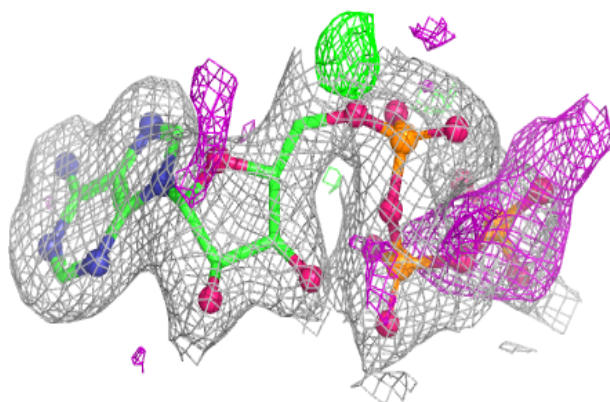
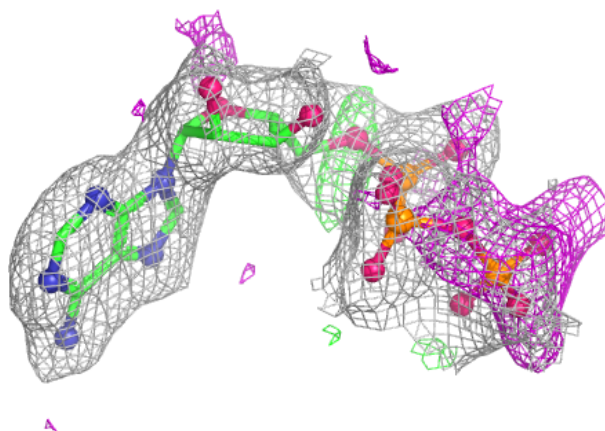
**Electron density around ATP F 301:**

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

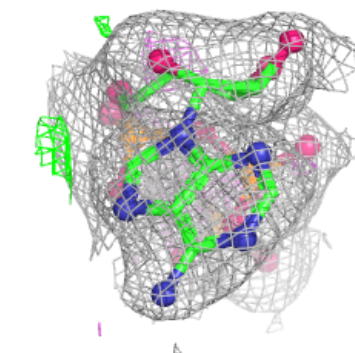
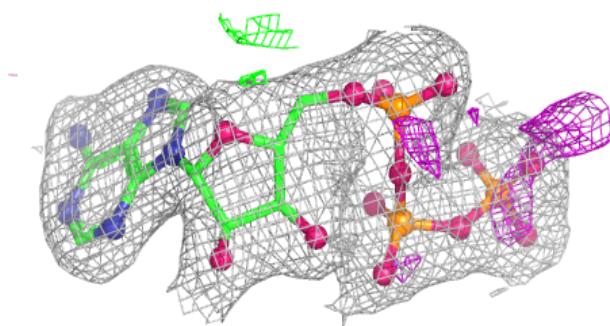
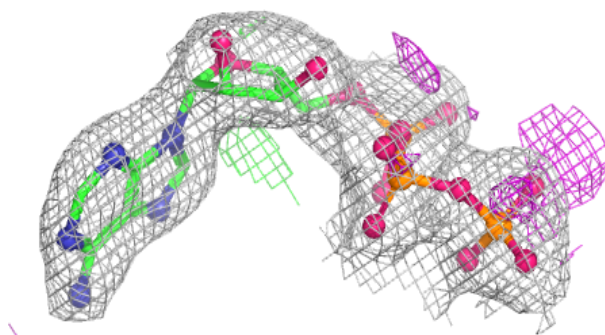


Electron density around ATP L 301:

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

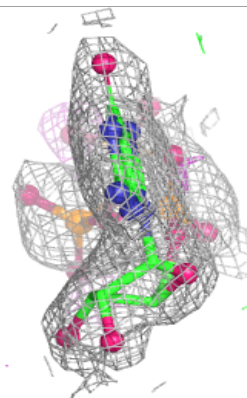
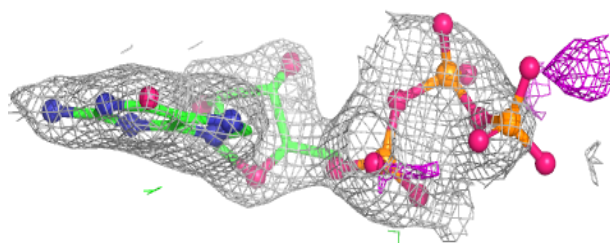
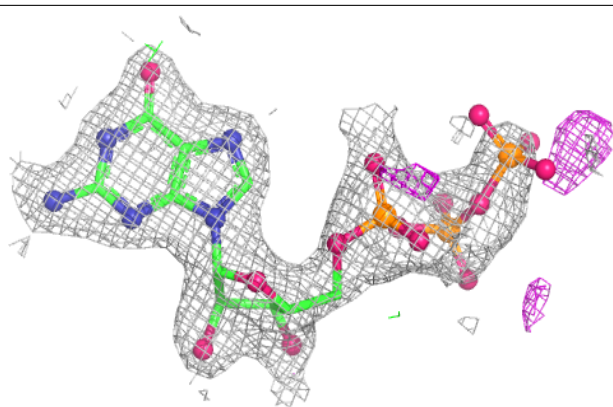
**Electron density around ATP N 301:**

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

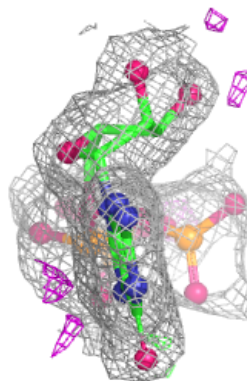
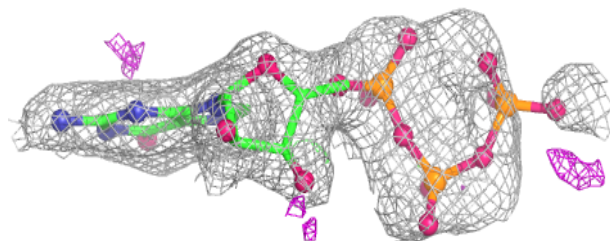
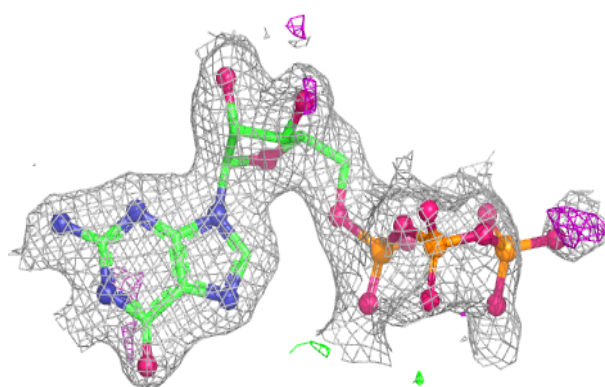


Electron density around GTP B 302:

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

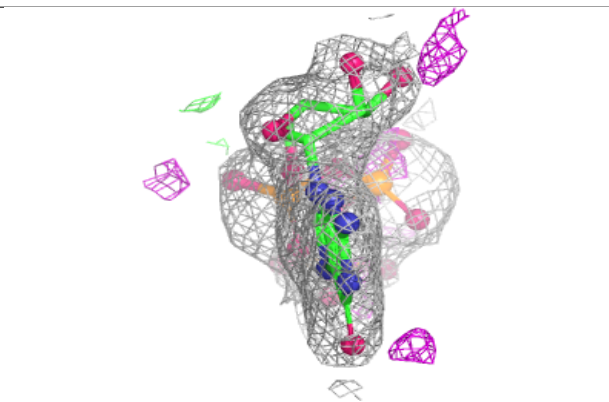
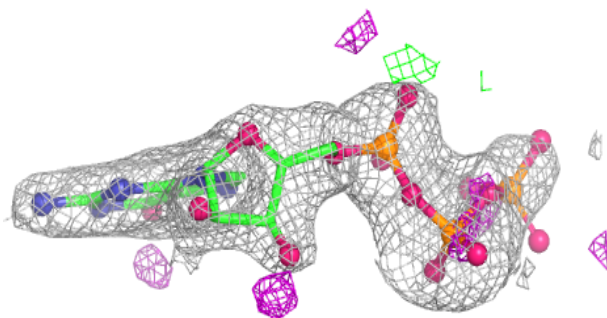
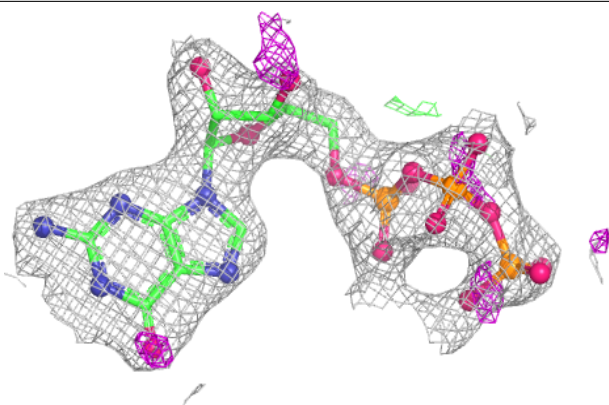
**Electron density around GTP D 302:**

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

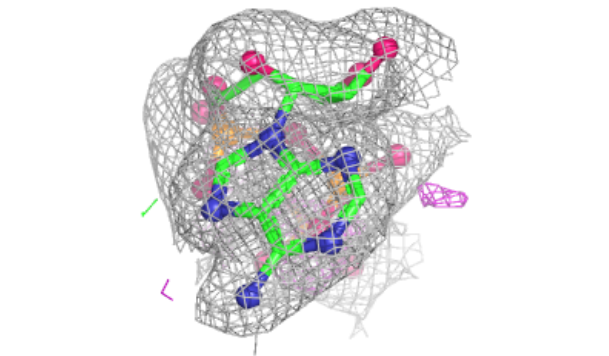
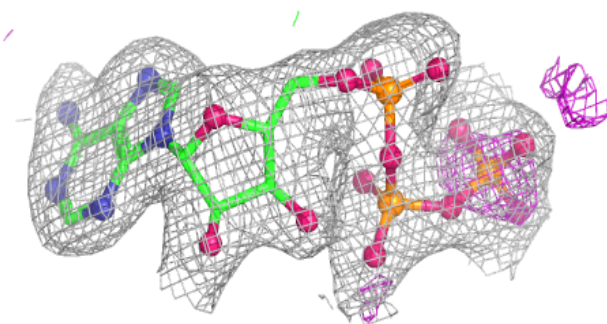
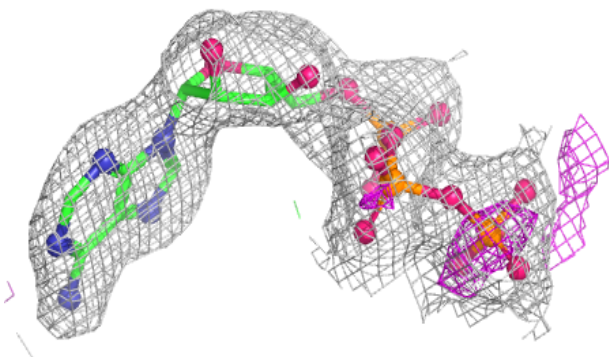


