



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 04:23 AM BST

PDB ID : 6TXC  
Title : Crystal structure of tetrameric human wt-SAMHD1 (residues 109-626) with GTP, dATP, dCMPNPP and Mg  
Authors : Morris, E.R.; Kunzelmann, S.; Caswell, S.J.; Arnold, L.H.; Purkiss, A.; Kelly, G.; Taylor, I.A.  
Deposited on : 2020-01-14  
Resolution : 2.84 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

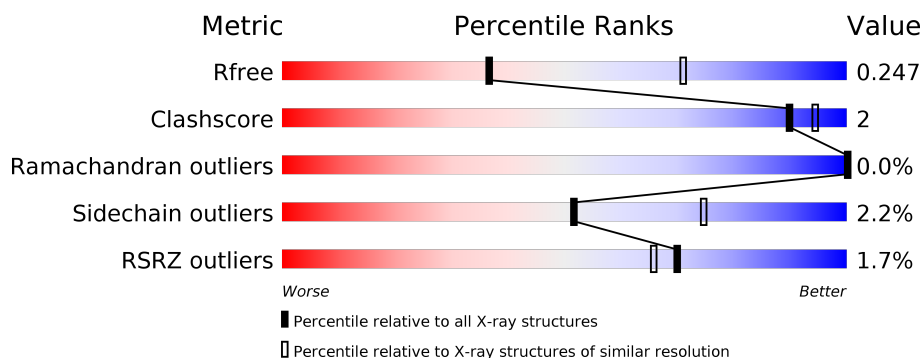
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.84 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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

Mol	Chain	Length	Quality of chain
1	A	520	 85% 7% • 8%
1	B	520	 85% 7% • 8%
1	C	520	 85% 7% • 8%
1	D	520	 85% 6% • 8%
1	E	520	 3% 86% 5% • 8%
1	F	520	 3% 84% • • 11%

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Mol	Chain	Length	Quality of chain
1	G	520	<div><div></div><div>3%</div><div>84%</div><div>5%</div><div>11%</div></div>
1	H	520	<div><div></div><div>%</div><div>87%</div><div>5%</div><div>8%</div></div>
1	I	520	<div><div></div><div></div><div>86%</div><div>5%</div><div>8%</div></div>
1	J	520	<div><div></div><div></div><div>86%</div><div>6%</div><div>8%</div></div>
1	K	520	<div><div></div><div></div><div>86%</div><div>5%</div><div>8%</div></div>
1	L	520	<div><div></div><div>%</div><div>86%</div><div>5%</div><div>9%</div></div>
1	M	520	<div><div></div><div>5%</div><div>86%</div><div></div><div>9%</div></div>
1	N	520	<div><div></div><div>2%</div><div>86%</div><div>5%</div><div>9%</div></div>
1	O	520	<div><div></div><div>4%</div><div>84%</div><div>5%</div><div>11%</div></div>
1	P	520	<div><div></div><div>3%</div><div>83%</div><div>5%</div><div>11%</div></div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 61950 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	0	0
			3840	2458	657	705	20			
1	B	478	Total	C	N	O	S	0	0	0
			3825	2449	662	694	20			
1	C	480	Total	C	N	O	S	0	0	0
			3854	2468	666	700	20			
1	D	481	Total	C	N	O	S	0	0	0
			3846	2462	663	701	20			
1	E	478	Total	C	N	O	S	0	0	0
			3799	2432	655	692	20			
1	F	463	Total	C	N	O	S	0	0	0
			3695	2364	633	678	20			
1	G	463	Total	C	N	O	S	0	0	0
			3668	2347	626	675	20			
1	H	478	Total	C	N	O	S	0	0	0
			3845	2461	665	699	20			
1	I	477	Total	C	N	O	S	0	0	0
			3822	2446	660	696	20			
1	J	479	Total	C	N	O	S	0	0	0
			3837	2456	662	699	20			
1	K	480	Total	C	N	O	S	0	0	0
			3839	2455	659	705	20			
1	L	475	Total	C	N	O	S	0	0	0
			3756	2406	642	689	19			
1	M	471	Total	C	N	O	S	0	0	0
			3704	2367	636	681	20			
1	N	475	Total	C	N	O	S	0	0	0
			3757	2403	642	692	20			
1	O	465	Total	C	N	O	S	0	0	0
			3680	2352	629	679	20			
1	P	461	Total	C	N	O	S	0	0	0
			3640	2330	618	672	20			



There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	GLY	-	expression tag	UNP Q9Y3Z3
A	108	SER	-	expression tag	UNP Q9Y3Z3
B	107	GLY	-	expression tag	UNP Q9Y3Z3
B	108	SER	-	expression tag	UNP Q9Y3Z3
C	107	GLY	-	expression tag	UNP Q9Y3Z3
C	108	SER	-	expression tag	UNP Q9Y3Z3
D	107	GLY	-	expression tag	UNP Q9Y3Z3
D	108	SER	-	expression tag	UNP Q9Y3Z3
E	107	GLY	-	expression tag	UNP Q9Y3Z3
E	108	SER	-	expression tag	UNP Q9Y3Z3
F	107	GLY	-	expression tag	UNP Q9Y3Z3
F	108	SER	-	expression tag	UNP Q9Y3Z3
G	107	GLY	-	expression tag	UNP Q9Y3Z3
G	108	SER	-	expression tag	UNP Q9Y3Z3
H	107	GLY	-	expression tag	UNP Q9Y3Z3
H	108	SER	-	expression tag	UNP Q9Y3Z3
I	107	GLY	-	expression tag	UNP Q9Y3Z3
I	108	SER	-	expression tag	UNP Q9Y3Z3
J	107	GLY	-	expression tag	UNP Q9Y3Z3
J	108	SER	-	expression tag	UNP Q9Y3Z3
K	107	GLY	-	expression tag	UNP Q9Y3Z3
K	108	SER	-	expression tag	UNP Q9Y3Z3
L	107	GLY	-	expression tag	UNP Q9Y3Z3
L	108	SER	-	expression tag	UNP Q9Y3Z3
M	107	GLY	-	expression tag	UNP Q9Y3Z3
M	108	SER	-	expression tag	UNP Q9Y3Z3
N	107	GLY	-	expression tag	UNP Q9Y3Z3
N	108	SER	-	expression tag	UNP Q9Y3Z3
O	107	GLY	-	expression tag	UNP Q9Y3Z3
O	108	SER	-	expression tag	UNP Q9Y3Z3
P	107	GLY	-	expression tag	UNP Q9Y3Z3
P	108	SER	-	expression tag	UNP Q9Y3Z3

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	P	1	Total Fe 1 1	0	0
2	G	1	Total Fe 1 1	0	0

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by author).

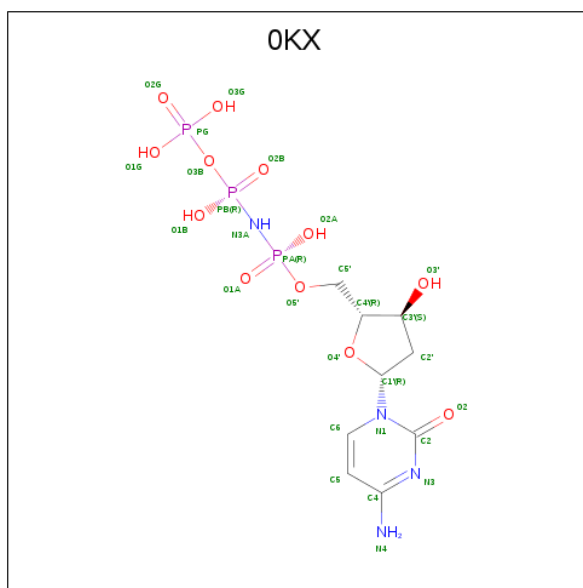
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	3	Total 3	Mg 3	0	0
3	G	3	Total 3	Mg 3	0	0
3	J	2	Total 2	Mg 2	0	0
3	D	3	Total 3	Mg 3	0	0
3	K	3	Total 3	Mg 3	0	0

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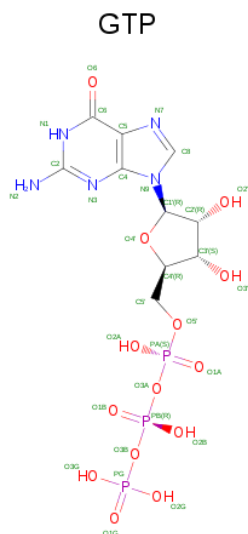
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	2	Total 2	Mg 2	0	0
3	H	2	Total 2	Mg 2	0	0
3	B	3	Total 3	Mg 3	0	0
3	I	3	Total 3	Mg 3	0	0
3	C	3	Total 3	Mg 3	0	0
3	A	3	Total 3	Mg 3	0	0
3	N	2	Total 2	Mg 2	0	0
3	O	2	Total 2	Mg 2	0	0
3	L	3	Total 3	Mg 3	0	0
3	F	2	Total 2	Mg 2	0	0
3	M	3	Total 3	Mg 3	0	0

- Molecule 4 is 2'-deoxy-5'-O-[(R)-hydroxy{[(R)-hydroxy(phosphonooxy)phosphoryl]amino}phosphoryl]cytidine (three-letter code: 0KX) (formula: C<sub>9</sub>H<sub>17</sub>N<sub>4</sub>O<sub>12</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			28	9	4	12	3		
4	B	1	Total	C	N	O	P	0	0
			28	9	4	12	3		
4	C	1	Total	C	N	O	P	0	0
			28	9	4	12	3		
4	D	1	Total	C	N	O	P	0	0
			28	9	4	12	3		
4	E	1	Total	C	N	O	P	0	0
			28	9	4	12	3		
4	F	1	Total	C	N	O	P	0	0
			28	9	4	12	3		
4	G	1	Total	C	N	O	P	0	0
			28	9	4	12	3		
4	H	1	Total	C	N	O	P	0	0
			28	9	4	12	3		
4	I	1	Total	C	N	O	P	0	0
			28	9	4	12	3		
4	J	1	Total	C	N	O	P	0	0
			28	9	4	12	3		
4	K	1	Total	C	N	O	P	0	0
			28	9	4	12	3		
4	L	1	Total	C	N	O	P	0	0
			28	9	4	12	3		
4	M	1	Total	C	N	O	P	0	0
			28	9	4	12	3		
4	N	1	Total	C	N	O	P	0	0
			28	9	4	12	3		
4	O	1	Total	C	N	O	P	0	0
			28	9	4	12	3		
4	P	1	Total	C	N	O	P	0	0
			28	9	4	12	3		

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ) (labeled as "Ligand of Interest" by author).



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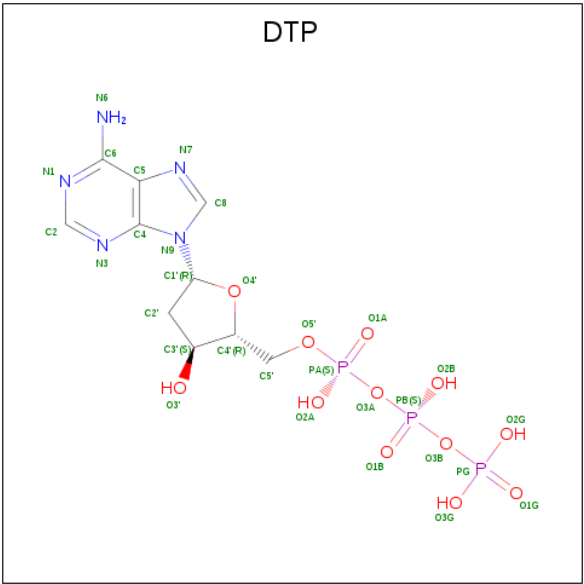
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	O	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	O	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 6 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		
6	I	1	Total	O	S	0	0
			5	4	1		
6	J	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
7	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
7	C	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
7	D	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
7	E	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
7	F	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
7	G	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
7	H	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
7	I	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
7	J	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
7	K	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
7	L	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

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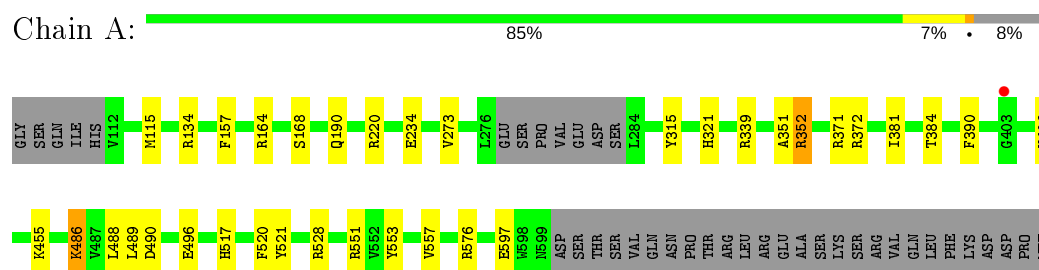
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	M	1	Total 30	C 10	N 5	O 12	P 3	0	0
7	N	1	Total 30	C 10	N 5	O 12	P 3	0	0
7	O	1	Total 30	C 10	N 5	O 12	P 3	0	0
7	P	1	Total 30	C 10	N 5	O 12	P 3	0	0



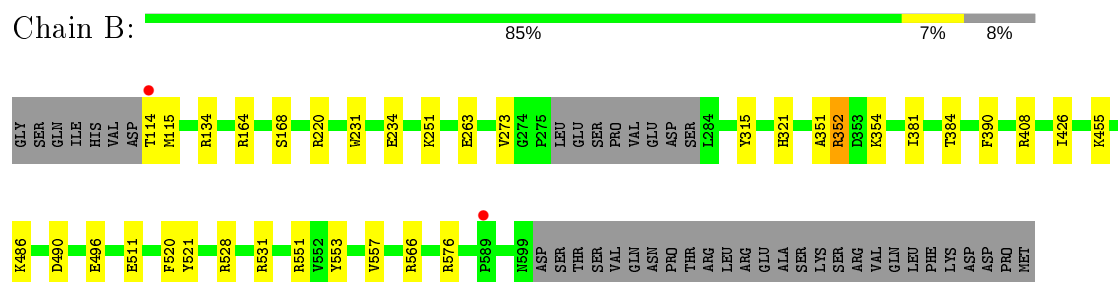
### 3 Residue-property plots [i](#)

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

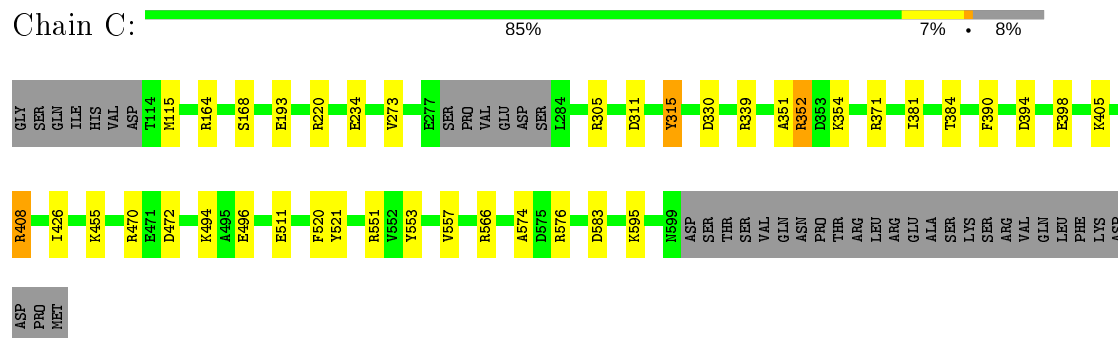
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



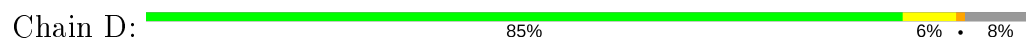
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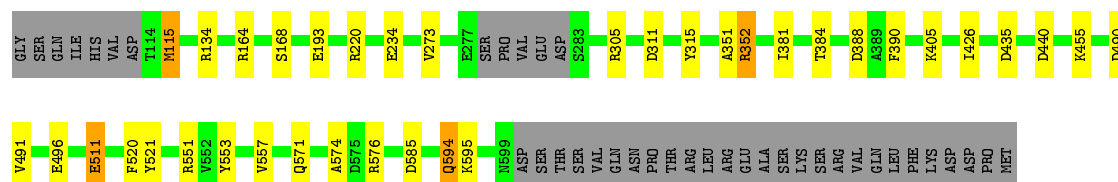


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

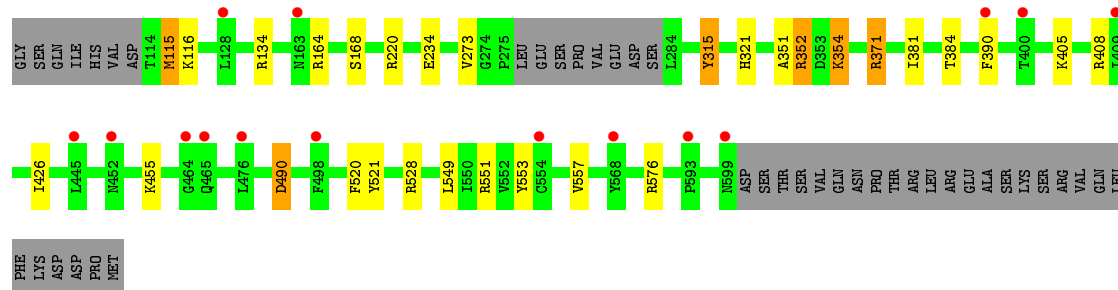
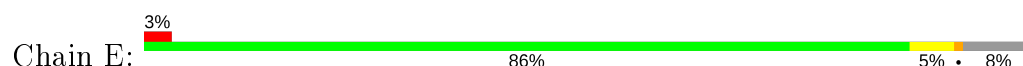


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

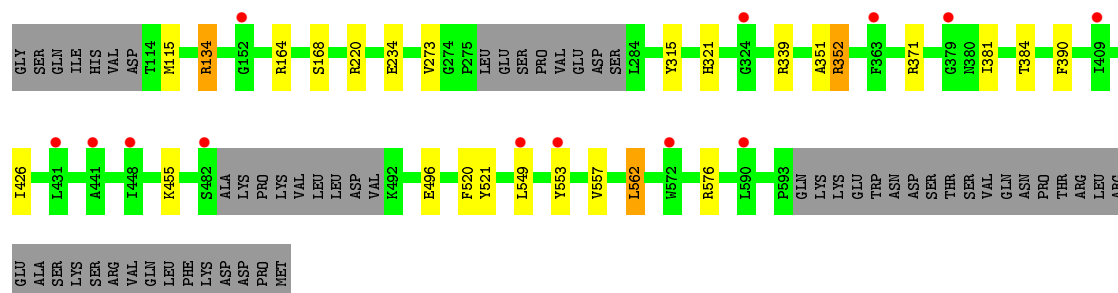
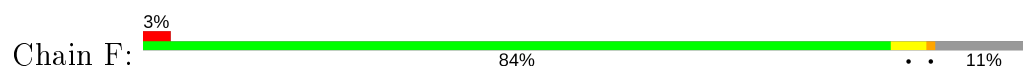




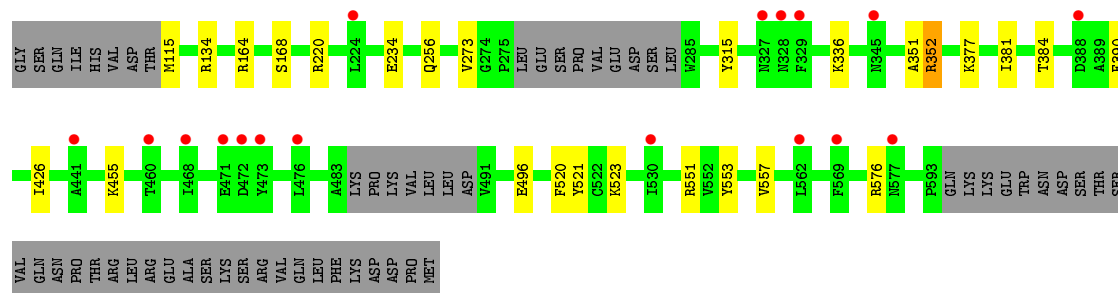
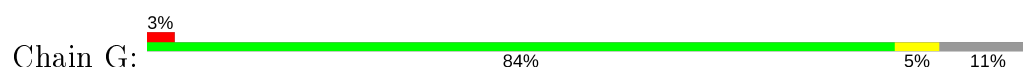
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



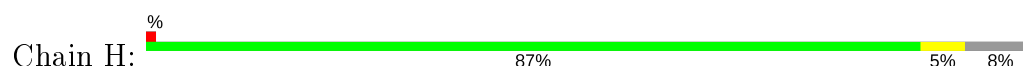
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

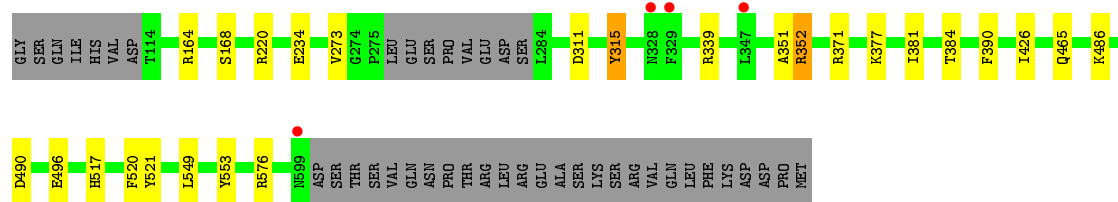


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



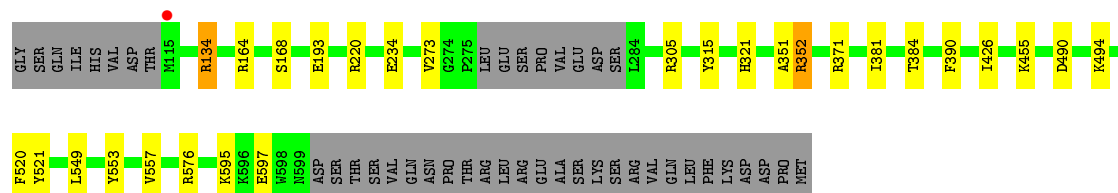
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





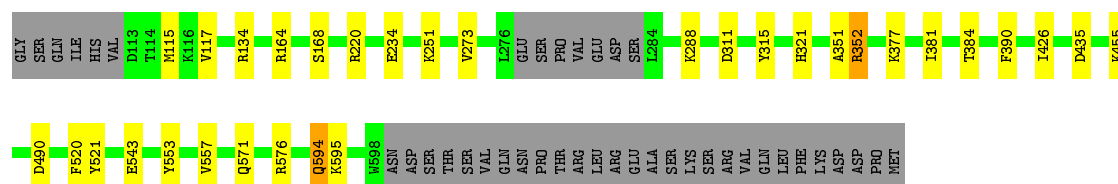
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain I: 86% 5% 8%



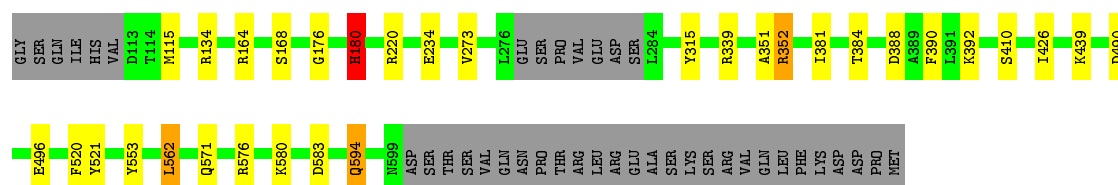
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain J: 86% 6% 8%



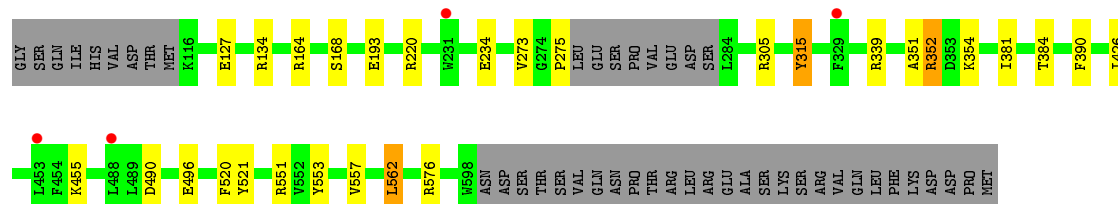
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain K: 86% 5% 8%

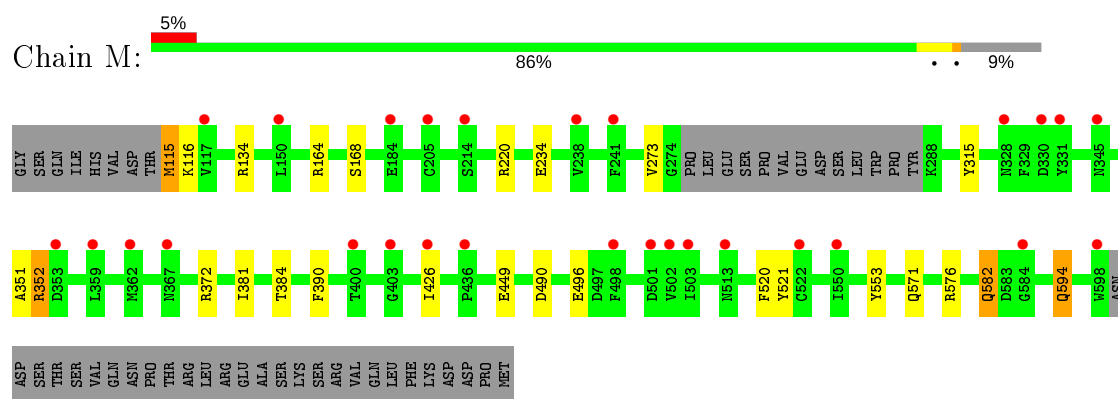


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

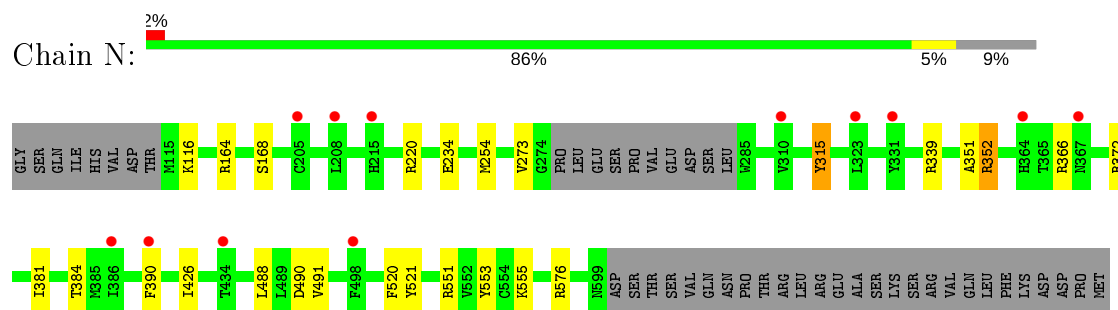
Chain L: 86% 5% 9%



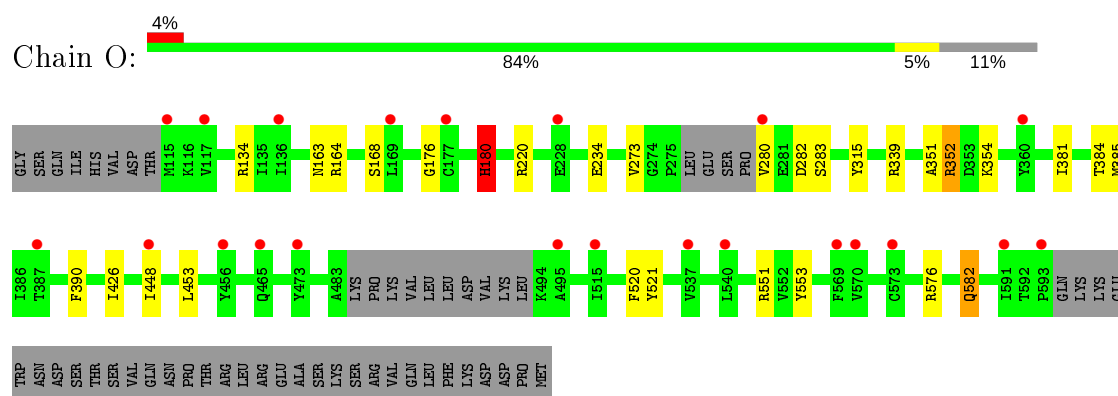
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



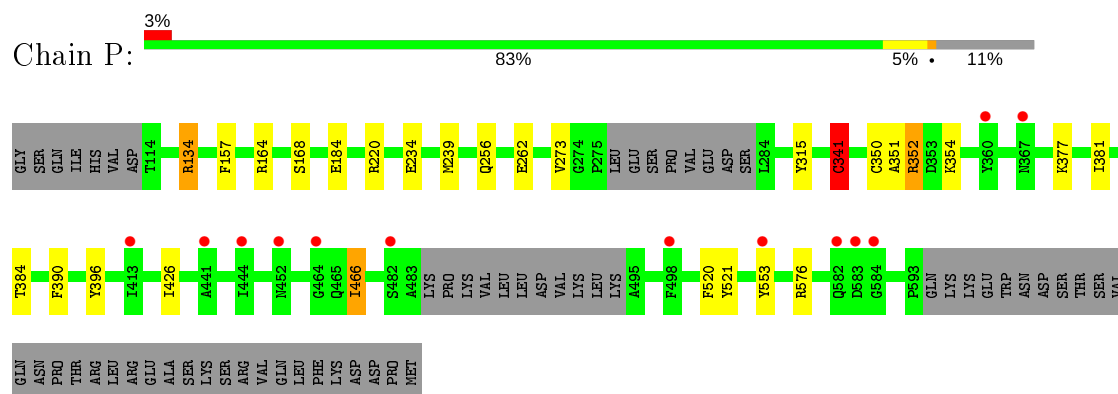
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.11Å 175.24Å 277.27Å 90.00° 94.81° 90.00°	Depositor
Resolution (Å)	276.29 – 2.84 276.29 – 2.82	Depositor EDS
% Data completeness (in resolution range)	72.7 (276.29-2.84) 71.3 (276.29-2.82)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.228 , 0.249 0.227 , 0.247	Depositor DCC
$R_{free}$ test set	8050 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.2	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 22.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	61950	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 0KX, GTP, SO4, DTP, FE

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	0.72	2/3933 (0.1%)	0.89	6/5335 (0.1%)
1	B	0.73	2/3918 (0.1%)	0.92	10/5310 (0.2%)
1	C	0.71	1/3947 (0.0%)	0.89	10/5346 (0.2%)
1	D	0.73	5/3939 (0.1%)	0.95	11/5339 (0.2%)
1	E	0.64	0/3892	0.88	10/5282 (0.2%)
1	F	0.65	0/3784	0.84	4/5129 (0.1%)
1	G	0.63	2/3757 (0.1%)	0.86	5/5099 (0.1%)
1	H	0.67	2/3938 (0.1%)	0.90	3/5333 (0.1%)
1	I	0.66	0/3915	0.86	5/5306 (0.1%)
1	J	0.69	2/3930 (0.1%)	0.93	7/5327 (0.1%)
1	K	0.69	1/3932 (0.0%)	0.88	9/5333 (0.2%)
1	L	0.66	6/3849 (0.2%)	0.90	6/5230 (0.1%)
1	M	0.64	0/3792	0.86	8/5151 (0.2%)
1	N	0.66	2/3849 (0.1%)	0.91	8/5229 (0.2%)
1	O	0.66	0/3769	0.89	8/5116 (0.2%)
1	P	0.68	6/3729 (0.2%)	0.90	6/5064 (0.1%)
All	All	0.68	31/61873 (0.1%)	0.89	116/83929 (0.1%)

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

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

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	341	CYS	CB-SG	8.66	1.97	1.82
1	L	193	GLU	CD-OE2	6.61	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	489	LEU	C-O	-6.56	1.10	1.23
1	K	410	SER	CB-OG	-6.51	1.33	1.42
1	L	275	PRO	C-O	-6.38	1.10	1.23

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	164	ARG	NE-CZ-NH1	23.34	131.97	120.30
1	D	164	ARG	NE-CZ-NH1	23.28	131.94	120.30
1	N	164	ARG	NE-CZ-NH1	22.96	131.78	120.30
1	P	164	ARG	NE-CZ-NH1	22.90	131.75	120.30
1	L	164	ARG	NE-CZ-NH1	22.63	131.61	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	486	LYS	Mainchain

## 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	3840	0	3707	15	0
1	B	3825	0	3715	11	0
1	C	3854	0	3758	17	1
1	D	3846	0	3732	15	0
1	E	3799	0	3656	14	0
1	F	3695	0	3560	12	0
1	G	3668	0	3505	13	0
1	H	3845	0	3751	15	0
1	I	3822	0	3705	13	0
1	J	3837	0	3723	15	0
1	K	3839	0	3704	12	0
1	L	3756	0	3583	12	0
1	M	3704	0	3524	10	0
1	N	3757	0	3573	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	3680	0	3508	12	0
1	P	3640	0	3463	14	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	3	0	0	0	0
3	H	2	0	0	0	0
3	I	3	0	0	0	0
3	J	2	0	0	0	0
3	K	3	0	0	0	0
3	L	3	0	0	0	0
3	M	3	0	0	0	0
3	N	2	0	0	0	0
3	O	2	0	0	0	0
3	P	3	0	0	0	0
4	A	28	0	16	0	0
4	B	28	0	16	1	0
4	C	28	0	16	2	0
4	D	28	0	17	1	0
4	E	28	0	17	1	0
4	F	28	0	17	0	0
4	G	28	0	16	0	0
4	H	28	0	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	28	0	15	0	0
4	J	28	0	17	0	0
4	K	28	0	15	0	0
4	L	28	0	16	2	0
4	M	28	0	17	0	0
4	N	28	0	17	2	0
4	O	28	0	17	0	0
4	P	28	0	16	0	0
5	A	32	0	12	0	0
5	B	32	0	12	0	0
5	C	32	0	12	0	0
5	D	32	0	12	1	0
5	E	32	0	12	1	0
5	F	32	0	12	1	0
5	G	32	0	12	1	0
5	H	32	0	12	0	0
5	I	32	0	12	0	0
5	J	32	0	12	1	0
5	K	32	0	12	0	0
5	L	32	0	12	0	0
5	M	32	0	12	0	0
5	N	32	0	12	1	0
5	O	64	0	24	2	0
6	A	5	0	0	1	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	1	0
6	H	5	0	0	1	0
6	I	5	0	0	0	0
6	J	5	0	0	0	0
6	L	5	0	0	0	0
6	M	5	0	0	0	0
7	A	30	0	12	0	0
7	B	30	0	12	2	0
7	C	30	0	12	1	0
7	D	30	0	12	1	0
7	E	30	0	12	3	0
7	F	30	0	12	2	0
7	G	30	0	12	2	0
7	H	30	0	12	2	0
7	I	30	0	12	0	0
7	J	30	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	K	30	0	12	2	0
7	L	30	0	12	1	0
7	M	30	0	12	4	0
7	N	30	0	12	1	0
7	O	30	0	12	1	0
7	P	30	0	12	2	0
All	All	61950	0	58812	213	1

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 213 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:352:ARG:NH1	7:N:706:DTP:O3G	2.20	0.71
1:M:352:ARG:NH1	7:M:708:DTP:O3G	2.21	0.70
7:E:706:DTP:O2G	5:G:707:GTP:O1B	2.13	0.67
1:I:595:LYS:HZ2	1:I:597:GLU:HG2	1.62	0.65
7:M:708:DTP:O1B	5:O:706:GTP:H5"	1.97	0.64

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:472:ASP:OD1	1:P:396:TYR:OH[1_565]	1.97	0.23

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	477/520 (92%)	463 (97%)	13 (3%)	1 (0%)	47 69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	474/520 (91%)	459 (97%)	14 (3%)	1 (0%)	47	69
1	C	476/520 (92%)	462 (97%)	14 (3%)	0	100	100
1	D	477/520 (92%)	462 (97%)	15 (3%)	0	100	100
1	E	474/520 (91%)	457 (96%)	17 (4%)	0	100	100
1	F	457/520 (88%)	443 (97%)	14 (3%)	0	100	100
1	G	457/520 (88%)	442 (97%)	15 (3%)	0	100	100
1	H	474/520 (91%)	458 (97%)	16 (3%)	0	100	100
1	I	473/520 (91%)	460 (97%)	13 (3%)	0	100	100
1	J	475/520 (91%)	459 (97%)	16 (3%)	0	100	100
1	K	476/520 (92%)	460 (97%)	16 (3%)	0	100	100
1	L	471/520 (91%)	455 (97%)	16 (3%)	0	100	100
1	M	467/520 (90%)	453 (97%)	14 (3%)	0	100	100
1	N	471/520 (91%)	457 (97%)	14 (3%)	0	100	100
1	O	459/520 (88%)	441 (96%)	17 (4%)	1 (0%)	47	69
1	P	455/520 (88%)	441 (97%)	14 (3%)	0	100	100
All	All	7513/8320 (90%)	7272 (97%)	238 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	283	SER
1	A	486	LYS
1	B	486	LYS

### 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	406/464 (88%)	394 (97%)	12 (3%)	41	65
1	B	404/464 (87%)	395 (98%)	9 (2%)	52	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	409/464 (88%)	399 (98%)	10 (2%)	49	72
1	D	407/464 (88%)	397 (98%)	10 (2%)	47	71
1	E	398/464 (86%)	390 (98%)	8 (2%)	55	76
1	F	390/464 (84%)	381 (98%)	9 (2%)	50	73
1	G	384/464 (83%)	378 (98%)	6 (2%)	62	81
1	H	409/464 (88%)	401 (98%)	8 (2%)	55	76
1	I	404/464 (87%)	397 (98%)	7 (2%)	60	80
1	J	406/464 (88%)	398 (98%)	8 (2%)	55	76
1	K	406/464 (88%)	393 (97%)	13 (3%)	39	63
1	L	391/464 (84%)	383 (98%)	8 (2%)	55	76
1	M	384/464 (83%)	374 (97%)	10 (3%)	46	70
1	N	391/464 (84%)	384 (98%)	7 (2%)	59	78
1	O	385/464 (83%)	376 (98%)	9 (2%)	50	73
1	P	380/464 (82%)	373 (98%)	7 (2%)	59	78
All	All	6354/7424 (86%)	6213 (98%)	141 (2%)	52	75

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	576	ARG
1	I	576	ARG
1	O	339	ARG
1	H	315	TYR
1	H	576	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	375	GLN
1	I	380	ASN
1	O	380	ASN
1	G	380	ASN
1	H	380	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 115 ligands modelled in this entry, 58 are monoatomic - leaving 57 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
5	GTP	M	706	3	26,34,34	0.95	1 (3%)	33,54,54	2.32	10 (30%)
5	GTP	C	707	3	26,34,34	1.04	1 (3%)	33,54,54	2.21	9 (27%)
6	SO4	L	708	-	4,4,4	0.62	0	6,6,6	0.70	0
7	DTP	H	701	3	26,32,32	1.25	2 (7%)	30,50,50	1.68	8 (26%)
7	DTP	G	701	3	26,32,32	0.94	0	30,50,50	1.56	7 (23%)
5	GTP	A	706	3	26,34,34	1.06	2 (7%)	33,54,54	1.96	13 (39%)
7	DTP	F	706	3	26,32,32	1.09	2 (7%)	30,50,50	1.53	7 (23%)
7	DTP	P	701	3	26,32,32	1.14	3 (11%)	30,50,50	1.35	4 (13%)
4	OKX	G	706	3,2	26,29,29	1.36	3 (11%)	33,45,45	2.08	8 (24%)
7	DTP	B	708	3	26,32,32	1.35	4 (15%)	30,50,50	1.77	9 (30%)
7	DTP	E	706	3	26,32,32	1.12	3 (11%)	30,50,50	1.23	3 (10%)
7	DTP	I	708	3	26,32,32	0.84	0	30,50,50	1.66	9 (30%)
7	DTP	D	701	3	26,32,32	1.14	4 (15%)	30,50,50	1.47	4 (13%)
4	OKX	A	705	3,2	26,29,29	1.18	3 (11%)	33,45,45	1.76	6 (18%)
6	SO4	C	708	-	4,4,4	0.70	0	6,6,6	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	DTP	N	706	3	26,32,32	1.06	2 (7%)	30,50,50	1.47	5 (16%)
6	SO4	H	707	-	4,4,4	0.45	0	6,6,6	0.51	0
4	OKX	E	704	3,2	26,29,29	1.46	4 (15%)	33,45,45	1.52	3 (9%)
6	SO4	B	707	-	4,4,4	0.59	0	6,6,6	0.87	0
4	OKX	P	706	3,2	26,29,29	1.54	4 (15%)	33,45,45	1.55	5 (15%)
5	GTP	G	707	3	26,34,34	1.15	3 (11%)	33,54,54	2.06	8 (24%)
5	GTP	B	706	3	26,34,34	1.26	2 (7%)	33,54,54	2.39	12 (36%)
4	OKX	K	706	3,2	26,29,29	1.29	3 (11%)	33,45,45	1.96	8 (24%)
4	OKX	J	704	3,2	26,29,29	1.32	3 (11%)	33,45,45	1.69	7 (21%)
7	DTP	O	701	3	26,32,32	0.96	1 (3%)	30,50,50	1.63	8 (26%)
6	SO4	A	707	-	4,4,4	0.47	0	6,6,6	0.98	1 (16%)
6	SO4	D	708	-	4,4,4	0.53	0	6,6,6	0.27	0
6	SO4	M	707	-	4,4,4	0.47	0	6,6,6	0.18	0
5	GTP	K	707	3	26,34,34	1.04	2 (7%)	33,54,54	2.35	11 (33%)
7	DTP	K	701	3	26,32,32	0.89	1 (3%)	30,50,50	1.62	8 (26%)
5	GTP	F	705	3	26,34,34	1.19	2 (7%)	33,54,54	2.25	11 (33%)
4	OKX	I	705	3,2	26,29,29	1.19	3 (11%)	33,45,45	1.89	5 (15%)
4	OKX	O	705	3,2	26,29,29	1.28	3 (11%)	33,45,45	1.52	5 (15%)
5	GTP	I	706	3	26,34,34	1.23	2 (7%)	33,54,54	2.57	12 (36%)
5	GTP	H	706	3	26,34,34	1.41	2 (7%)	33,54,54	2.02	10 (30%)
6	SO4	I	707	-	4,4,4	0.43	0	6,6,6	0.81	0
4	OKX	L	706	3,2	26,29,29	1.55	3 (11%)	33,45,45	1.83	6 (18%)
5	GTP	E	705	3	26,34,34	1.17	2 (7%)	33,54,54	2.44	11 (33%)
4	OKX	F	704	3,2	26,29,29	1.16	3 (11%)	33,45,45	2.00	6 (18%)
4	OKX	C	706	3	26,29,29	1.22	3 (11%)	33,45,45	1.61	4 (12%)
5	GTP	N	705	3	26,34,34	1.06	2 (7%)	33,54,54	2.26	10 (30%)
5	GTP	O	707	3	26,34,34	0.97	2 (7%)	33,54,54	2.18	13 (39%)
7	DTP	J	707	3	26,32,32	1.11	1 (3%)	30,50,50	1.99	8 (26%)
5	GTP	J	705	3	26,34,34	1.26	4 (15%)	33,54,54	1.63	7 (21%)
5	GTP	O	706	3	26,34,34	1.22	2 (7%)	33,54,54	2.34	12 (36%)
7	DTP	A	708	3	26,32,32	0.82	1 (3%)	30,50,50	1.48	5 (16%)
4	OKX	D	706	3,2	26,29,29	1.55	5 (19%)	33,45,45	2.02	7 (21%)
6	SO4	J	706	-	4,4,4	0.64	0	6,6,6	0.45	0
7	DTP	M	708	3	26,32,32	1.12	3 (11%)	30,50,50	1.27	4 (13%)
7	DTP	L	701	3	26,32,32	1.12	3 (11%)	30,50,50	2.01	7 (23%)
5	GTP	D	707	3	26,34,34	1.19	4 (15%)	33,54,54	1.62	9 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	0KX	H	705	3,2	26,29,29	1.11	3 (11%)	33,45,45	1.57	6 (18%)
5	GTP	L	707	3	26,34,34	1.23	3 (11%)	33,54,54	2.13	10 (30%)
4	0KX	B	705	3,2	26,29,29	1.60	6 (23%)	33,45,45	2.06	8 (24%)
4	0KX	N	704	3,2	26,29,29	1.28	3 (11%)	33,45,45	1.63	5 (15%)
4	0KX	M	705	3,2	26,29,29	1.24	3 (11%)	33,45,45	1.79	7 (21%)
7	DTP	C	701	3	26,32,32	0.86	1 (3%)	30,50,50	2.02	12 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	M	706	3	-	1/18/38/38	0/3/3/3
5	GTP	C	707	3	-	4/18/38/38	0/3/3/3
7	DTP	H	701	3	-	6/18/34/34	0/3/3/3
7	DTP	G	701	3	-	1/18/34/34	0/3/3/3
5	GTP	A	706	3	-	1/18/38/38	0/3/3/3
7	DTP	P	701	3	-	1/18/34/34	0/3/3/3
4	0KX	G	706	3,2	-	6/16/34/34	0/2/2/2
7	DTP	B	708	3	-	2/18/34/34	0/3/3/3
7	DTP	E	706	3	-	2/18/34/34	0/3/3/3
7	DTP	I	708	3	-	5/18/34/34	0/3/3/3
7	DTP	D	701	3	-	3/18/34/34	0/3/3/3
4	0KX	A	705	3,2	-	2/16/34/34	0/2/2/2
7	DTP	N	706	3	-	2/18/34/34	0/3/3/3
5	GTP	G	707	3	-	2/18/38/38	0/3/3/3
4	0KX	E	704	3,2	-	5/16/34/34	0/2/2/2
4	0KX	H	705	3,2	-	4/16/34/34	0/2/2/2
4	0KX	P	706	3,2	-	7/16/34/34	0/2/2/2
5	GTP	B	706	3	-	4/18/38/38	0/3/3/3
4	0KX	K	706	3,2	-	3/16/34/34	0/2/2/2
4	0KX	J	704	3,2	-	2/16/34/34	0/2/2/2
7	DTP	O	701	3	-	5/18/34/34	0/3/3/3
5	GTP	N	705	3	-	3/18/38/38	0/3/3/3
5	GTP	K	707	3	-	2/18/38/38	0/3/3/3
7	DTP	K	701	3	-	0/18/34/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	F	705	3	-	0/18/38/38	0/3/3/3
4	0KX	I	705	3,2	-	4/16/34/34	0/2/2/2
4	0KX	O	705	3,2	-	3/16/34/34	0/2/2/2
5	GTP	I	706	3	-	2/18/38/38	0/3/3/3
5	GTP	H	706	3	-	1/18/38/38	0/3/3/3
4	0KX	L	706	3,2	-	5/16/34/34	0/2/2/2
5	GTP	E	705	3	-	1/18/38/38	0/3/3/3
4	0KX	F	704	3,2	-	6/16/34/34	0/2/2/2
4	0KX	C	706	3	-	3/16/34/34	0/2/2/2
5	GTP	O	707	3	-	2/18/38/38	0/3/3/3
7	DTP	J	707	3	-	4/18/34/34	0/3/3/3
5	GTP	J	705	3	-	0/18/38/38	0/3/3/3
5	GTP	O	706	3	-	3/18/38/38	0/3/3/3
7	DTP	A	708	3	-	4/18/34/34	0/3/3/3
4	0KX	D	706	3,2	-	5/16/34/34	0/2/2/2
5	GTP	L	707	3	-	2/18/38/38	0/3/3/3
7	DTP	M	708	3	-	2/18/34/34	0/3/3/3
7	DTP	L	701	3	-	3/18/34/34	0/3/3/3
5	GTP	D	707	3	-	2/18/38/38	0/3/3/3
7	DTP	F	706	3	-	0/18/34/34	0/3/3/3
4	0KX	B	705	3,2	-	5/16/34/34	0/2/2/2
4	0KX	N	704	3,2	-	2/16/34/34	0/2/2/2
4	0KX	M	705	3,2	-	1/16/34/34	0/2/2/2
7	DTP	C	701	3	-	4/18/34/34	0/3/3/3

The worst 5 of 122 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	705	0KX	PB-O2B	5.22	1.54	1.46
4	L	706	0KX	PB-O2B	4.96	1.54	1.46
4	D	706	0KX	PB-O2B	4.66	1.53	1.46
4	P	706	0KX	PB-O2B	4.65	1.53	1.46
5	O	706	GTP	C6-C5	4.42	1.49	1.41

The worst 5 of 373 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	705	0KX	O2B-PB-N3A	-7.11	101.30	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	701	DTP	C4-C5-N7	-6.77	102.34	109.40
5	M	706	GTP	C2-N3-C4	6.54	122.82	115.36
4	B	705	OKX	O1B-PB-O2B	6.53	123.61	109.92
5	I	706	GTP	C6-C5-C4	-6.50	114.59	120.80

There are no chirality outliers.

5 of 137 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	705	OKX	PG-O3B-PB-O1B
4	A	705	OKX	PG-O3B-PB-O2B
4	I	705	OKX	PA-N3A-PB-O3B
4	I	705	OKX	PB-N3A-PA-O1A
4	I	705	OKX	O4'-C1'-N1-C6

There are no ring outliers.

