wwPDB X-ray Structure Validation Summary Report ⓘ

May 19, 2022 – 03:41 pm BST

PDB ID	:	7PMZ
Title	:	Crystal structure of Streptomyces coelicolor guaB (IMP dehydrogenase) bound to ATP and ppGpp at 2.0 A resolution
Authors	:	Fernandez-Justel, D.; Revuelta, J.L.; Buey, R.M.
Deposited on	:	2021-09-04
Resolution	:	2.03 Å(reported)

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

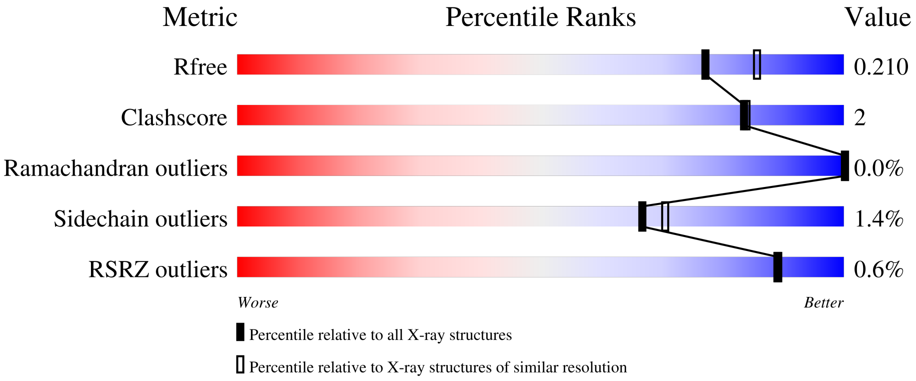
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

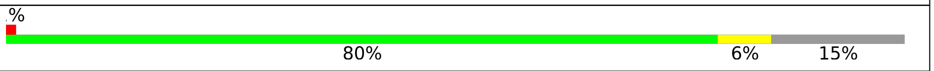
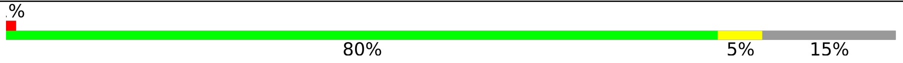
The reported resolution of this entry is 2.03 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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 <=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	504	
1	B	504	
1	C	504	
1	D	504	
1	E	504	

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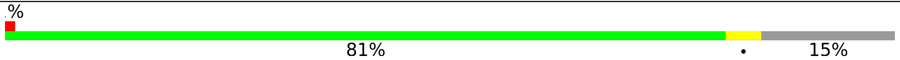
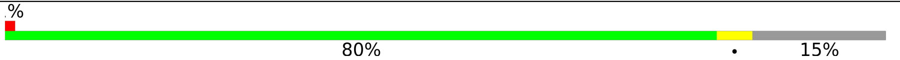
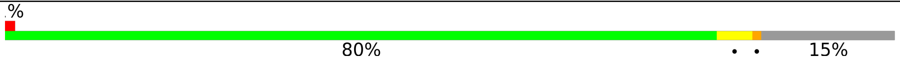
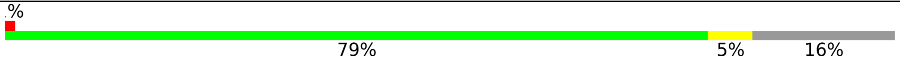
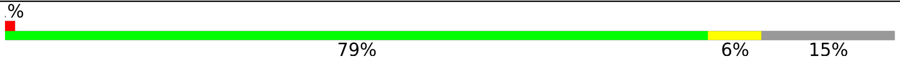
Mol	Chain	Length	Quality of chain
1	F	504	
1	G	504	
1	H	504	
1	I	504	
1	J	504	
1	K	504	
1	L	504	
1	M	504	
1	N	504	
1	O	504	
1	P	504	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 101645 atoms, of which 48699 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Inosine-5'-monophosphate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	428	Total	C	H	N	O	S	0	0	0
			6157	1912	3101	547	582	15			
1	B	430	Total	C	H	N	O	S	0	0	0
			6058	1894	3025	540	585	14			
1	C	427	Total	C	H	N	O	S	0	0	0
			5937	1860	2959	532	572	14			
1	D	428	Total	C	H	N	O	S	0	0	0
			6102	1902	3062	539	584	15			
1	E	428	Total	C	H	N	O	S	0	0	0
			6173	1916	3103	550	589	15			
1	F	428	Total	C	H	N	O	S	0	0	0
			6214	1924	3131	551	593	15			
1	G	426	Total	C	H	N	O	S	0	0	0
			5871	1852	2915	529	560	15			
1	H	428	Total	C	H	N	O	S	0	0	0
			6211	1923	3132	551	590	15			
1	I	427	Total	C	H	N	O	S	0	0	0
			5740	1818	2829	518	561	14			
1	J	428	Total	C	H	N	O	S	0	0	0
			6056	1893	3032	534	582	15			
1	K	428	Total	C	H	N	O	S	0	0	0
			6098	1903	3062	536	582	15			
1	L	427	Total	C	H	N	O	S	0	0	0
			6111	1901	3073	543	579	15			
1	M	428	Total	C	H	N	O	S	0	0	0
			6137	1908	3085	545	584	15			
1	N	428	Total	C	H	N	O	S	0	0	0
			6067	1893	3041	536	582	15			
1	O	425	Total	C	H	N	O	S	0	0	0
			5780	1831	2850	522	565	12			
1	P	428	Total	C	H	N	O	S	0	0	0
			5922	1864	2947	528	568	15			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q9L0I7
A	-1	SER	-	expression tag	UNP Q9L0I7
A	0	HIS	-	expression tag	UNP Q9L0I7
B	-2	GLY	-	expression tag	UNP Q9L0I7
B	-1	SER	-	expression tag	UNP Q9L0I7
B	0	HIS	-	expression tag	UNP Q9L0I7
C	-2	GLY	-	expression tag	UNP Q9L0I7
C	-1	SER	-	expression tag	UNP Q9L0I7
C	0	HIS	-	expression tag	UNP Q9L0I7
D	-2	GLY	-	expression tag	UNP Q9L0I7
D	-1	SER	-	expression tag	UNP Q9L0I7
D	0	HIS	-	expression tag	UNP Q9L0I7
E	-2	GLY	-	expression tag	UNP Q9L0I7
E	-1	SER	-	expression tag	UNP Q9L0I7
E	0	HIS	-	expression tag	UNP Q9L0I7
F	-2	GLY	-	expression tag	UNP Q9L0I7
F	-1	SER	-	expression tag	UNP Q9L0I7
F	0	HIS	-	expression tag	UNP Q9L0I7
G	-2	GLY	-	expression tag	UNP Q9L0I7
G	-1	SER	-	expression tag	UNP Q9L0I7
G	0	HIS	-	expression tag	UNP Q9L0I7
H	-2	GLY	-	expression tag	UNP Q9L0I7
H	-1	SER	-	expression tag	UNP Q9L0I7
H	0	HIS	-	expression tag	UNP Q9L0I7
I	-2	GLY	-	expression tag	UNP Q9L0I7
I	-1	SER	-	expression tag	UNP Q9L0I7
I	0	HIS	-	expression tag	UNP Q9L0I7
J	-2	GLY	-	expression tag	UNP Q9L0I7
J	-1	SER	-	expression tag	UNP Q9L0I7
J	0	HIS	-	expression tag	UNP Q9L0I7
K	-2	GLY	-	expression tag	UNP Q9L0I7
K	-1	SER	-	expression tag	UNP Q9L0I7
K	0	HIS	-	expression tag	UNP Q9L0I7
L	-2	GLY	-	expression tag	UNP Q9L0I7
L	-1	SER	-	expression tag	UNP Q9L0I7
L	0	HIS	-	expression tag	UNP Q9L0I7
M	-2	GLY	-	expression tag	UNP Q9L0I7
M	-1	SER	-	expression tag	UNP Q9L0I7
M	0	HIS	-	expression tag	UNP Q9L0I7
N	-2	GLY	-	expression tag	UNP Q9L0I7
N	-1	SER	-	expression tag	UNP Q9L0I7
N	0	HIS	-	expression tag	UNP Q9L0I7

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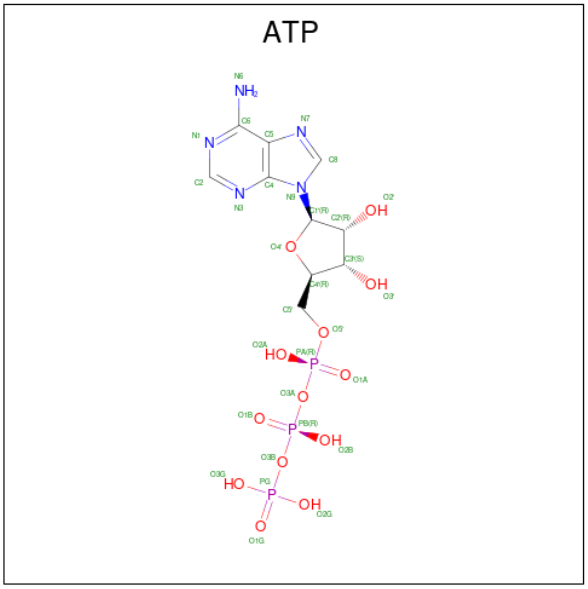
Chain	Residue	Modelled	Actual	Comment	Reference
O	-2	GLY	-	expression tag	UNP Q9L0I7
O	-1	SER	-	expression tag	UNP Q9L0I7
O	0	HIS	-	expression tag	UNP Q9L0I7
P	-2	GLY	-	expression tag	UNP Q9L0I7
P	-1	SER	-	expression tag	UNP Q9L0I7
P	0	HIS	-	expression tag	UNP Q9L0I7

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: 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	A	1	Total 42	C 10	H 11	N 5	O 13	P 3	0	0
2	B	1	Total 42	C 10	H 11	N 5	O 13	P 3	0	0
2	C	1	Total 42	C 10	H 11	N 5	O 13	P 3	0	0
2	D	1	Total 42	C 10	H 11	N 5	O 13	P 3	0	0
2	E	1	Total 42	C 10	H 11	N 5	O 13	P 3	0	0
2	F	1	Total 42	C 10	H 11	N 5	O 13	P 3	0	0
2	G	1	Total 42	C 10	H 11	N 5	O 13	P 3	0	0
2	H	1	Total 42	C 10	H 11	N 5	O 13	P 3	0	0

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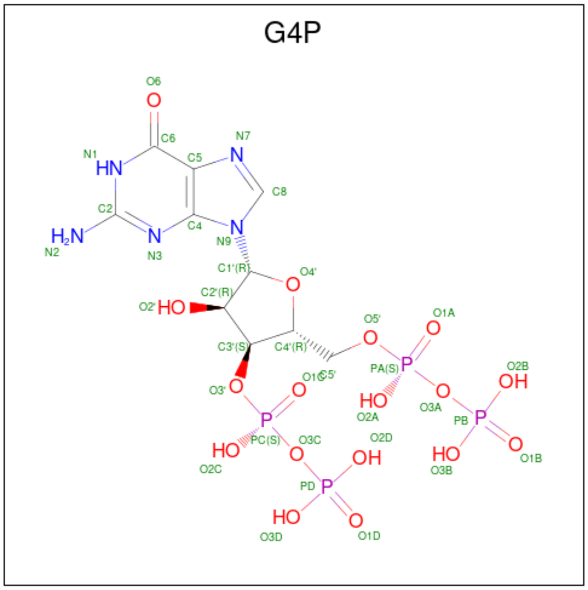
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	I	1	Total C H N O P 42 10 11 5 13 3	0	0
2	J	1	Total C H N O P 42 10 11 5 13 3	0	0
2	K	1	Total C H N O P 42 10 11 5 13 3	0	0
2	L	1	Total C H N O P 42 10 11 5 13 3	0	0
2	M	1	Total C H N O P 42 10 11 5 13 3	0	0
2	N	1	Total C H N O P 42 10 11 5 13 3	0	0
2	O	1	Total C H N O P 42 10 11 5 13 3	0	0
2	P	1	Total C H N O P 42 10 11 5 13 3	0	0

- Molecule 3 is GUANOSINE-5',3'-TETRAPHOSPHATE (three-letter code: G4P) (formula: $C_{10}H_{17}N_5O_{17}P_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H N O P 47 10 11 5 17 4	0	0
3	B	1	Total C H N O P 47 10 11 5 17 4	0	0
3	C	1	Total C H N O P 47 10 11 5 17 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C H N O P 47 10 11 5 17 4	0	0
3	E	1	Total C H N O P 47 10 11 5 17 4	0	0
3	F	1	Total C H N O P 47 10 11 5 17 4	0	0
3	G	1	Total C H N O P 47 10 11 5 17 4	0	0
3	H	1	Total C H N O P 47 10 11 5 17 4	0	0
3	I	1	Total C H N O P 47 10 11 5 17 4	0	0
3	J	1	Total C H N O P 47 10 11 5 17 4	0	0
3	K	1	Total C H N O P 47 10 11 5 17 4	0	0
3	L	1	Total C H N O P 47 10 11 5 17 4	0	0
3	M	1	Total C H N O P 47 10 11 5 17 4	0	0
3	N	1	Total C H N O P 47 10 11 5 17 4	0	0
3	O	1	Total C H N O P 47 10 11 5 17 4	0	0
3	P	1	Total C H N O P 47 10 11 5 17 4	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mg 2 2	0	0
4	B	2	Total Mg 2 2	0	0
4	C	2	Total Mg 2 2	0	0
4	D	2	Total Mg 2 2	0	0
4	E	2	Total Mg 2 2	0	0
4	F	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	2	Total Mg 2 2	0	0
4	H	2	Total Mg 2 2	0	0
4	I	2	Total Mg 2 2	0	0
4	J	2	Total Mg 2 2	0	0
4	K	2	Total Mg 2 2	0	0
4	L	2	Total Mg 2 2	0	0
4	M	2	Total Mg 2 2	0	0
4	N	2	Total Mg 2 2	0	0
4	O	2	Total Mg 2 2	0	0
4	P	2	Total Mg 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	264	Total O 264 264	0	0
5	B	237	Total O 237 237	0	0
5	C	223	Total O 223 223	0	0
5	D	240	Total O 240 240	0	0
5	E	299	Total O 299 299	0	0
5	F	279	Total O 279 279	0	0
5	G	192	Total O 192 192	0	0
5	H	273	Total O 273 273	0	0
5	I	174	Total O 174 174	0	0

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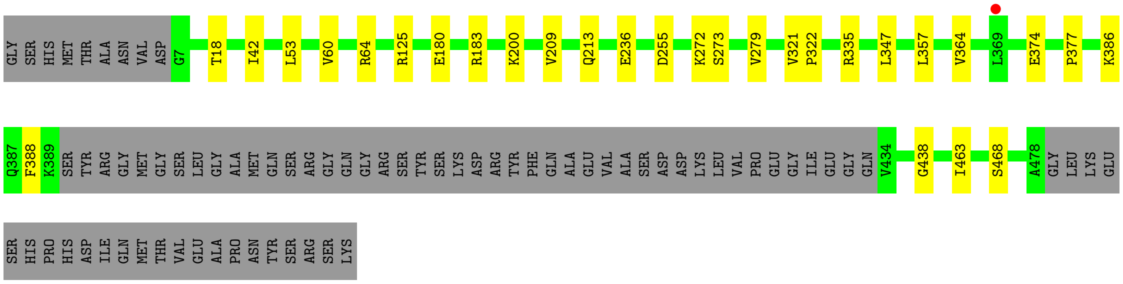
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	J	192	Total O 192 192	0	0
5	K	245	Total O 245 245	0	0
5	L	238	Total O 238 238	0	0
5	M	222	Total O 222 222	0	0
5	N	172	Total O 172 172	0	0
5	O	153	Total O 153 153	0	0
5	P	152	Total O 152 152	0	0

3 Residue-property plots

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

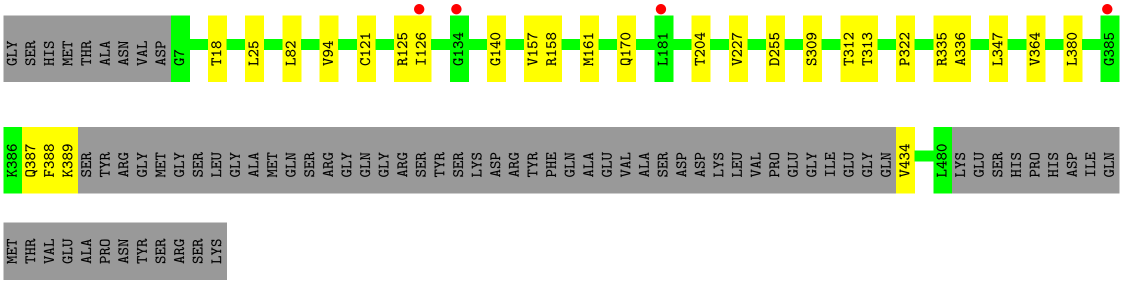
- Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain A:



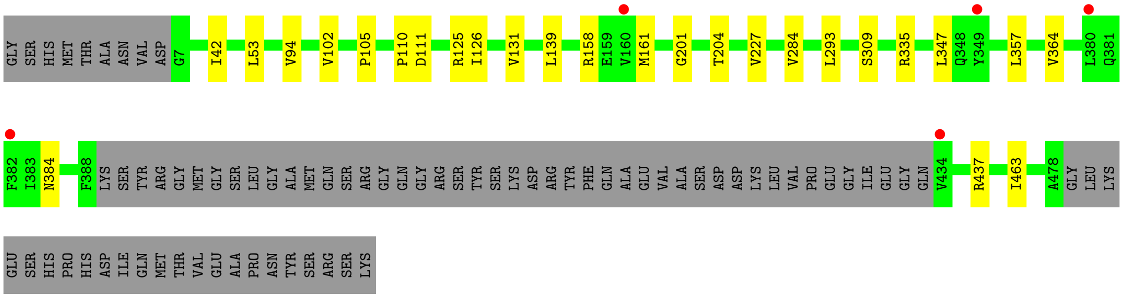
- Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain B:

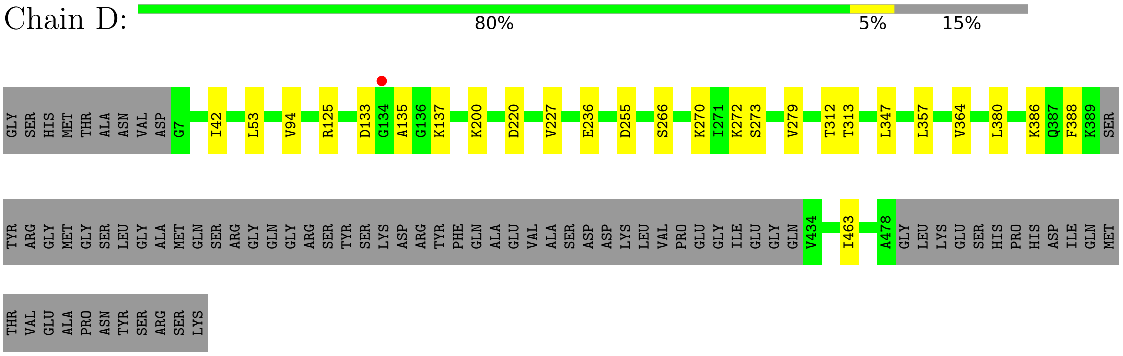


- Molecule 1: Inosine-5'-monophosphate dehydrogenase

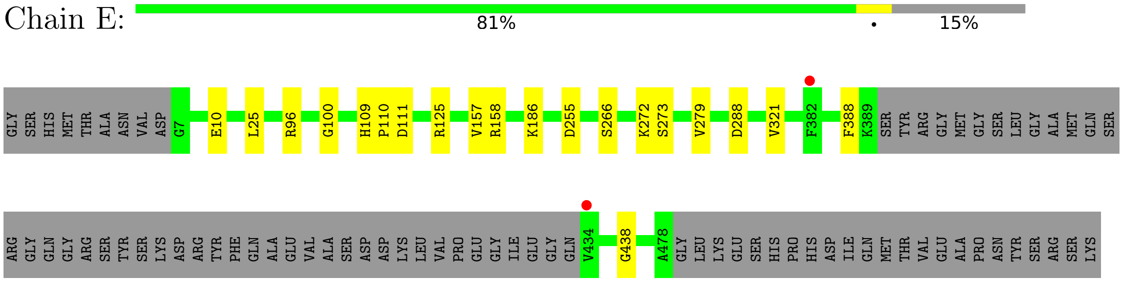
Chain C:



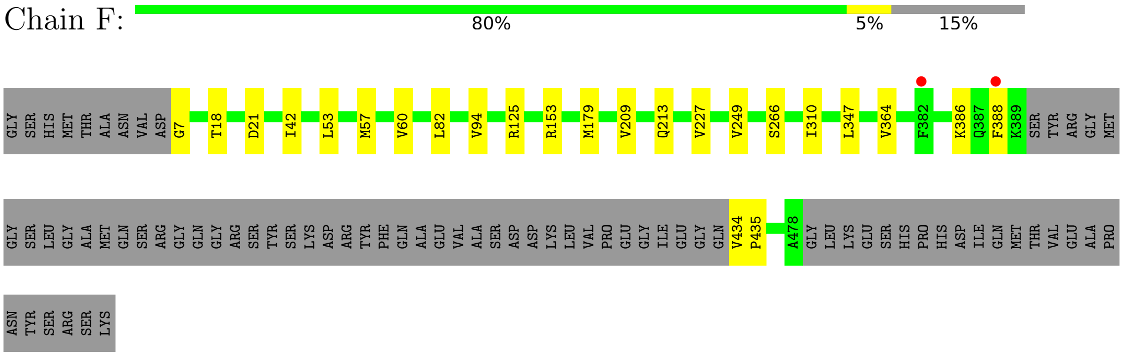
- Molecule 1: Inosine-5'-monophosphate dehydrogenase



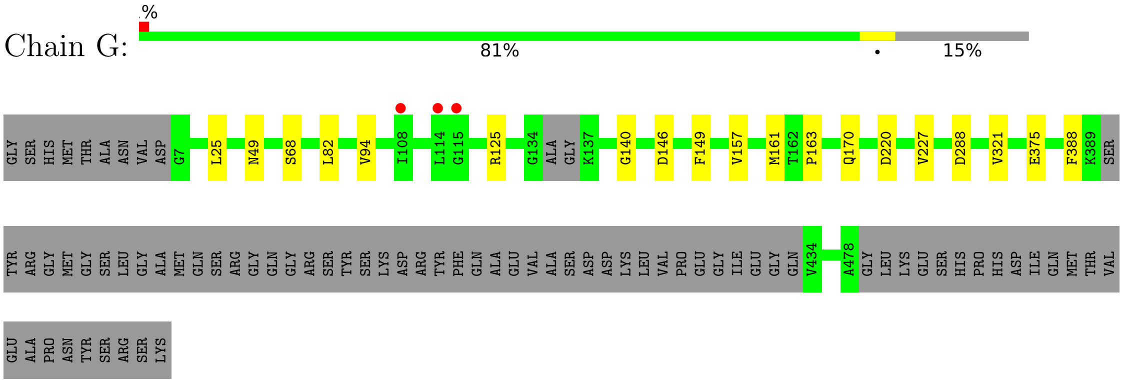
- Molecule 1: Inosine-5'-monophosphate dehydrogenase



- Molecule 1: Inosine-5'-monophosphate dehydrogenase

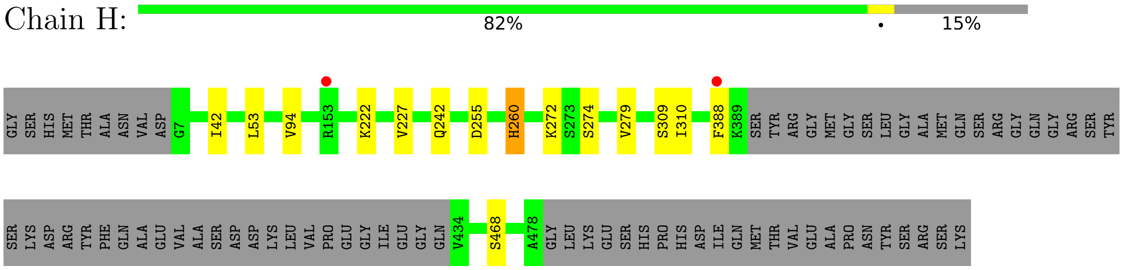


- Molecule 1: Inosine-5'-monophosphate dehydrogenase



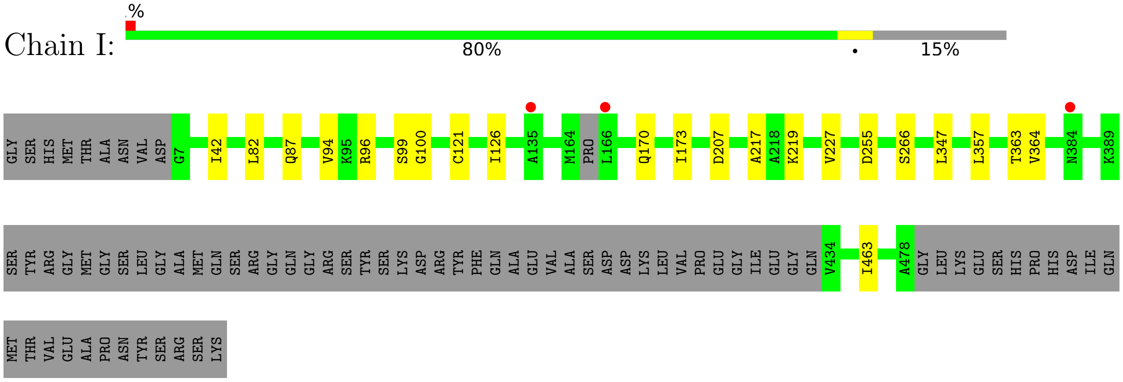
- Molecule 1: Inosine-5’-monophosphate dehydrogenase

Chain H:



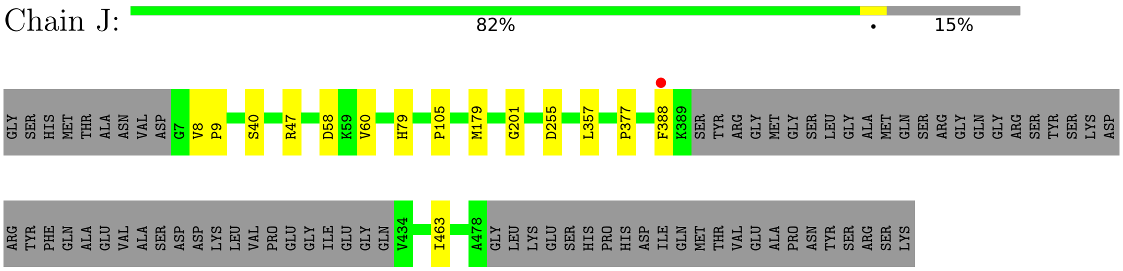
- Molecule 1: Inosine-5’-monophosphate dehydrogenase

Chain I:



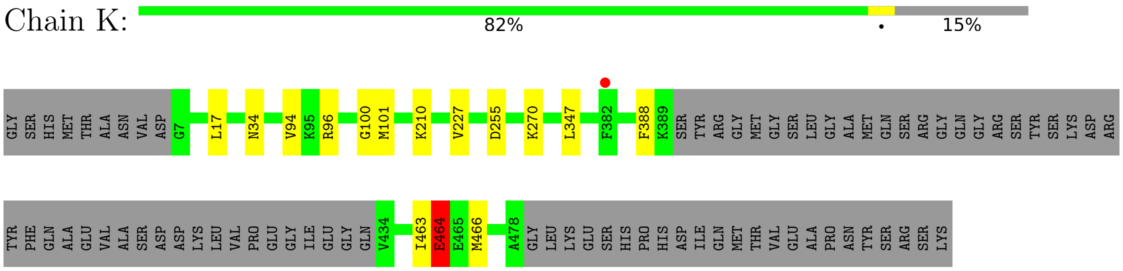
- Molecule 1: Inosine-5’-monophosphate dehydrogenase

Chain J:



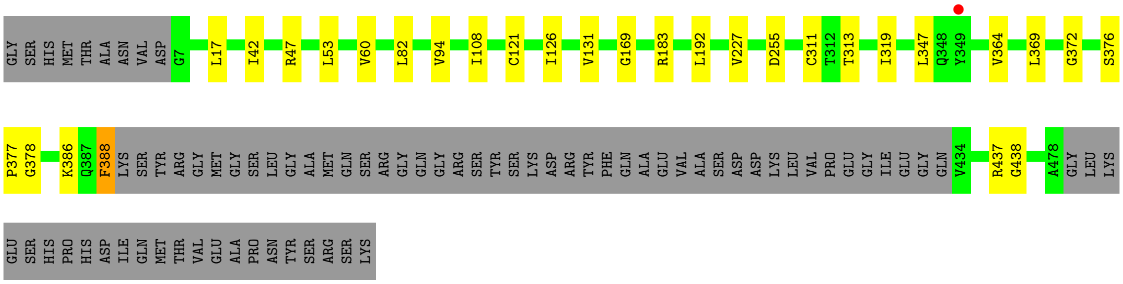
- Molecule 1: Inosine-5’-monophosphate dehydrogenase

Chain K:



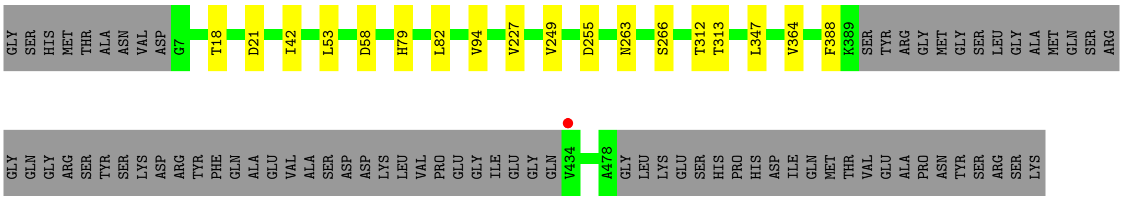
- Molecule 1: Inosine-5’-monophosphate dehydrogenase

Chain L:



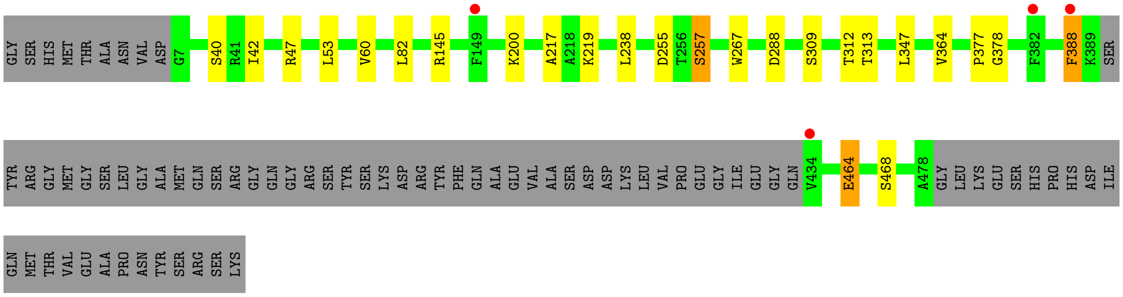
- Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain M:



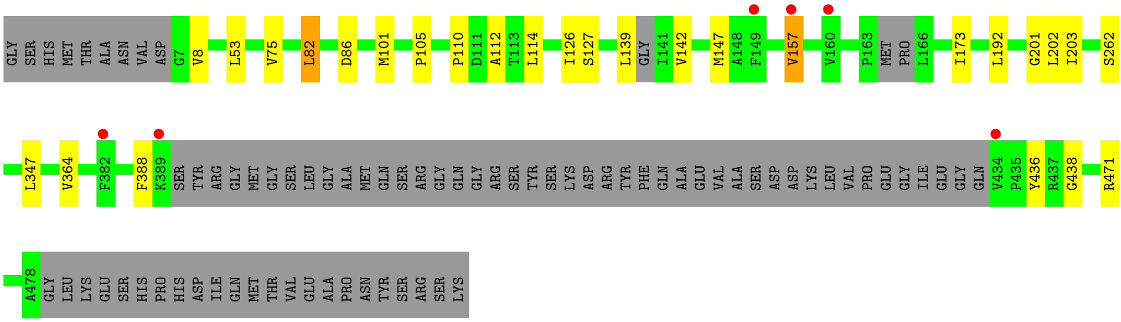
- Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain N:



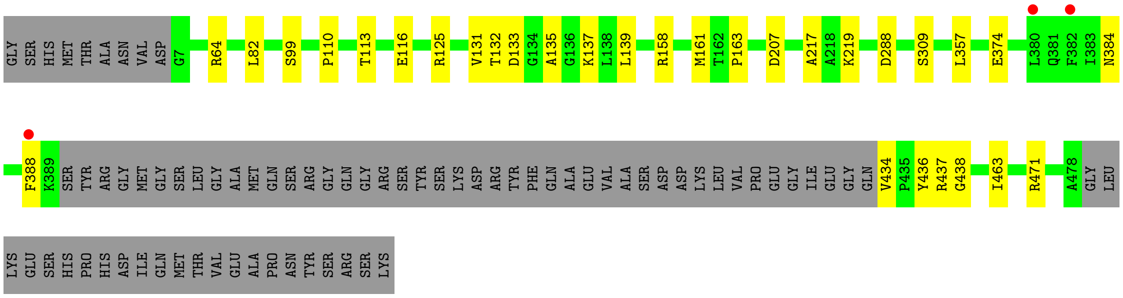
- Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain O:



- Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain P:


GLY
SER
HIS
MET
THR
ALA
ASN
VAL
ASP
G7
R64
L82
S99
P110
T113
E116
R125
V131
T132
D133
G134
A135
G136
K137
L138
L139
R158
M161
T162
P163
D207
A217
A218
K219
D288
S309
L357
E374
L380
Q381
F382
I383
N384
F388
K389
SER
TYR
ARG
GLY
MET
GLY
SER
LEU
GLY
ALA
MET
GLN
SER
ARG
GLY
GLN
GLY
ARG
SER
TYR
SER
LYS
ASP
ARG
TYR
PHE
GLN
ALA
GLU
VAL
ALA
SER
ASP
ASP
LYS
LEU
VAL
PRO
GLU
GLY
ILE
GLU
GLY
GLN
V434
P435
Y436
R437
G438
I463
R471
A478
GLY
LEU
LYS
GLU
SER
HIS
PRO
HIS
ASP
ILE
GLN
MET
THR
VAL
GLU
ALA
PRO
ASN
TYR
SER
ARG
SER
LYS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	119.29Å 300.90Å 123.09Å 90.00° 90.28° 90.00°	Depositor
Resolution (Å)	85.88 – 2.03 150.45 – 2.03	Depositor EDS
% Data completeness (in resolution range)	84.9 (85.88-2.03) 84.9 (150.45-2.03)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.180 , 0.212 0.180 , 0.210	Depositor DCC
R_{free} test set	23525 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	32.0	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.003 for l,k,-h 0.137 for h,-k,-l 0.015 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	101645	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG, G4P

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	0.26	0/3094	0.54	0/4196
1	B	0.32	0/3072	0.55	0/4173
1	C	0.34	0/3014	0.56	0/4099
1	D	0.30	0/3078	0.54	0/4177
1	E	0.28	0/3109	0.56	0/4216
1	F	0.32	0/3122	0.56	0/4232
1	G	0.32	0/2993	0.55	0/4067
1	H	0.32	0/3118	0.59	1/4226 (0.0%)
1	I	0.37	0/2944	0.59	0/4007
1	J	0.29	0/3062	0.54	0/4158
1	K	0.34	0/3074	0.56	1/4173 (0.0%)
1	L	0.34	0/3076	0.56	0/4173
1	M	0.28	0/3091	0.54	0/4193
1	N	0.33	0/3064	0.57	1/4161 (0.0%)
1	O	0.34	0/2965	0.55	0/4033
1	P	0.39	0/3013	0.57	0/4100
All	All	0.32	0/48889	0.56	3/66384 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	257	SER	CB-CA-C	6.93	123.27	110.10
1	H	222	LYS	CA-CB-CG	6.15	126.93	113.40
1	K	464	GLU	CG-CD-OE2	-6.14	106.02	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3056	3101	3101	18	0
1	B	3033	3025	3025	28	0
1	C	2978	2959	2959	19	0
1	D	3040	3062	3062	16	0
1	E	3070	3103	3103	16	0
1	F	3083	3131	3131	12	0
1	G	2956	2915	2915	14	0
1	H	3079	3132	3132	7	0
1	I	2911	2829	2829	13	0
1	J	3024	3032	3032	9	0
1	K	3036	3062	3062	8	0
1	L	3038	3073	3071	23	0
1	M	3052	3085	3085	9	0
1	N	3026	3041	3041	13	0
1	O	2930	2850	2849	22	0
1	P	2975	2947	2947	18	0
2	A	31	11	12	0	0
2	B	31	11	12	0	0
2	C	31	11	12	0	0
2	D	31	11	12	0	0
2	E	31	11	12	0	0
2	F	31	11	12	0	0
2	G	31	11	12	1	0
2	H	31	11	12	0	0
2	I	31	11	12	0	0
2	J	31	11	12	0	0
2	K	31	11	12	0	0
2	L	31	11	12	0	0
2	M	31	11	12	0	0
2	N	31	11	12	1	0
2	O	31	11	12	0	0
2	P	31	11	12	0	0
3	A	36	11	11	1	0
3	B	36	11	11	3	0
3	C	36	11	11	1	0
3	D	36	11	11	2	0
3	E	36	11	11	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	36	11	11	1	0
3	G	36	11	11	1	0
3	H	36	11	11	1	0
3	I	36	11	11	0	0
3	J	36	11	11	0	0
3	K	36	11	11	0	0
3	L	36	11	11	0	0
3	M	36	11	11	0	0
3	N	36	11	11	0	0
3	O	36	11	11	1	0
3	P	36	11	11	1	0
4	A	2	0	0	0	0
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	2	0	0	0	0
4	N	2	0	0	0	0
4	O	2	0	0	0	0
4	P	2	0	0	0	0
5	A	264	0	0	0	0
5	B	237	0	0	4	0
5	C	223	0	0	1	0
5	D	240	0	0	1	0
5	E	299	0	0	3	0
5	F	279	0	0	1	0
5	G	192	0	0	1	0
5	H	273	0	0	2	0
5	I	174	0	0	0	0
5	J	192	0	0	0	0
5	K	245	0	0	2	0
5	L	238	0	0	1	0
5	M	222	0	0	1	0
5	N	172	0	0	1	0
5	O	153	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	152	0	0	0	0
All	All	52946	48699	48712	233	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 2.

The worst 5 of 233 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)
3:H:601:G4P:O4'	3:H:601:G4P:C1'	1.63	1.18
3:O:601:G4P:O4'	3:O:601:G4P:C1'	1.64	1.16
1:B:125:ARG:NH1	3:B:601:G4P:O3B	2.01	0.94
1:O:101:MET:HE1	1:O:126:ILE:HD12	1.53	0.88
1:E:111:ASP:OD1	1:E:158:ARG:NH1	2.07	0.88

There are no symmetry-related clashes.

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	424/504 (84%)	415 (98%)	9 (2%)	0	100	100
1	B	426/504 (84%)	418 (98%)	8 (2%)	0	100	100
1	C	423/504 (84%)	413 (98%)	9 (2%)	1 (0%)	47	43
1	D	424/504 (84%)	415 (98%)	9 (2%)	0	100	100
1	E	424/504 (84%)	415 (98%)	9 (2%)	0	100	100
1	F	424/504 (84%)	414 (98%)	10 (2%)	0	100	100
1	G	420/504 (83%)	412 (98%)	8 (2%)	0	100	100
1	H	424/504 (84%)	416 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	421/504 (84%)	413 (98%)	8 (2%)	0	100	100
1	J	424/504 (84%)	415 (98%)	9 (2%)	0	100	100
1	K	424/504 (84%)	416 (98%)	8 (2%)	0	100	100
1	L	423/504 (84%)	414 (98%)	9 (2%)	0	100	100
1	M	424/504 (84%)	415 (98%)	9 (2%)	0	100	100
1	N	424/504 (84%)	416 (98%)	8 (2%)	0	100	100
1	O	417/504 (83%)	405 (97%)	12 (3%)	0	100	100
1	P	424/504 (84%)	415 (98%)	8 (2%)	1 (0%)	47	43
All	All	6770/8064 (84%)	6627 (98%)	141 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	384	ASN
1	C	384	ASN

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	311/389 (80%)	306 (98%)	5 (2%)	62	66
1	B	304/389 (78%)	300 (99%)	4 (1%)	69	72
1	C	293/389 (75%)	292 (100%)	1 (0%)	92	94
1	D	308/389 (79%)	303 (98%)	5 (2%)	62	66
1	E	314/389 (81%)	311 (99%)	3 (1%)	76	80
1	F	319/389 (82%)	313 (98%)	6 (2%)	57	59
1	G	285/389 (73%)	281 (99%)	4 (1%)	67	70
1	H	318/389 (82%)	315 (99%)	3 (1%)	78	82
1	I	273/389 (70%)	271 (99%)	2 (1%)	84	87
1	J	304/389 (78%)	302 (99%)	2 (1%)	84	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	307/389 (79%)	302 (98%)	5 (2%)	62	66
1	L	307/389 (79%)	303 (99%)	4 (1%)	69	72
1	M	311/389 (80%)	306 (98%)	5 (2%)	62	66
1	N	306/389 (79%)	298 (97%)	8 (3%)	46	46
1	O	279/389 (72%)	274 (98%)	5 (2%)	59	61
1	P	291/389 (75%)	285 (98%)	6 (2%)	53	55
All	All	4830/6224 (78%)	4762 (99%)	68 (1%)	67	70

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	82	LEU
1	O	262	SER
1	P	388	PHE
1	G	82	LEU
1	F	388	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	260	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 64 ligands modelled in this entry, 32 are monoatomic - leaving 32 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	G4P	P	601	4	30,38,38	5.14	12 (40%)	43,61,61	1.75	9 (20%)
3	G4P	D	601	4	30,38,38	5.05	12 (40%)	43,61,61	1.68	8 (18%)
3	G4P	N	601	4	30,38,38	5.13	12 (40%)	43,61,61	1.72	7 (16%)
3	G4P	H	601	4	30,38,38	5.14	12 (40%)	43,61,61	1.64	7 (16%)
2	ATP	K	600	4	26,33,33	0.62	0	31,52,52	1.03	2 (6%)
2	ATP	F	600	4	26,33,33	0.62	0	31,52,52	1.02	1 (3%)
3	G4P	C	601	4	30,38,38	5.12	12 (40%)	43,61,61	1.71	8 (18%)
2	ATP	E	600	4	26,33,33	0.63	0	31,52,52	1.01	1 (3%)
2	ATP	M	600	4	26,33,33	0.62	0	31,52,52	0.99	1 (3%)
2	ATP	O	600	4	26,33,33	0.62	0	31,52,52	1.04	3 (9%)
2	ATP	N	600	4	26,33,33	0.62	0	31,52,52	1.05	2 (6%)
3	G4P	O	601	4	30,38,38	5.14	12 (40%)	43,61,61	1.68	6 (13%)
2	ATP	P	600	4	26,33,33	0.61	0	31,52,52	1.04	2 (6%)
2	ATP	G	600	4	26,33,33	0.62	0	31,52,52	1.03	2 (6%)
3	G4P	G	601	4	30,38,38	5.09	12 (40%)	43,61,61	1.70	7 (16%)
3	G4P	K	601	4	30,38,38	5.08	12 (40%)	43,61,61	1.61	8 (18%)
2	ATP	J	600	4	26,33,33	0.62	0	31,52,52	1.04	2 (6%)
3	G4P	J	601	4	30,38,38	5.11	12 (40%)	43,61,61	1.75	8 (18%)
2	ATP	H	600	4	26,33,33	0.61	0	31,52,52	1.00	1 (3%)
2	ATP	D	600	4	26,33,33	0.60	0	31,52,52	1.00	1 (3%)
3	G4P	E	601	4	30,38,38	5.03	12 (40%)	43,61,61	1.70	7 (16%)
2	ATP	L	600	4	26,33,33	0.60	0	31,52,52	1.01	2 (6%)
3	G4P	F	601	4	30,38,38	5.02	12 (40%)	43,61,61	1.71	9 (20%)
3	G4P	L	601	4	30,38,38	5.08	12 (40%)	43,61,61	1.67	8 (18%)
2	ATP	B	600	4	26,33,33	0.61	0	31,52,52	1.02	1 (3%)
2	ATP	C	600	4	26,33,33	0.62	0	31,52,52	1.17	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	ATP	A	600	4	26,33,33	0.60	0	31,52,52	1.01	1 (3%)
2	ATP	I	600	4	26,33,33	0.60	0	31,52,52	1.03	2 (6%)
3	G4P	M	601	4	30,38,38	5.10	12 (40%)	43,61,61	1.63	8 (18%)
3	G4P	B	601	4	30,38,38	5.05	12 (40%)	43,61,61	1.74	8 (18%)
3	G4P	A	601	4	30,38,38	5.03	12 (40%)	43,61,61	1.57	7 (16%)
3	G4P	I	601	4	30,38,38	5.13	12 (40%)	43,61,61	1.67	7 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	G4P	P	601	4	-	1/23/43/43	0/3/3/3
3	G4P	D	601	4	-	2/23/43/43	0/3/3/3
3	G4P	N	601	4	-	2/23/43/43	0/3/3/3
3	G4P	H	601	4	-	1/23/43/43	0/3/3/3
2	ATP	K	600	4	-	2/18/38/38	0/3/3/3
2	ATP	F	600	4	-	1/18/38/38	0/3/3/3
3	G4P	C	601	4	-	2/23/43/43	0/3/3/3
2	ATP	E	600	4	-	1/18/38/38	0/3/3/3
2	ATP	M	600	4	-	1/18/38/38	0/3/3/3
2	ATP	O	600	4	-	1/18/38/38	0/3/3/3
2	ATP	N	600	4	-	5/18/38/38	0/3/3/3
3	G4P	O	601	4	-	8/23/43/43	0/3/3/3
2	ATP	P	600	4	-	0/18/38/38	0/3/3/3
2	ATP	G	600	4	-	1/18/38/38	0/3/3/3
3	G4P	G	601	4	-	2/23/43/43	0/3/3/3
3	G4P	K	601	4	-	2/23/43/43	0/3/3/3
2	ATP	J	600	4	-	2/18/38/38	0/3/3/3
3	G4P	J	601	4	-	4/23/43/43	0/3/3/3
2	ATP	H	600	4	-	1/18/38/38	0/3/3/3
2	ATP	D	600	4	-	2/18/38/38	0/3/3/3
3	G4P	E	601	4	-	2/23/43/43	0/3/3/3
2	ATP	L	600	4	-	2/18/38/38	0/3/3/3
3	G4P	F	601	4	-	1/23/43/43	0/3/3/3
3	G4P	L	601	4	-	2/23/43/43	0/3/3/3
2	ATP	B	600	4	-	0/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	C	600	4	-	0/18/38/38	0/3/3/3
2	ATP	A	600	4	-	1/18/38/38	0/3/3/3
2	ATP	I	600	4	-	1/18/38/38	0/3/3/3
3	G4P	M	601	4	-	2/23/43/43	0/3/3/3
3	G4P	B	601	4	-	2/23/43/43	0/3/3/3
3	G4P	A	601	4	-	2/23/43/43	0/3/3/3
3	G4P	I	601	4	-	5/23/43/43	0/3/3/3

The worst 5 of 192 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	601	G4P	O4'-C1'	16.41	1.64	1.41
3	H	601	G4P	O4'-C1'	16.10	1.63	1.41
3	N	601	G4P	O4'-C1'	15.97	1.63	1.41
3	M	601	G4P	O4'-C1'	15.97	1.63	1.41
3	I	601	G4P	O4'-C1'	15.94	1.63	1.41

The worst 5 of 150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	601	G4P	N3-C2-N1	-5.59	119.76	127.22
3	C	601	G4P	N3-C2-N1	-5.56	119.81	127.22
3	I	601	G4P	N3-C2-N1	-5.54	119.83	127.22
3	P	601	G4P	N3-C2-N1	-5.54	119.84	127.22
3	O	601	G4P	N3-C2-N1	-5.49	119.90	127.22

There are no chirality outliers.