Electron density around GTP G 302:

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

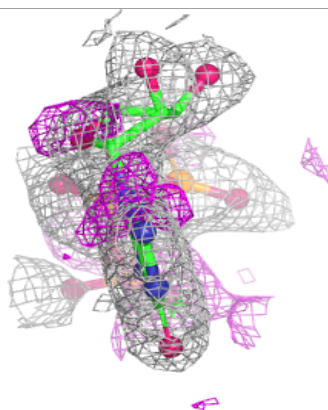
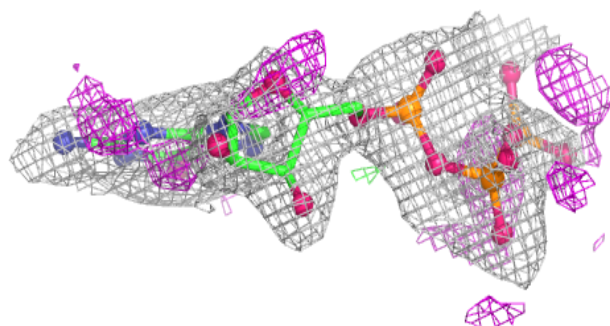
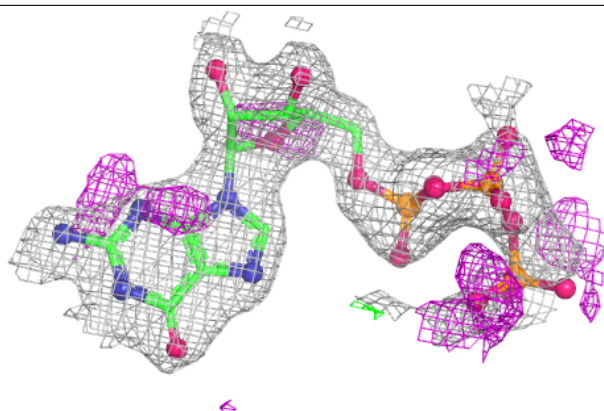
**Electron density around ATP B 301:**

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

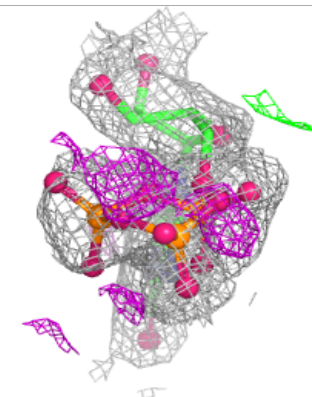
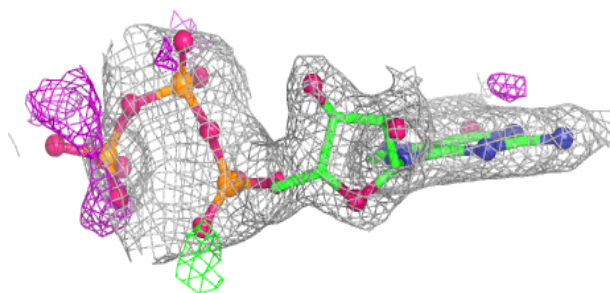
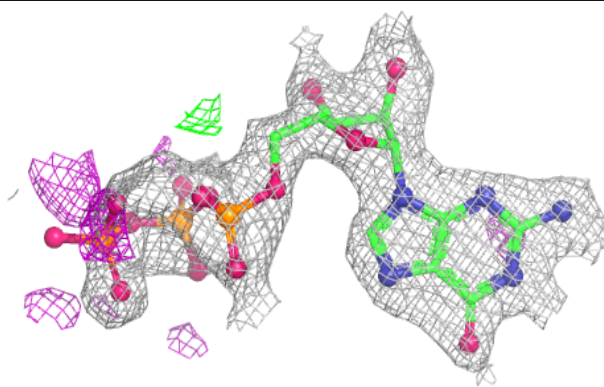


Electron density around GTP J 302:

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

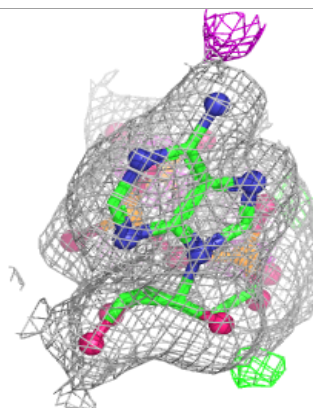
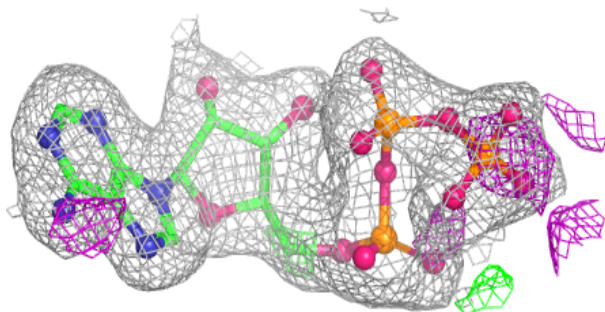
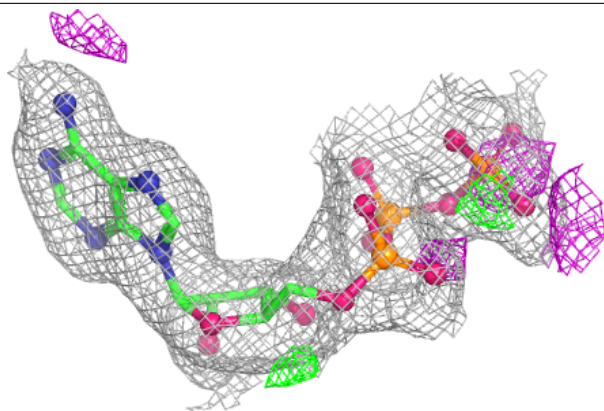
**Electron density around GTP K 302:**

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

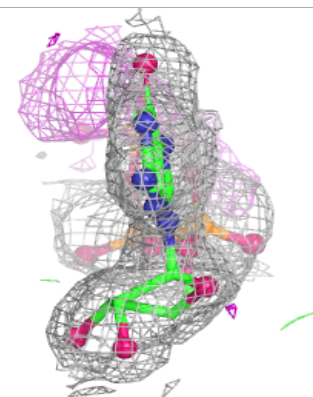
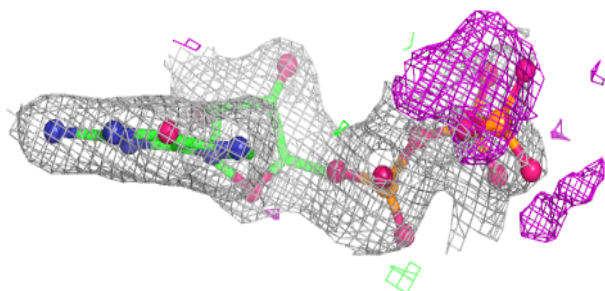
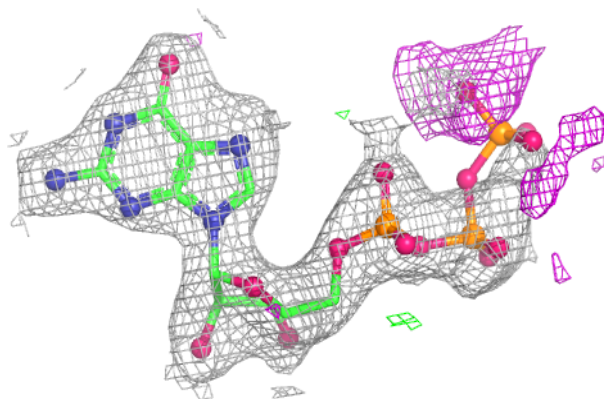


Electron density around ATP K 301:

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

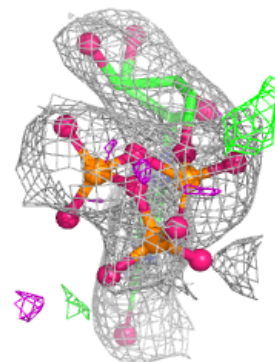
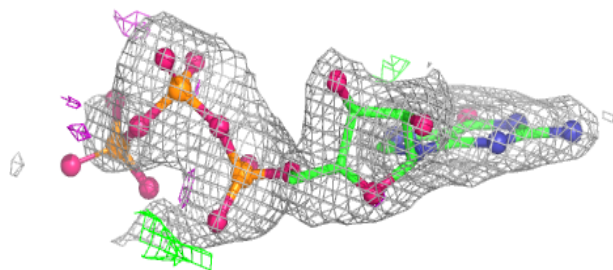
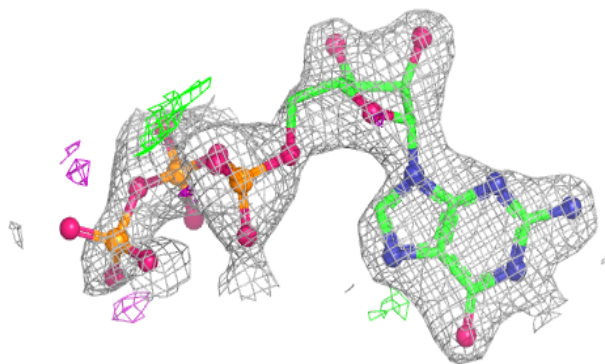
**Electron density around GTP A 302:**

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

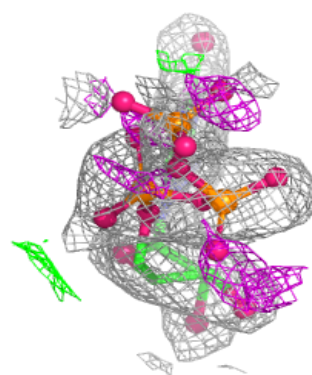
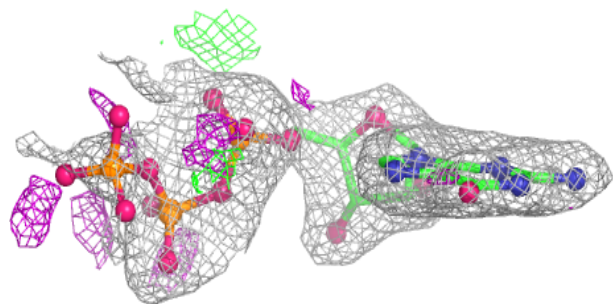
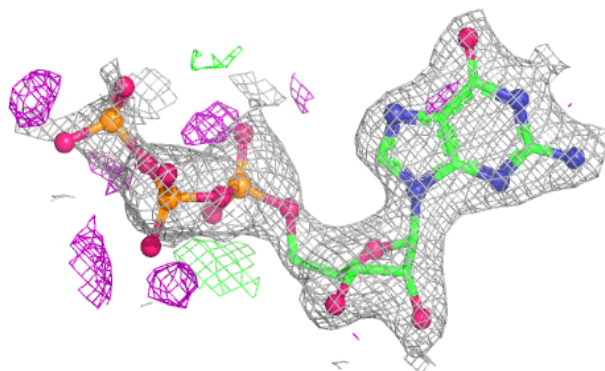