32 monomers are involved in 42 short contacts:

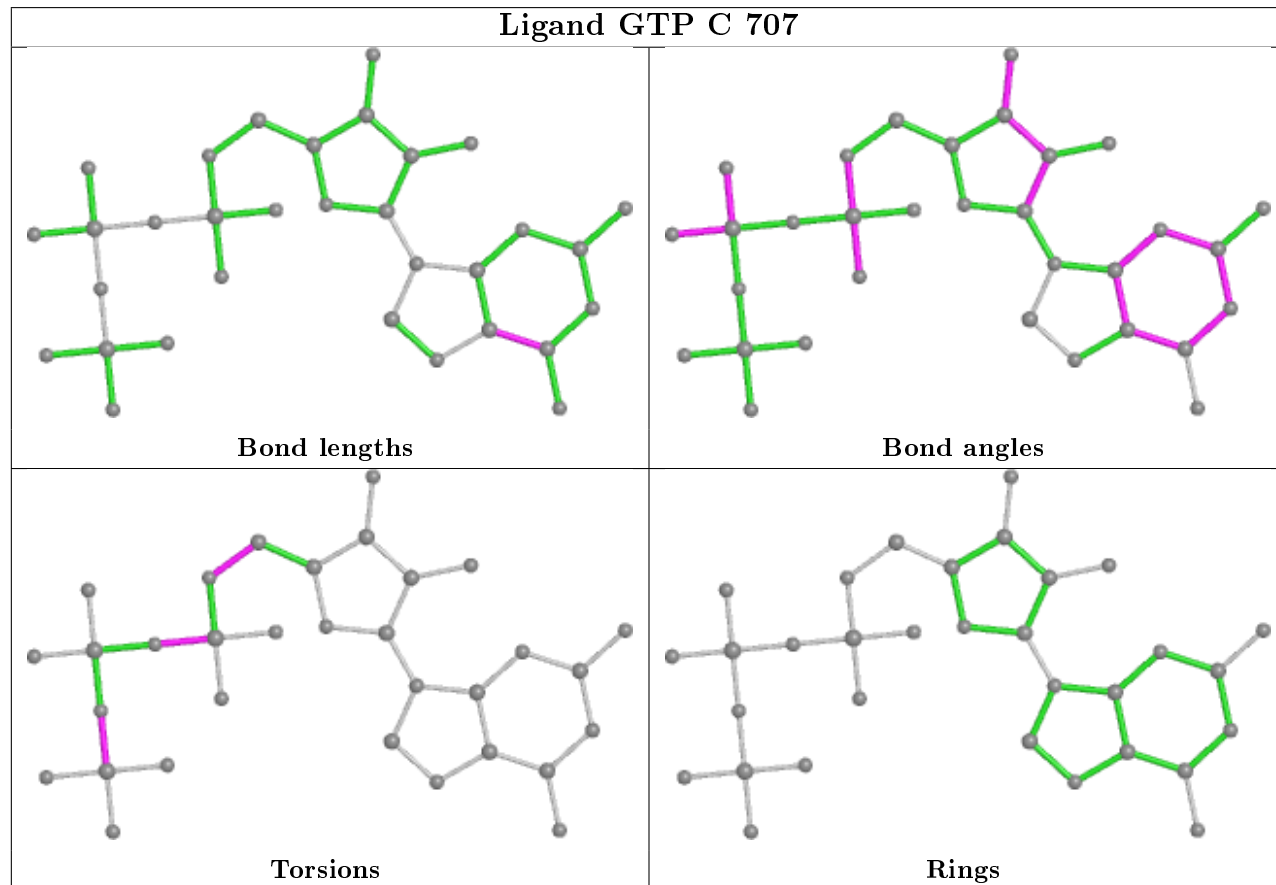
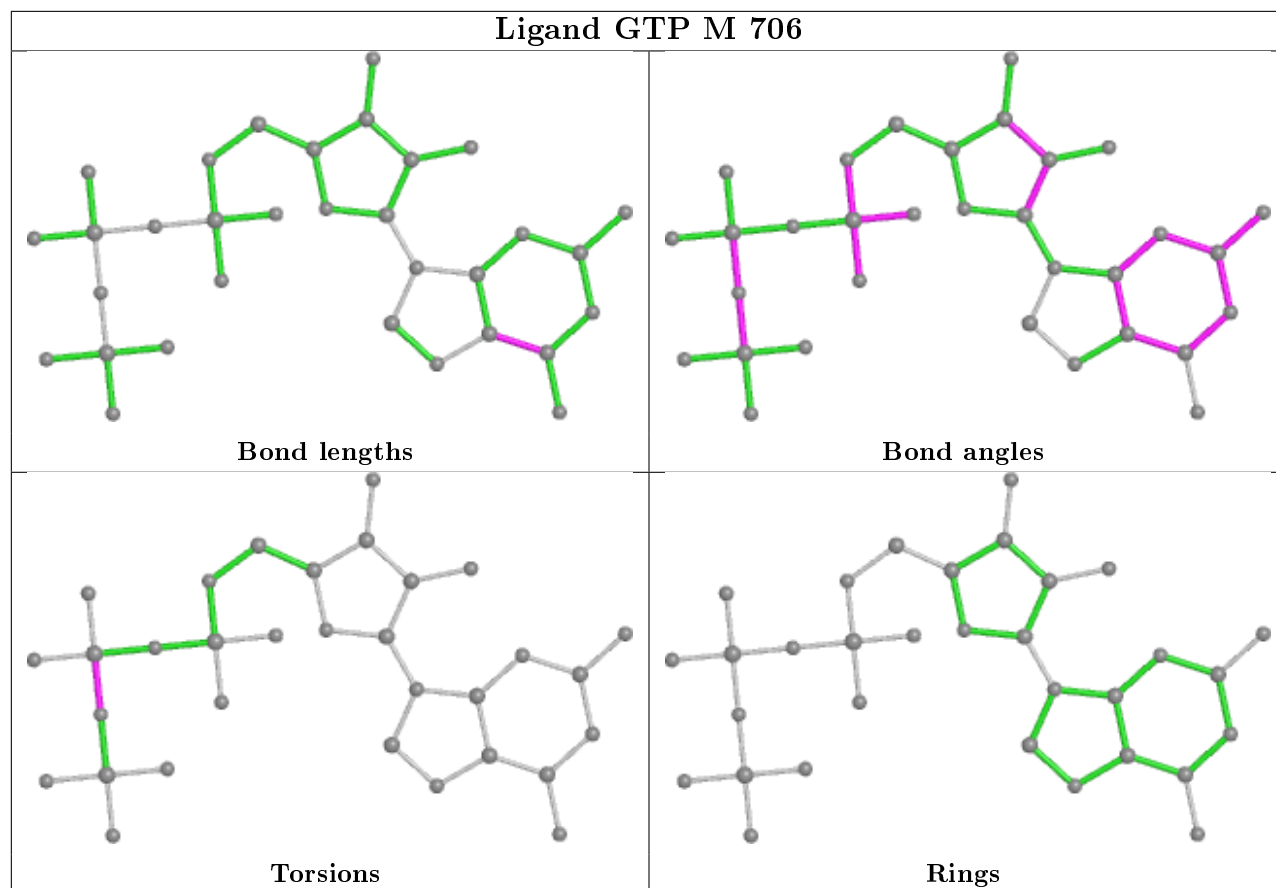
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	701	DTP	2	0
7	G	701	DTP	2	0
7	F	706	DTP	2	0
7	P	701	DTP	2	0
7	B	708	DTP	2	0
7	E	706	DTP	3	0
7	D	701	DTP	1	0
7	N	706	DTP	1	0
6	H	707	SO4	1	0
4	E	704	OKX	1	0
5	G	707	GTP	1	0
7	O	701	DTP	1	0
6	A	707	SO4	1	0
6	D	708	SO4	1	0
7	K	701	DTP	2	0
5	F	705	GTP	1	0
4	L	706	OKX	2	0
5	E	705	GTP	1	0
4	C	706	OKX	2	0
5	N	705	GTP	1	0
5	O	707	GTP	1	0
7	J	707	DTP	1	0

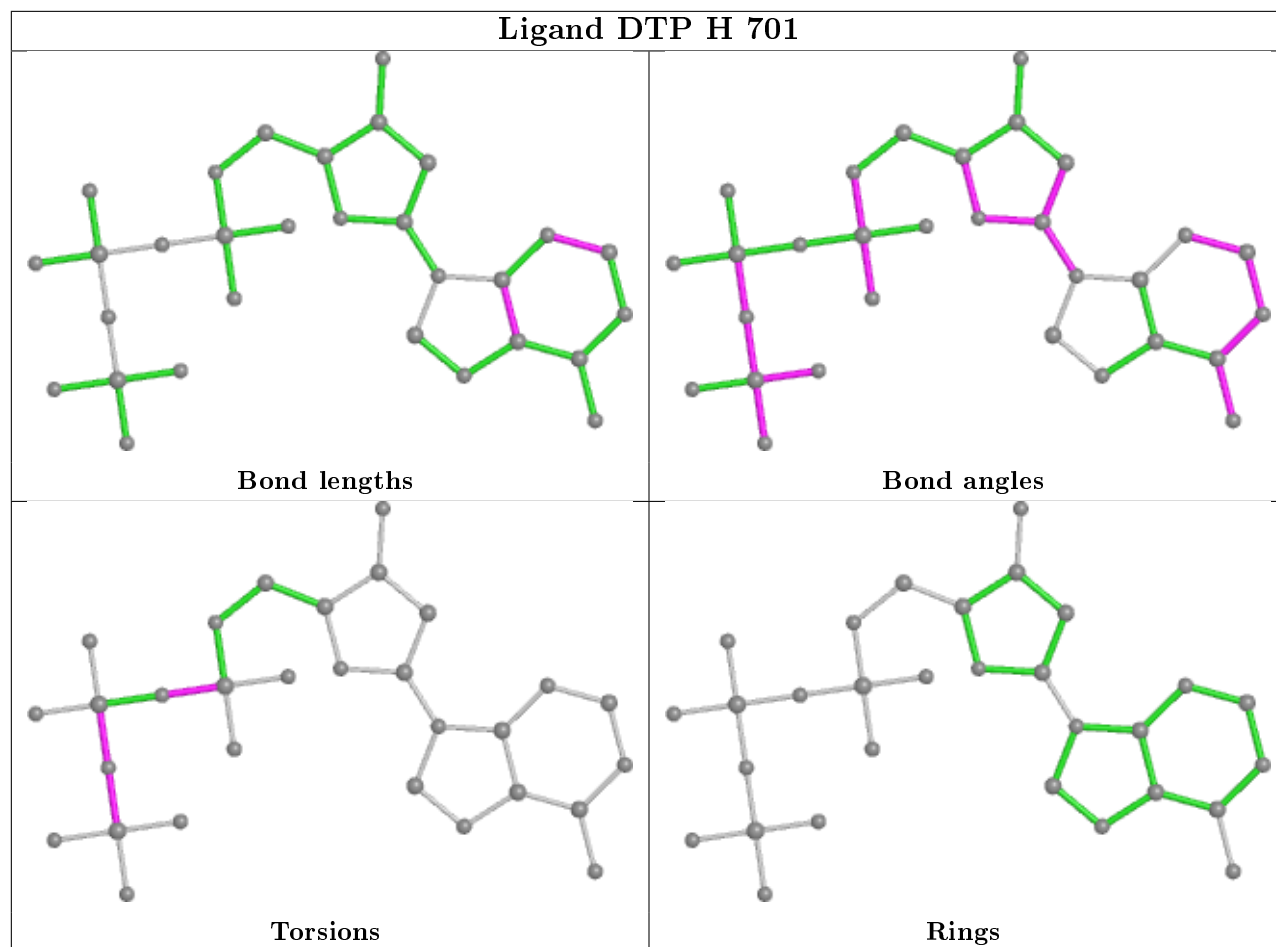
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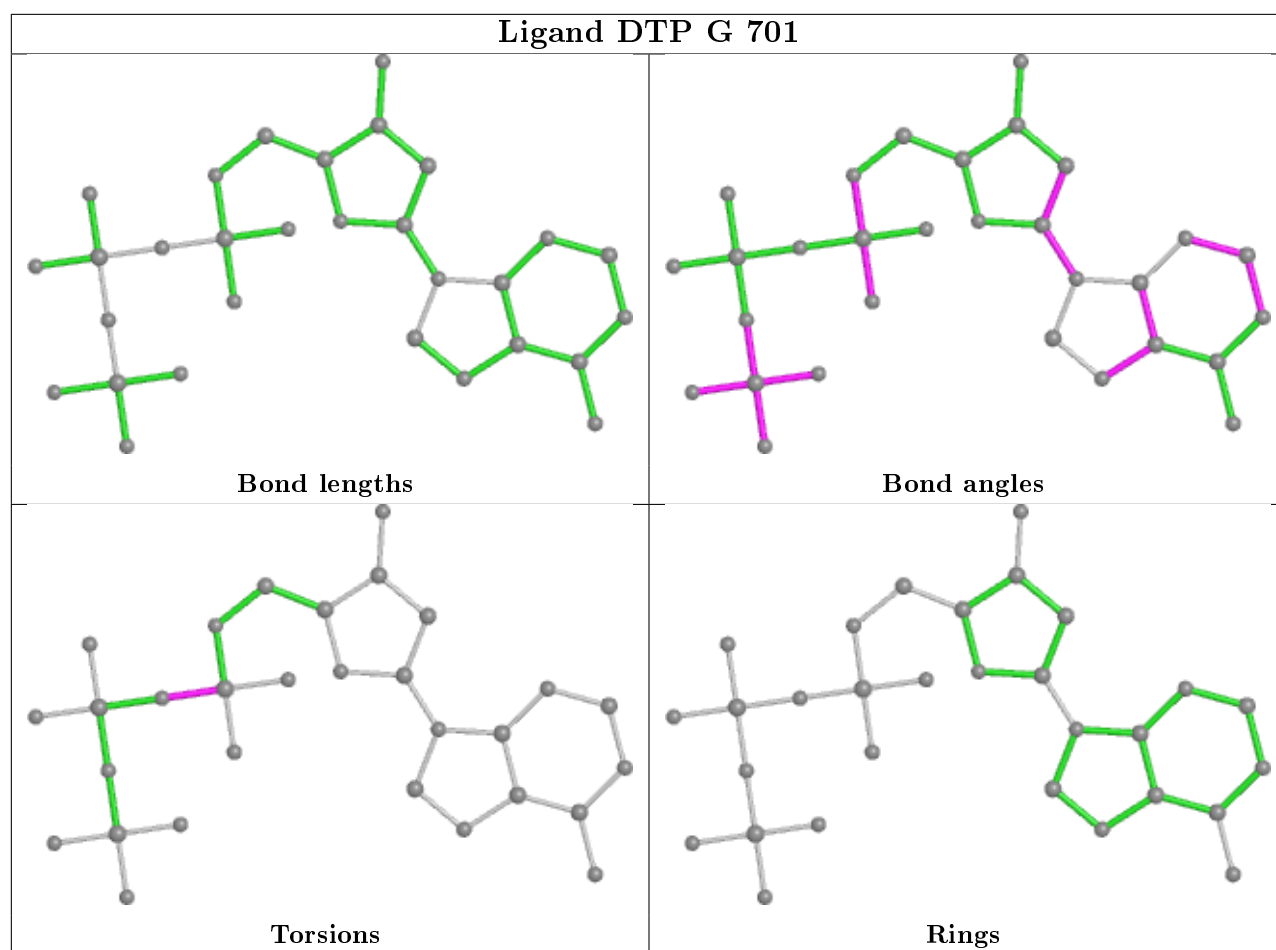
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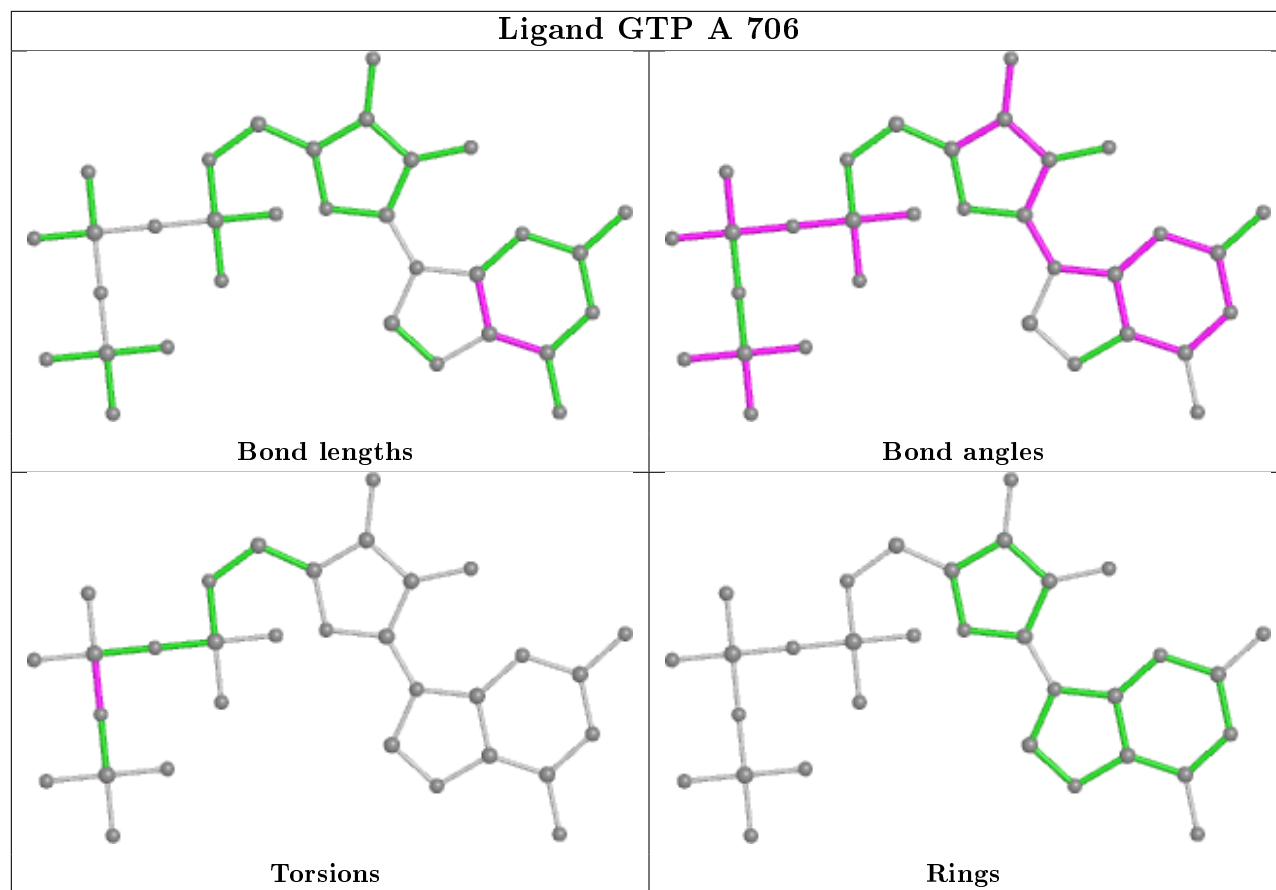
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	705	GTP	1	0
5	O	706	GTP	1	0
4	D	706	0KX	1	0
7	M	708	DTP	4	0
7	L	701	DTP	1	0
5	D	707	GTP	1	0
4	H	705	0KX	1	0
4	B	705	0KX	1	0
4	N	704	0KX	2	0
7	C	701	DTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

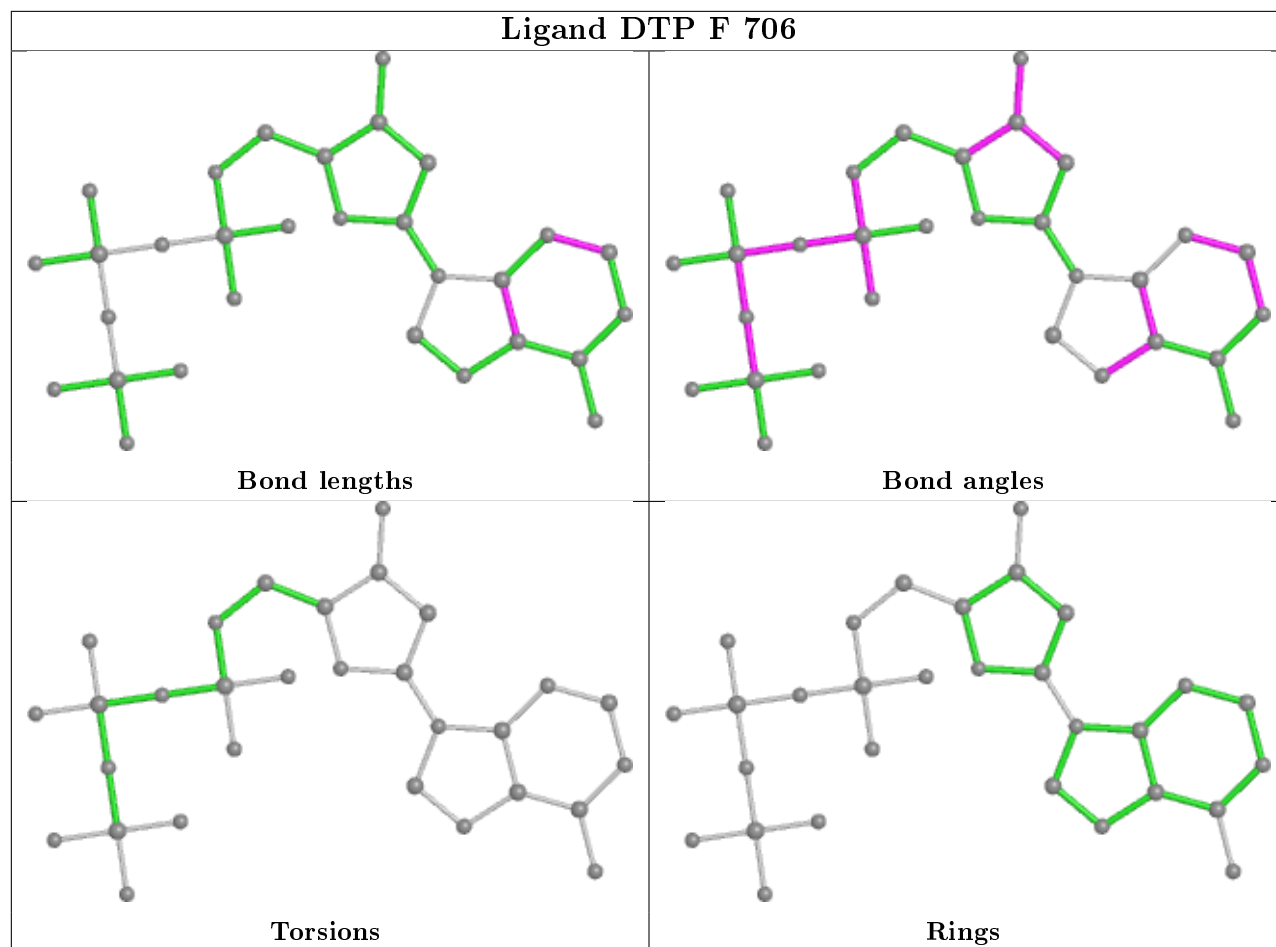




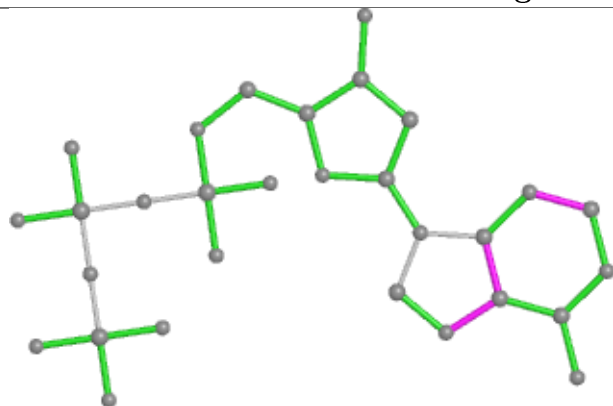




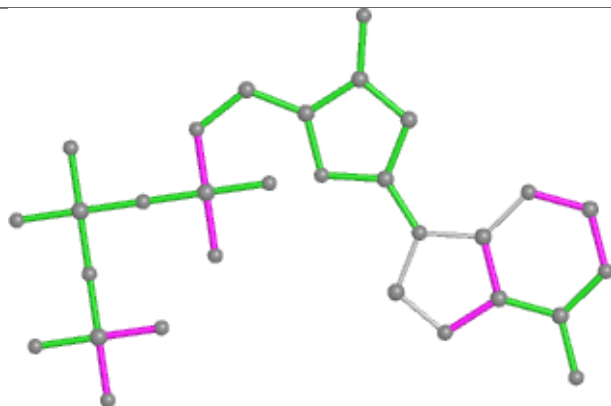
## Ligand DTP F 706



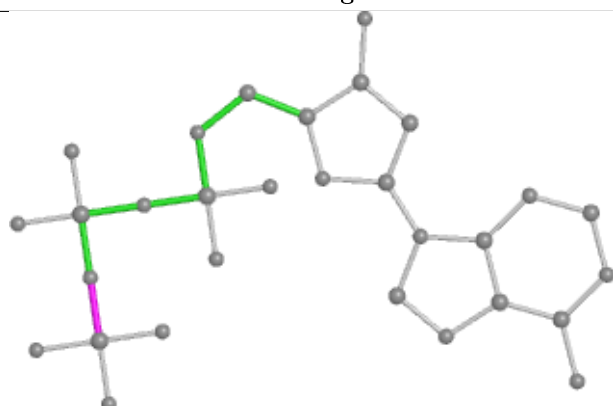
## Ligand DTP P 701



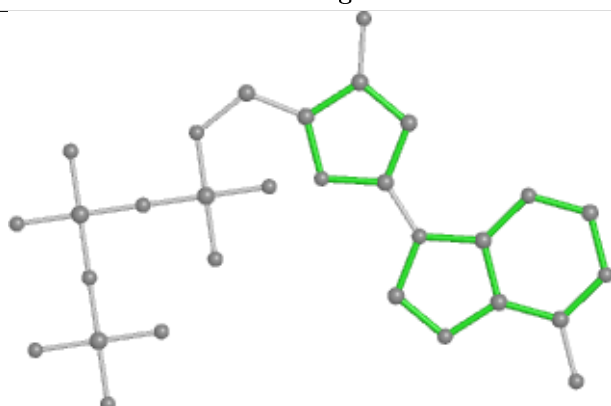
Bond lengths



Bond angles

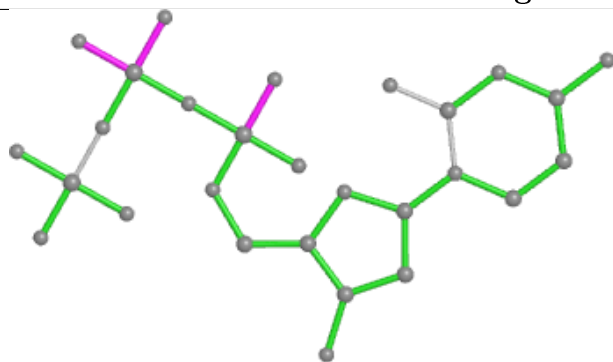


Torsions

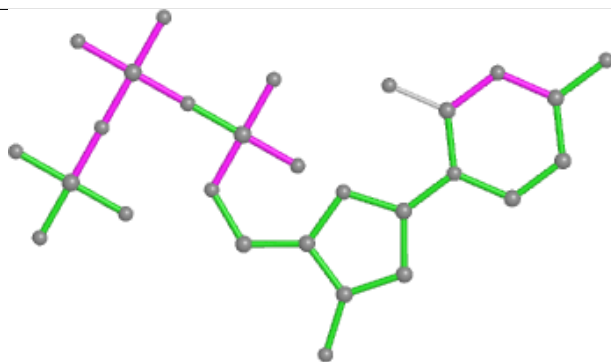


Rings

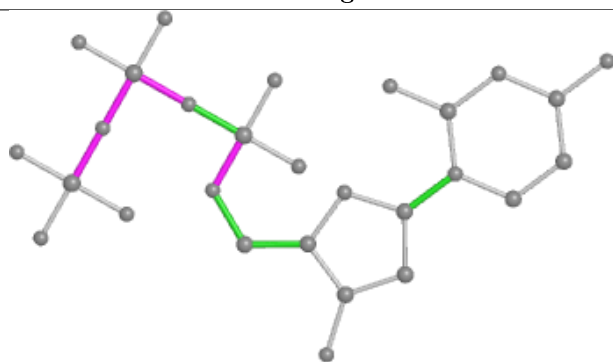
## Ligand 0KX G 706



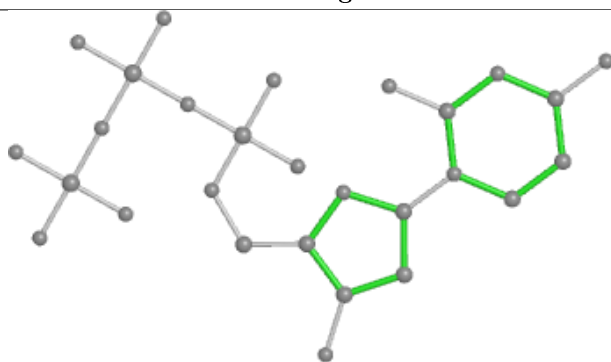
Bond lengths



Bond angles

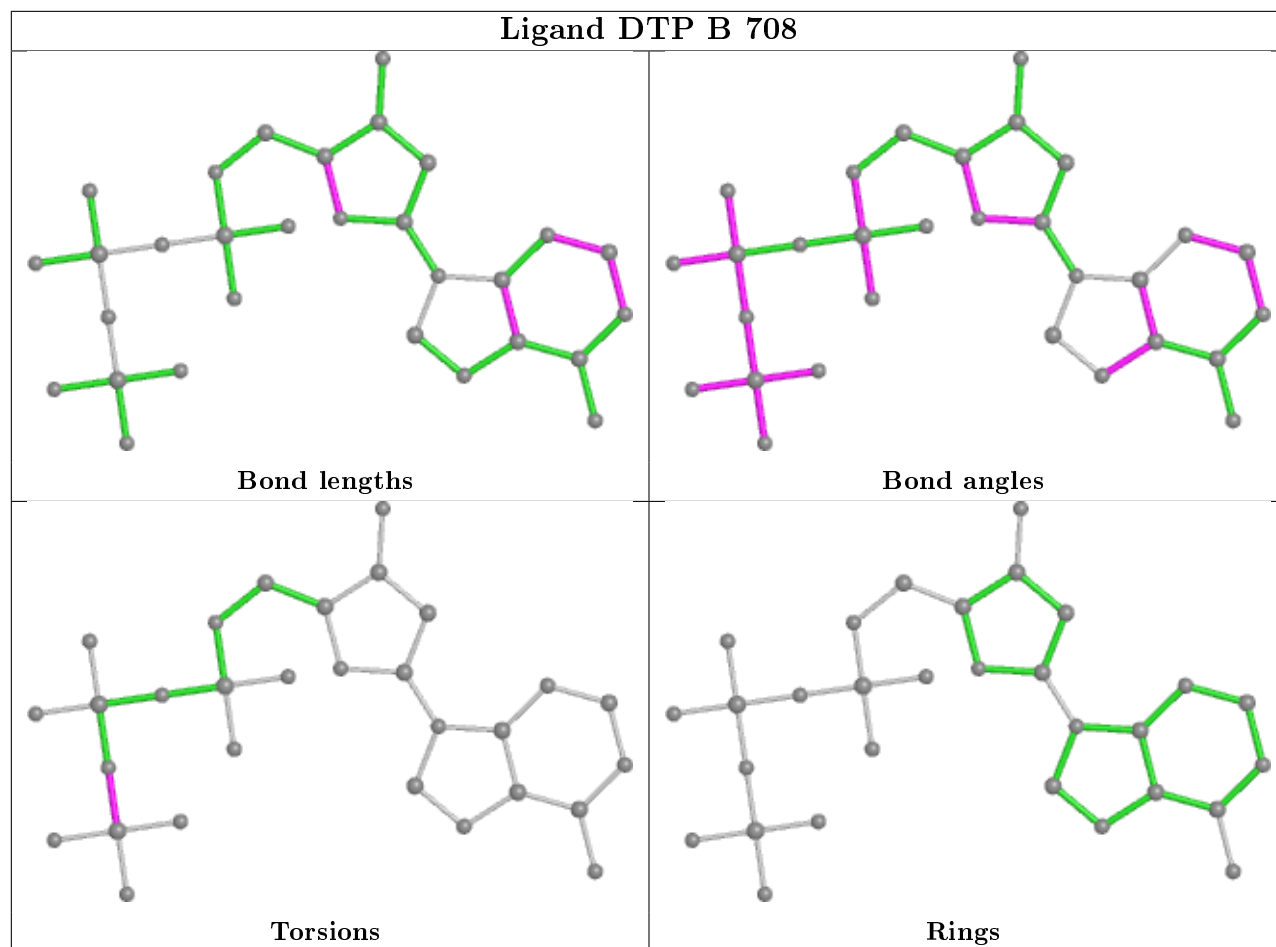


Torsions

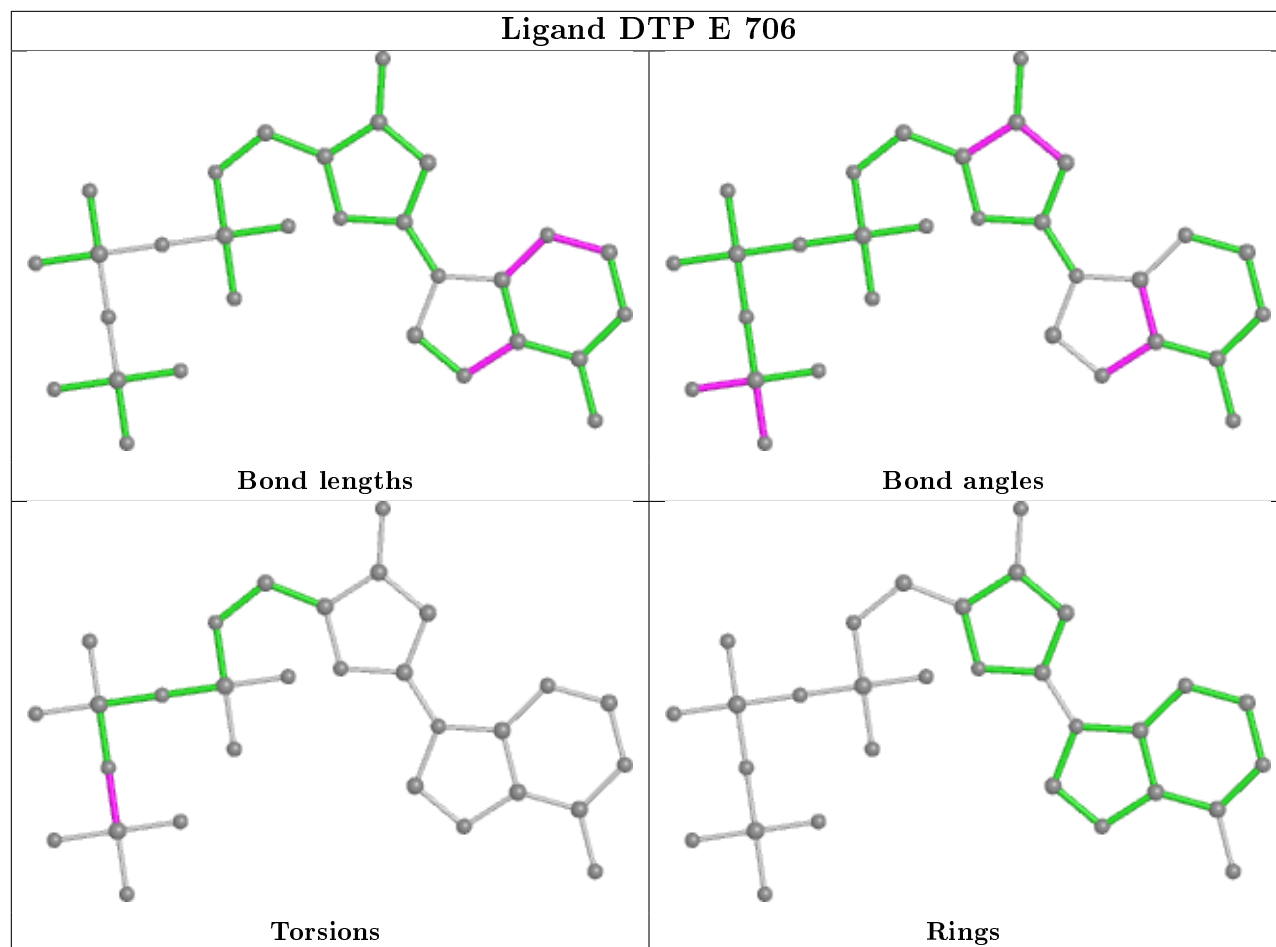


Rings

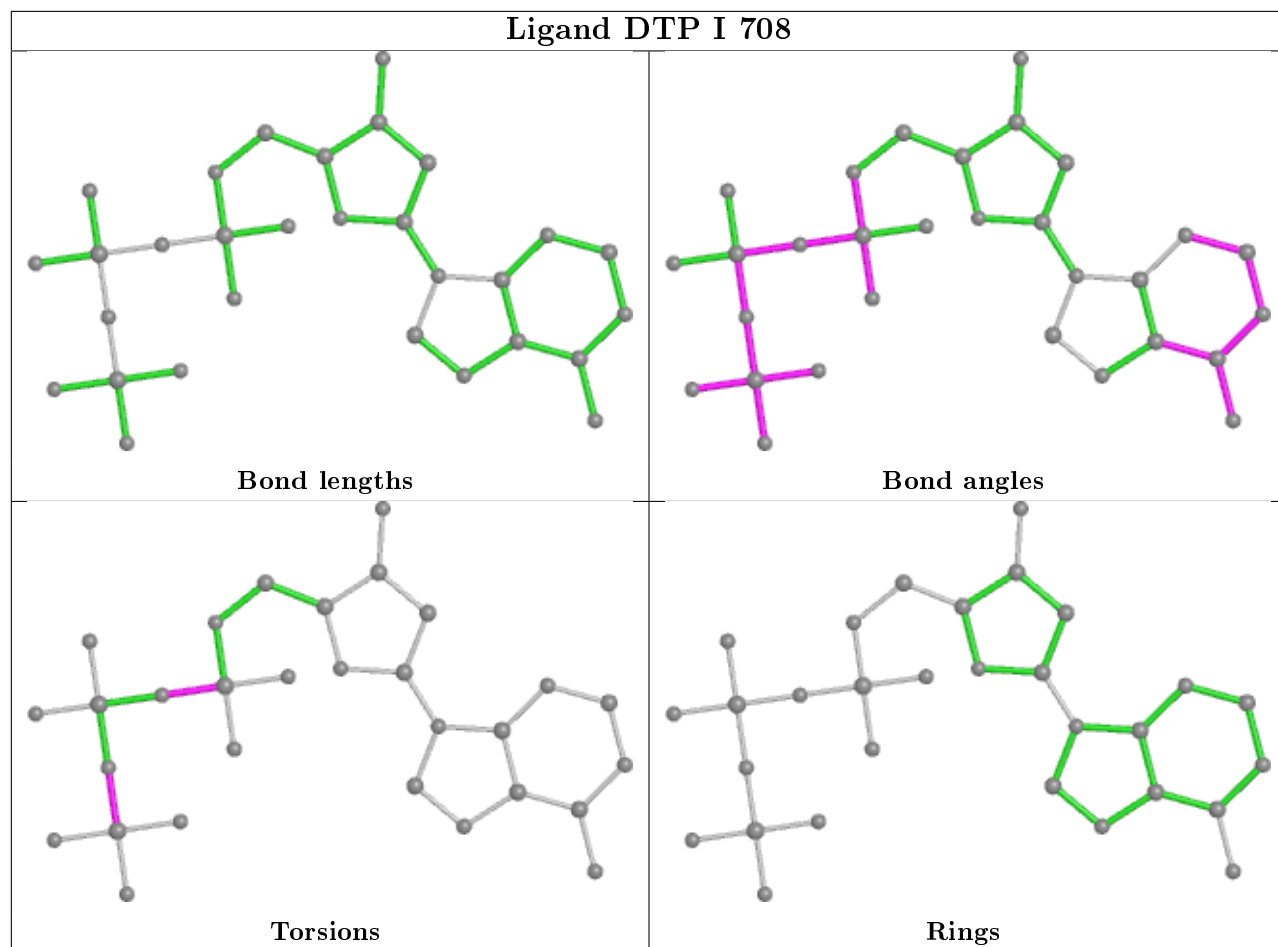


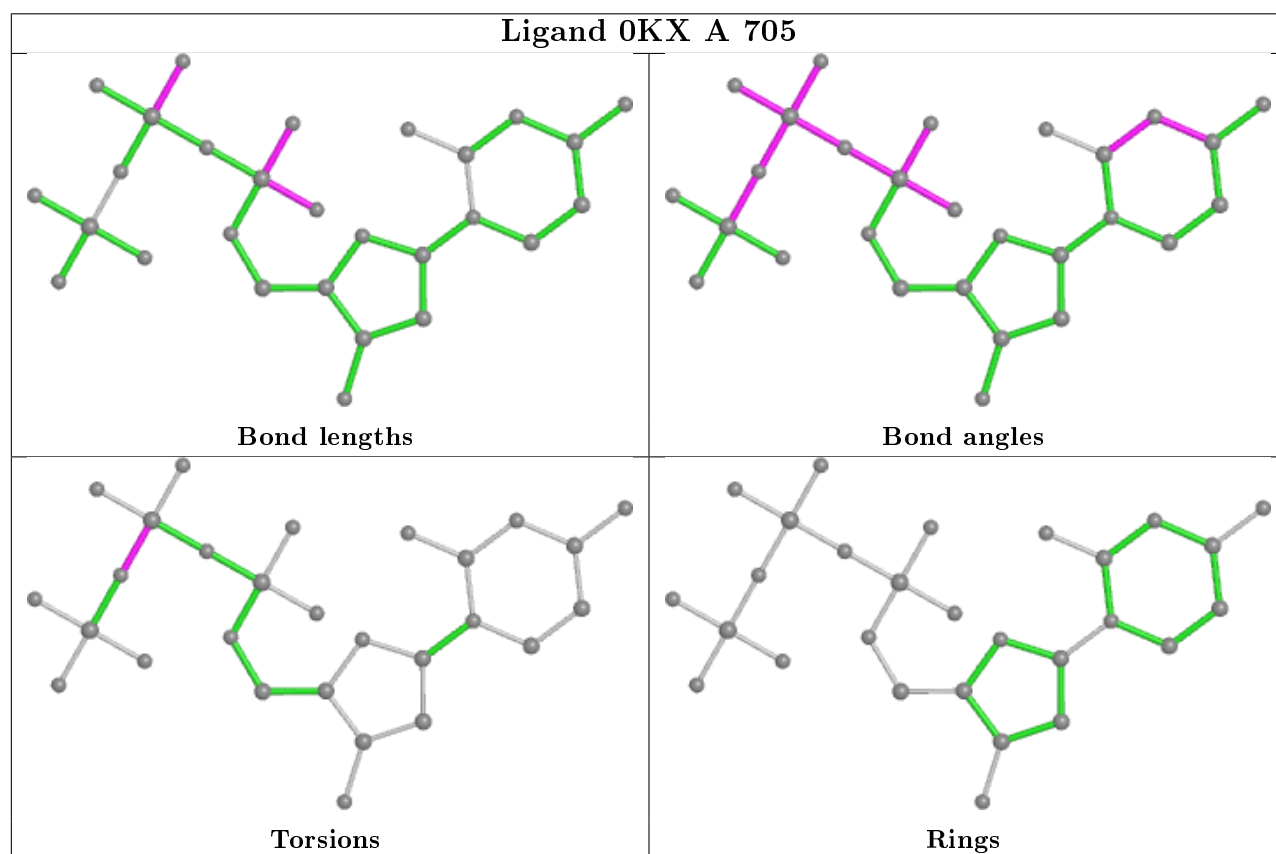
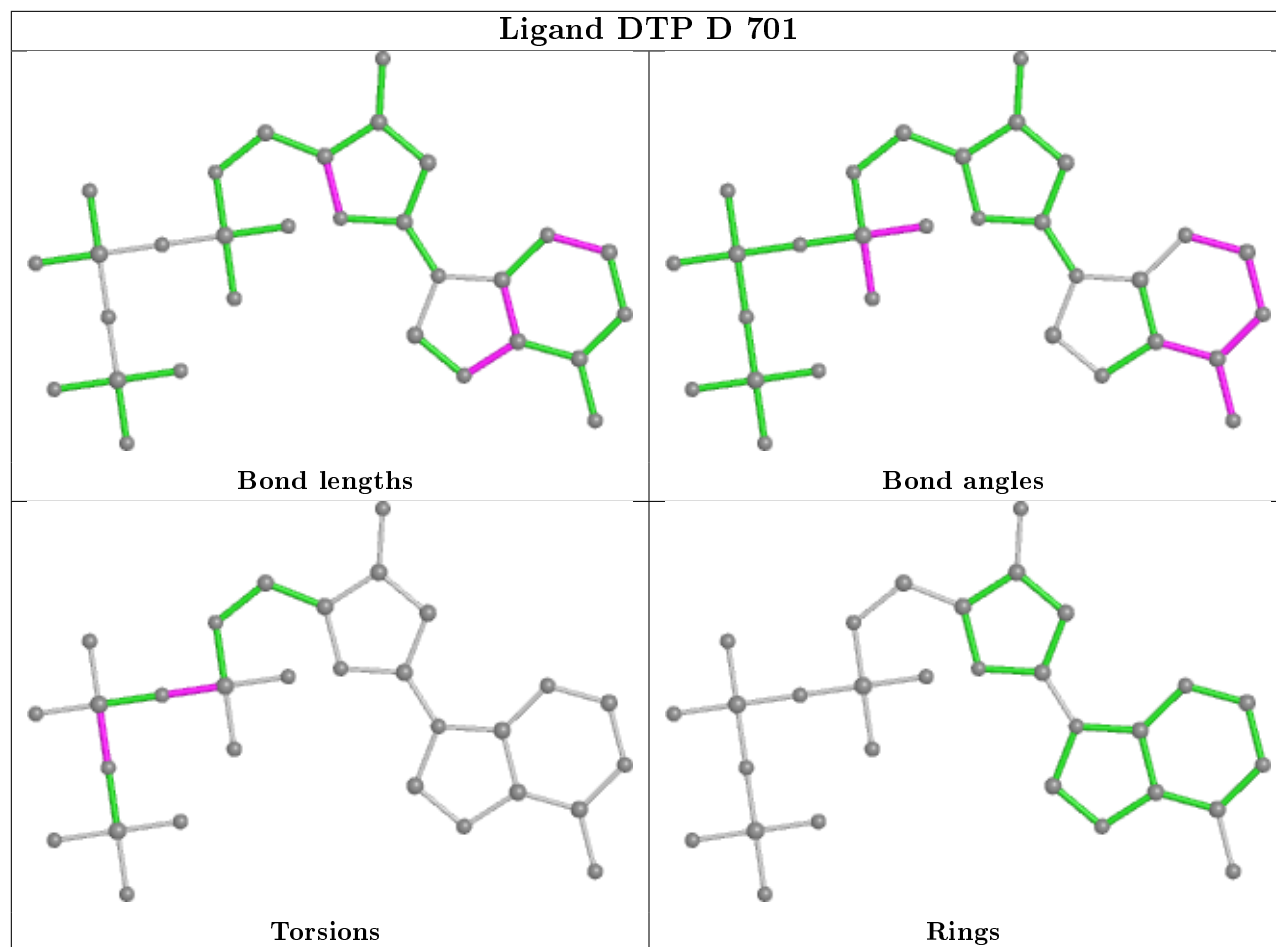