5 of 61 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	N	600	ATP	PB-O3A-PA-O5'
3	A	601	G4P	C5'-O5'-PA-O3A
3	A	601	G4P	C5'-O5'-PA-O1A
3	B	601	G4P	C5'-O5'-PA-O1A
3	C	601	G4P	C5'-O5'-PA-O3A

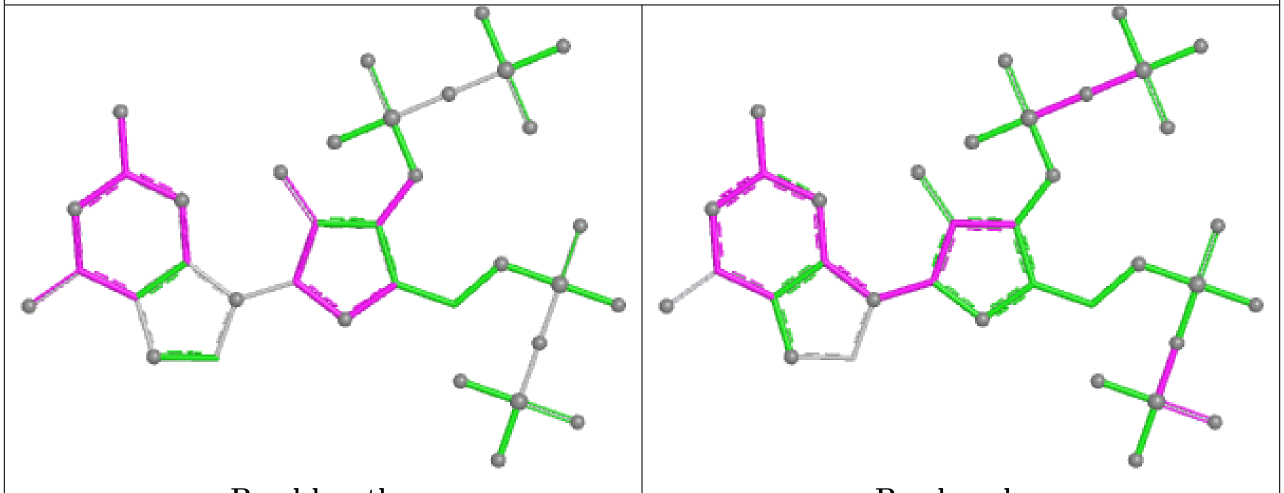
There are no ring outliers.

12 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	601	G4P	1	0
3	D	601	G4P	2	0
3	H	601	G4P	1	0
3	C	601	G4P	1	0
2	N	600	ATP	1	0
3	O	601	G4P	1	0
2	G	600	ATP	1	0
3	G	601	G4P	1	0
3	E	601	G4P	1	0
3	F	601	G4P	1	0
3	B	601	G4P	3	0
3	A	601	G4P	1	0

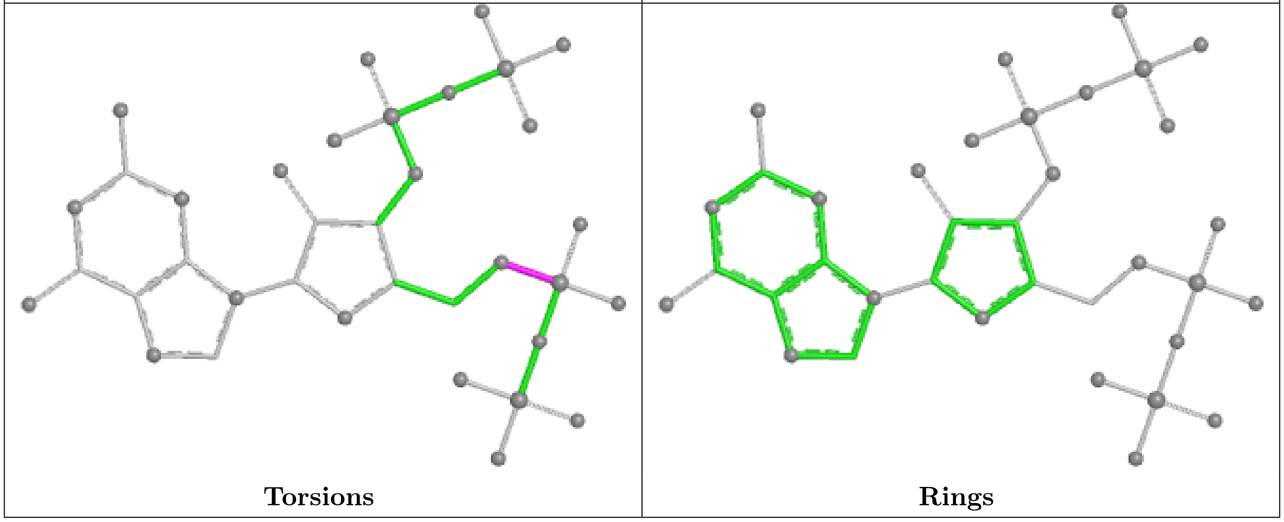
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 G4P P 601



Bond lengths

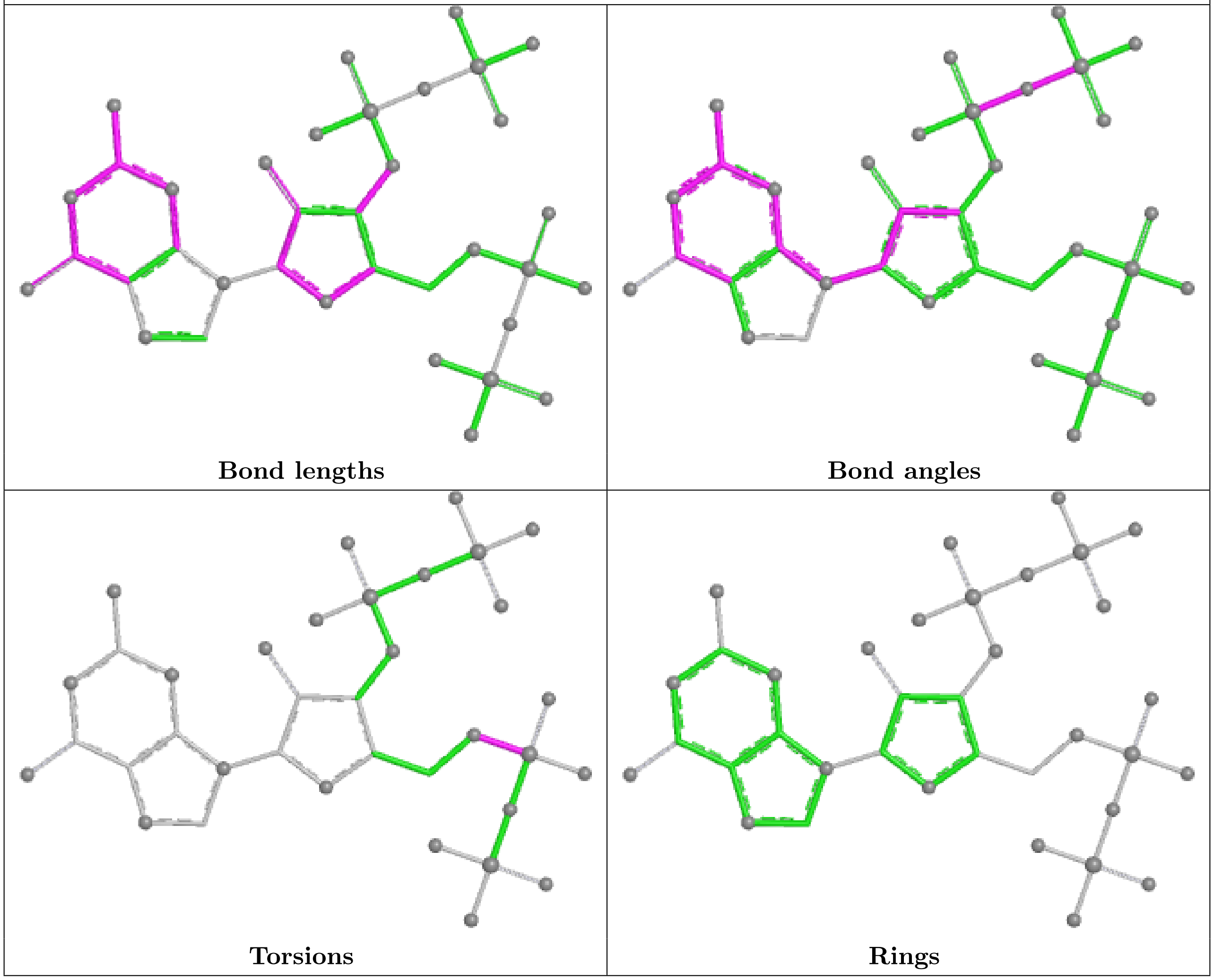
Bond angles



Torsions

Rings

Ligand G4P D 601



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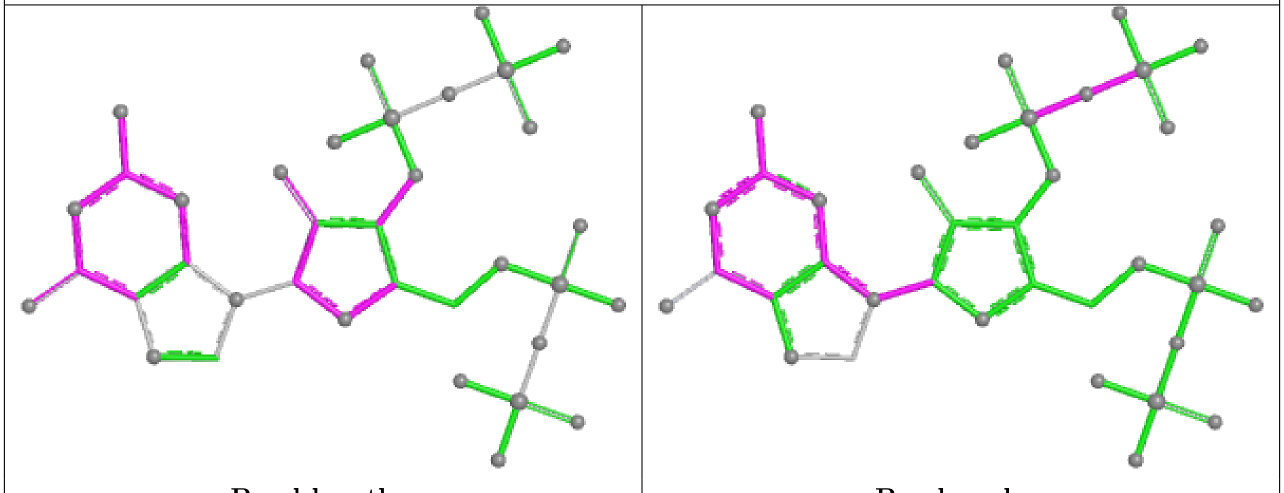
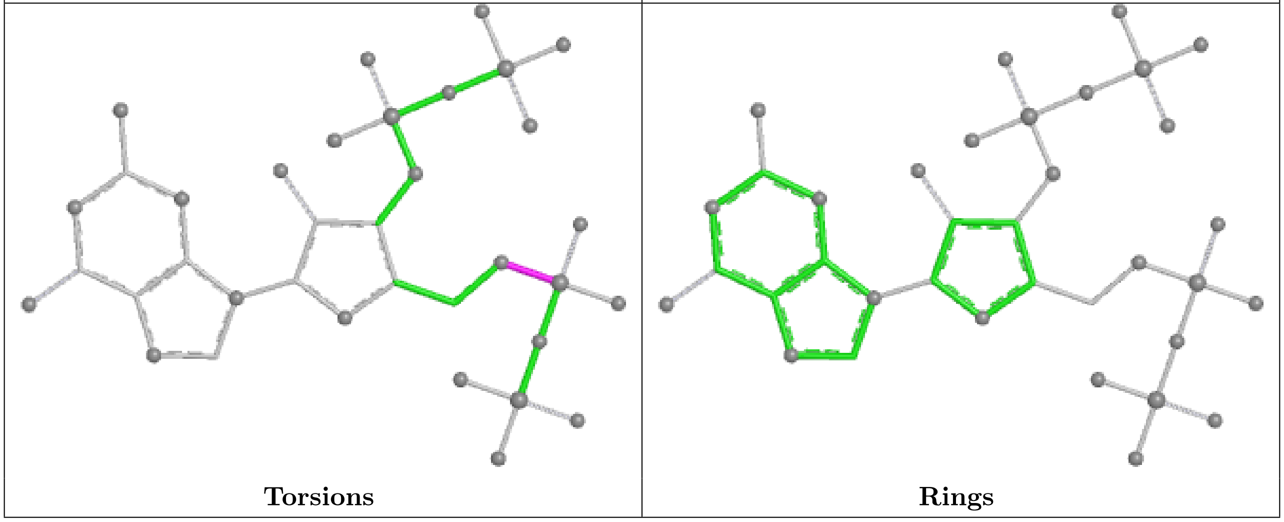
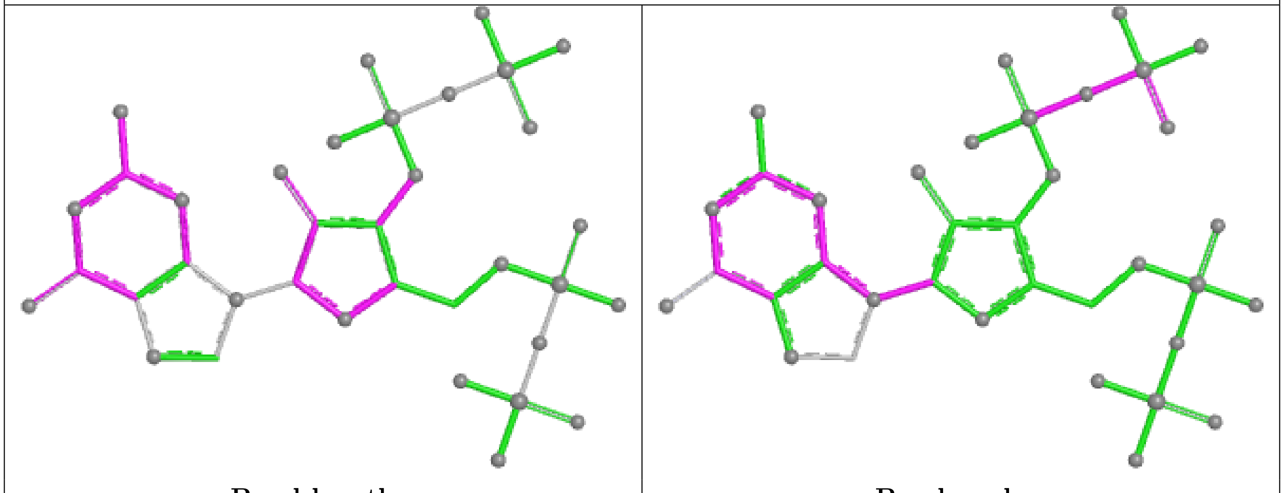


Bond lengths Bond angles



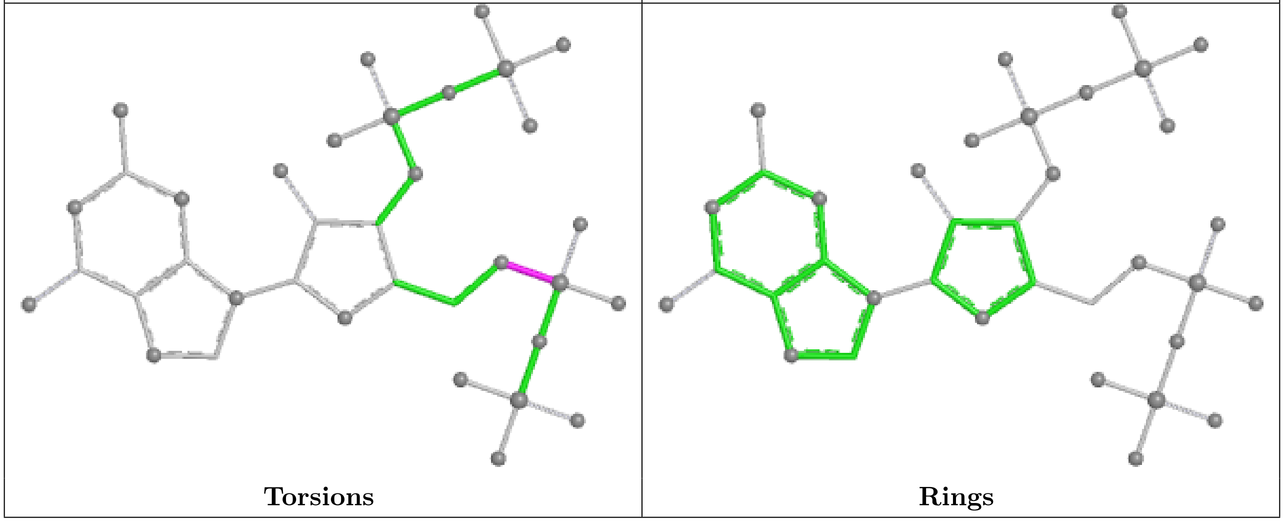
Torsions Rings

Ligand G4P H 601



Bond lengths

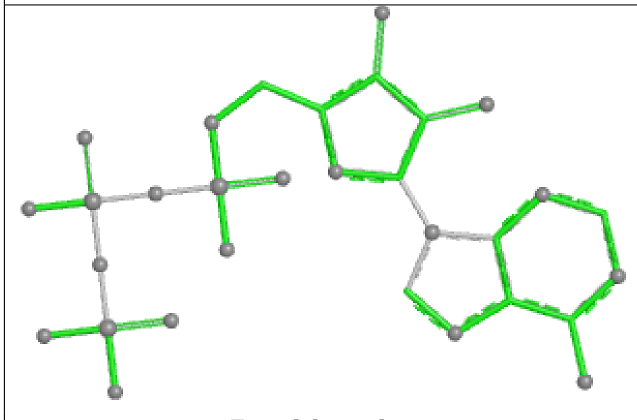
Bond angles



Torsions

Rings

Ligand ATP K 600



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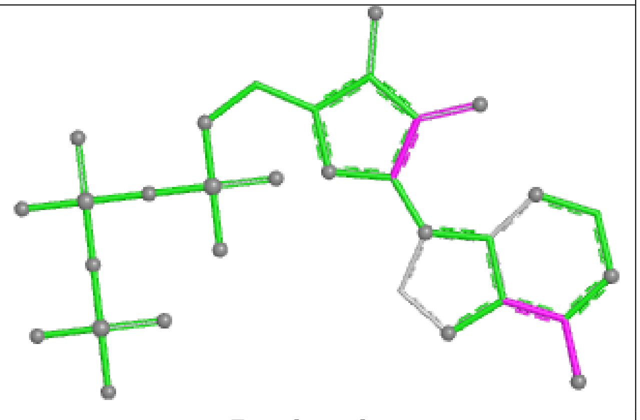
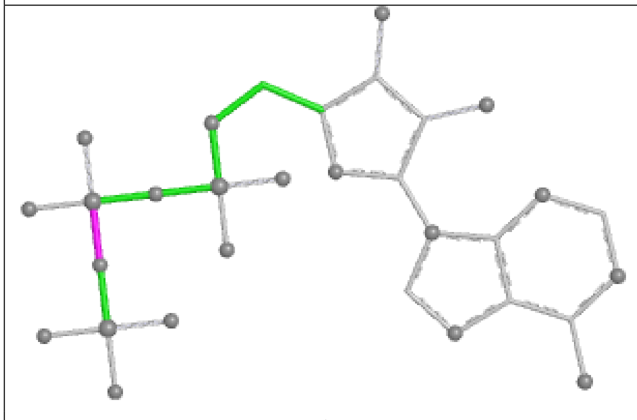
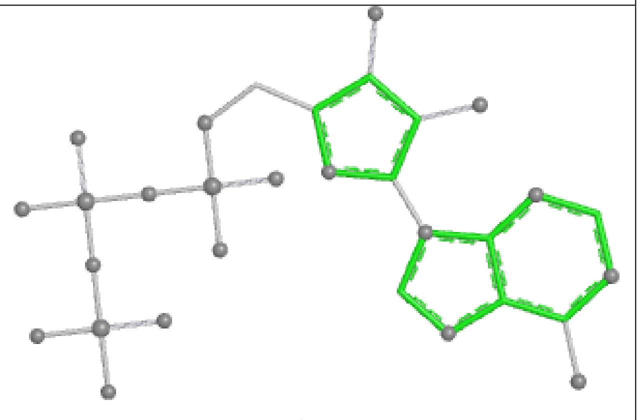


Bond angles

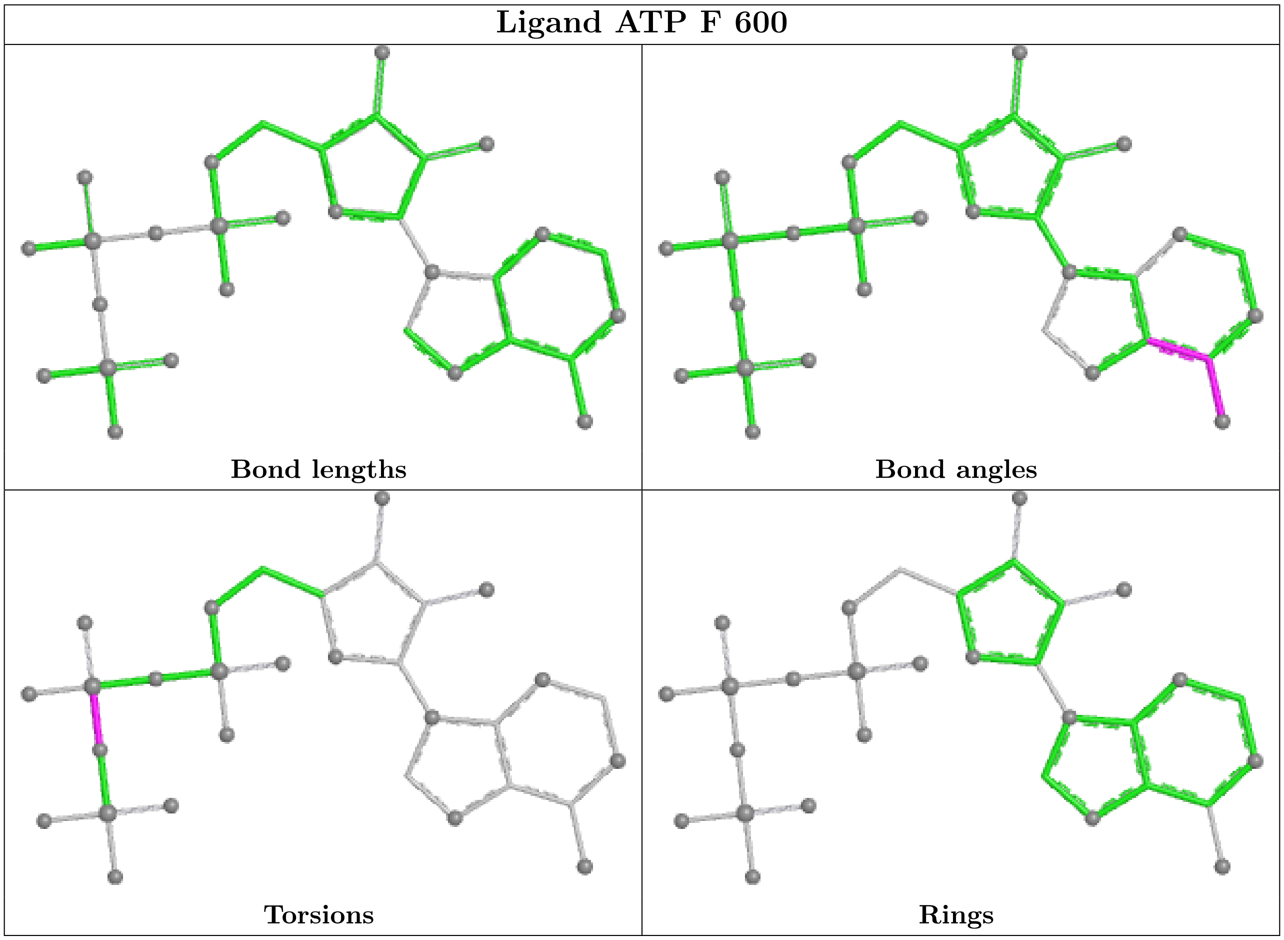


Torsions



Rings

Ligand ATP F 600



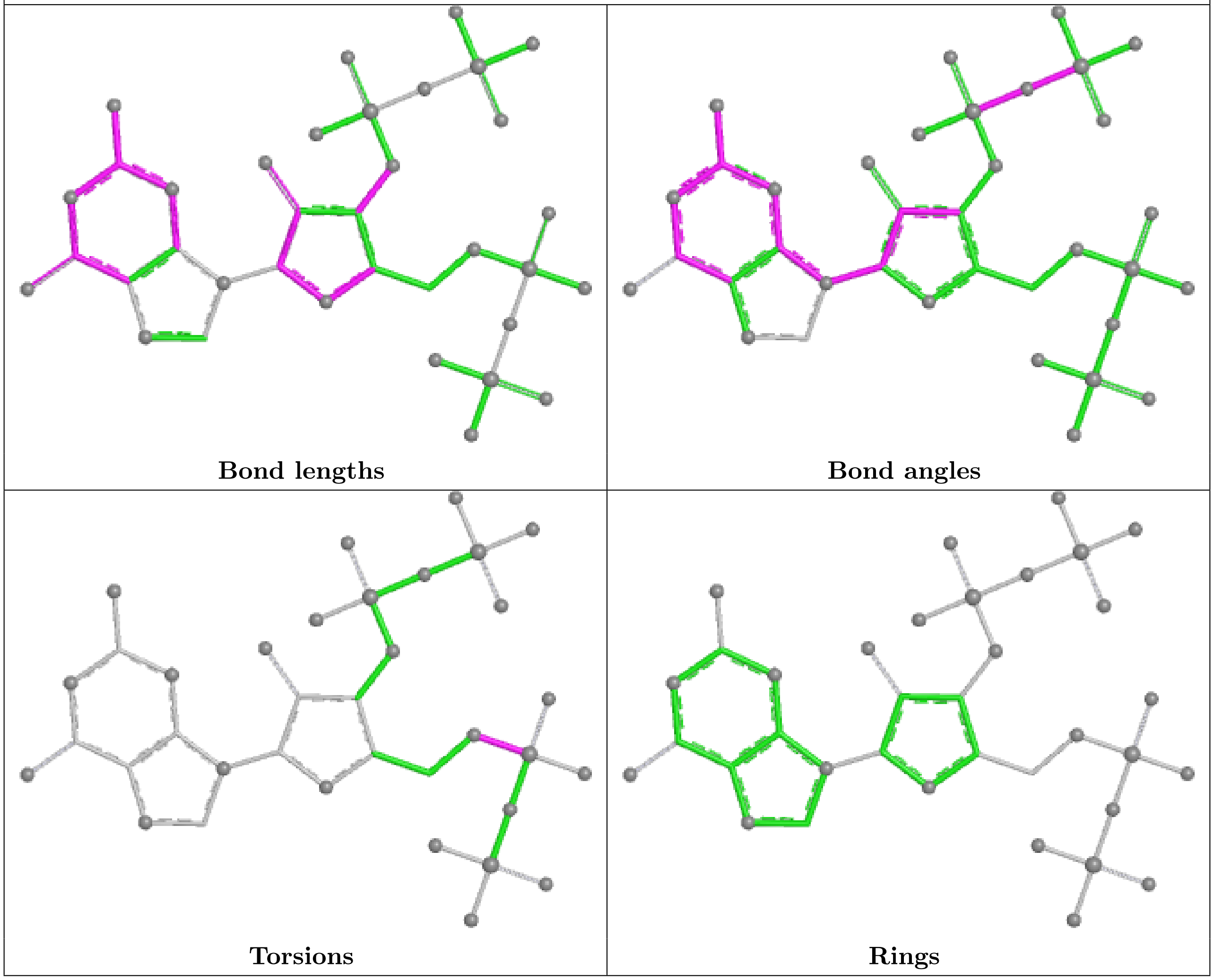
Bond lengths

Bond angles

Torsions

Rings

Ligand G4P C 601



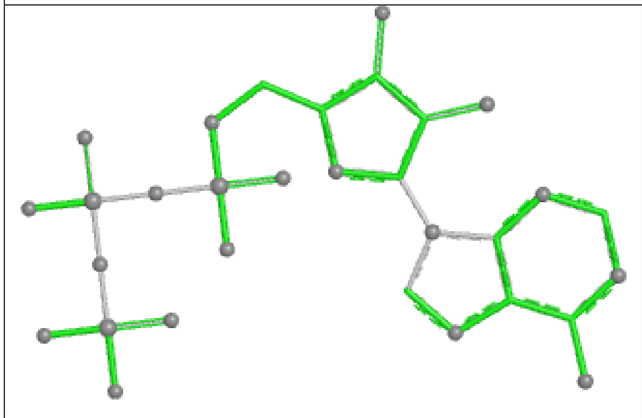
Bond lengths

Bond angles

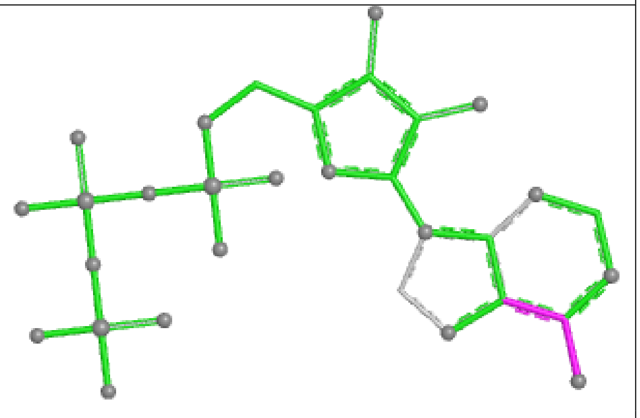
Torsions

Rings

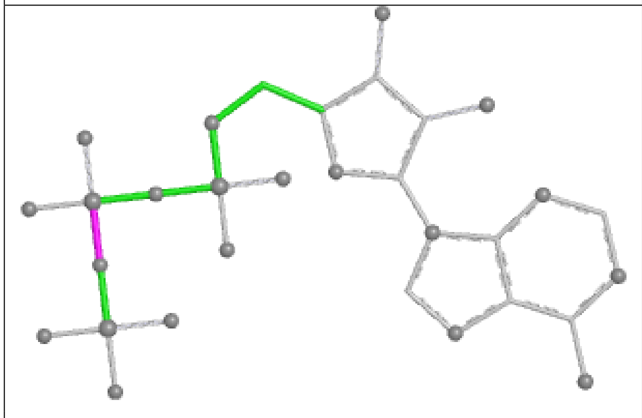
Ligand ATP E 600



Bond lengths



Bond angles



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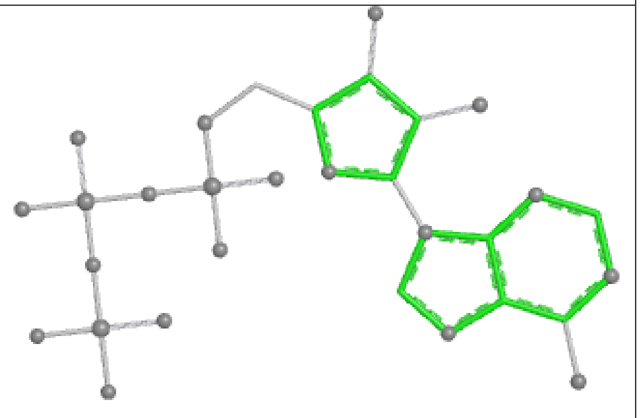
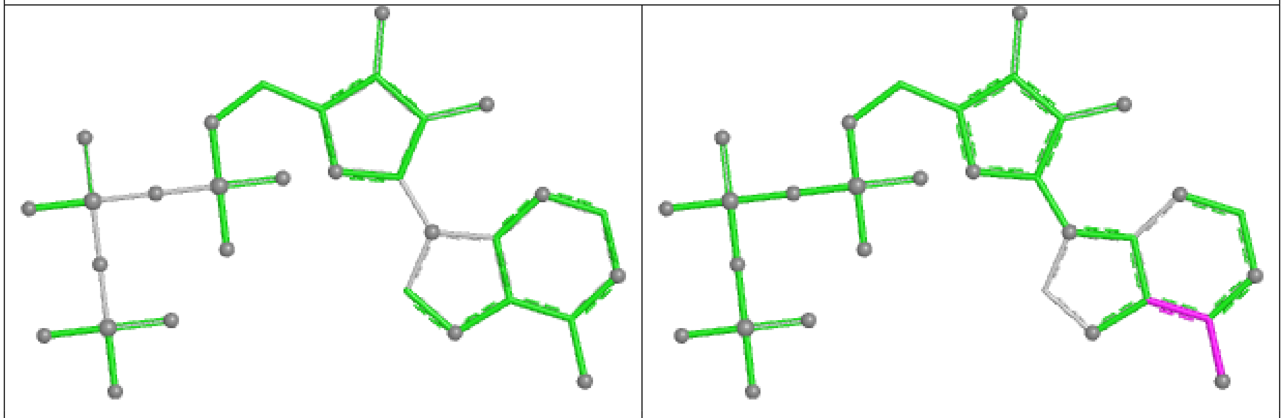


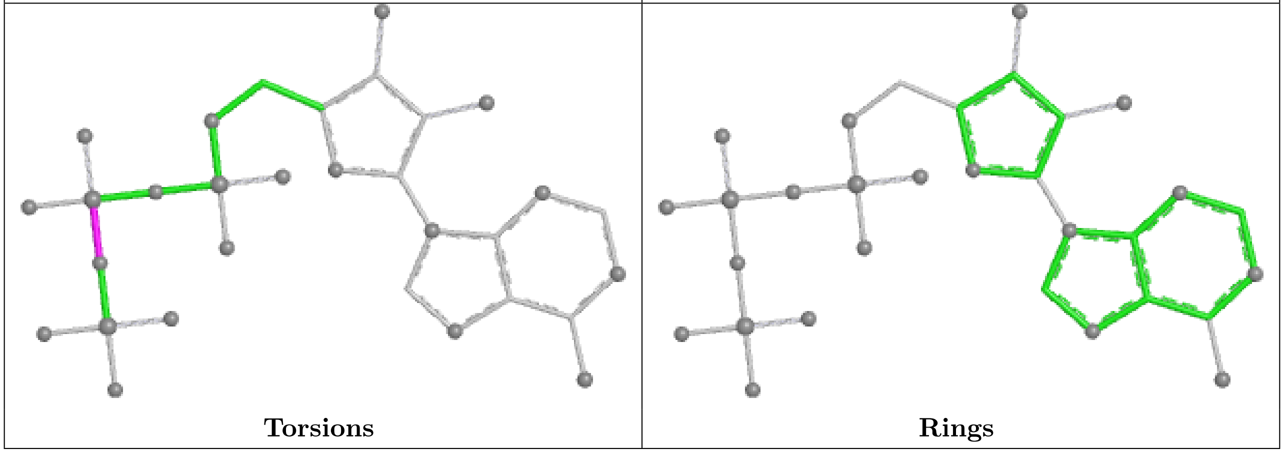
Rings

Ligand ATP M 600



Bond lengths

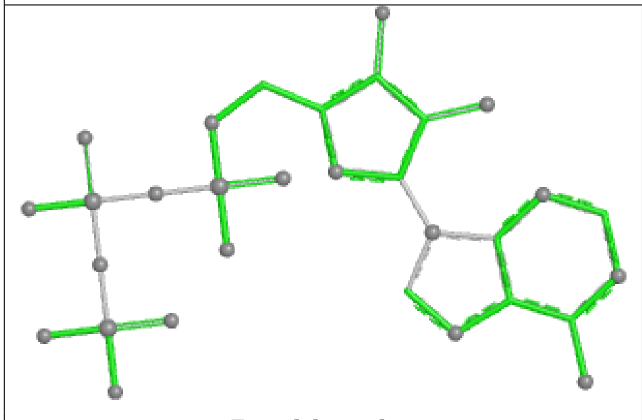
Bond angles

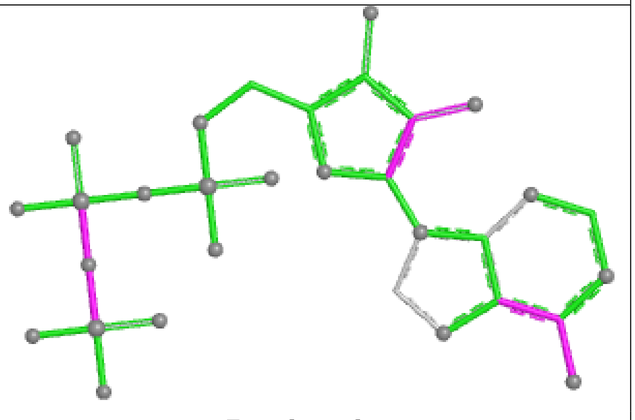


Torsions

Rings

Ligand ATP O 600


Bond lengths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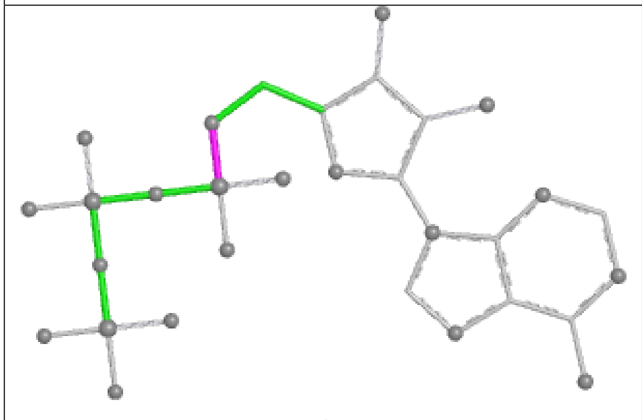
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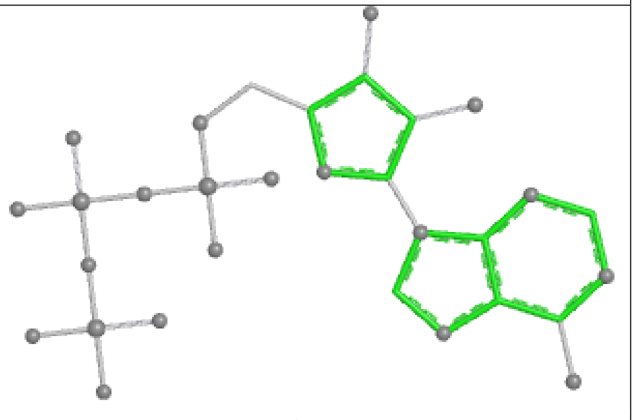
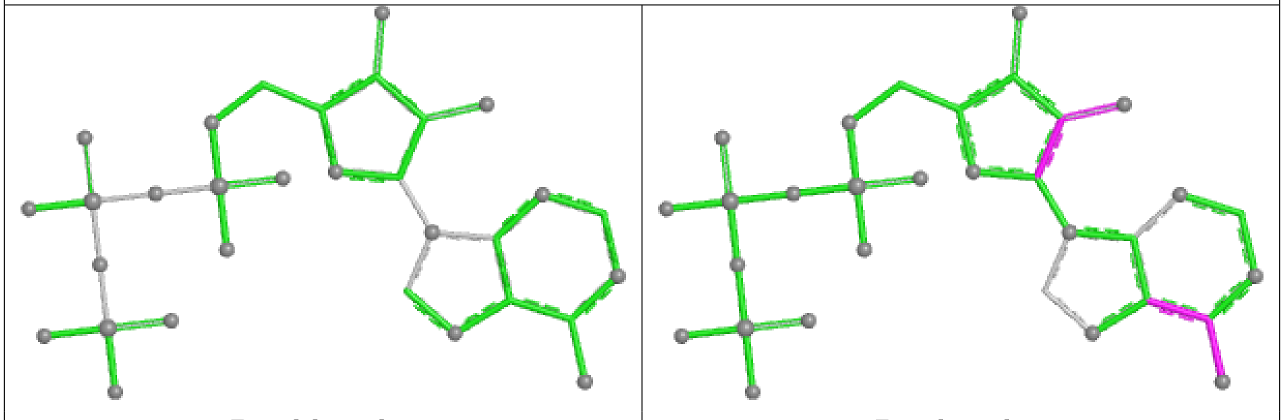

Rings

Ligand ATP N 600



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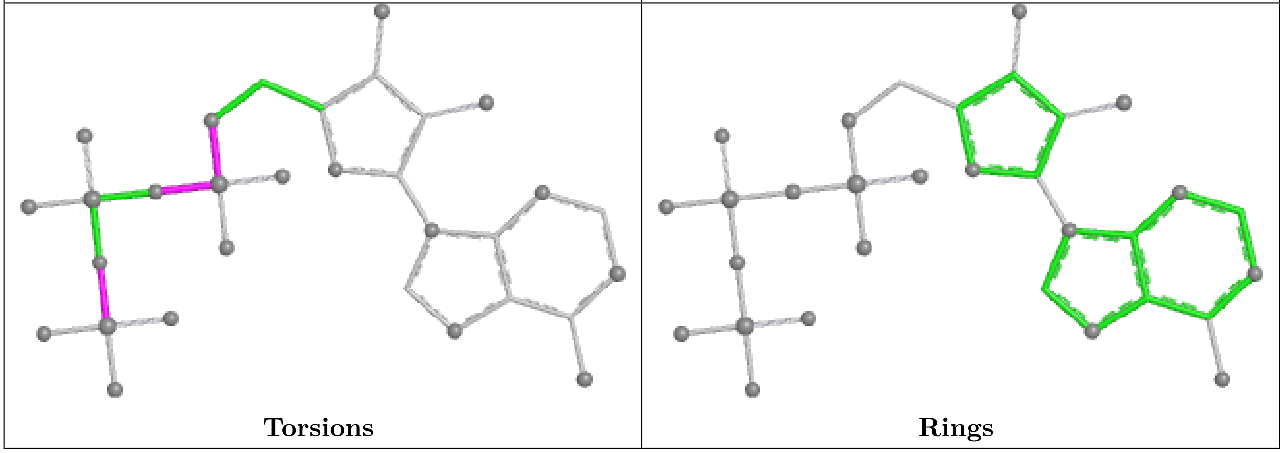
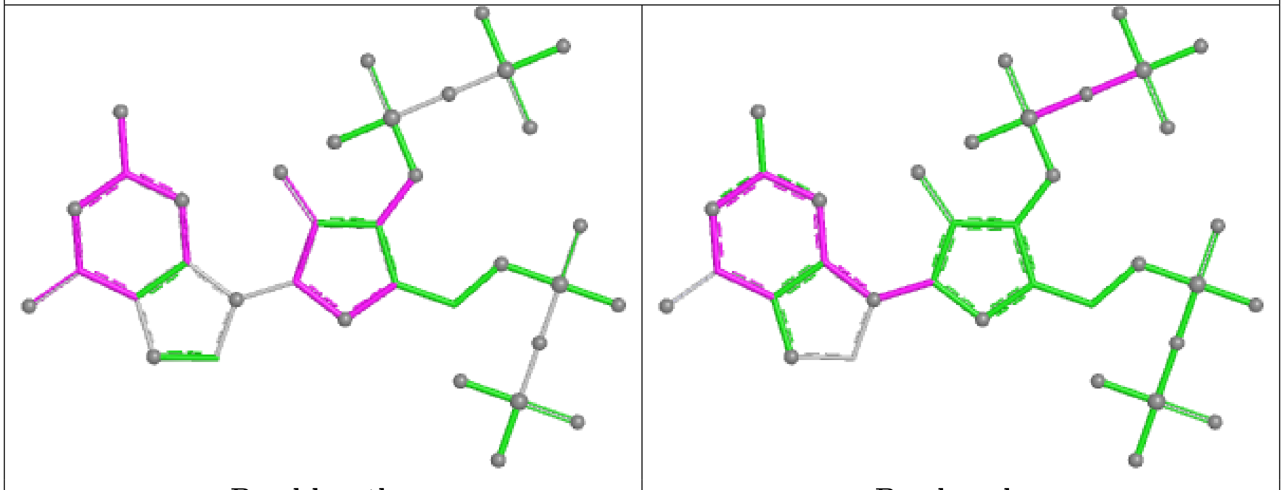