Electron density around GTP C 302:

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

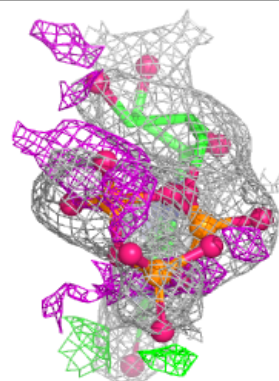
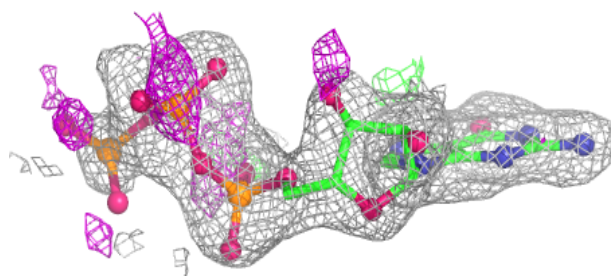
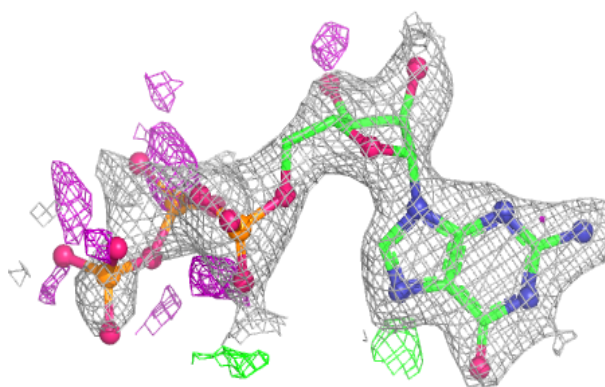
**Electron density around GTP E 302:**

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

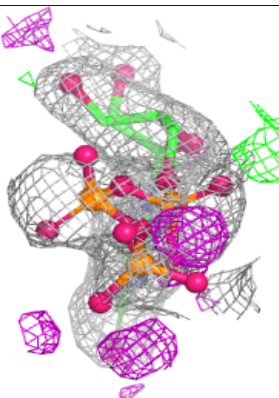
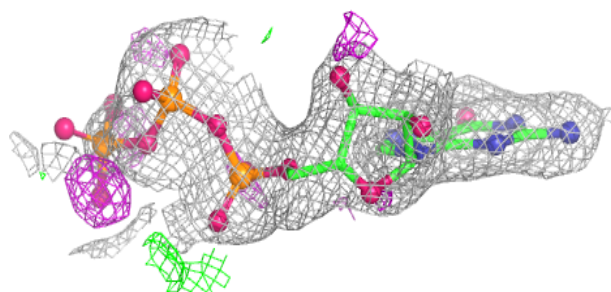
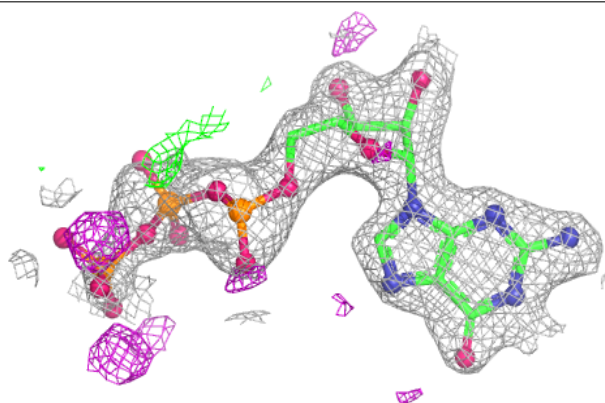


Electron density around GTP F 302:

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

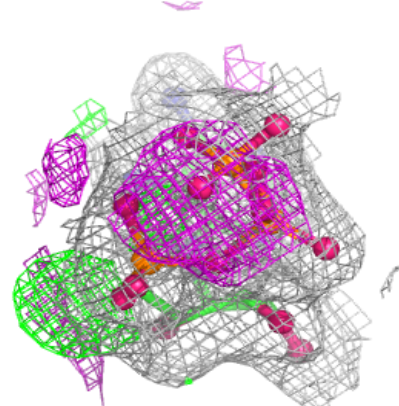
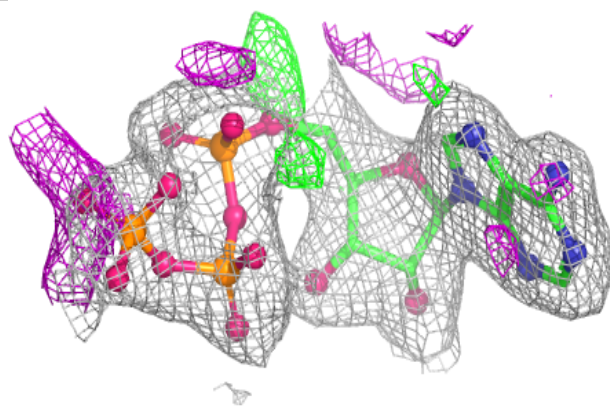
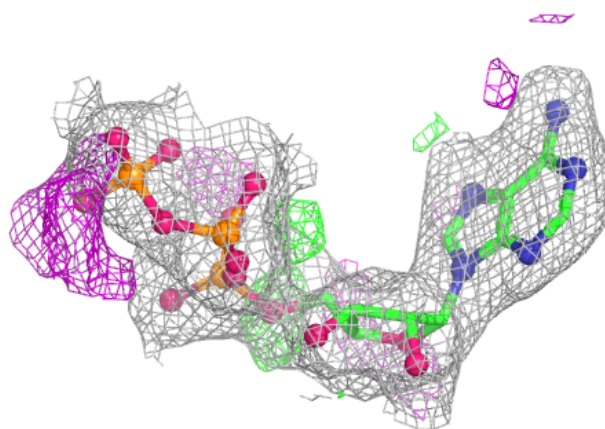
**Electron density around GTP H 302:**

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

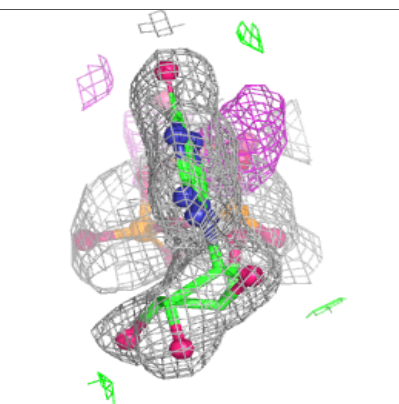
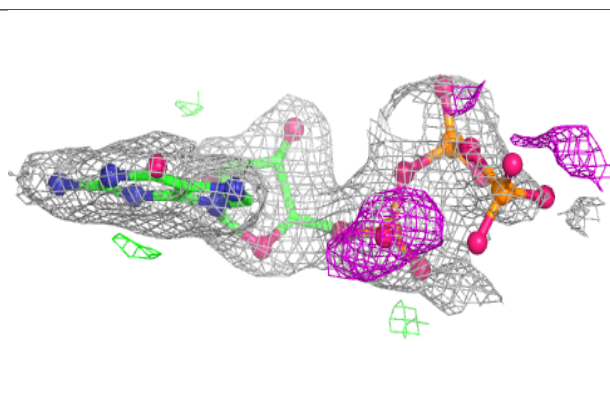
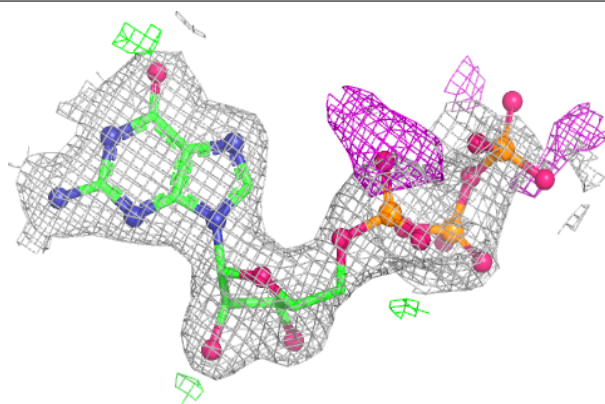


Electron density around ATP M 301:

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

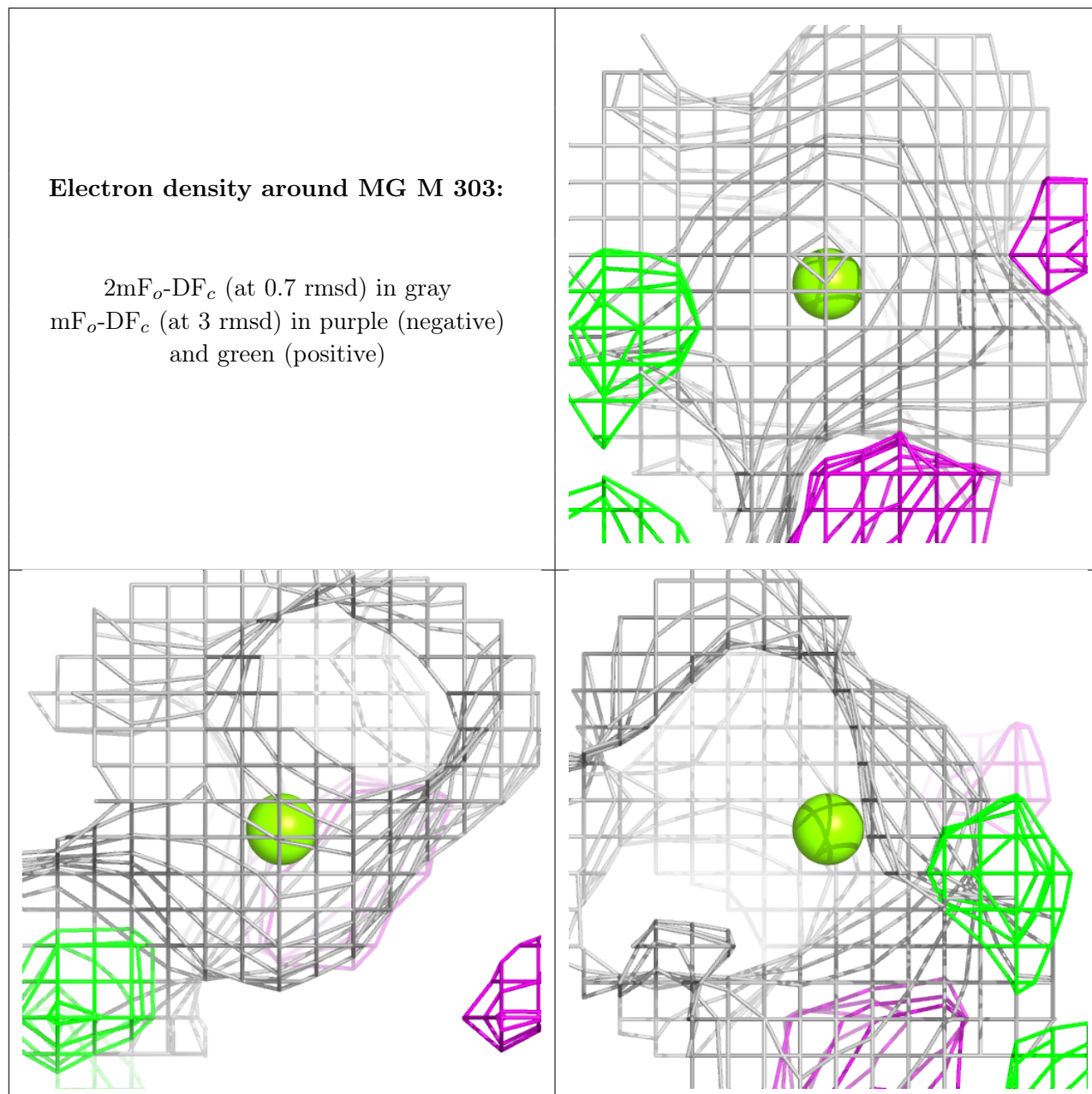
**Electron density around GTP N 302:**

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



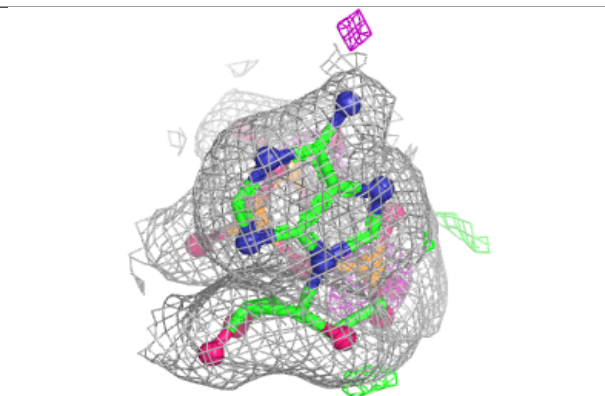
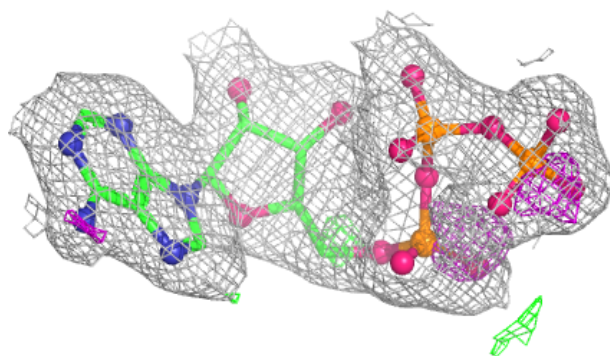
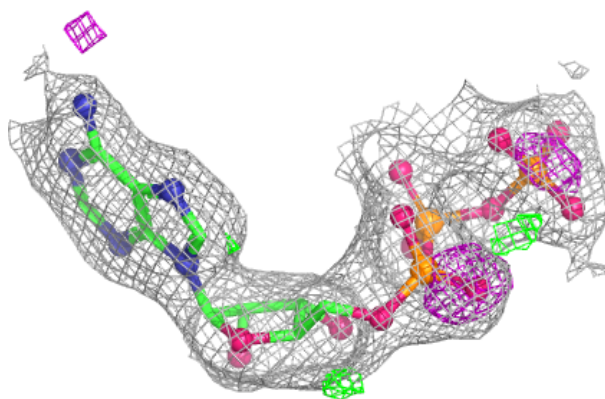
Electron density around MG M 303:

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

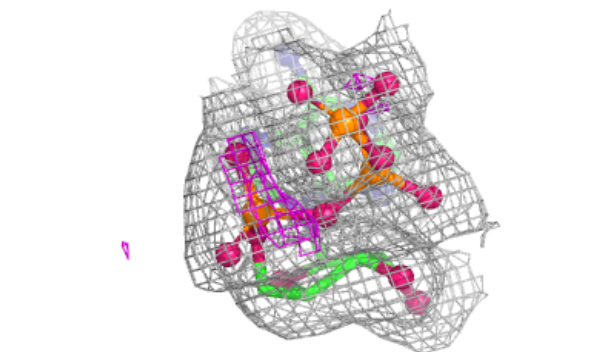
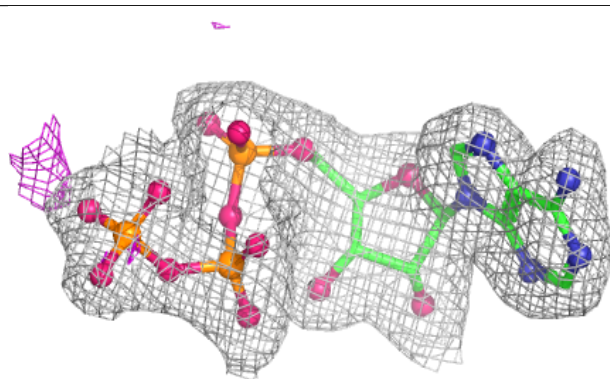
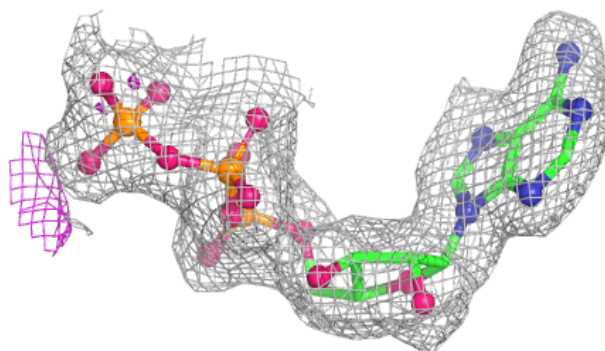


Electron density around ATP C 301:

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

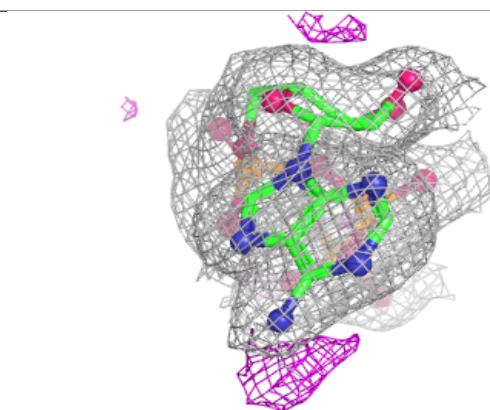
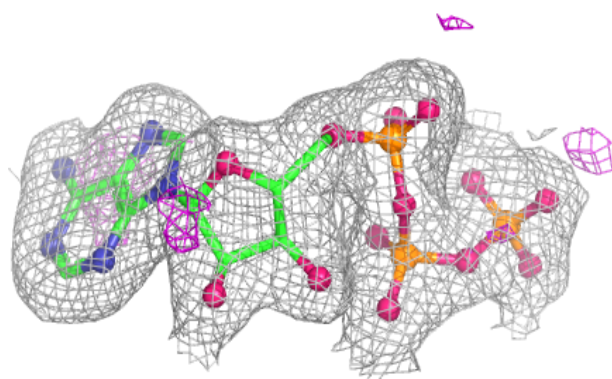
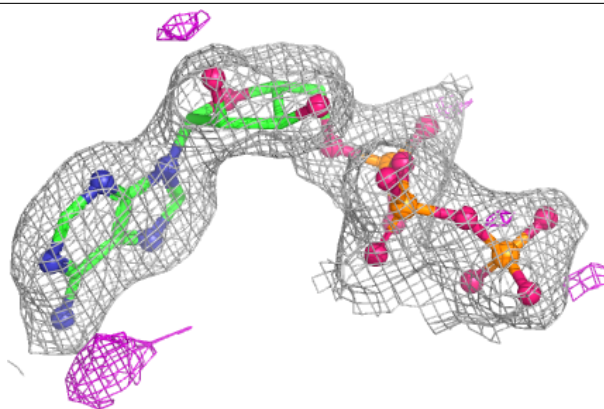
**Electron density around ATP G 301:**

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

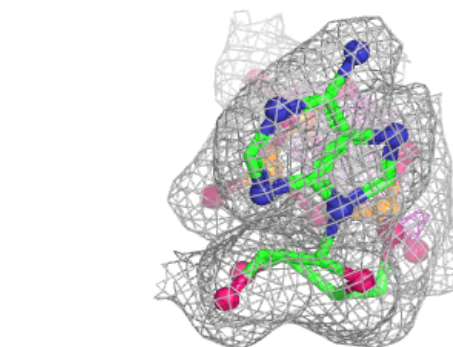
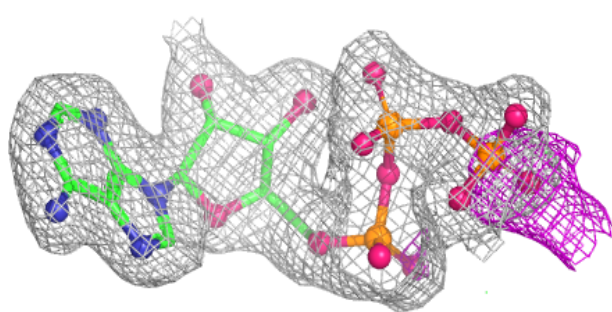
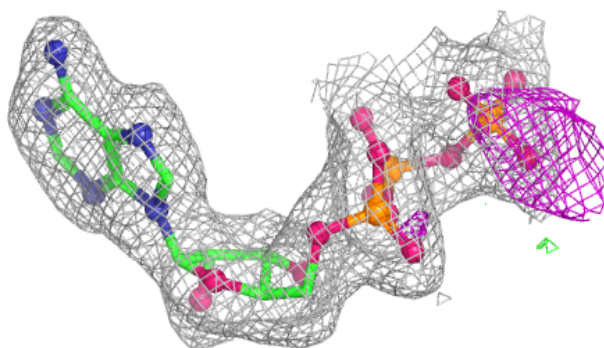


Electron density around ATP A 301:

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

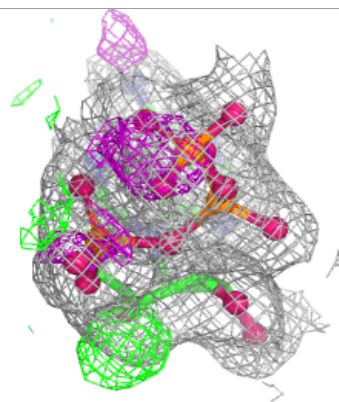
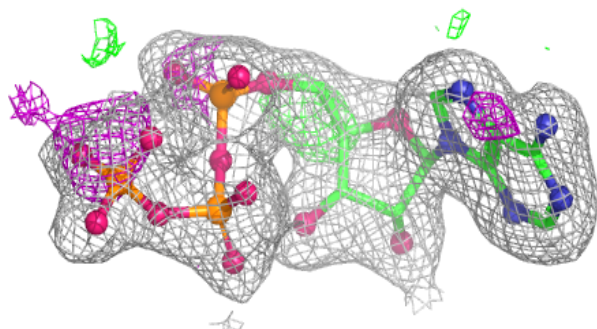
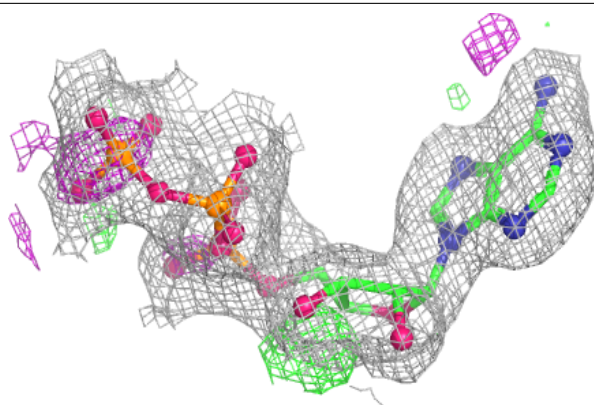
**Electron density around ATP I 301:**