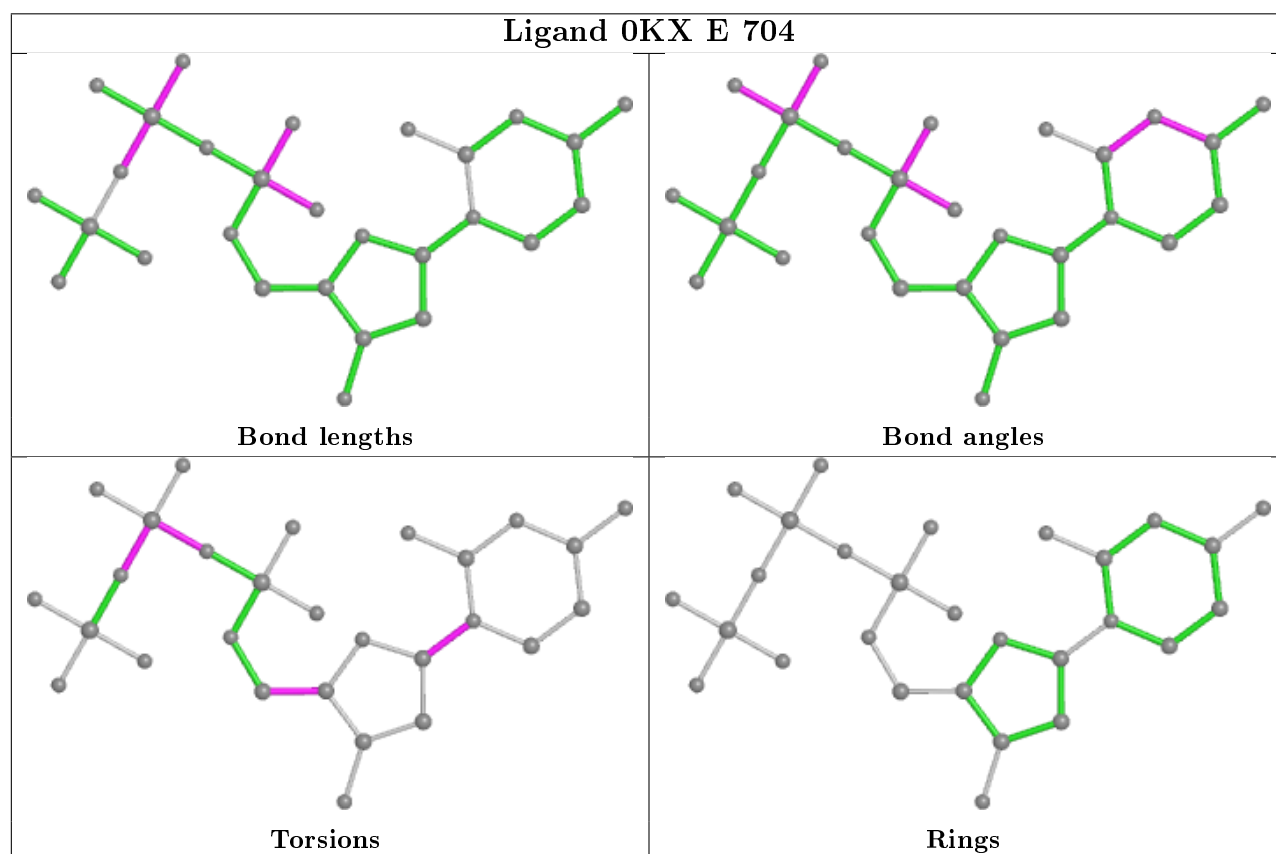
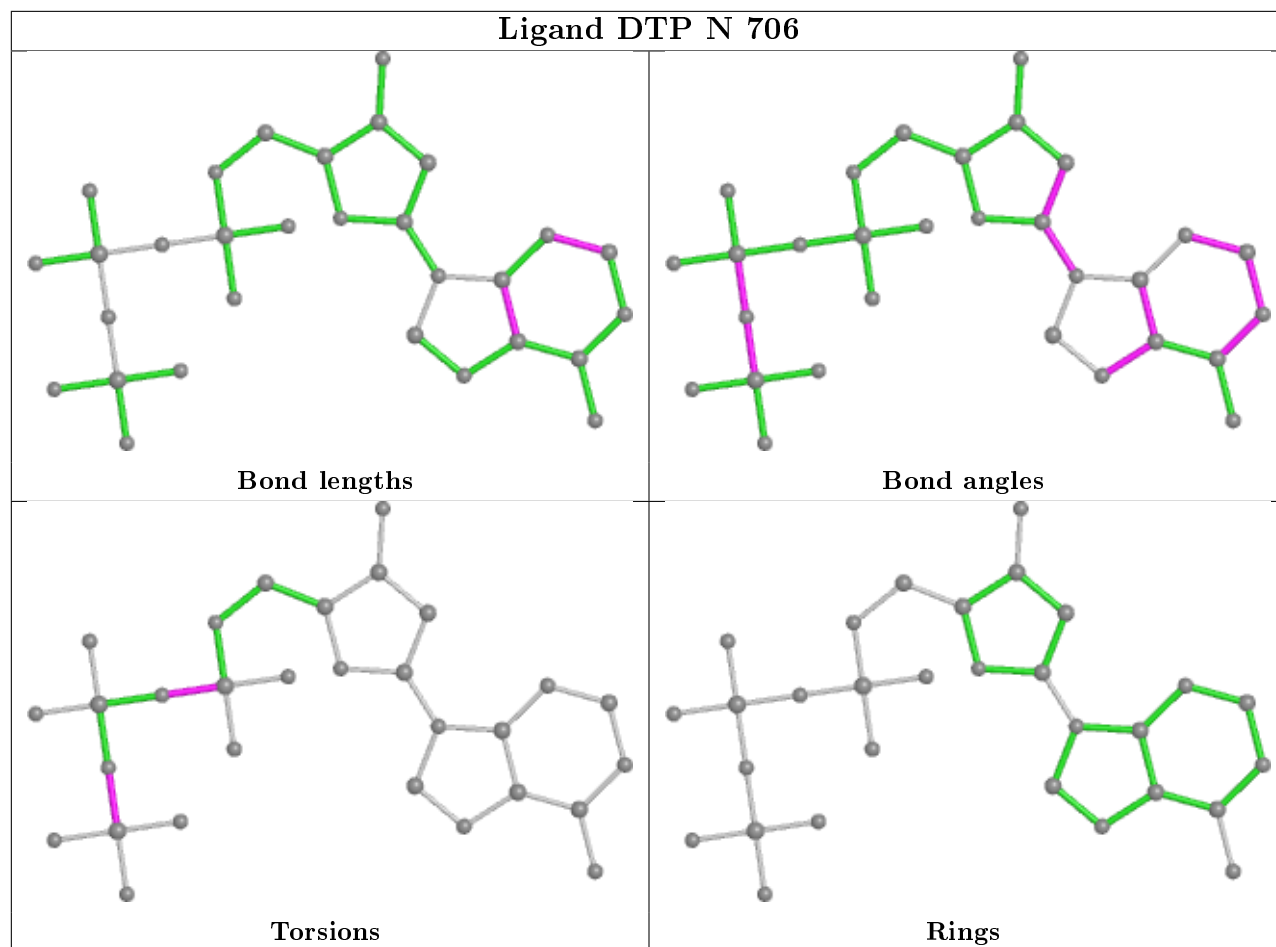
## Ligand DTP E 706



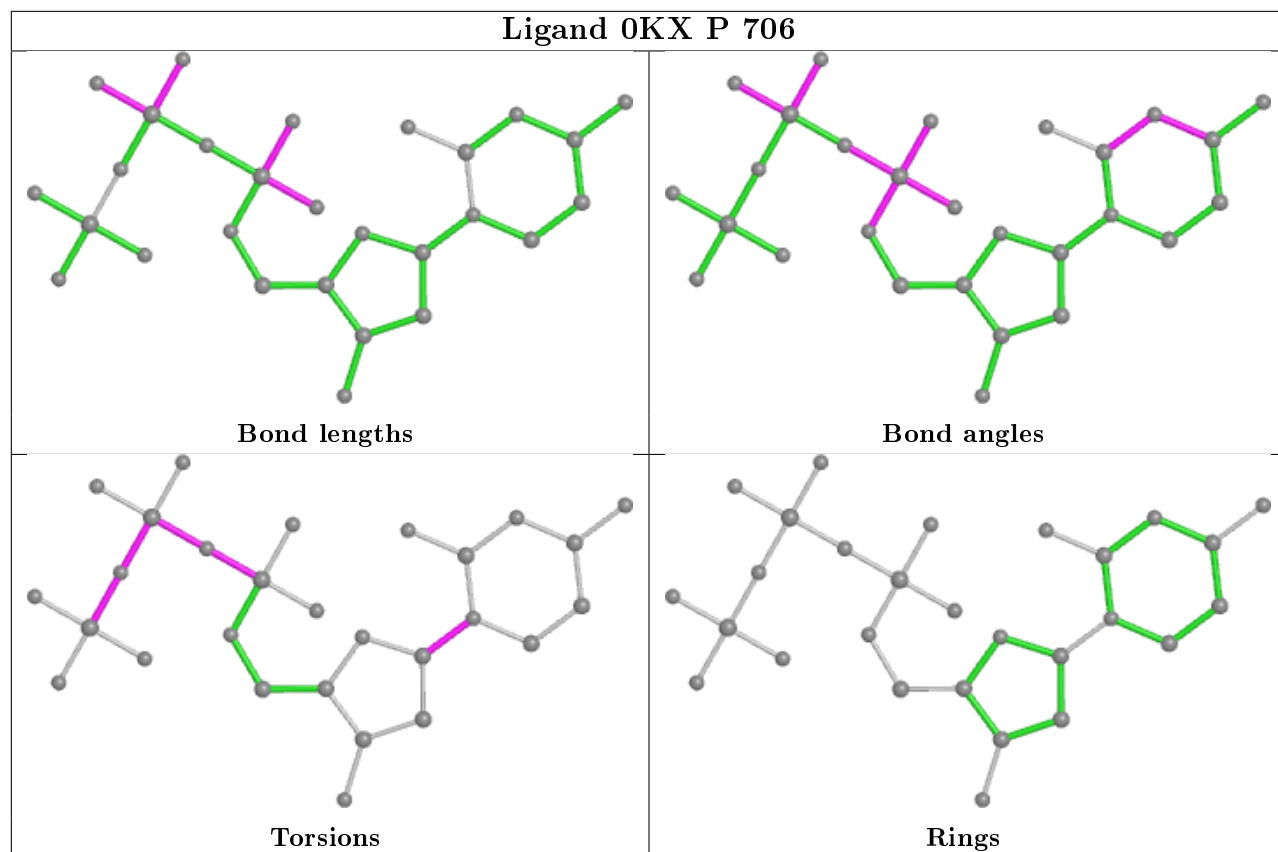
## Ligand DTP I 708



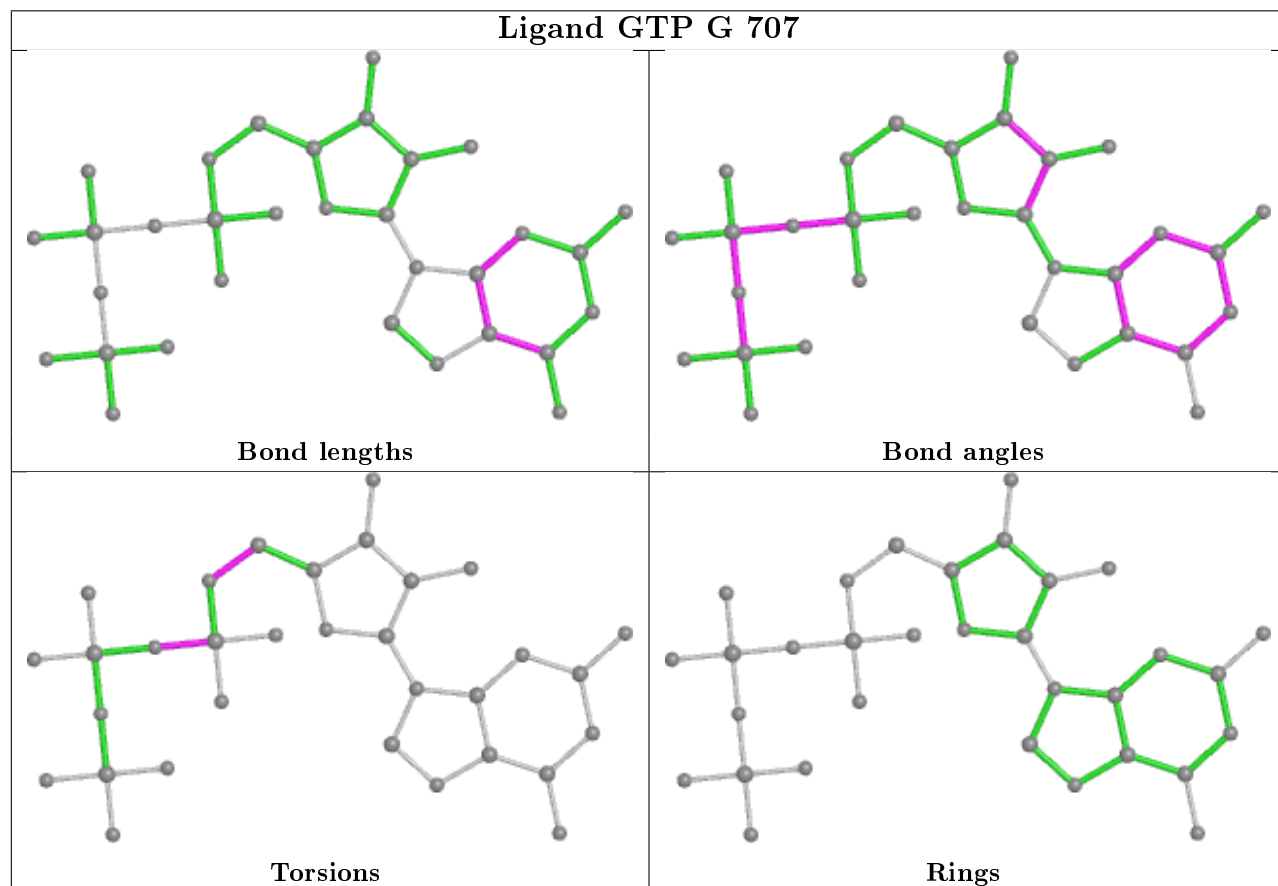


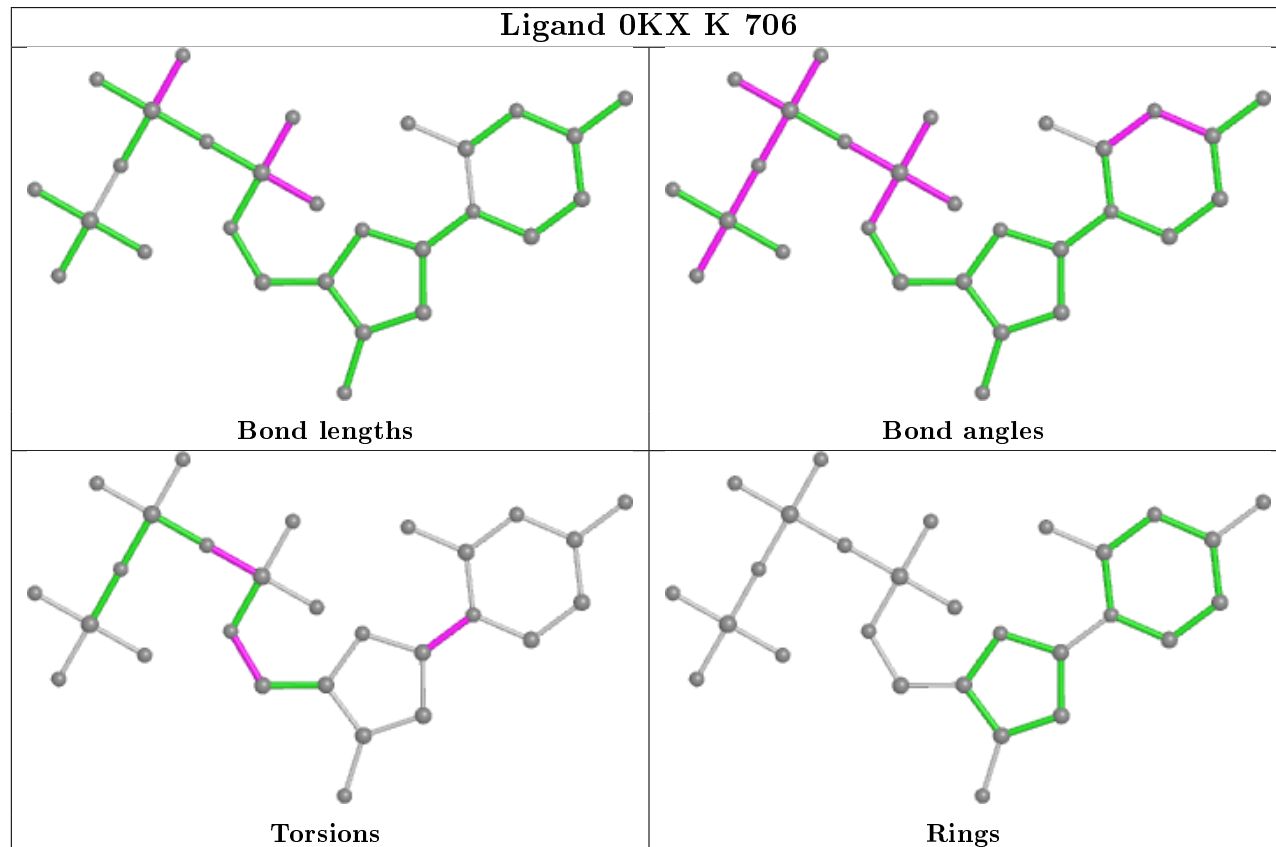
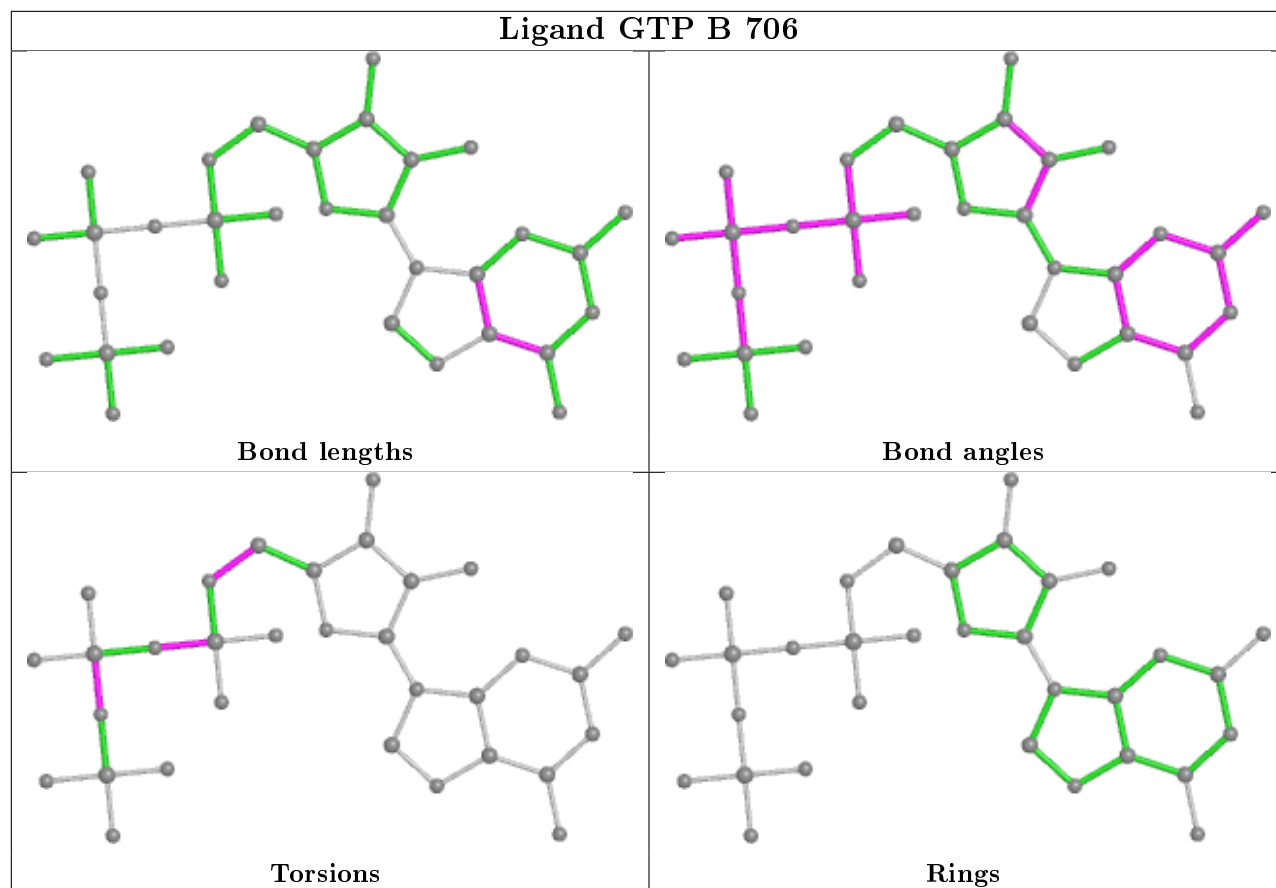


## Ligand 0KX P 706

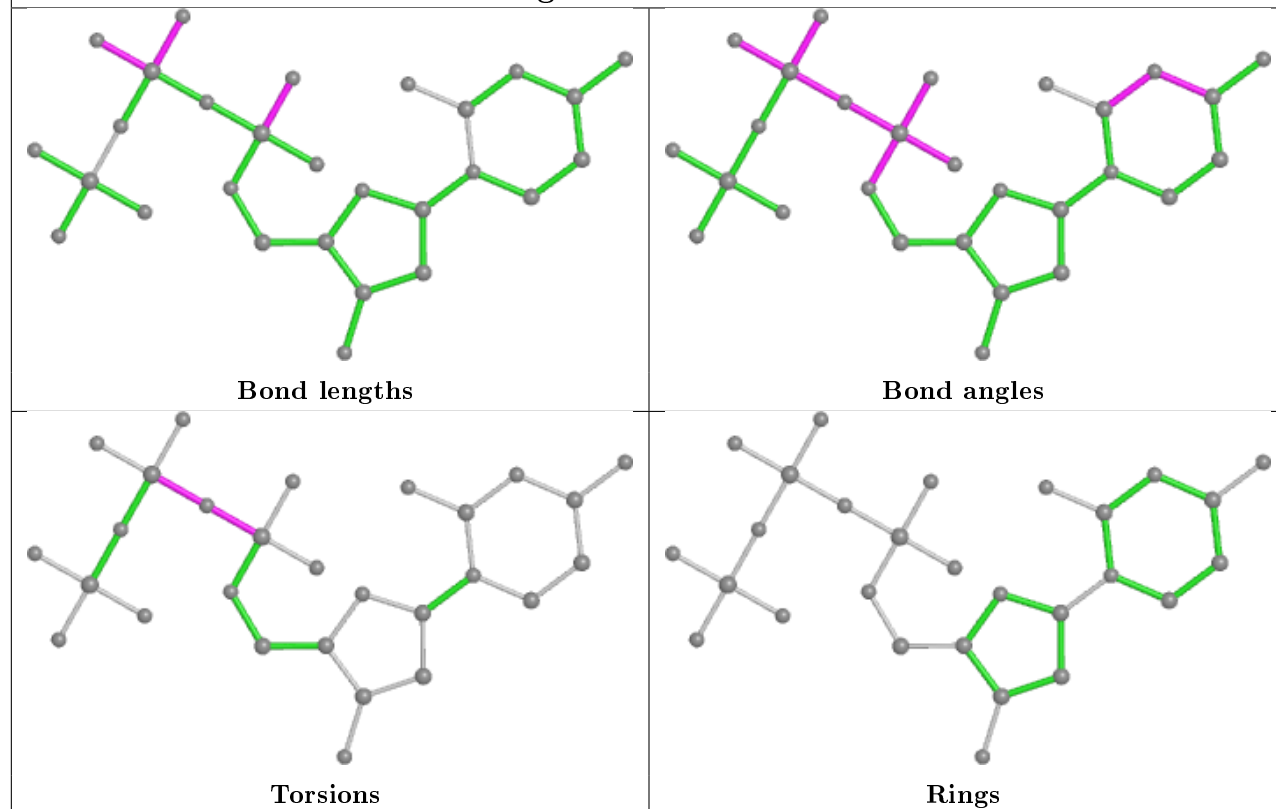


## Ligand GTP G 707

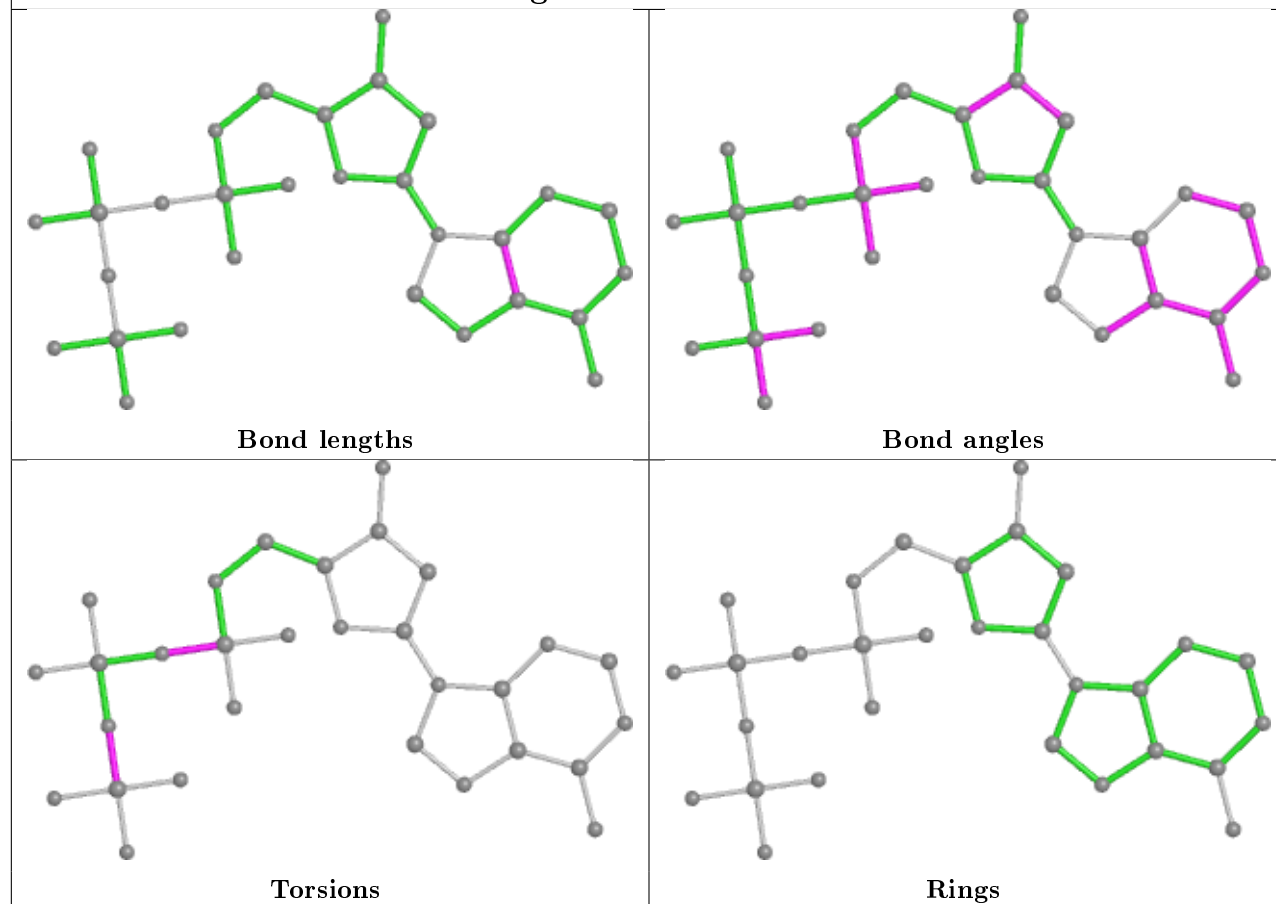




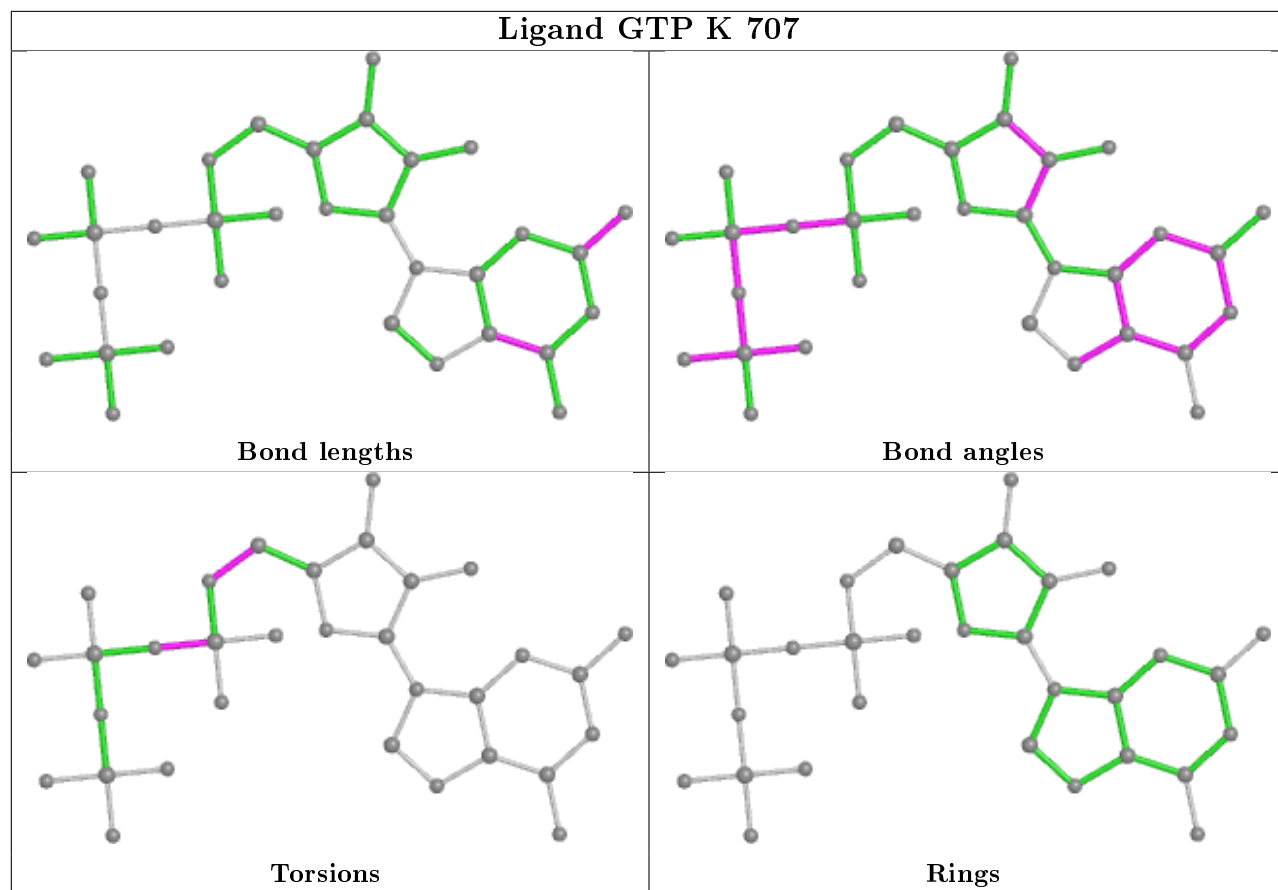
## Ligand 0KX J 704

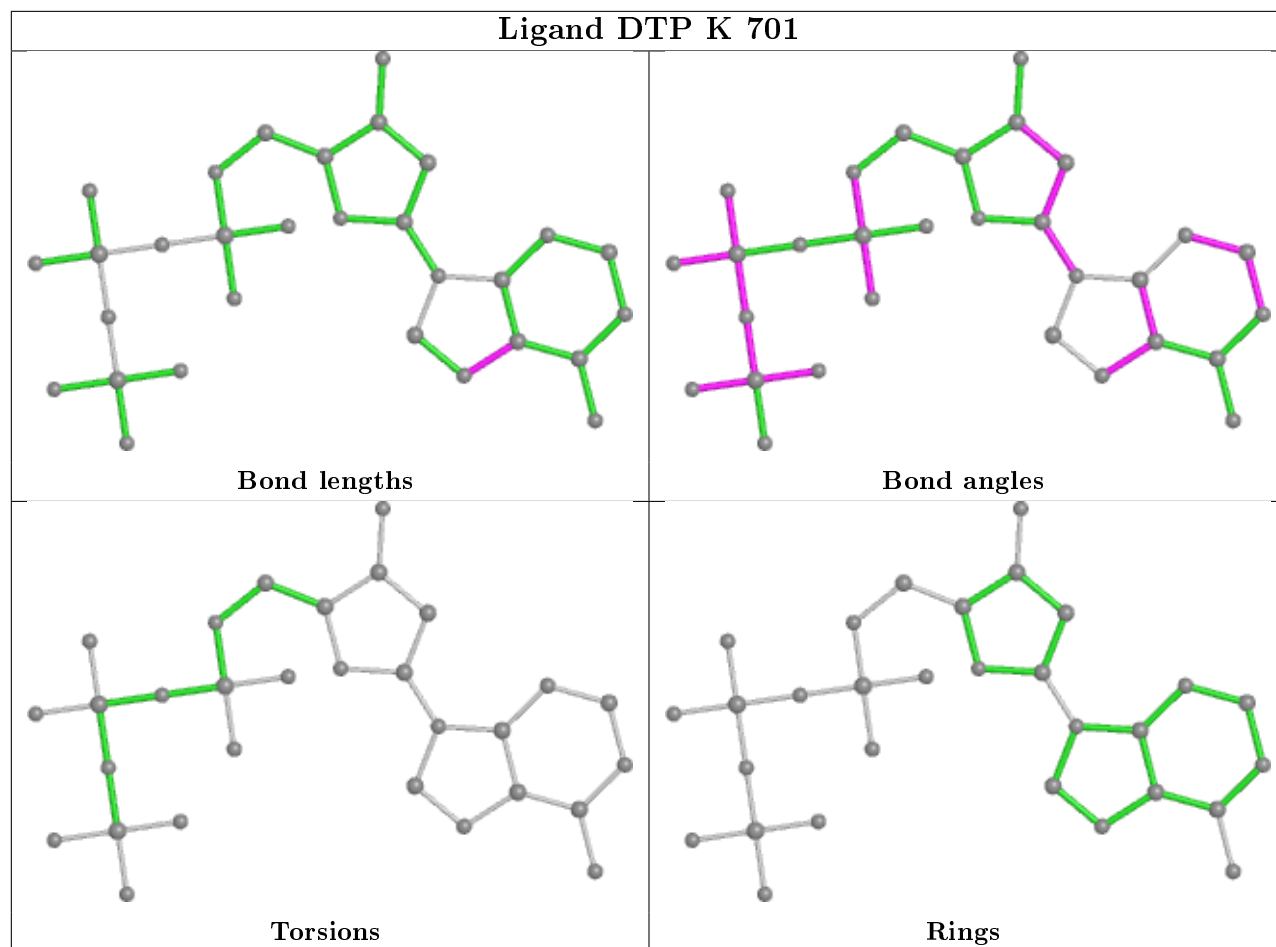


## Ligand DTP O 701

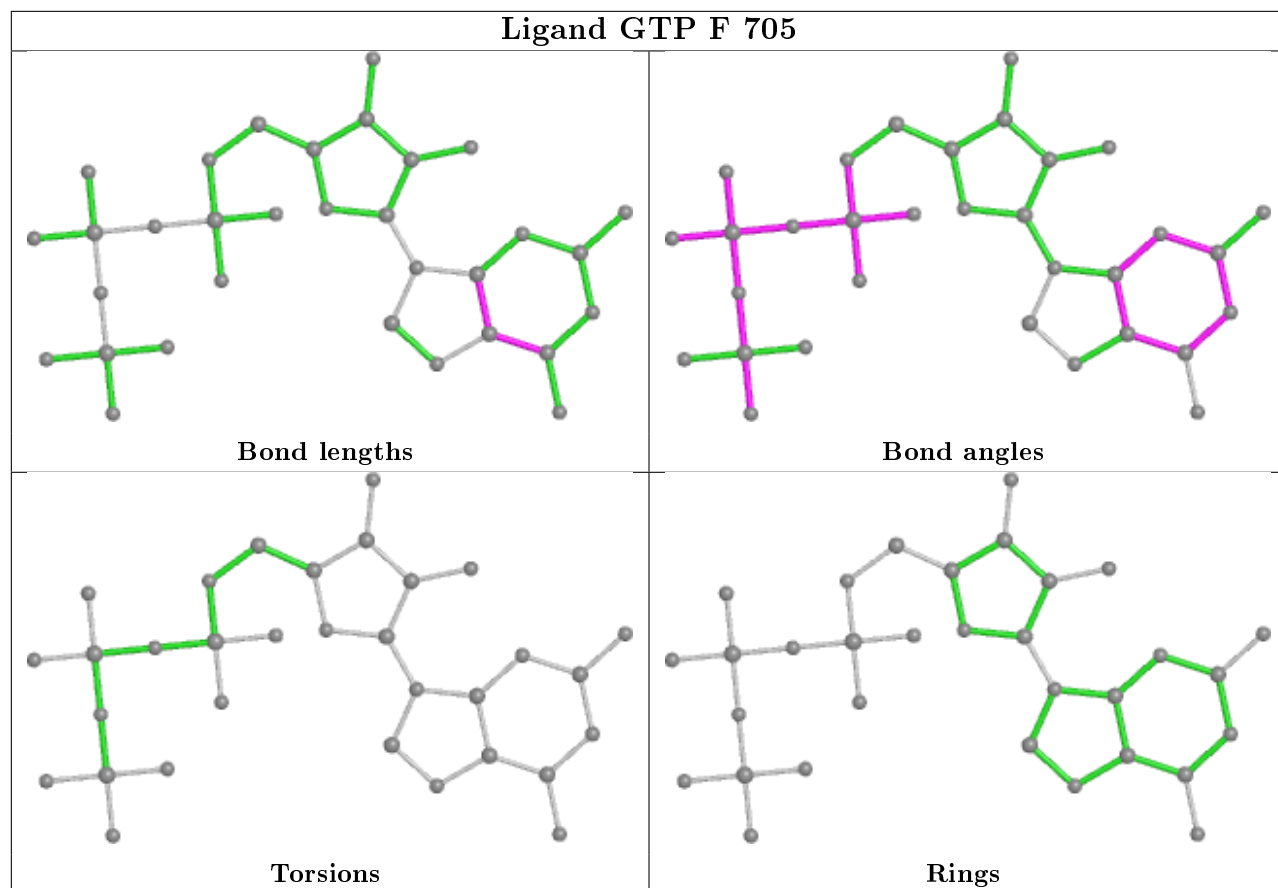




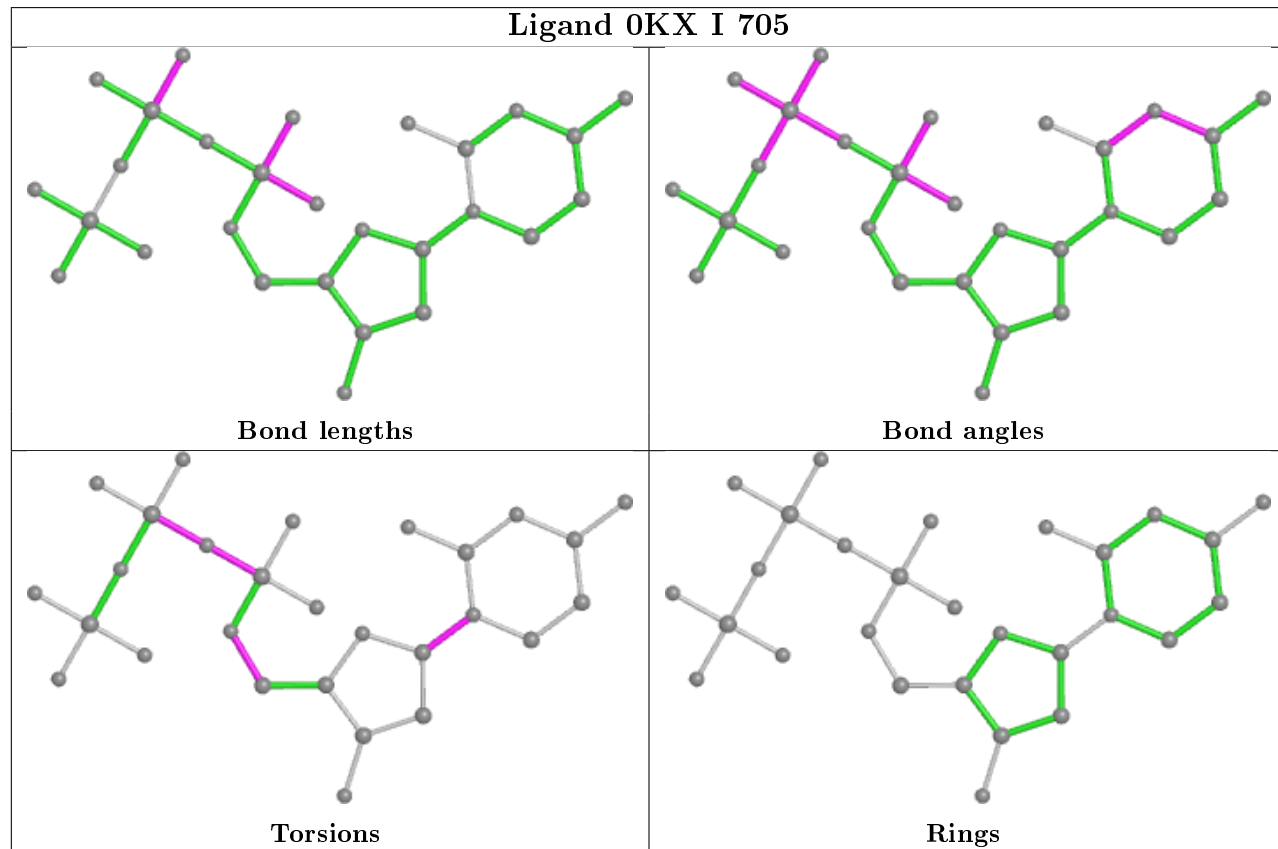




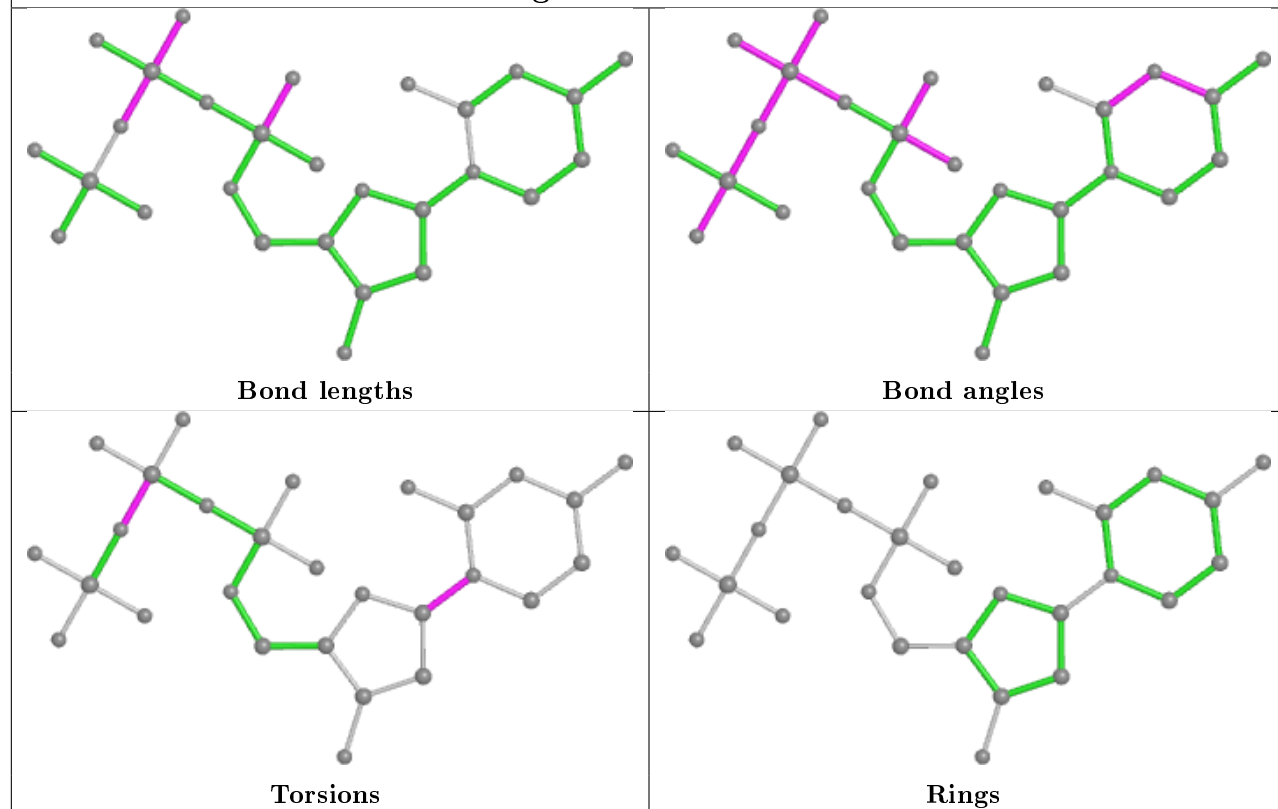
## Ligand GTP F 705



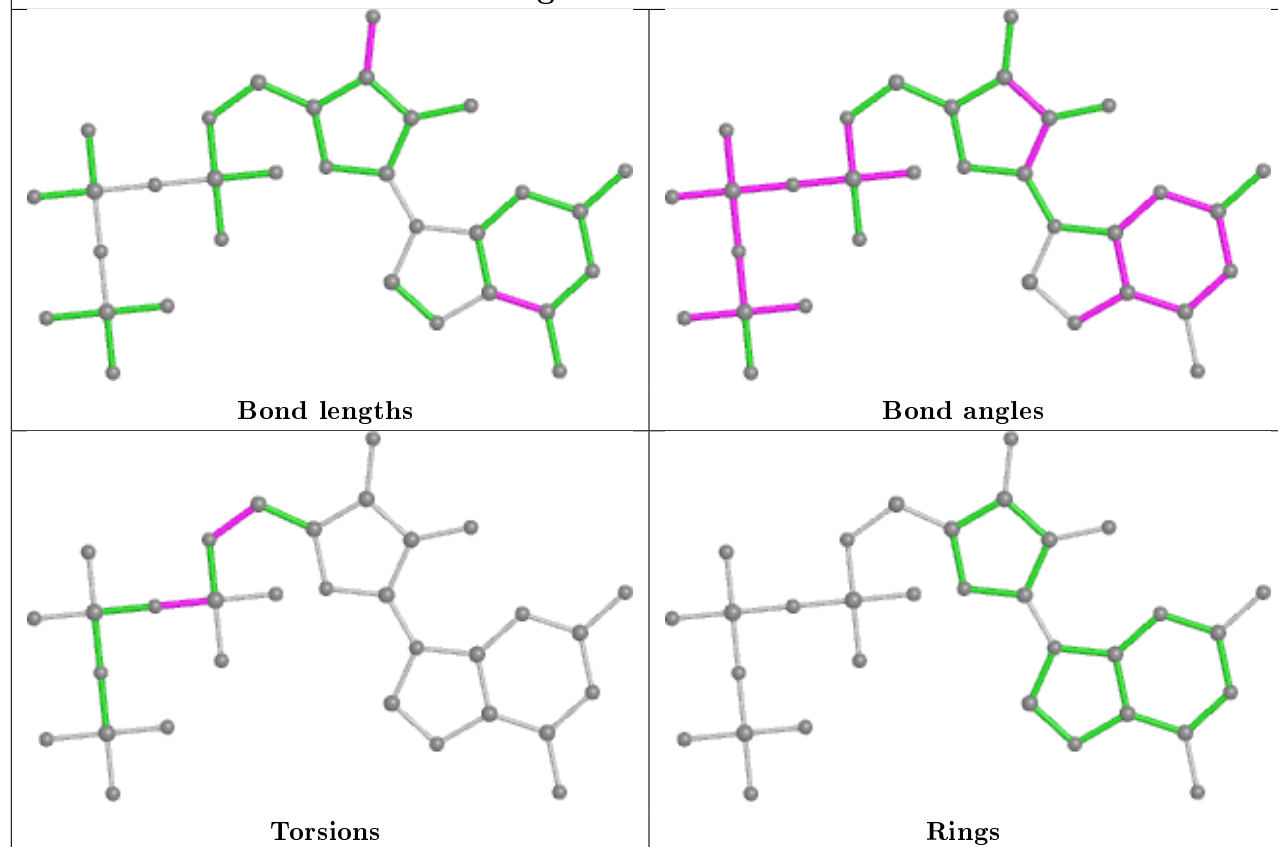
## Ligand OKX I 705

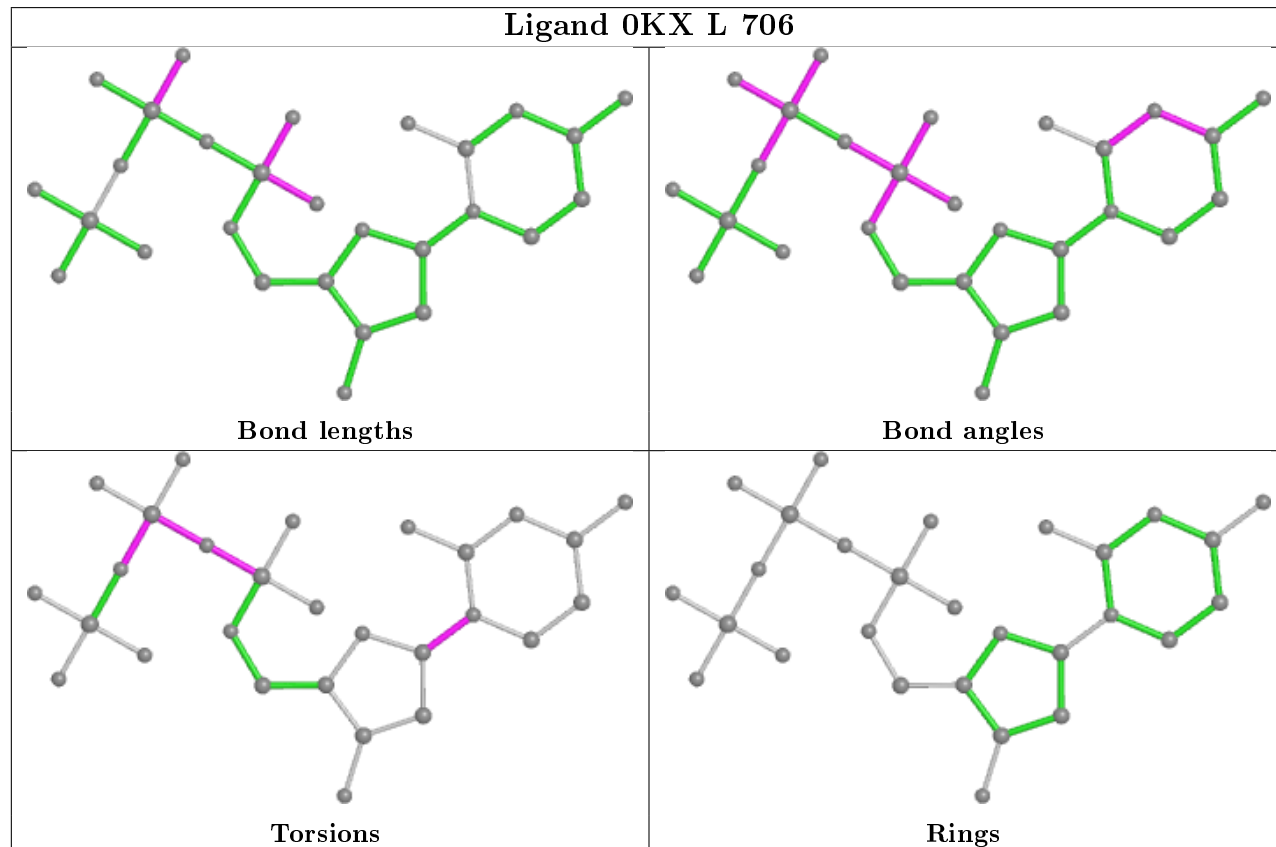
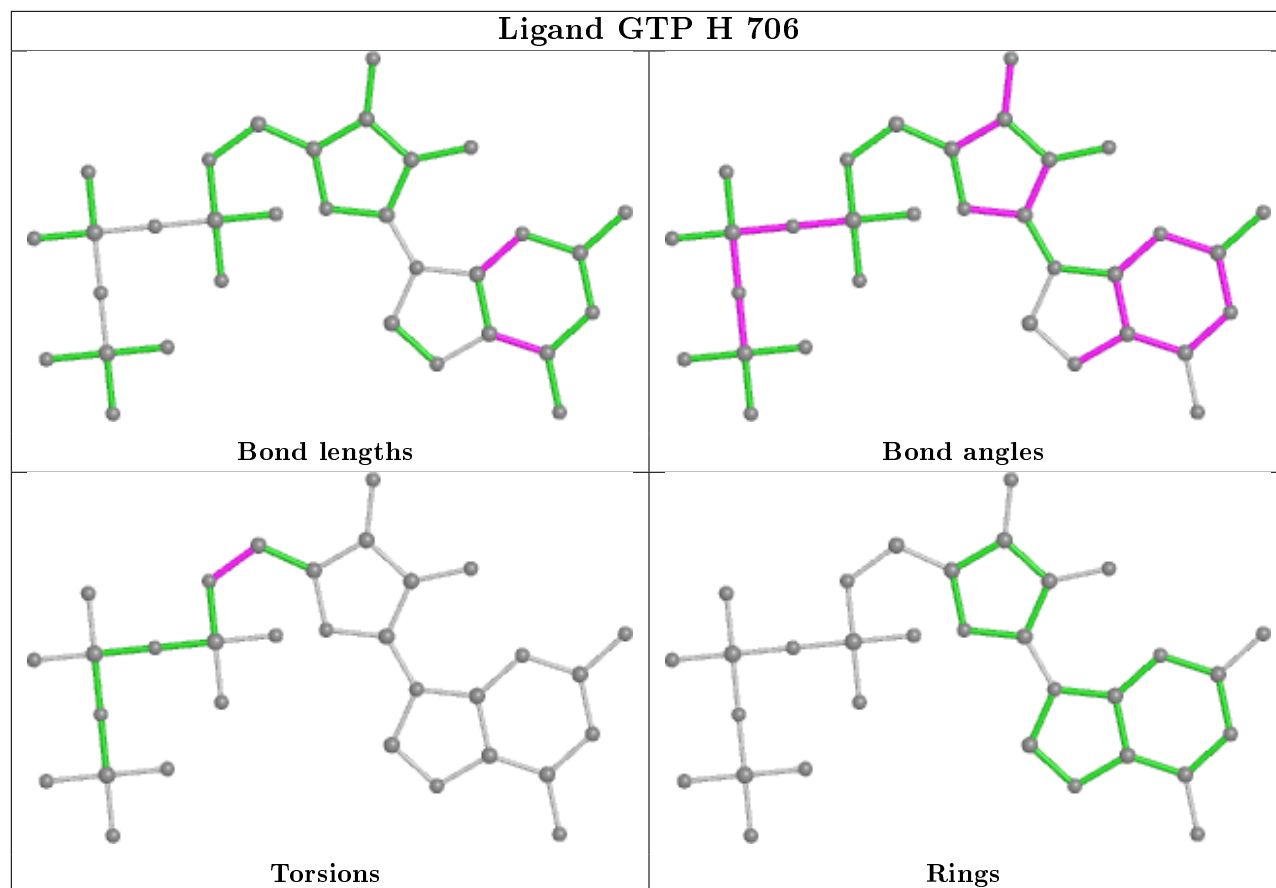