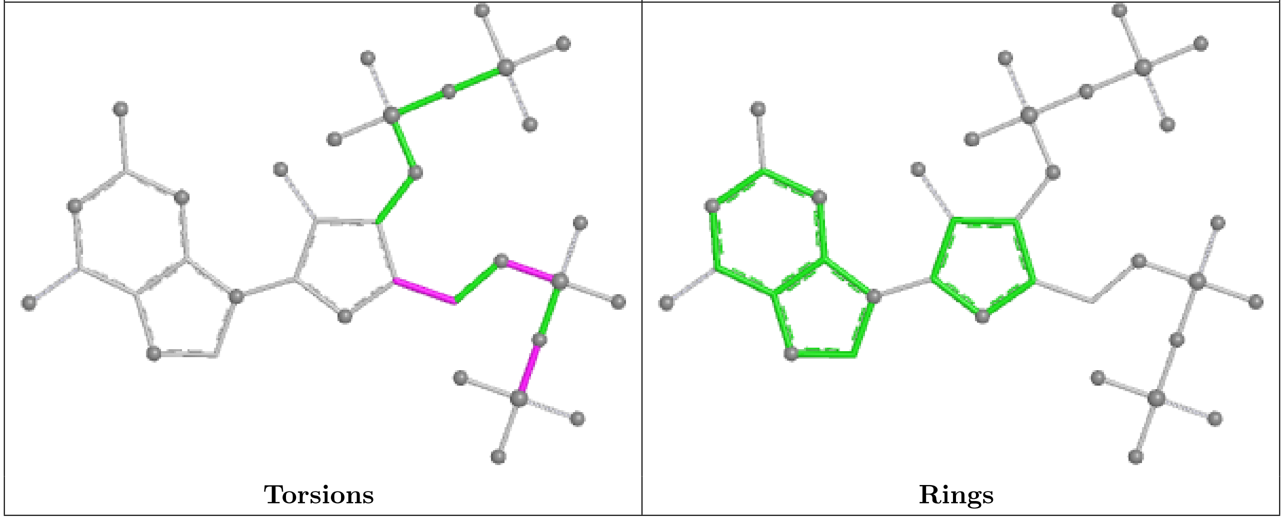
Torsions

Rings

Ligand G4P O 601

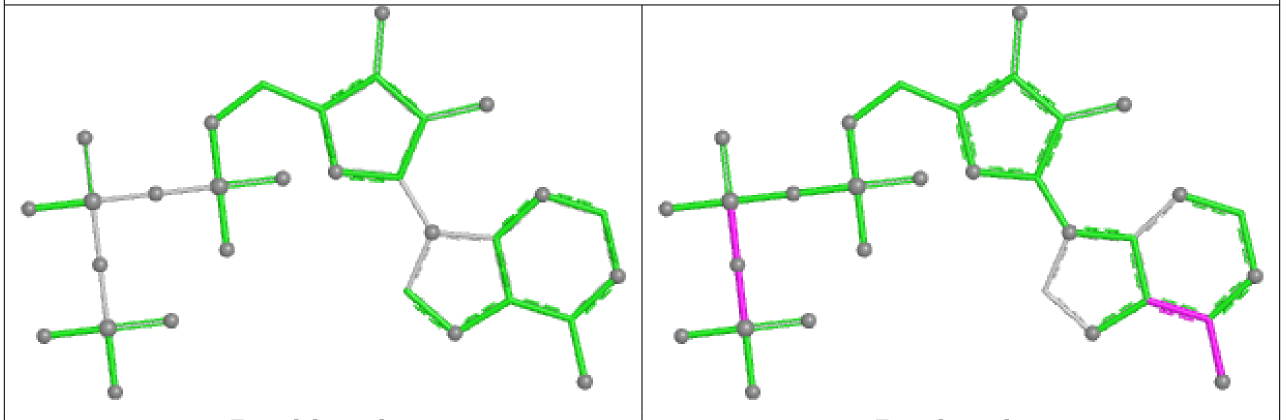


Bond lengths Bond angles



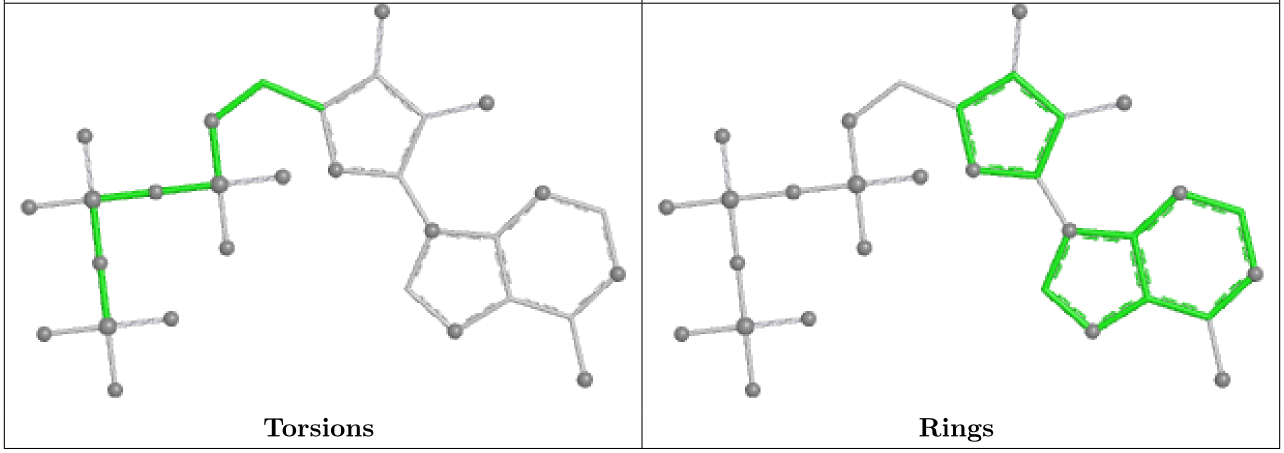
Torsions Rings

Ligand ATP P 600



Bond lengths

Bond angles



Torsions

Rings

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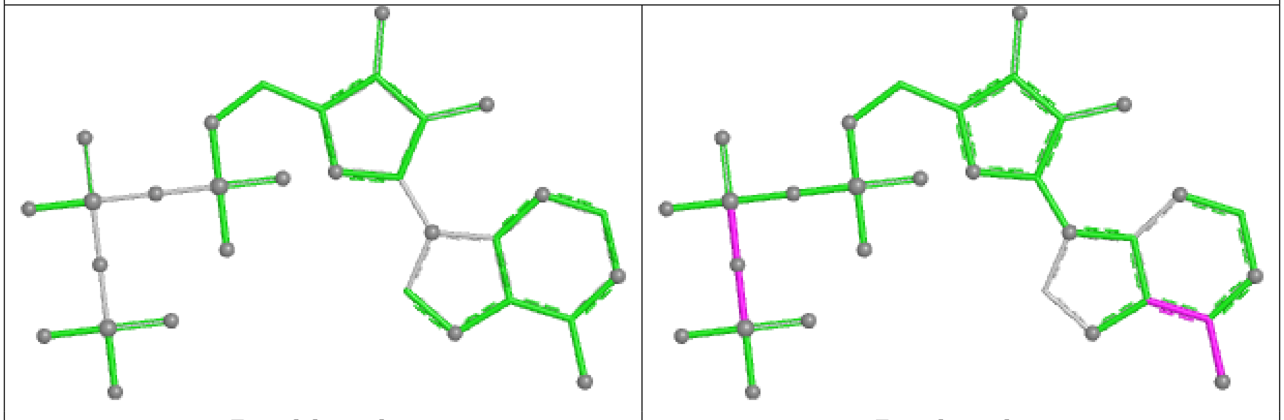
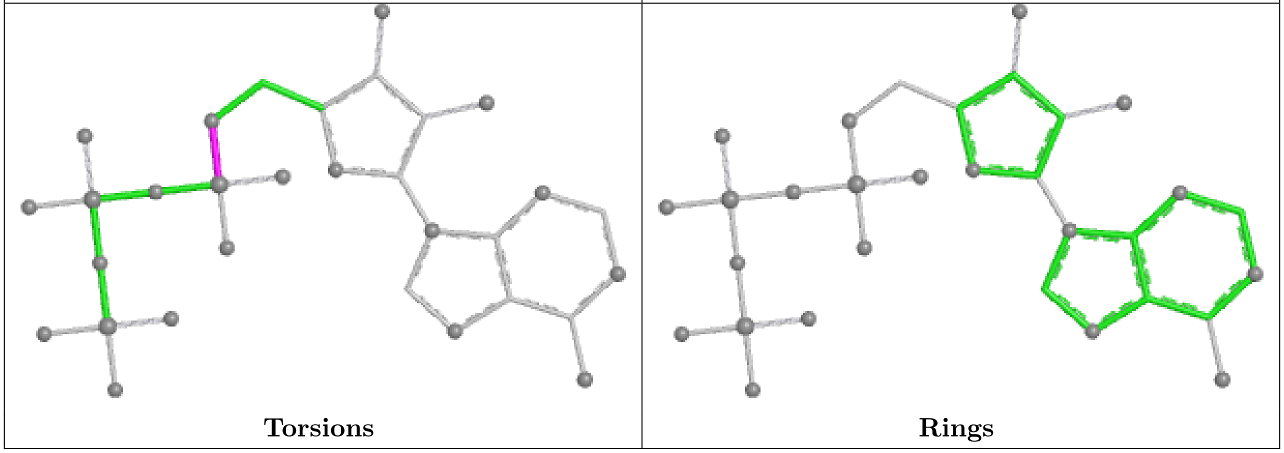


Bond lengths

Bond angles



Torsions

Rings

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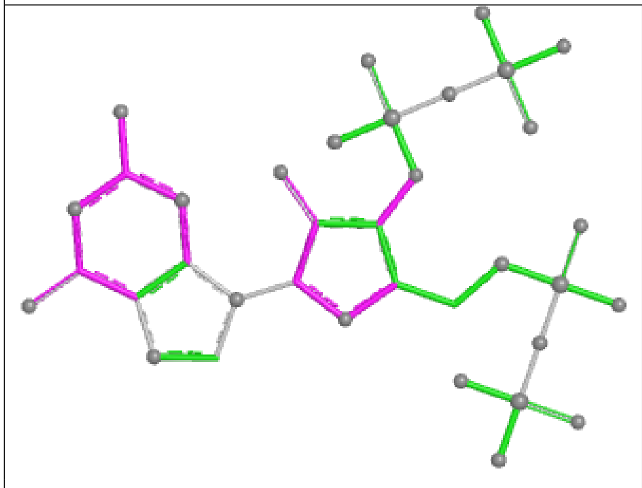

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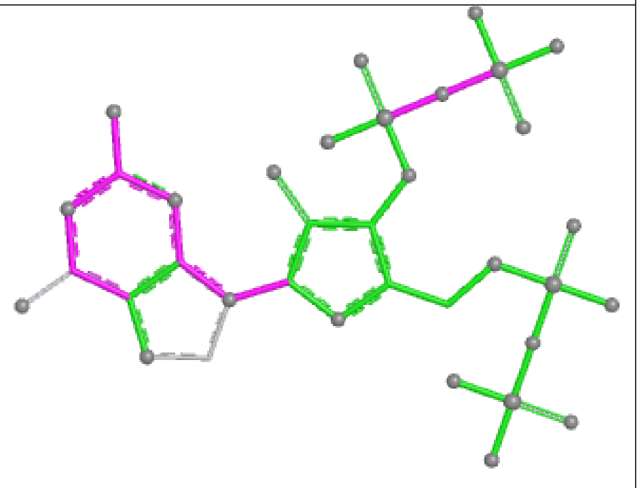

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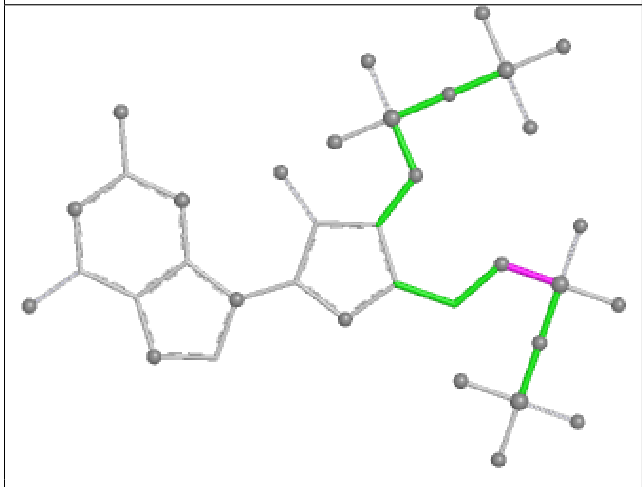

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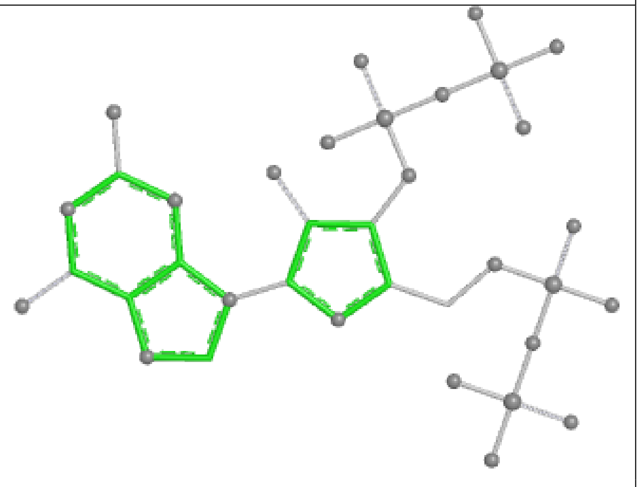

Rings

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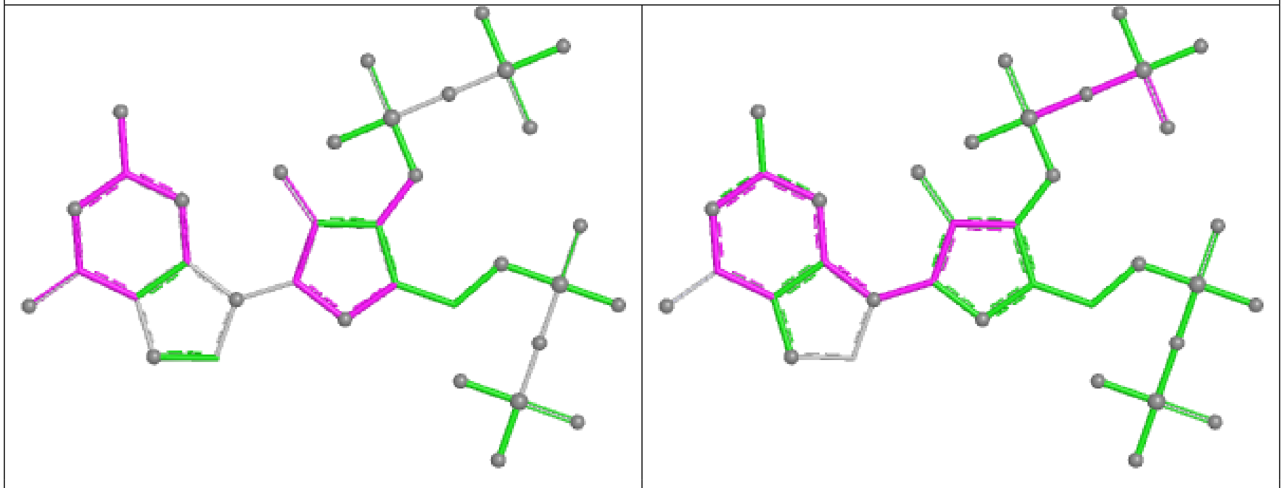
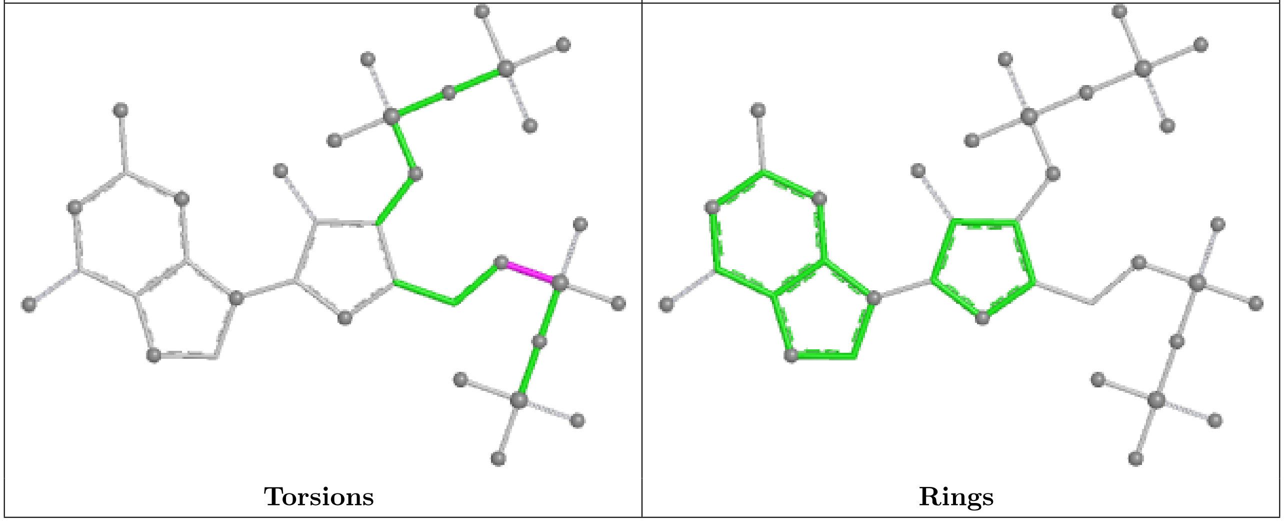


Bond lengths

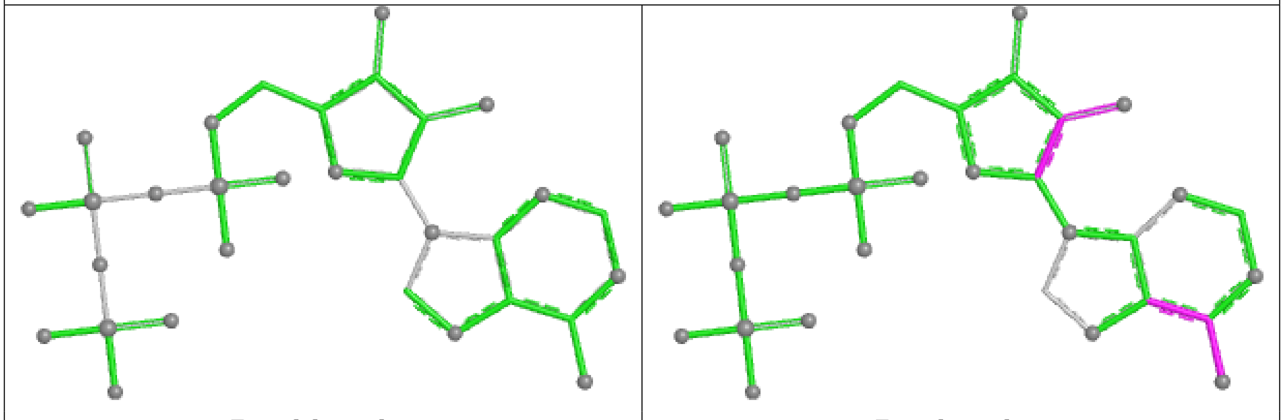
Bond angles



Torsions

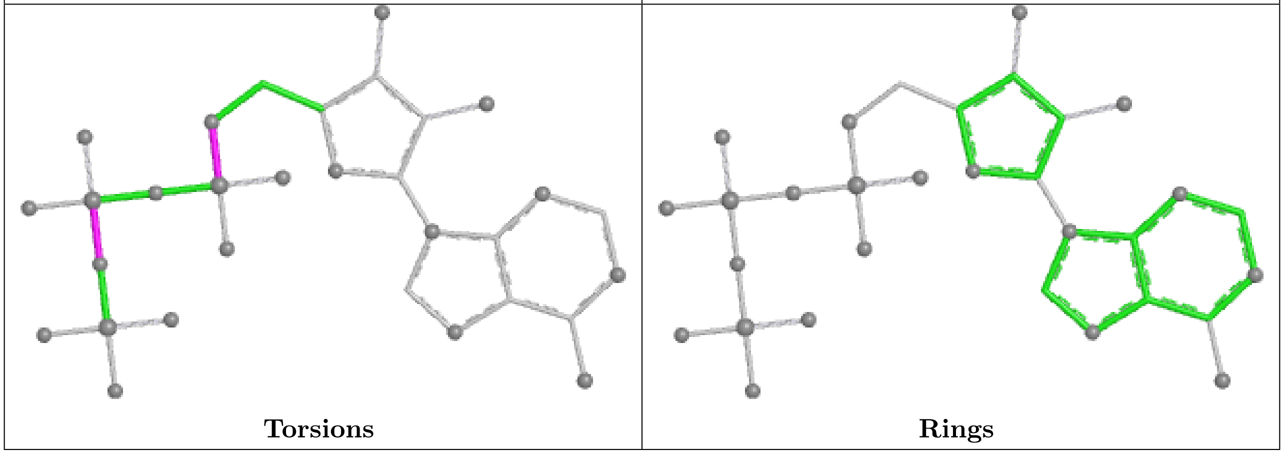
Rings

Ligand ATP J 600



Bond lengths

Bond angles



Torsions

Rings

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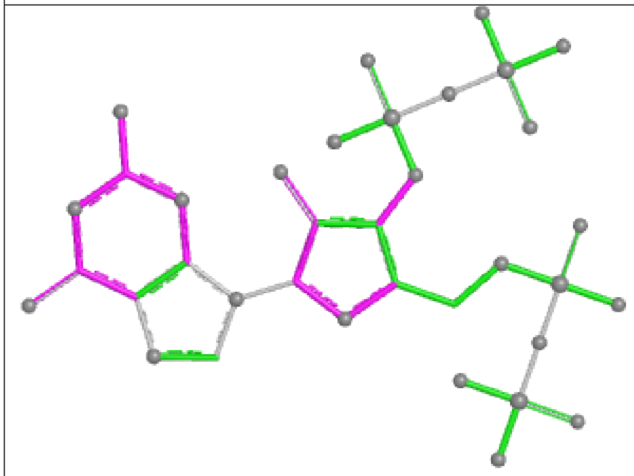

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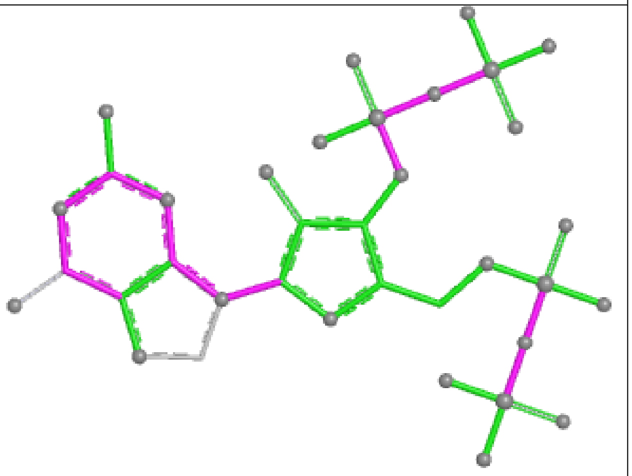

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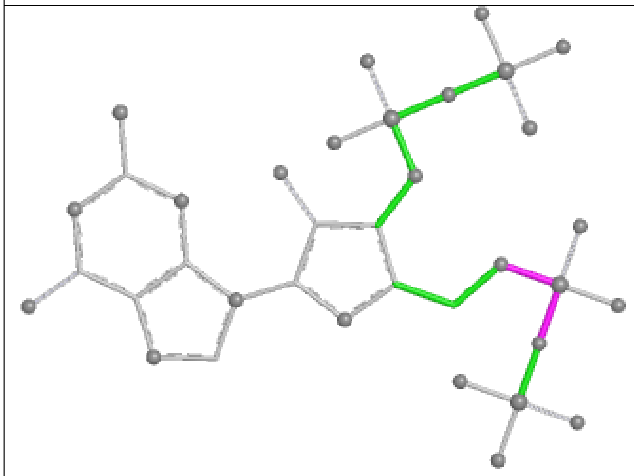

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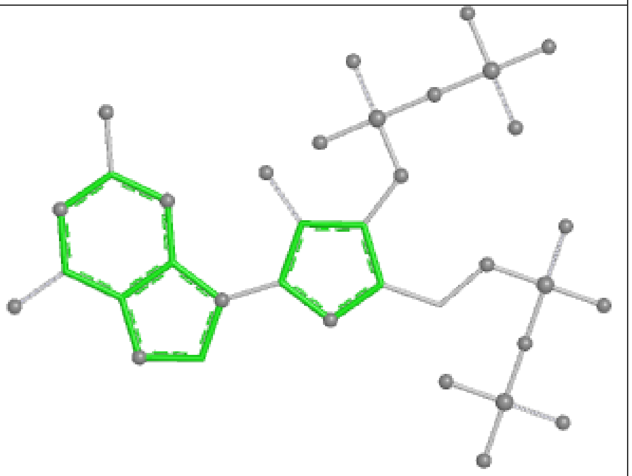
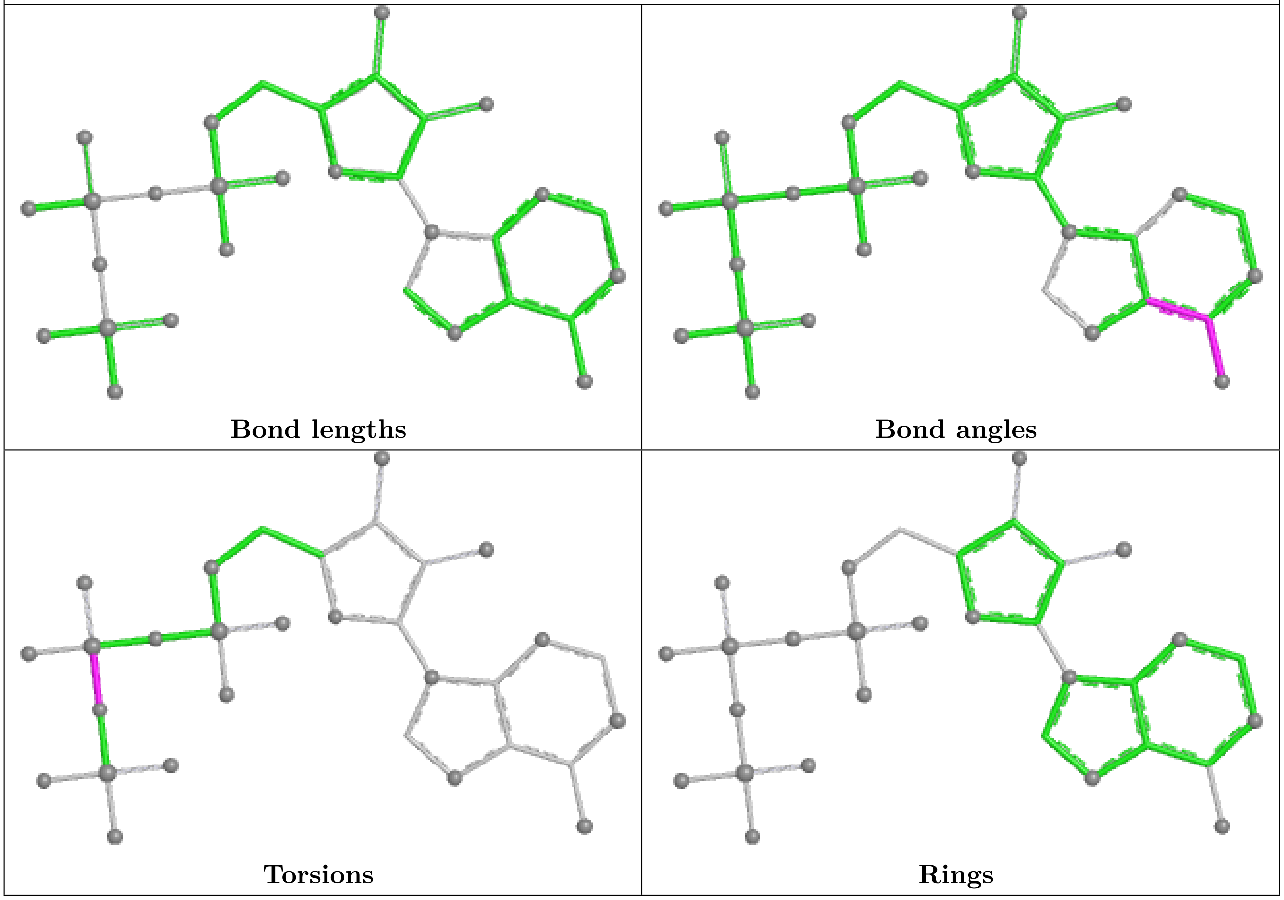


Rings

Ligand ATP H 600



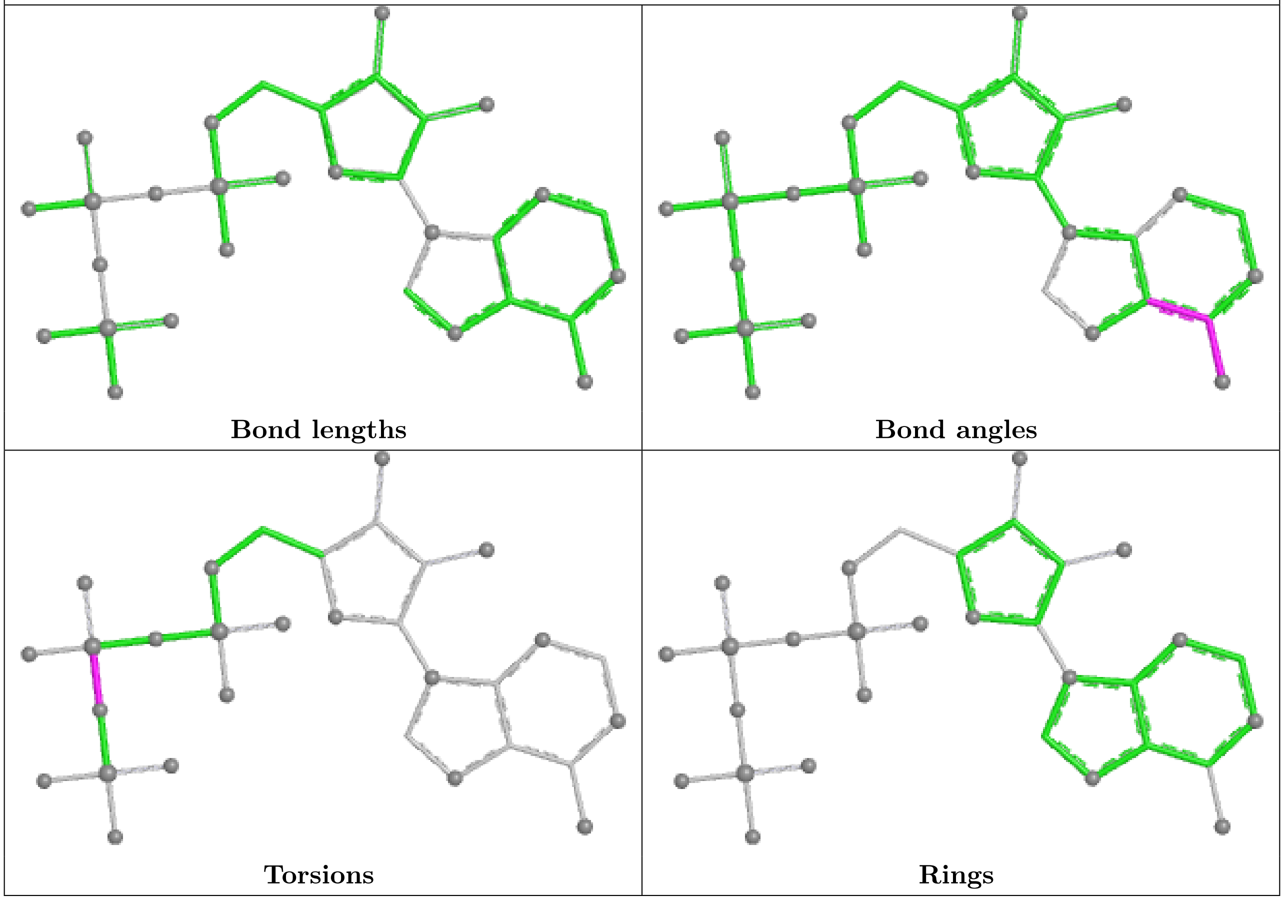
Bond lengths

Bond angles

Torsions

Rings

Ligand ATP D 600



Bond lengths

Bond angles

Torsions

Rings

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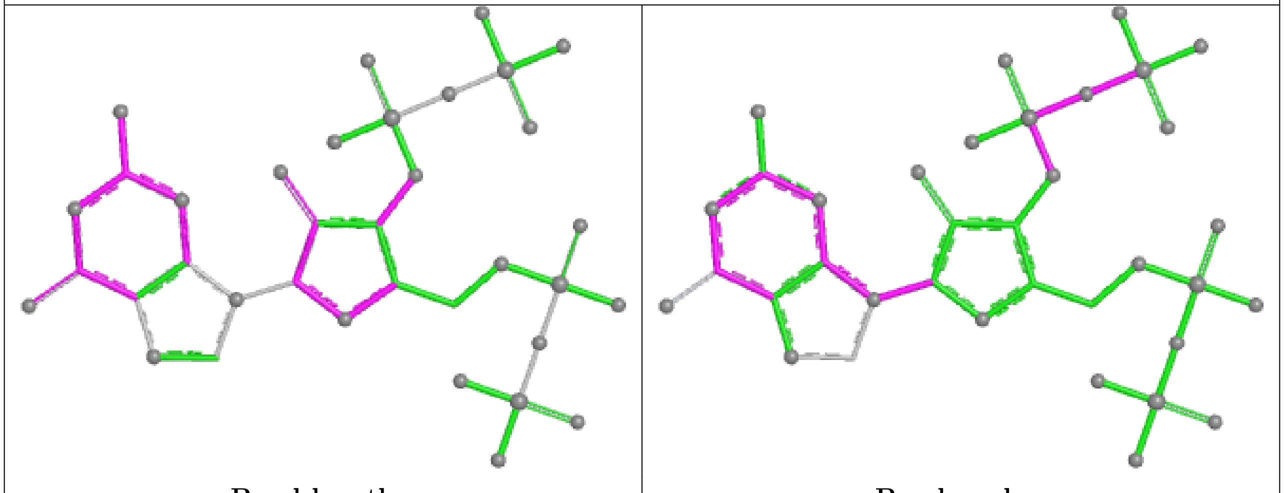

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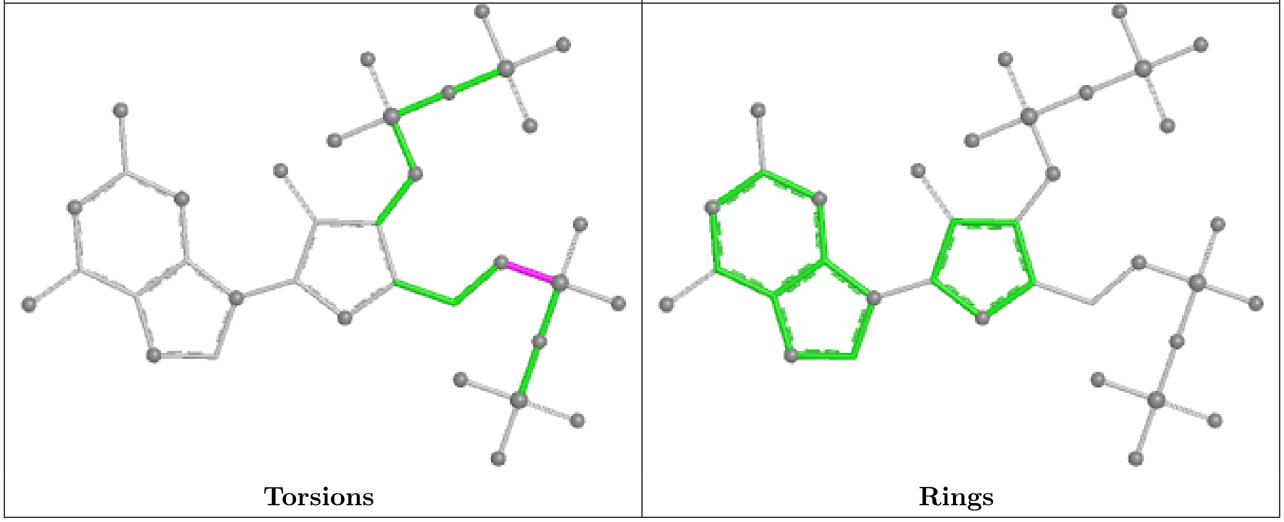
Bond angles



Torsions

Rings

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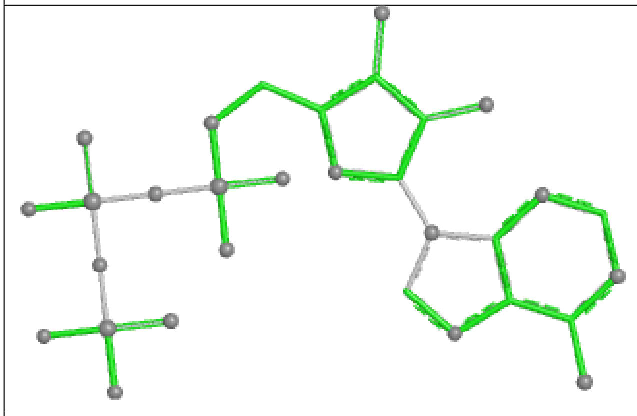

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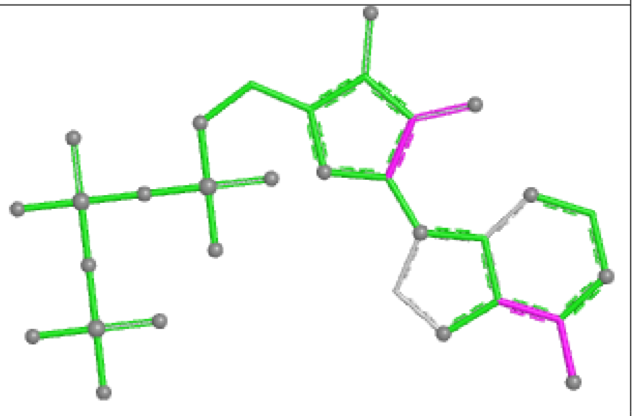
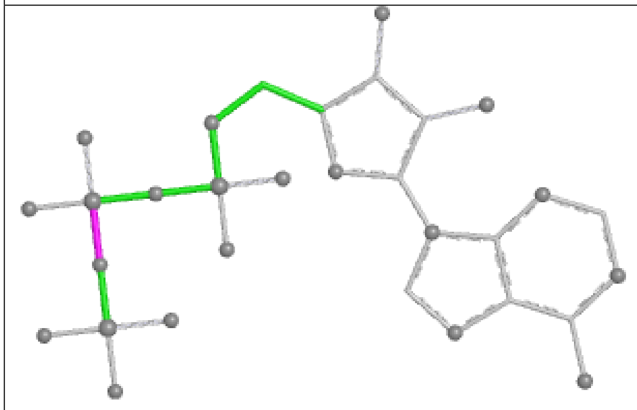


Bond angles



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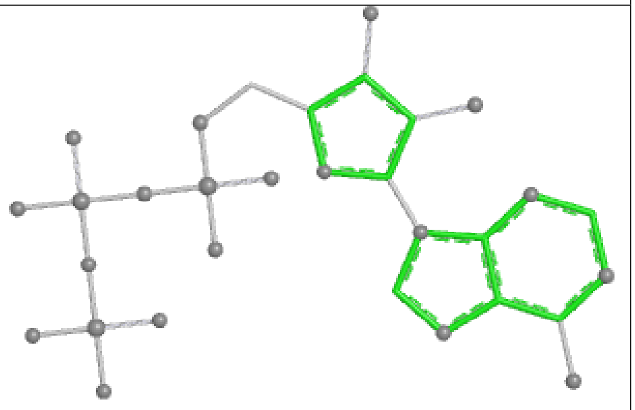
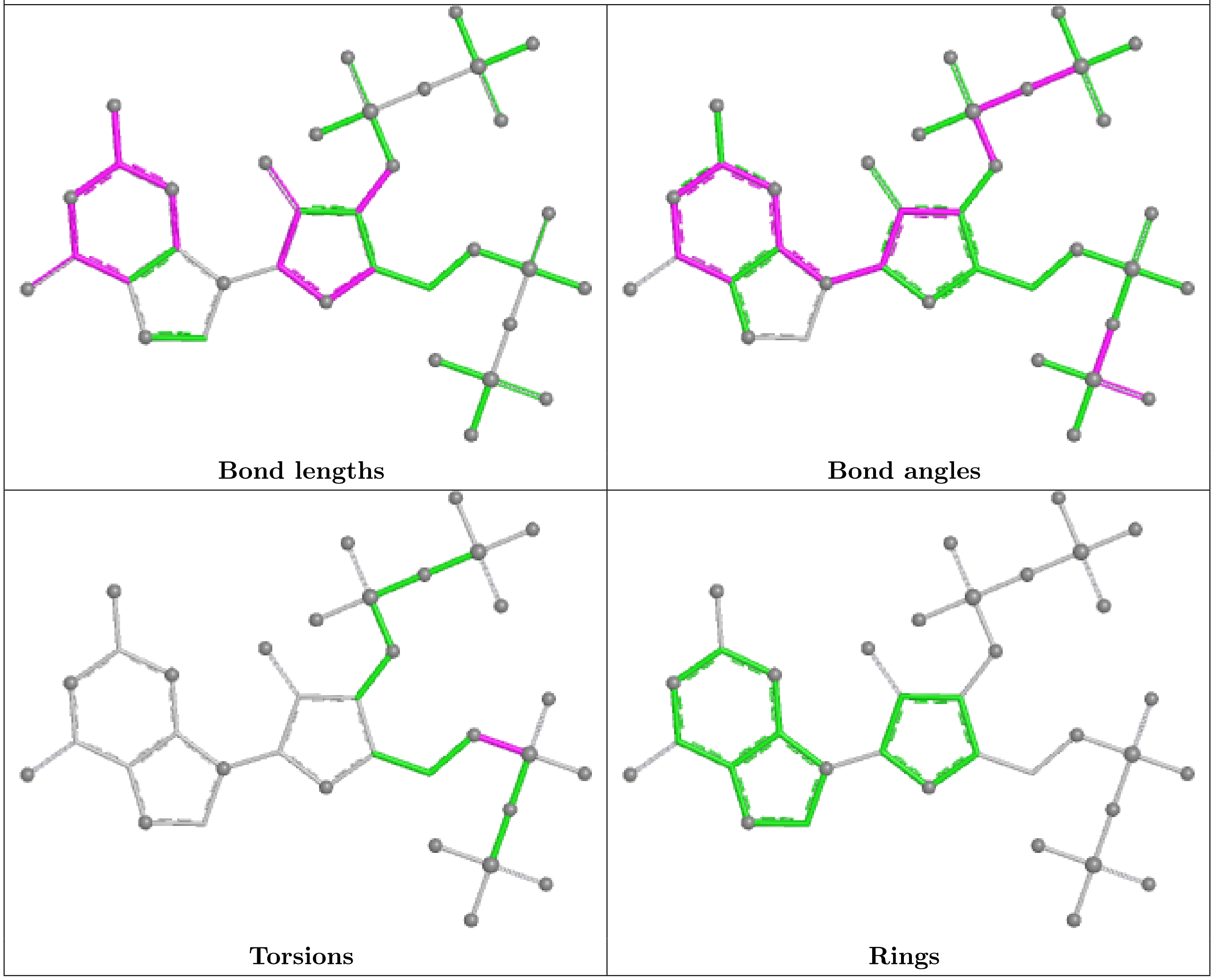


Rings

Ligand G4P F 601



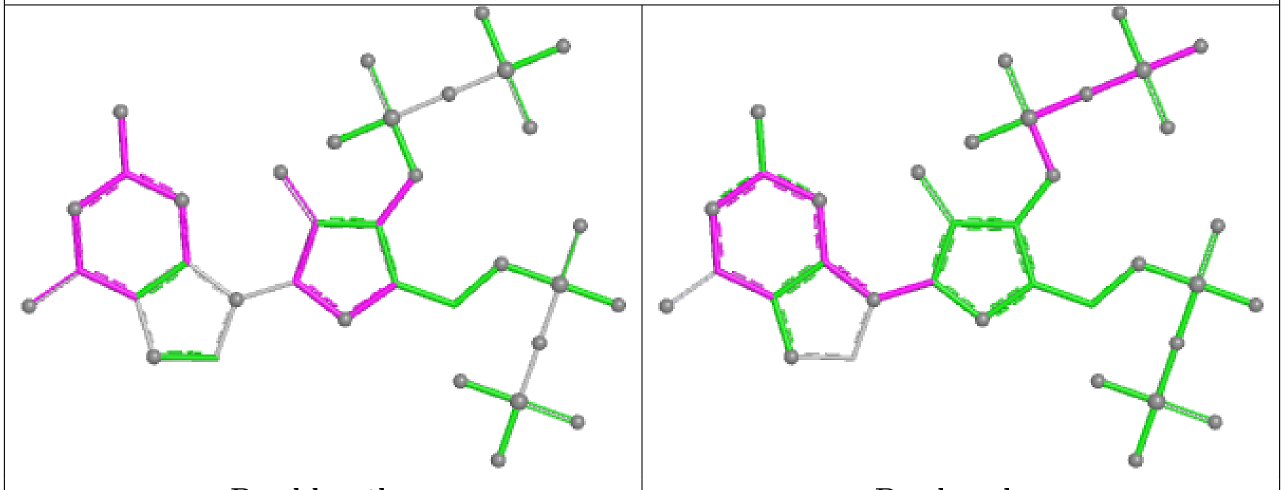
Bond lengths

Bond angles

Torsions

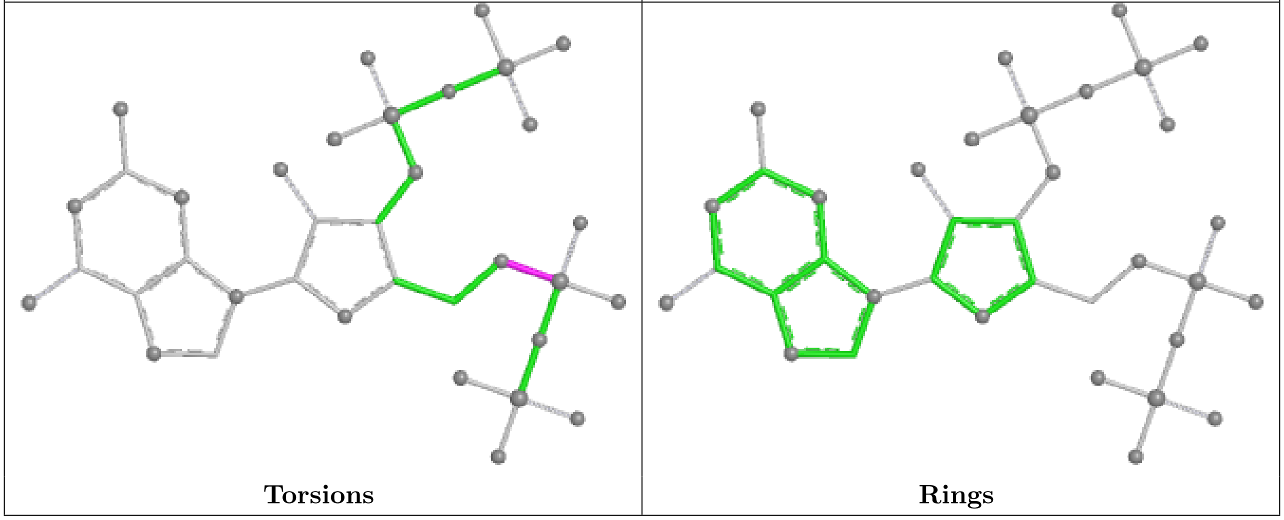
Rings

Ligand G4P L 601



Bond lengths

Bond angles



Torsions

Rings

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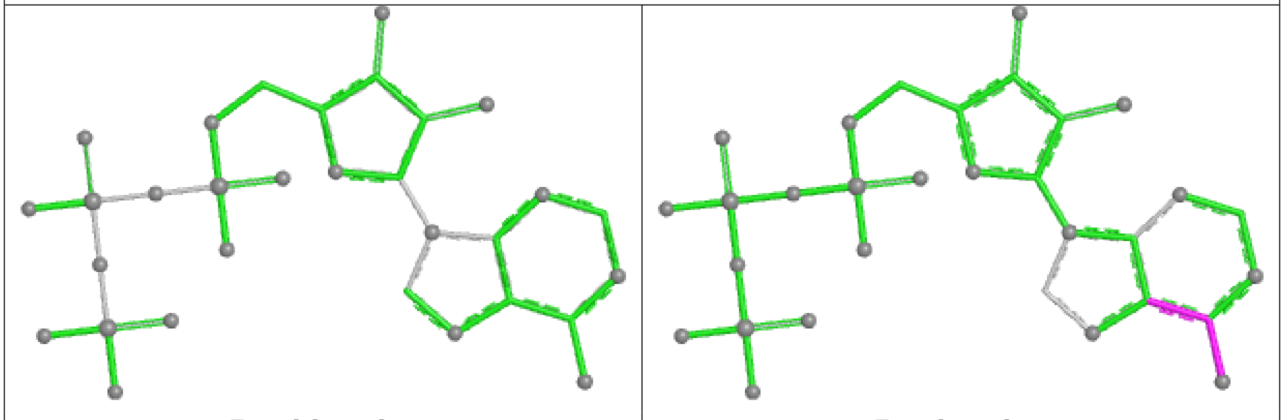
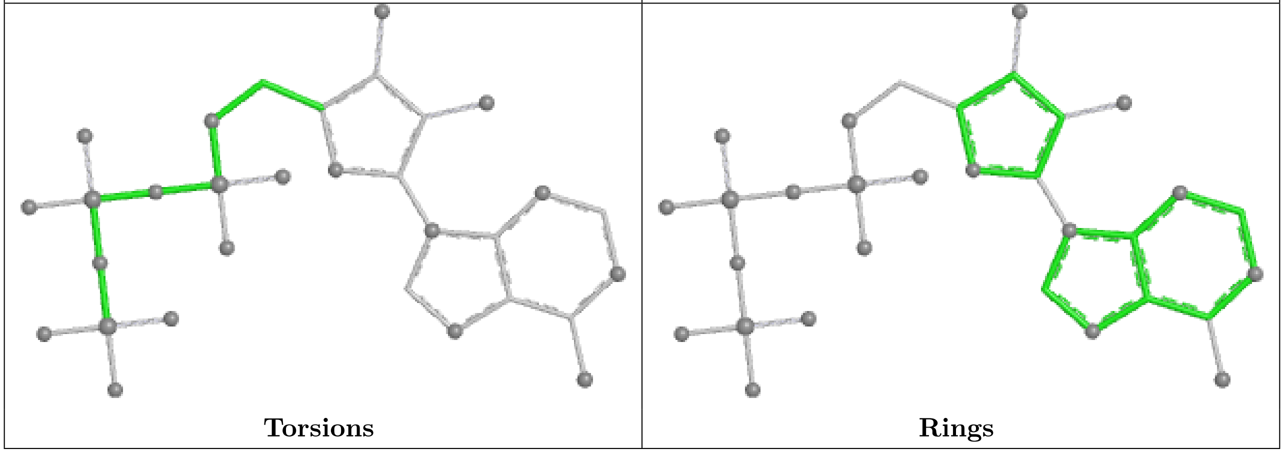