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



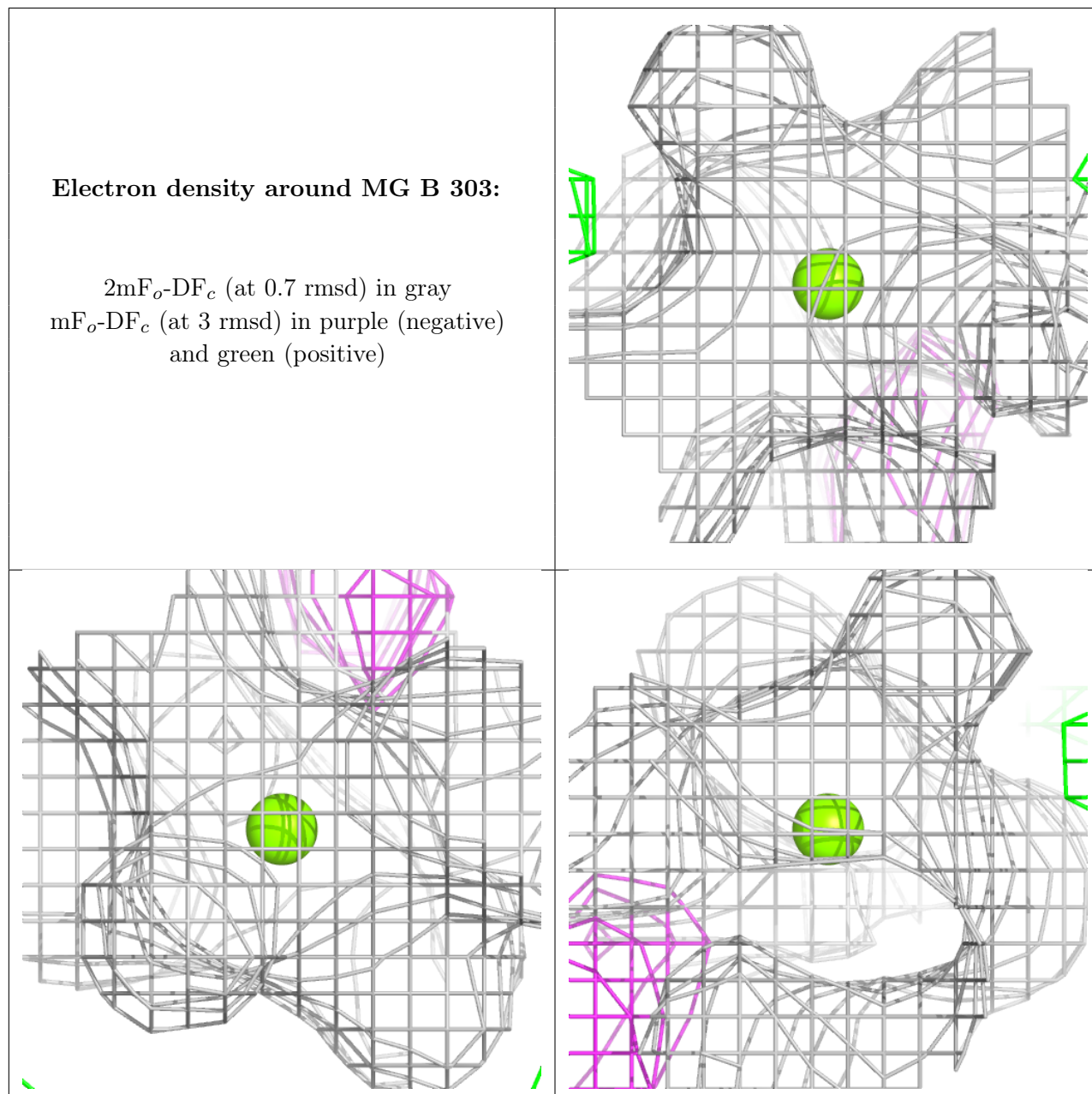
Electron density around ATP J 301:

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



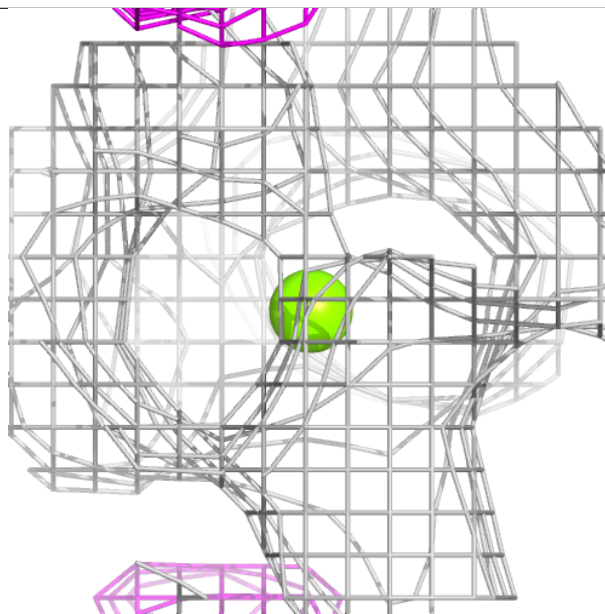
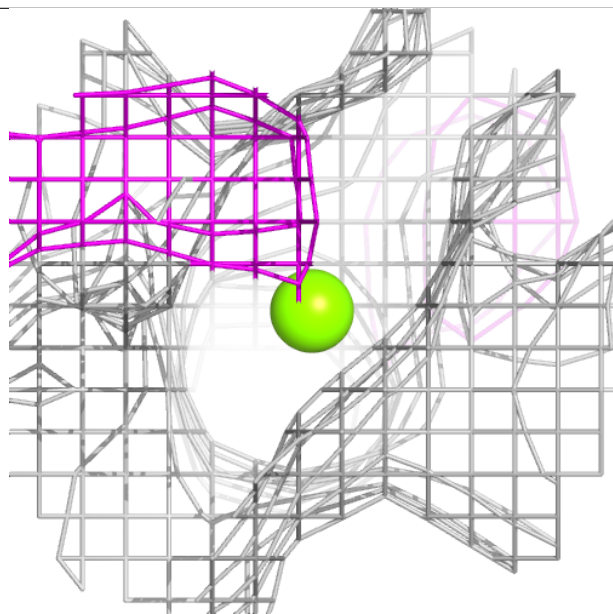
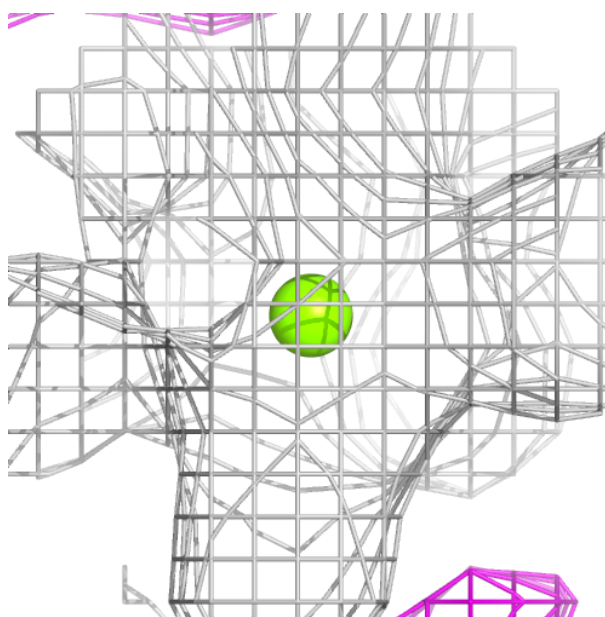
Electron density around MG B 303:

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



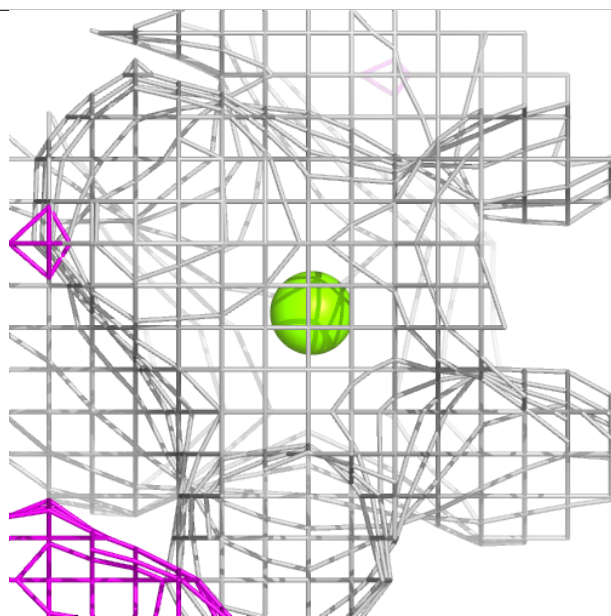
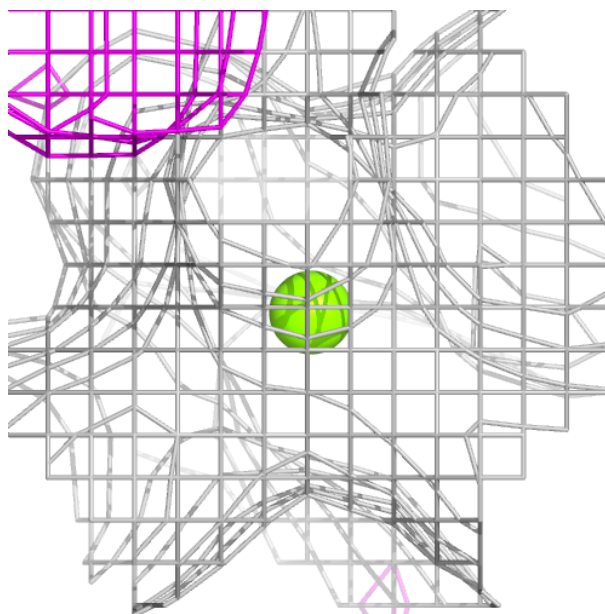
Electron density around MG D 303:

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



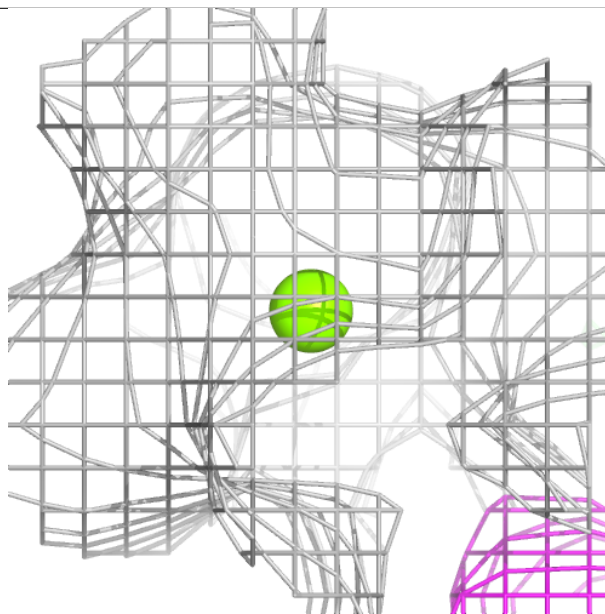
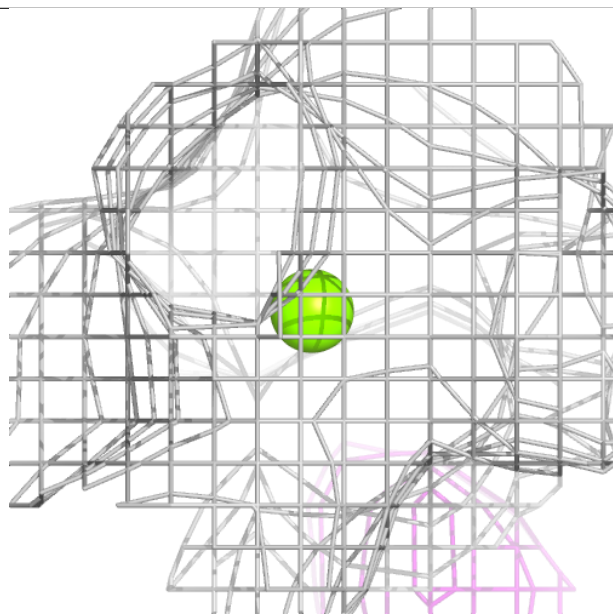
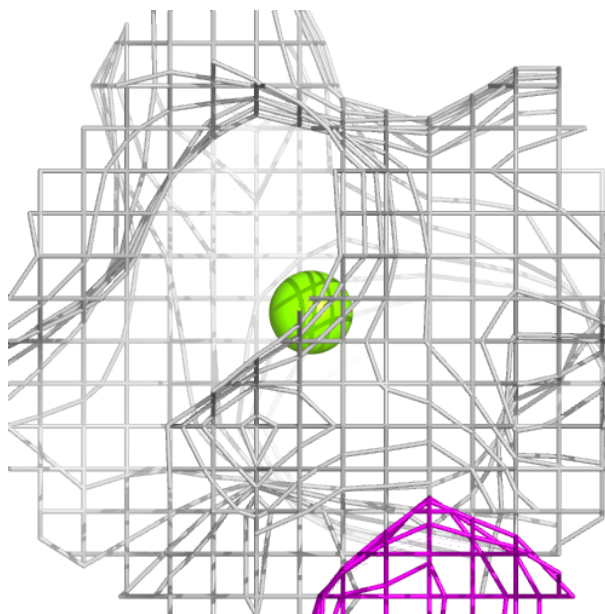
Electron density around MG G 303:

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



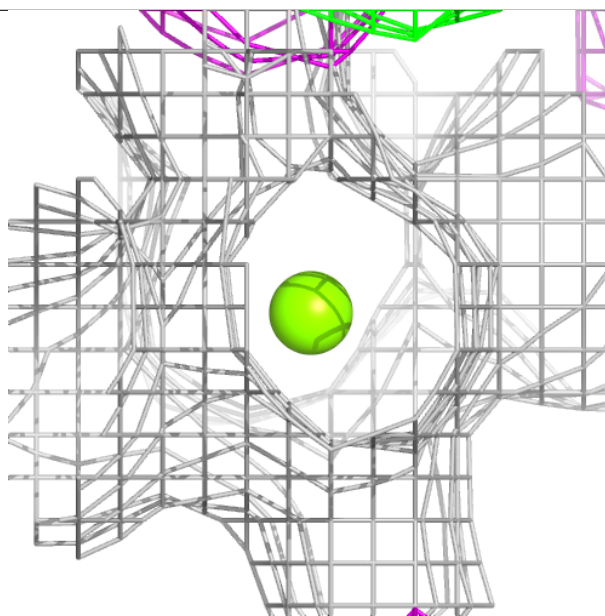
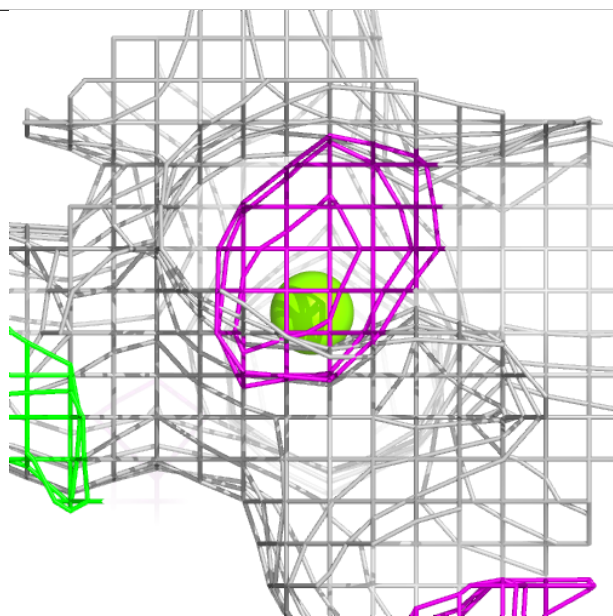
Electron density around MG I 303:

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



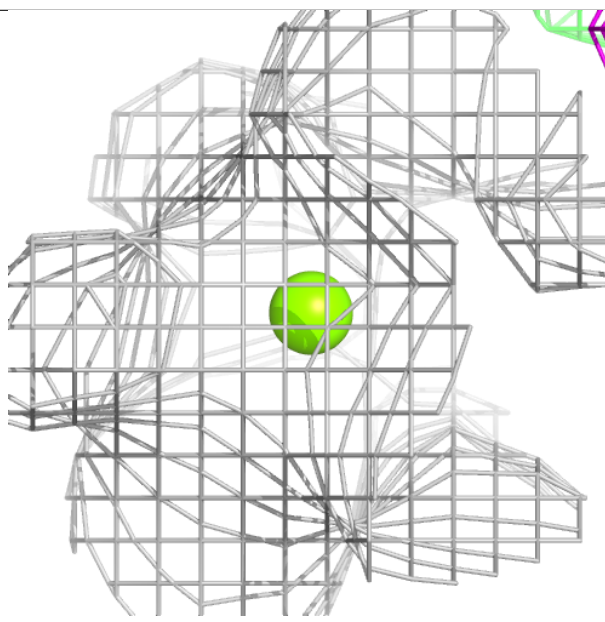
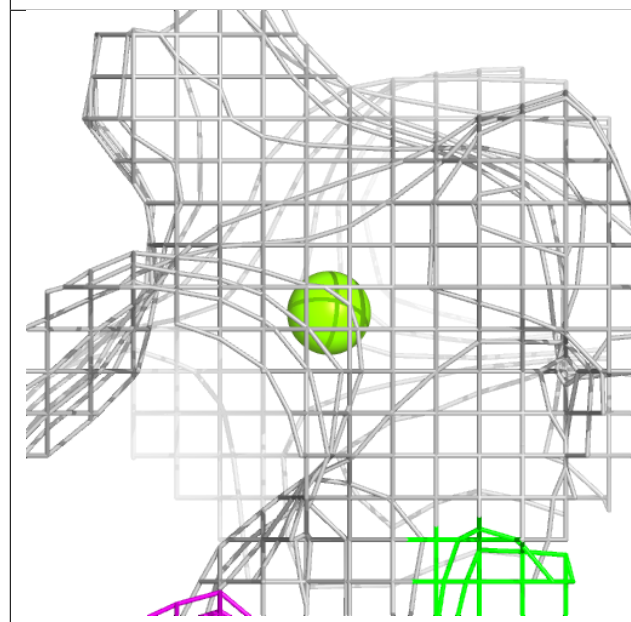
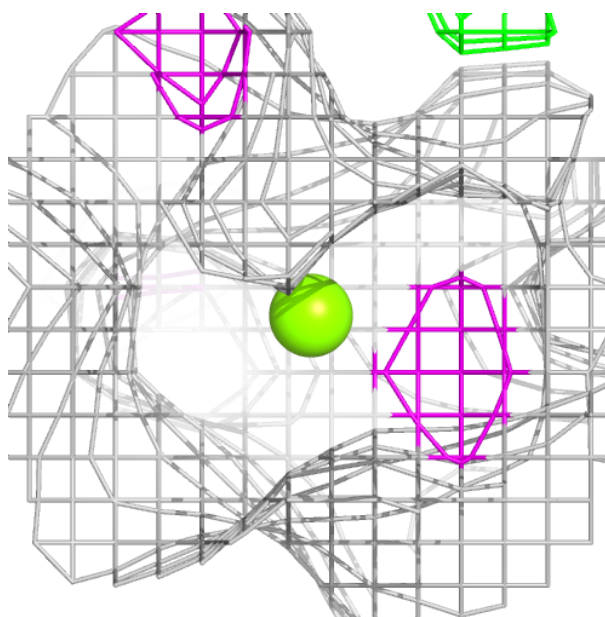
Electron density around MG J 303:

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



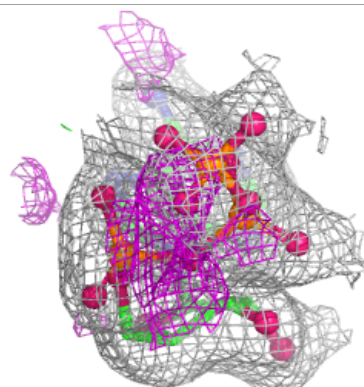
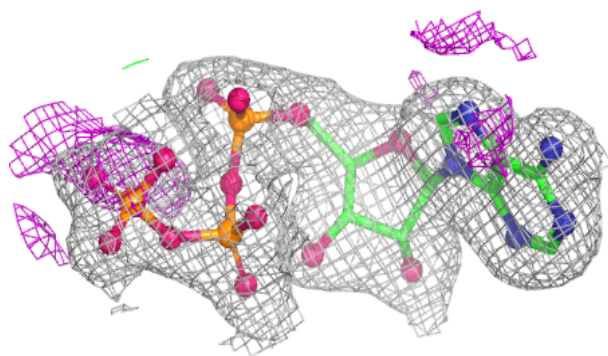
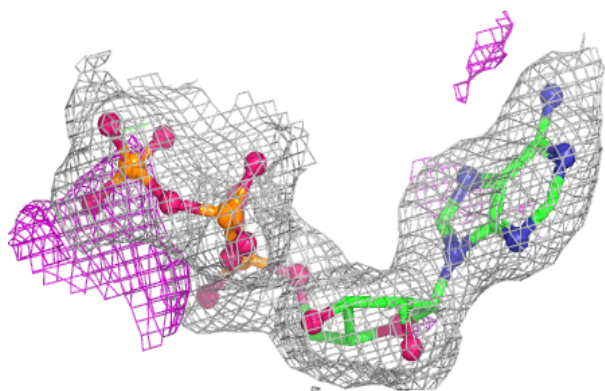
Electron density around MG K 303:

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



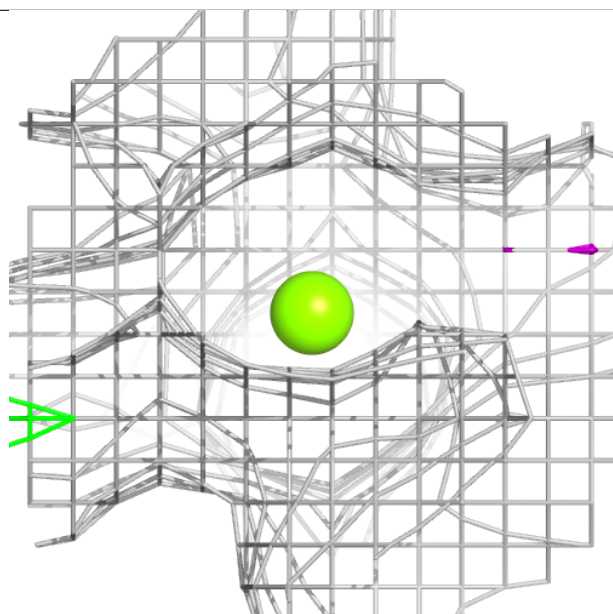
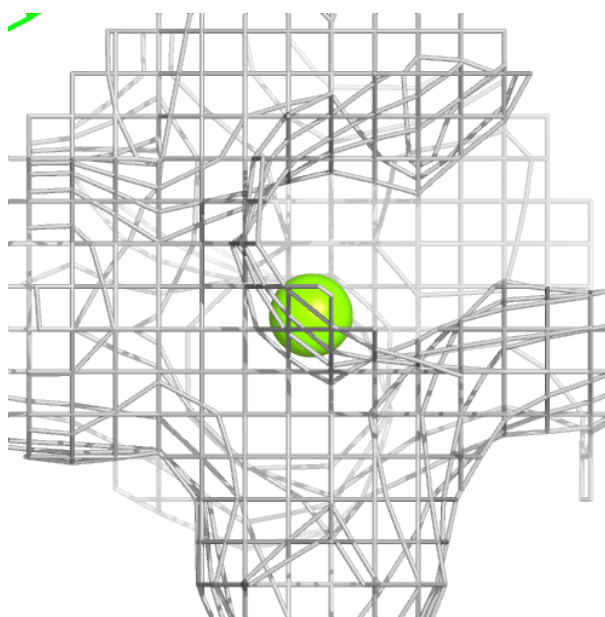
Electron density around ATP D 301:

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



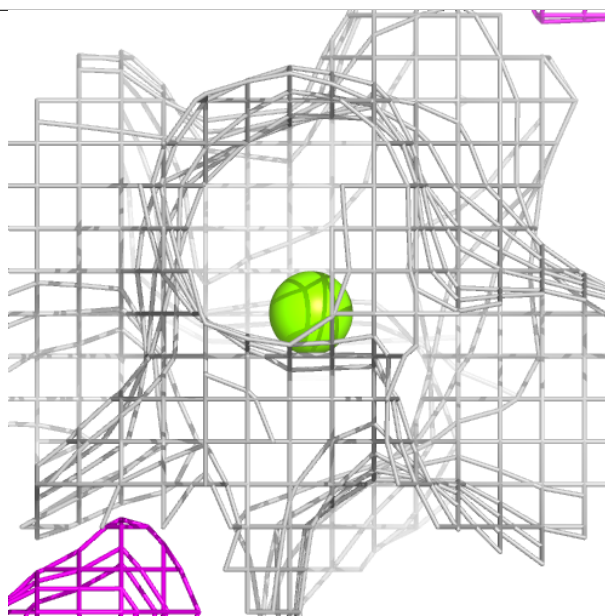
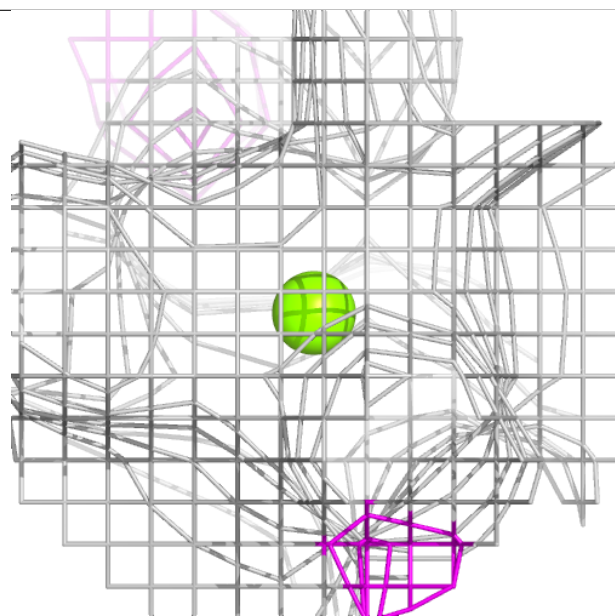
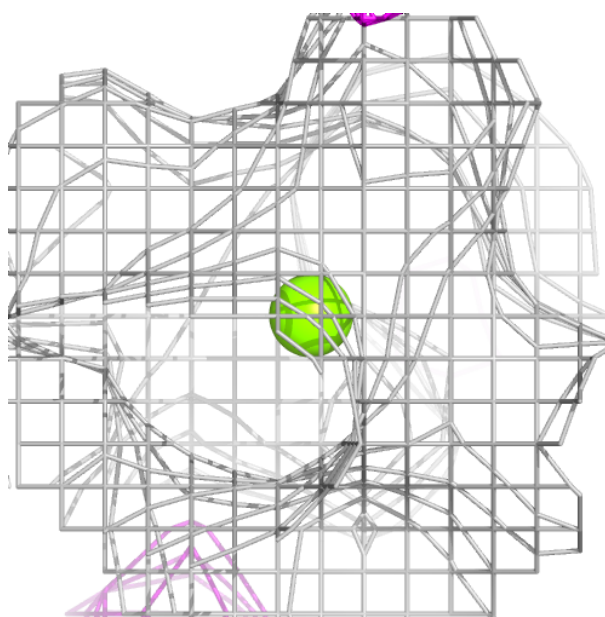
Electron density around MG A 303:

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



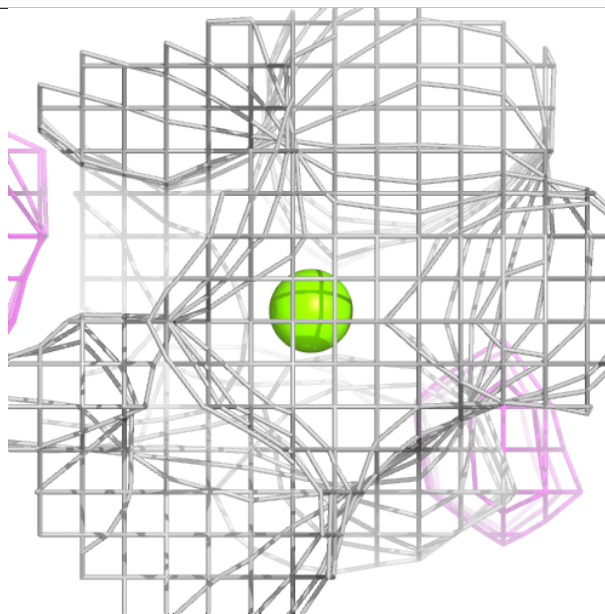
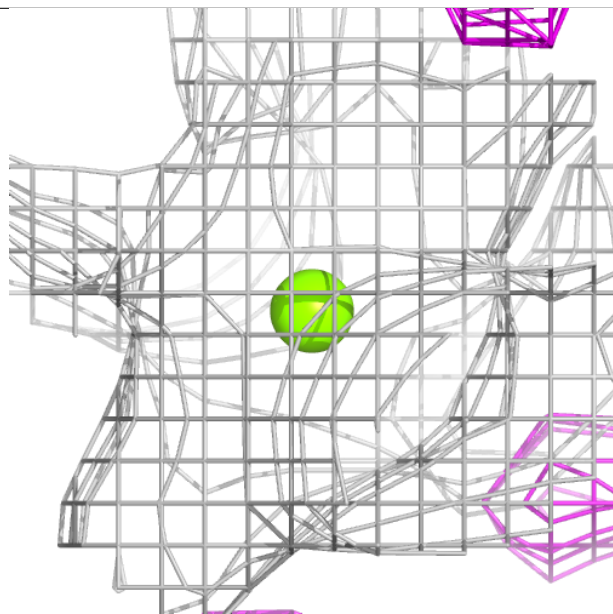
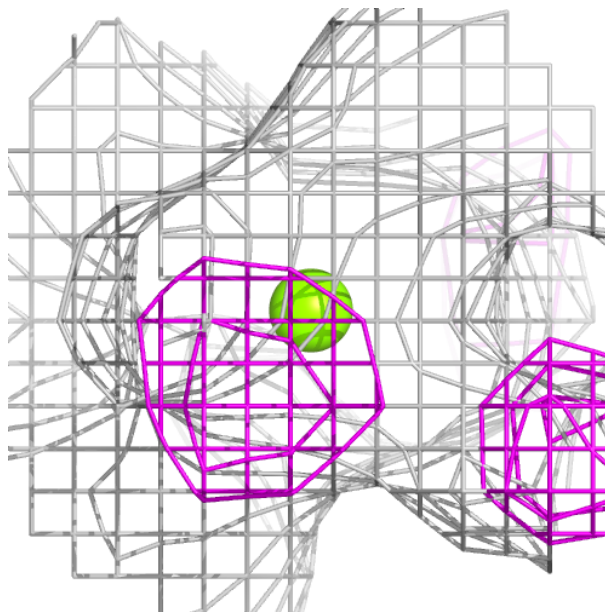
Electron density around MG C 303:

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



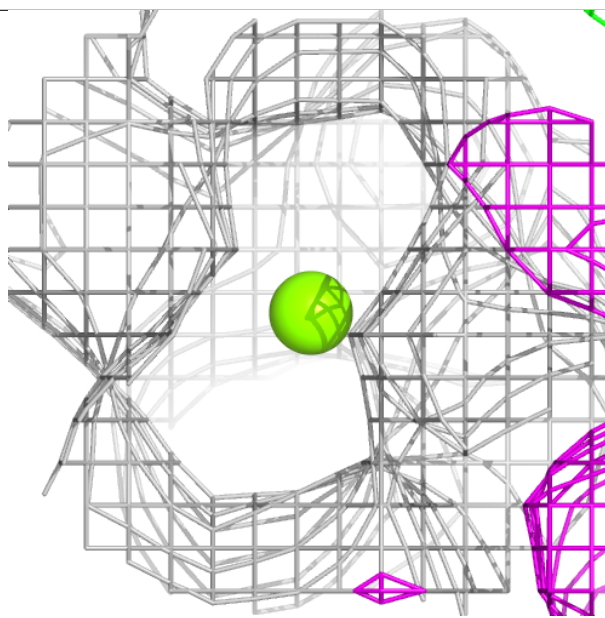
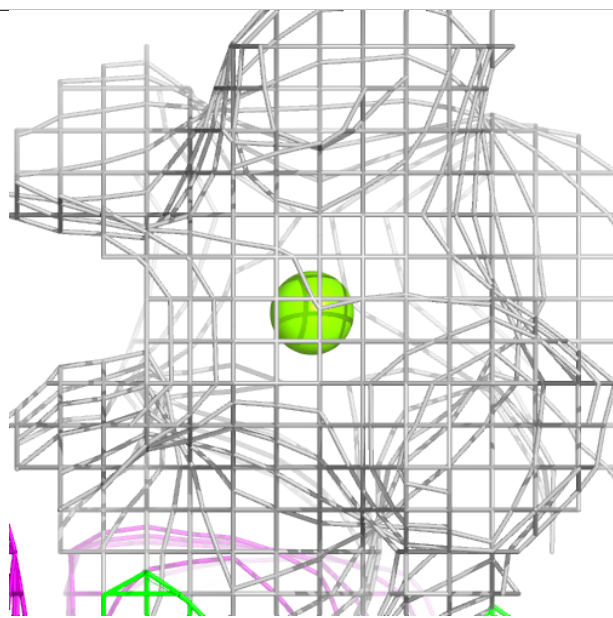
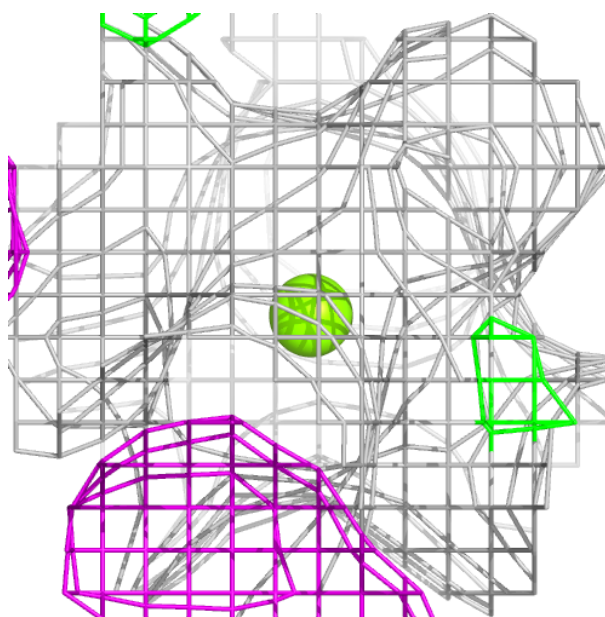
Electron density around MG E 303:

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



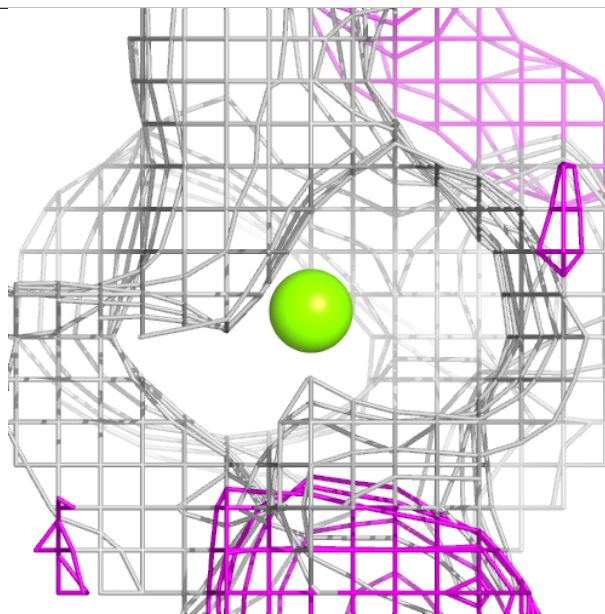
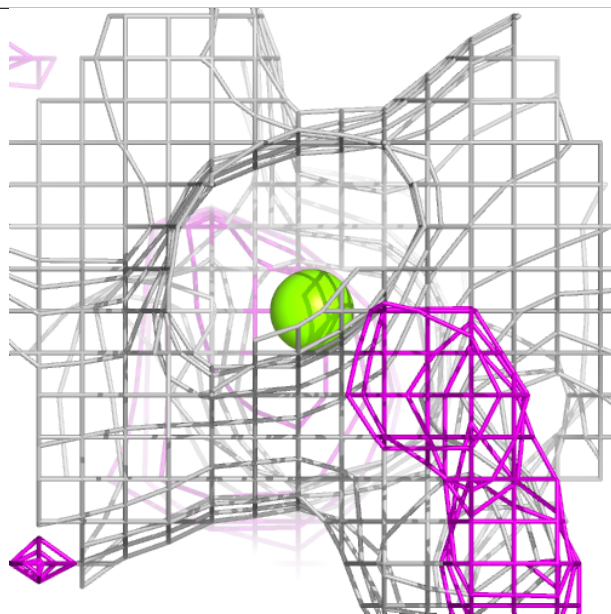
Electron density around MG F 303:

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



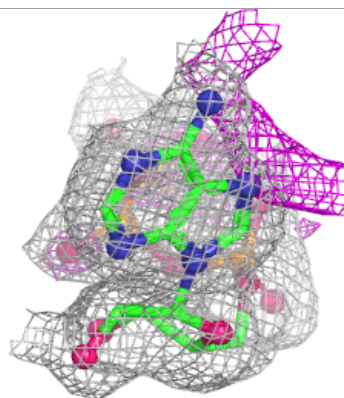
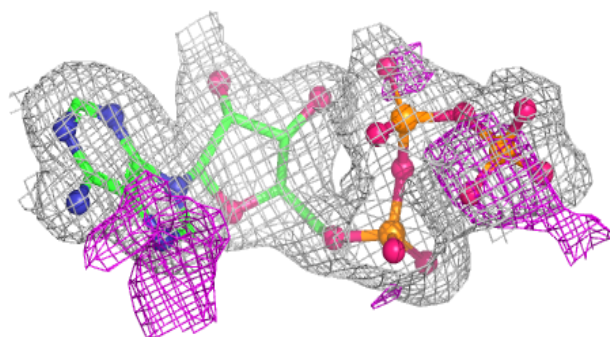
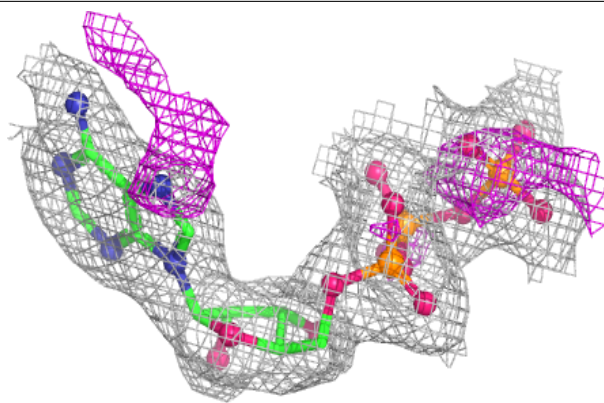
Electron density around MG H 303:

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



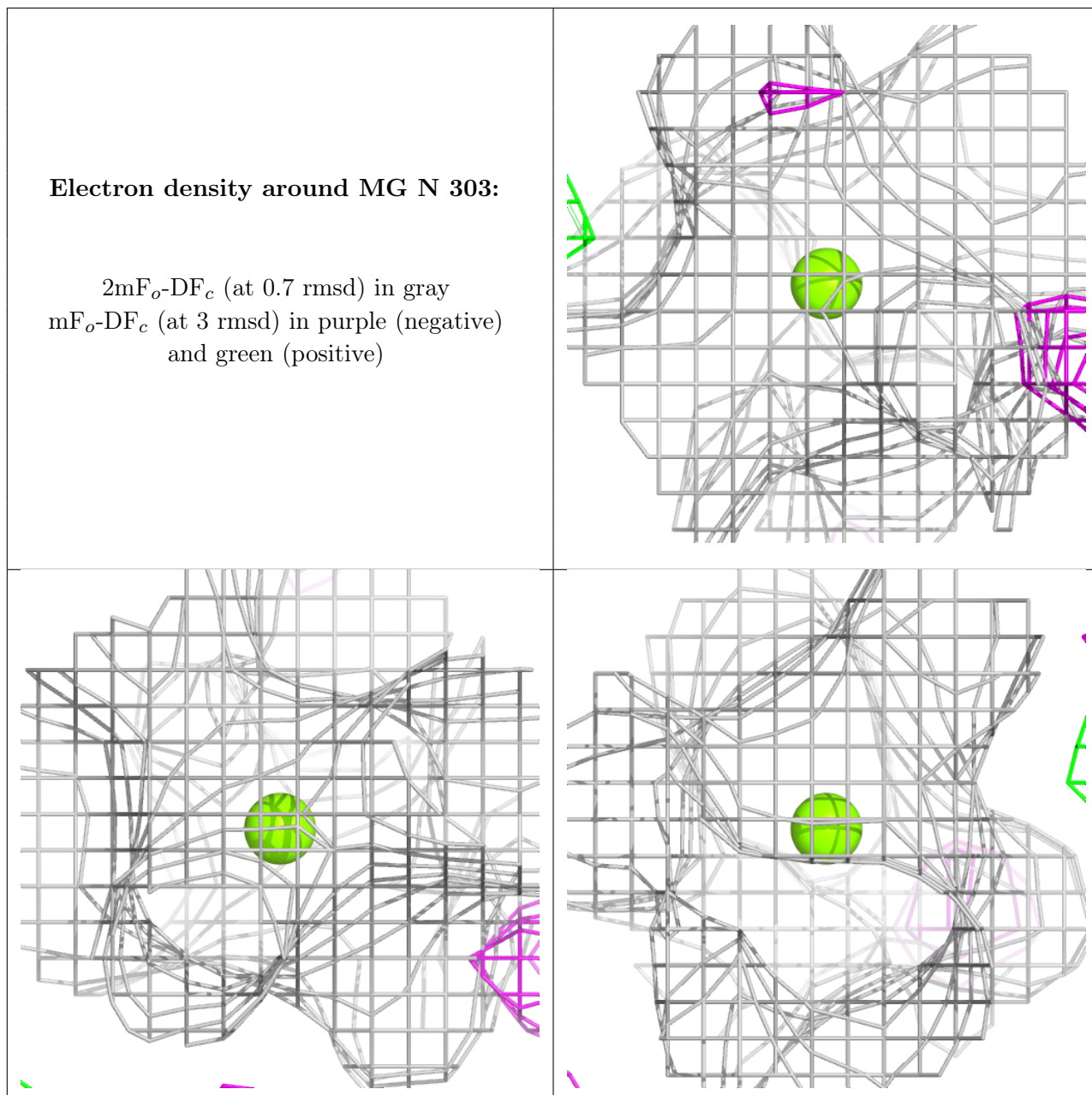
Electron density around ATP H 301:

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



Electron density around MG N 303:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.