## Ligand 0KX O 705

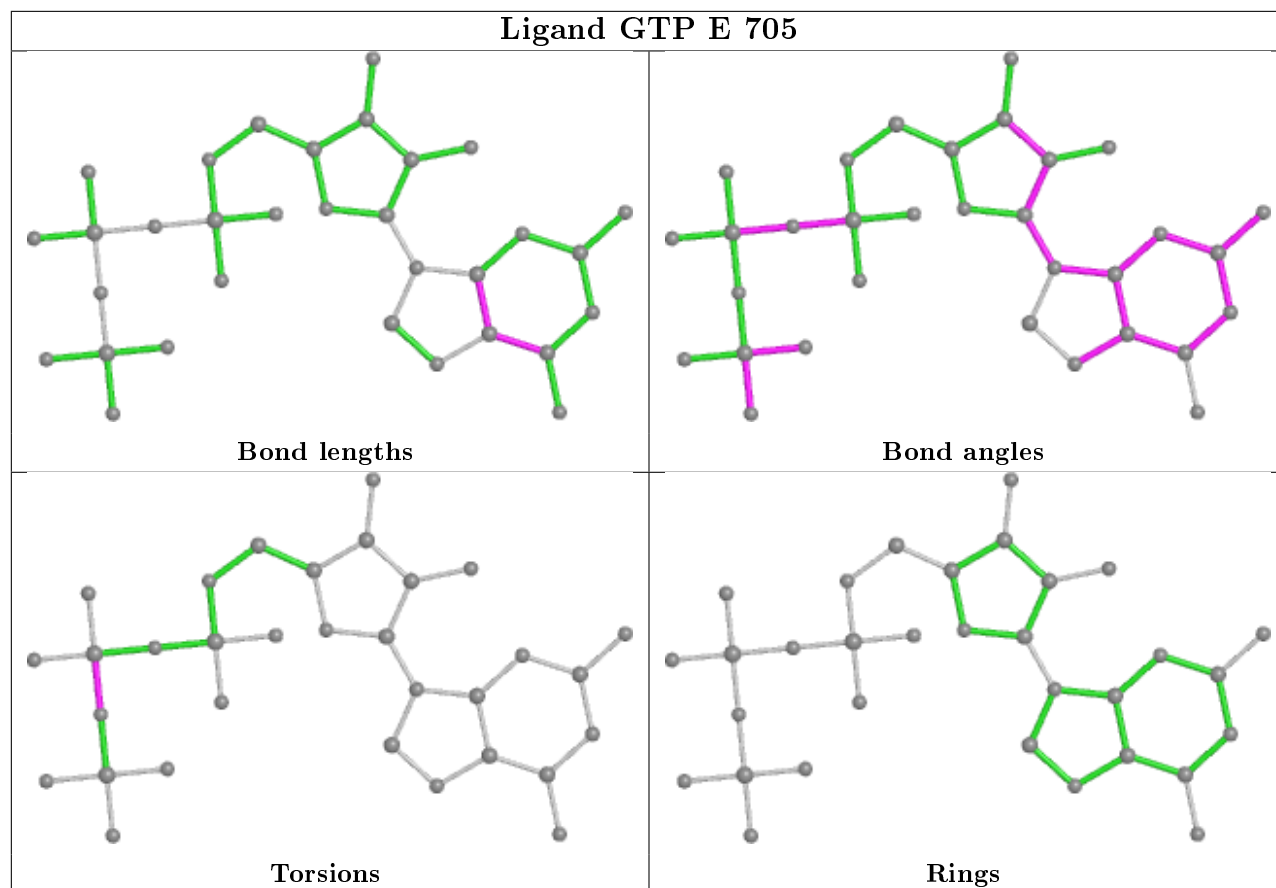


## Ligand GTP I 706

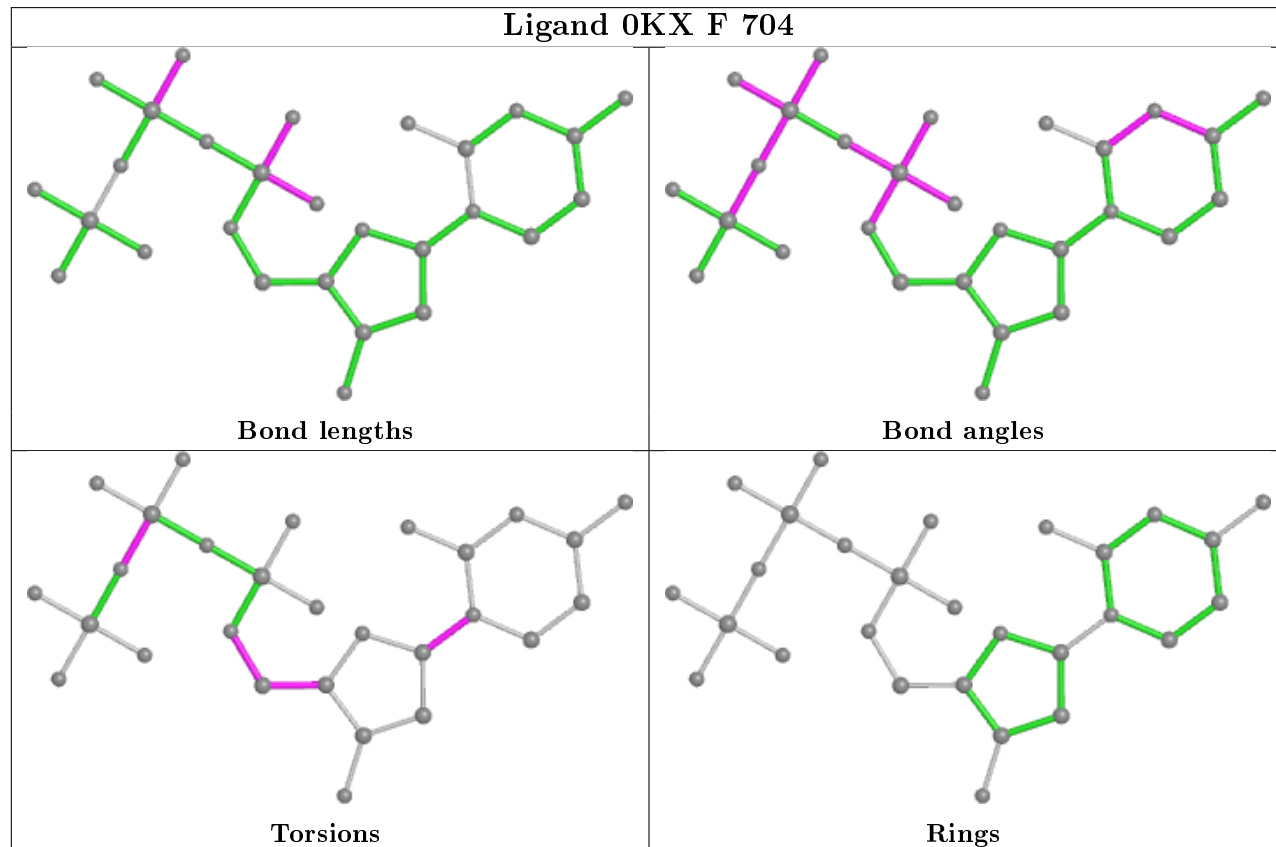




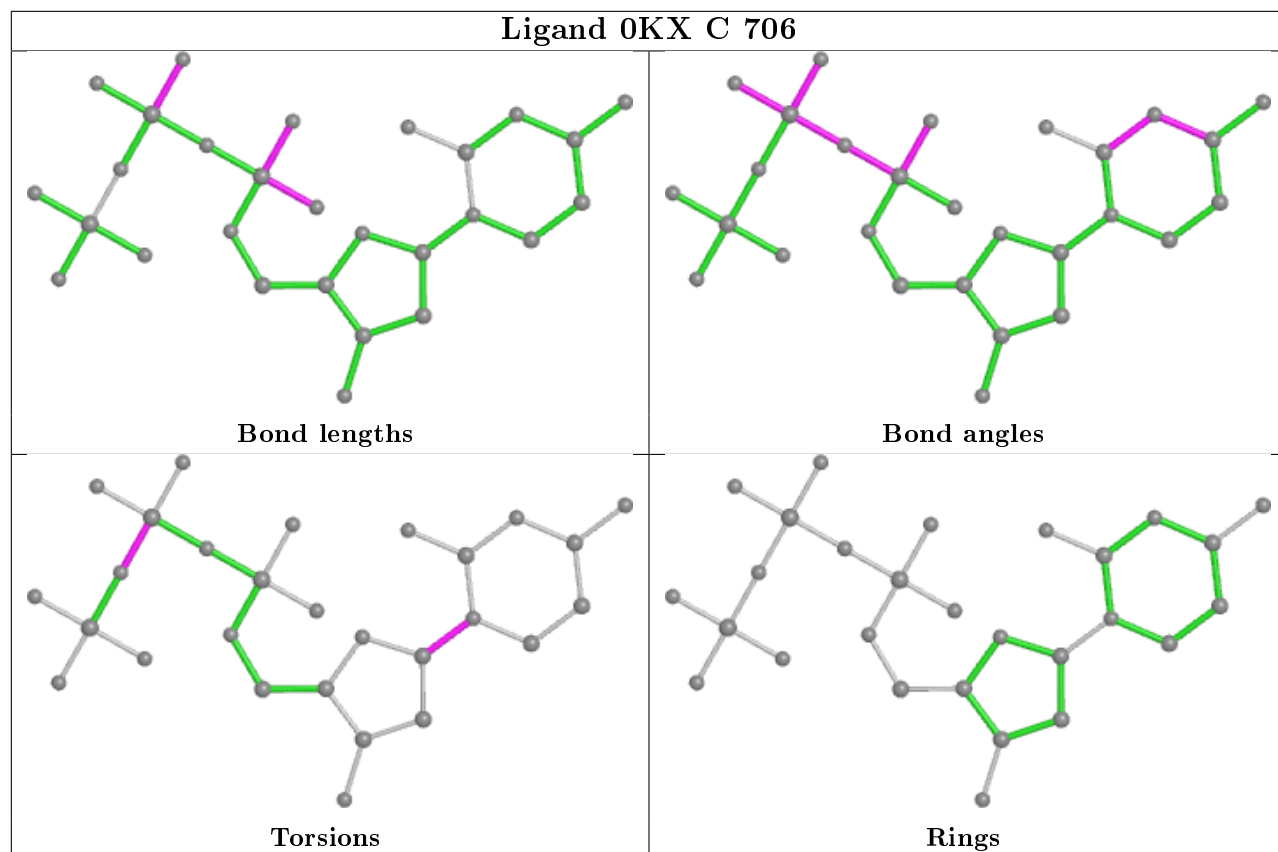
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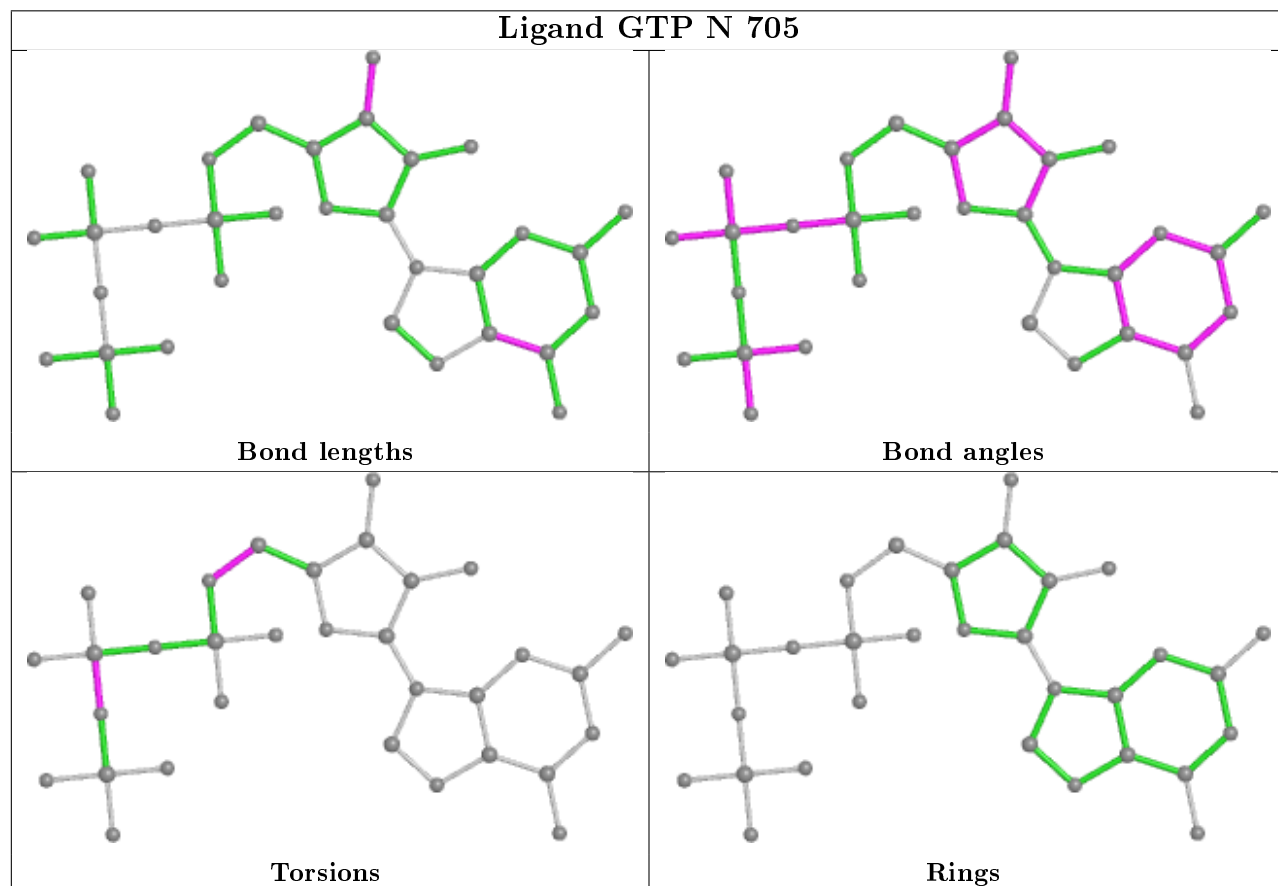
## Ligand OKX F 704

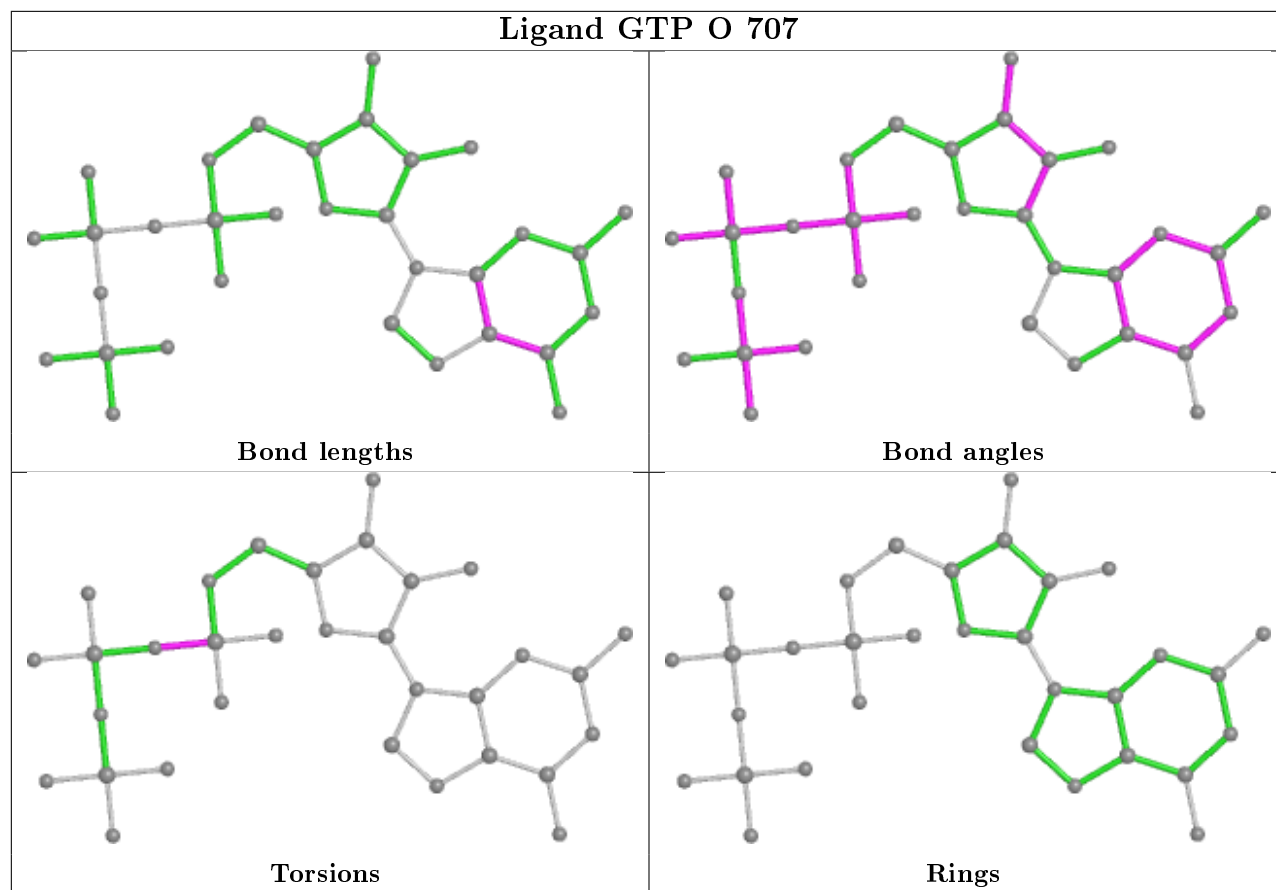


## Ligand 0KX C 706

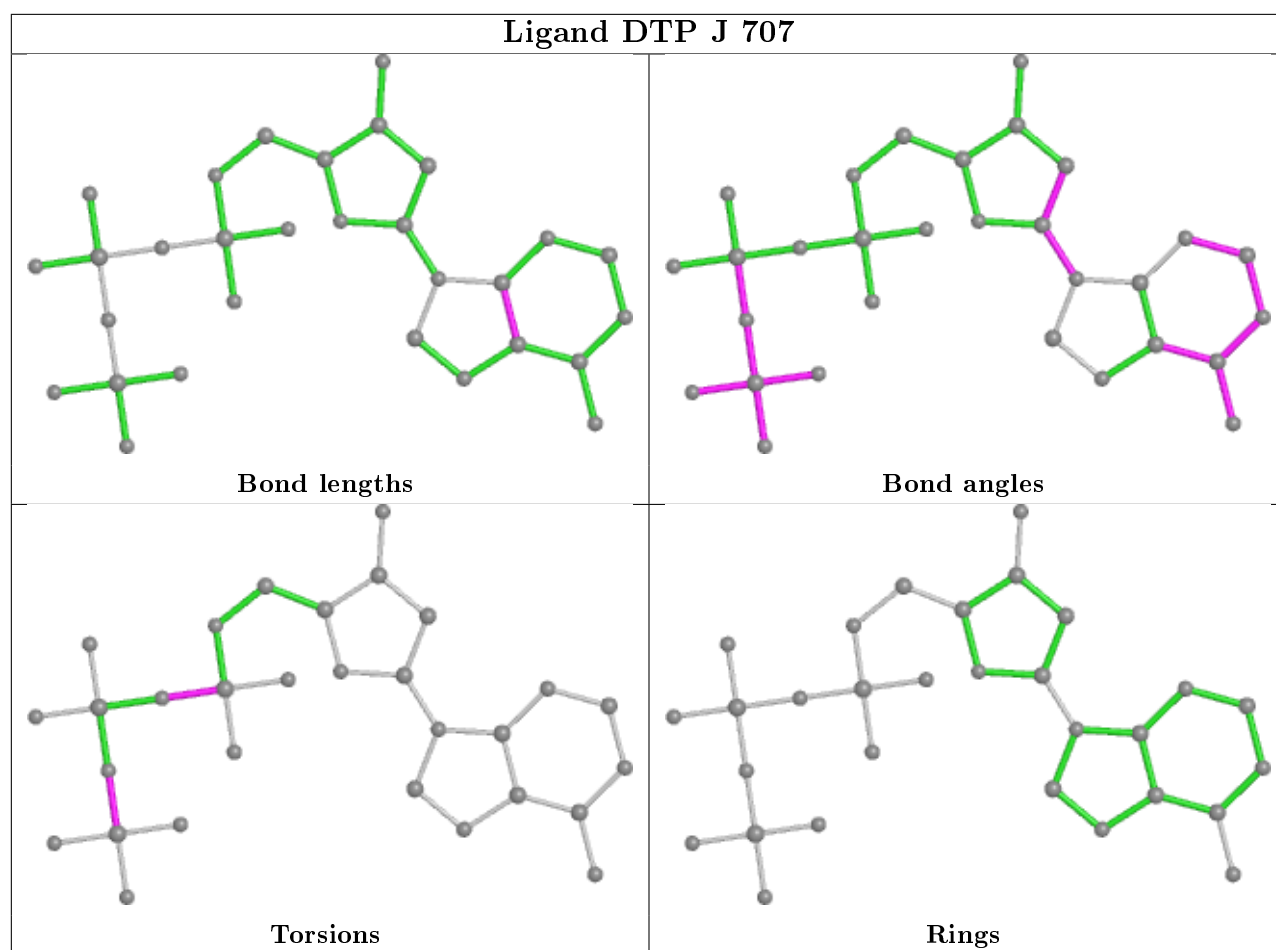


## Ligand GTP N 705

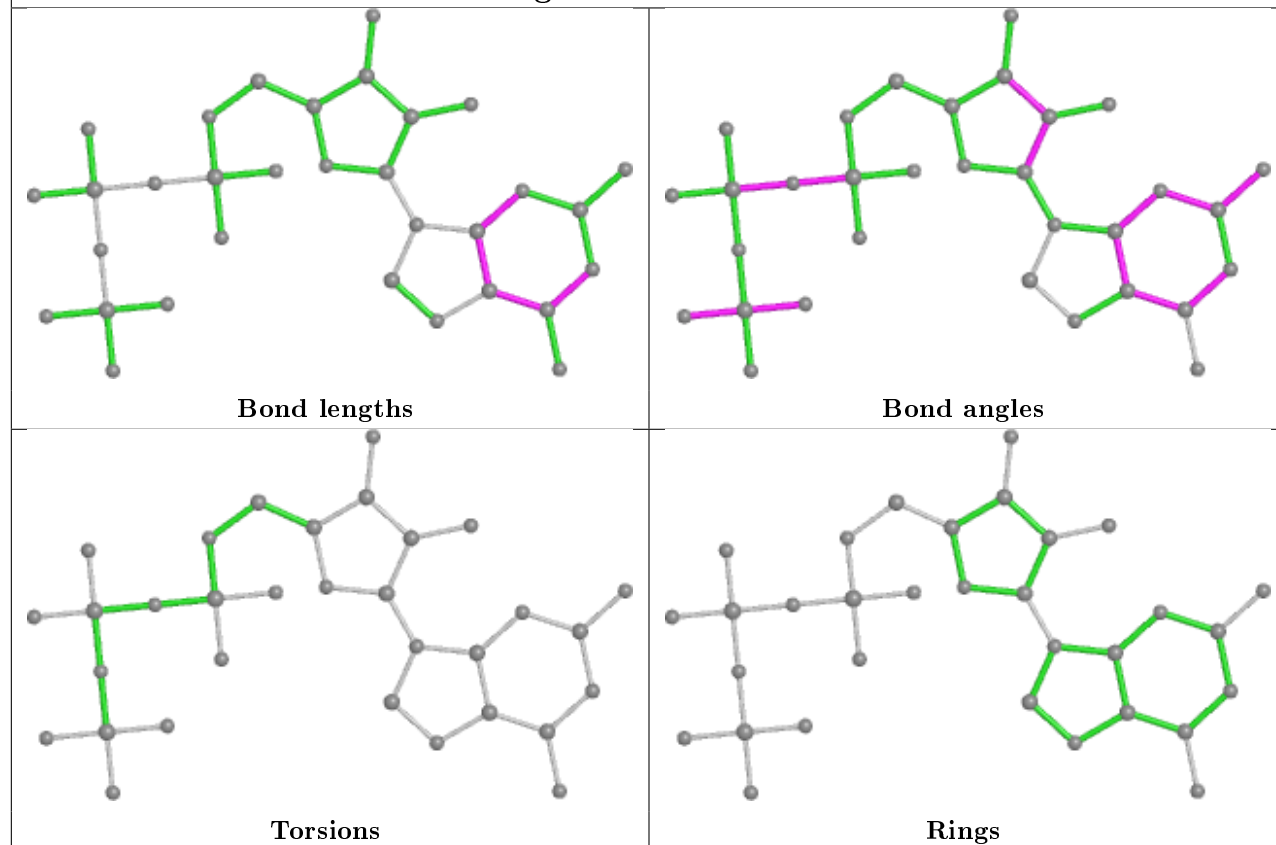




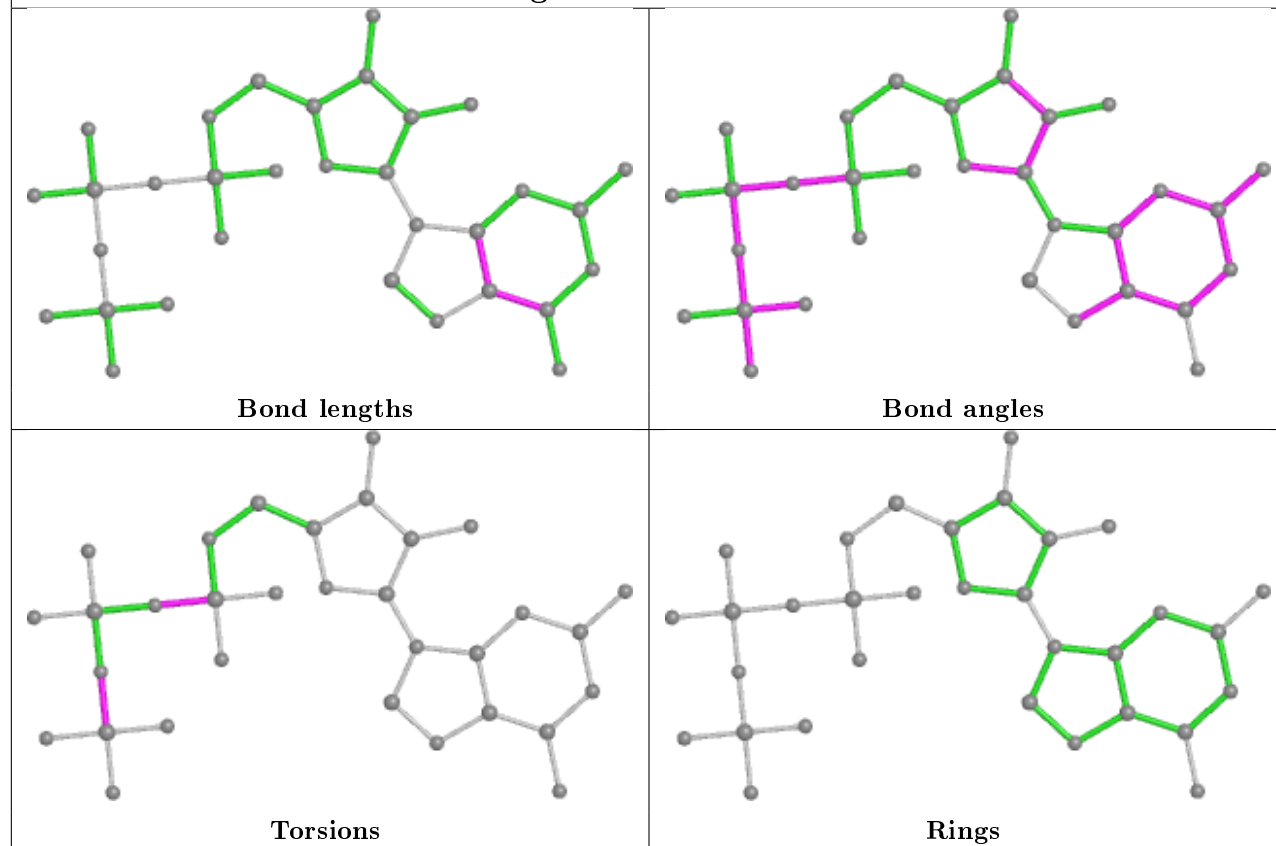


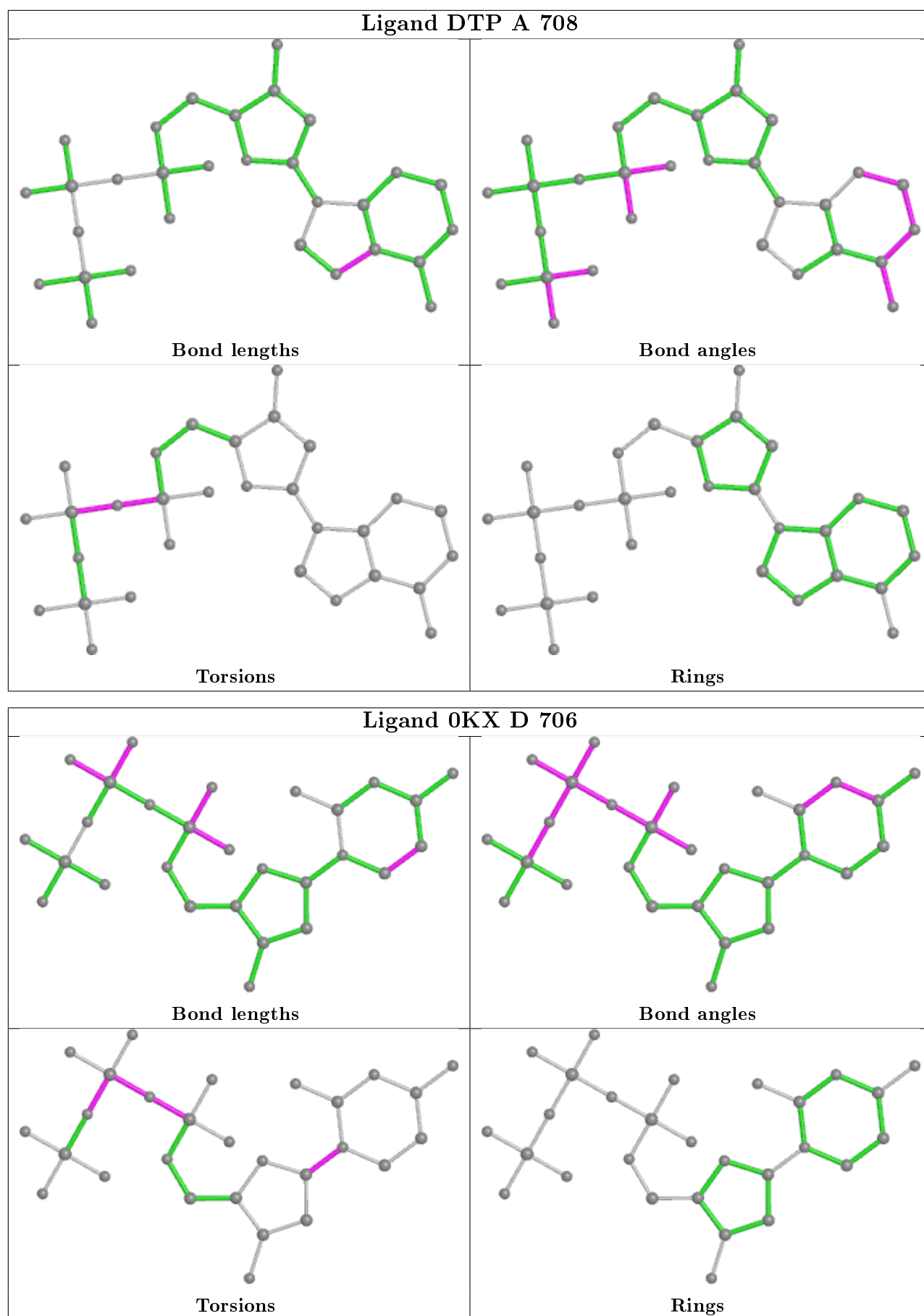


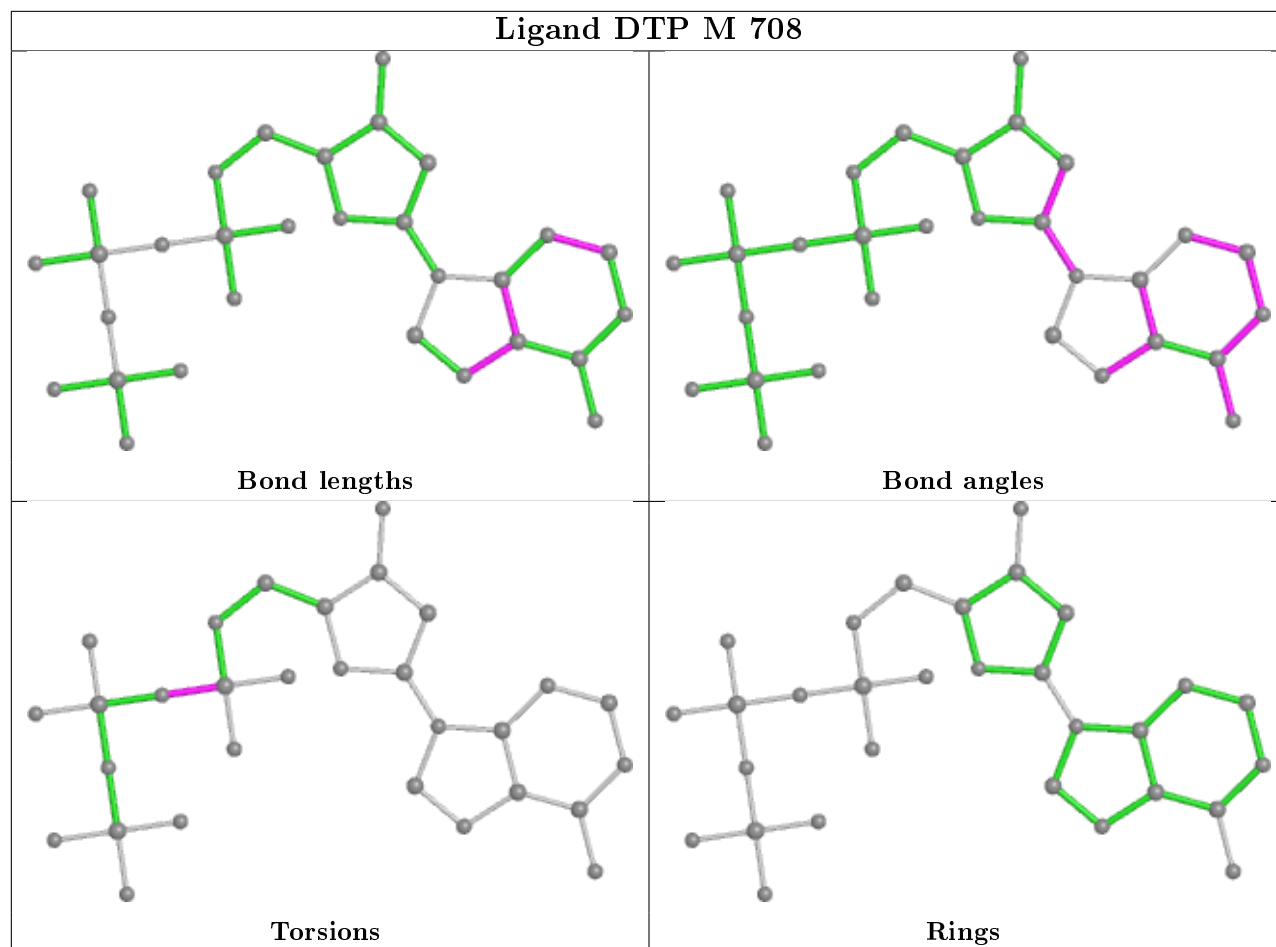
## Ligand GTP J 705



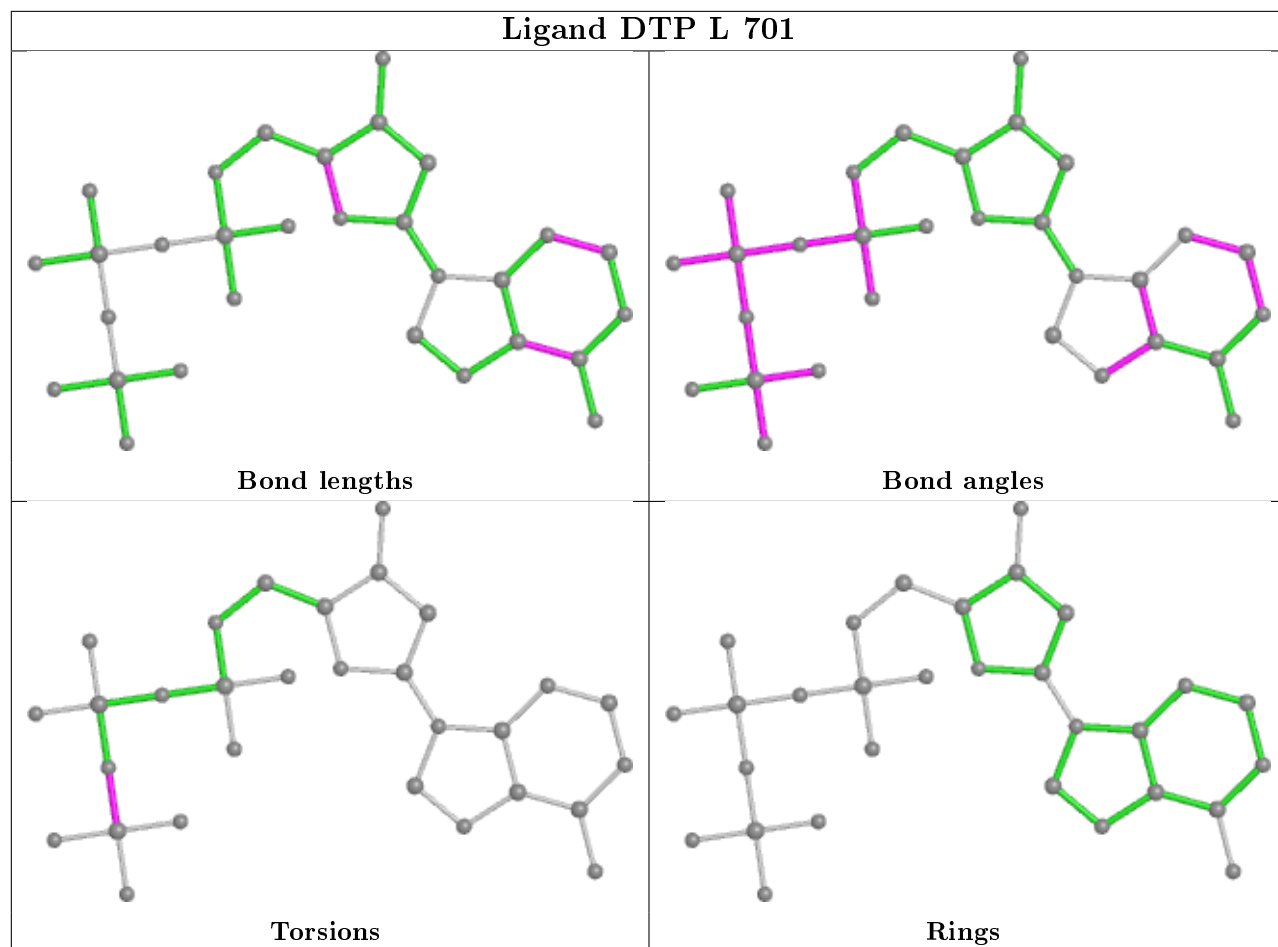
## Ligand GTP O 706

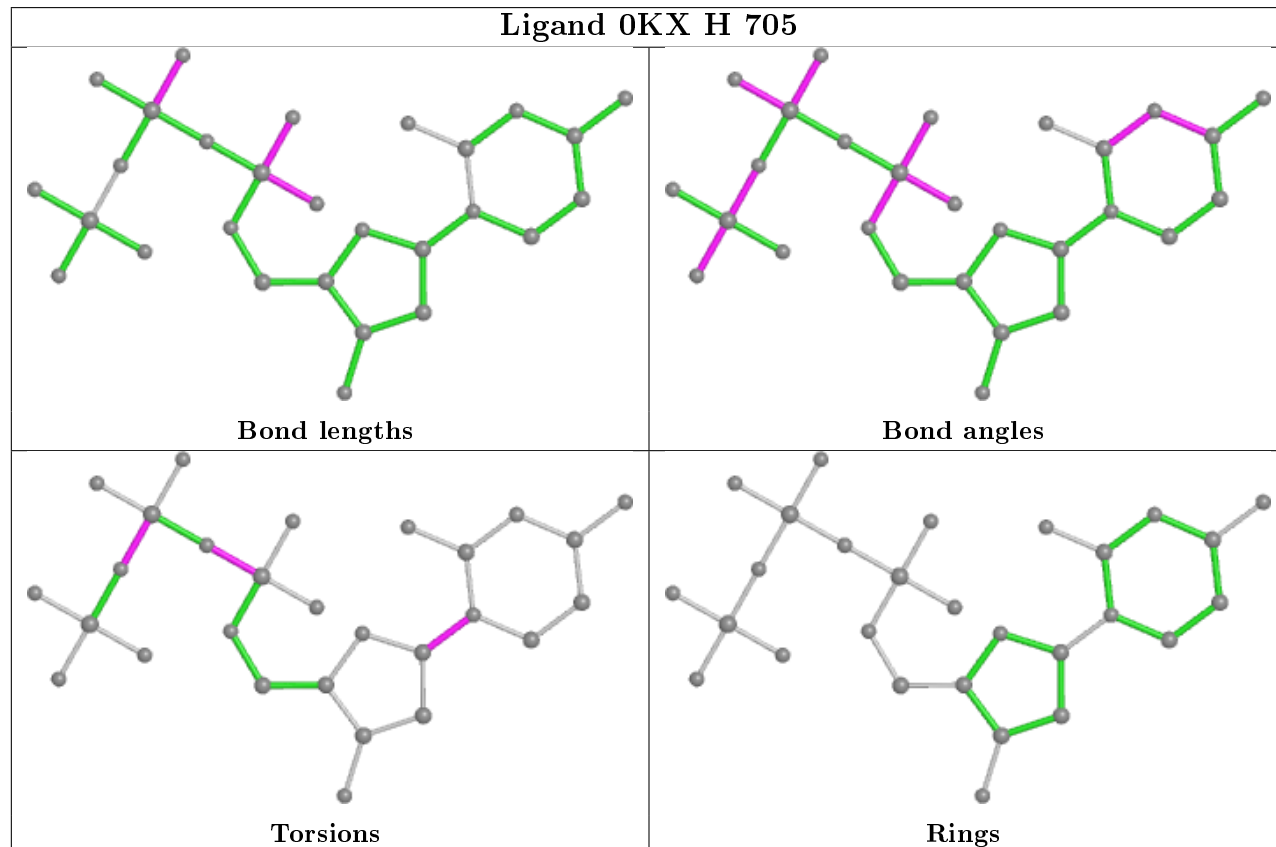
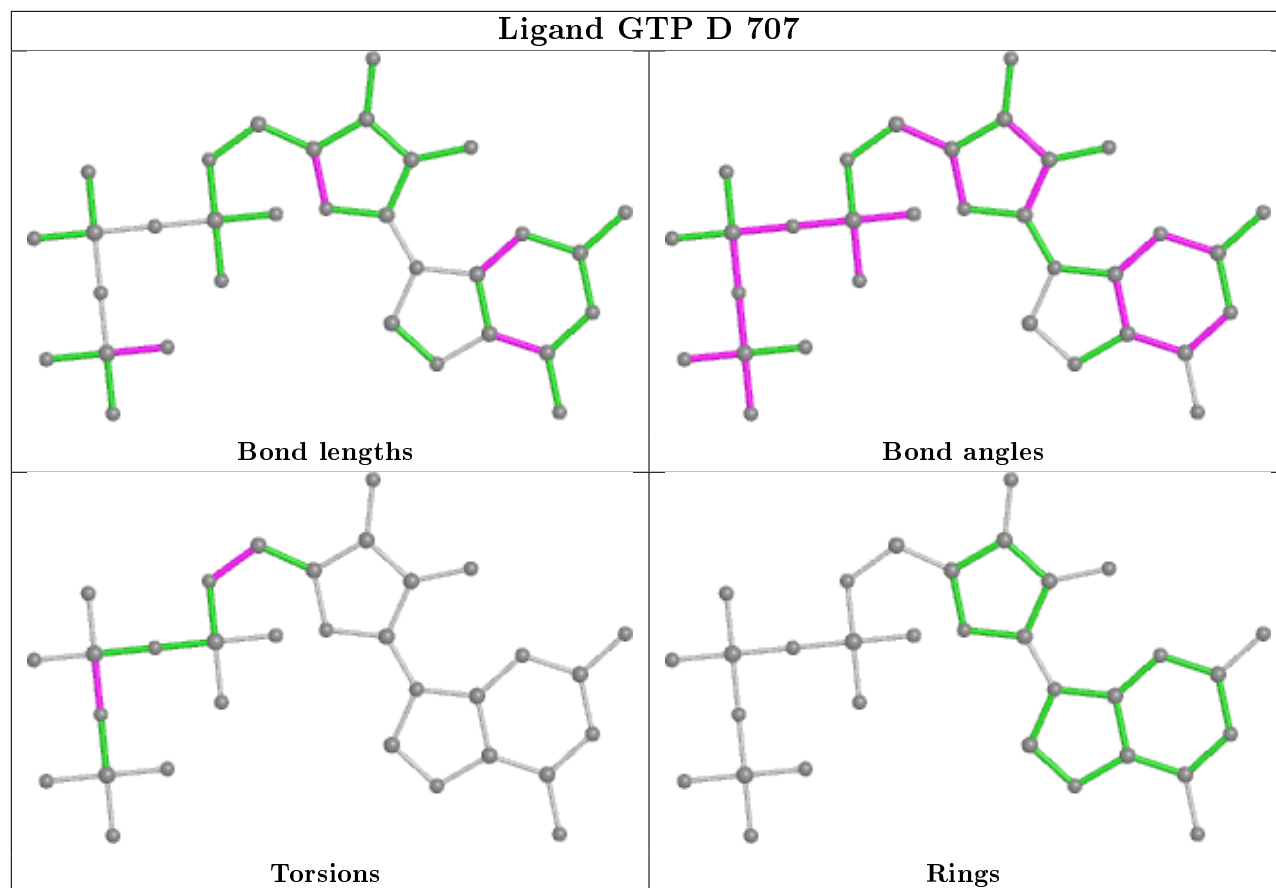