Bond lengths

Bond angles



Torsions

Rings

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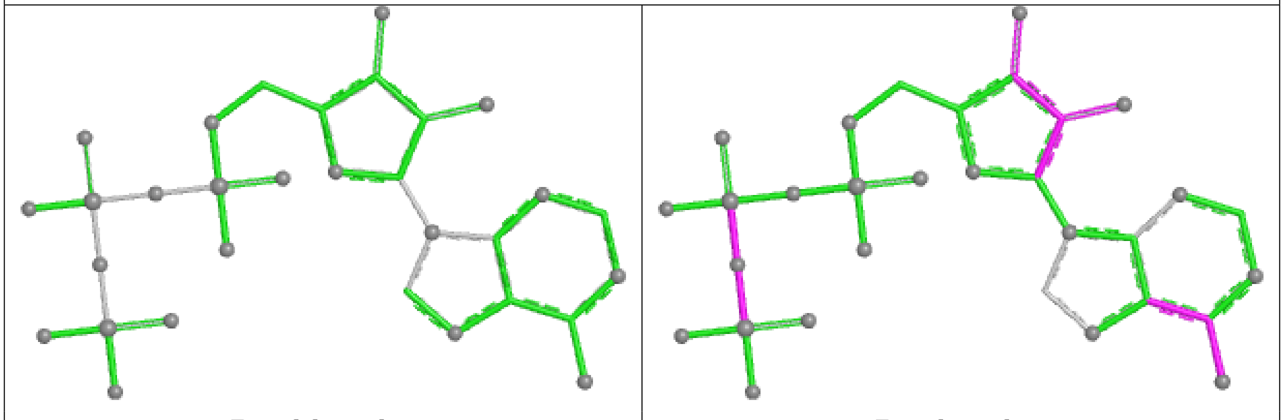
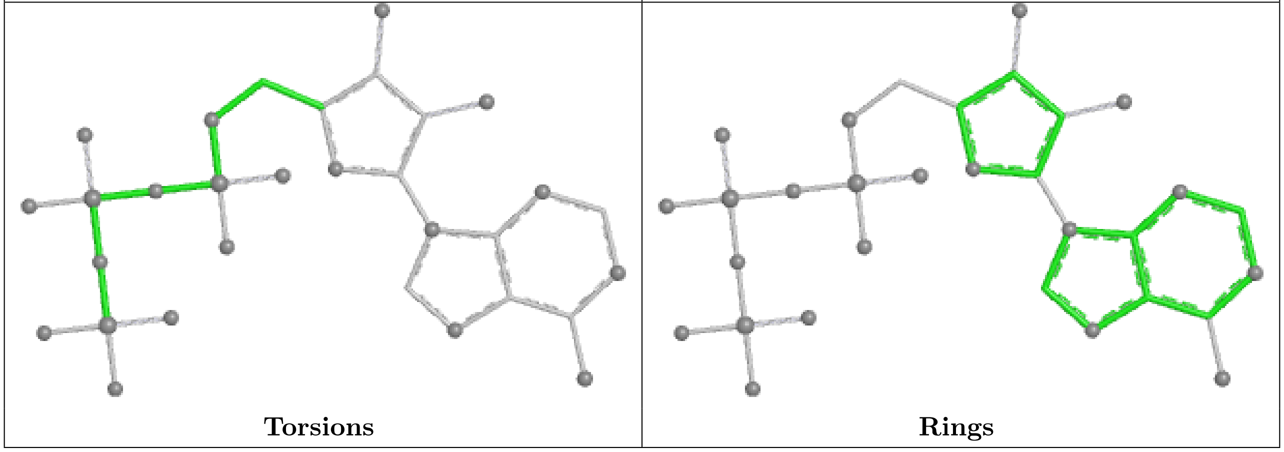
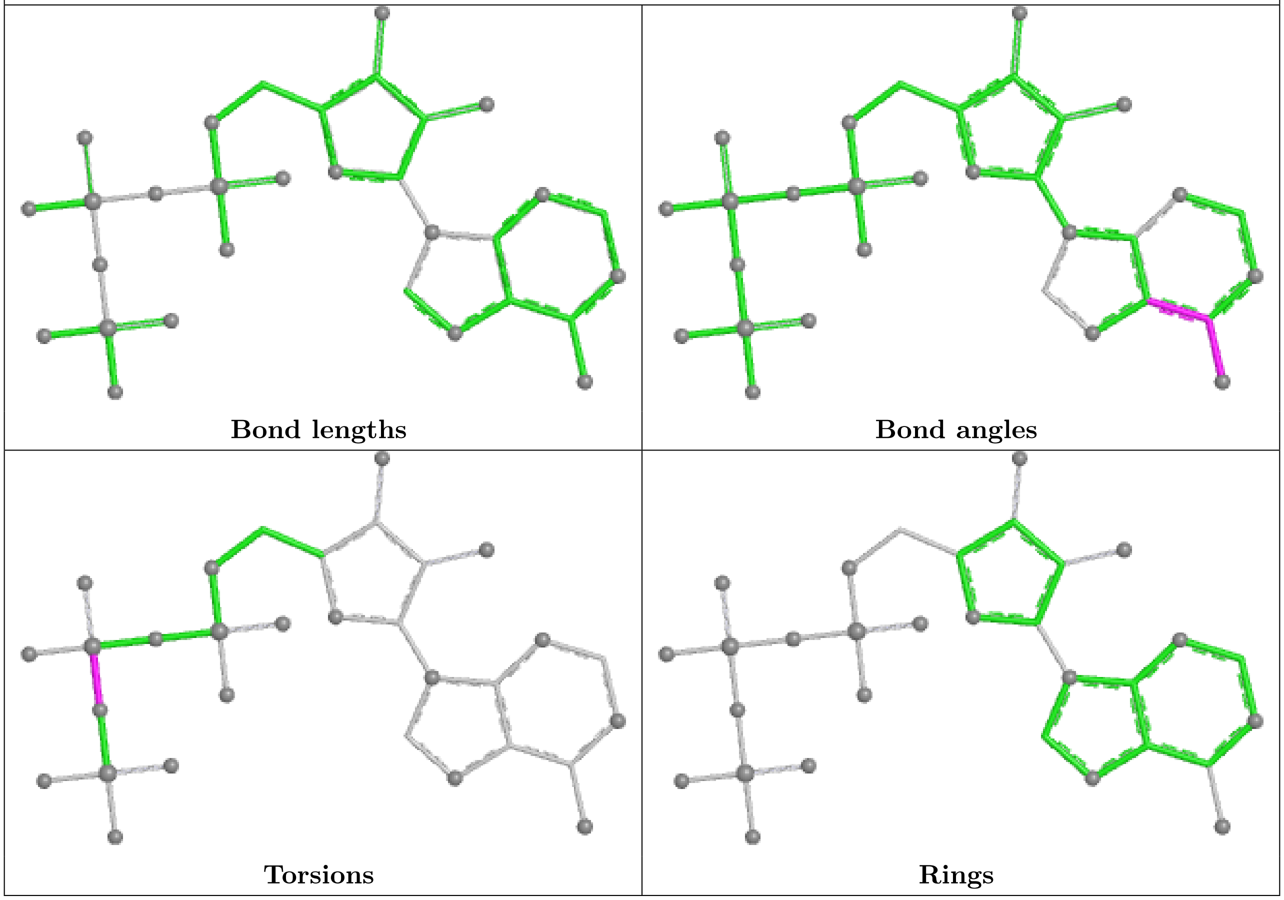


Bond lengths **Bond angles**



Torsions **Rings**

Ligand ATP A 600



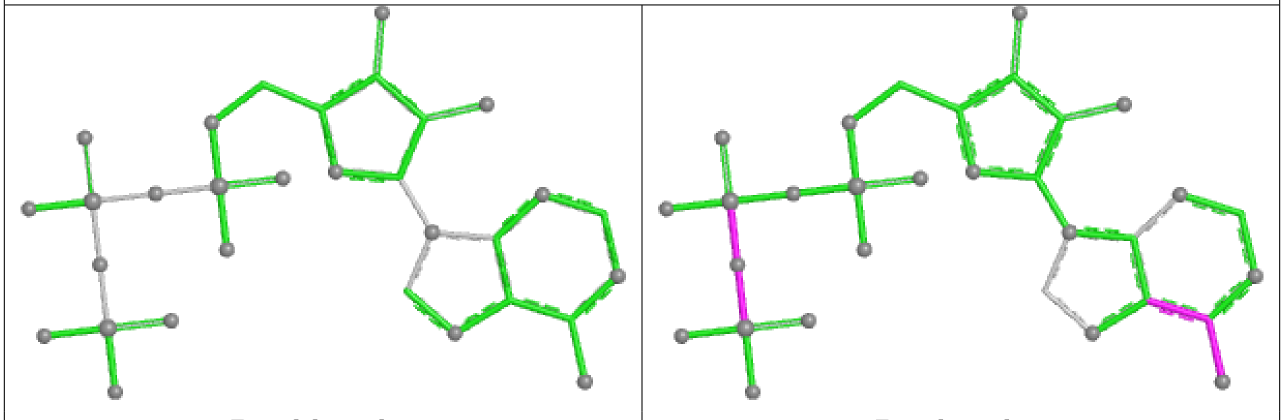
Bond lengths

Bond angles

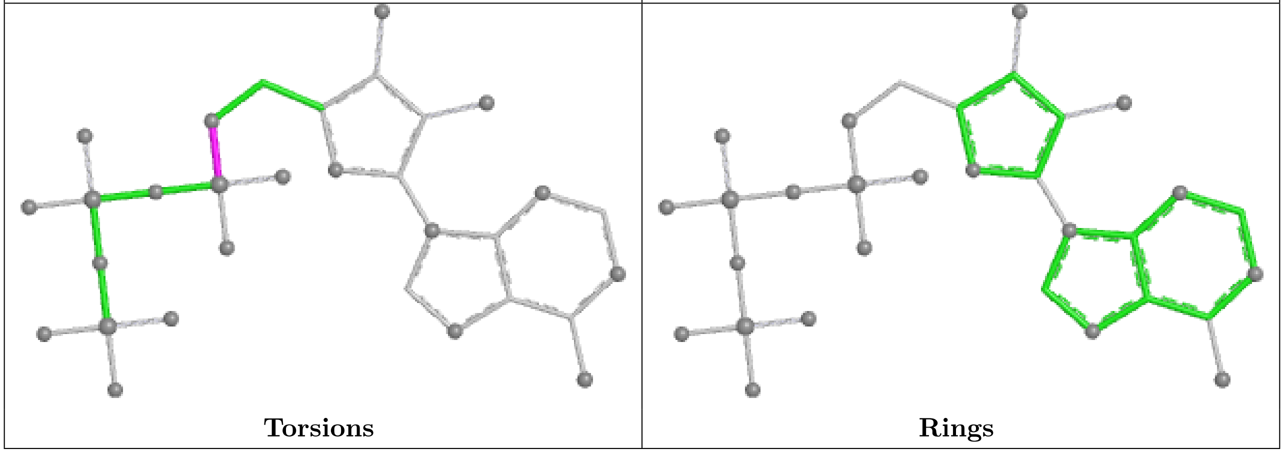
Torsions

Rings

Ligand ATP I 600

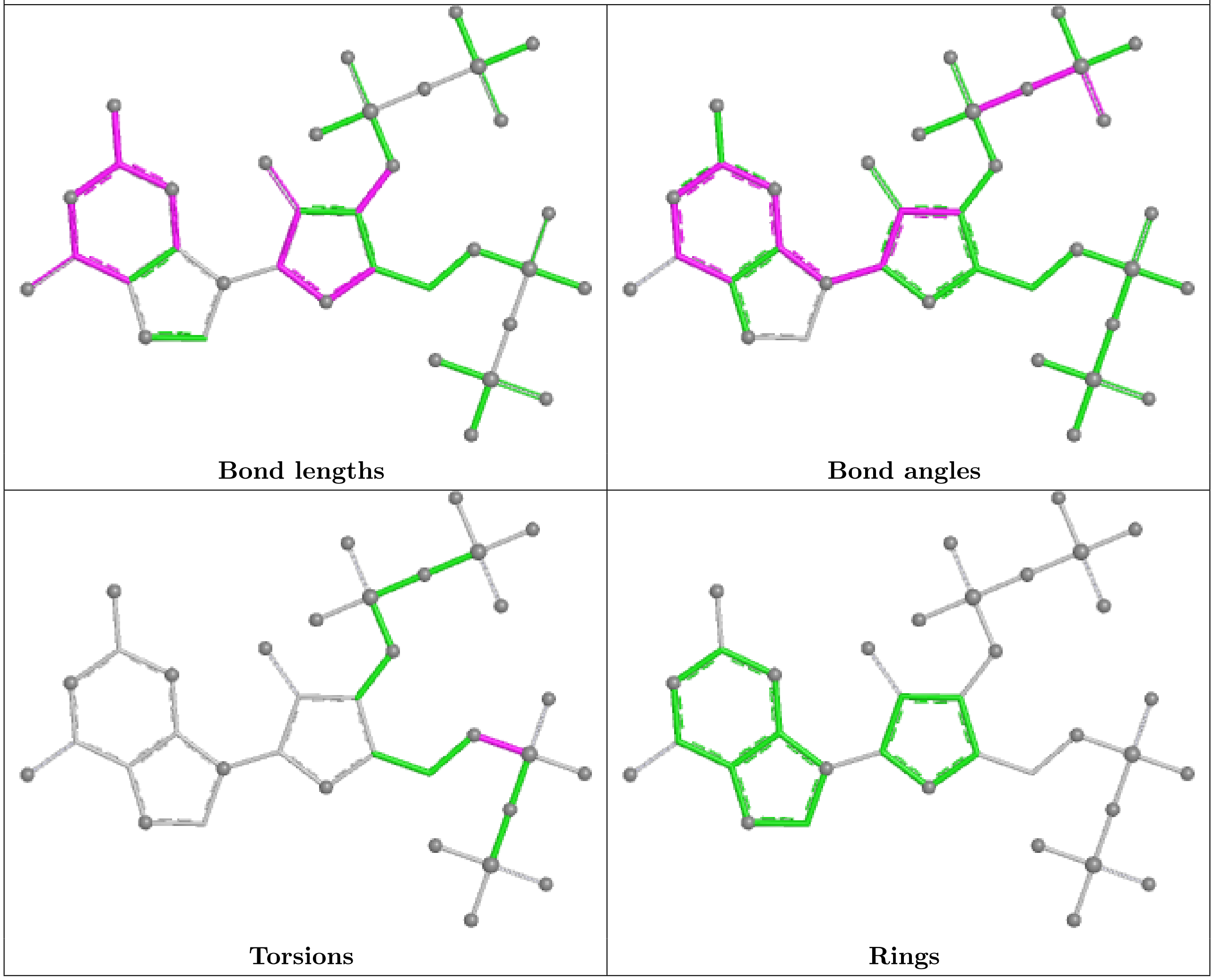


Bond lengths **Bond angles**



Torsions **Rings**

Ligand G4P M 601



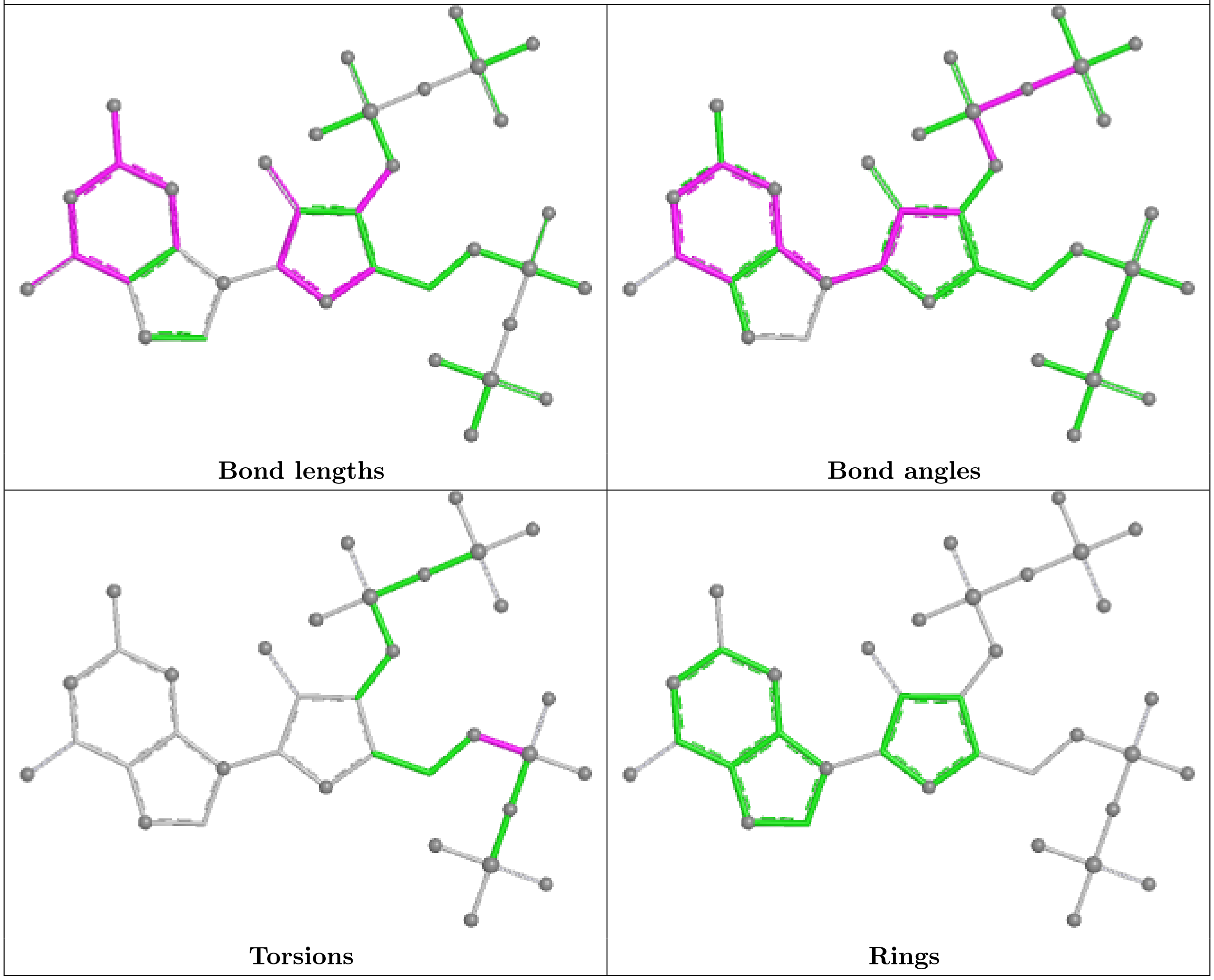
Bond lengths

Bond angles

Torsions

Rings

Ligand G4P B 601



Bond lengths

Bond angles

Torsions

Rings

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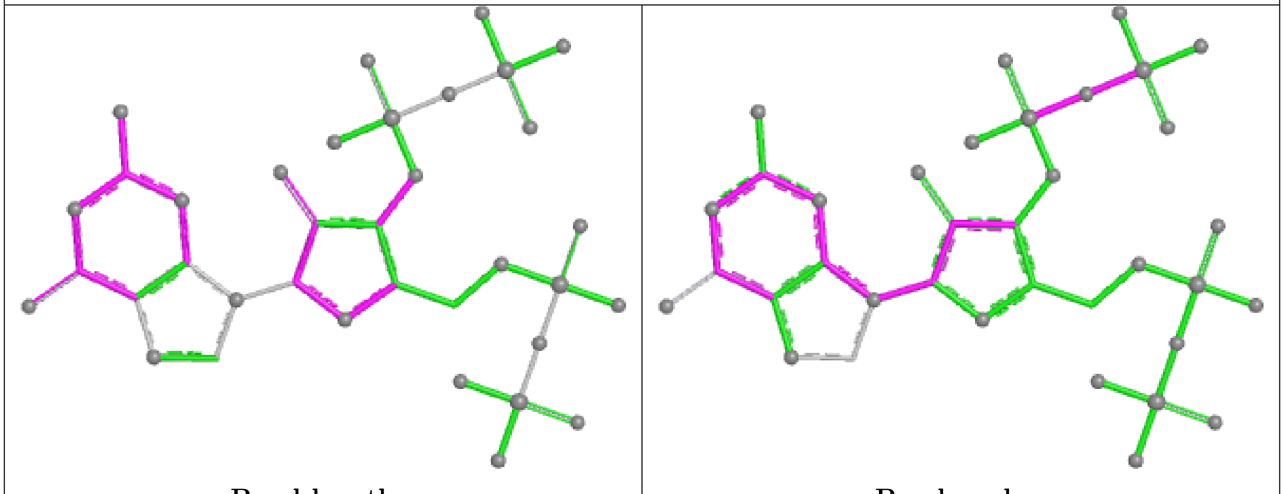
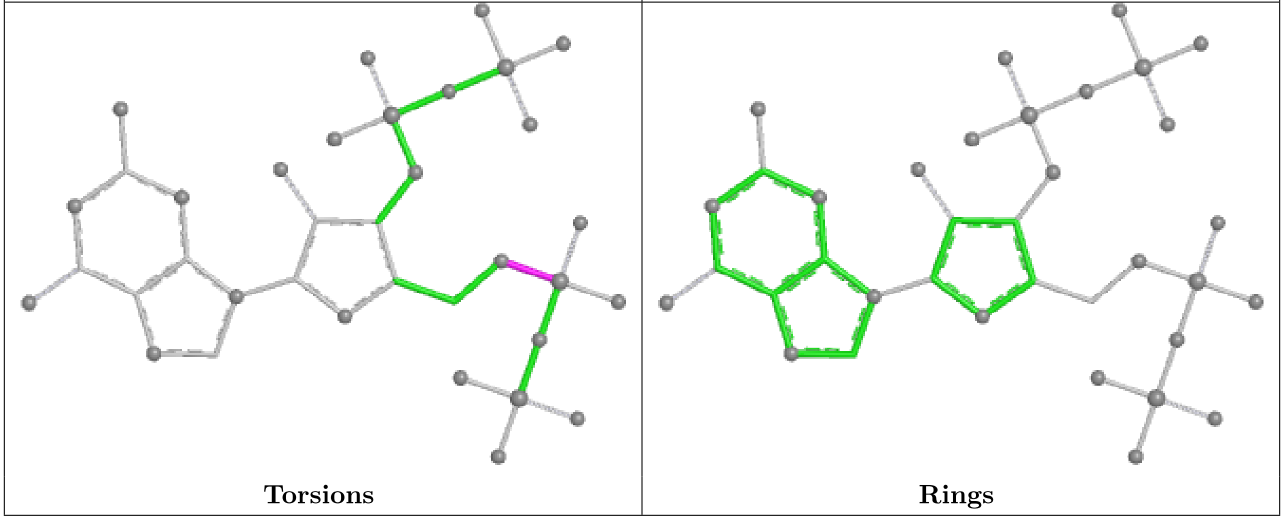


Bond lengths

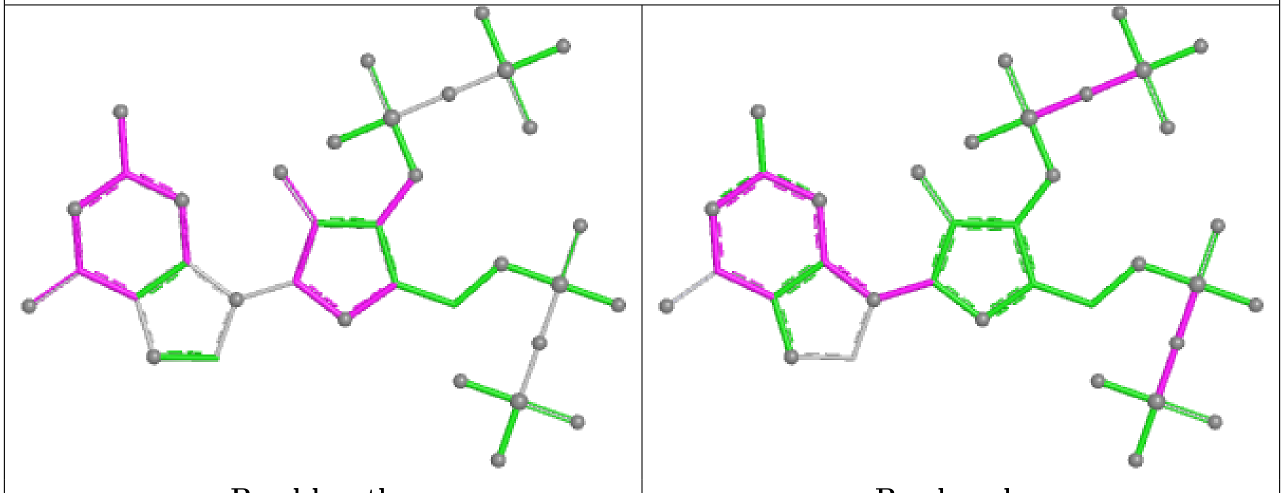
Bond angles



Torsions

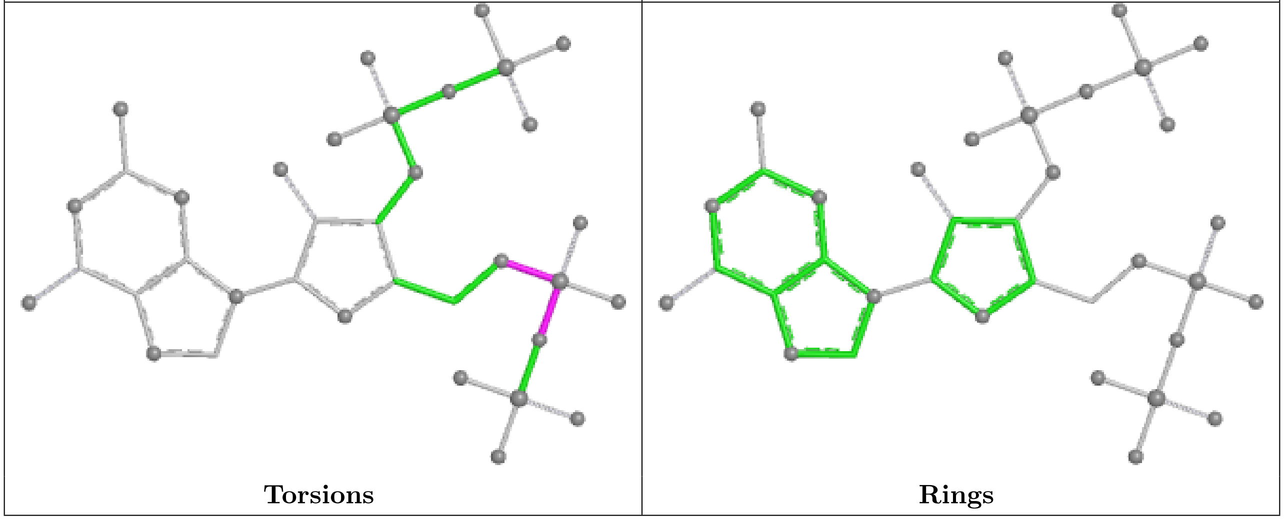
Rings

Ligand G4P I 601



Bond lengths

Bond angles



Torsions

Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	428/504 (84%)	-0.28	1 (0%)	95	94	16, 32, 55, 69	0
1	B	430/504 (85%)	-0.13	4 (0%)	84	83	18, 33, 70, 80	0
1	C	427/504 (84%)	-0.13	5 (1%)	79	78	18, 33, 67, 81	0
1	D	428/504 (84%)	-0.24	1 (0%)	95	94	19, 33, 61, 81	0
1	E	428/504 (84%)	-0.21	2 (0%)	91	91	21, 31, 49, 68	0
1	F	428/504 (84%)	-0.24	2 (0%)	91	91	21, 32, 52, 71	0
1	G	426/504 (84%)	-0.17	3 (0%)	87	87	20, 37, 79, 93	0
1	H	428/504 (84%)	-0.24	2 (0%)	91	91	20, 33, 52, 71	0
1	I	427/504 (84%)	-0.14	3 (0%)	87	87	21, 39, 76, 92	0
1	J	428/504 (84%)	-0.18	1 (0%)	95	94	22, 39, 66, 78	0
1	K	428/504 (84%)	-0.22	1 (0%)	95	94	23, 35, 53, 64	0
1	L	427/504 (84%)	-0.25	1 (0%)	95	94	22, 34, 52, 66	0
1	M	428/504 (84%)	-0.29	1 (0%)	95	94	25, 37, 54, 65	0
1	N	428/504 (84%)	-0.17	4 (0%)	84	83	27, 42, 64, 78	0
1	O	425/504 (84%)	-0.09	6 (1%)	75	74	27, 44, 76, 90	0
1	P	428/504 (84%)	-0.13	3 (0%)	87	87	27, 42, 73, 94	0
All	All	6842/8064 (84%)	-0.19	40 (0%)	89	89	16, 36, 66, 94	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	181	LEU	4.1
1	C	382	PHE	3.8
1	P	382	PHE	3.8
1	P	388	PHE	3.8
1	C	380	LEU	3.2

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
4	MG	N	603	1/1	0.92	0.16	45,45,45,45	0
4	MG	G	602	1/1	0.93	0.17	45,45,45,45	0
4	MG	P	602	1/1	0.93	0.13	41,41,41,41	0
2	ATP	N	600	31/31	0.95	0.14	30,42,56,76	0
4	MG	G	603	1/1	0.95	0.15	40,40,40,40	0
2	ATP	G	600	31/31	0.96	0.13	34,49,63,68	0
4	MG	I	602	1/1	0.96	0.13	45,45,45,45	0
3	G4P	J	601	36/36	0.97	0.11	32,47,58,69	0
3	G4P	O	601	36/36	0.97	0.11	39,52,63,73	0
4	MG	B	603	1/1	0.97	0.14	36,36,36,36	0
2	ATP	B	600	31/31	0.97	0.11	34,49,63,71	0
2	ATP	I	600	31/31	0.97	0.13	40,57,71,72	0
2	ATP	J	600	31/31	0.97	0.12	33,43,55,60	0
2	ATP	C	600	31/31	0.97	0.14	32,54,69,77	0
4	MG	O	602	1/1	0.97	0.17	45,45,45,45	0
2	ATP	O	600	31/31	0.97	0.12	42,58,73,77	0
3	G4P	E	601	36/36	0.98	0.12	18,28,43,72	0
3	G4P	F	601	36/36	0.98	0.13	18,31,45,62	0
3	G4P	G	601	36/36	0.98	0.11	34,45,70,74	0
3	G4P	H	601	36/36	0.98	0.12	23,32,46,68	0
3	G4P	I	601	36/36	0.98	0.10	37,49,60,68	0
2	ATP	F	600	31/31	0.98	0.13	14,25,31,40	0
3	G4P	K	601	36/36	0.98	0.12	22,31,45,75	0
3	G4P	M	601	36/36	0.98	0.12	23,33,46,56	0
3	G4P	N	601	36/36	0.98	0.11	31,43,60,77	0
2	ATP	M	600	31/31	0.98	0.12	19,28,37,41	0
3	G4P	P	601	36/36	0.98	0.11	35,44,55,69	0

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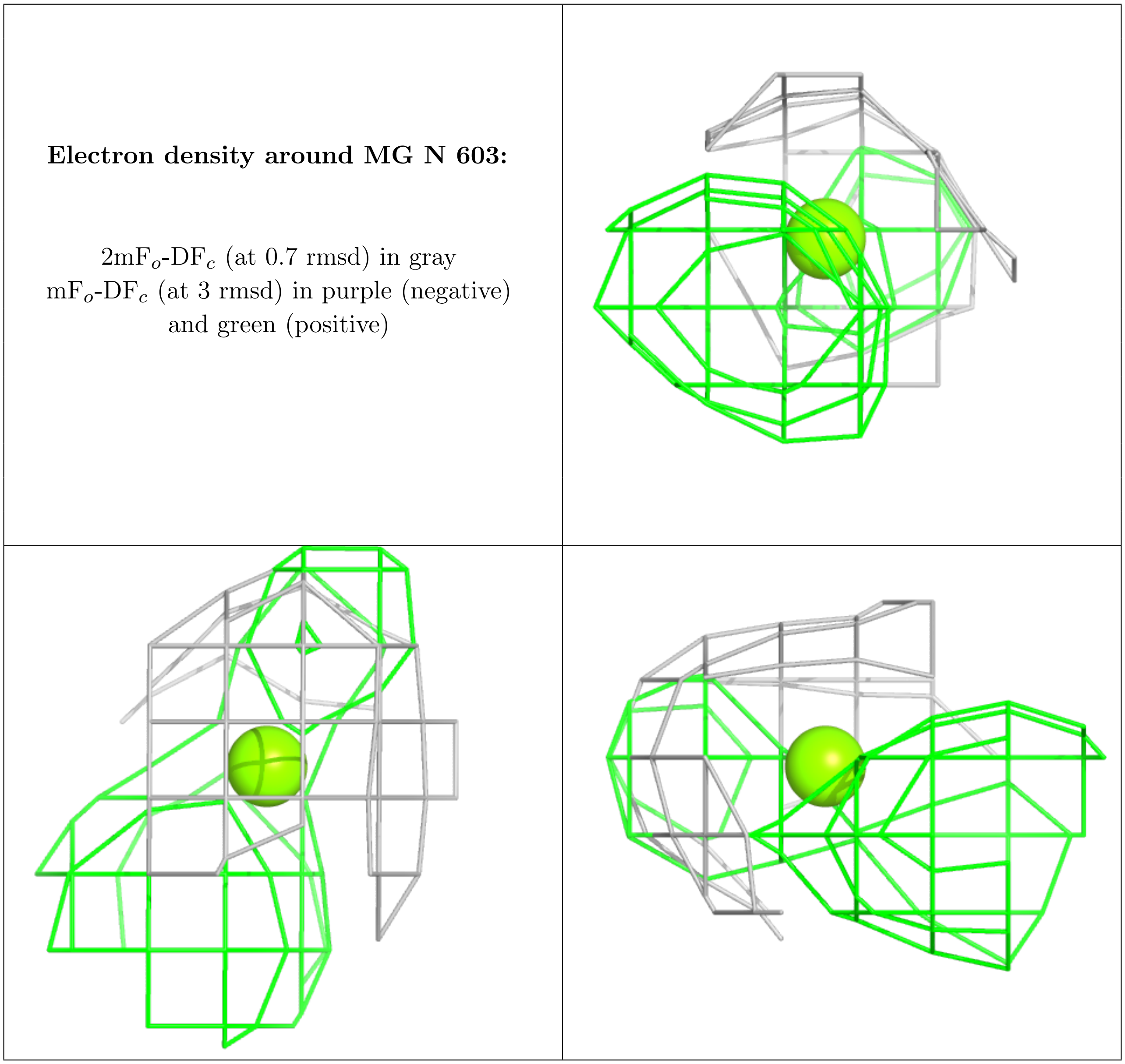
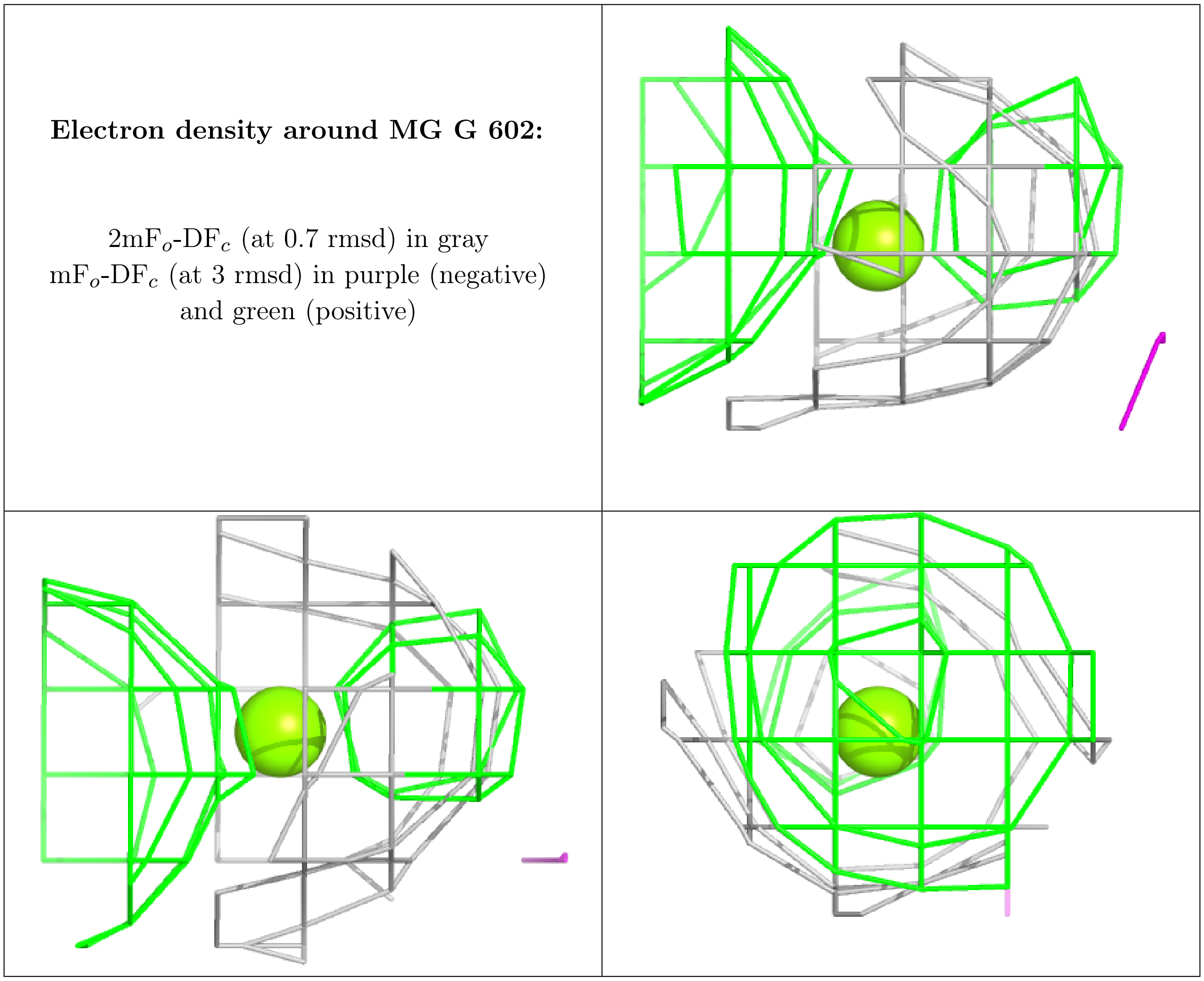
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	B	602	1/1	0.98	0.10	35,35,35,35	0
2	ATP	A	600	31/31	0.98	0.12	20,28,44,49	0
4	MG	C	602	1/1	0.98	0.12	38,38,38,38	0
4	MG	C	603	1/1	0.98	0.11	38,38,38,38	0
4	MG	D	603	1/1	0.98	0.15	26,26,26,26	0
4	MG	E	602	1/1	0.98	0.14	23,23,23,23	0
4	MG	F	603	1/1	0.98	0.17	22,22,22,22	0
2	ATP	D	600	31/31	0.98	0.12	21,36,51,59	0
2	ATP	P	600	31/31	0.98	0.10	29,52,70,76	0
4	MG	H	603	1/1	0.98	0.14	26,26,26,26	0
3	G4P	A	601	36/36	0.98	0.12	22,33,47,70	0
4	MG	J	602	1/1	0.98	0.14	41,41,41,41	0
4	MG	M	603	1/1	0.98	0.17	25,25,25,25	0
4	MG	N	602	1/1	0.98	0.12	35,35,35,35	0
3	G4P	B	601	36/36	0.98	0.11	30,40,55,65	0
3	G4P	C	601	36/36	0.98	0.12	34,41,54,67	0
4	MG	O	603	1/1	0.98	0.18	43,43,43,43	0
3	G4P	D	601	36/36	0.98	0.12	22,34,47,70	0
4	MG	P	603	1/1	0.98	0.14	37,37,37,37	0
2	ATP	E	600	31/31	0.99	0.12	15,25,30,35	0
2	ATP	H	600	31/31	0.99	0.12	20,27,33,40	0
4	MG	I	603	1/1	0.99	0.13	46,46,46,46	0
2	ATP	K	600	31/31	0.99	0.13	20,29,38,48	0
4	MG	J	603	1/1	0.99	0.13	42,42,42,42	0
4	MG	K	602	1/1	0.99	0.16	23,23,23,23	0
4	MG	K	603	1/1	0.99	0.15	25,25,25,25	0
4	MG	L	602	1/1	0.99	0.18	24,24,24,24	0
4	MG	L	603	1/1	0.99	0.16	23,23,23,23	0
4	MG	M	602	1/1	0.99	0.16	24,24,24,24	0
4	MG	A	602	1/1	0.99	0.14	27,27,27,27	0
4	MG	E	603	1/1	0.99	0.13	23,23,23,23	0
4	MG	F	602	1/1	0.99	0.13	25,25,25,25	0
4	MG	A	603	1/1	0.99	0.12	25,25,25,25	0
3	G4P	L	601	36/36	0.99	0.12	20,32,47,68	0
2	ATP	L	600	31/31	0.99	0.12	17,27,32,34	0
4	MG	H	602	1/1	0.99	0.13	23,23,23,23	0
4	MG	D	602	1/1	1.00	0.15	24,24,24,24	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 MG N 603:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

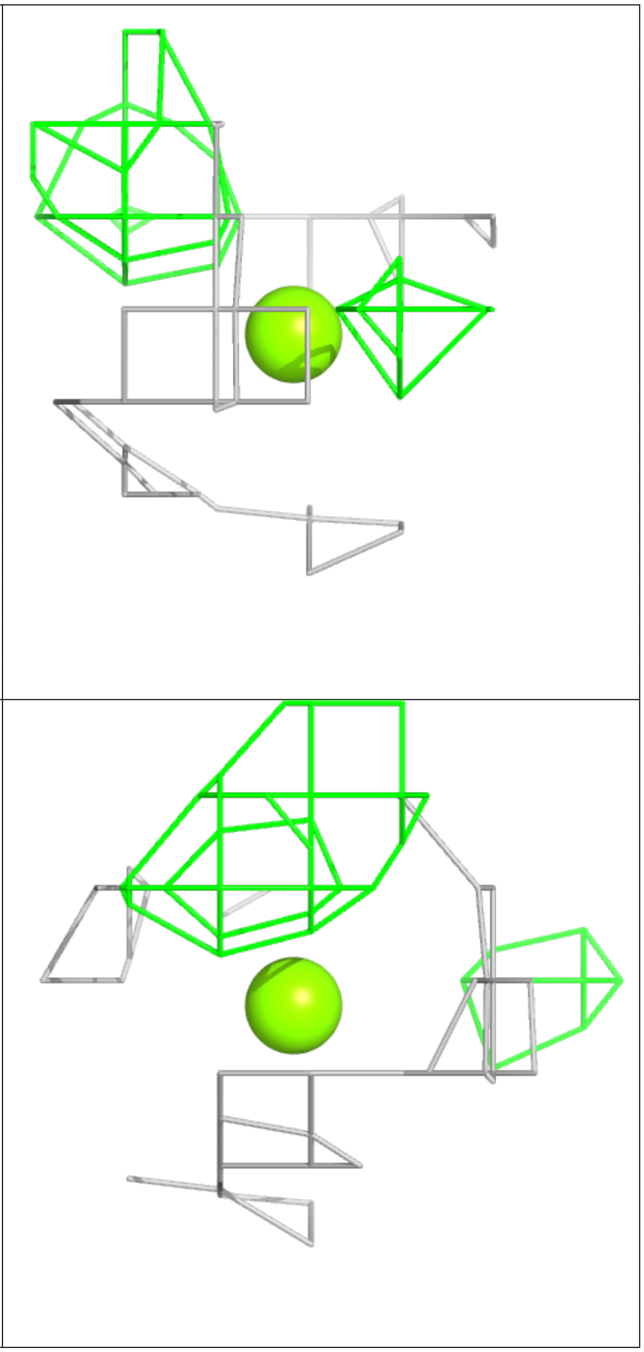


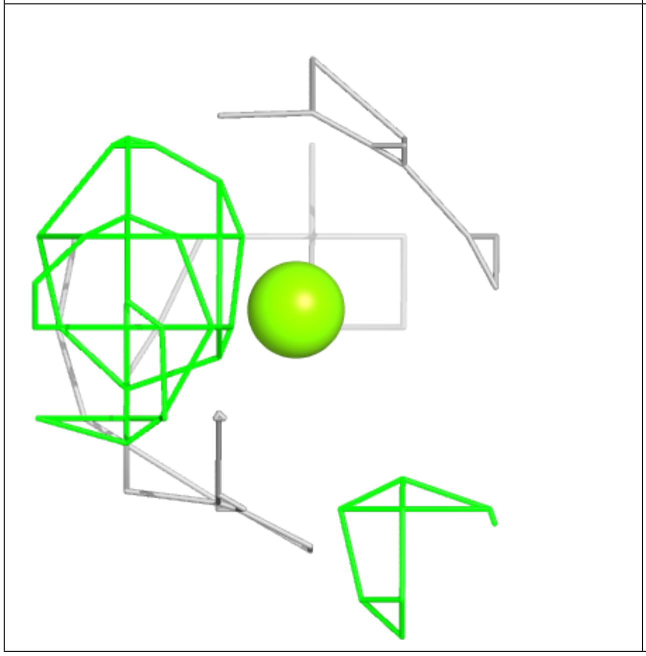
Electron density around MG G 602:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around MG P 602:

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





Electron density around ATP N 600:

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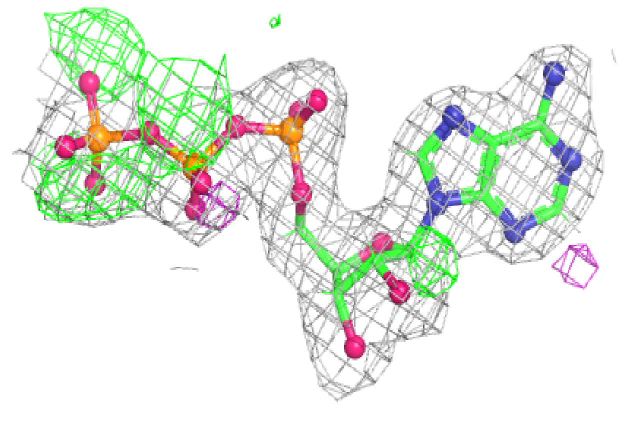
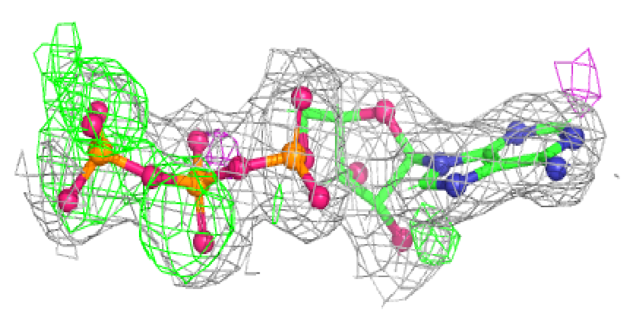
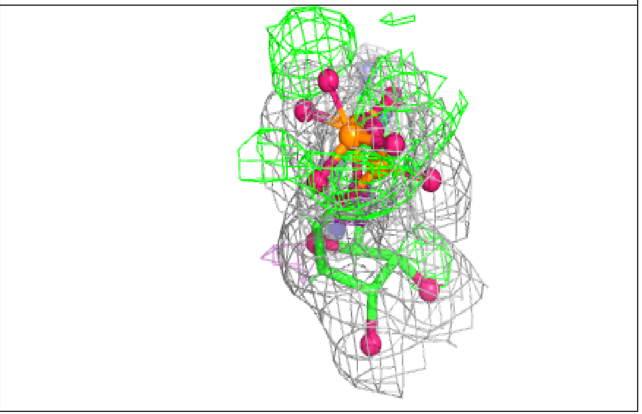
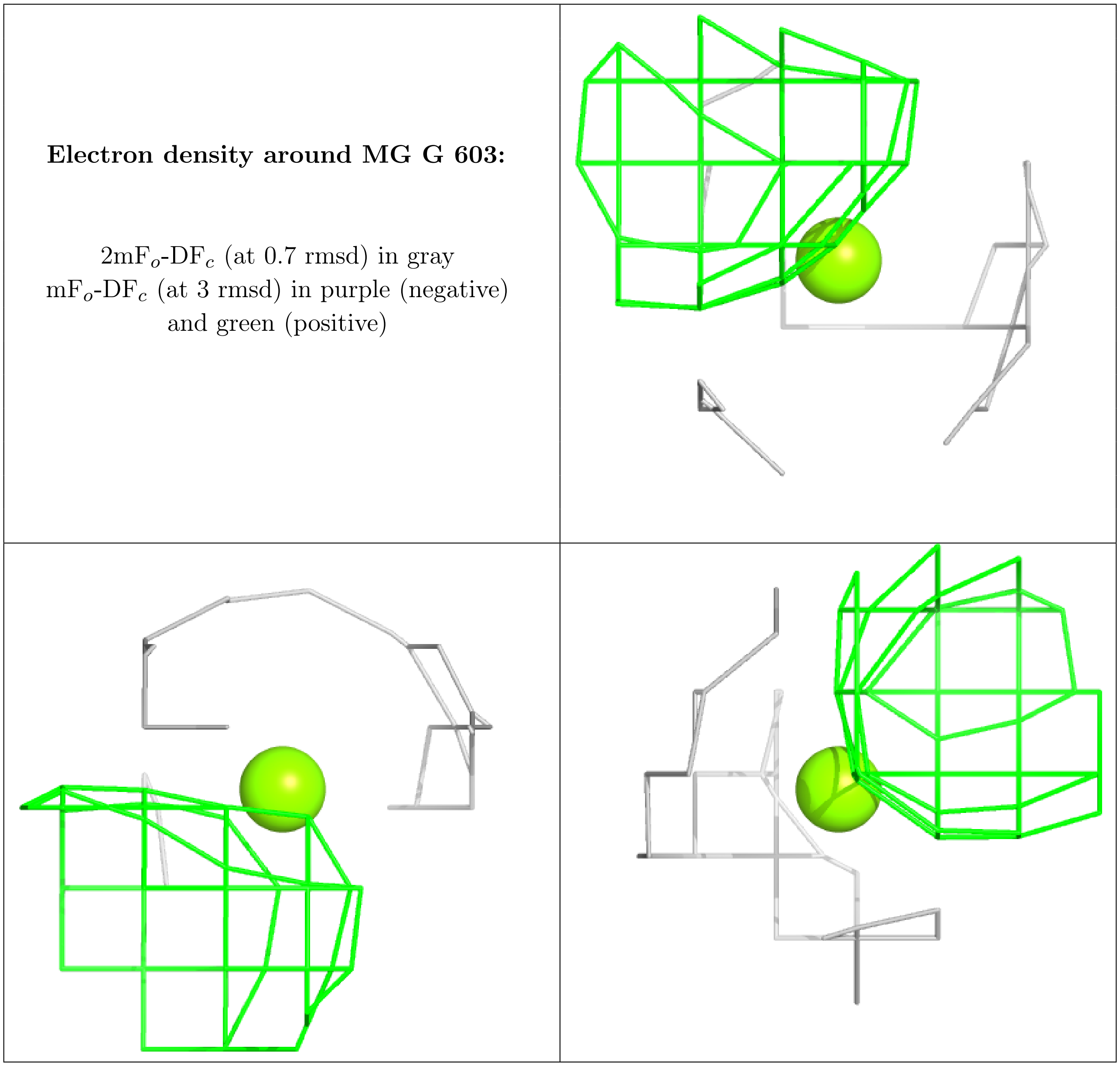
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)







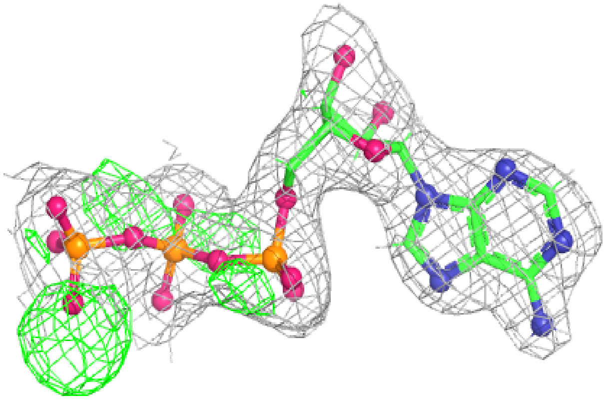


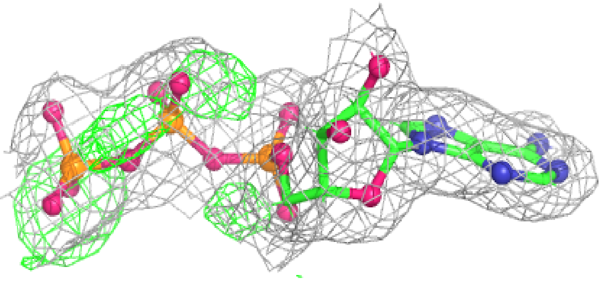
Electron density around MG G 603:

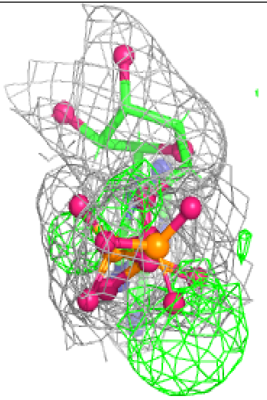
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

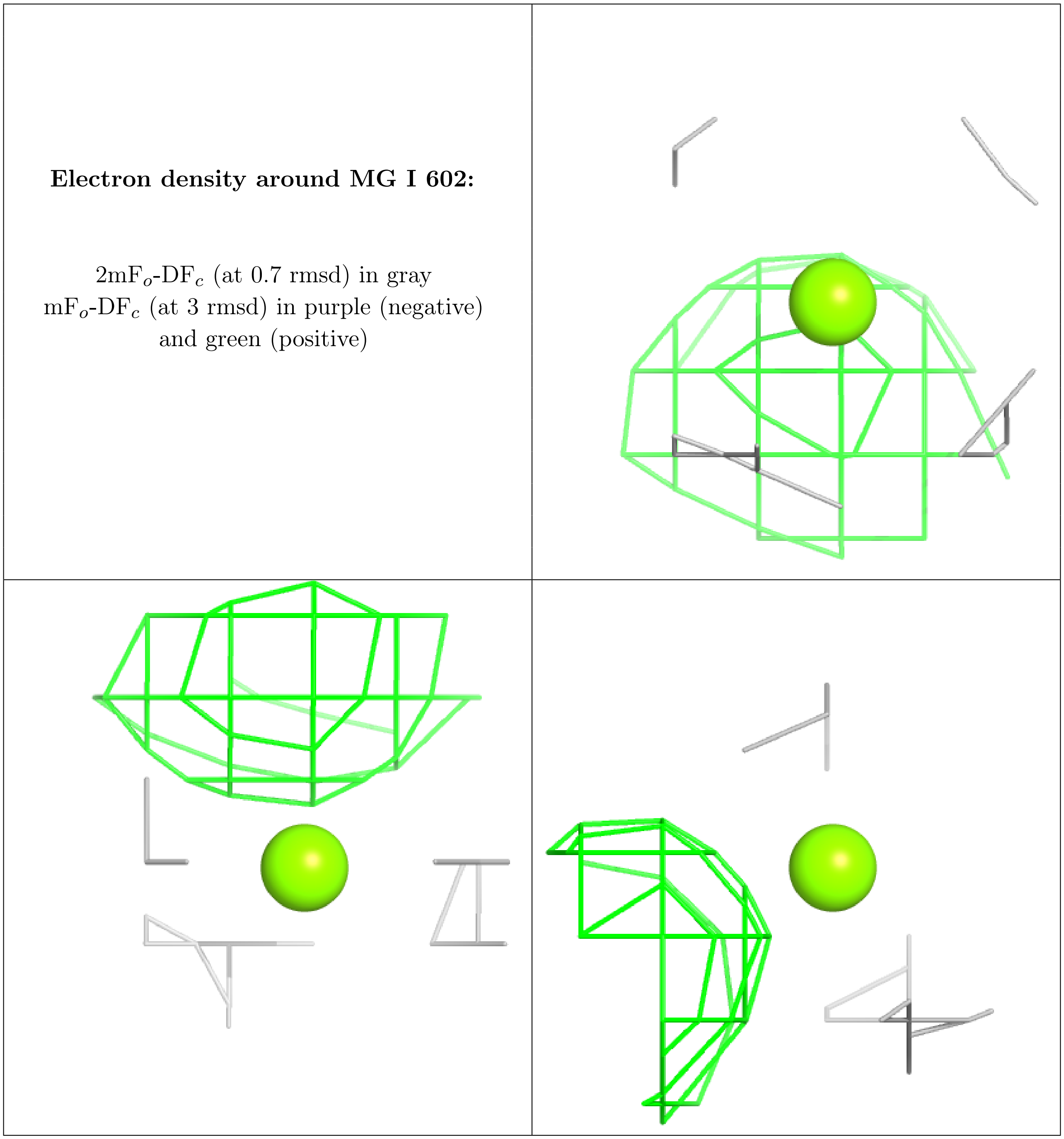
Electron density around ATP G 600:

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 602:

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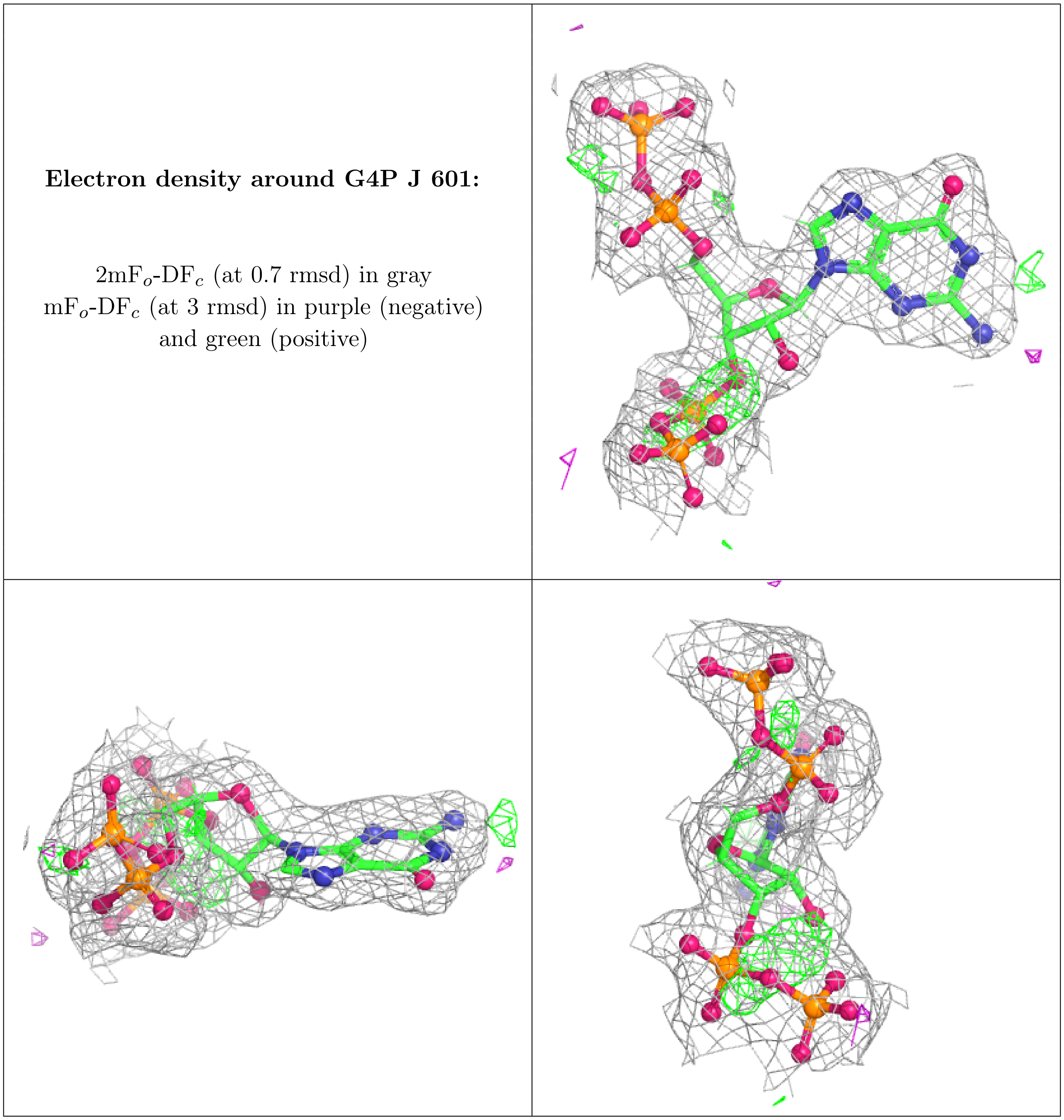
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

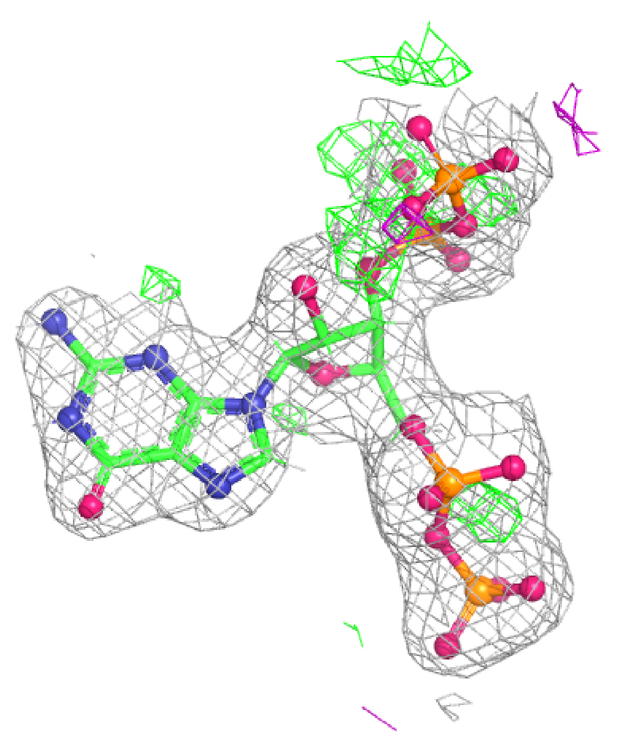


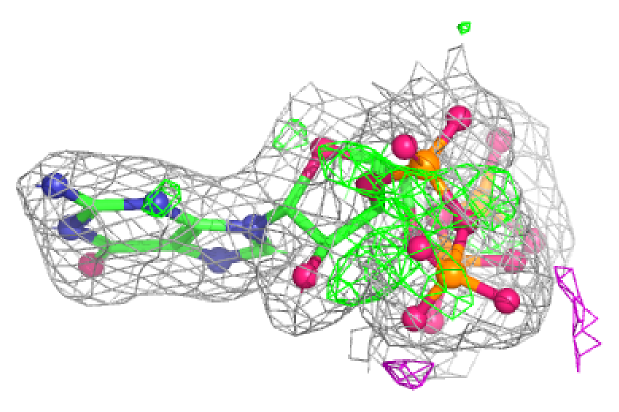
Electron density around G4P J 601:

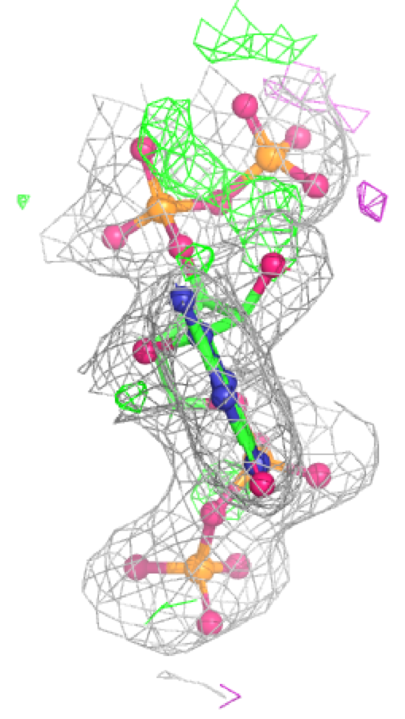
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around G4P O 601:

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







Electron density around MG B 603:

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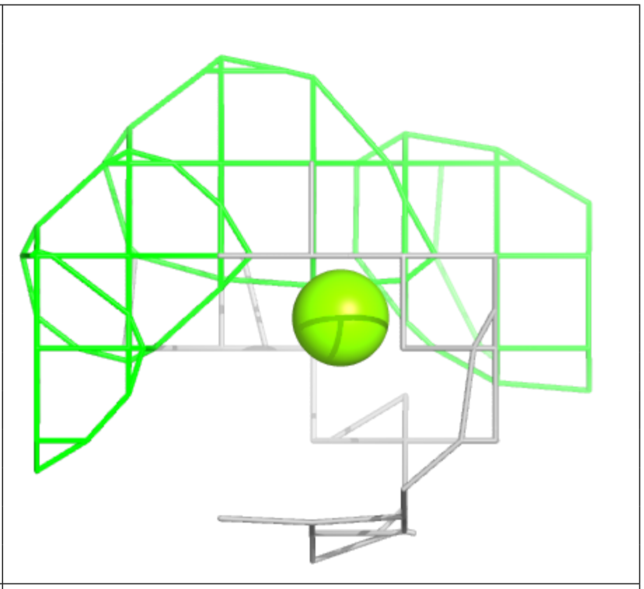
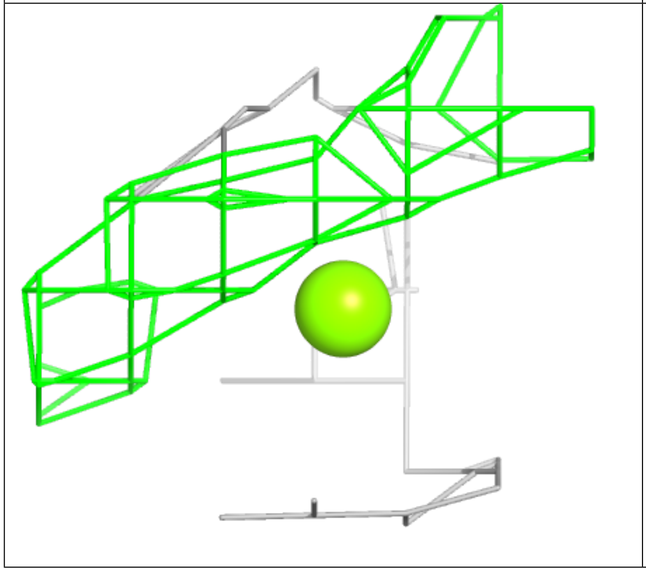
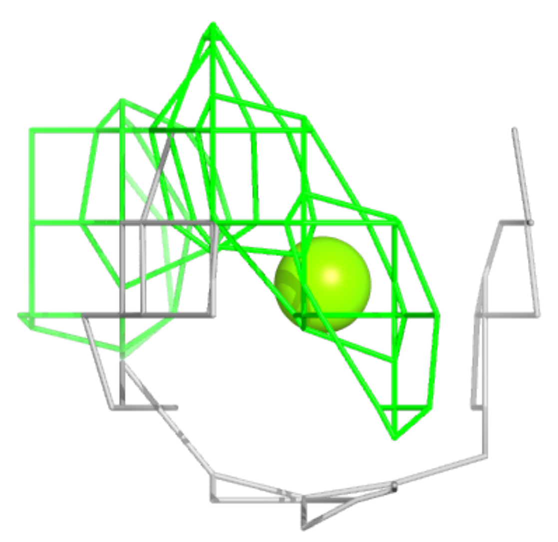
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around ATP B 600:

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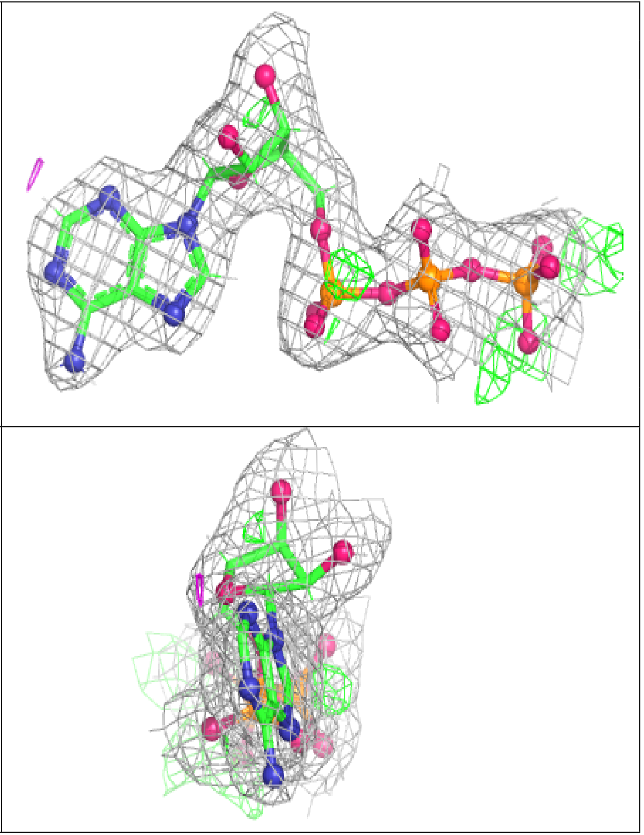
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ATP I 600:

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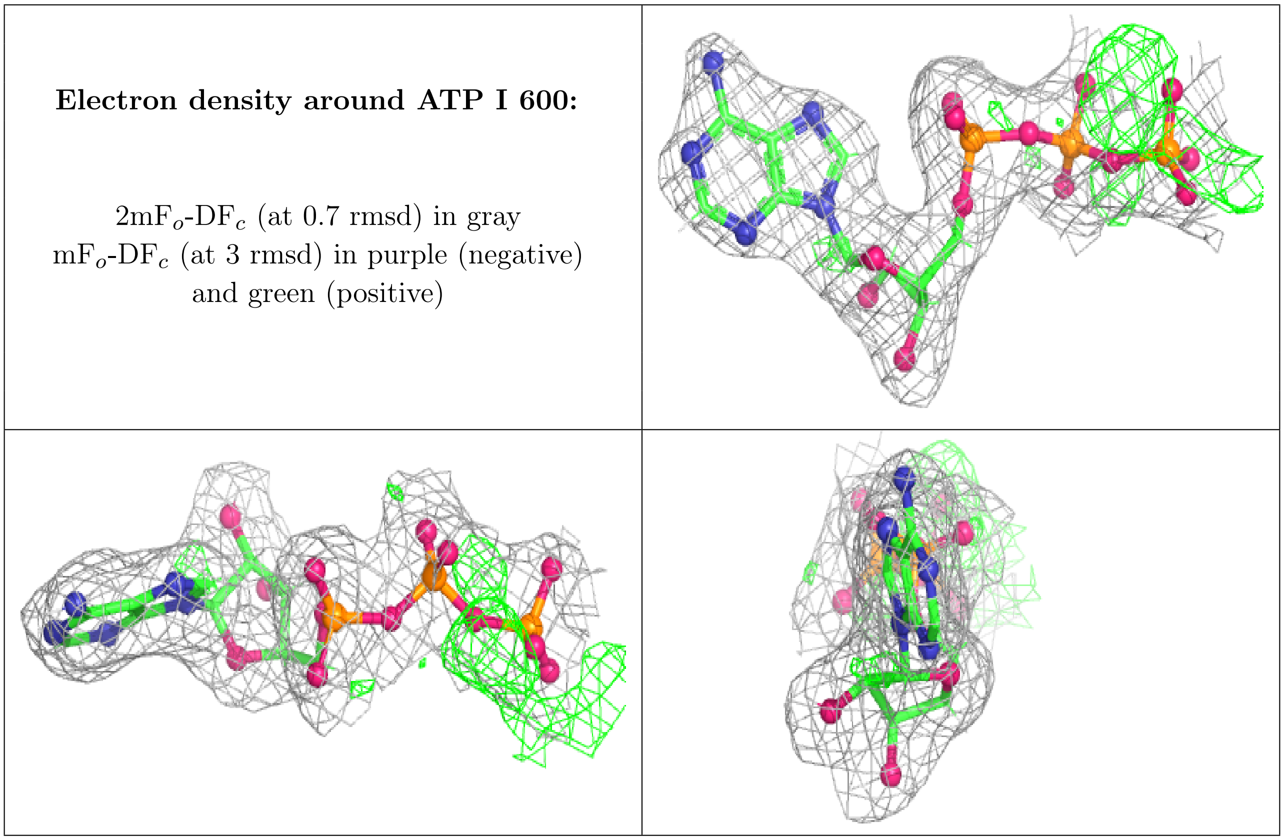

Electron density around ATP J 600:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
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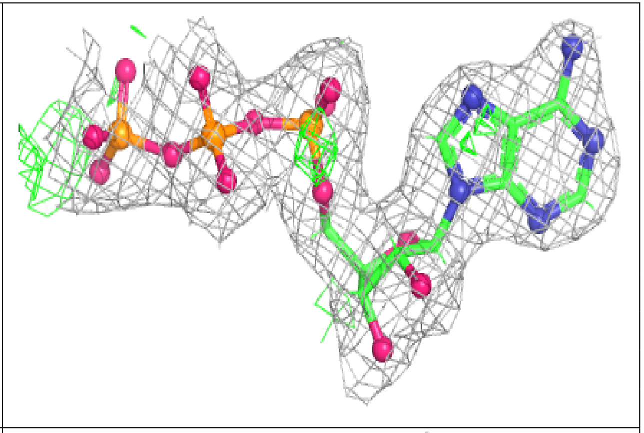

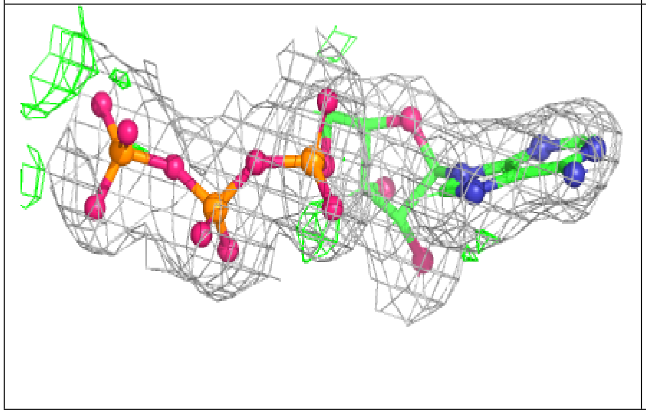

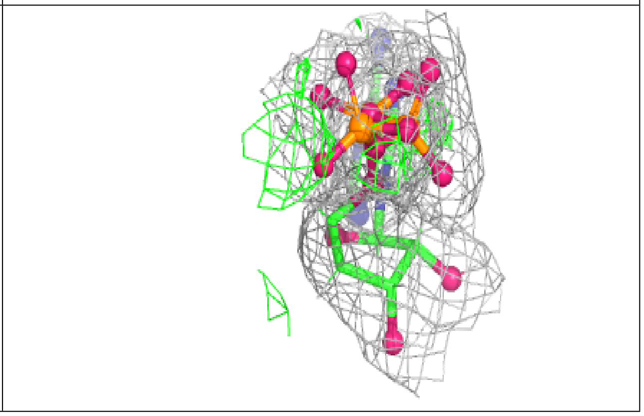

Electron density around ATP C 600:

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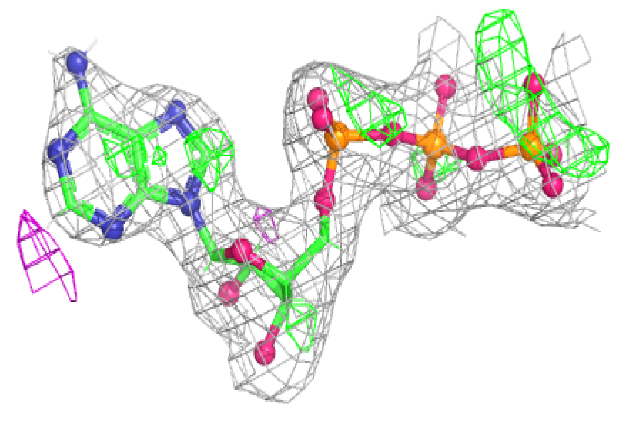
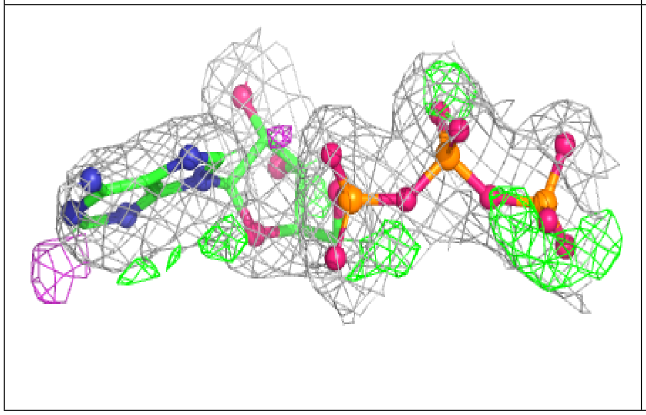
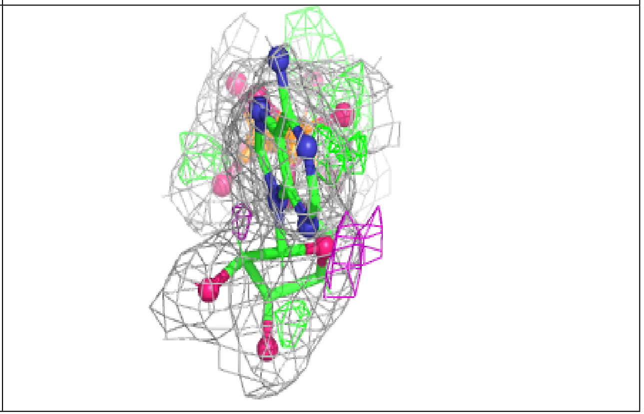
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

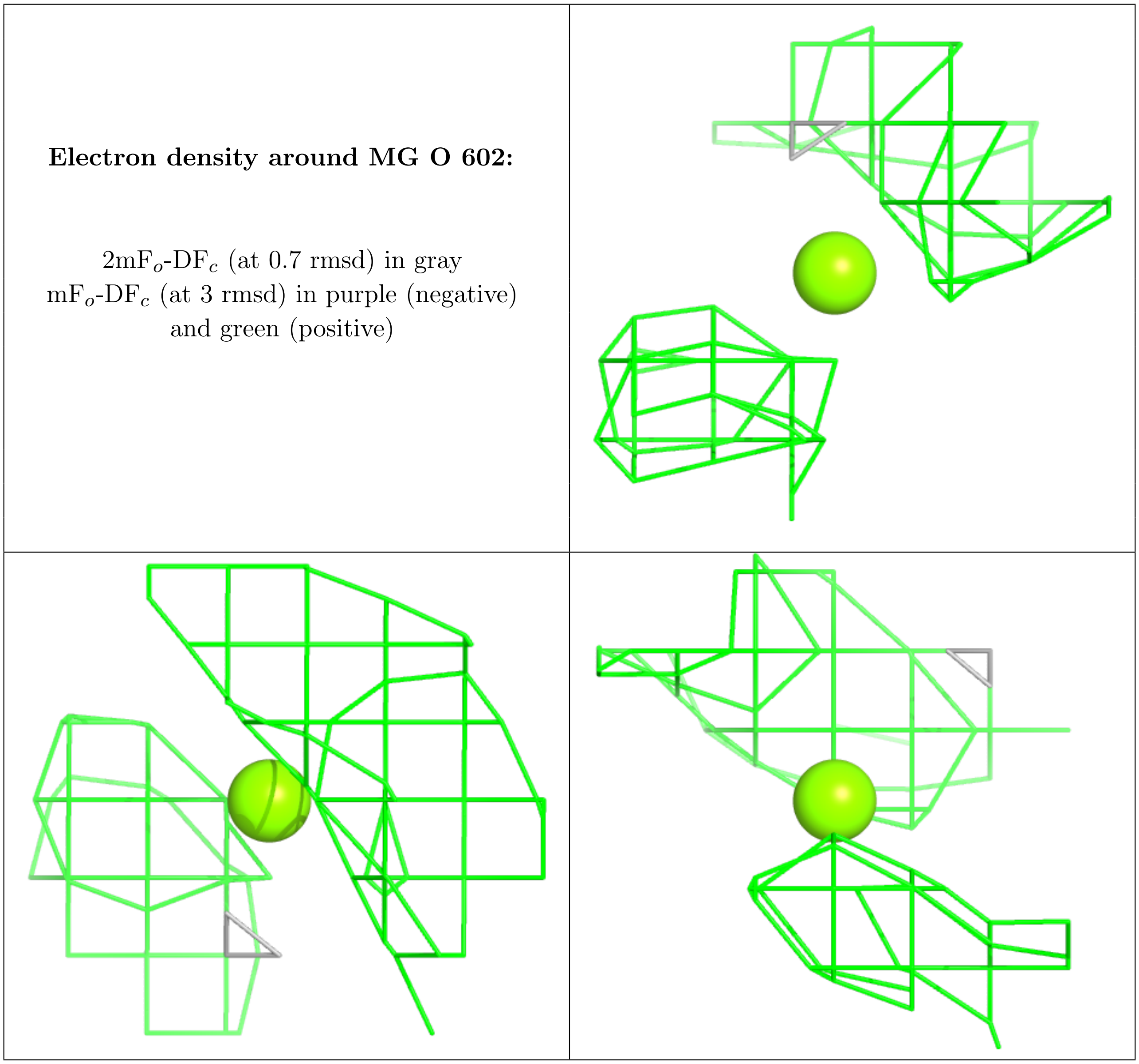






Electron density around MG O 602:

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



Electron density around ATP O 600:

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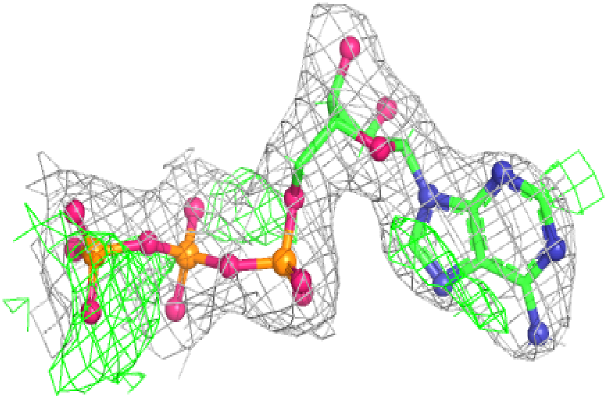
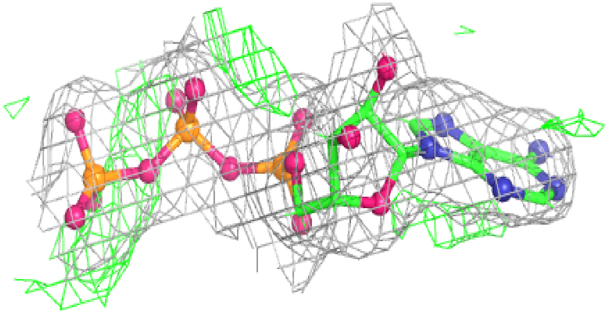
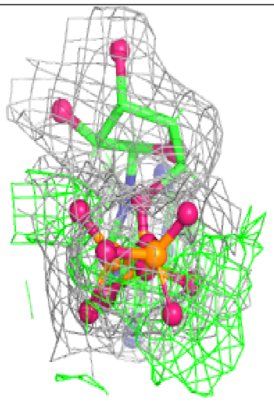
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

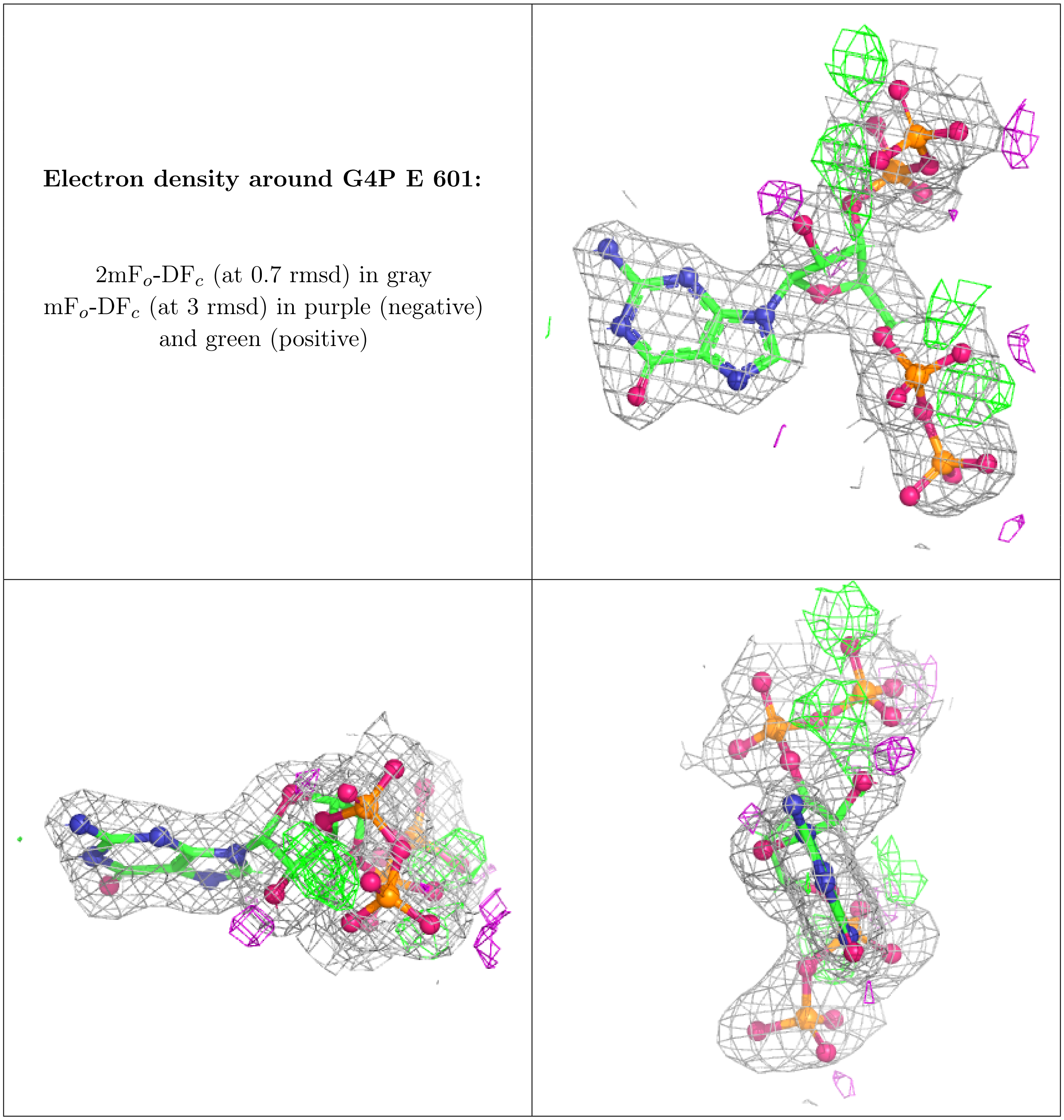






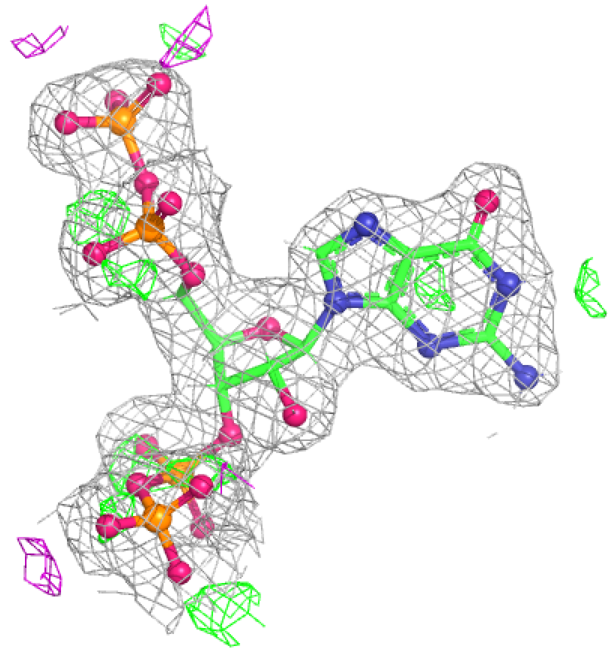
Electron density around G4P E 601:

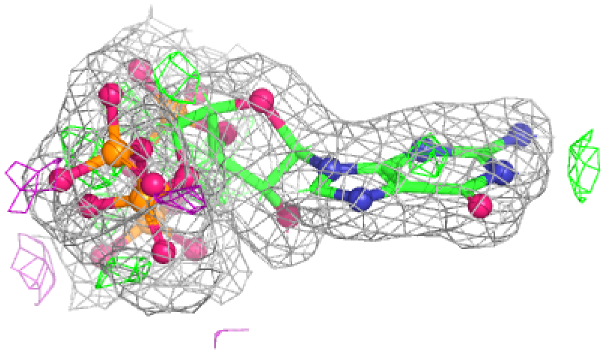
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

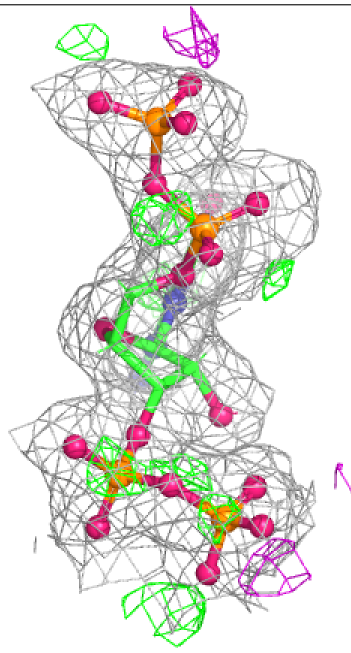


Electron density around G4P F 601:

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

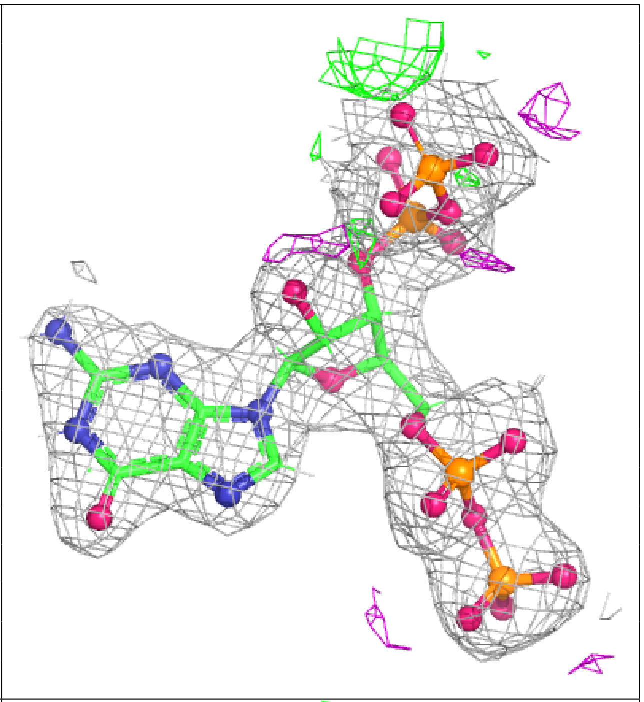


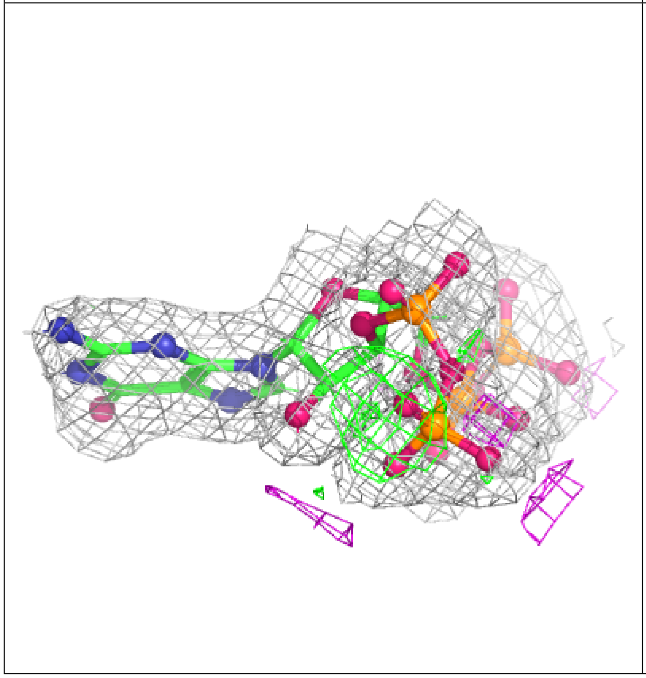


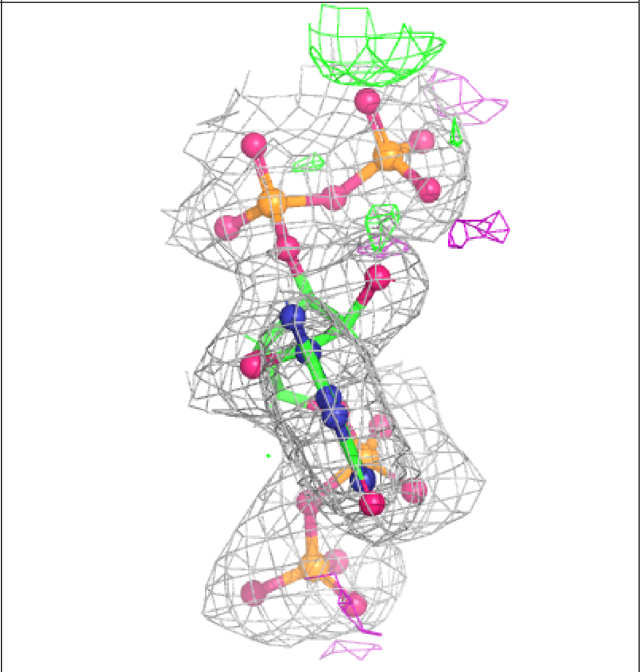


Electron density around G4P G 601:

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

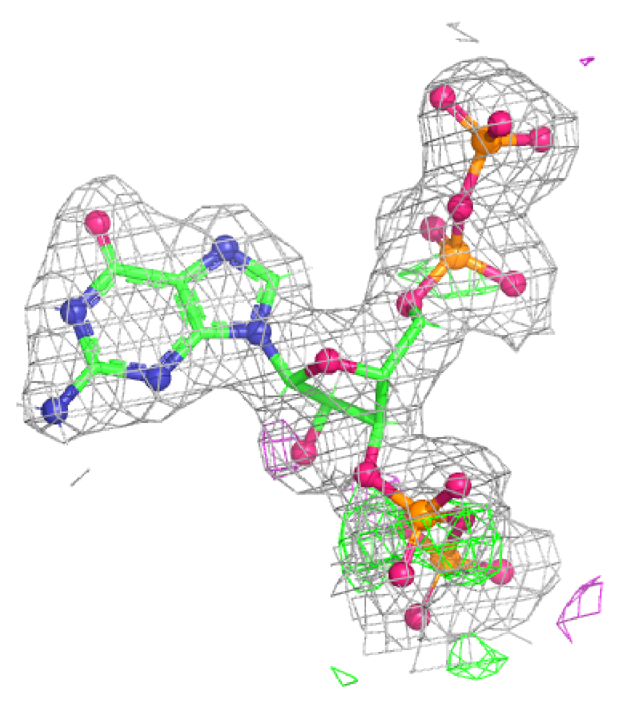


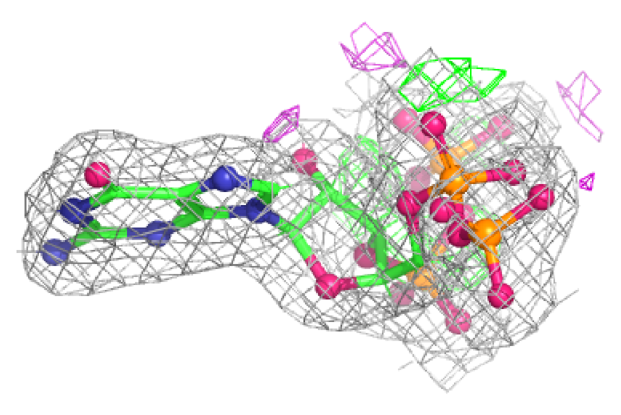


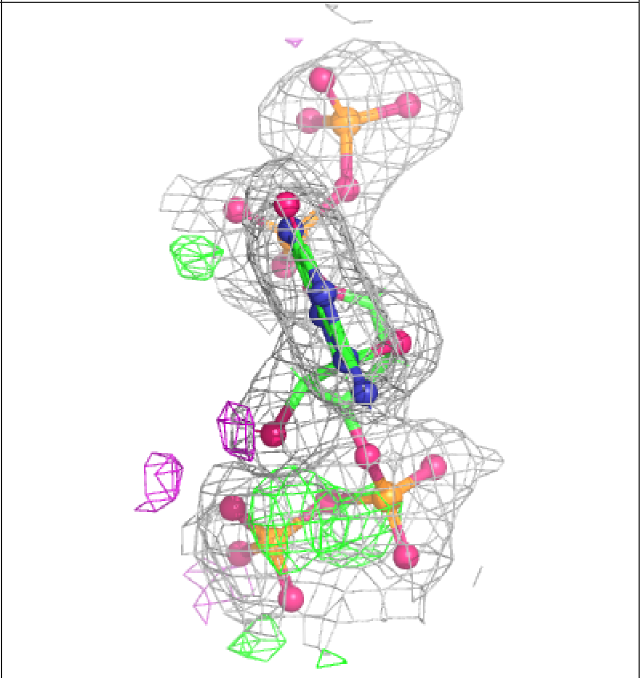


Electron density around G4P H 601:

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

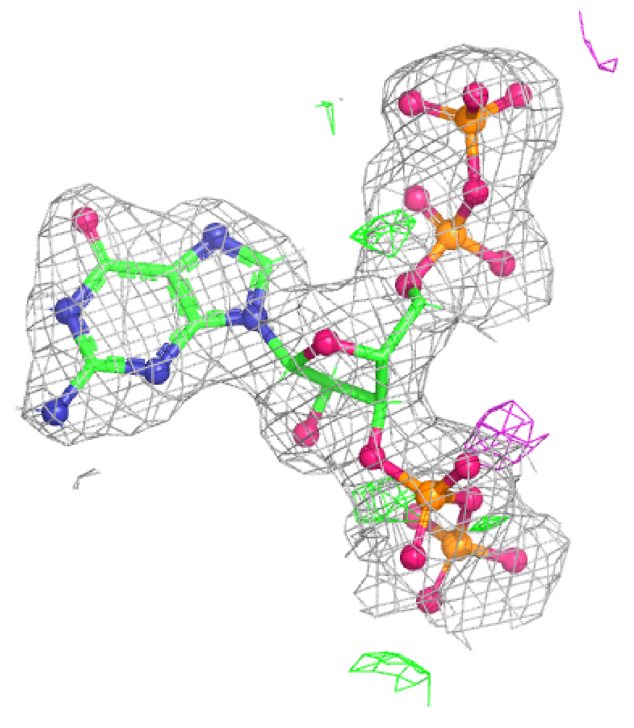


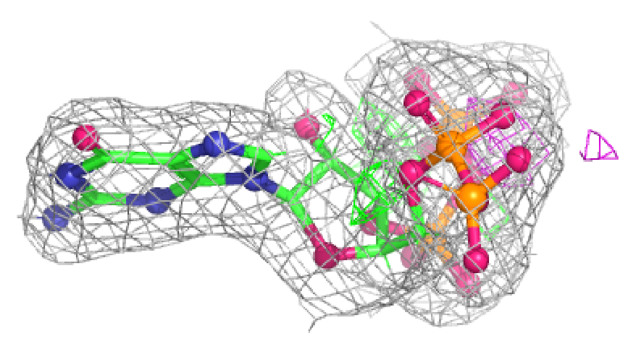


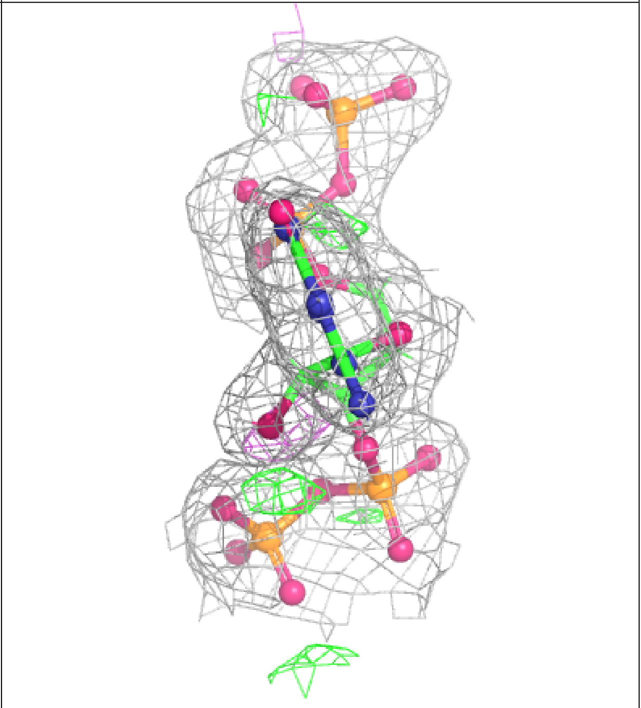


Electron density around G4P I 601:

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

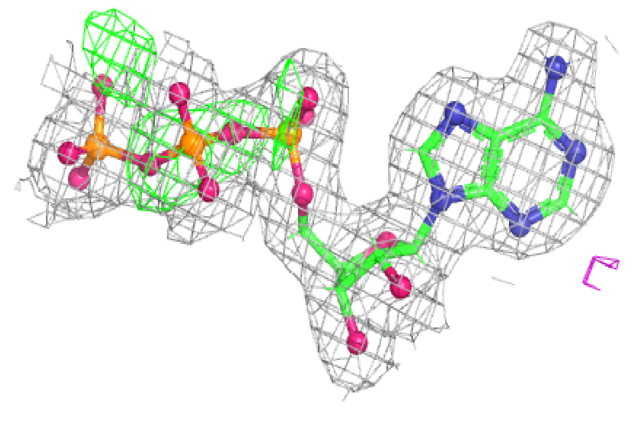


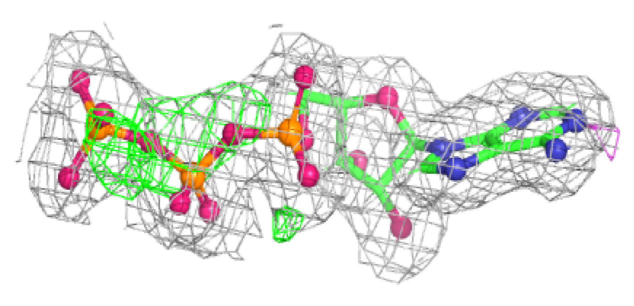


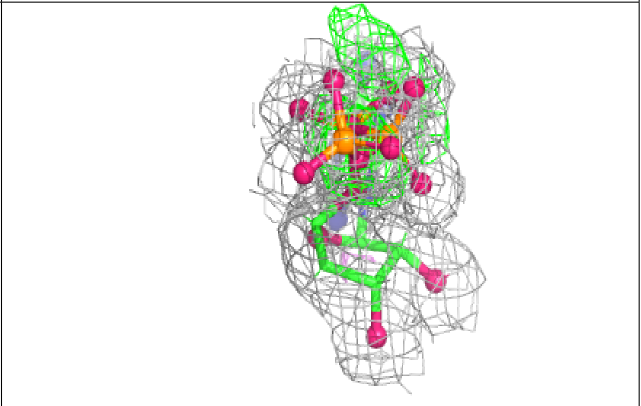


Electron density around ATP F 600:

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

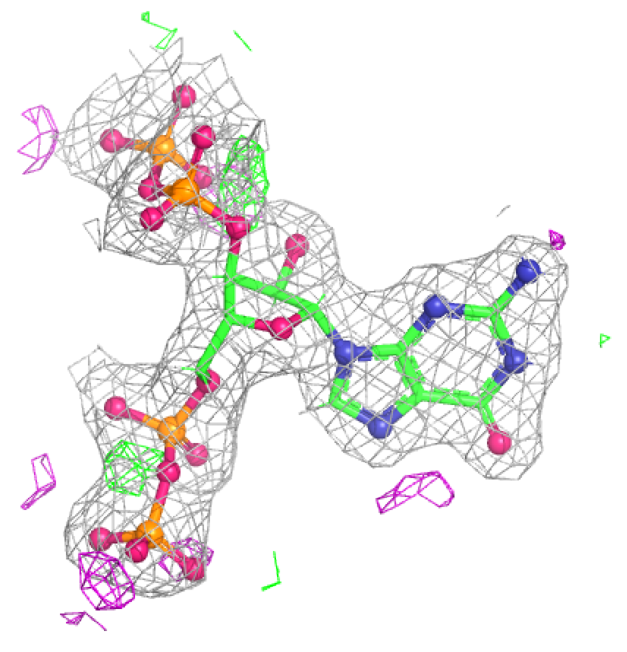


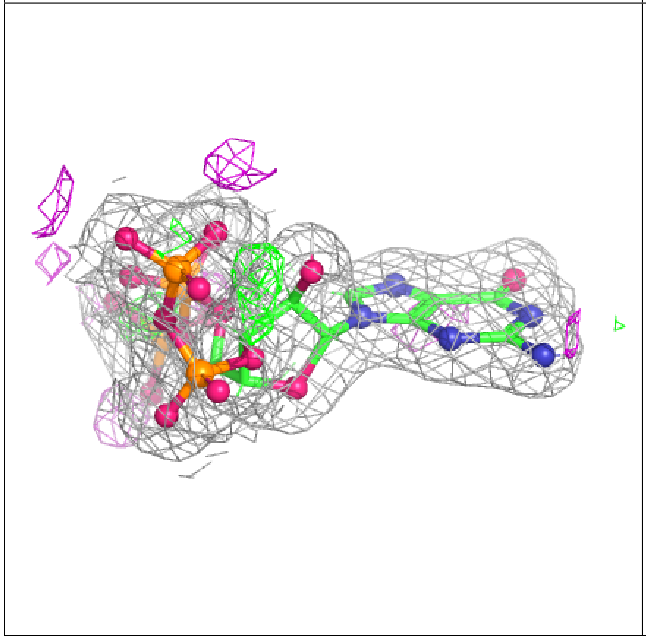


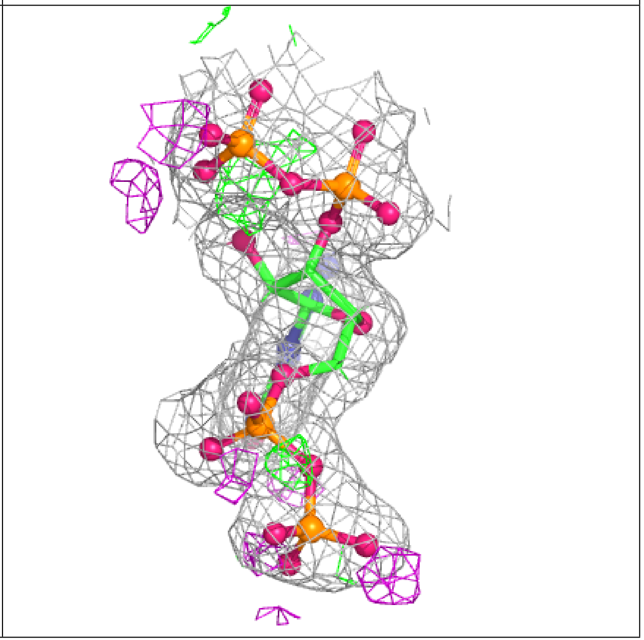


Electron density around G4P K 601:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

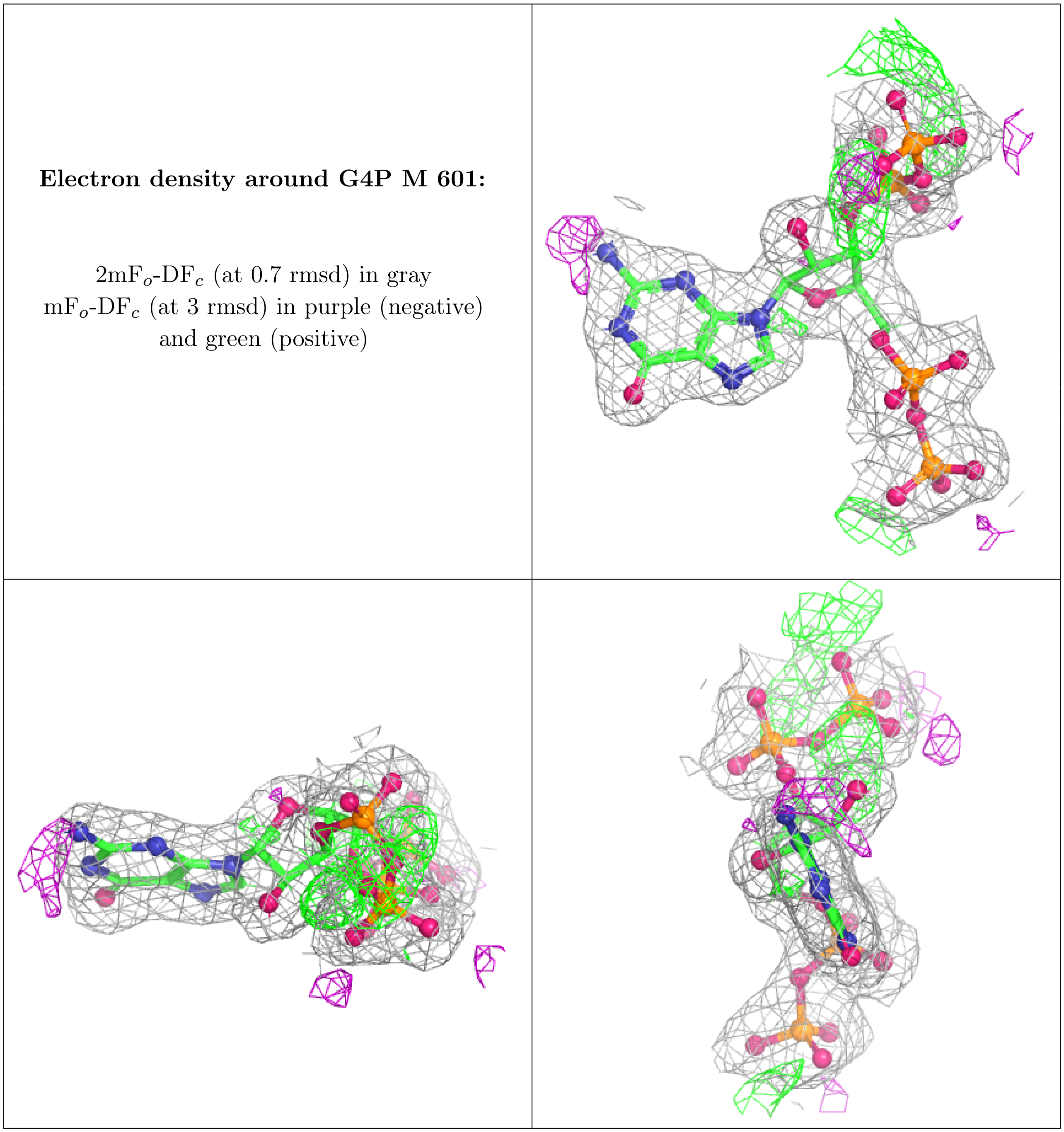






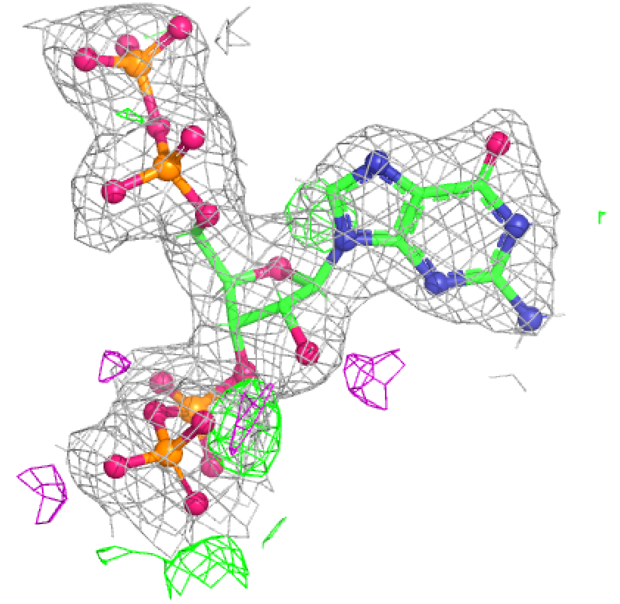
Electron density around G4P M 601:

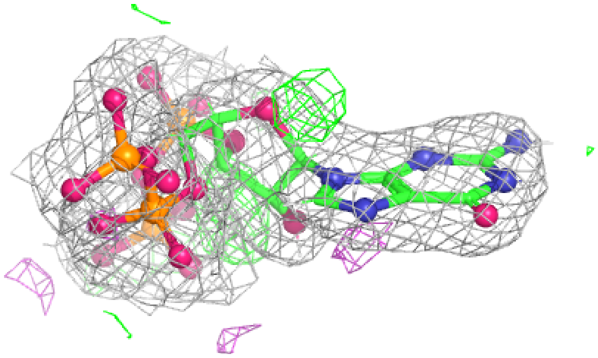
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

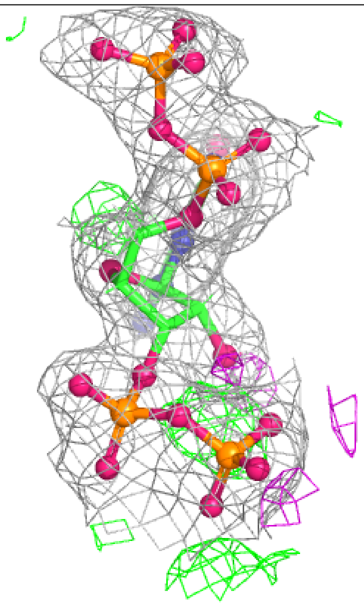


Electron density around G4P N 601:

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







Electron density around ATP M 600:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
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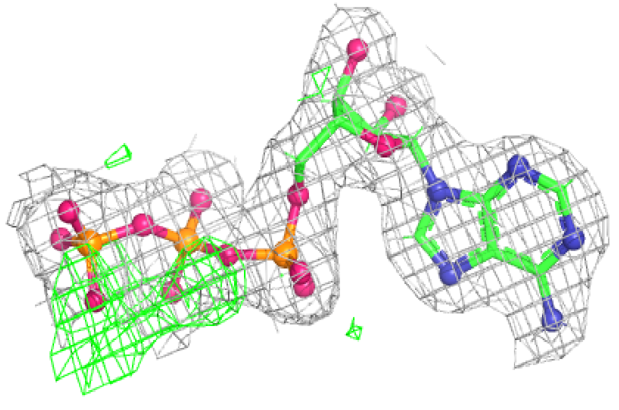
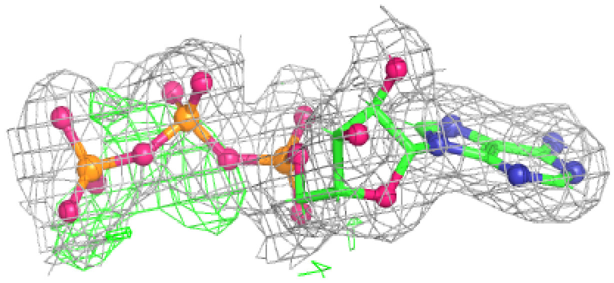
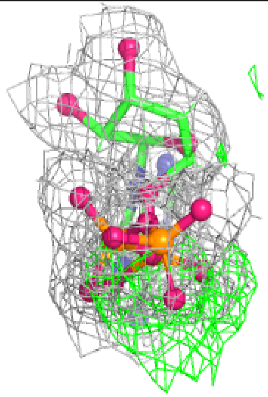
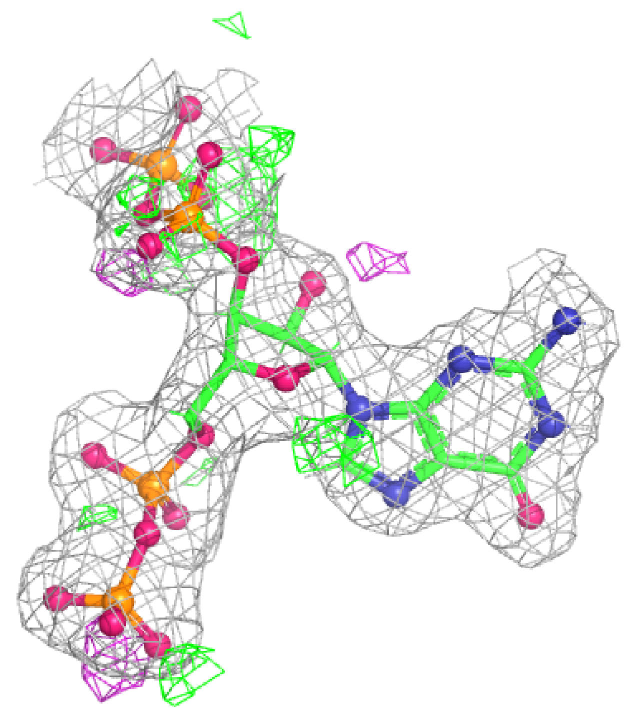


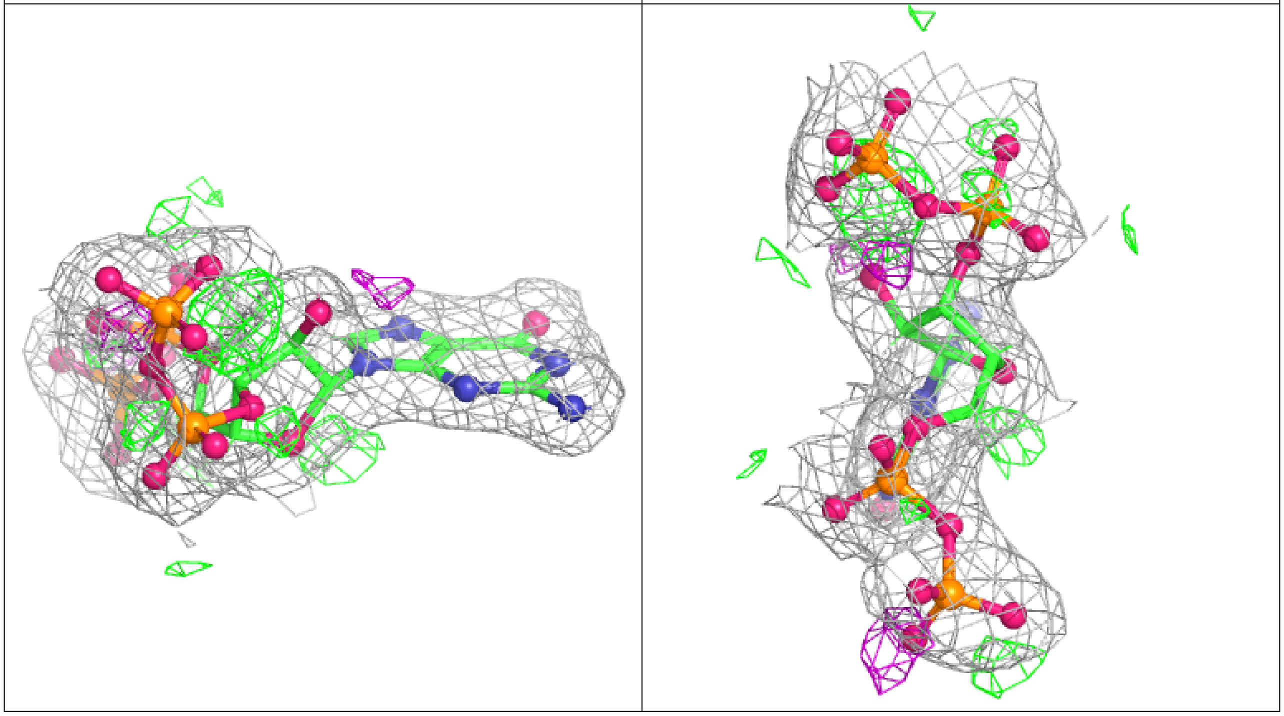




Electron density around G4P P 601:

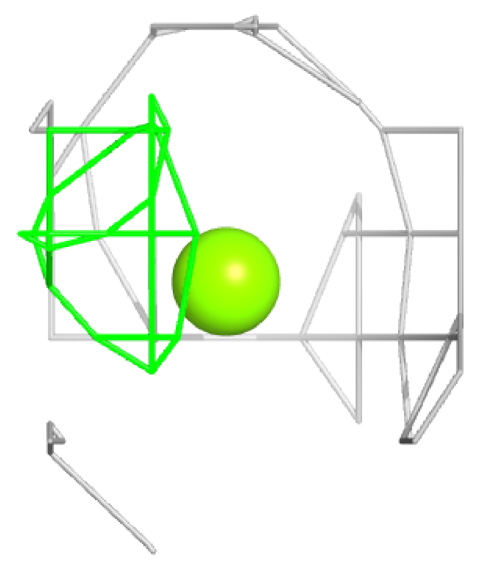
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

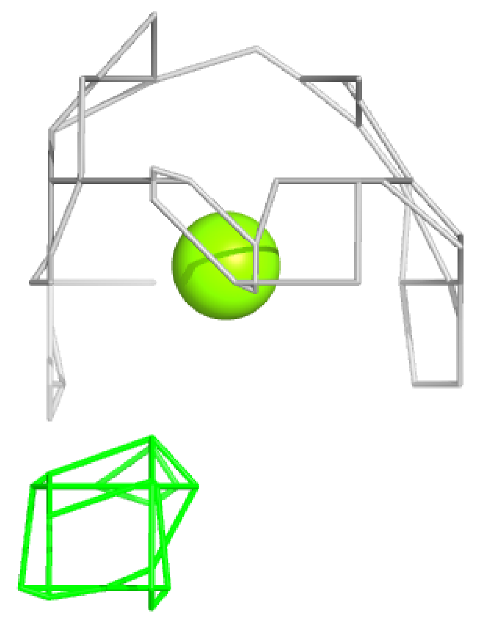


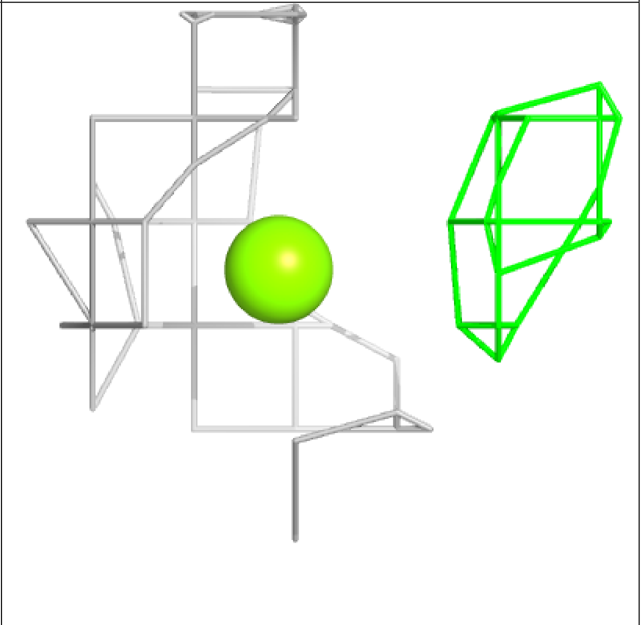


Electron density around MG B 602:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

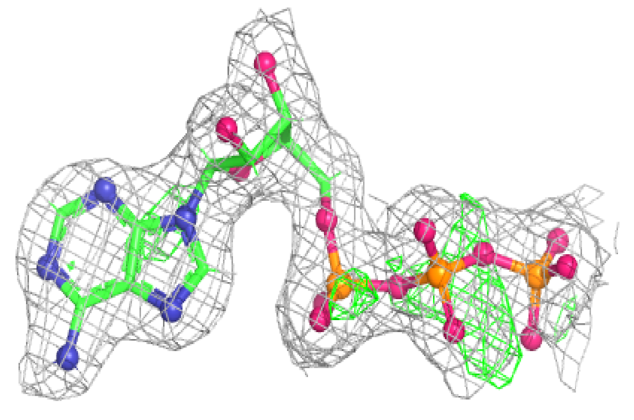


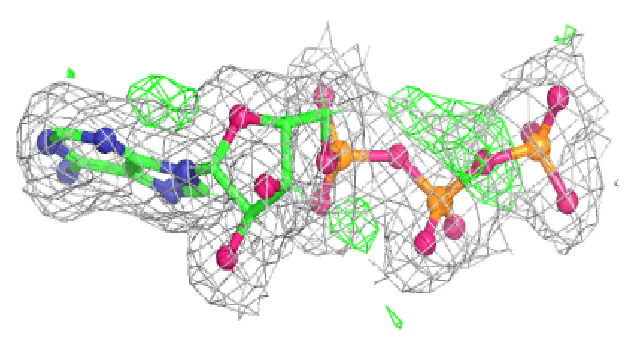


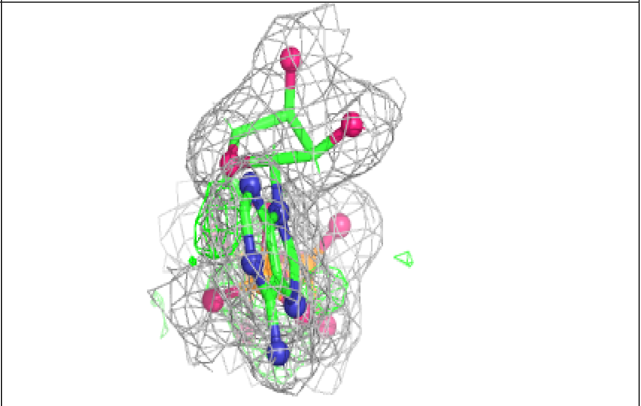


Electron density around ATP A 600:

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

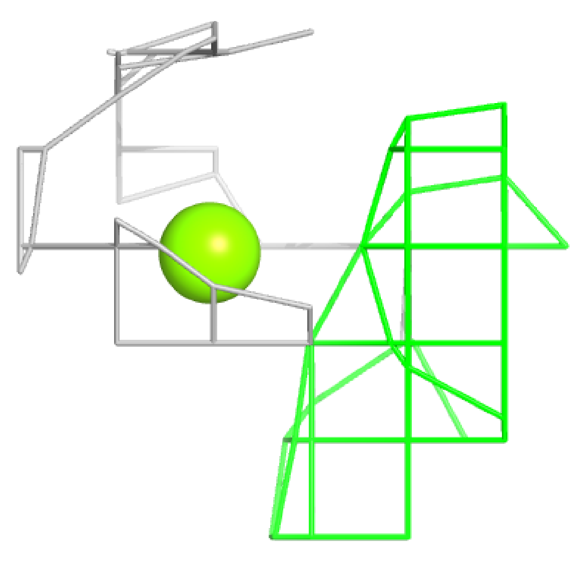


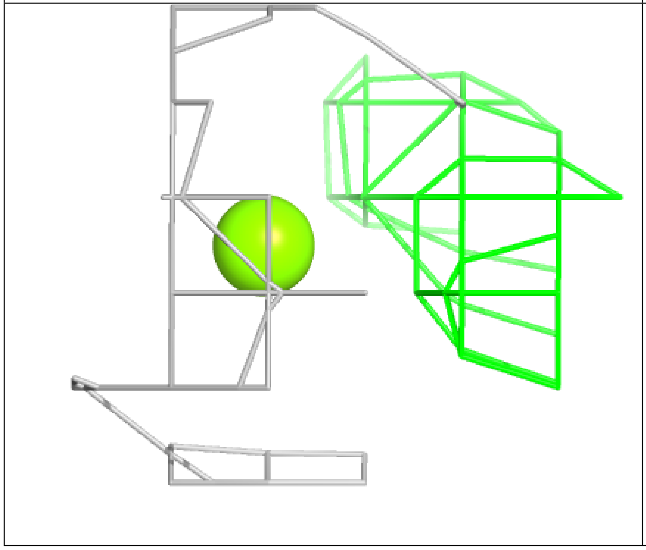


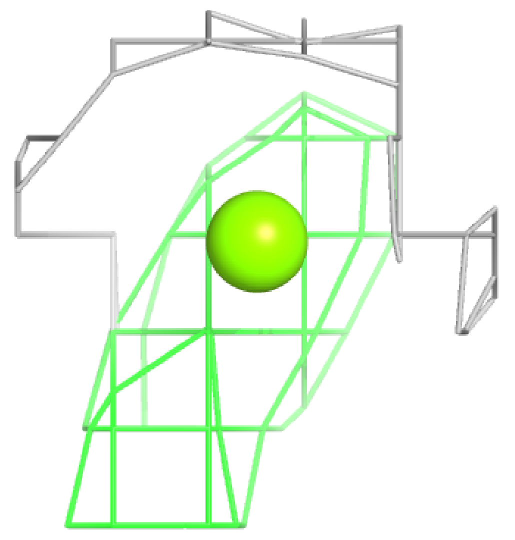


Electron density around MG C 602:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

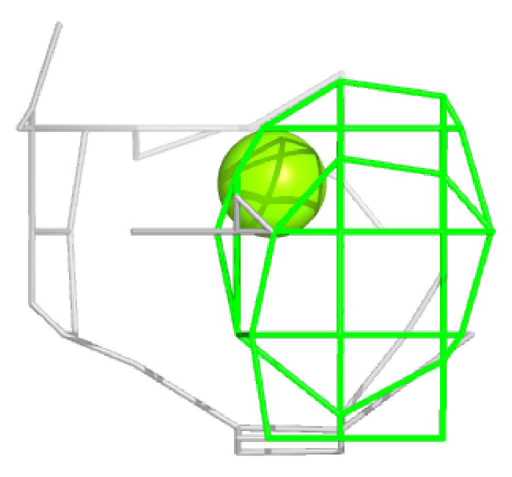


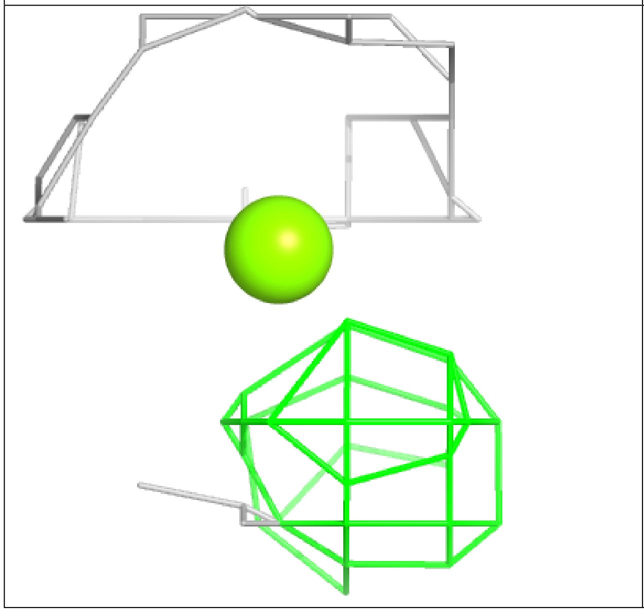


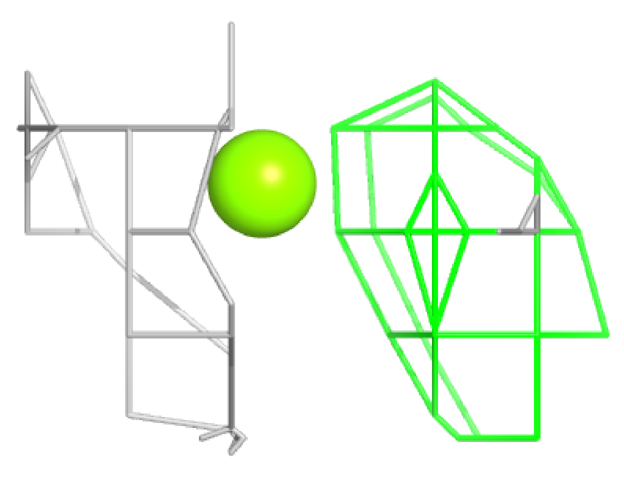


Electron density around MG C 603:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

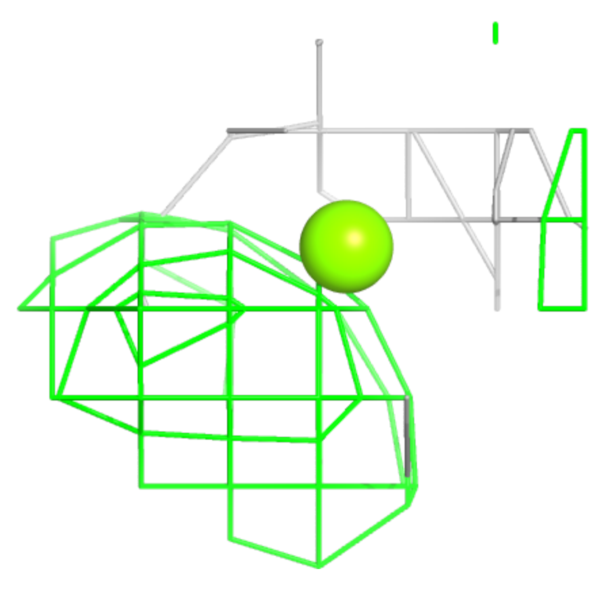


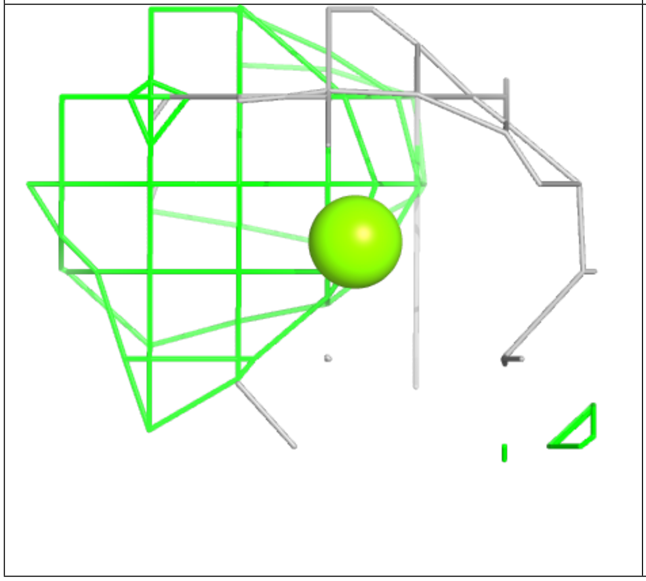


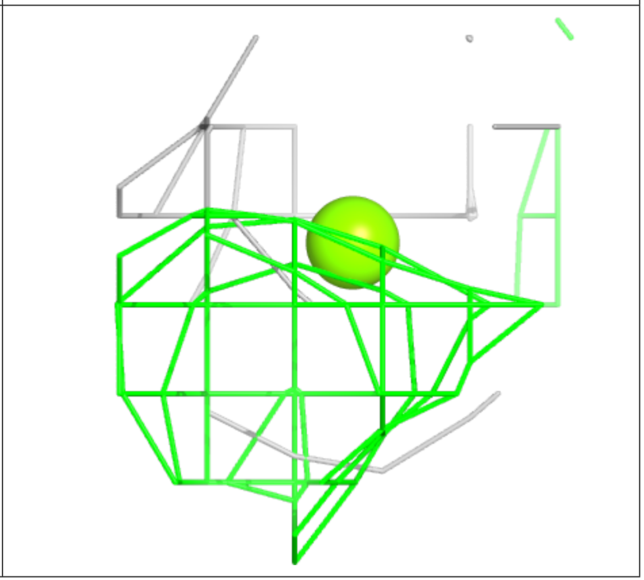


Electron density around MG D 603:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

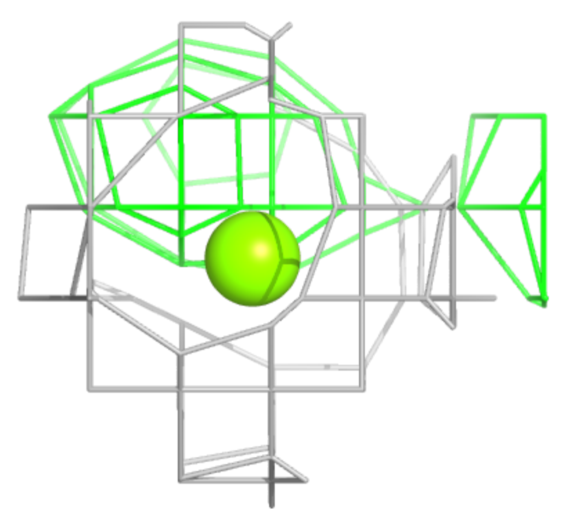


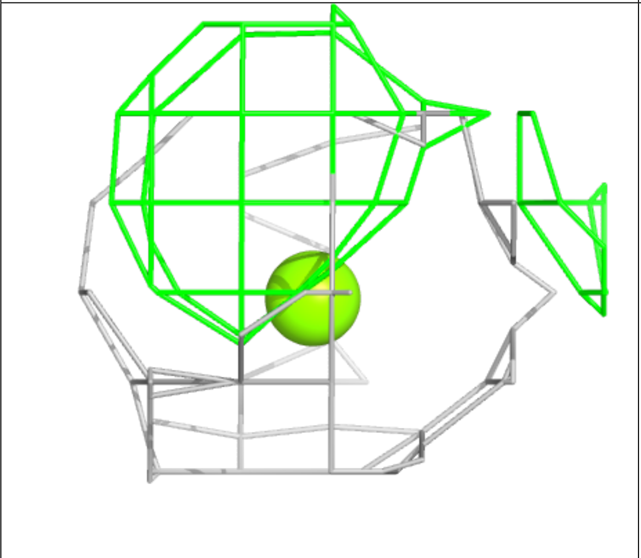


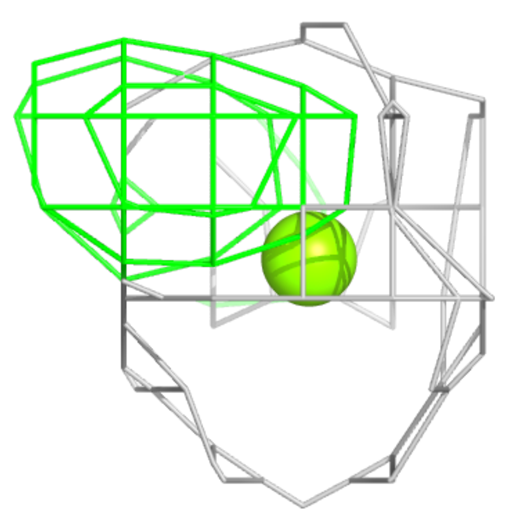


Electron density around MG E 602:

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

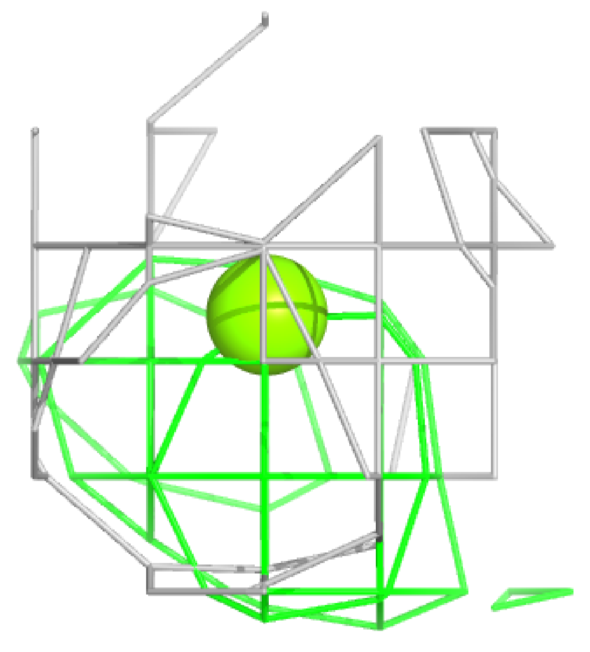


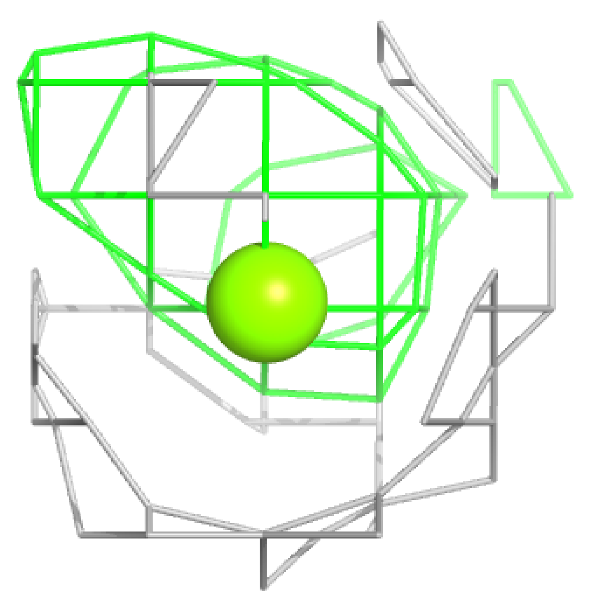


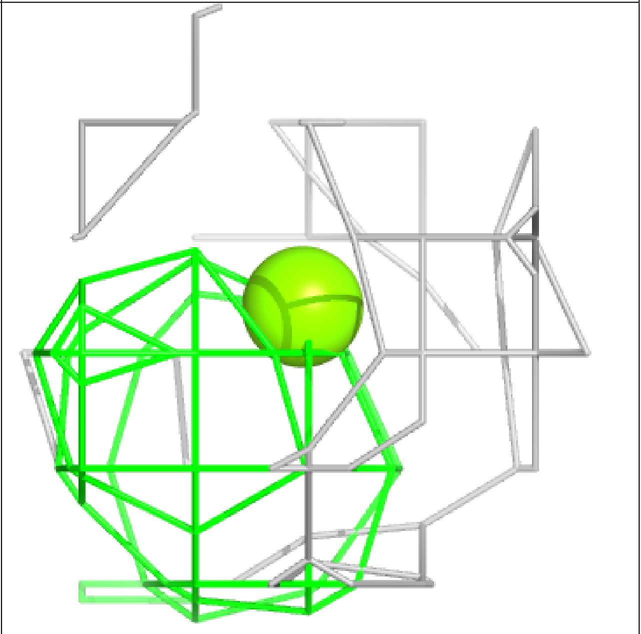


Electron density around MG F 603:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

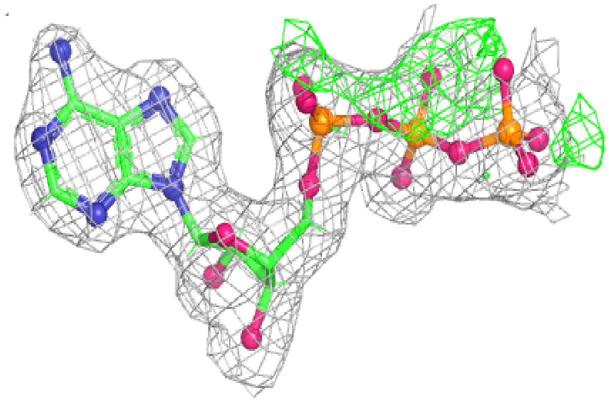


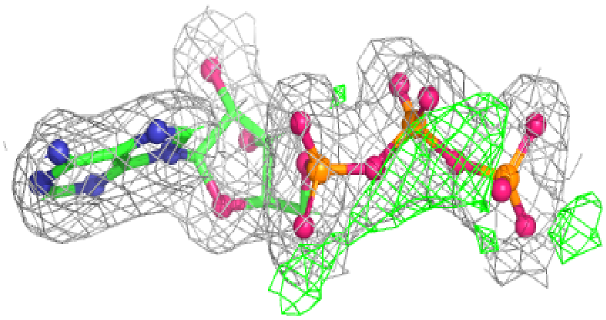


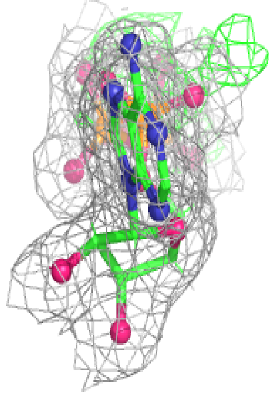


Electron density around ATP D 600:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

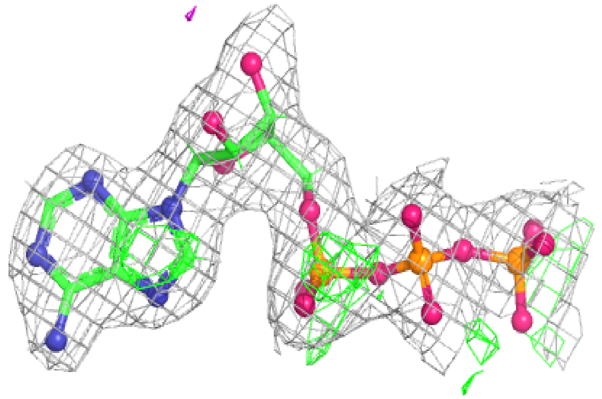


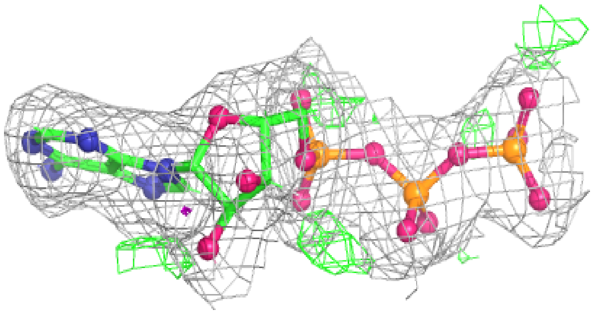


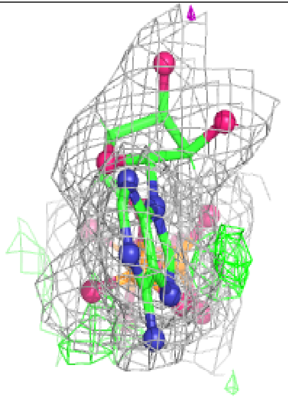


Electron density around ATP P 600:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

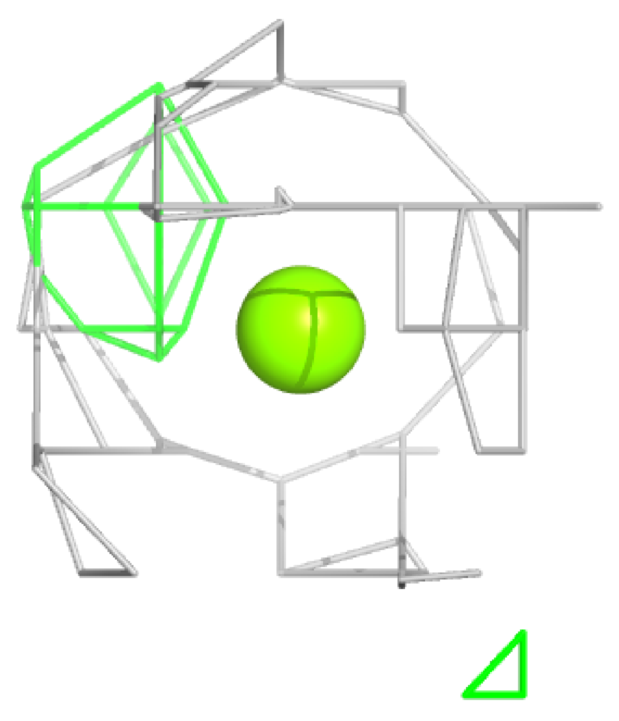


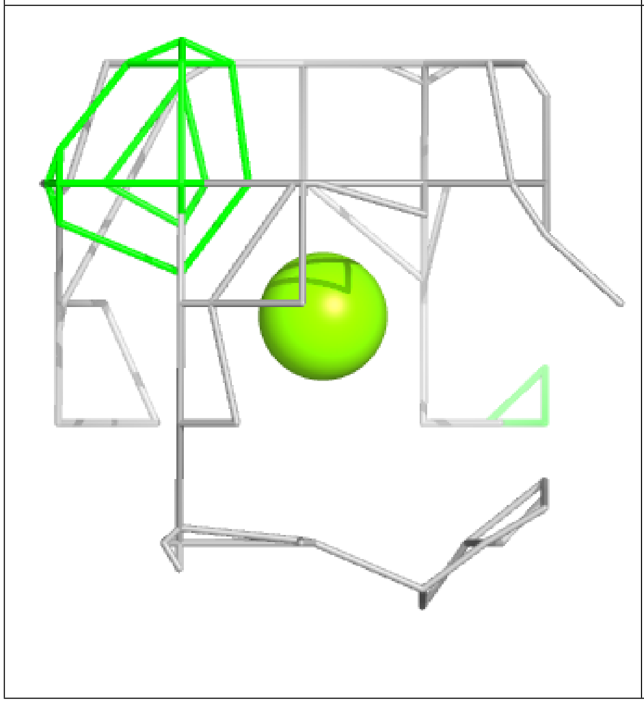


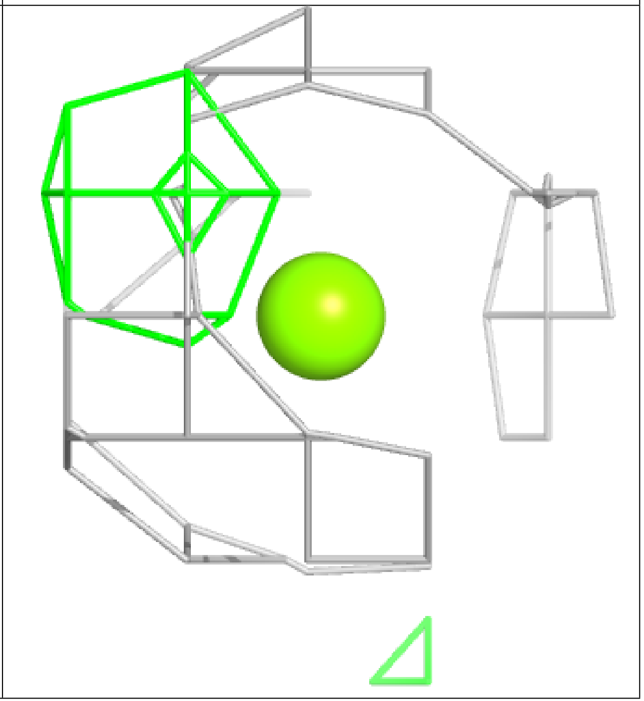


Electron density around MG H 603:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

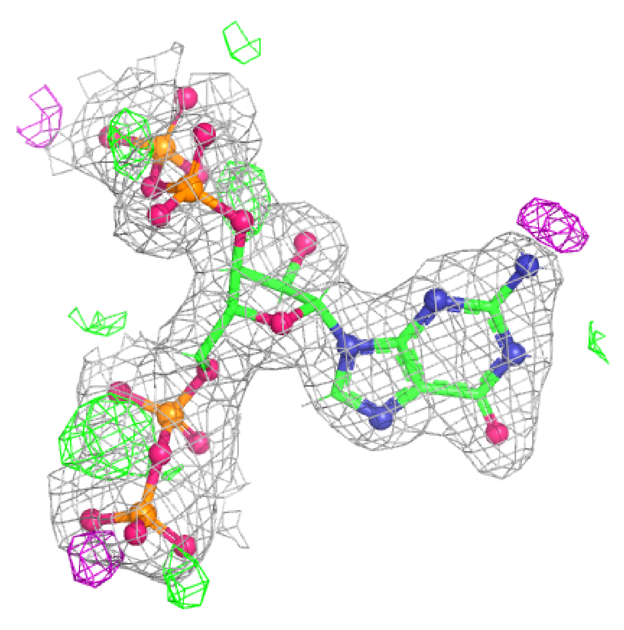


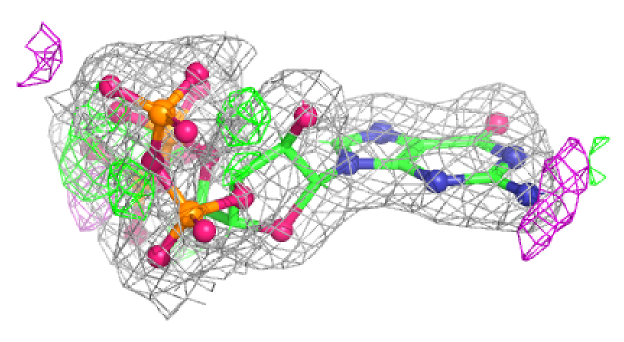


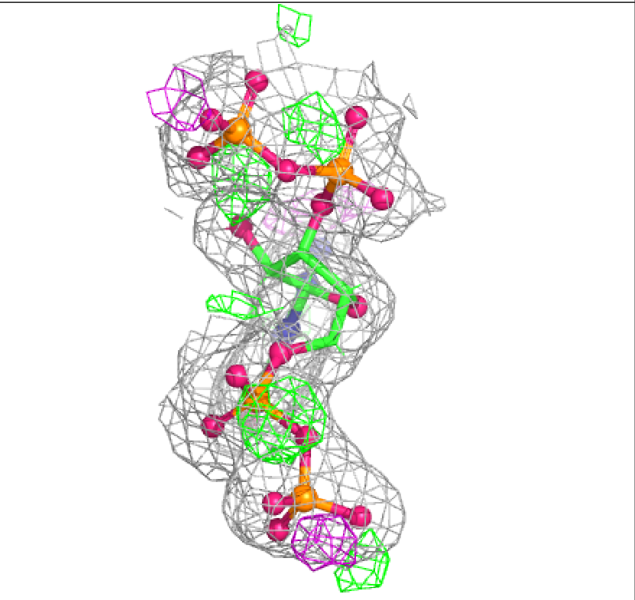


Electron density around G4P A 601:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

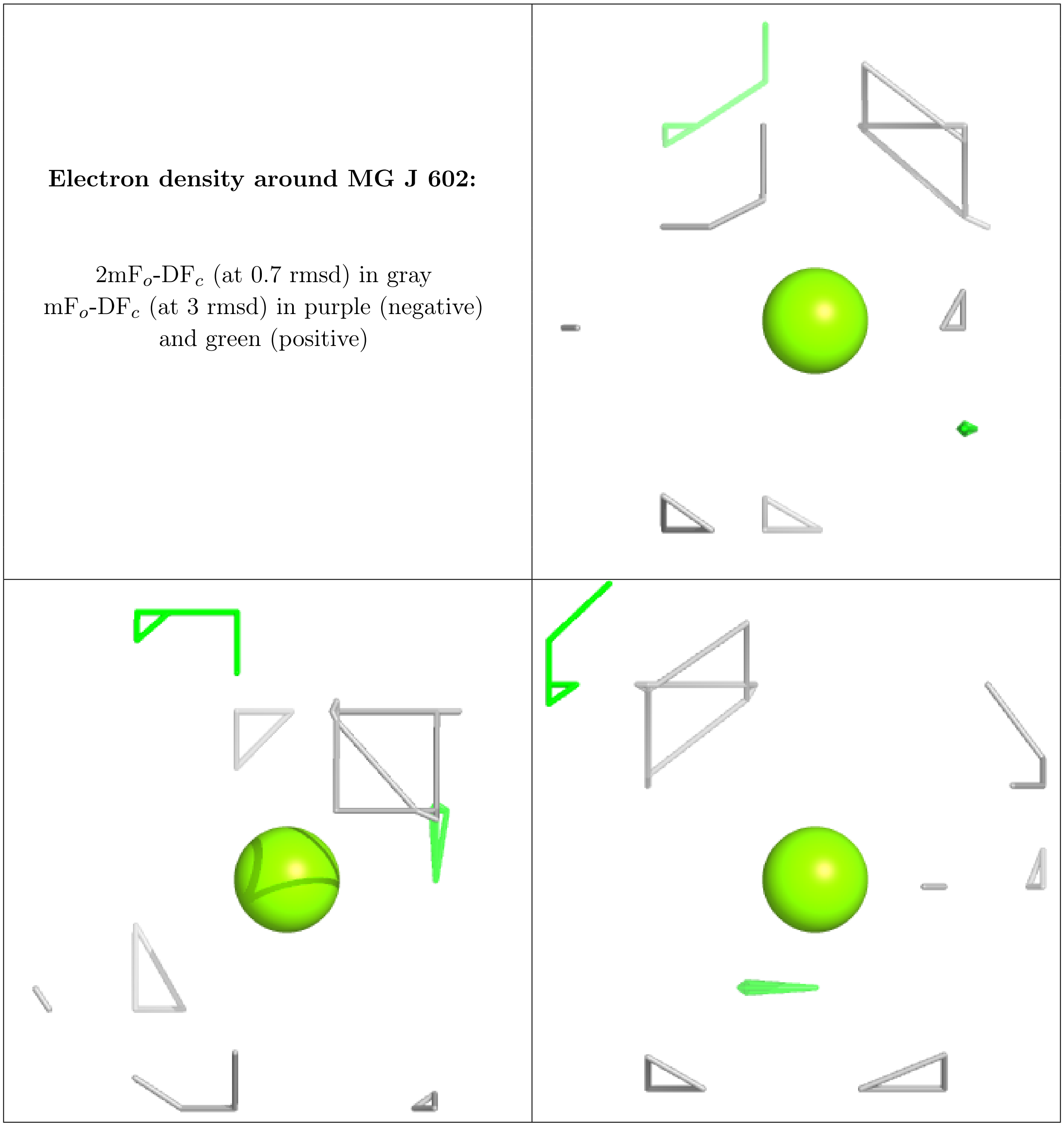






Electron density around MG J 602:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

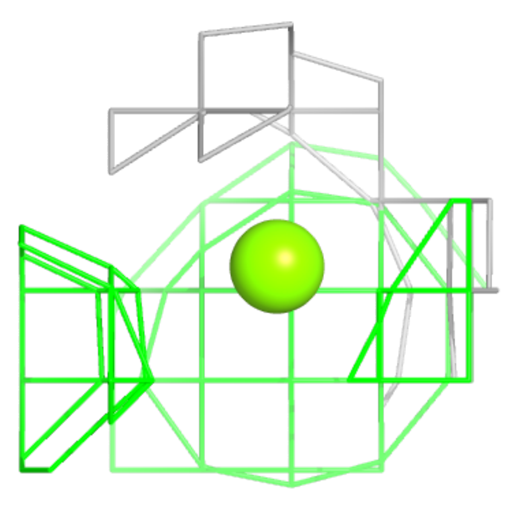


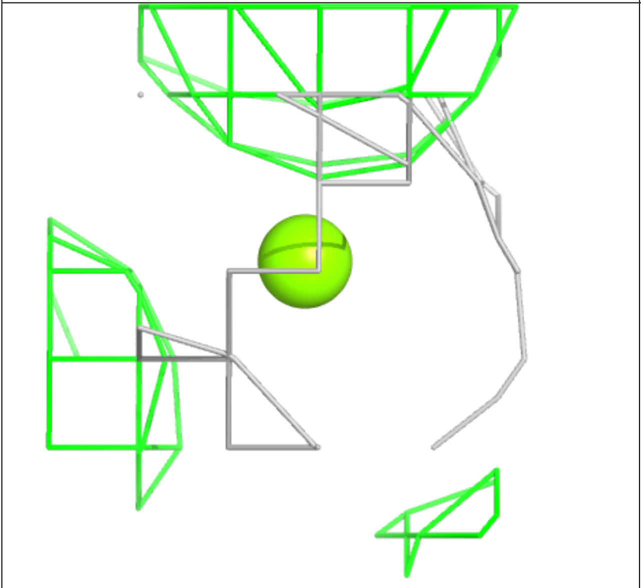
Electron density around MG M 603:

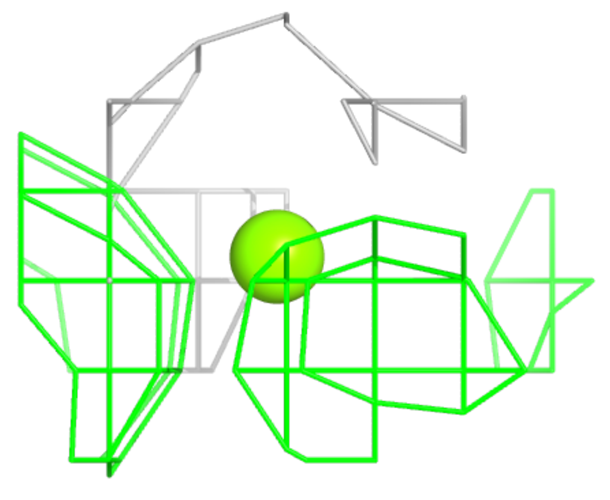
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around MG N 602:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

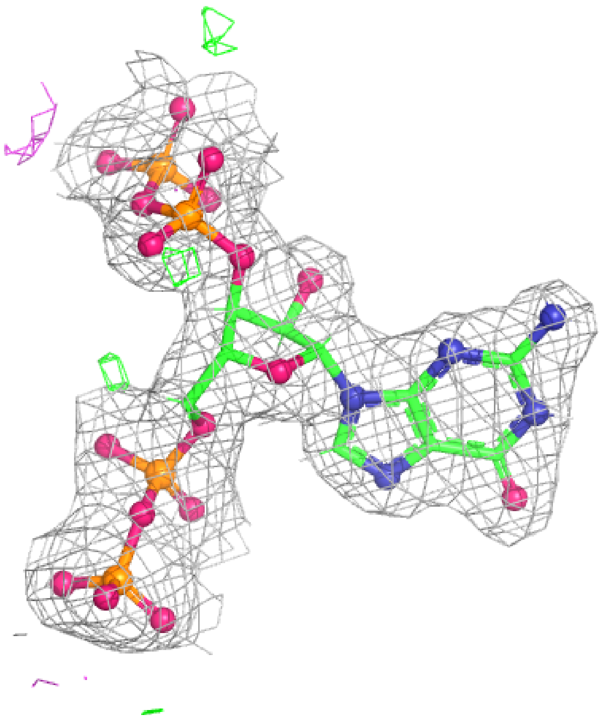


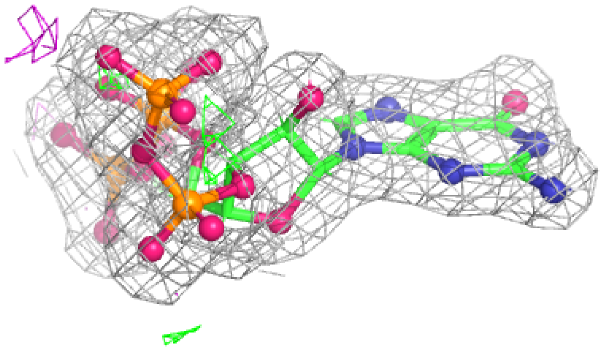


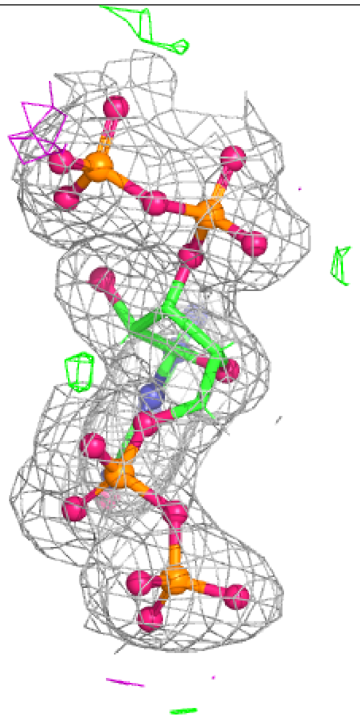


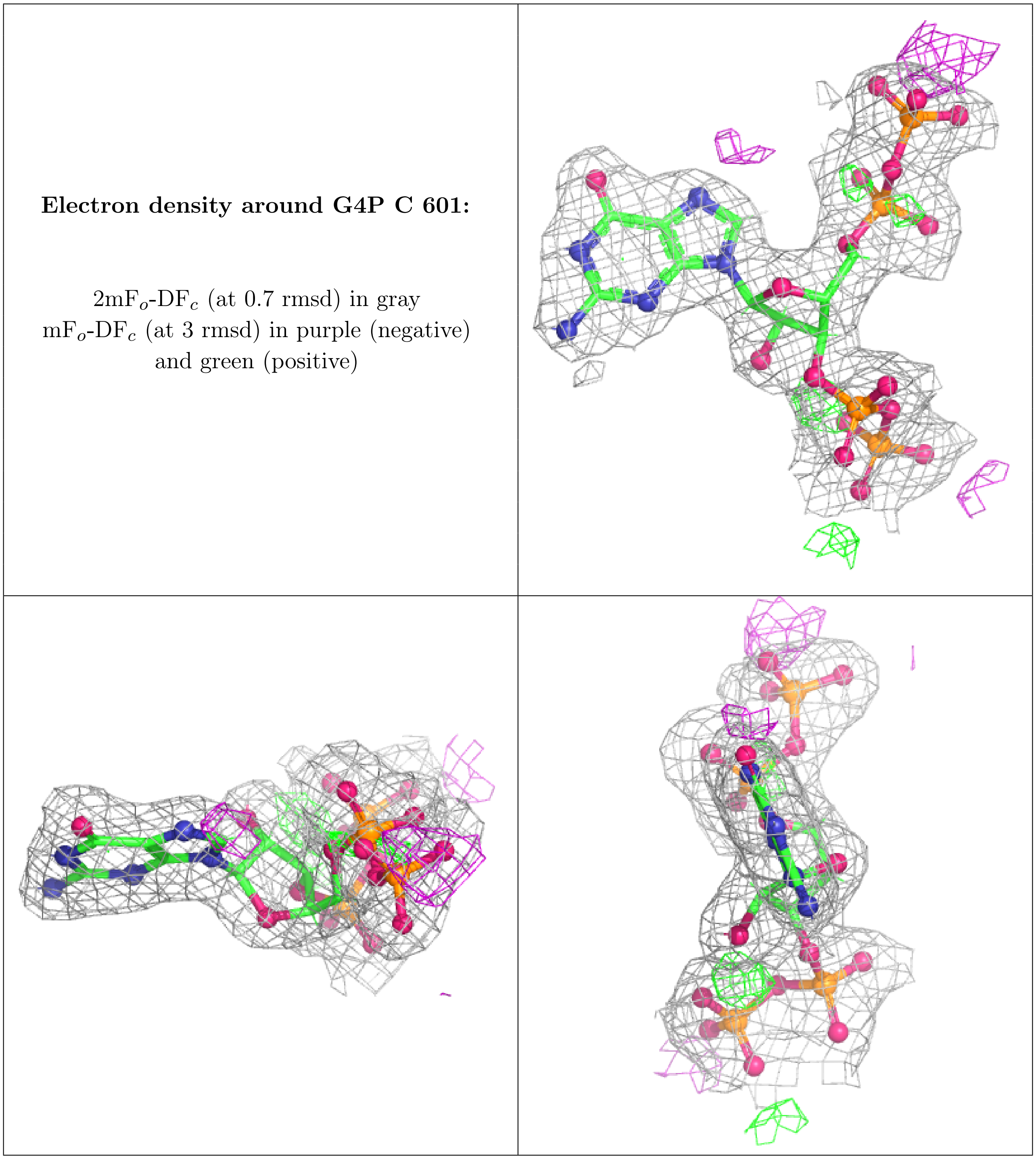
Electron density around G4P B 601:

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



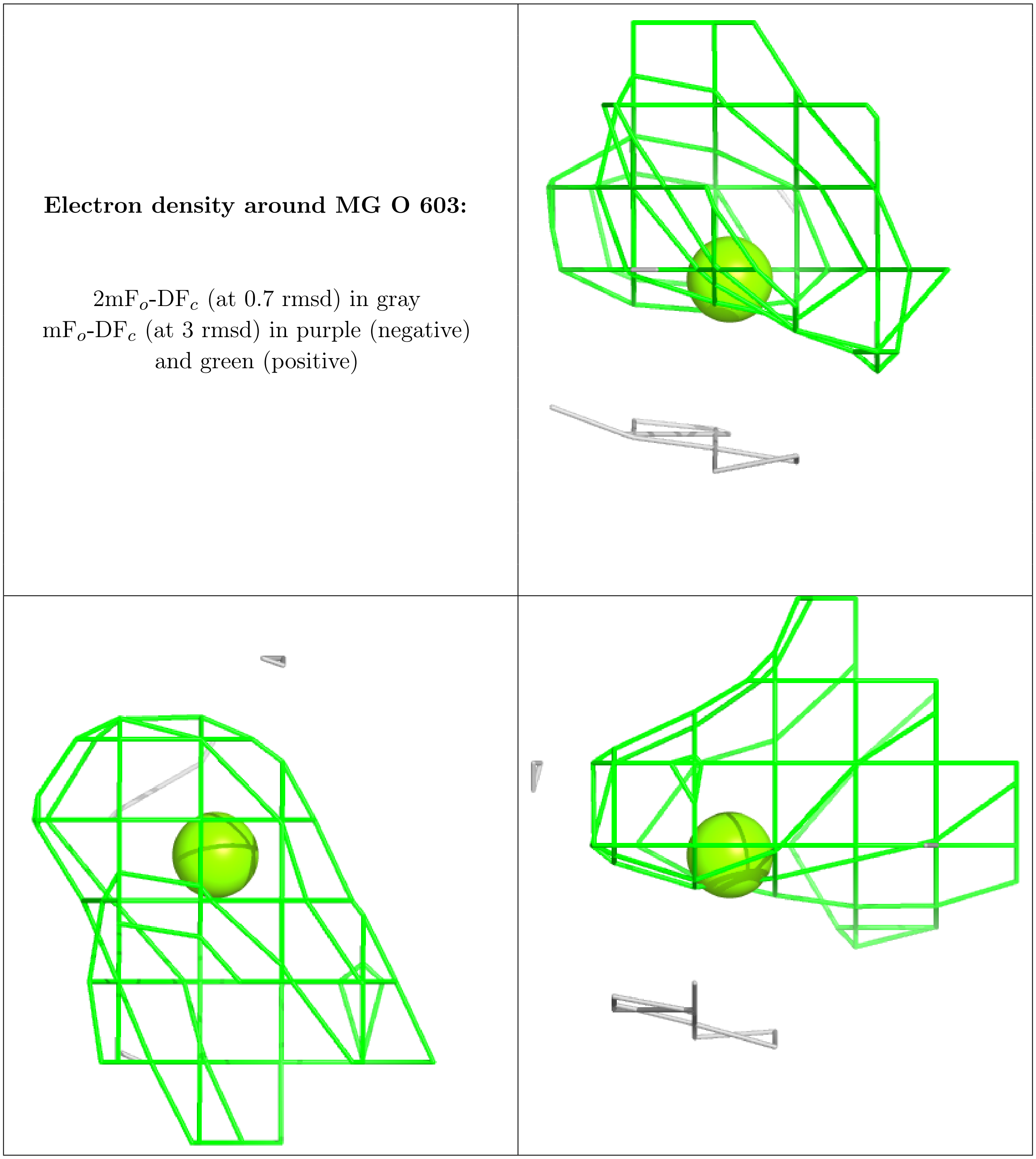






Electron density around G4P C 601:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

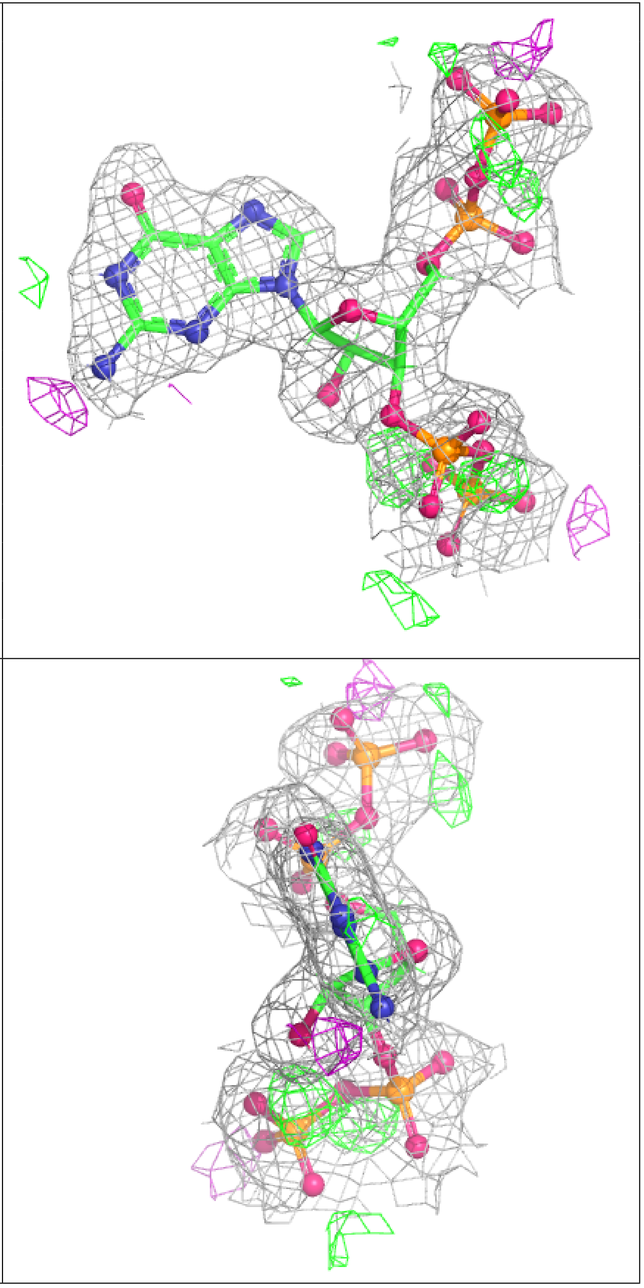


Electron density around MG O 603:

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

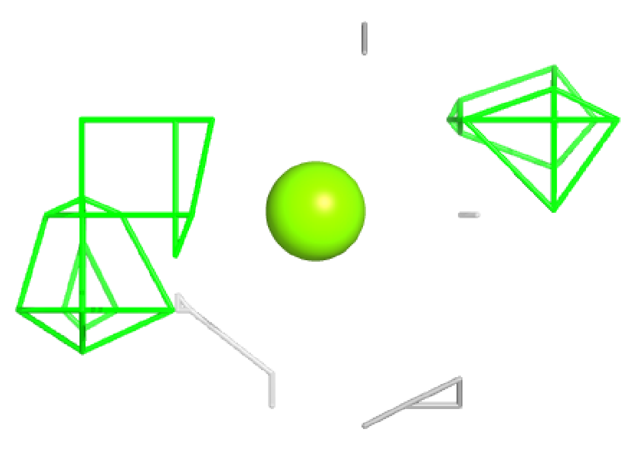
Electron density around G4P D 601:

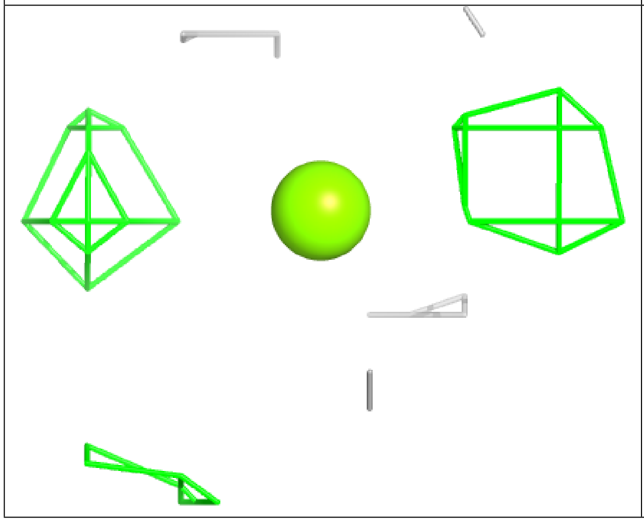
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

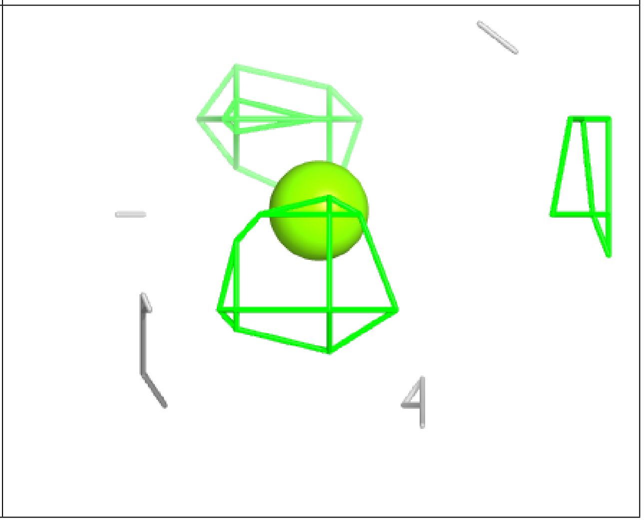


Electron density around MG P 603:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

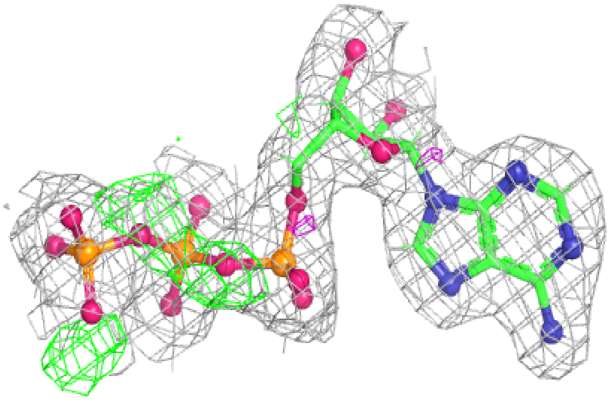


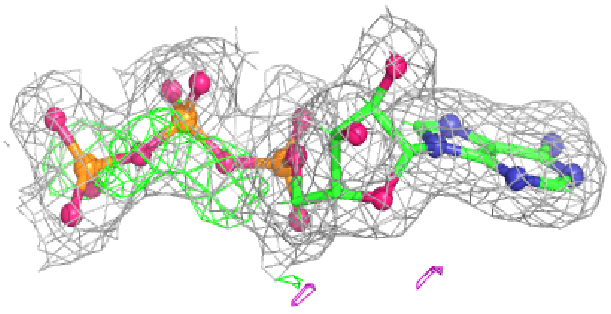


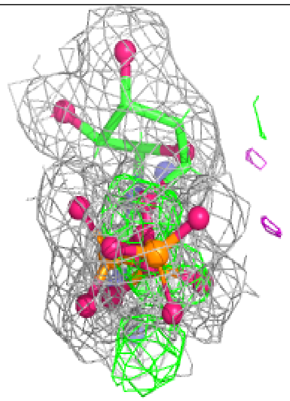


Electron density around ATP E 600:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

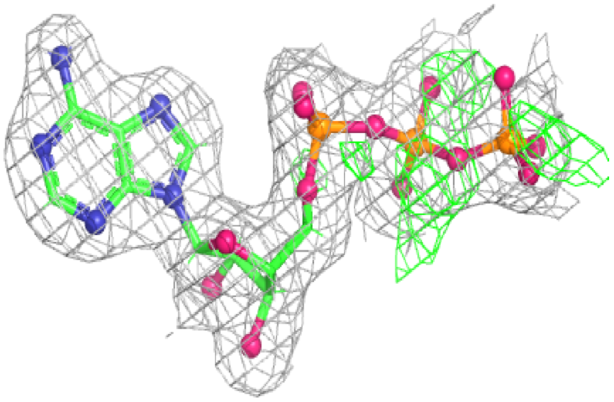


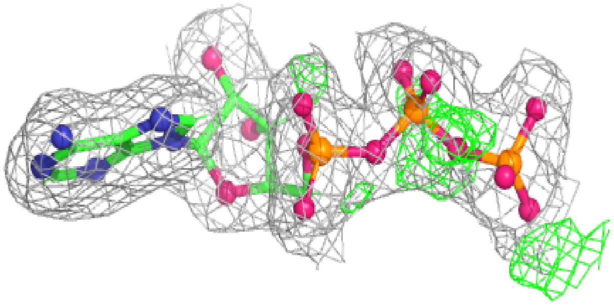


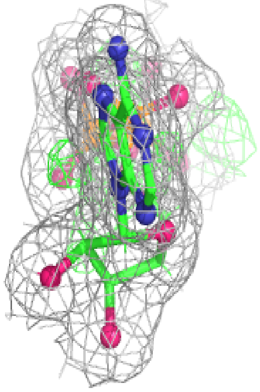


Electron density around ATP H 600:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

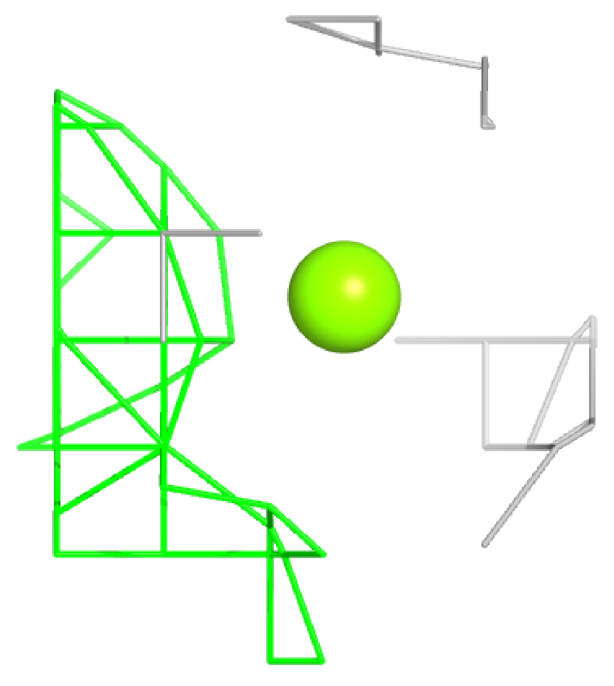


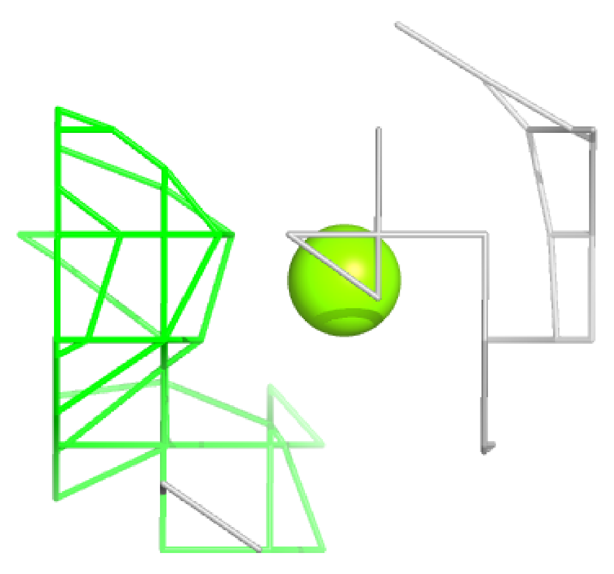


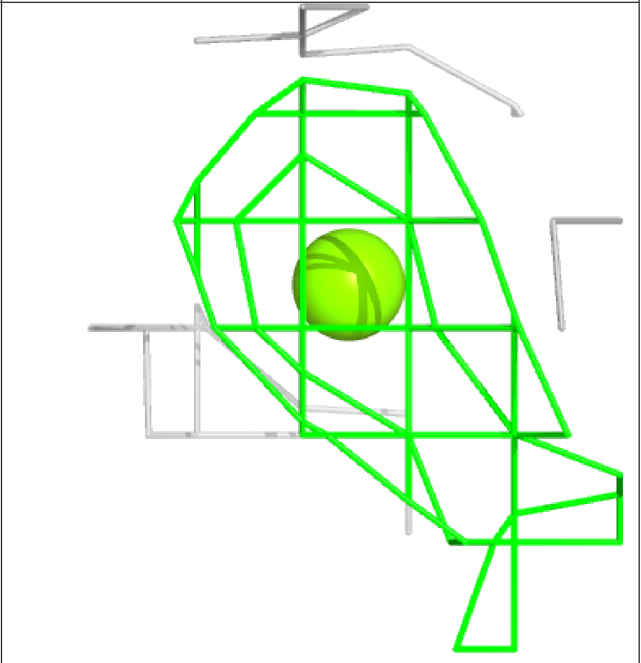


Electron density around MG I 603:

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

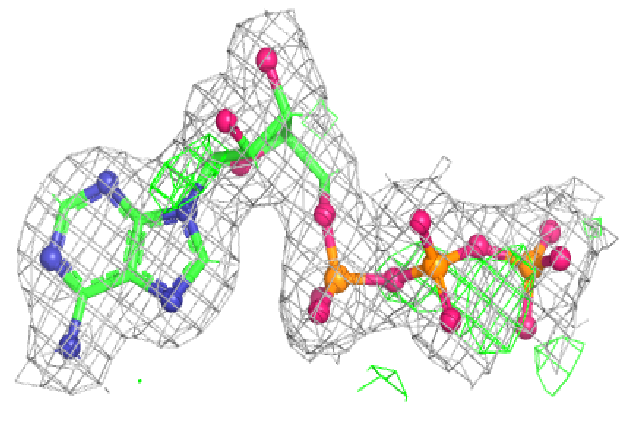


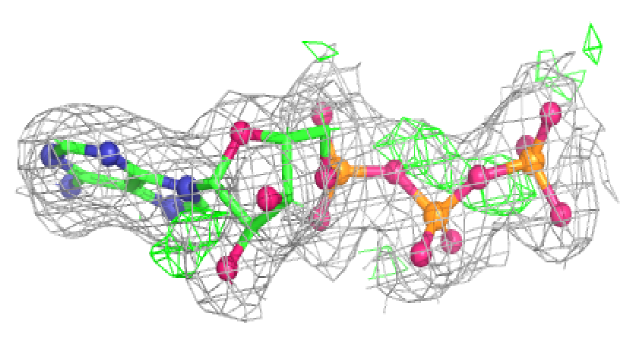


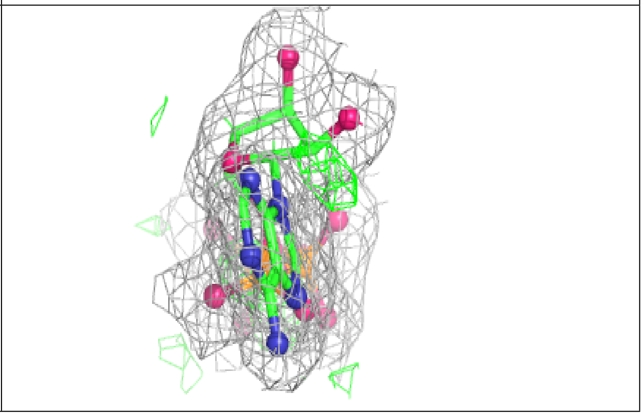


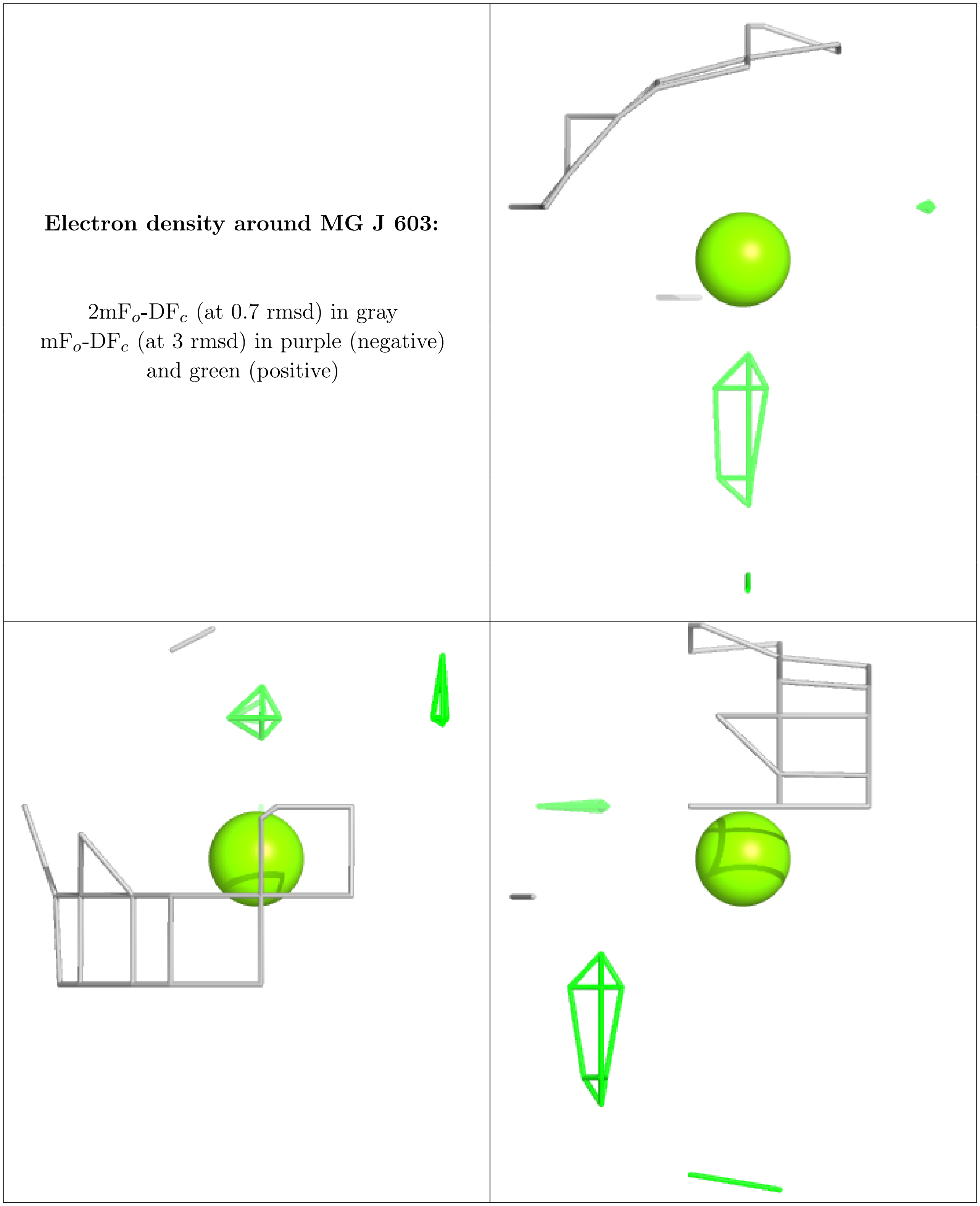
Electron density around ATP K 600:

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







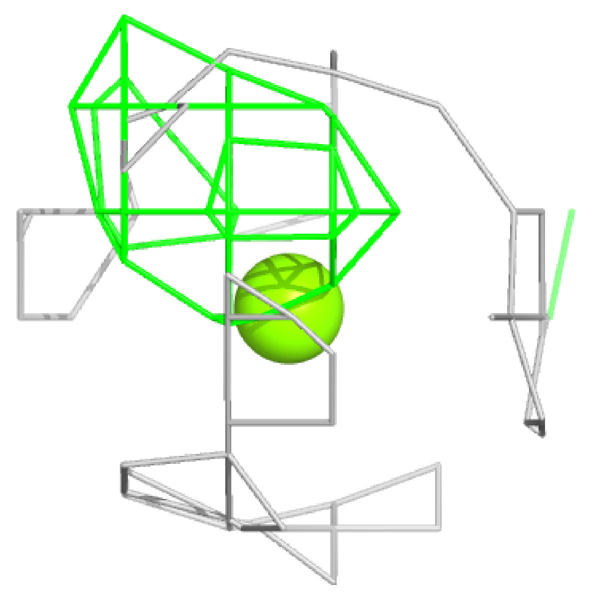


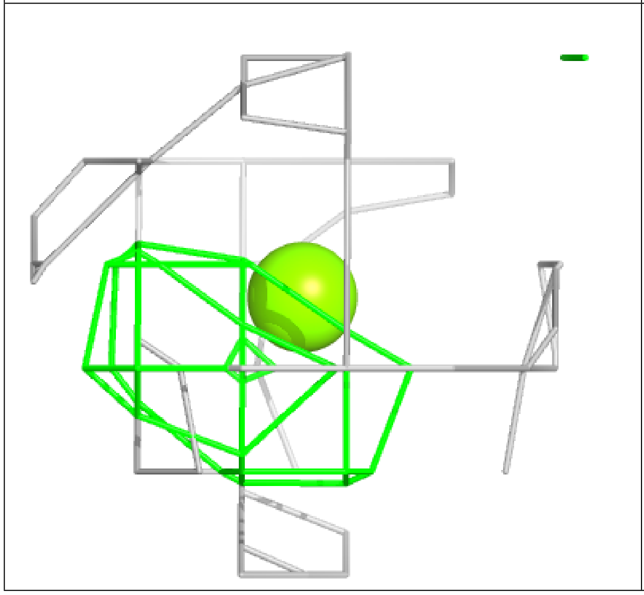
Electron density around MG J 603:

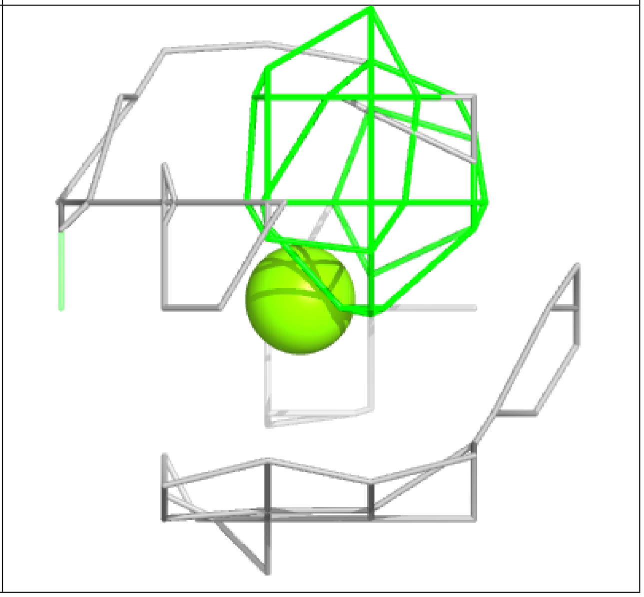
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around MG K 602:

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

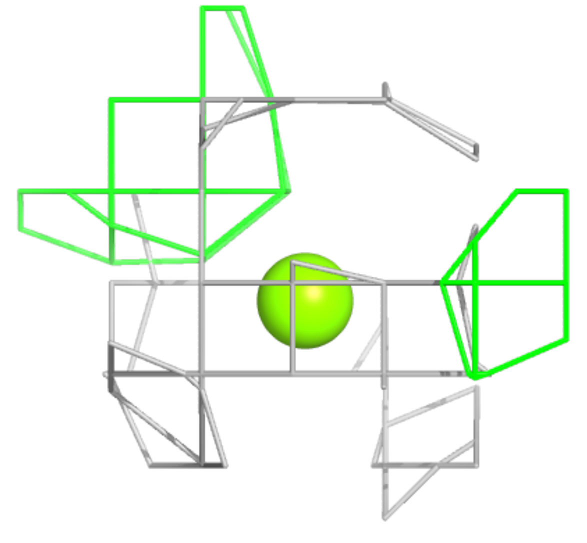


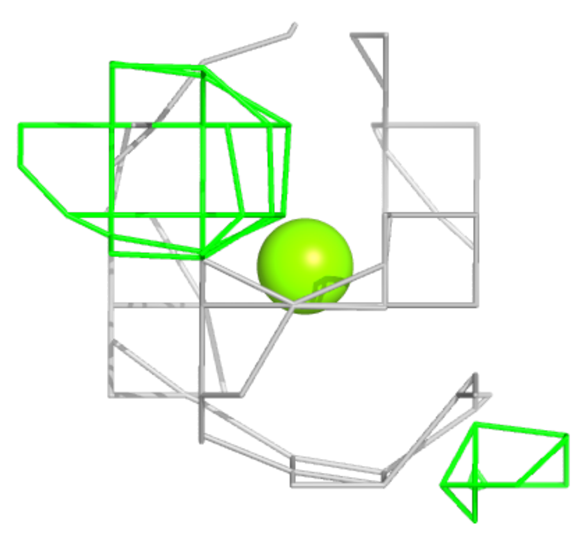


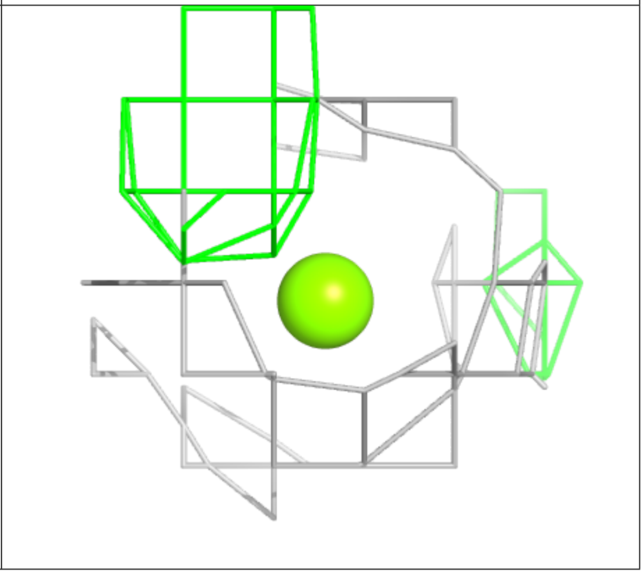


Electron density around MG K 603:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

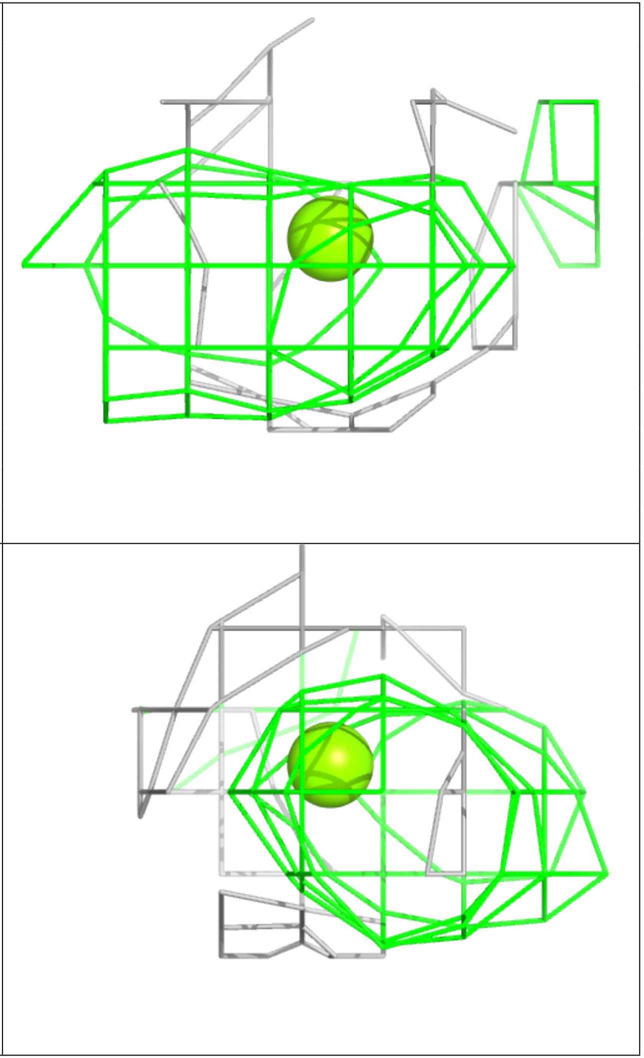


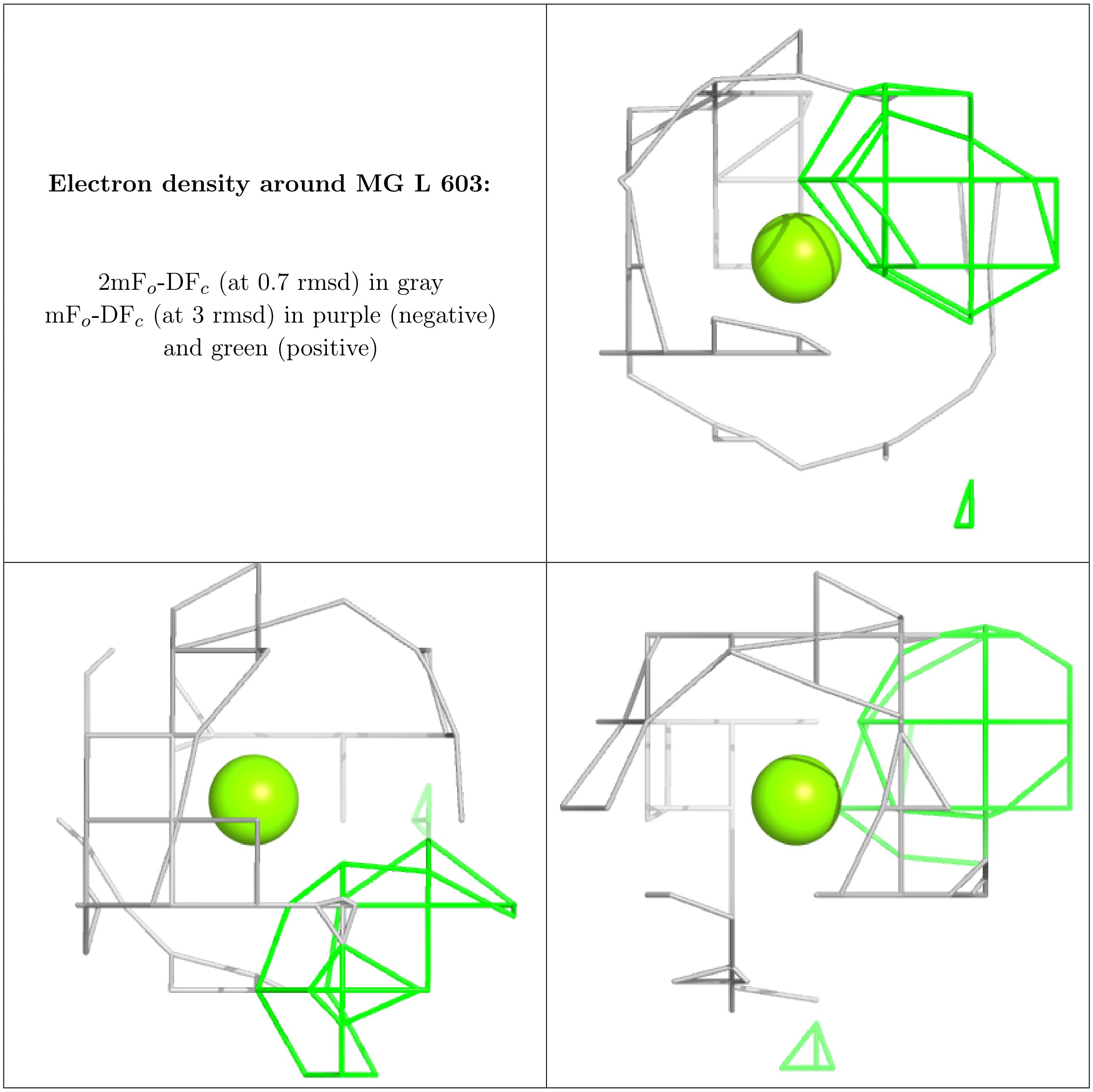




Electron density around MG L 602:

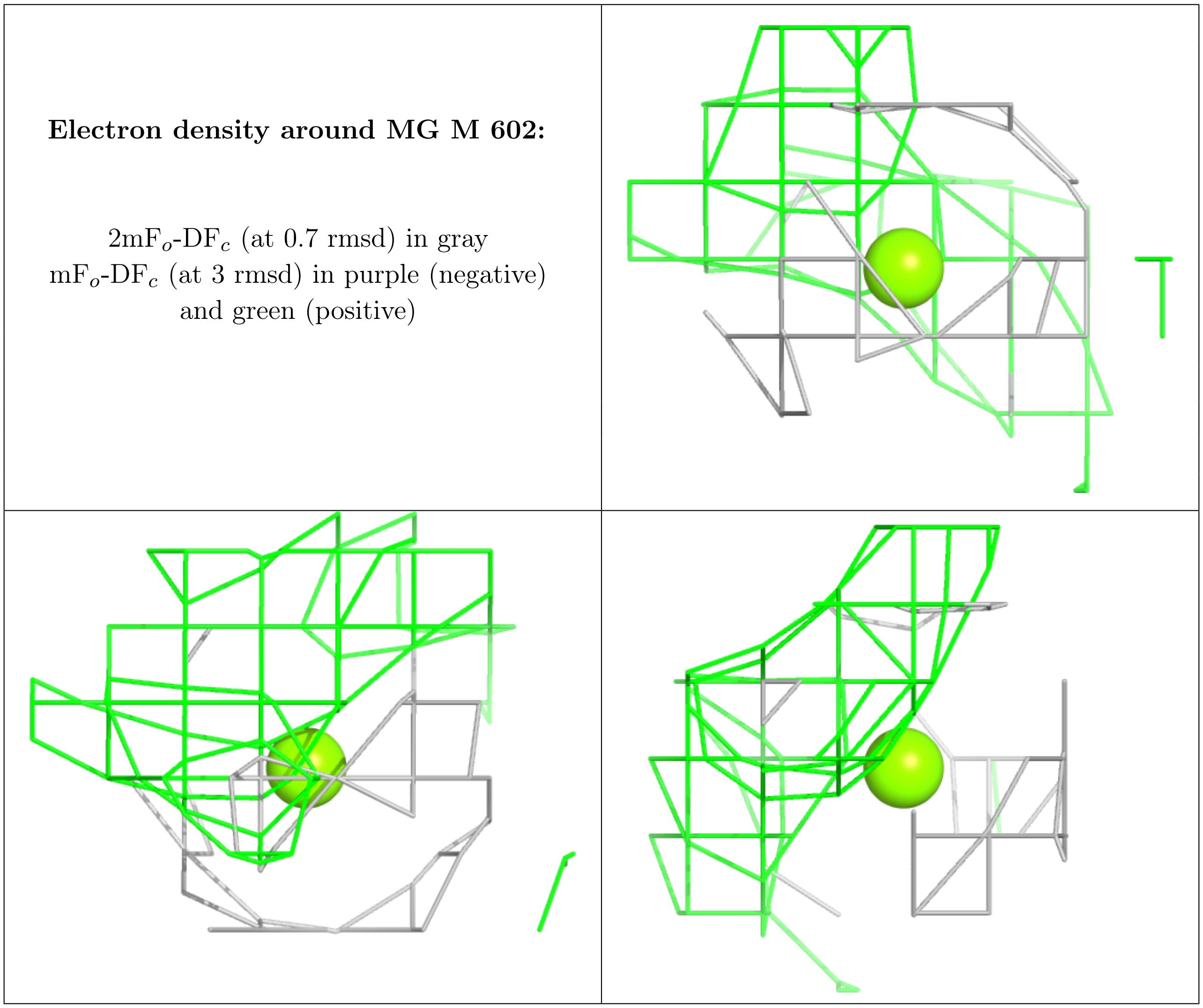
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around MG L 603:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

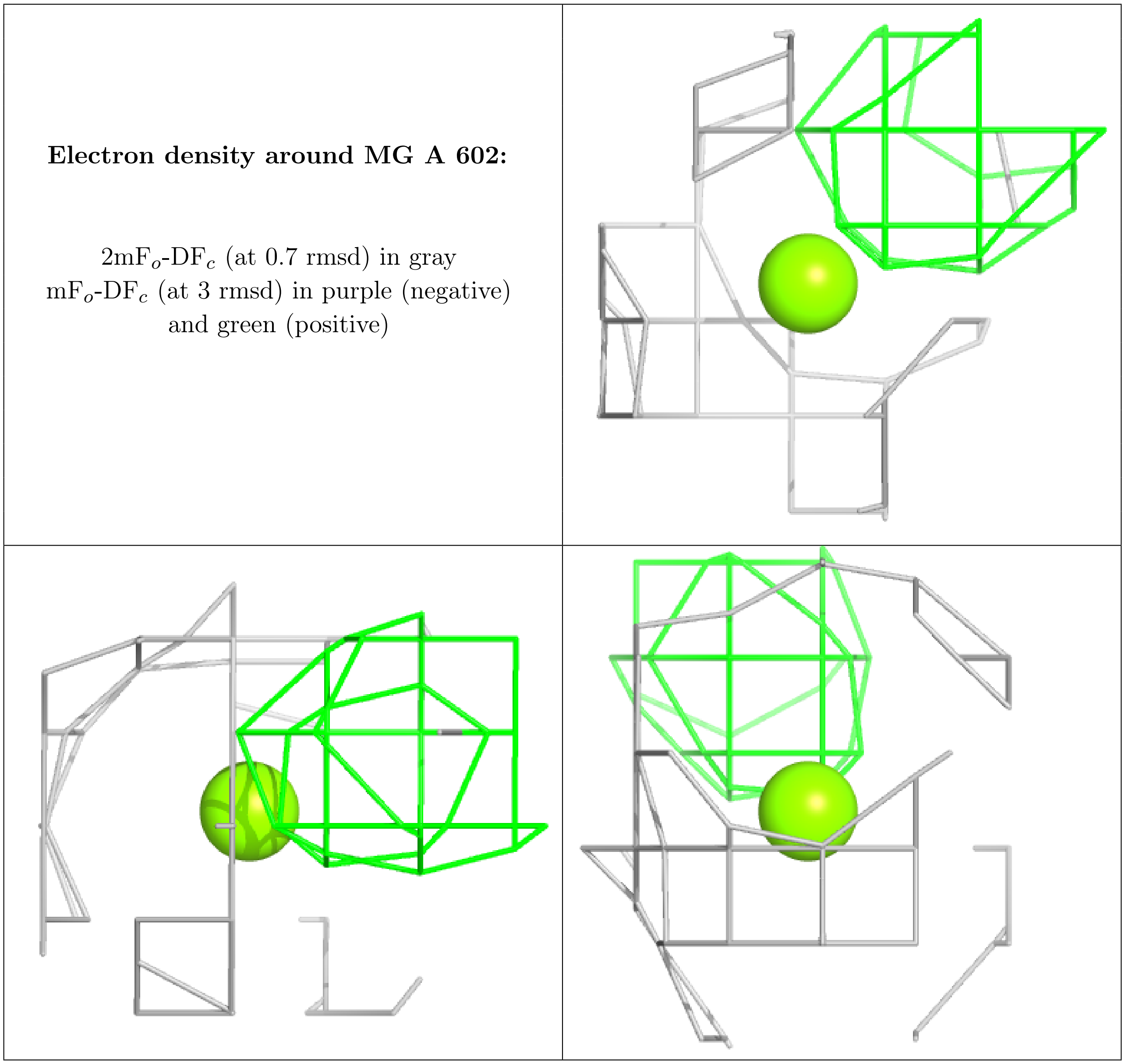


Electron density around MG M 602:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

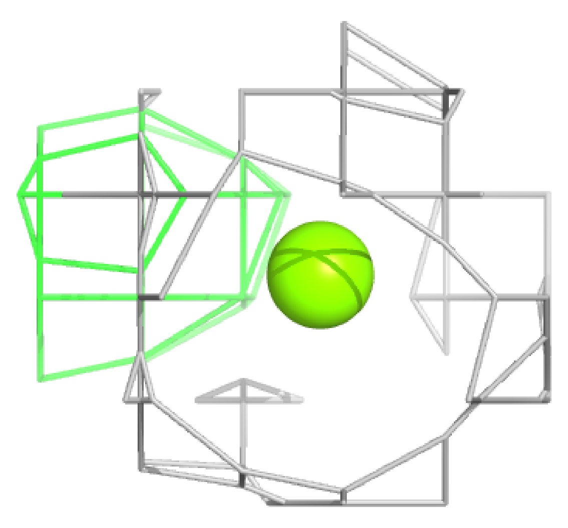
Electron density around MG A 602:

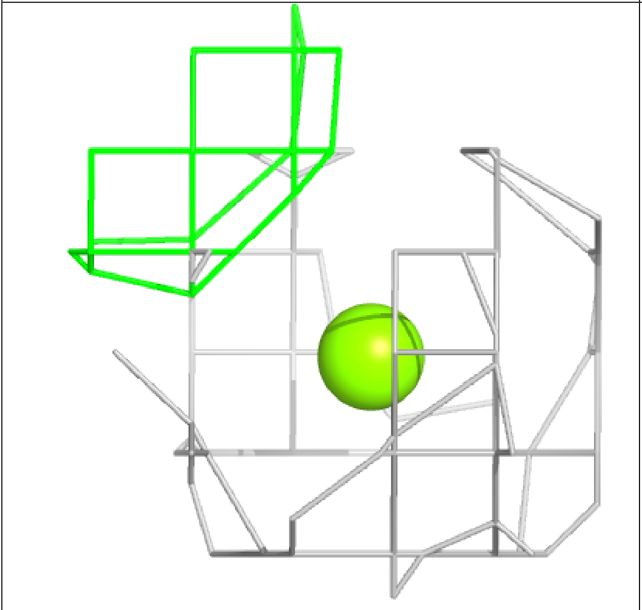
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

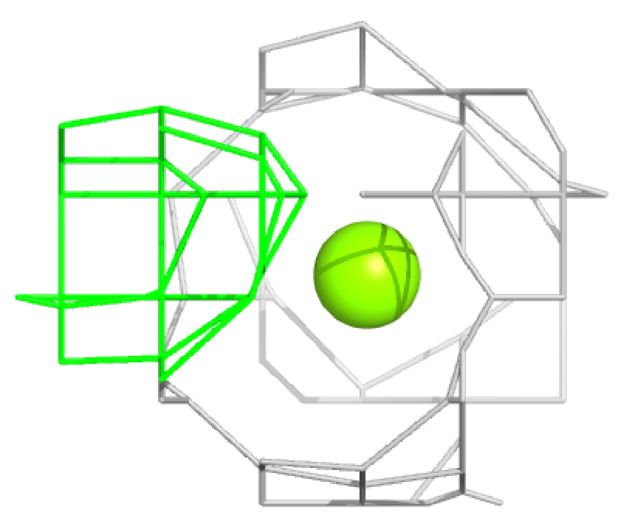


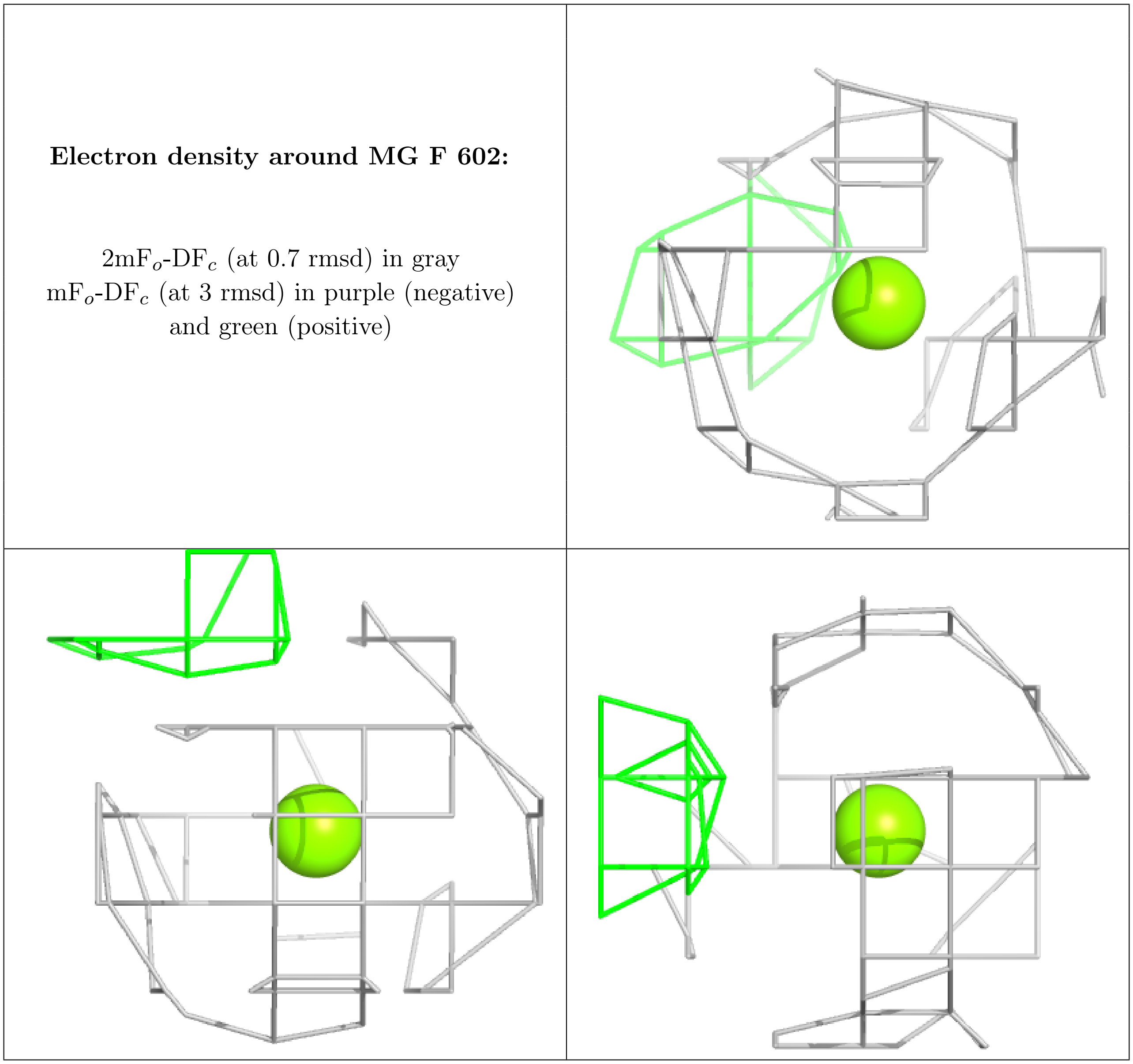
Electron density around MG E 603:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



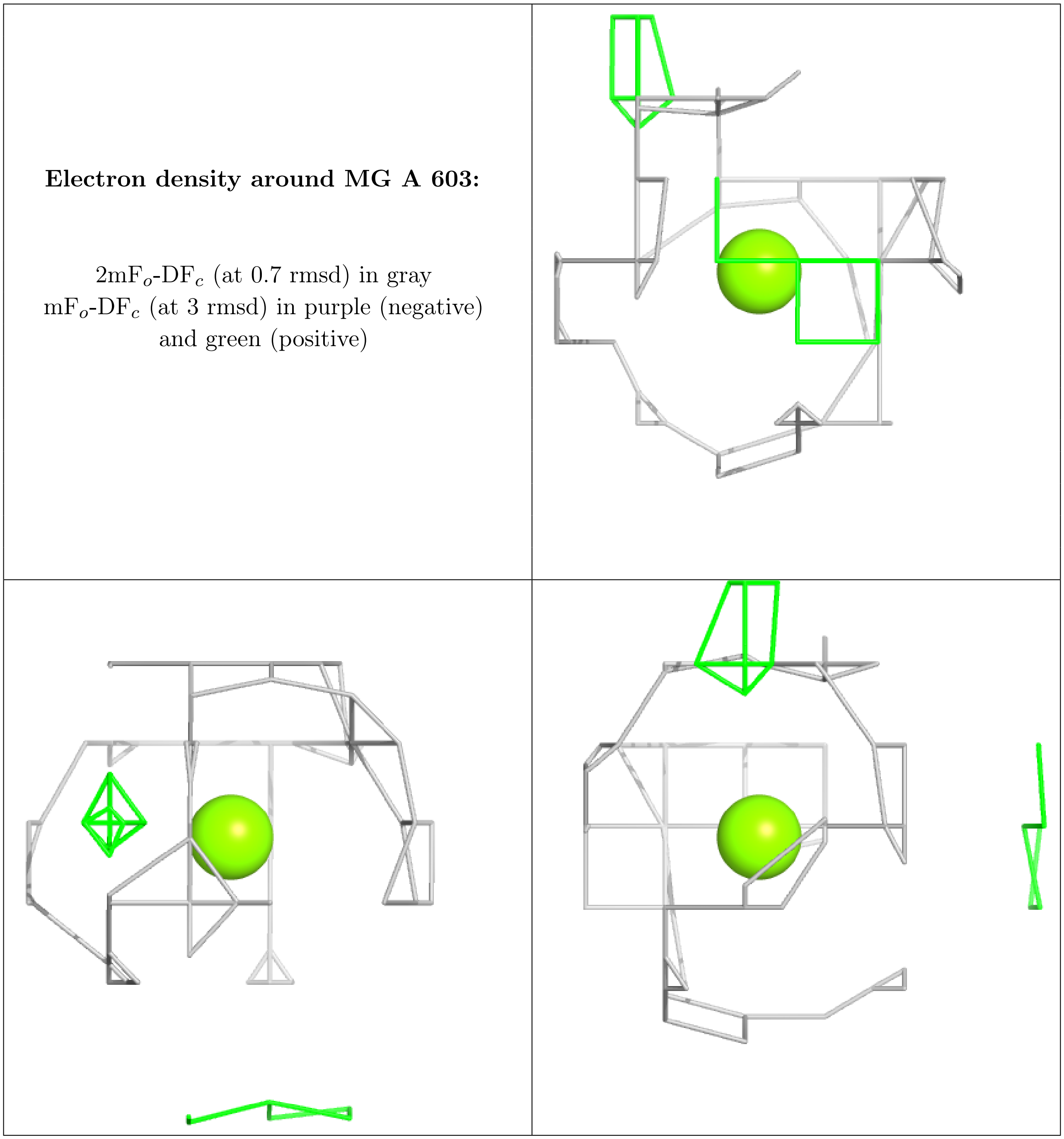






Electron density around MG F 602:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

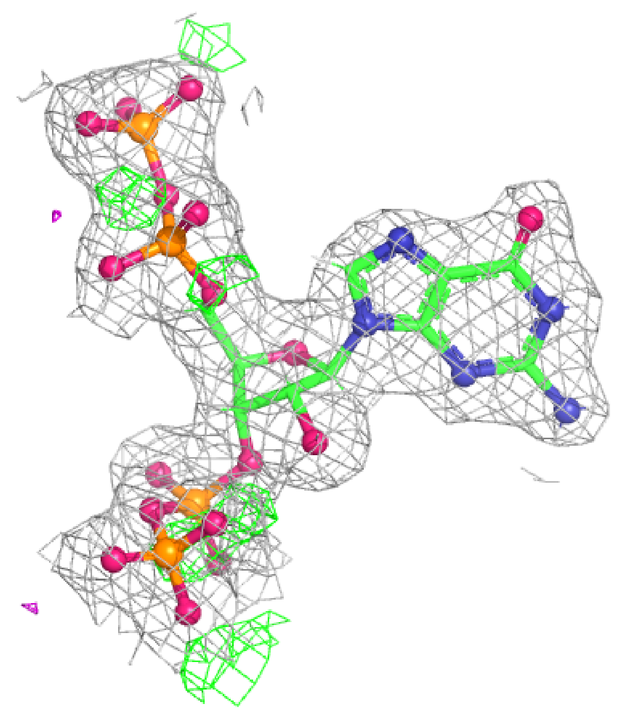


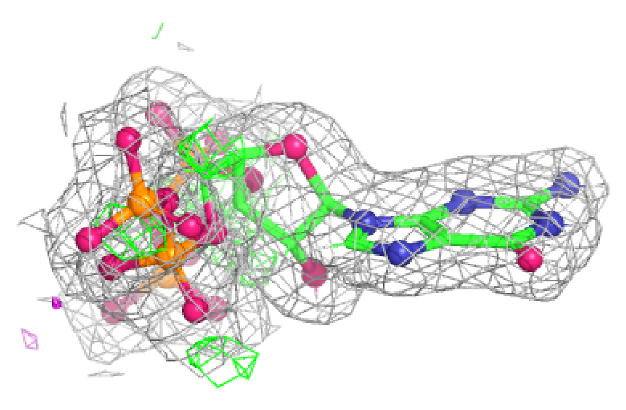
Electron density around MG A 603:

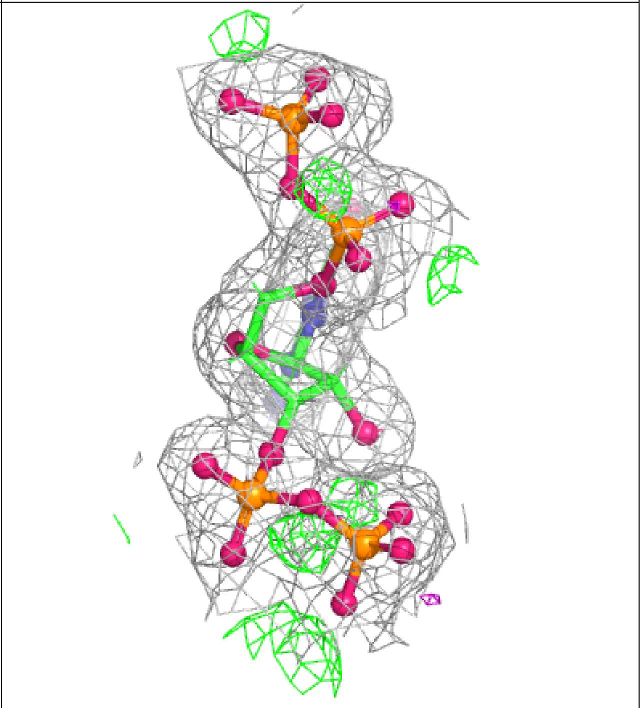
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around G4P L 601:

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

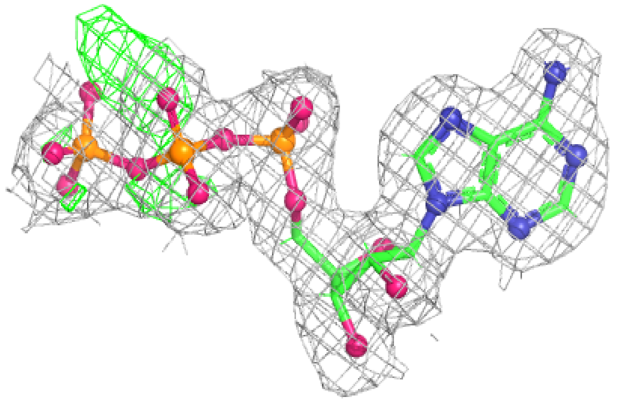


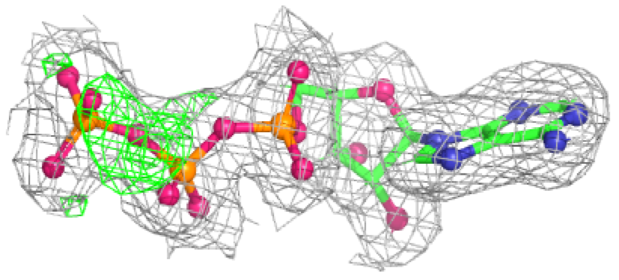


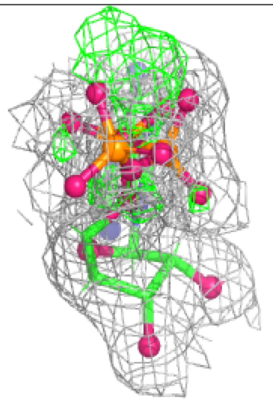


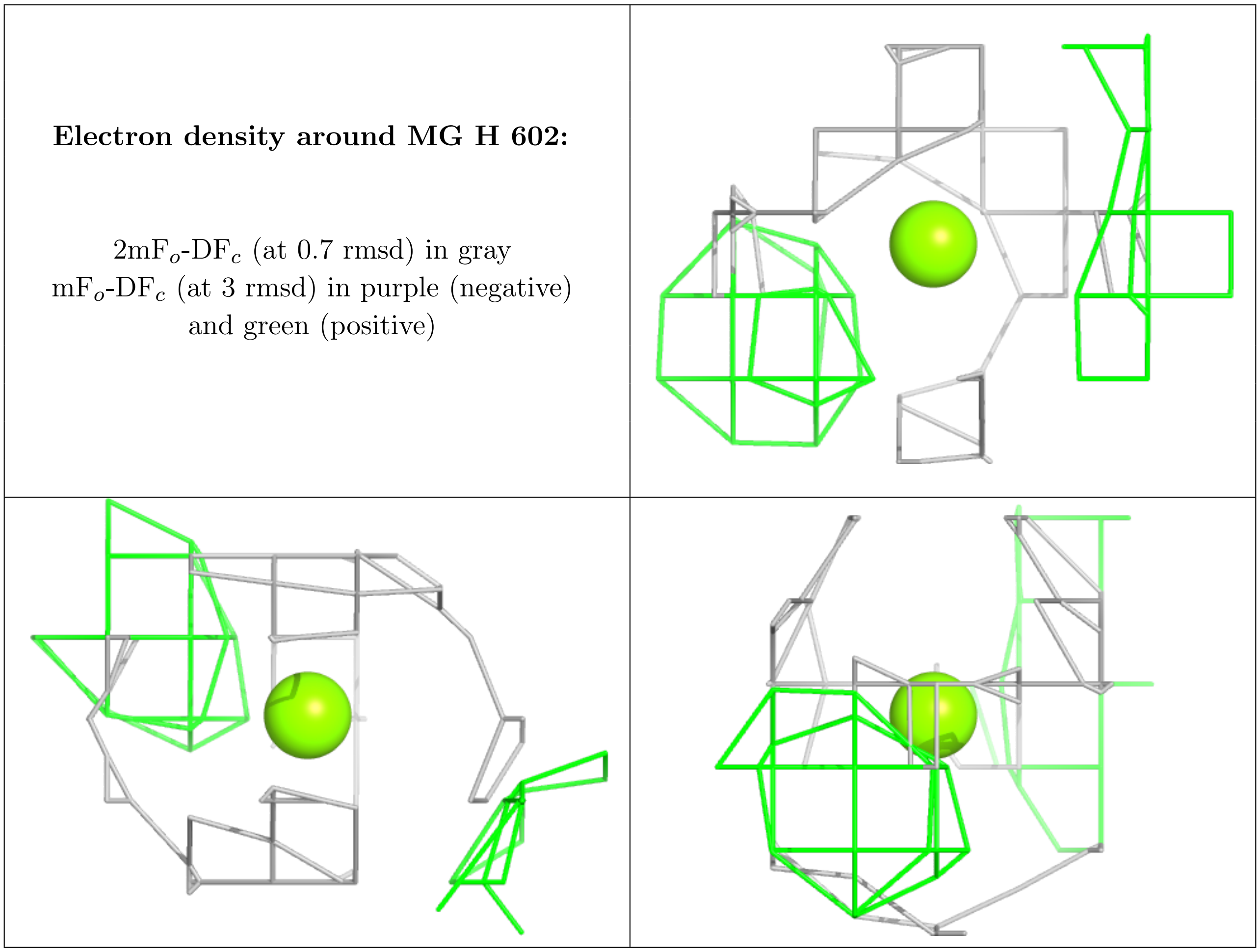
Electron density around ATP L 600:

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







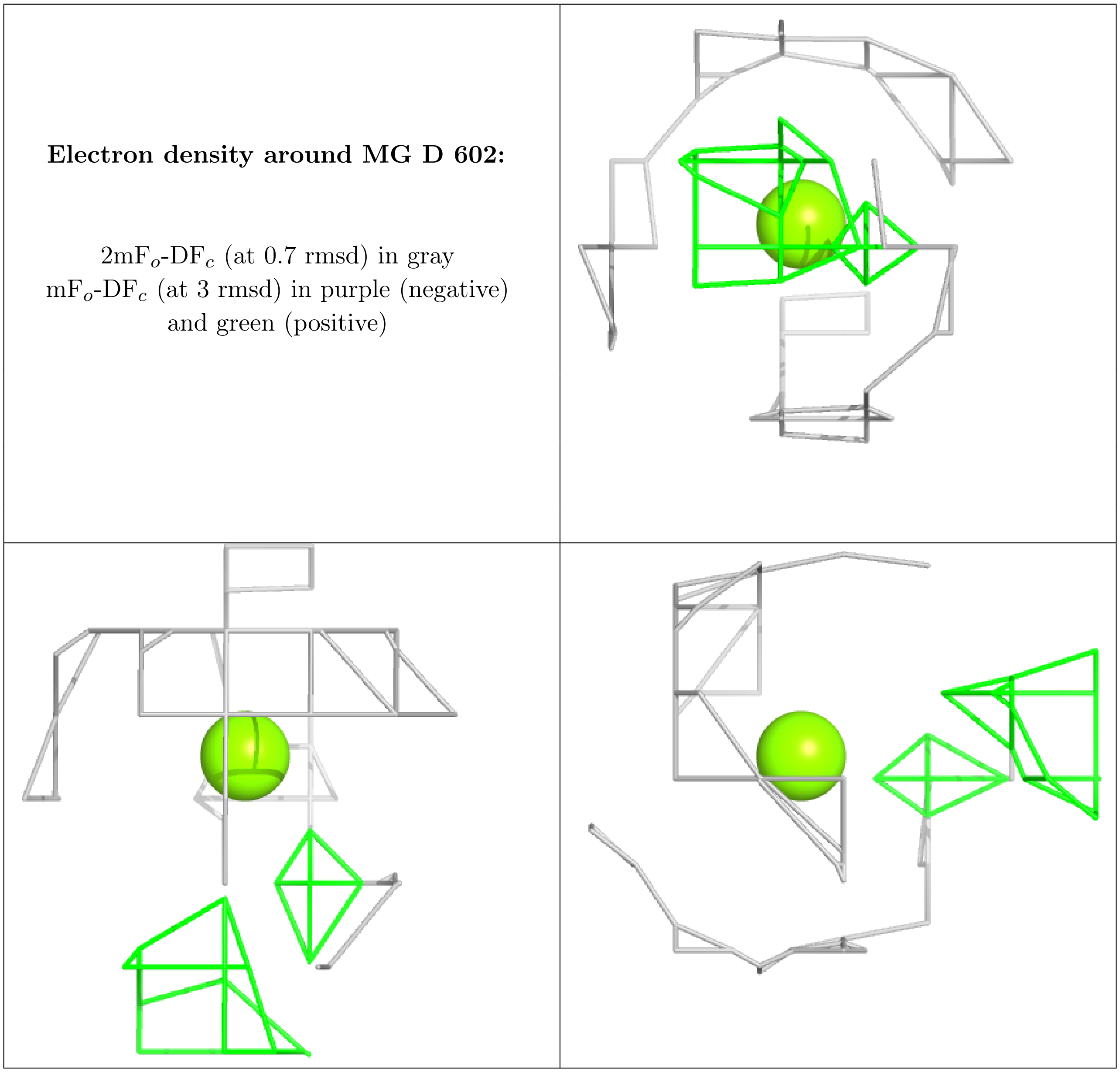


Electron density around MG H 602:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around MG D 602:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.