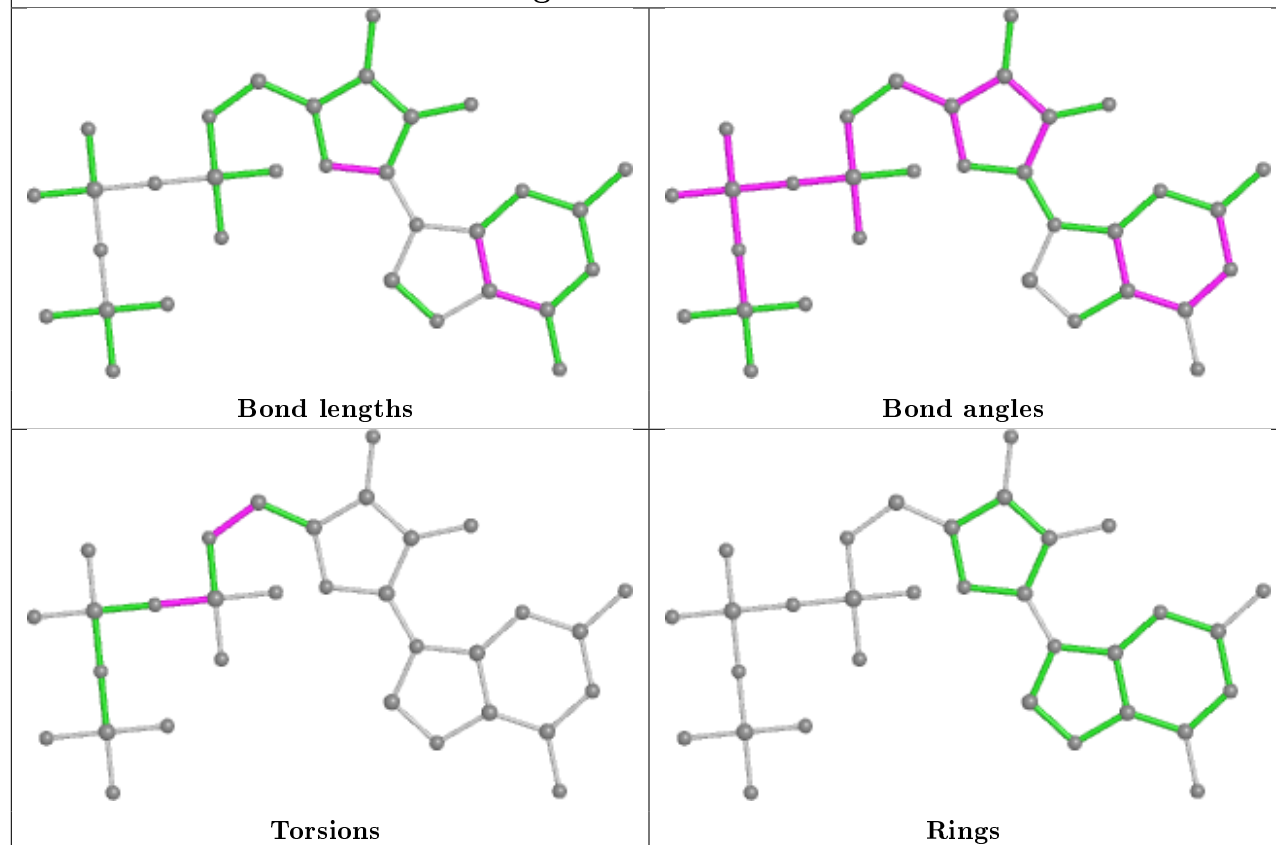


## Ligand DTP L 701

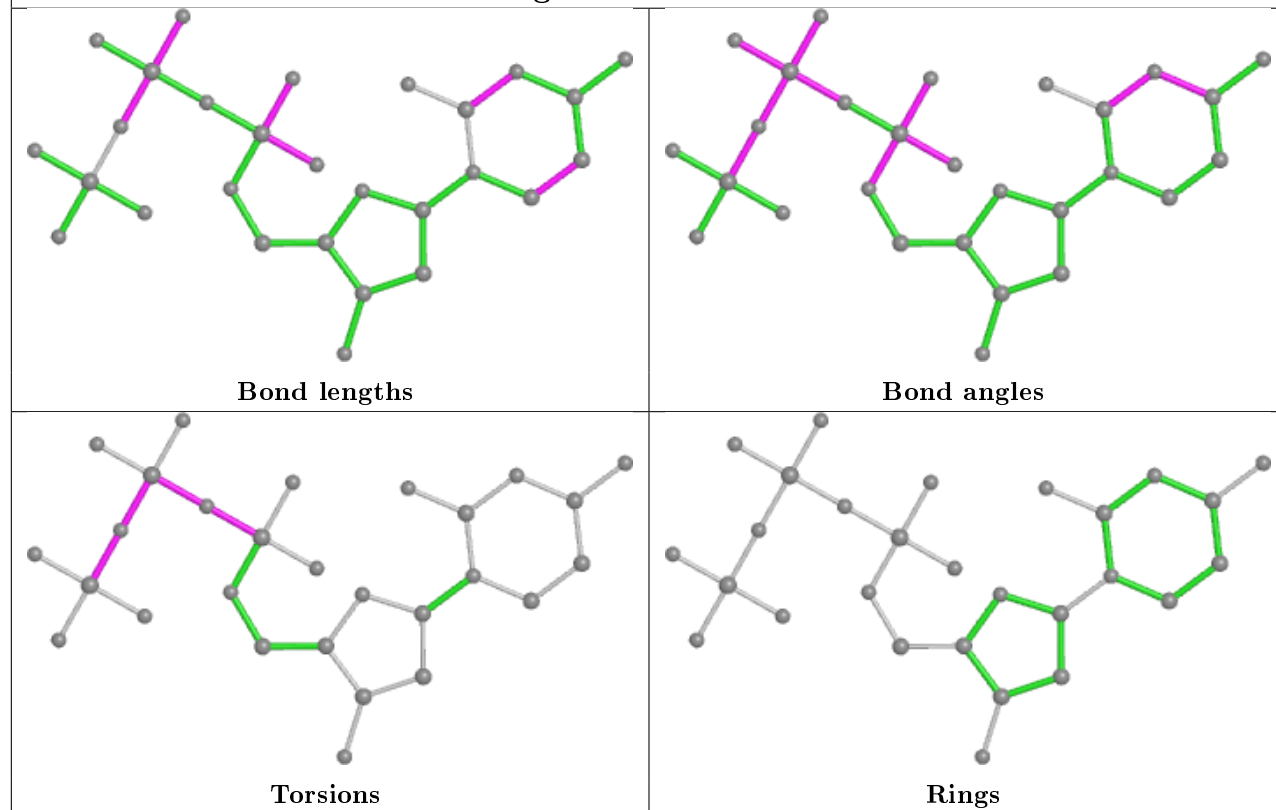




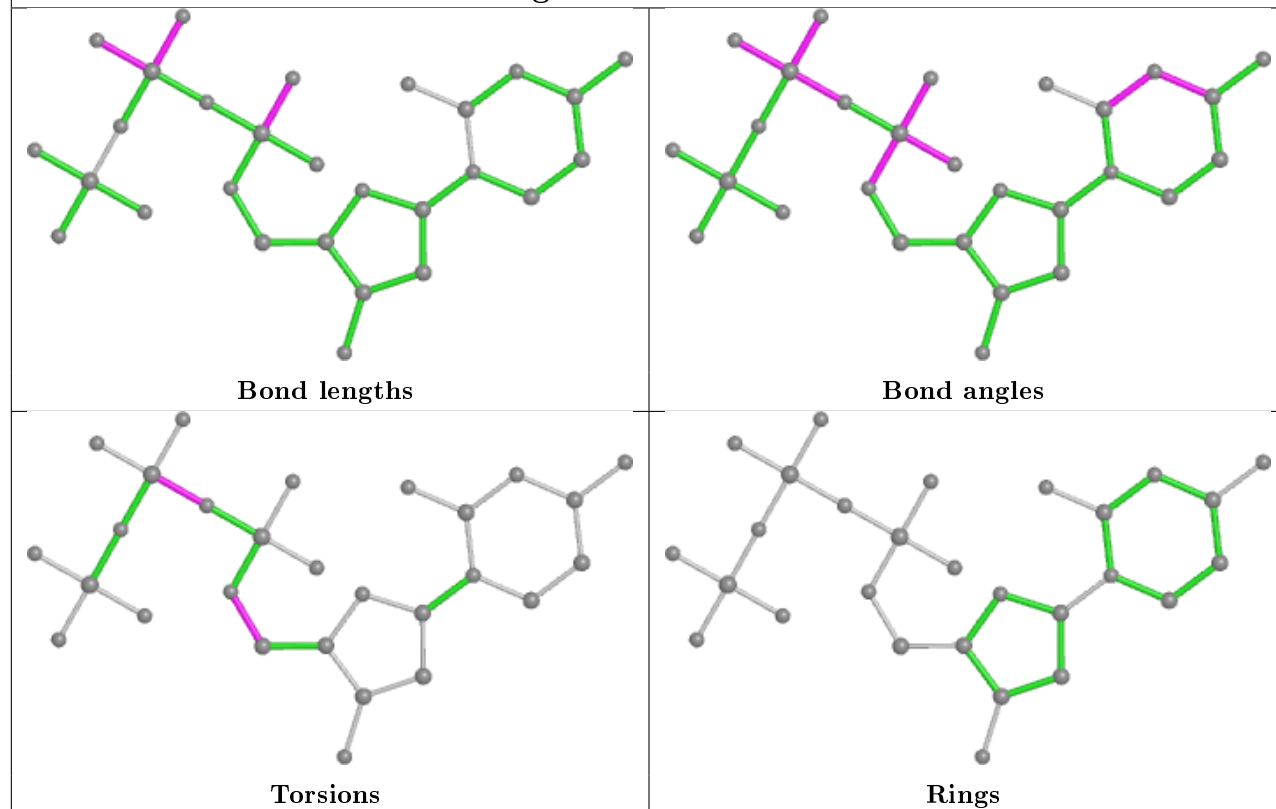
## Ligand GTP L 707



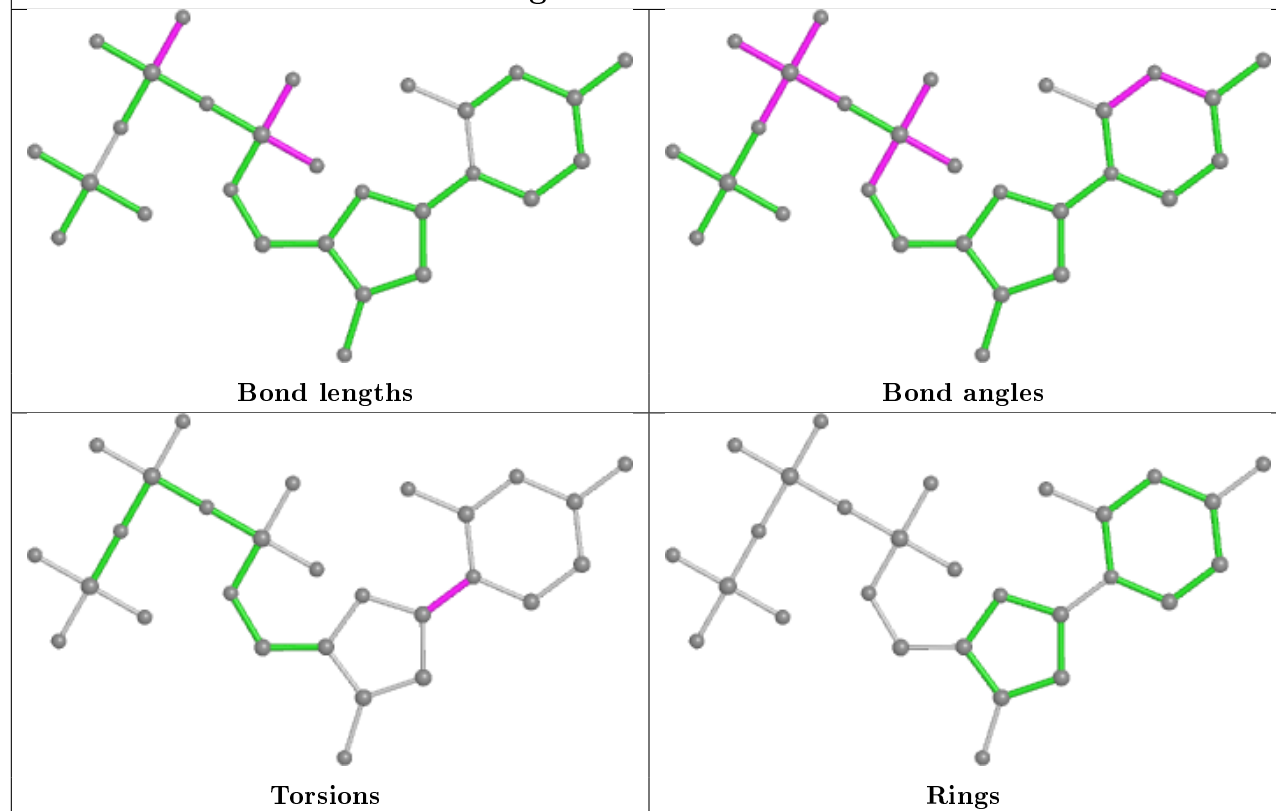
## Ligand 0KX B 705



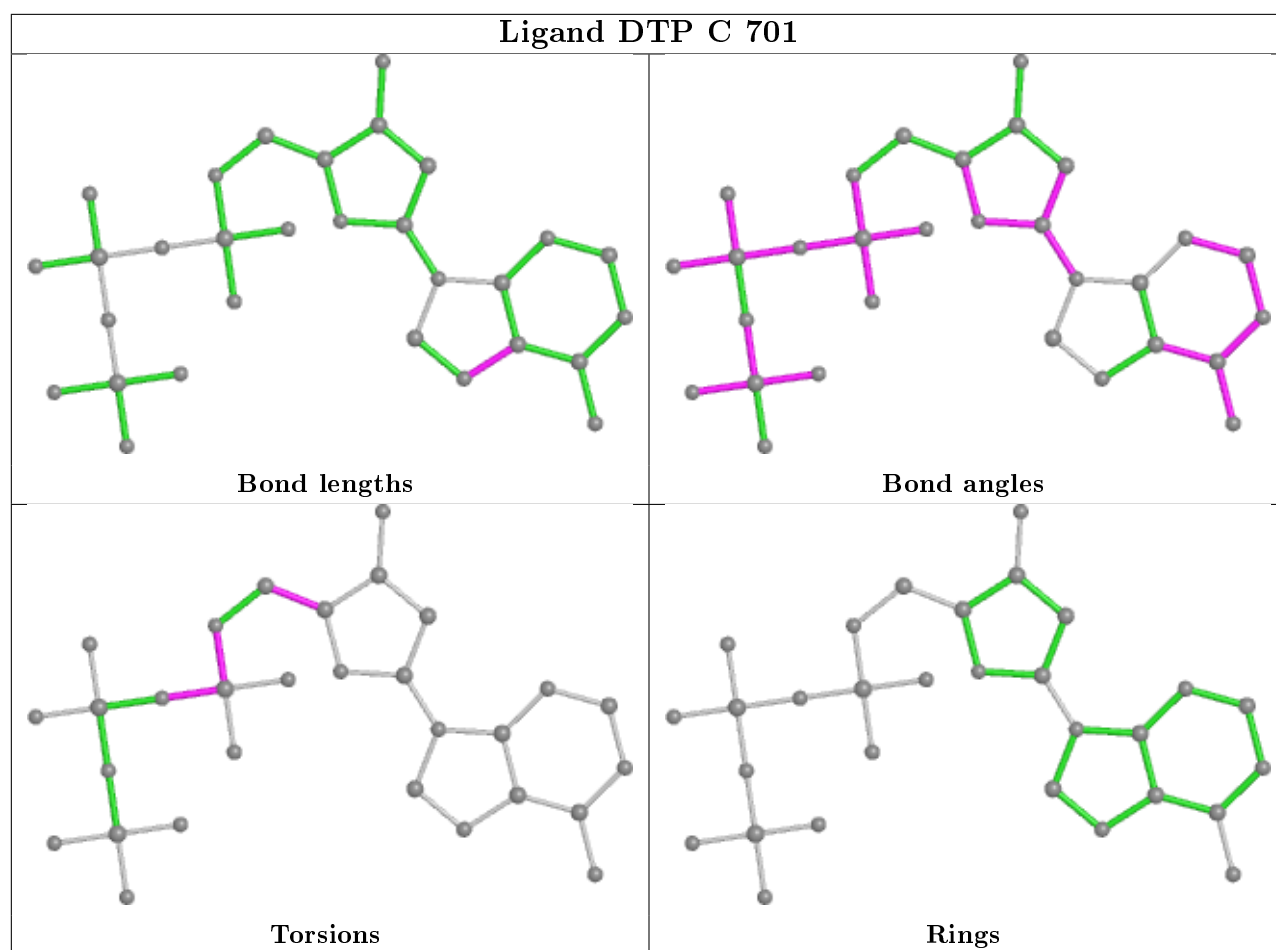
## Ligand 0KX N 704



## Ligand 0KX M 705







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	481/520 (92%)	0.01	1 (0%) 95 94	21, 41, 68, 81	0
1	B	478/520 (91%)	-0.00	2 (0%) 92 91	18, 37, 79, 110	0
1	C	480/520 (92%)	-0.01	0 100 100	17, 36, 58, 90	0
1	D	481/520 (92%)	-0.04	0 100 100	18, 37, 58, 83	0
1	E	478/520 (91%)	0.40	15 (3%) 49 42	36, 66, 114, 142	0
1	F	463/520 (89%)	0.41	13 (2%) 53 47	39, 64, 105, 120	0
1	G	463/520 (89%)	0.41	17 (3%) 41 33	35, 61, 107, 120	0
1	H	478/520 (91%)	0.16	4 (0%) 86 85	28, 50, 74, 86	0
1	I	477/520 (91%)	0.07	1 (0%) 95 94	25, 50, 74, 93	0
1	J	479/520 (92%)	0.02	0 100 100	21, 41, 72, 87	0
1	K	480/520 (92%)	0.04	0 100 100	25, 45, 68, 81	0
1	L	475/520 (91%)	0.14	4 (0%) 86 85	25, 49, 91, 120	0
1	M	471/520 (90%)	0.59	28 (5%) 22 16	49, 75, 98, 107	0
1	N	475/520 (91%)	0.44	12 (2%) 57 52	44, 68, 89, 105	0
1	O	465/520 (89%)	0.42	22 (4%) 31 24	36, 64, 104, 124	0
1	P	461/520 (88%)	0.37	13 (2%) 53 47	36, 57, 104, 120	0
All	All	7585/8320 (91%)	0.21	132 (1%) 70 66	17, 52, 95, 142	0

The worst 5 of 132 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	464	GLY	4.8
1	P	582	GLN	4.0
1	A	403	GLY	4.0
1	E	554	CYS	3.8
1	M	498	PHE	3.8

## 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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	SO4	I	707	5/5	0.81	0.15	92,93,97,97	0
3	MG	I	702	1/1	0.81	0.15	55,55,55,55	0
3	MG	G	703	1/1	0.86	0.13	52,52,52,52	0
3	MG	N	702	1/1	0.89	0.15	40,40,40,40	0
3	MG	B	702	1/1	0.89	0.31	61,61,61,61	0
6	SO4	L	708	5/5	0.89	0.17	72,75,77,80	0
3	MG	K	703	1/1	0.90	0.31	68,68,68,68	0
6	SO4	B	707	5/5	0.90	0.16	67,68,70,71	0
3	MG	N	703	1/1	0.91	0.11	40,40,40,40	0
6	SO4	J	706	5/5	0.92	0.14	70,72,73,74	0
6	SO4	A	707	5/5	0.92	0.17	83,84,84,85	0
3	MG	H	704	1/1	0.92	0.08	37,37,37,37	0
3	MG	K	705	1/1	0.93	0.08	30,30,30,30	0
6	SO4	M	707	5/5	0.93	0.15	88,89,90,92	0
3	MG	M	702	1/1	0.93	0.21	59,59,59,59	0
3	MG	E	702	1/1	0.93	0.23	32,32,32,32	0
3	MG	P	703	1/1	0.93	0.09	39,39,39,39	0
4	OKX	M	705	28/28	0.93	0.17	52,56,59,61	0
5	GTP	F	705	32/32	0.94	0.16	44,48,53,55	0
3	MG	D	703	1/1	0.94	0.15	32,32,32,32	0
3	MG	M	703	1/1	0.94	0.18	46,46,46,46	0
3	MG	H	703	1/1	0.94	0.17	25,25,25,25	0
6	SO4	H	707	5/5	0.94	0.14	94,94,94,95	0
3	MG	L	703	1/1	0.94	0.19	37,37,37,37	0
3	MG	L	704	1/1	0.94	0.17	20,20,20,20	0
5	GTP	H	706	32/32	0.95	0.13	36,39,43,45	0
5	GTP	O	706	32/32	0.95	0.15	45,50,58,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	SO4	D	708	5/5	0.95	0.11	69,71,72,73	0
5	GTP	M	706	32/32	0.95	0.17	48,51,56,56	0
3	MG	G	704	1/1	0.95	0.21	33,33,33,33	0
4	0KX	G	706	28/28	0.95	0.15	40,45,47,49	0
5	GTP	N	705	32/32	0.95	0.15	50,52,54,54	0
3	MG	F	703	1/1	0.95	0.09	44,44,44,44	0
7	DTP	P	701	30/30	0.96	0.16	44,45,49,51	0
3	MG	F	702	1/1	0.96	0.25	35,35,35,35	0
3	MG	C	703	1/1	0.96	0.16	32,32,32,32	0
7	DTP	E	706	30/30	0.96	0.14	28,29,34,34	0
7	DTP	F	706	30/30	0.96	0.15	36,39,45,47	0
3	MG	I	703	1/1	0.96	0.17	20,20,20,20	0
4	0KX	O	705	28/28	0.96	0.17	48,51,56,59	0
3	MG	P	705	1/1	0.96	0.08	43,43,43,43	0
5	GTP	O	707	32/32	0.96	0.14	37,41,47,48	0
7	DTP	G	701	30/30	0.96	0.17	41,44,52,54	0
4	0KX	N	704	28/28	0.96	0.16	51,54,55,55	0
5	GTP	G	707	32/32	0.97	0.12	30,31,32,33	0
4	0KX	H	705	28/28	0.97	0.14	38,40,42,44	0
4	0KX	E	704	28/28	0.97	0.13	42,45,48,50	0
2	FE	I	701	1/1	0.97	0.10	25,25,25,25	0
7	DTP	N	706	30/30	0.97	0.18	38,43,48,50	0
5	GTP	K	707	32/32	0.97	0.15	36,40,44,46	0
4	0KX	F	704	28/28	0.97	0.15	42,47,50,52	0
7	DTP	J	707	30/30	0.97	0.17	19,21,23,23	0
4	0KX	A	705	28/28	0.97	0.14	23,29,32,33	0
2	FE	P	702	1/1	0.97	0.12	30,30,30,30	0
7	DTP	L	701	30/30	0.97	0.15	26,28,31,32	0
3	MG	E	703	1/1	0.97	0.09	52,52,52,52	0
5	GTP	A	706	32/32	0.97	0.14	21,23,27,29	0
3	MG	A	702	1/1	0.97	0.15	48,48,48,48	0
4	0KX	C	706	28/28	0.97	0.14	19,21,26,27	0
4	0KX	I	705	28/28	0.97	0.14	28,31,33,34	0
3	MG	L	705	1/1	0.97	0.13	22,22,22,22	0
7	DTP	A	708	30/30	0.97	0.17	21,25,26,28	0
7	DTP	D	701	30/30	0.97	0.15	20,25,28,30	0
5	GTP	L	707	32/32	0.97	0.14	21,24,26,27	0
7	DTP	H	701	30/30	0.97	0.15	39,43,49,52	0
4	0KX	P	706	28/28	0.97	0.18	40,43,50,53	0
4	0KX	J	704	28/28	0.97	0.16	23,26,28,29	0
7	DTP	O	701	30/30	0.97	0.15	44,46,49,49	0
7	DTP	M	708	30/30	0.97	0.18	41,45,58,59	0

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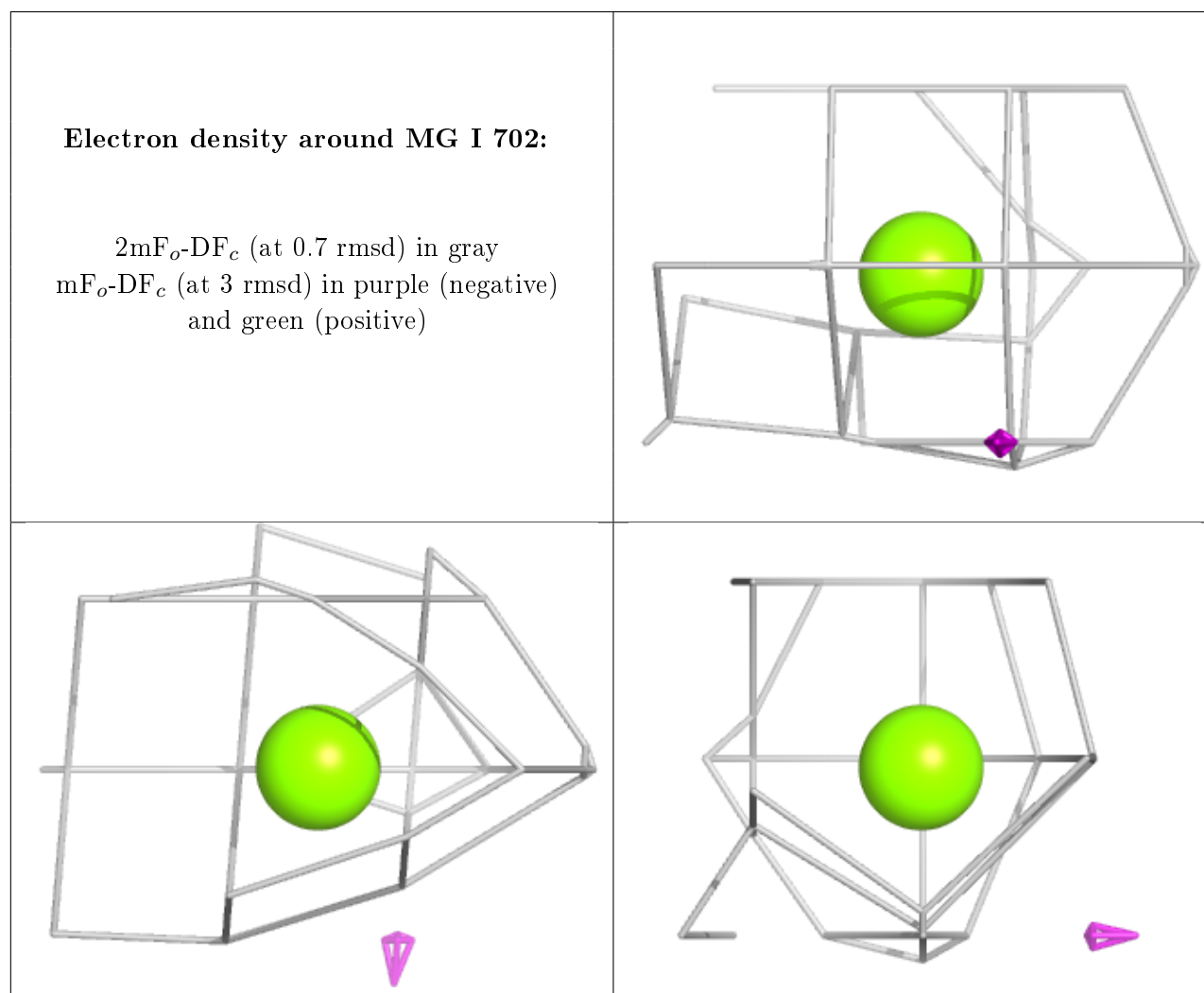
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	K	704	1/1	0.97	0.14	19,19,19,19	0
3	MG	D	705	1/1	0.97	0.11	23,23,23,23	0
4	OKX	L	706	28/28	0.97	0.13	31,35,39,41	0
5	GTP	E	705	32/32	0.97	0.12	45,49,55,57	0
3	MG	D	704	1/1	0.97	0.21	13,13,13,13	0
5	GTP	I	706	32/32	0.97	0.16	26,29,37,38	0
5	GTP	J	705	32/32	0.97	0.12	21,23,25,26	0
7	DTP	I	708	30/30	0.97	0.16	30,33,38,39	0
4	OKX	D	706	28/28	0.97	0.15	21,23,27,30	0
6	SO4	C	708	5/5	0.97	0.11	57,57,59,60	0
2	FE	N	701	1/1	0.98	0.09	38,38,38,38	0
7	DTP	C	701	30/30	0.98	0.14	16,18,23,24	0
4	OKX	K	706	28/28	0.98	0.16	31,34,38,40	0
7	DTP	B	708	30/30	0.98	0.15	15,16,19,19	0
5	GTP	C	707	32/32	0.98	0.14	21,23,26,27	0
7	DTP	K	701	30/30	0.98	0.14	25,28,30,30	0
3	MG	C	704	1/1	0.98	0.21	13,13,13,13	0
2	FE	G	702	1/1	0.98	0.10	30,30,30,30	0
3	MG	J	703	1/1	0.98	0.12	18,18,18,18	0
5	GTP	D	707	32/32	0.98	0.13	16,17,19,20	0
5	GTP	B	706	32/32	0.98	0.14	20,22,26,27	0
3	MG	I	704	1/1	0.98	0.09	23,23,23,23	0
3	MG	G	705	1/1	0.98	0.07	25,25,25,25	0
3	MG	A	704	1/1	0.98	0.08	20,20,20,20	0
3	MG	B	704	1/1	0.98	0.12	20,20,20,20	0
3	MG	B	703	1/1	0.98	0.15	13,13,13,13	0
3	MG	P	704	1/1	0.98	0.24	28,28,28,28	0
3	MG	O	703	1/1	0.98	0.13	31,31,31,31	0
3	MG	O	704	1/1	0.98	0.06	43,43,43,43	0
3	MG	J	702	1/1	0.98	0.09	17,17,17,17	0
4	OKX	B	705	28/28	0.98	0.14	19,22,24,25	0
2	FE	M	701	1/1	0.99	0.08	44,44,44,44	0
2	FE	A	701	1/1	0.99	0.12	22,22,22,22	0
2	FE	K	702	1/1	0.99	0.10	28,28,28,28	0
2	FE	D	702	1/1	0.99	0.14	14,14,14,14	0
2	FE	B	701	1/1	0.99	0.12	16,16,16,16	0
2	FE	E	701	1/1	0.99	0.09	42,42,42,42	0
2	FE	H	702	1/1	0.99	0.08	26,26,26,26	0
2	FE	L	702	1/1	0.99	0.10	25,25,25,25	0
2	FE	J	701	1/1	0.99	0.11	18,18,18,18	0
3	MG	M	704	1/1	0.99	0.05	49,49,49,49	0
2	FE	O	702	1/1	0.99	0.09	39,39,39,39	0

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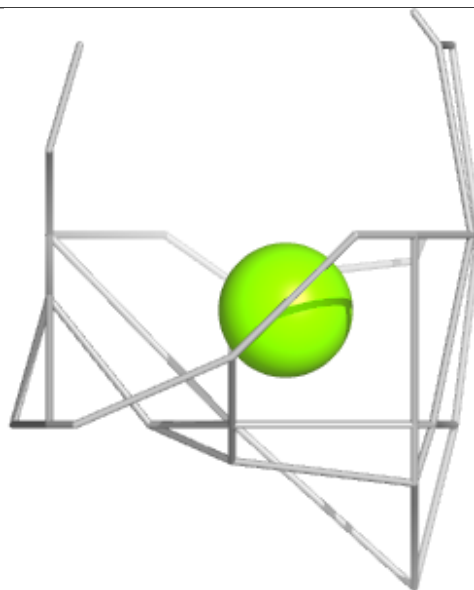
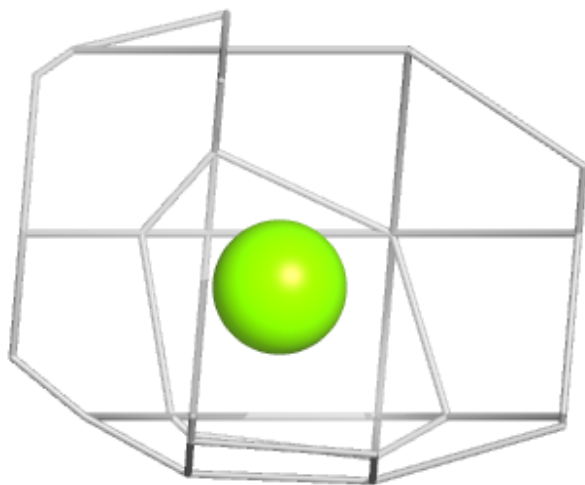
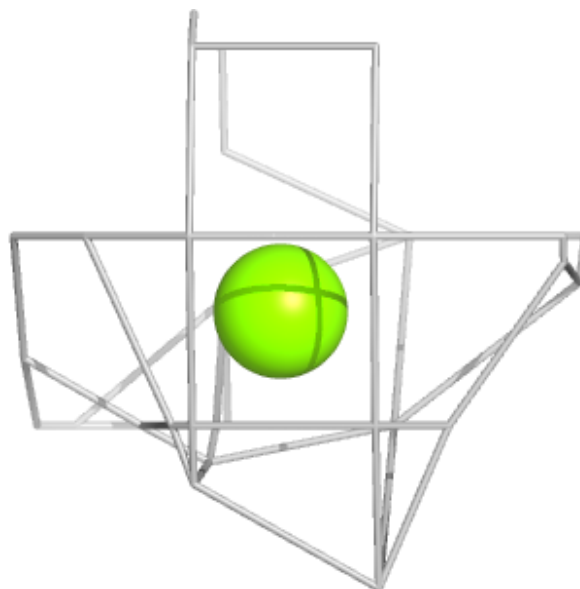
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	C	705	1/1	0.99	0.04	24,24,24,24	0
3	MG	A	703	1/1	0.99	0.23	16,16,16,16	0
2	FE	C	702	1/1	1.00	0.09	17,17,17,17	0
2	FE	F	701	1/1	1.00	0.10	33,33,33,33	0

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.



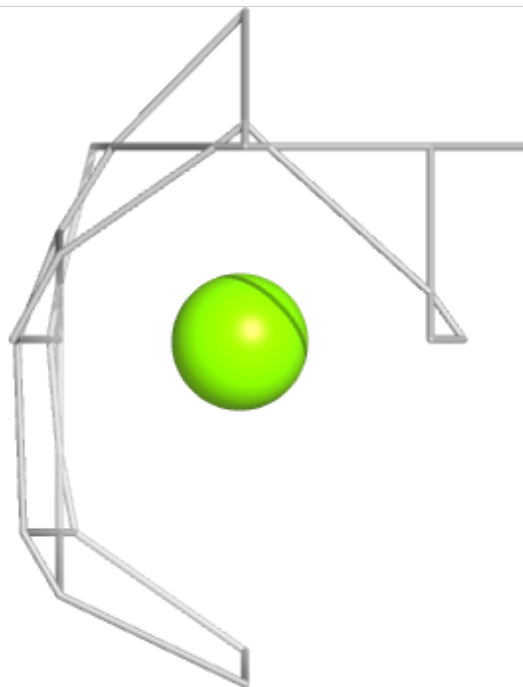
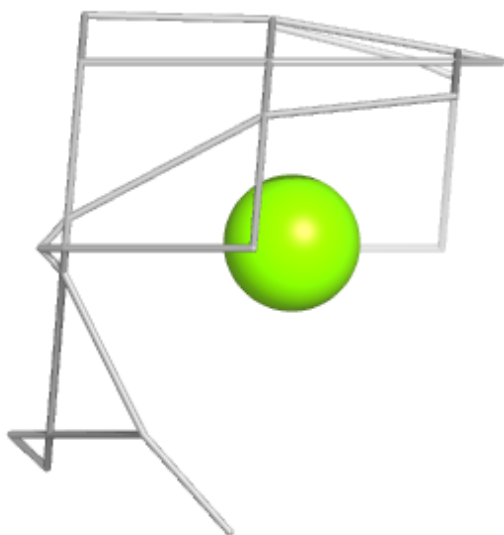
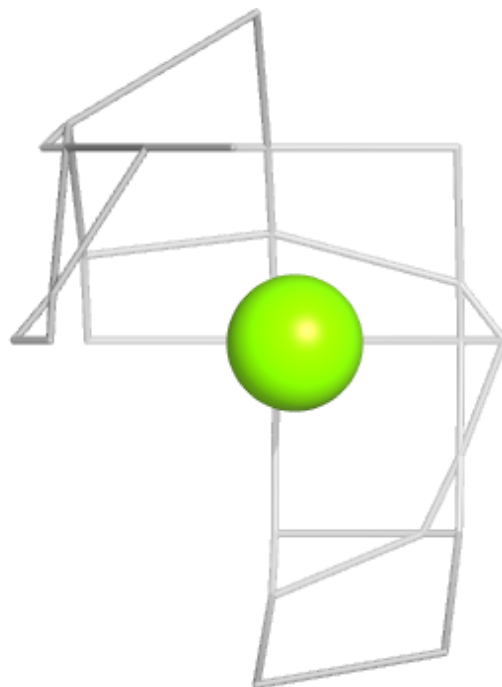
**Electron density around MG G 703:**

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



**Electron density around MG N 702:**

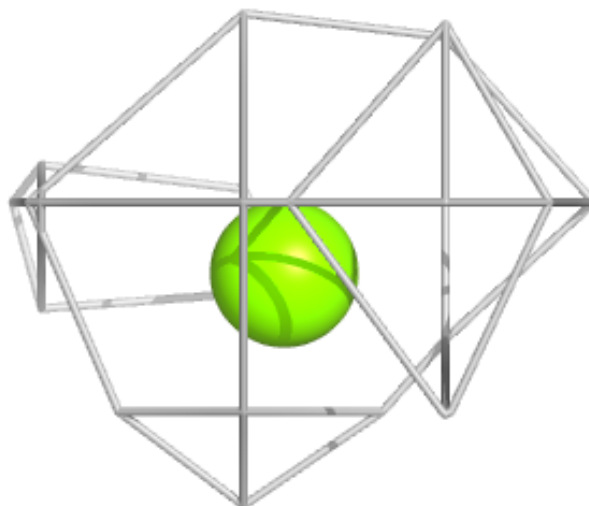
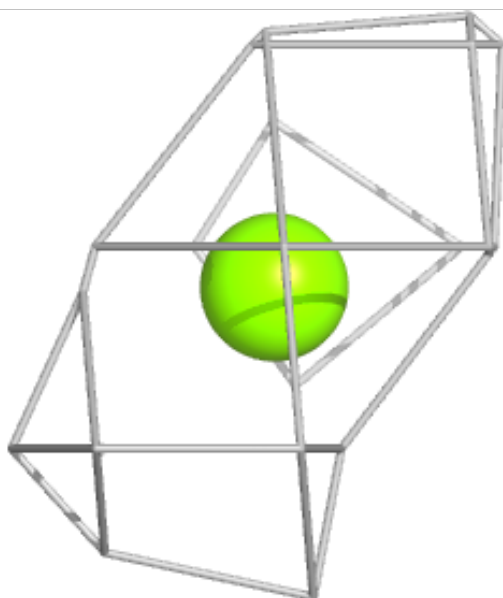
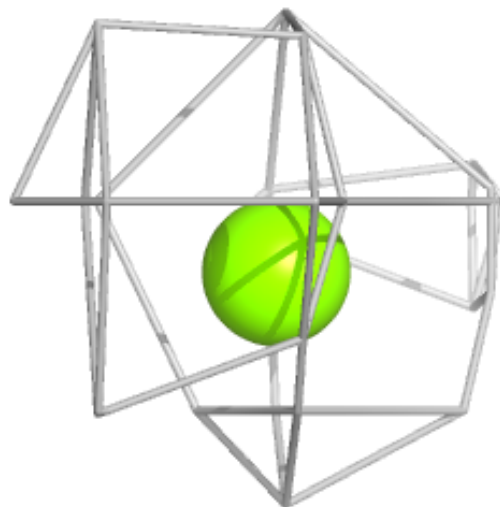
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





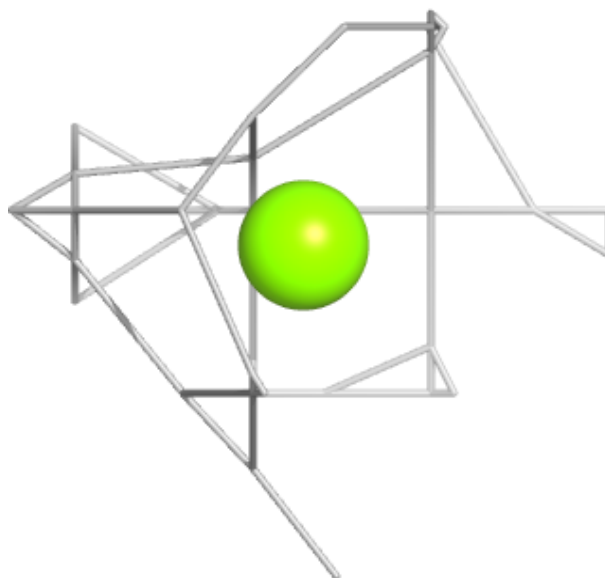
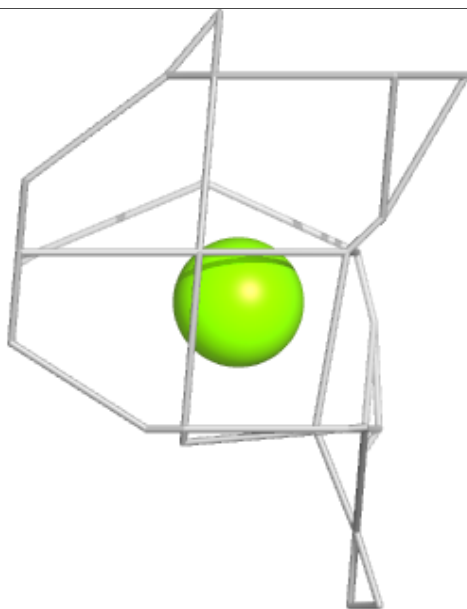
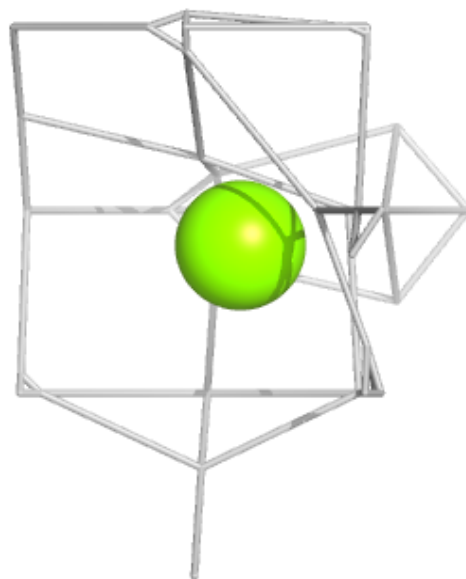
**Electron density around MG B 702:**

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and green (positive)



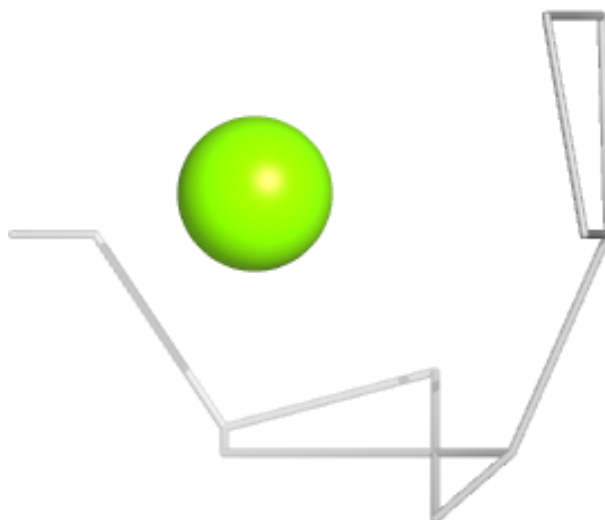
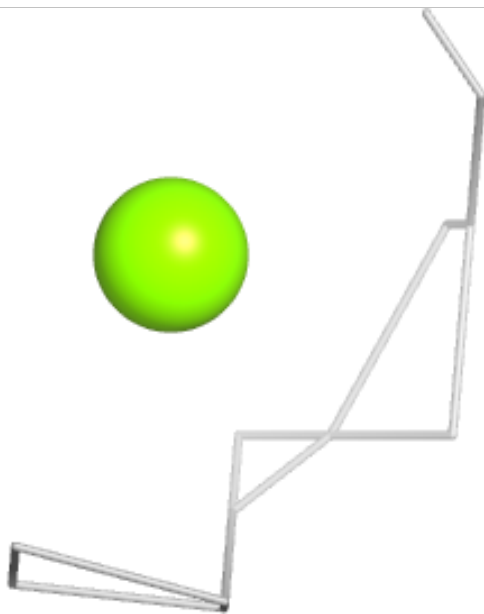
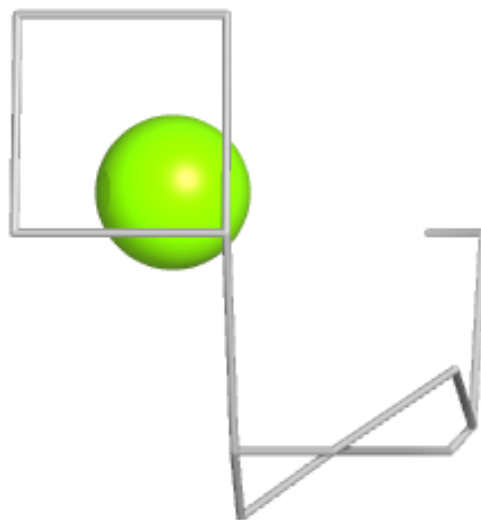
**Electron density around MG K 703:**

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



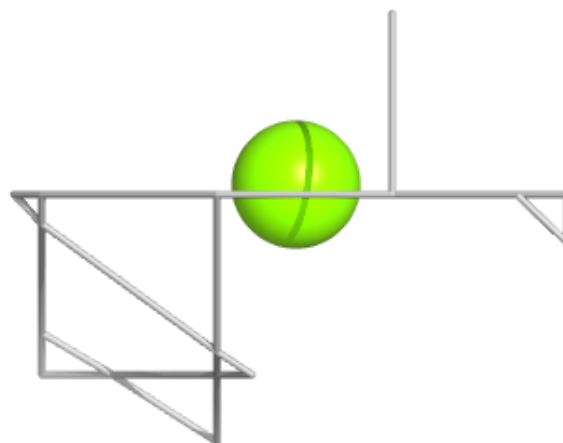
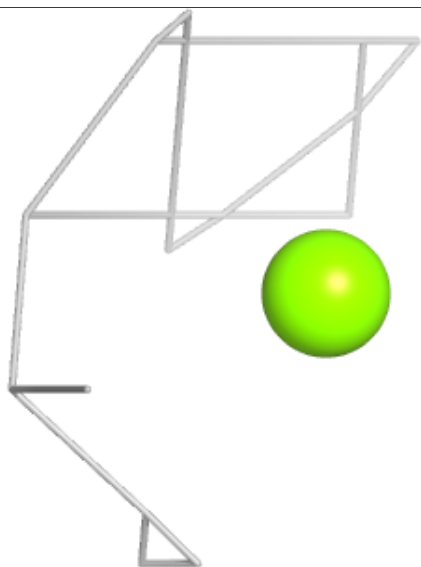
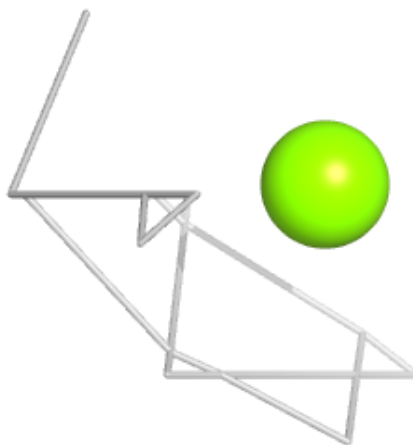
**Electron density around MG N 703:**

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



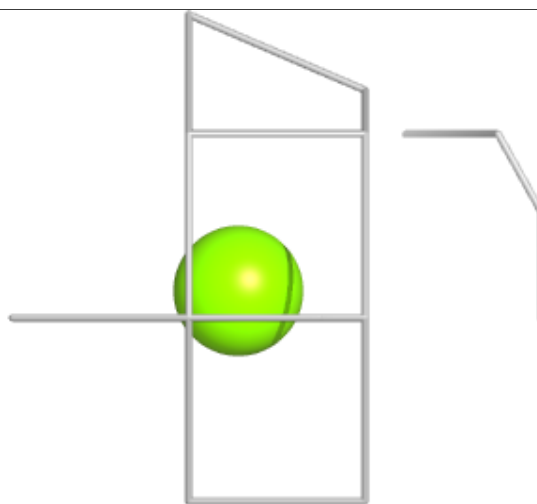
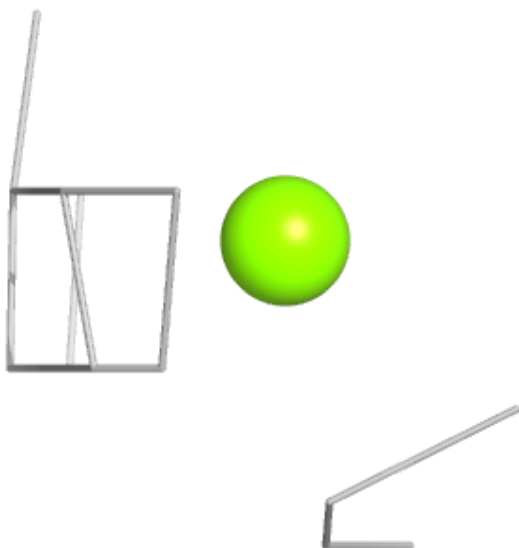
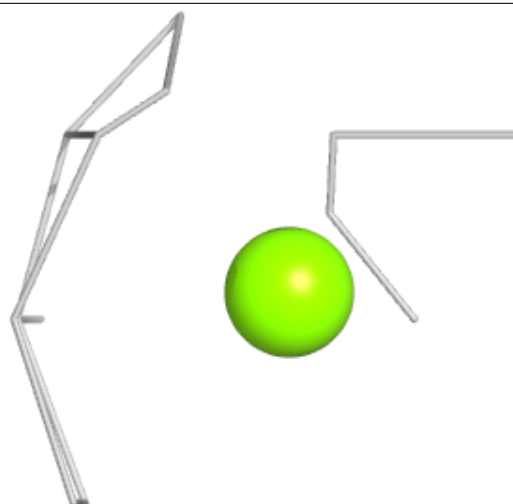
**Electron density around MG H 704:**

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and green (positive)



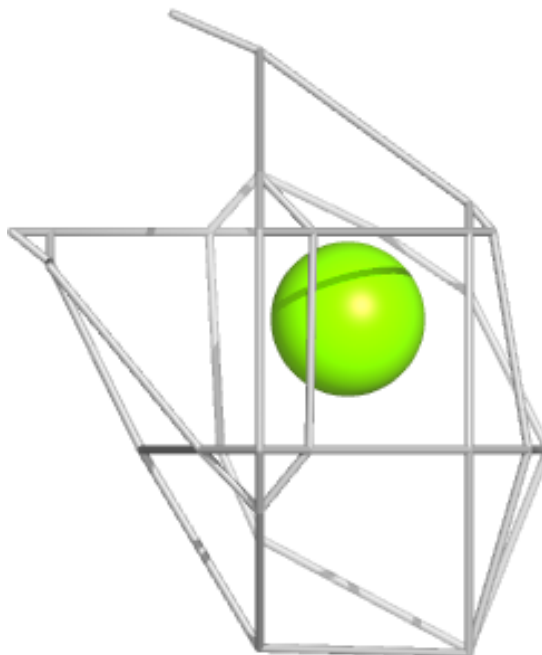
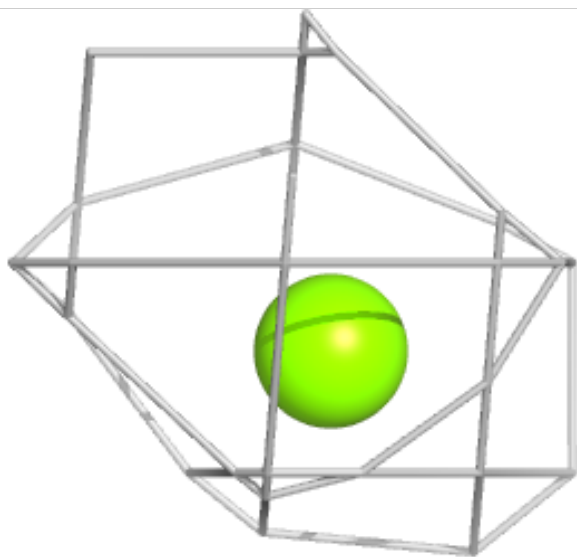
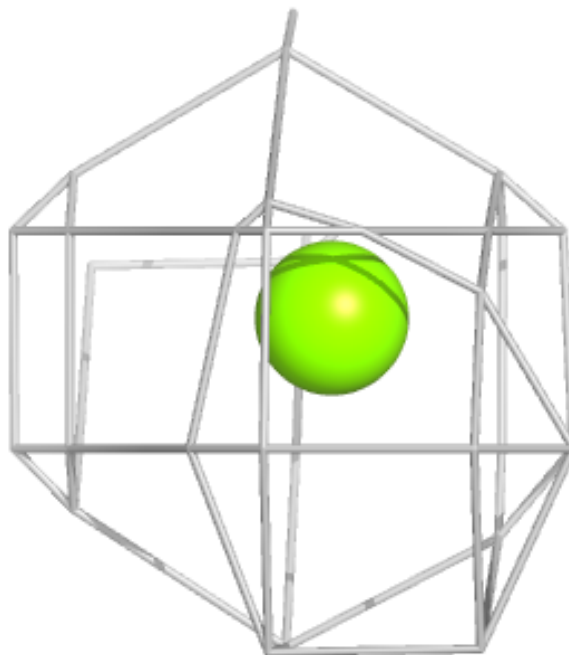
**Electron density around MG K 705:**

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



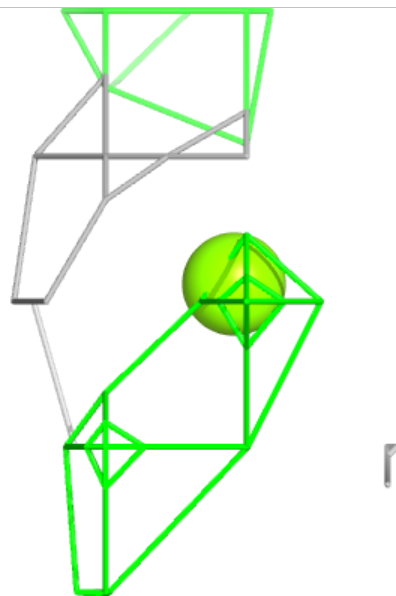
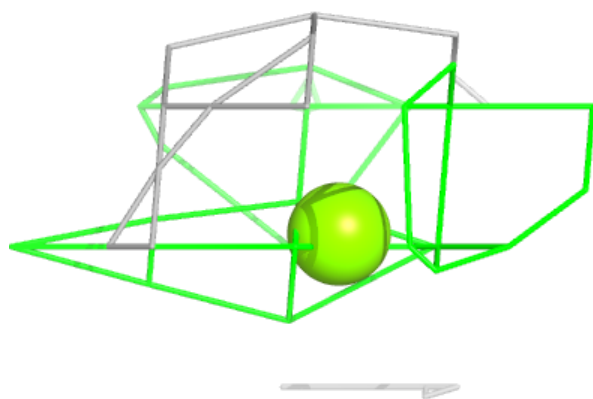
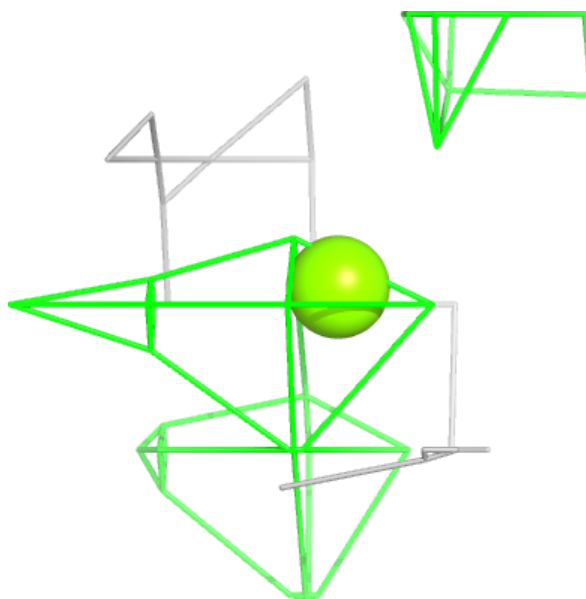
**Electron density around MG M 702:**

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and green (positive)



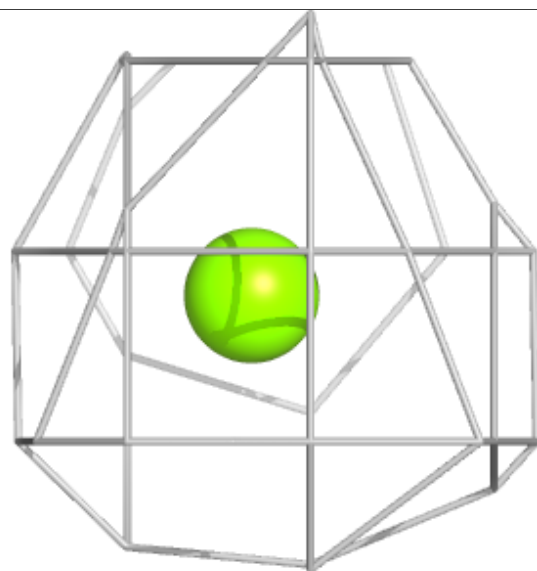
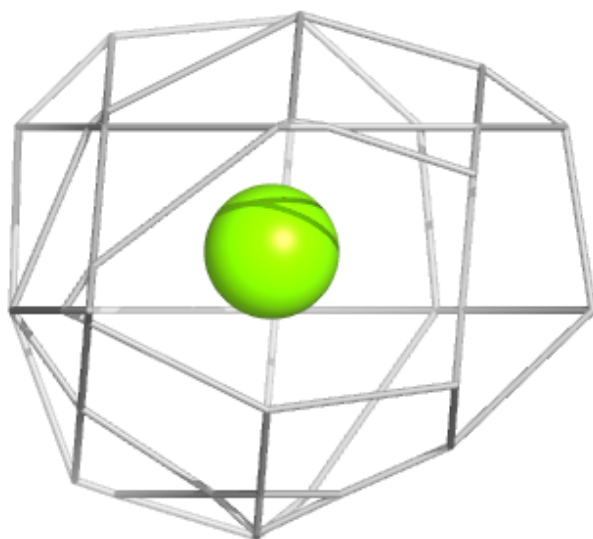
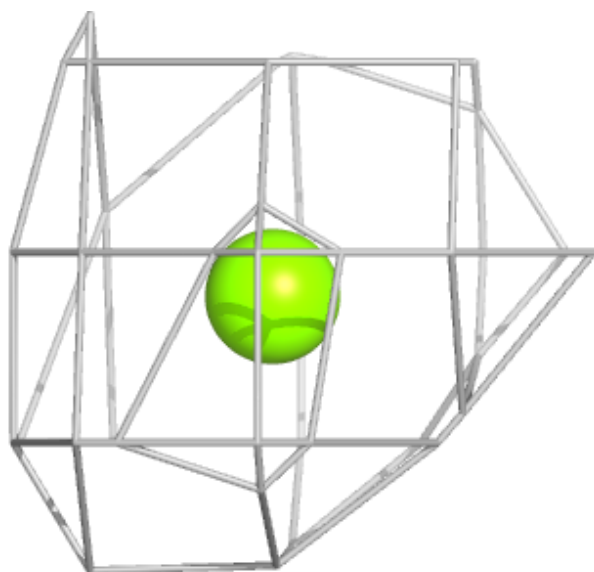
**Electron density around MG E 702:**

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and green (positive)



**Electron density around MG P 703:**

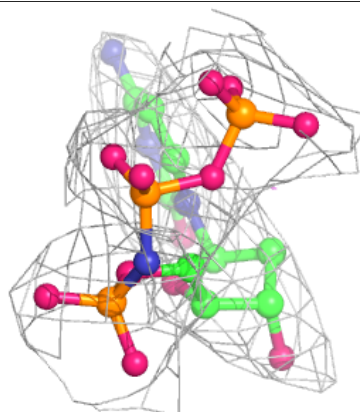
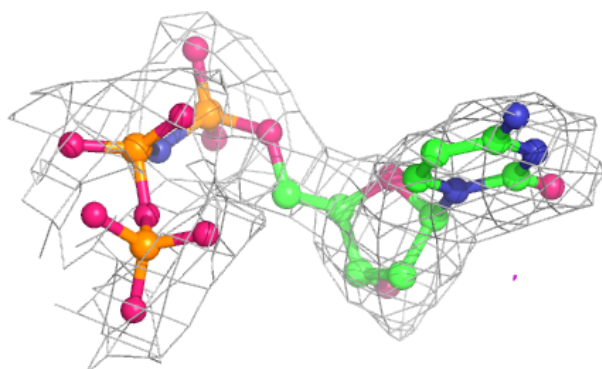
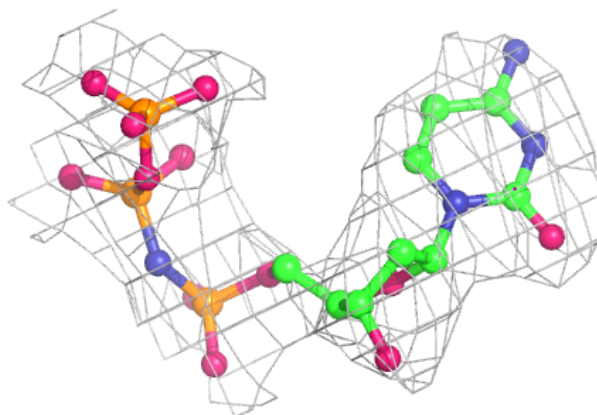
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



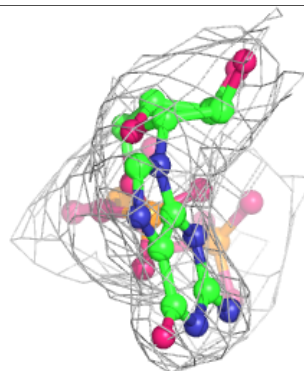
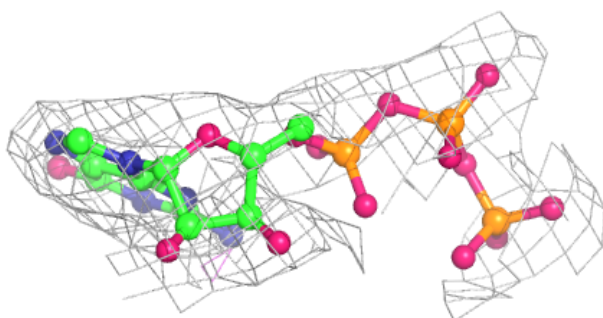
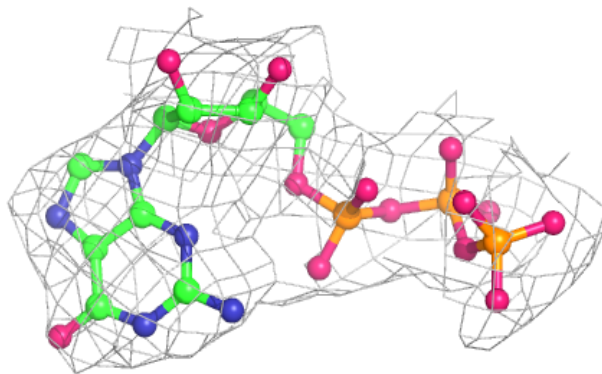


**Electron density around 0KX M 705:**

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

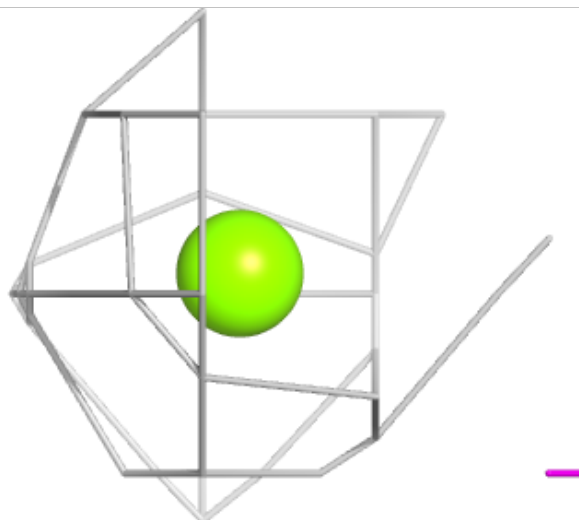
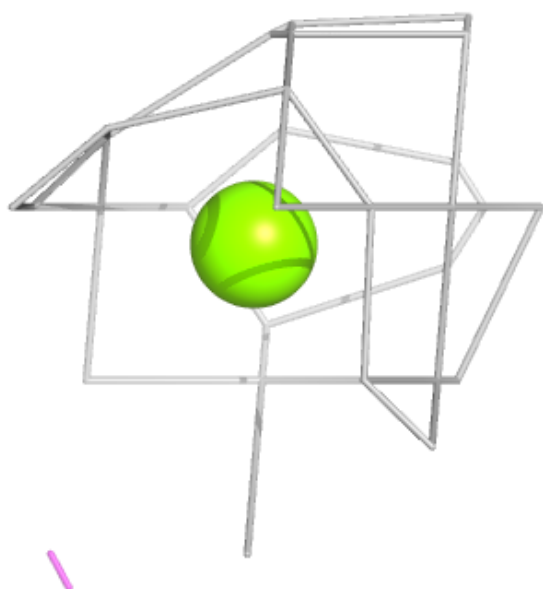
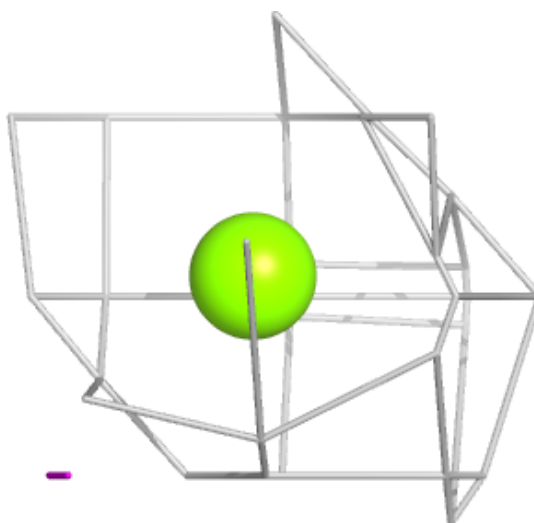
**Electron density around GTP F 705:**

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



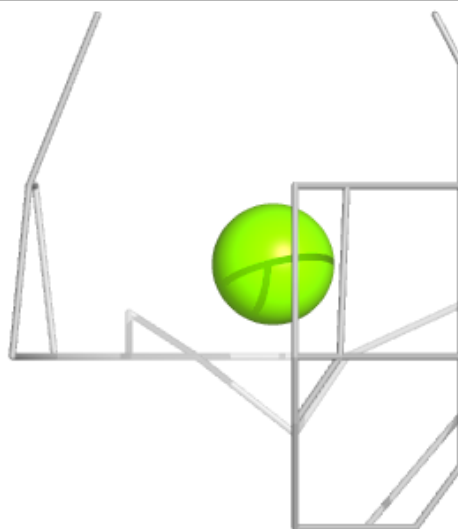
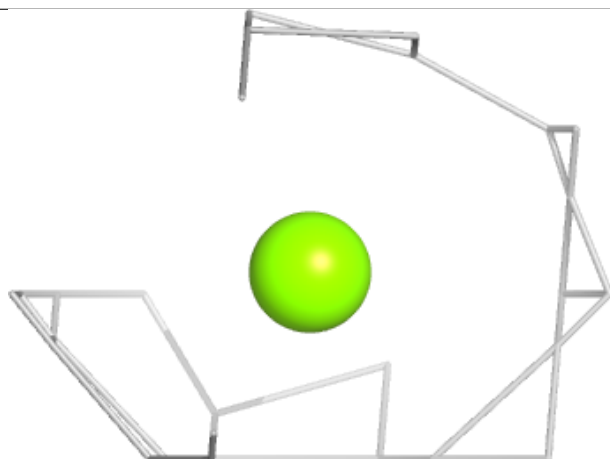
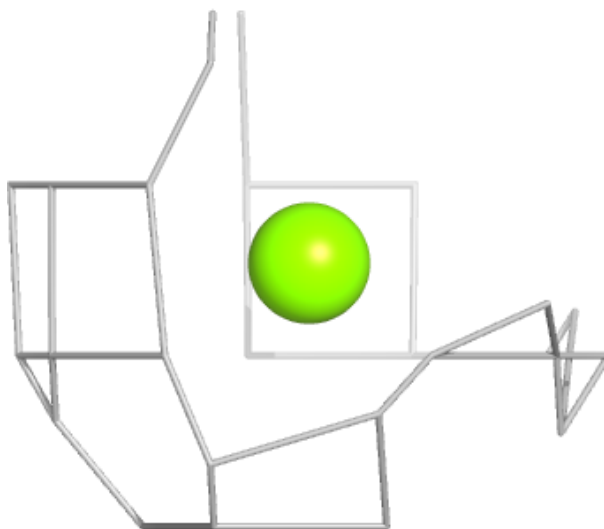
**Electron density around MG D 703:**

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



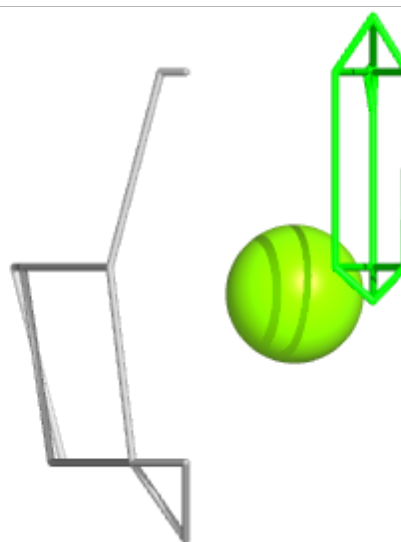
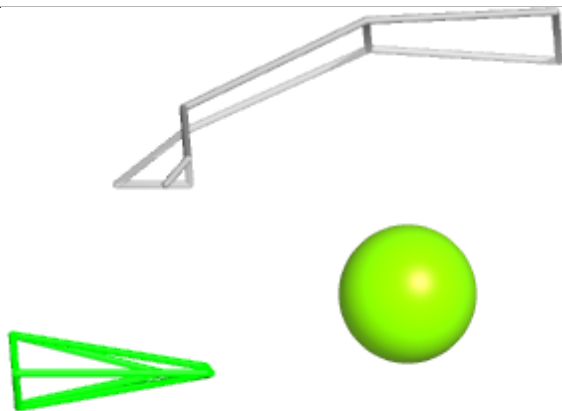
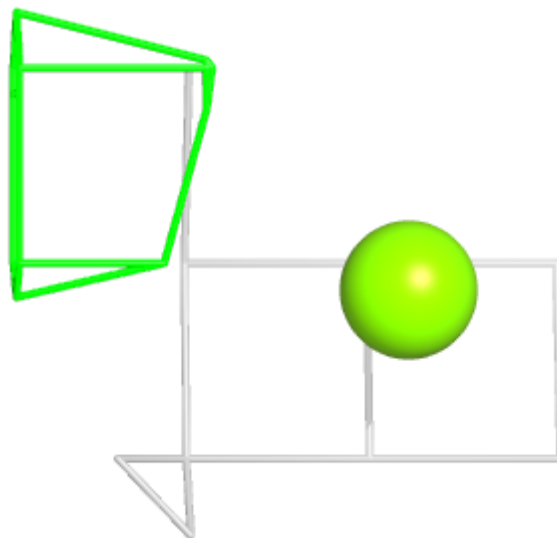
**Electron density around MG M 703:**

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



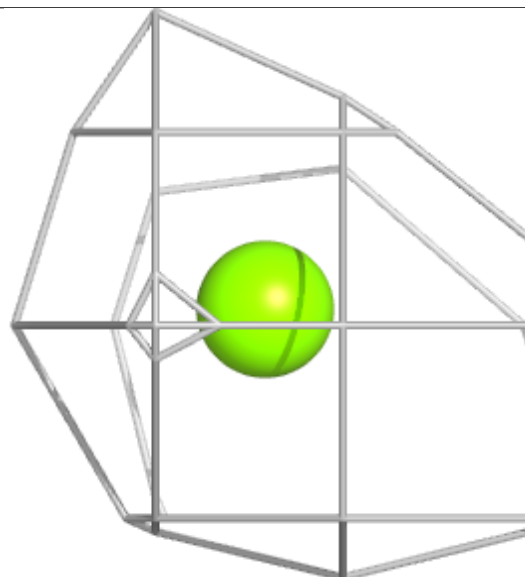
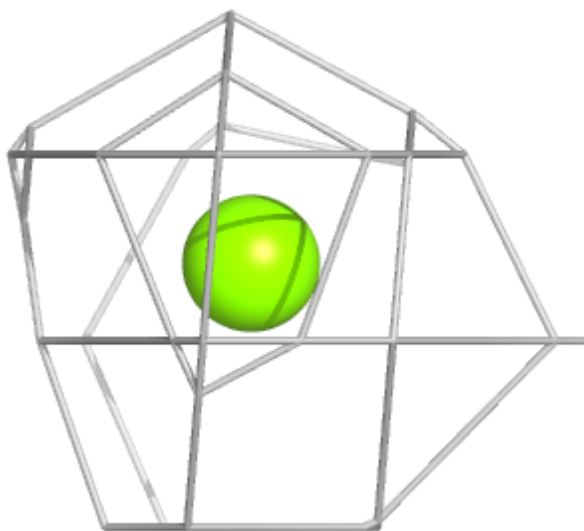
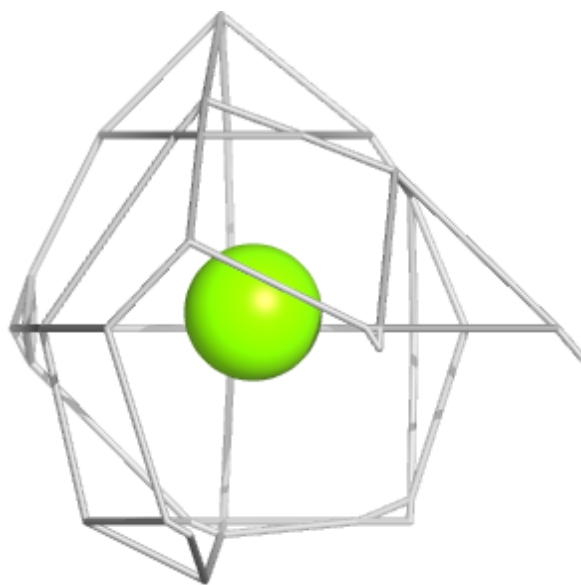
**Electron density around MG H 703:**

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



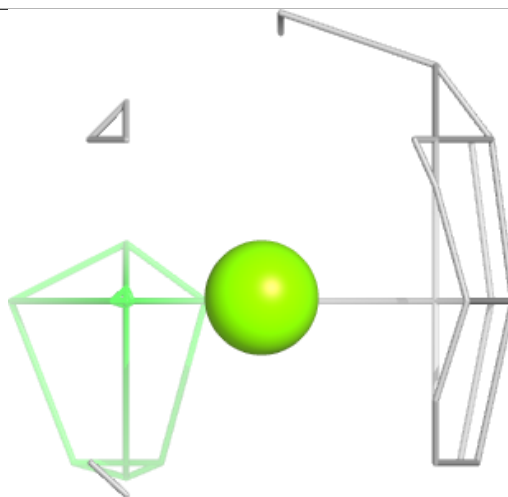
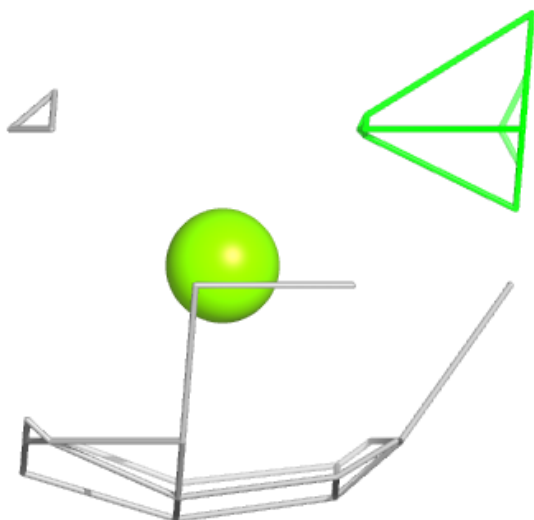
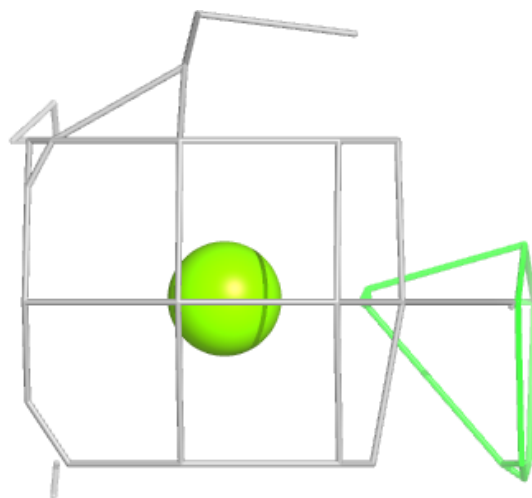
**Electron density around MG L 703:**

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



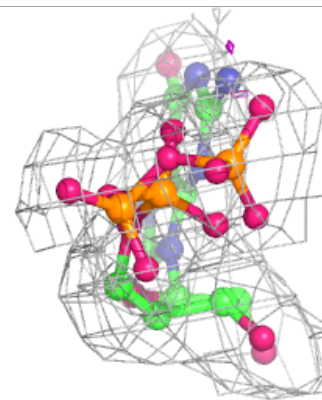
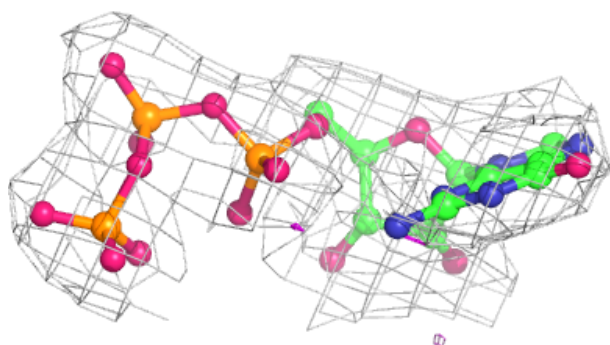
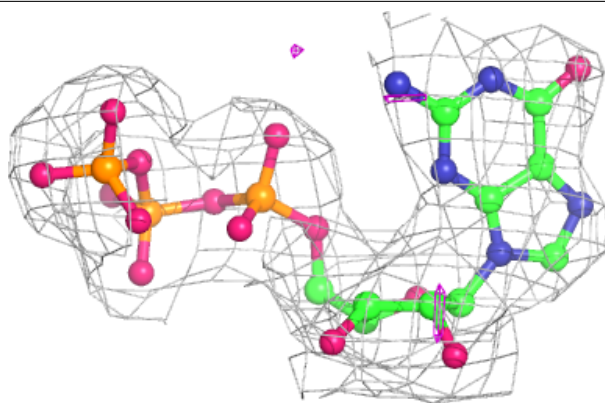
**Electron density around MG L 704:**

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

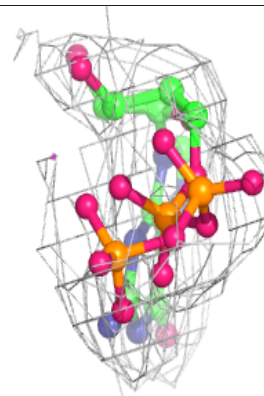
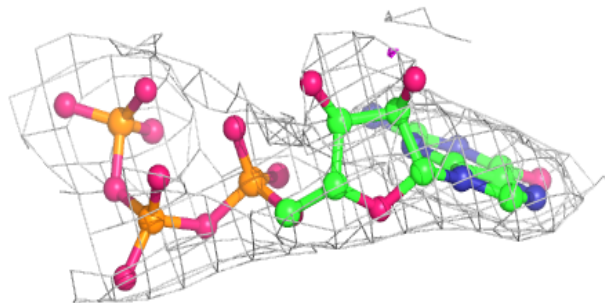
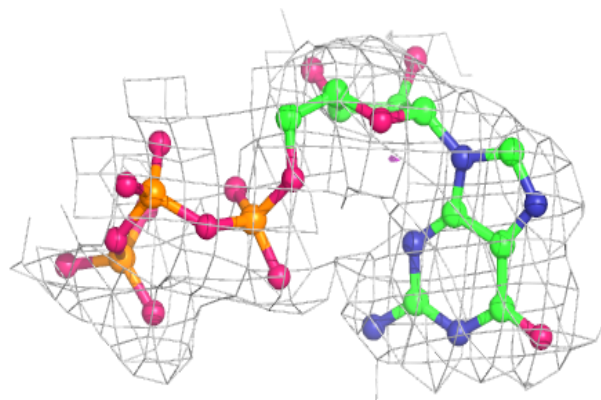


**Electron density around GTP H 706:**

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

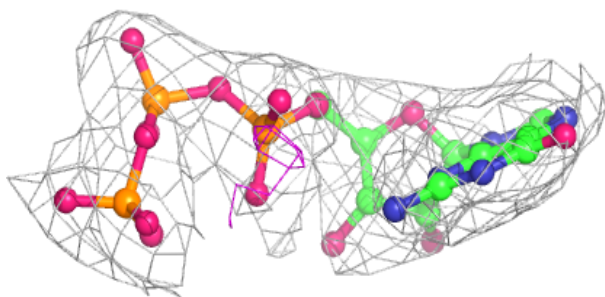
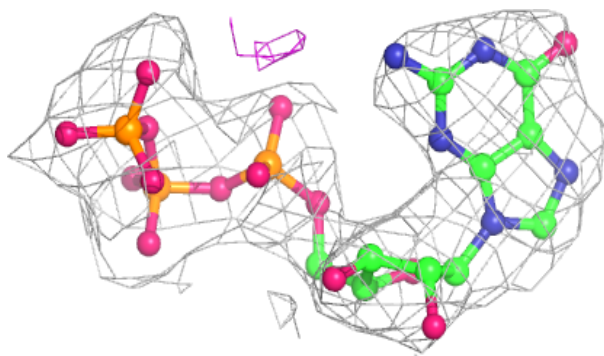
**Electron density around GTP O 706:**

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



**Electron density around GTP M 706:**

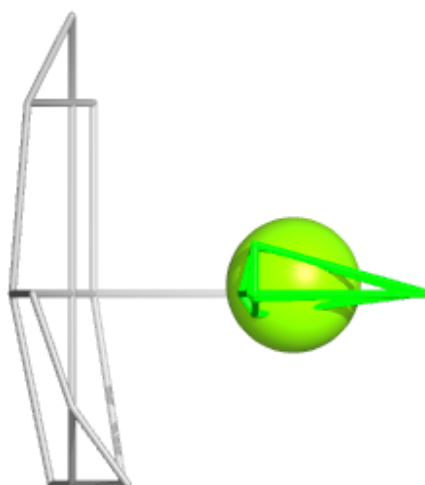
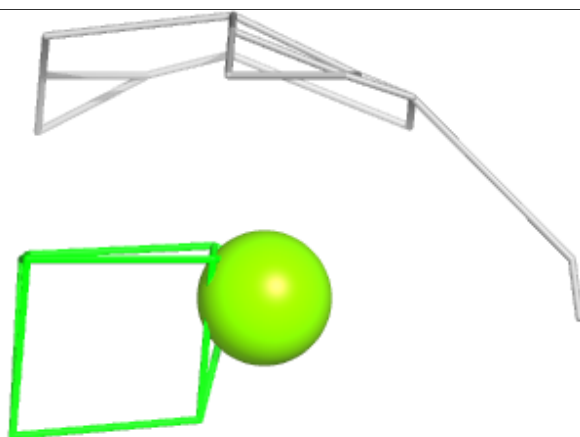
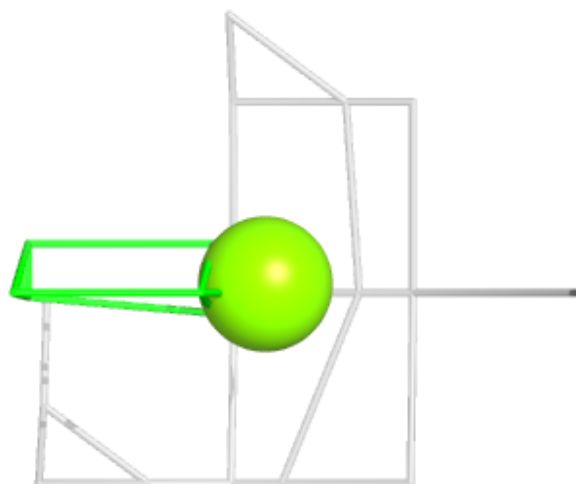
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





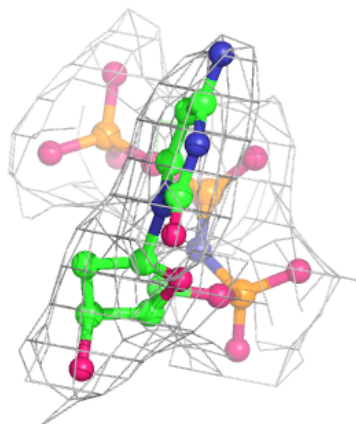
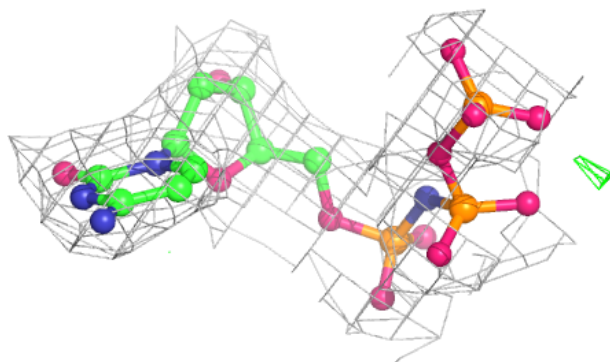
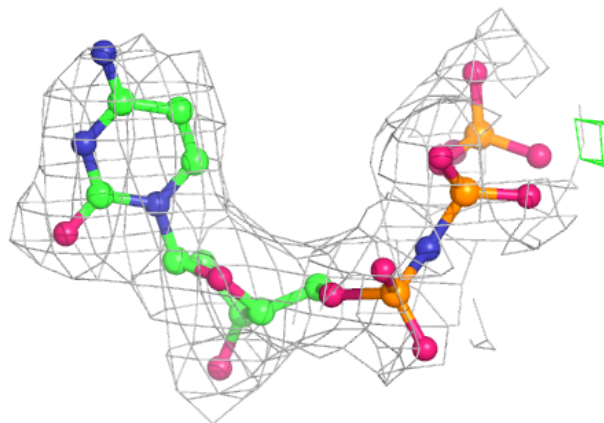
**Electron density around MG G 704:**

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



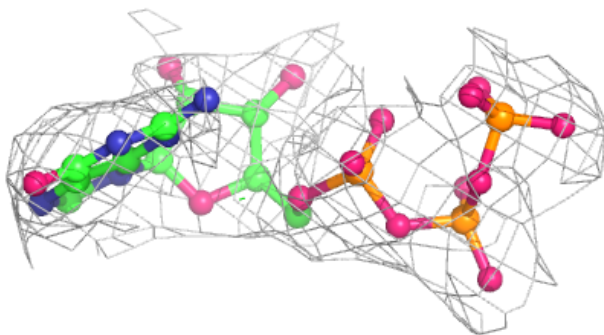
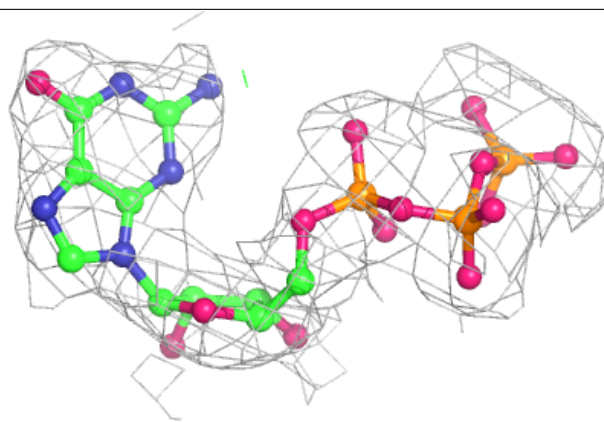
**Electron density around 0KX G 706:**

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



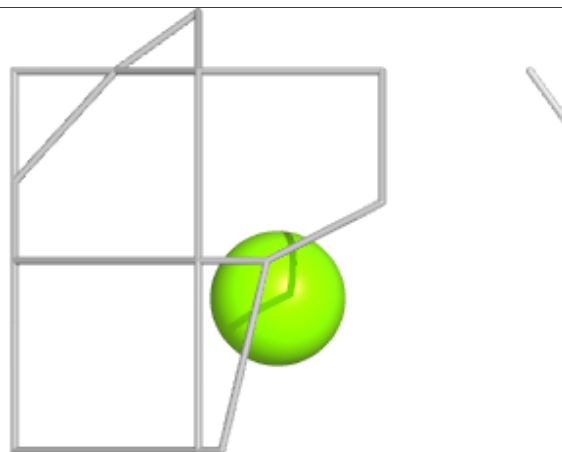
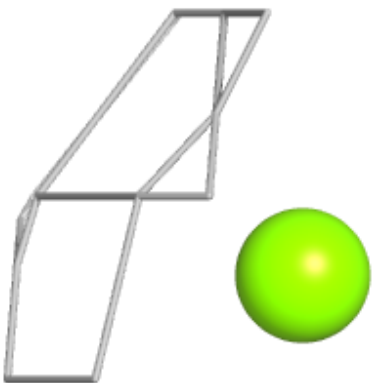
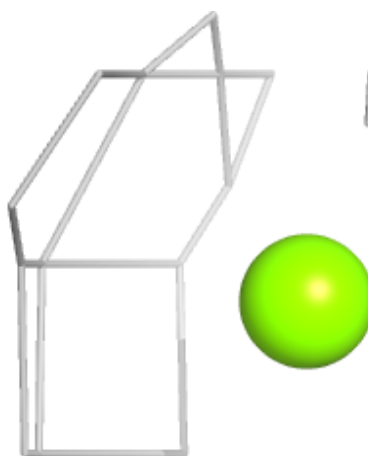
**Electron density around GTP N 705:**

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



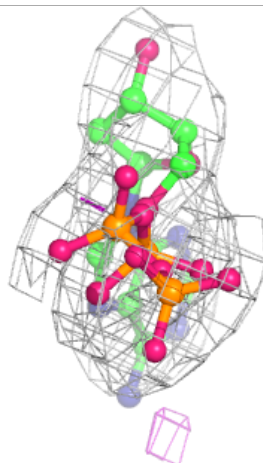
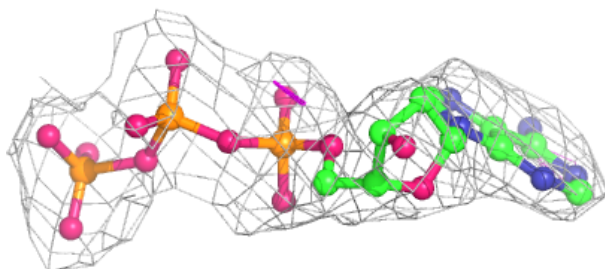
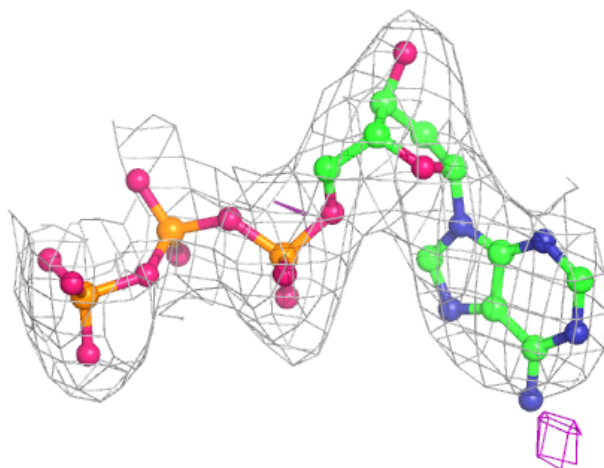
**Electron density around MG F 703:**

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



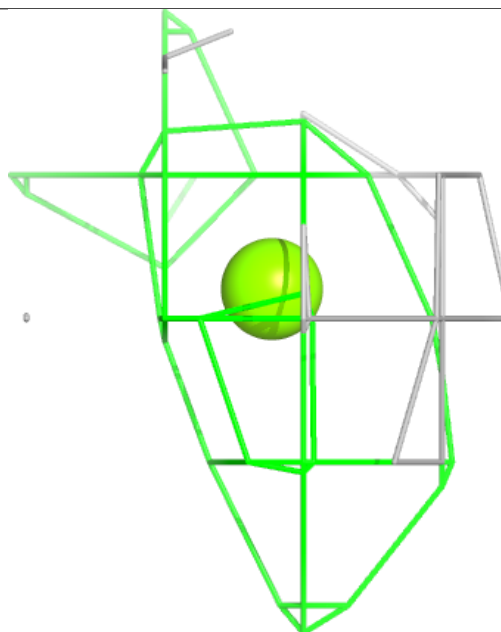
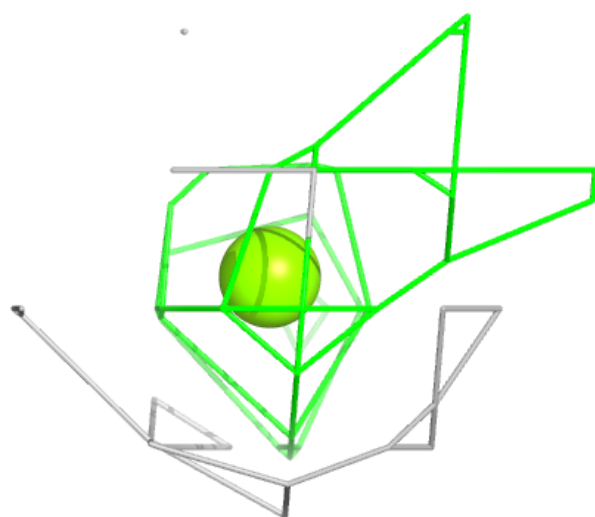
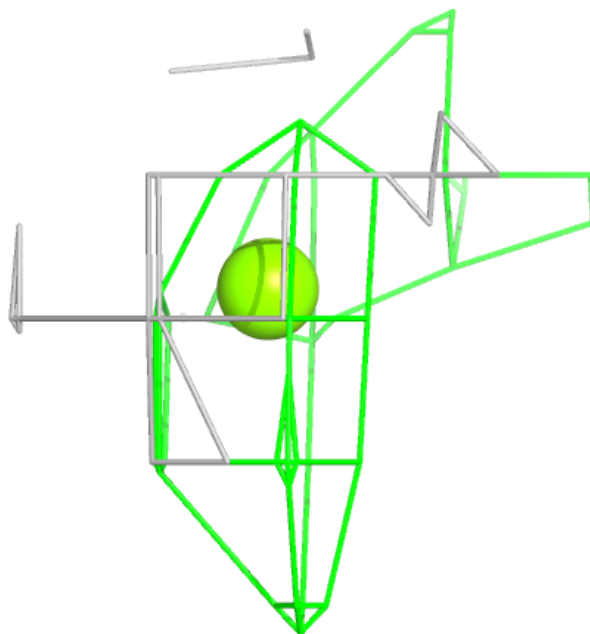
**Electron density around DTP P 701:**

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



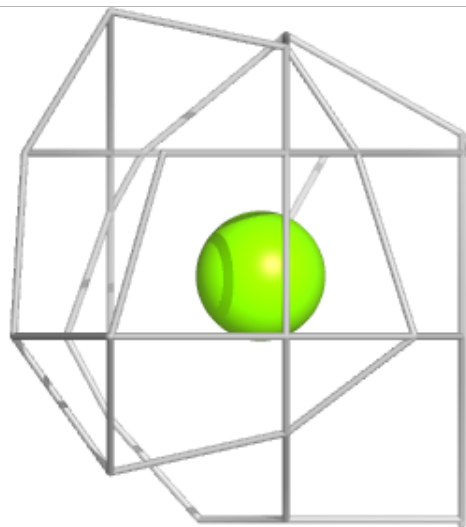
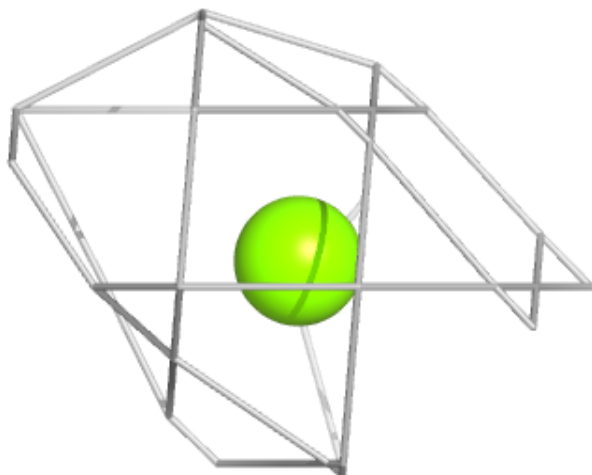
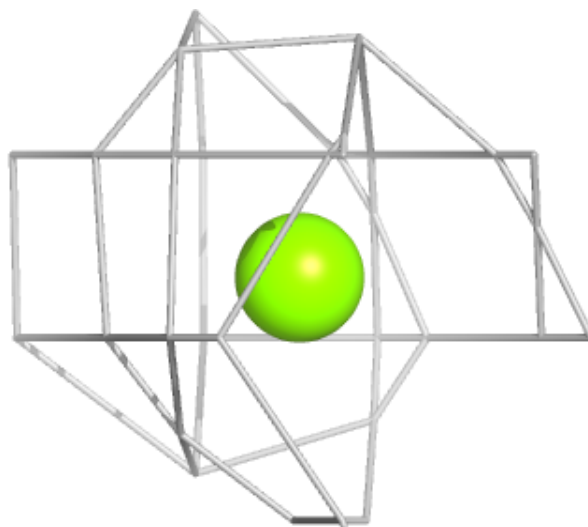
**Electron density around MG F 702:**

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



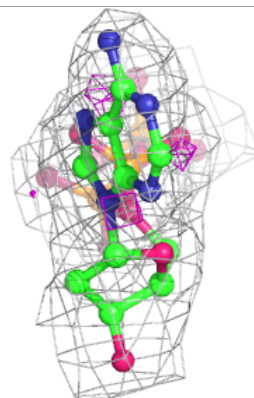
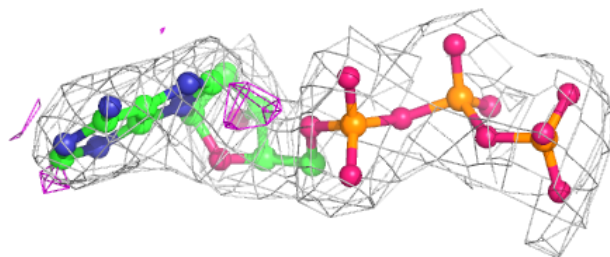
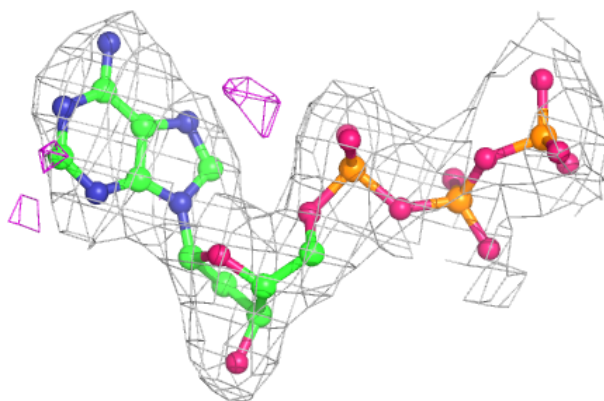
**Electron density around MG C 703:**

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

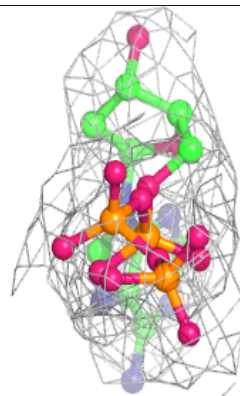
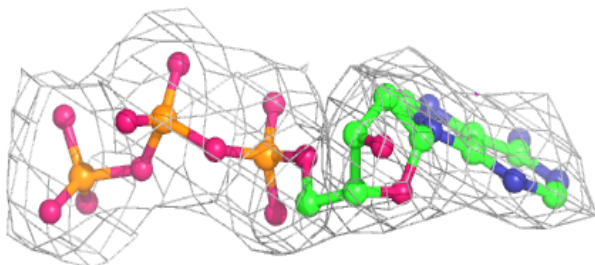
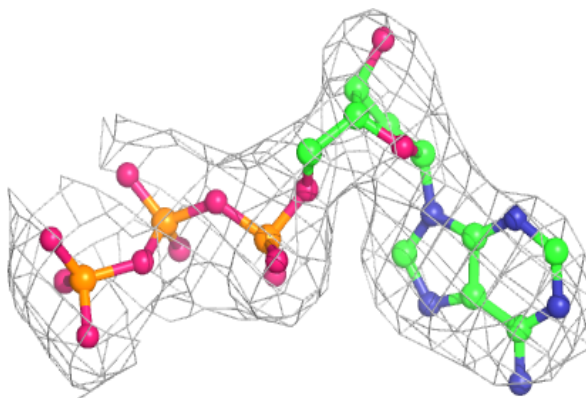


**Electron density around DTP E 706:**

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

**Electron density around DTP F 706:**

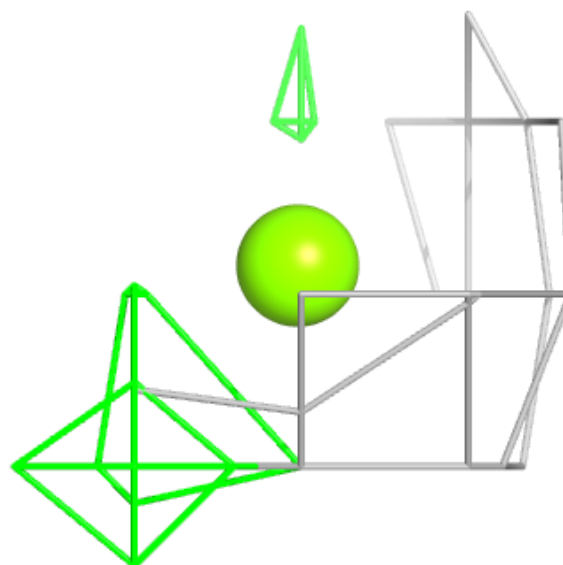
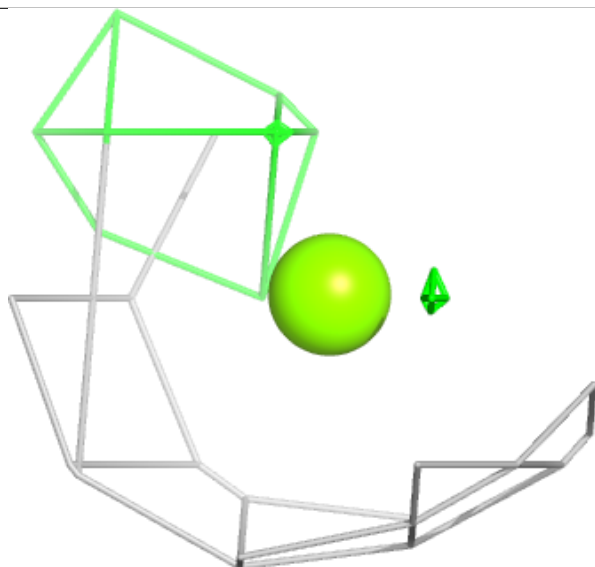
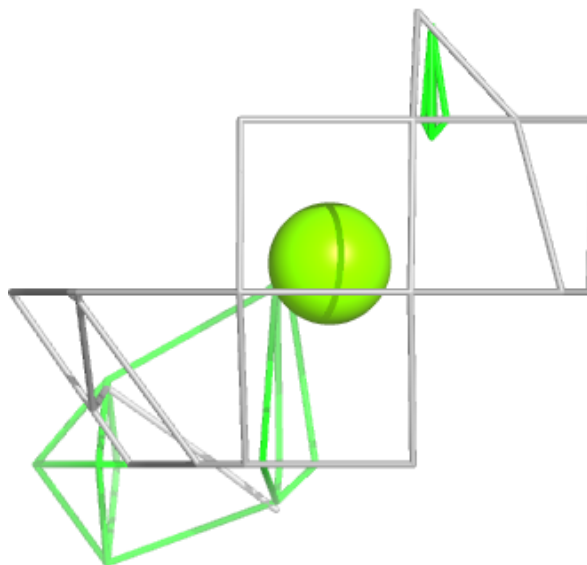
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





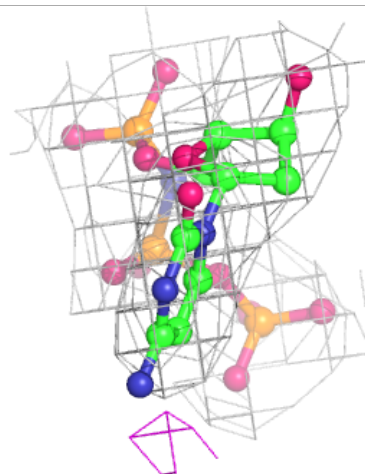
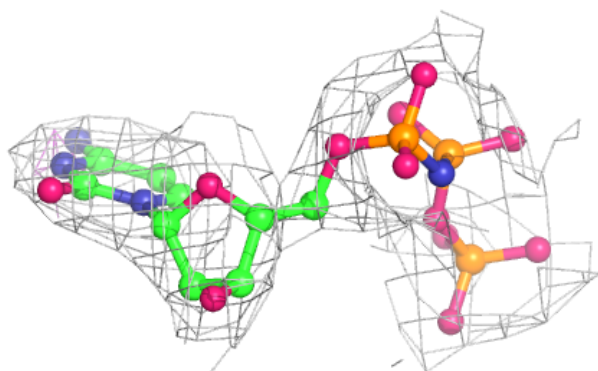
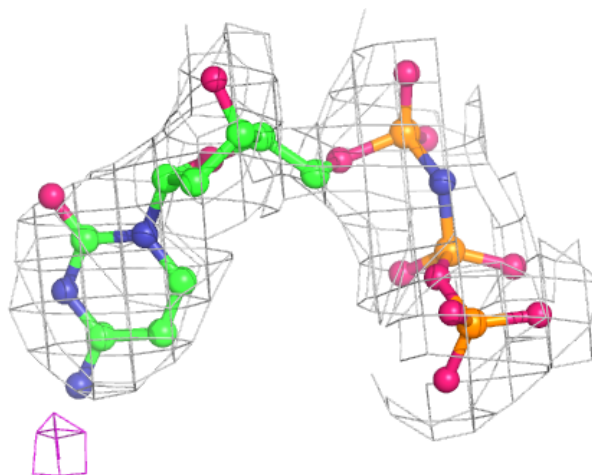
**Electron density around MG I 703:**

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



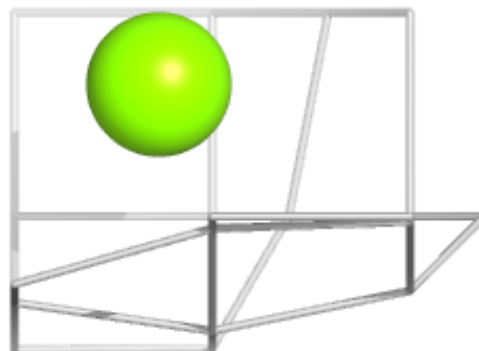
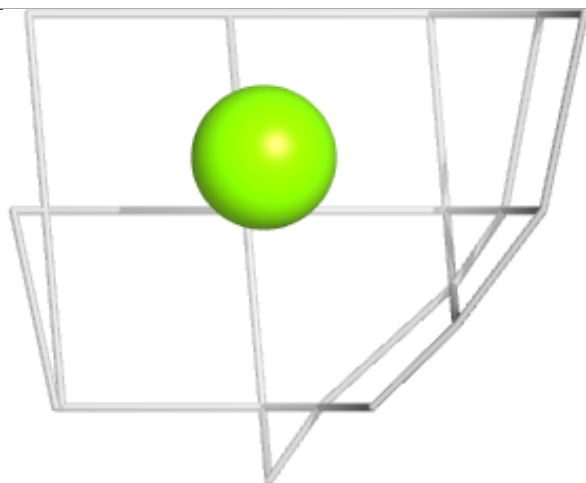
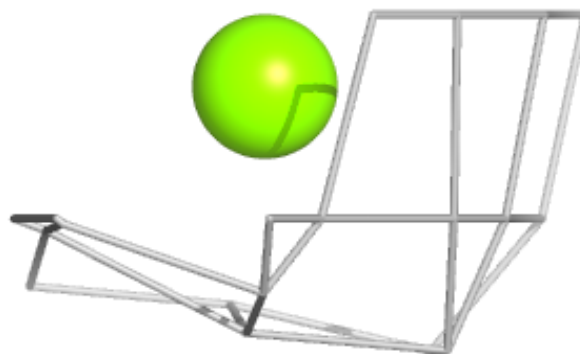
**Electron density around 0KX O 705:**

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



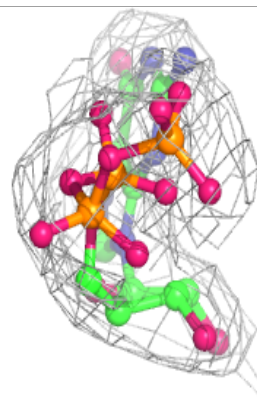
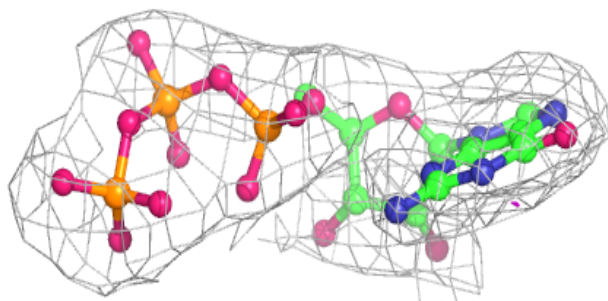
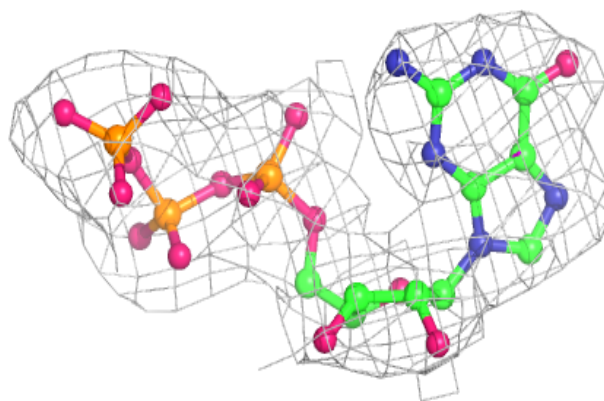
**Electron density around MG P 705:**

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

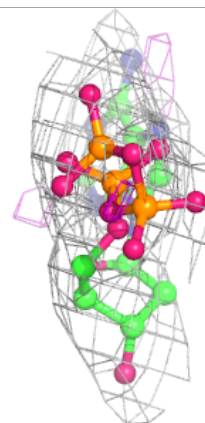
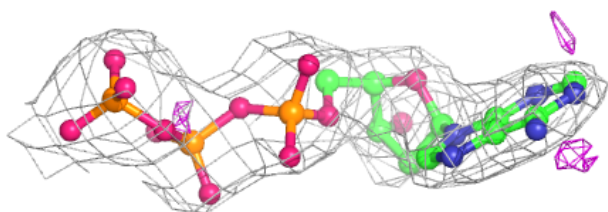
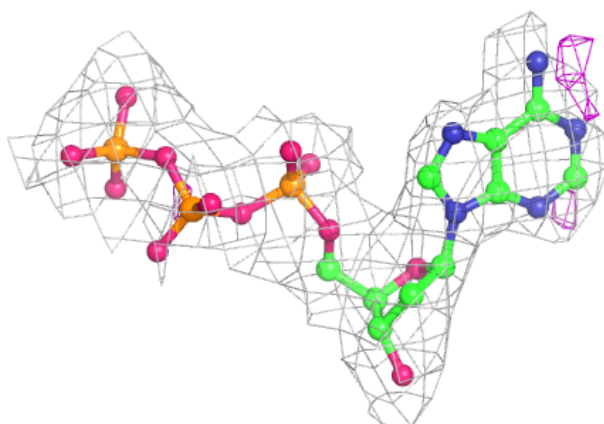


**Electron density around GTP O 707:**

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

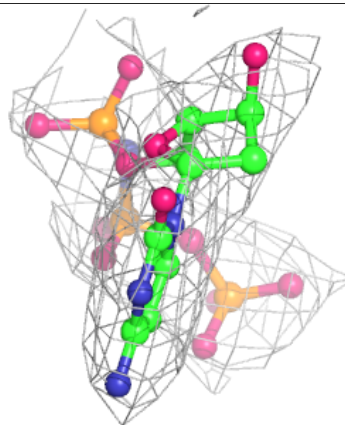
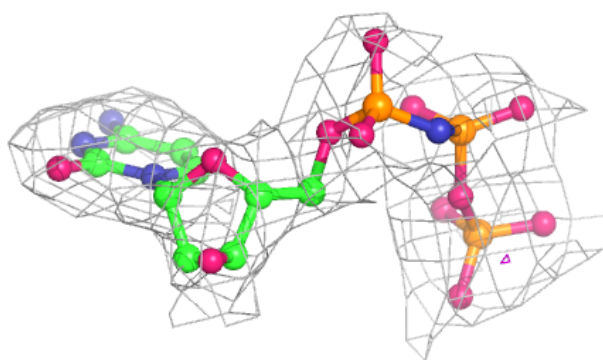
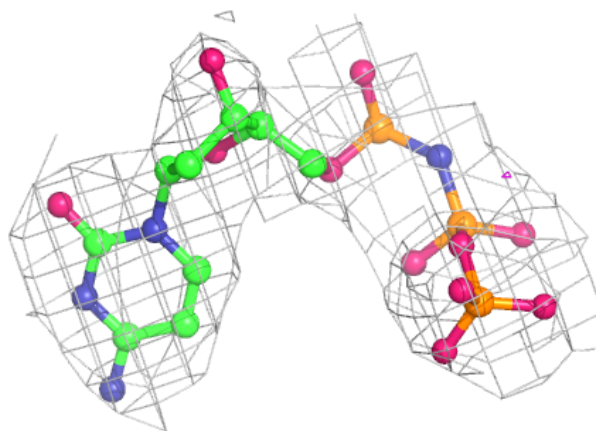
**Electron density around DTP G 701:**

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

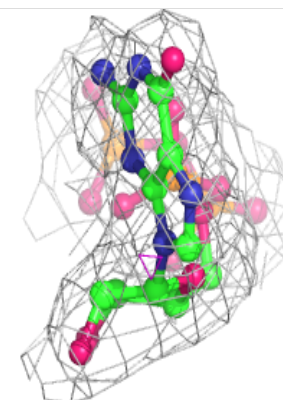
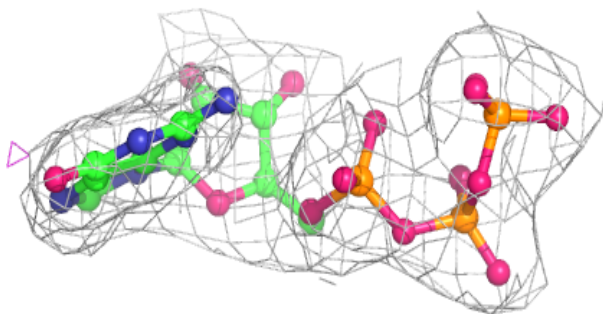
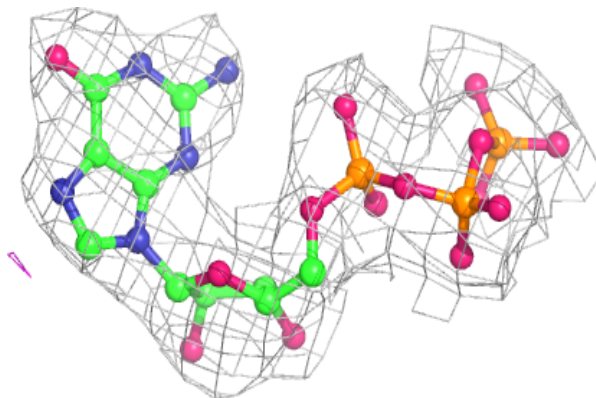


**Electron density around 0KX N 704:**

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

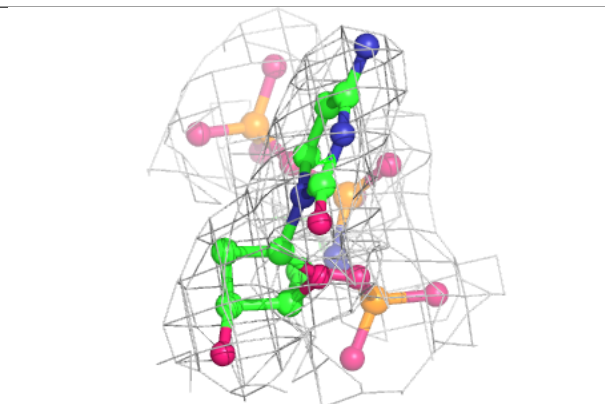
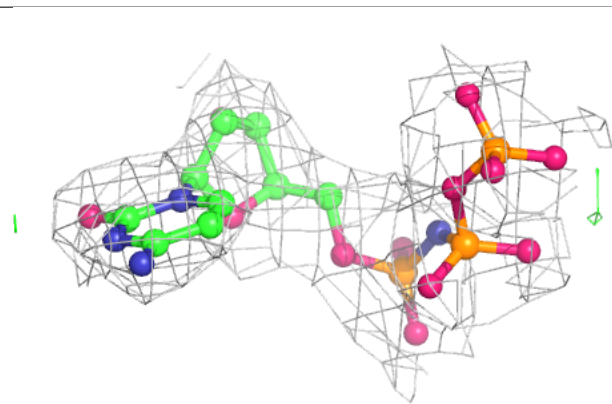
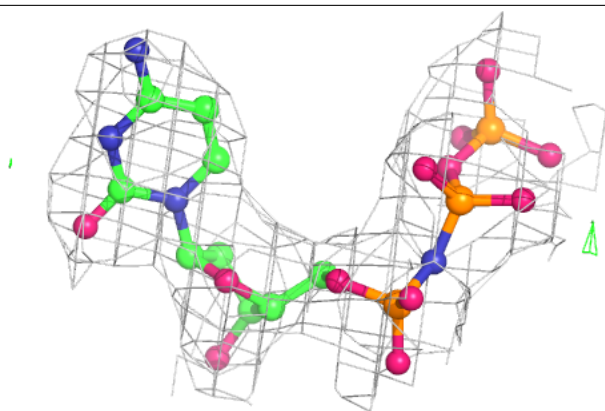
**Electron density around GTP G 707:**

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

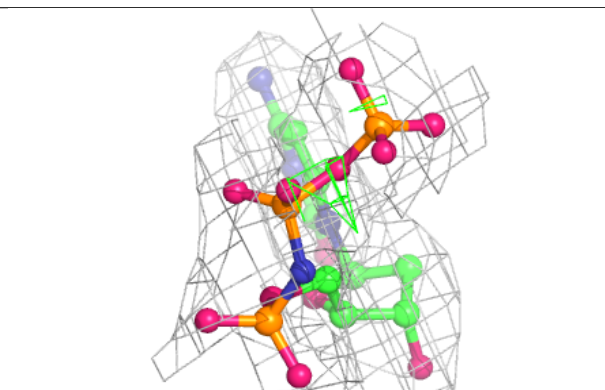
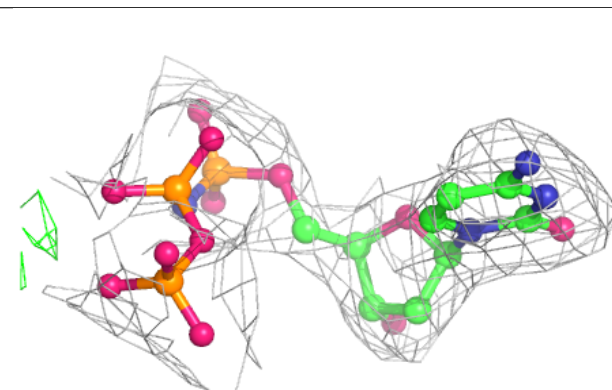
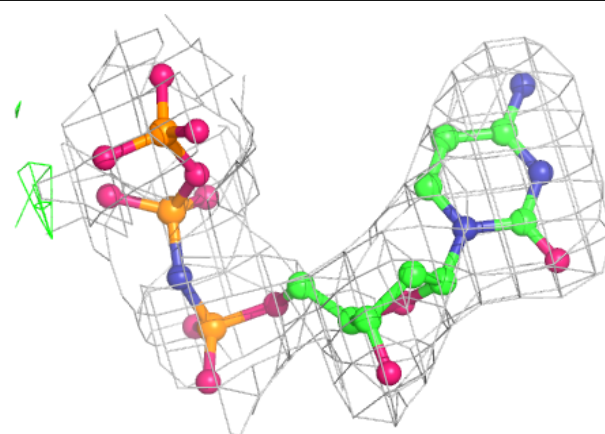


**Electron density around 0KX H 705:**

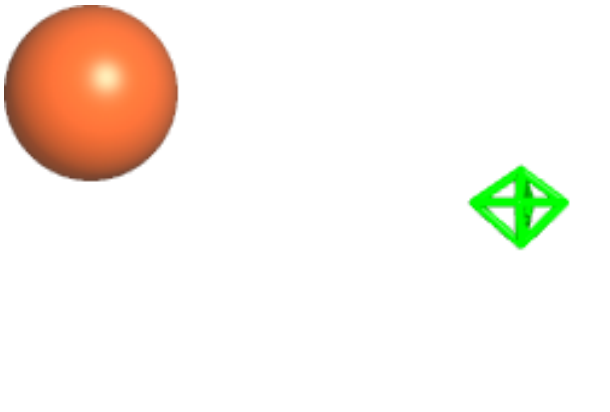
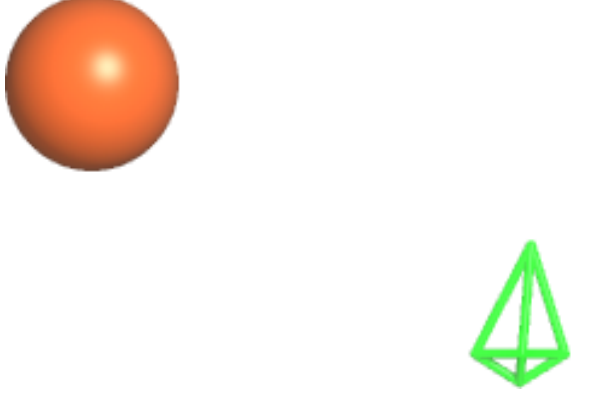
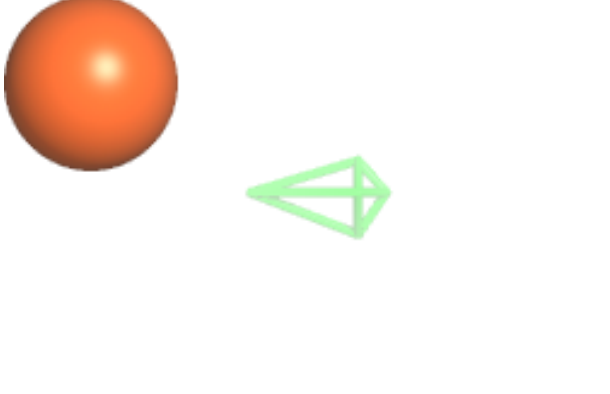
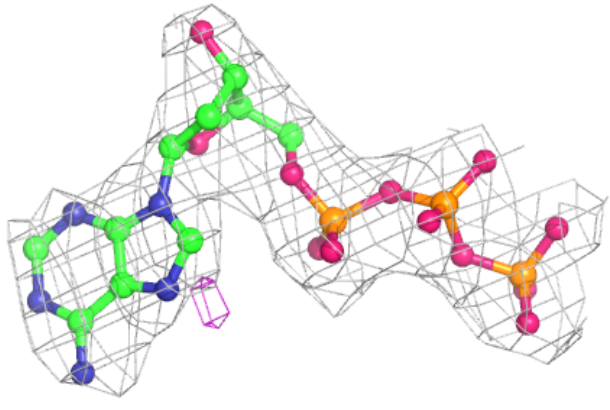
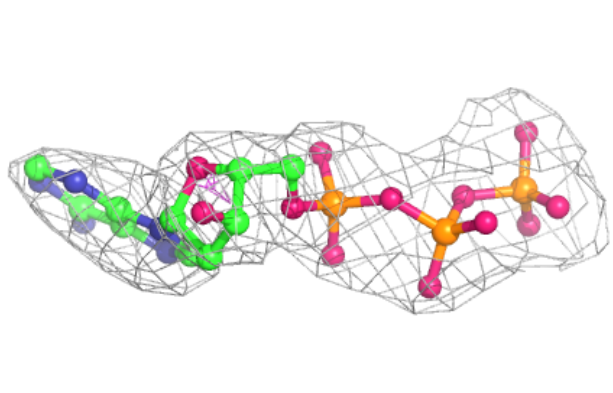
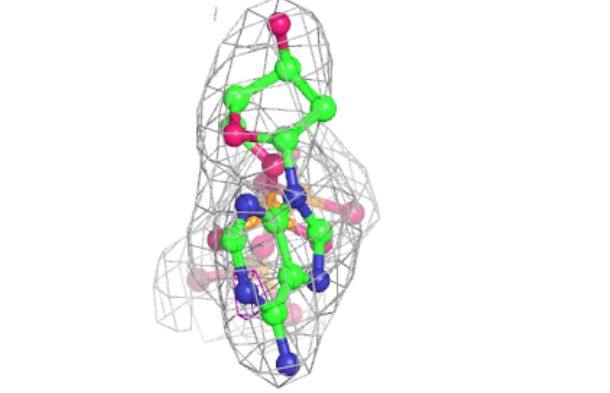
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around 0KX E 704:**

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

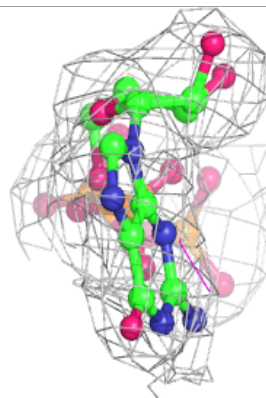
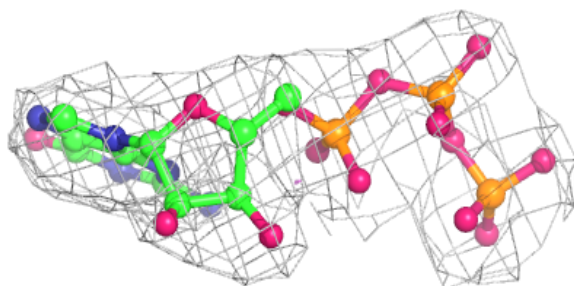
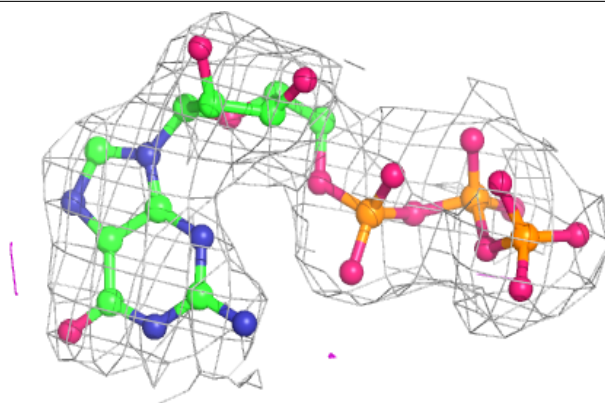




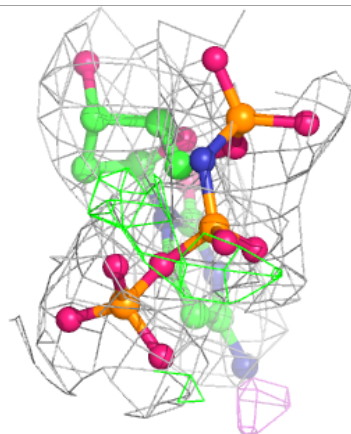
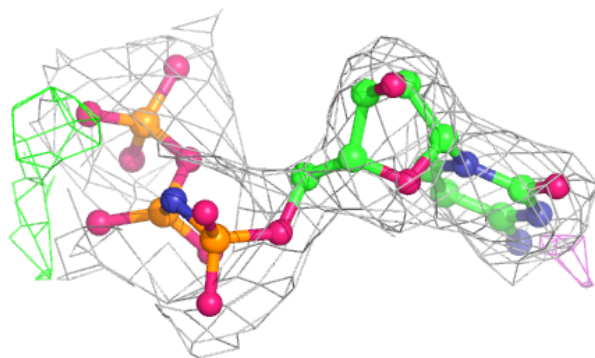
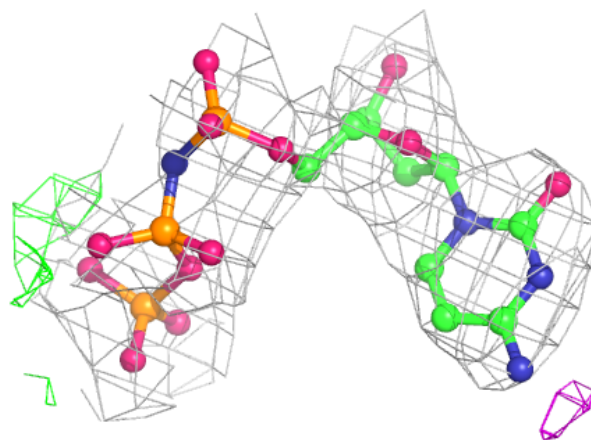
<p><b>Electron density around FE I 701:</b></p> <p><math>2mF_o-DF_c</math> (at 0.7 rmsd) in gray <math>mF_o-DF_c</math> (at 3 rmsd) in purple (negative) and green (positive)</p>	
	
<p><b>Electron density around DTP N 706:</b></p> <p><math>2mF_o-DF_c</math> (at 0.7 rmsd) in gray <math>mF_o-DF_c</math> (at 3 rmsd) in purple (negative) and green (positive)</p>	
	

**Electron density around GTP K 707:**

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

**Electron density around 0KX F 704:**

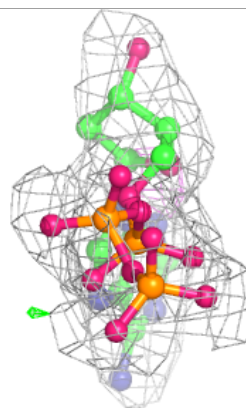
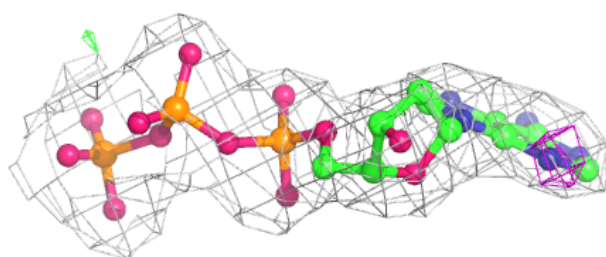
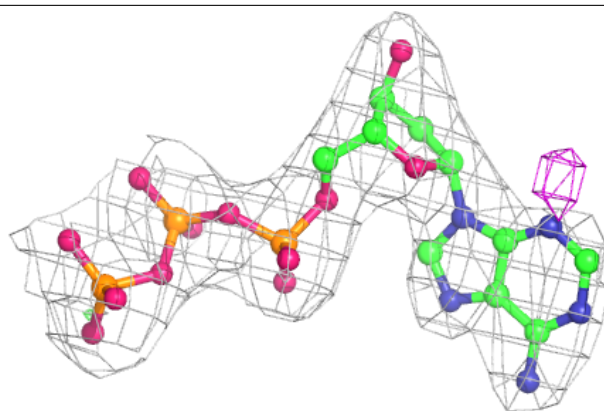
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



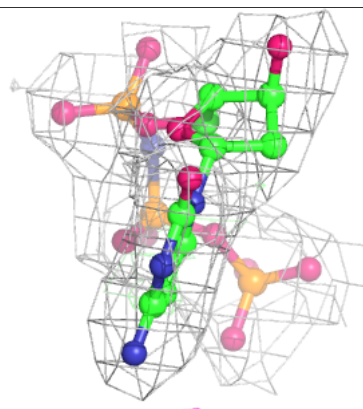
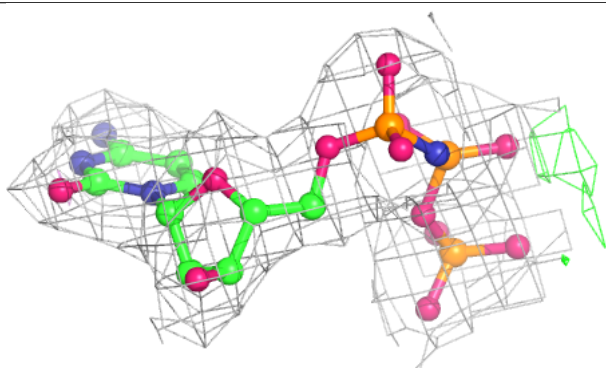
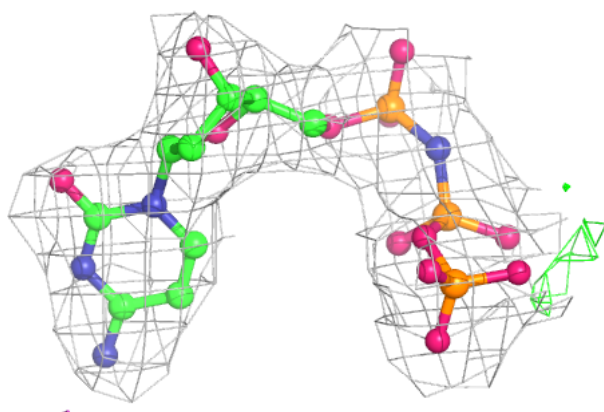


**Electron density around DTP J 707:**

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

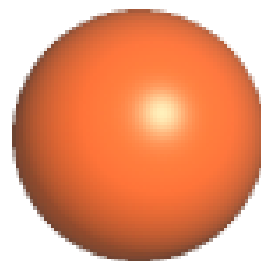
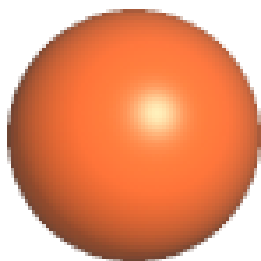
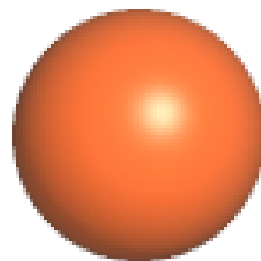
**Electron density around 0KX A 705:**

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



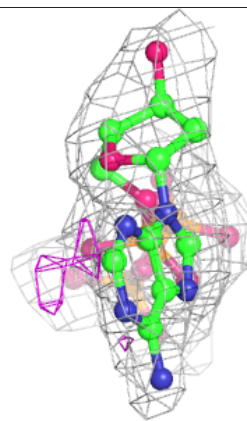
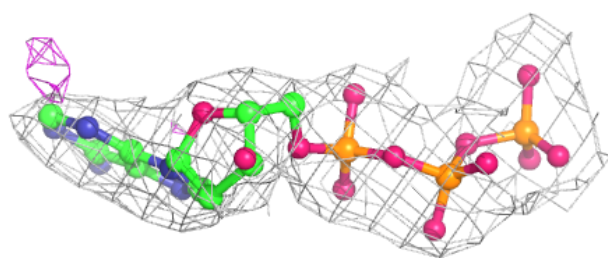
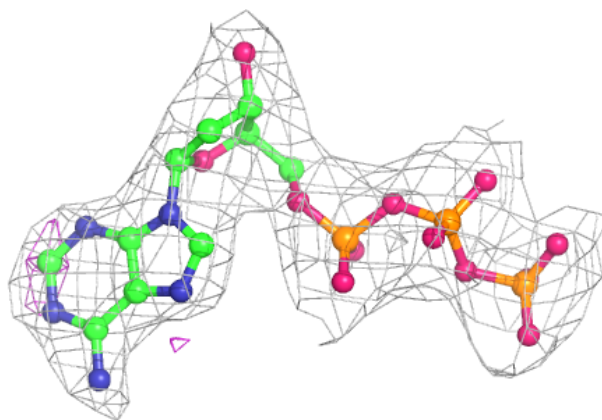
**Electron density around FE P 702:**

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



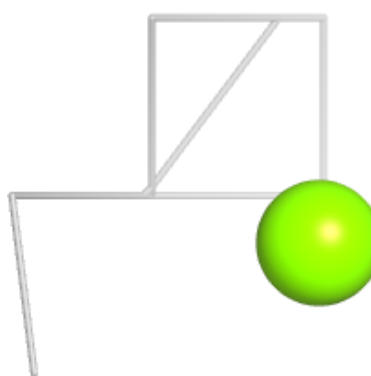
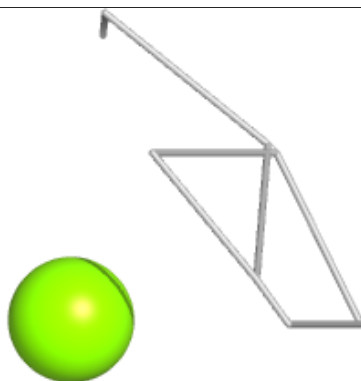
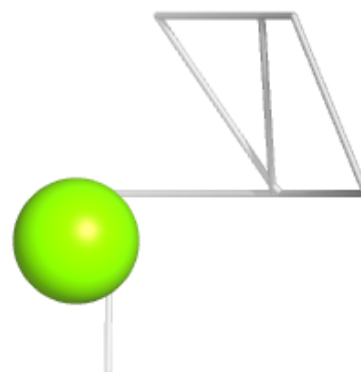
**Electron density around DTP L 701:**

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

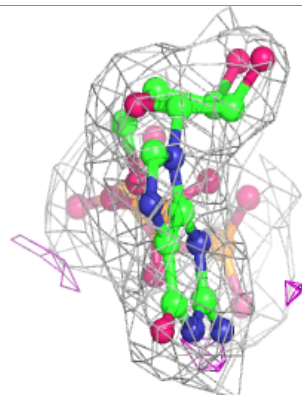
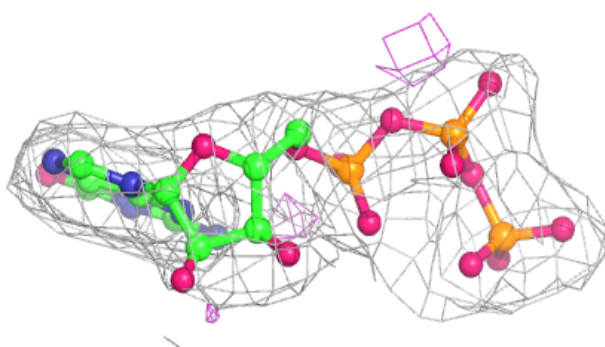
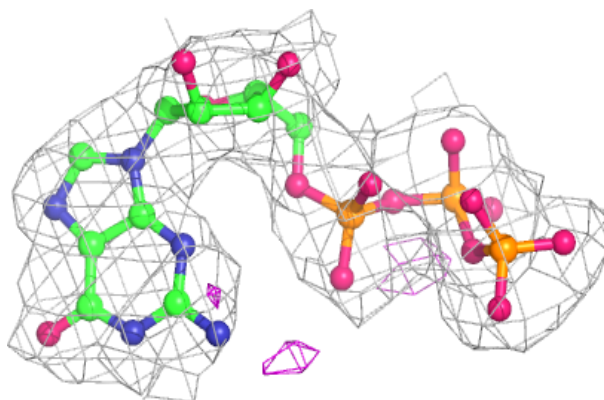


**Electron density around MG E 703:**

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

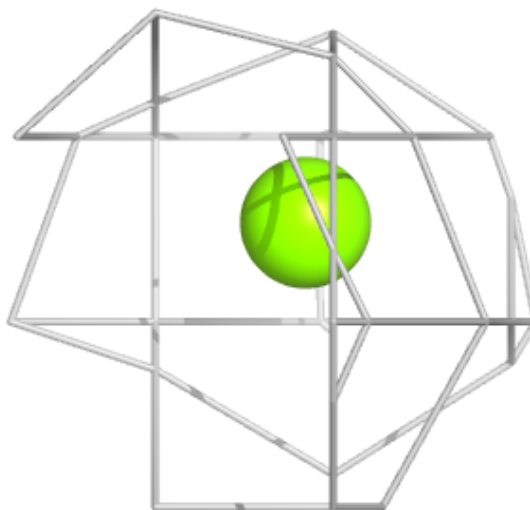
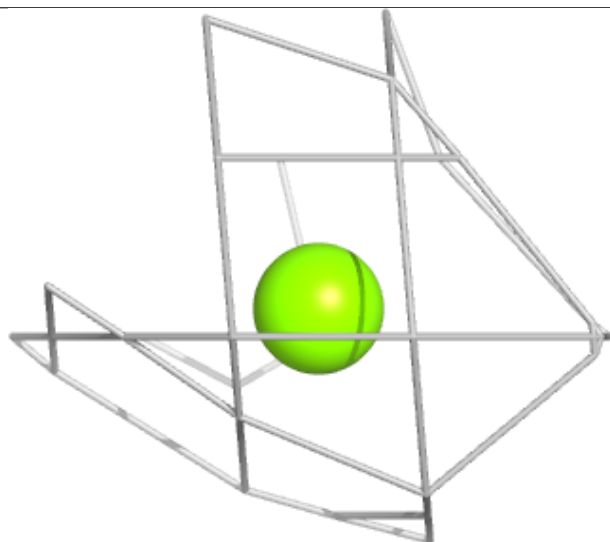
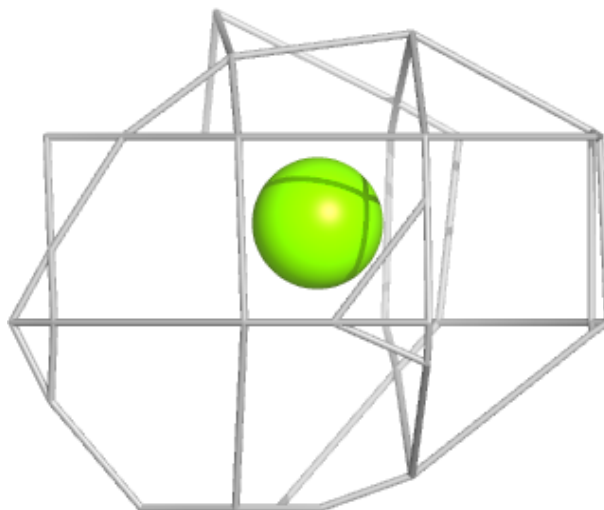
**Electron density around GTP A 706:**

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



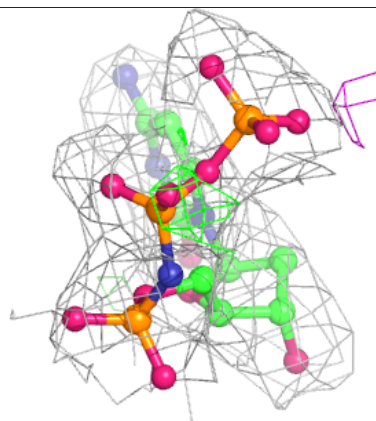
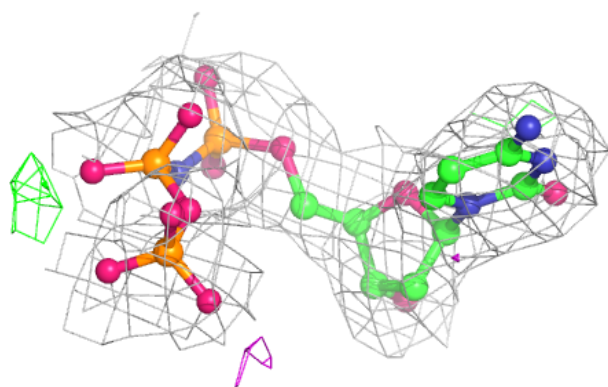
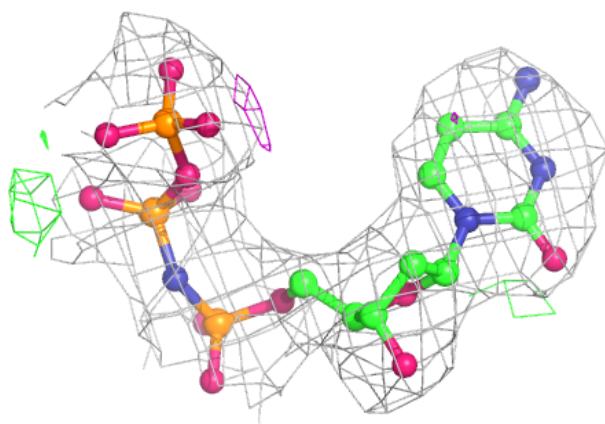
**Electron density around MG A 702:**

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

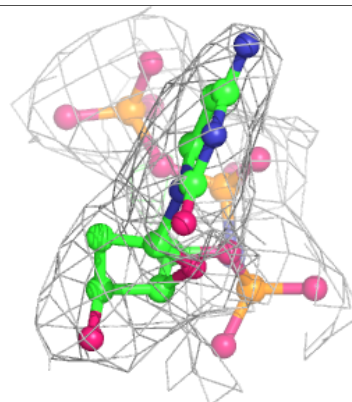
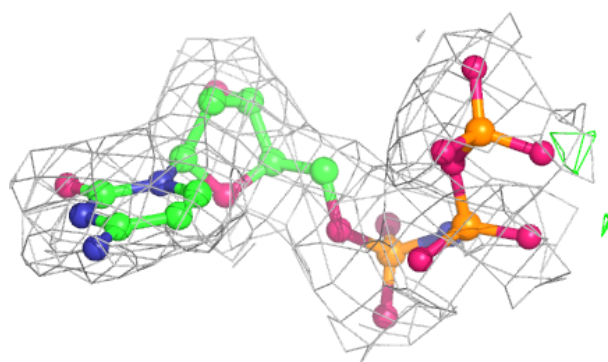
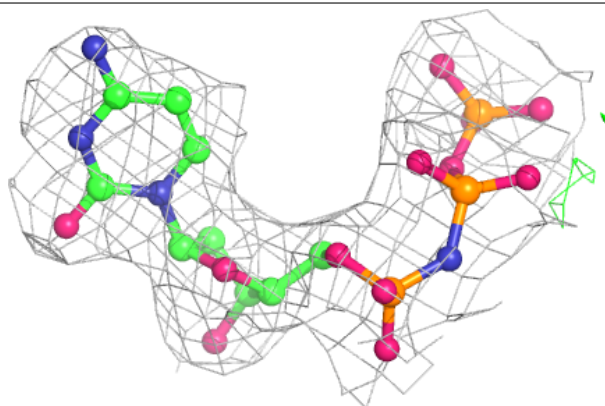


**Electron density around 0KX C 706:**

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

**Electron density around 0KX I 705:**

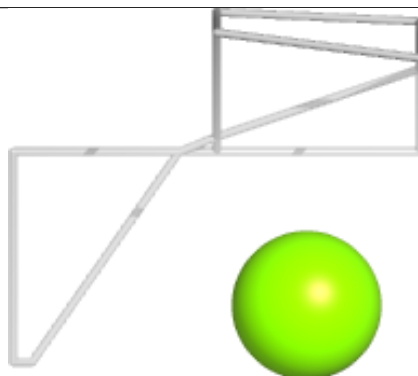
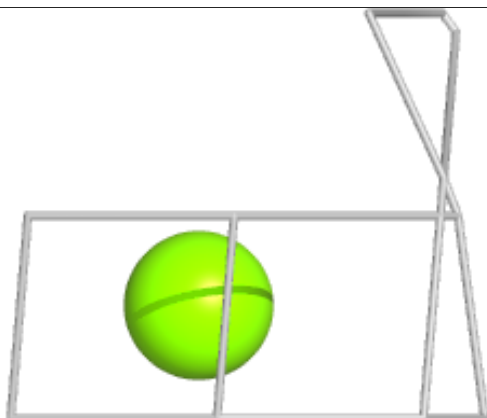
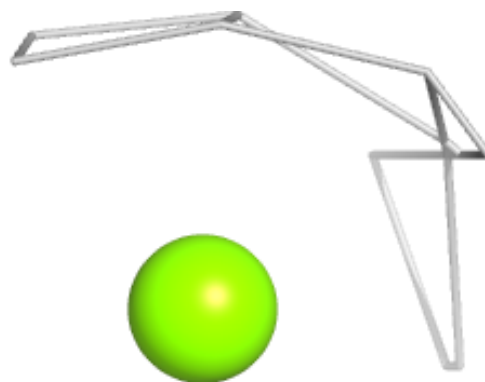
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



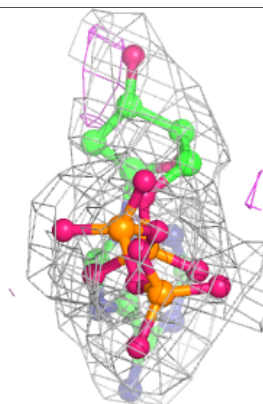
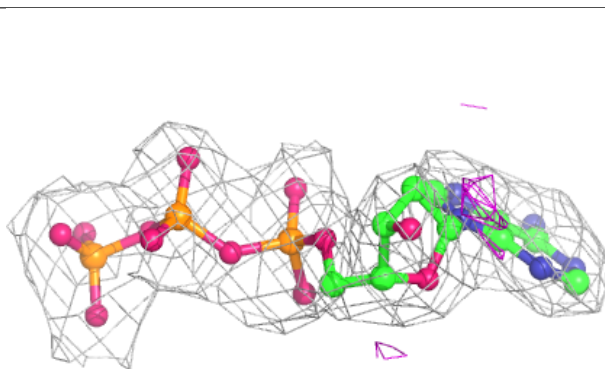
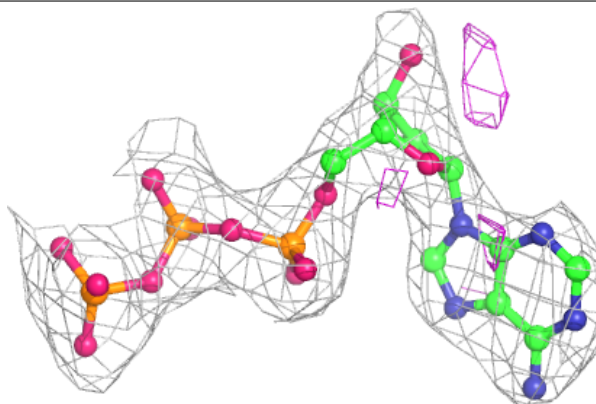


**Electron density around MG L 705:**

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

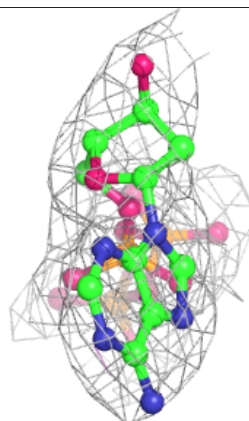
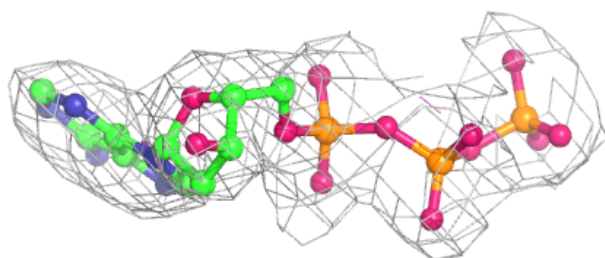
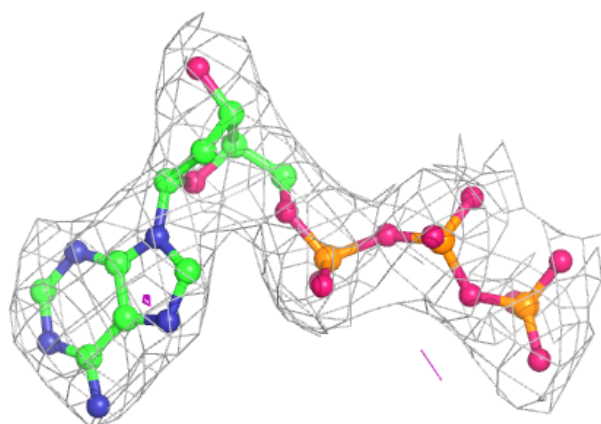
**Electron density around DTP A 708:**

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

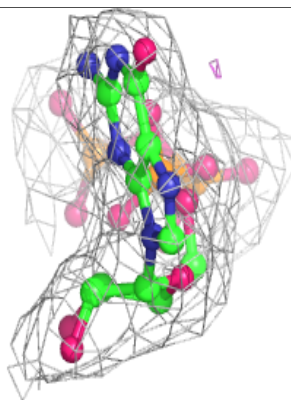
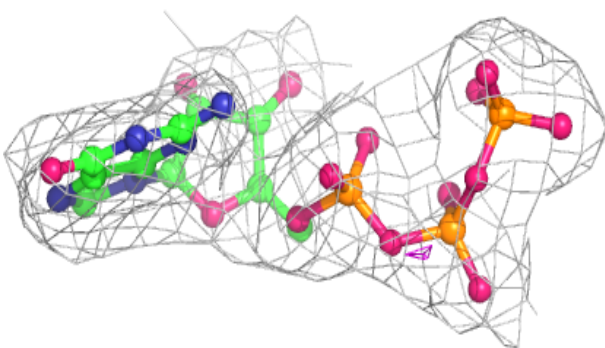
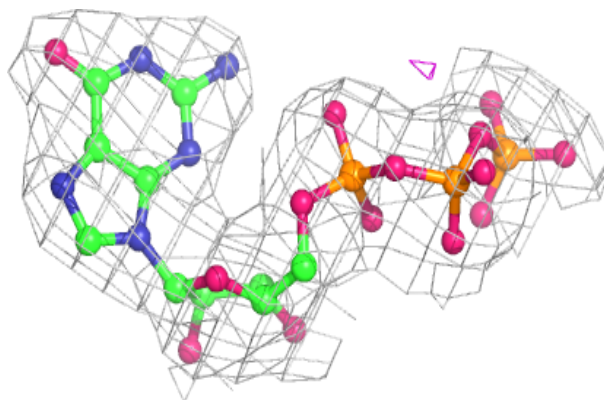


**Electron density around DTP D 701:**

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

**Electron density around GTP L 707:**

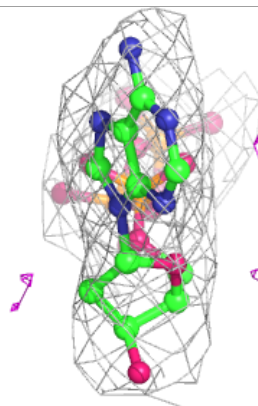
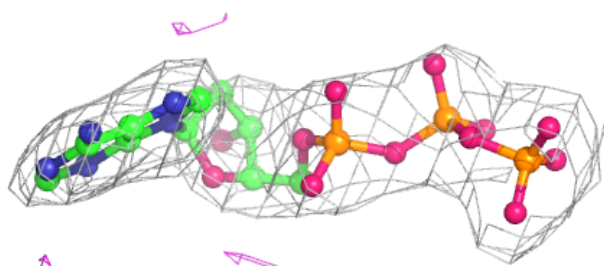
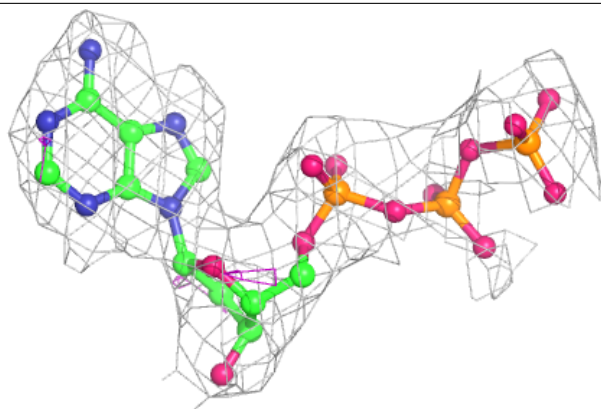
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



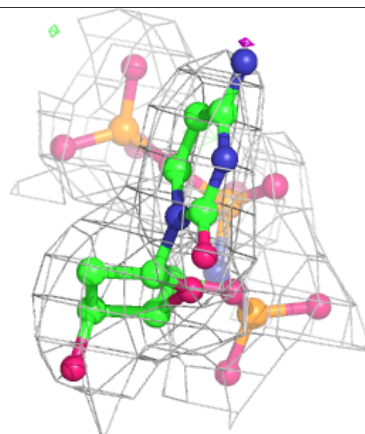
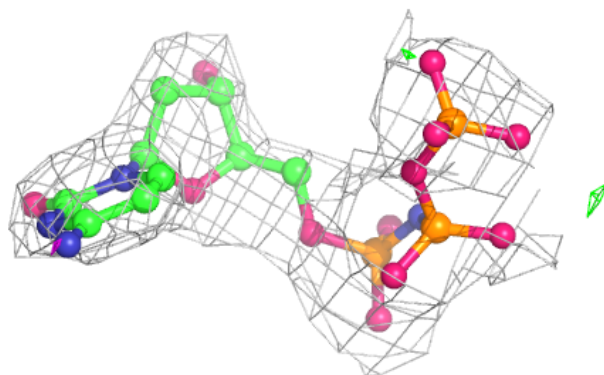
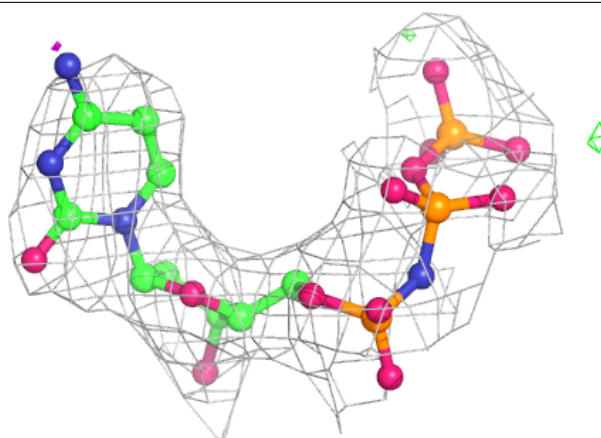


**Electron density around DTP H 701:**

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

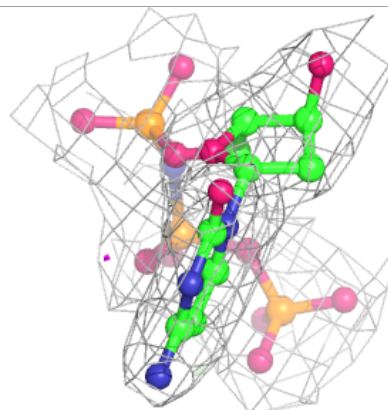
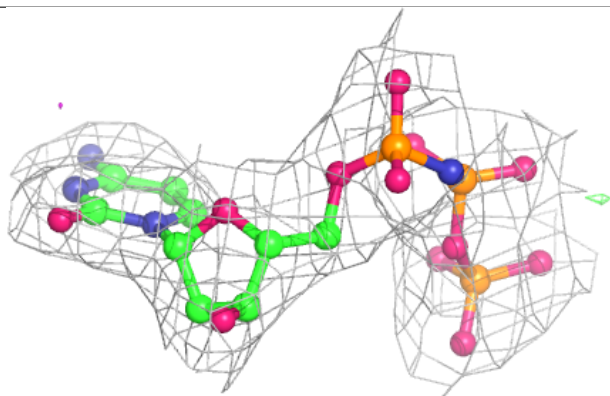
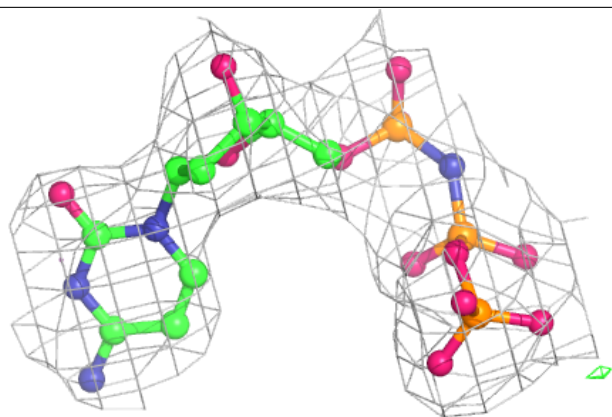
**Electron density around 0KX P 706:**

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

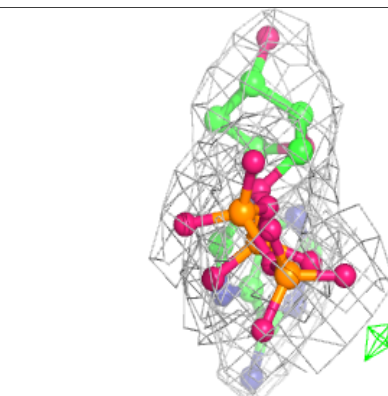
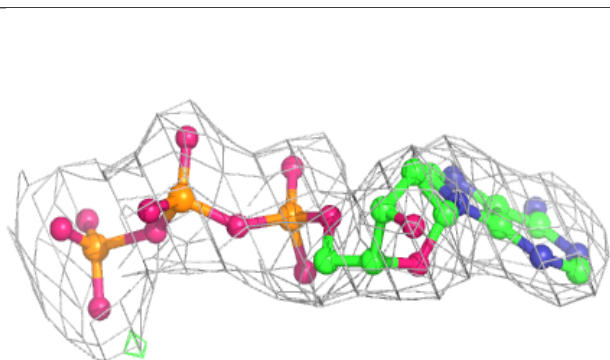
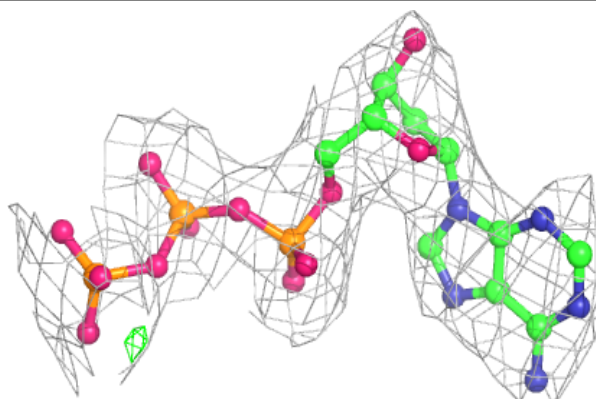


**Electron density around 0KX J 704:**

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

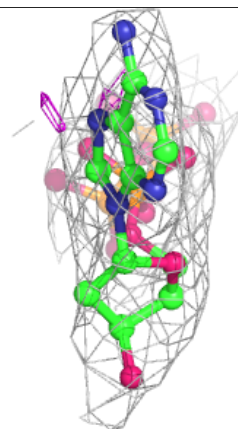
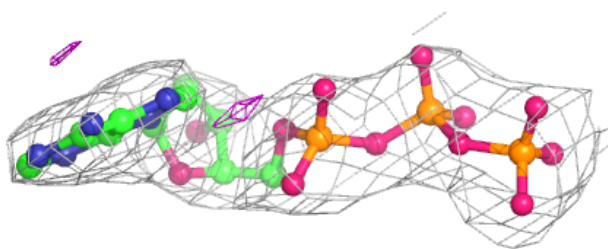
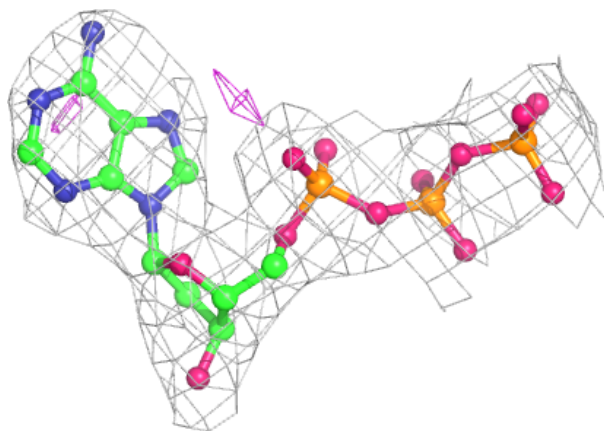
**Electron density around DTP O 701:**

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



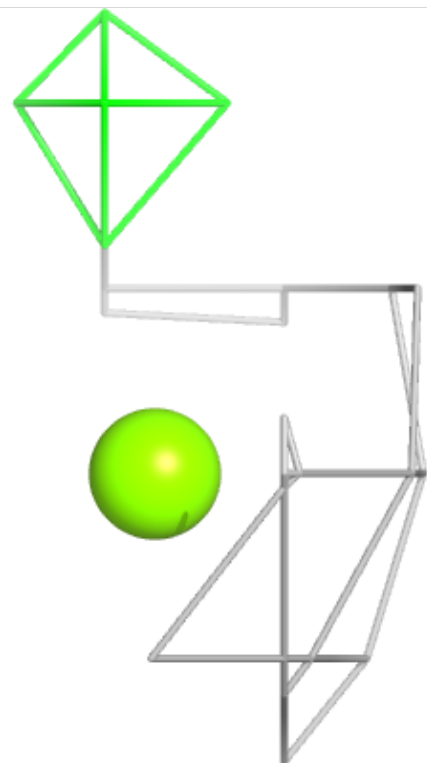
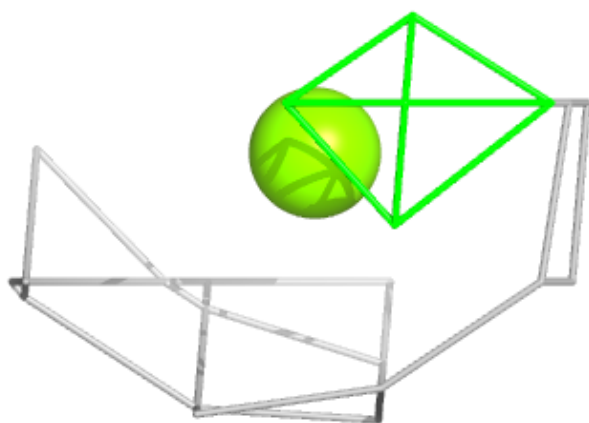
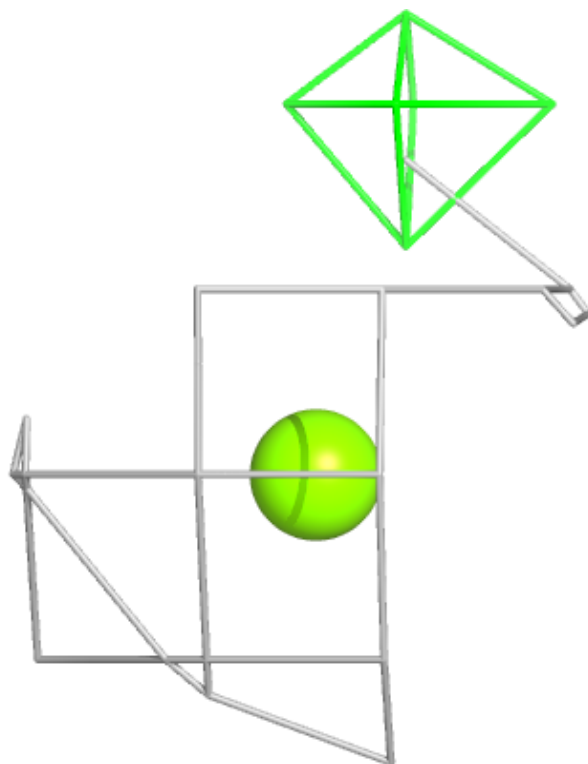
**Electron density around DTP M 708:**

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



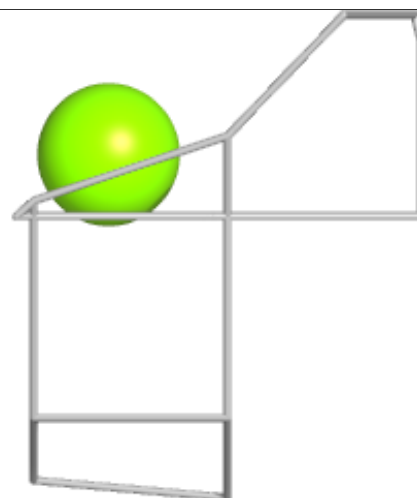
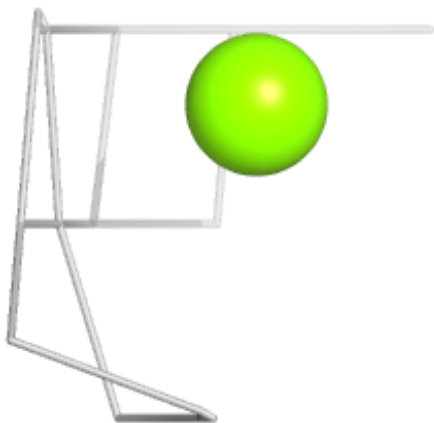
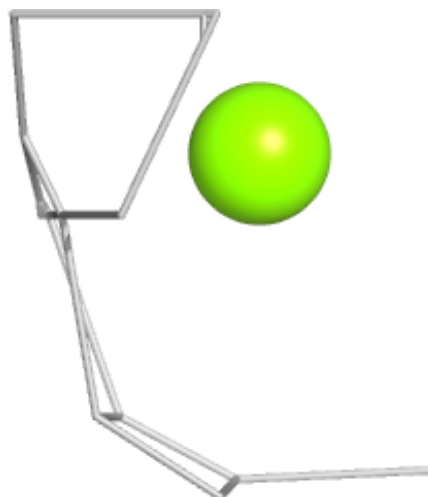
**Electron density around MG K 704:**

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



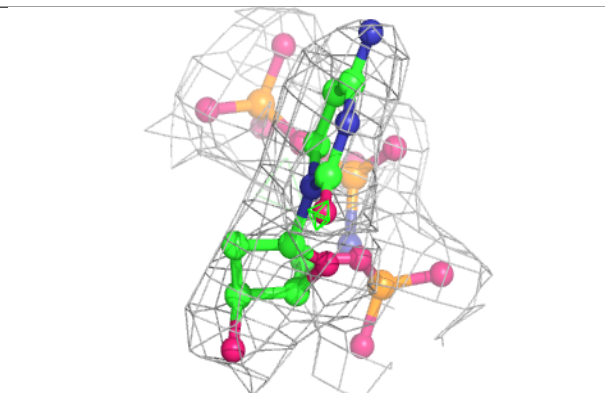
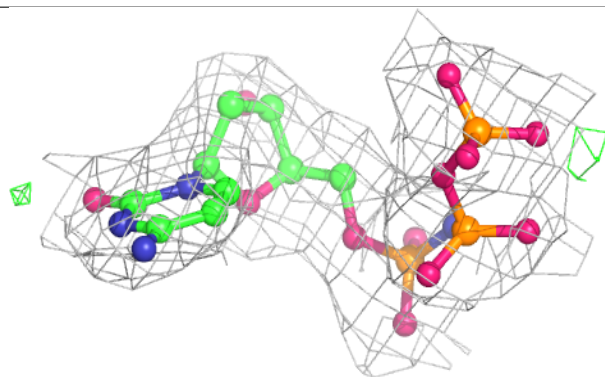
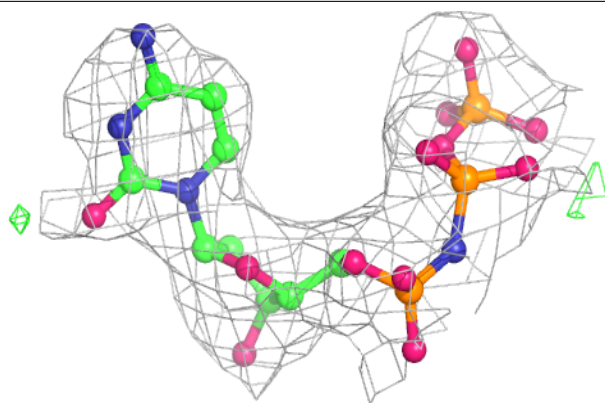
**Electron density around MG D 705:**

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

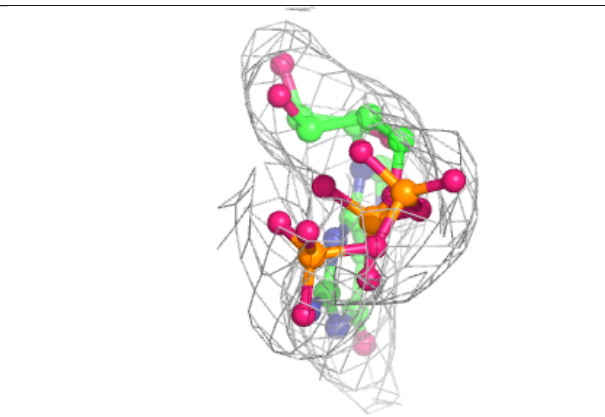
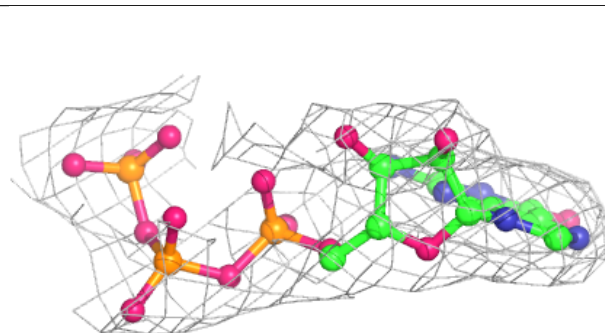
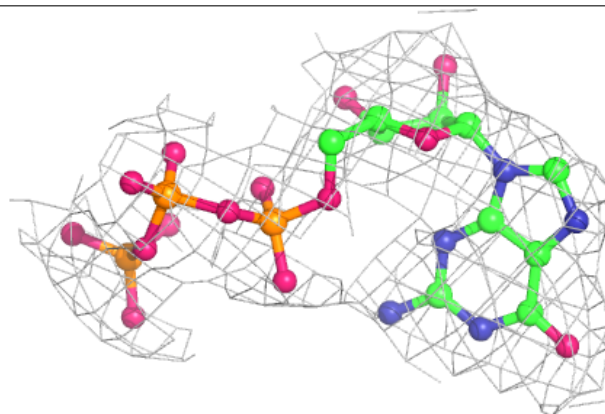


**Electron density around 0KX L 706:**

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

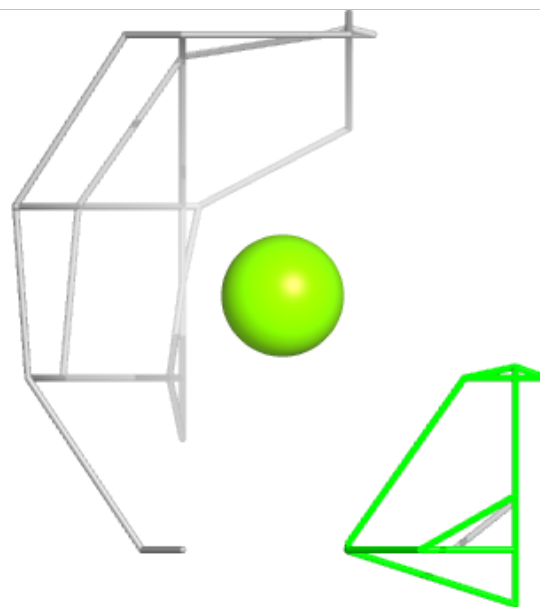
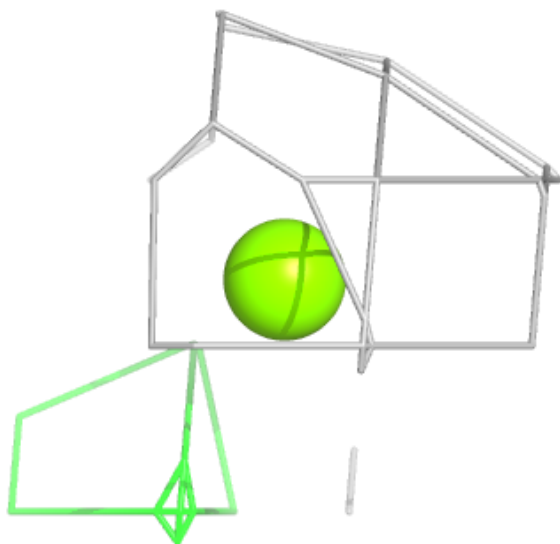
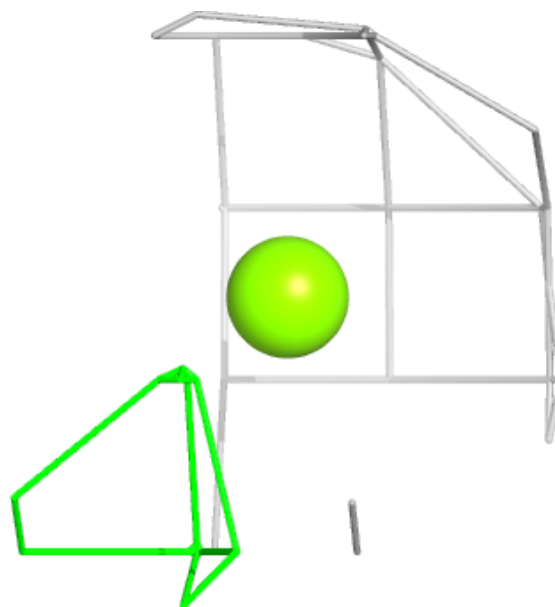
**Electron density around GTP E 705:**

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



**Electron density around MG D 704:**

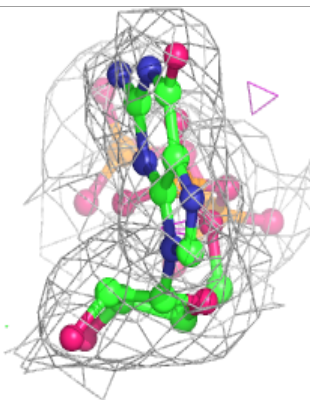
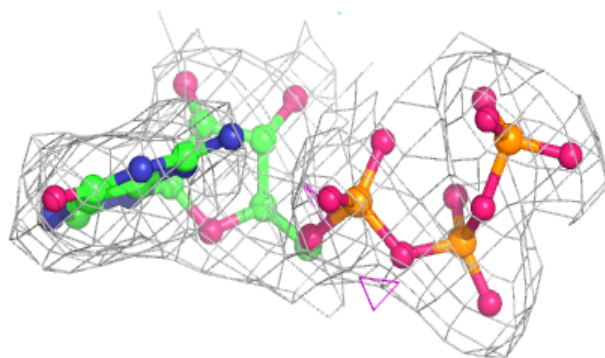
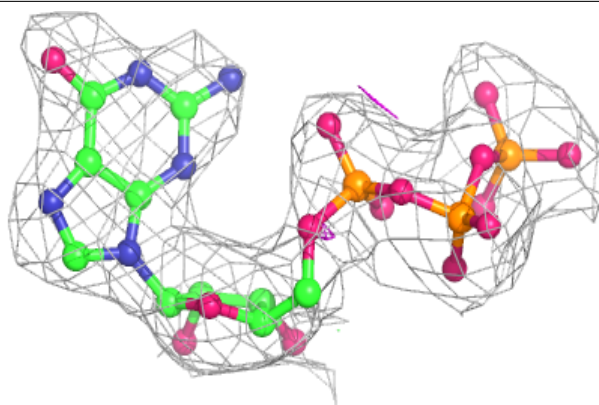
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



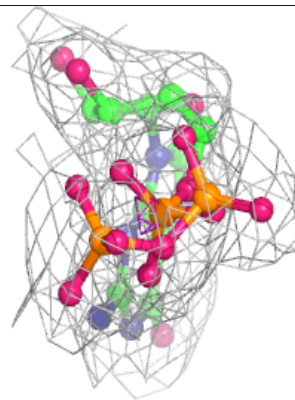
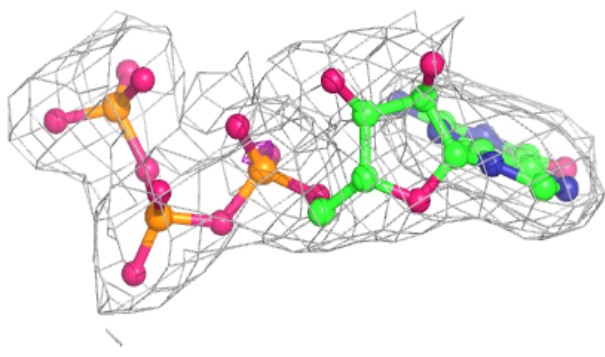
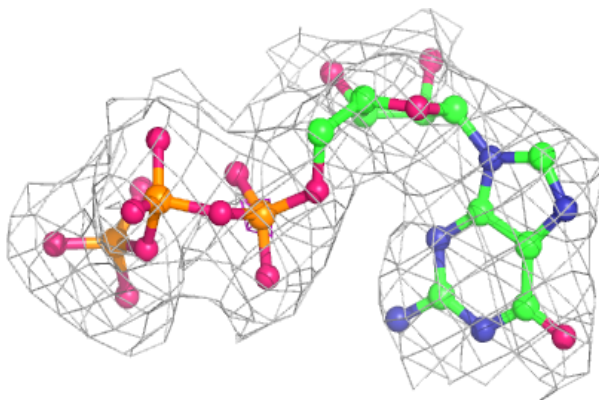


**Electron density around GTP I 706:**

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

**Electron density around GTP J 705:**

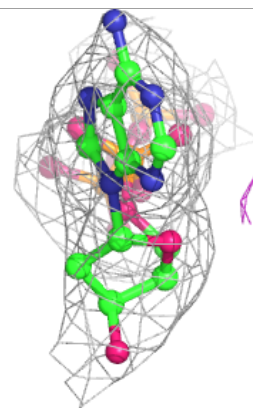
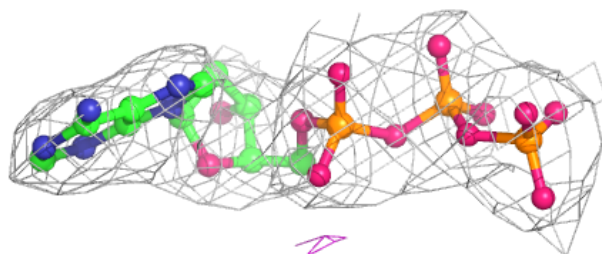
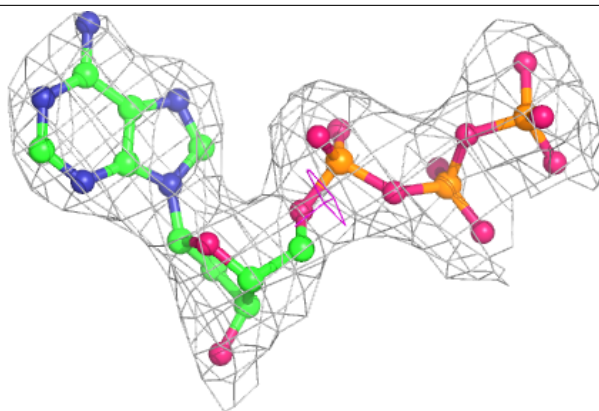
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





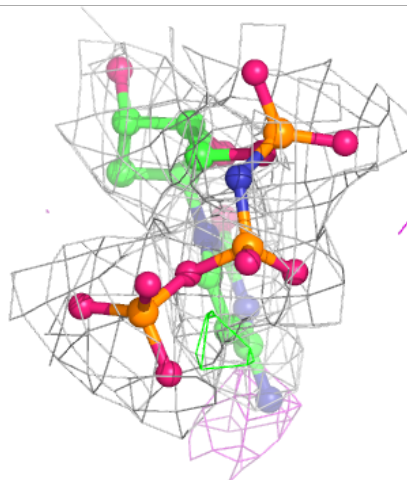
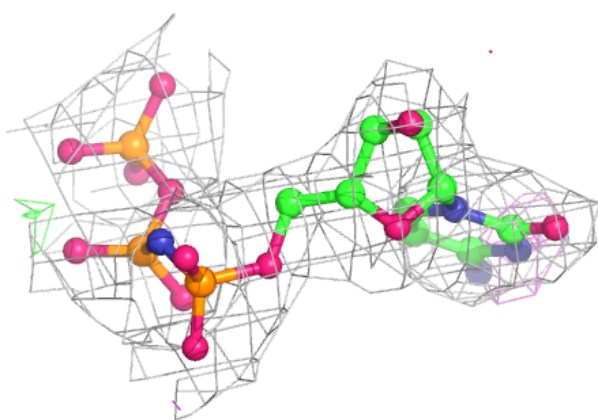
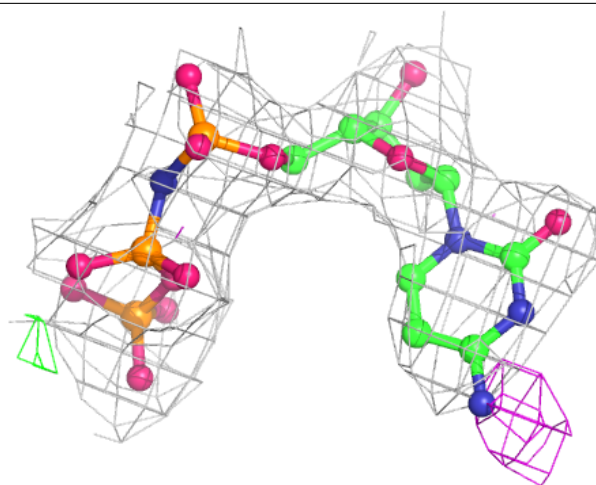
**Electron density around DTP I 708:**

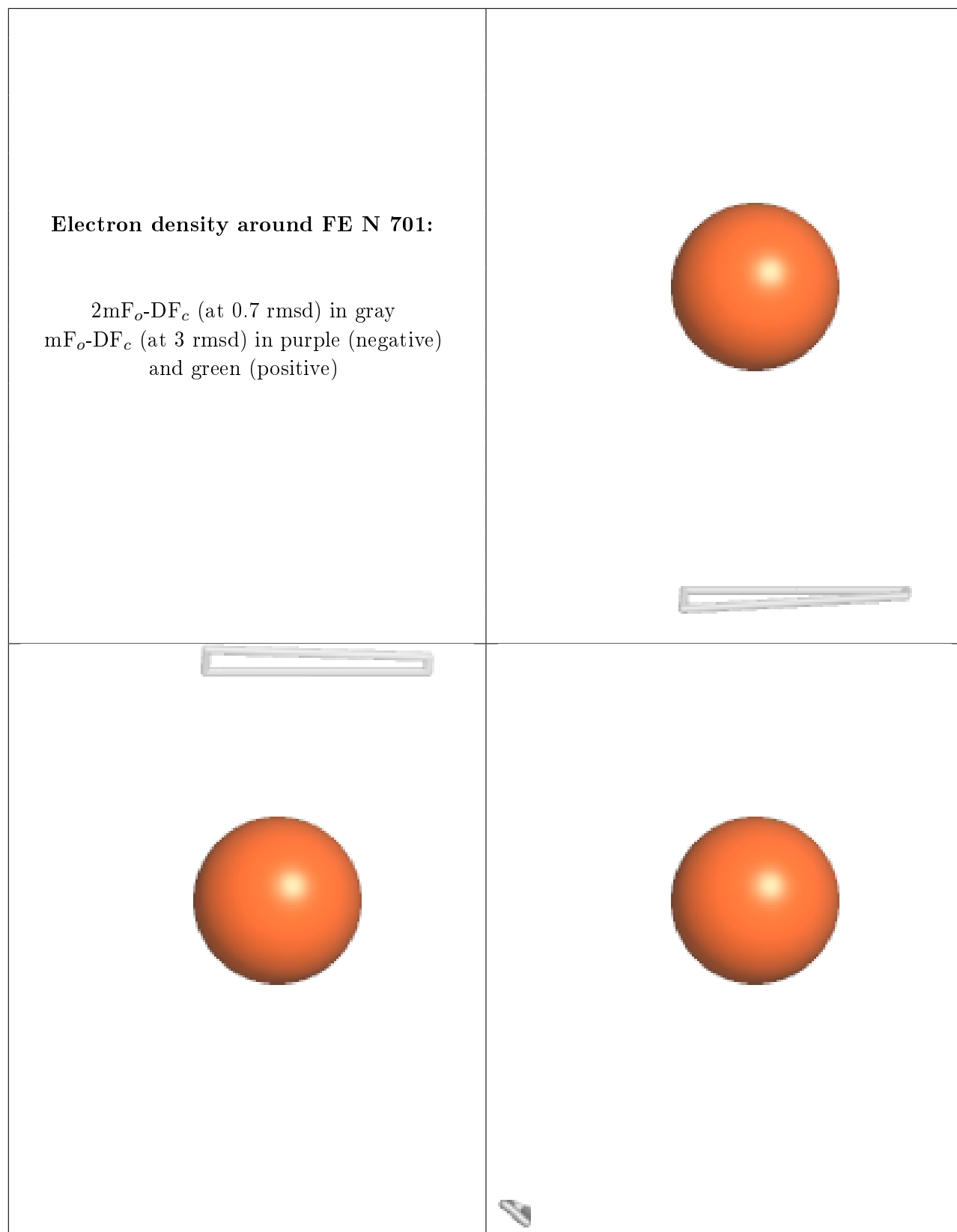
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 0KX D 706:**

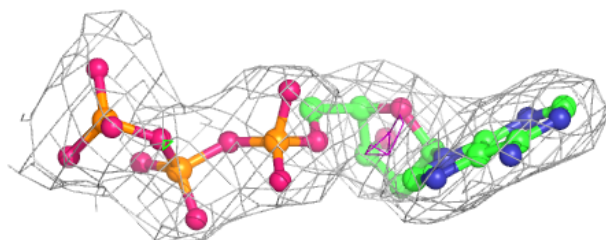
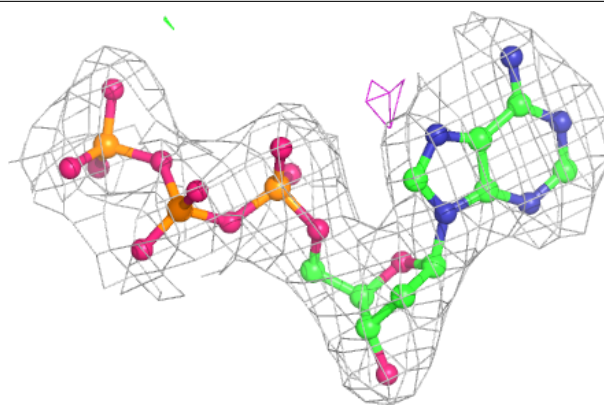
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



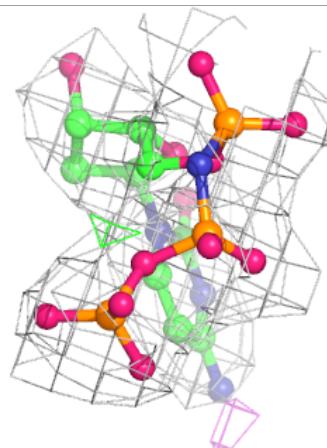
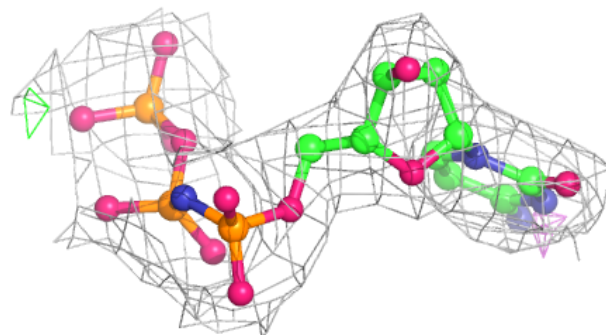
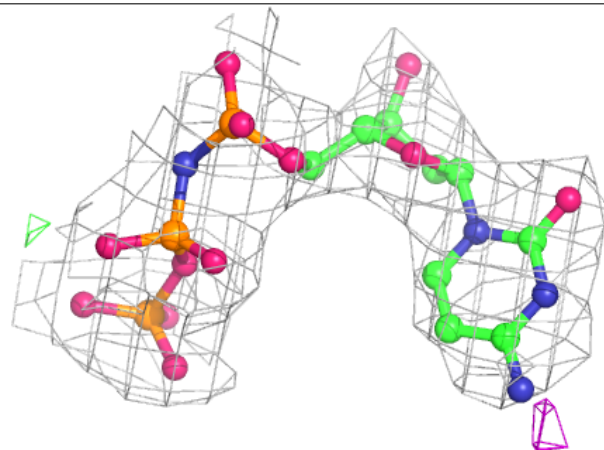


**Electron density around DTP C 701:**

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

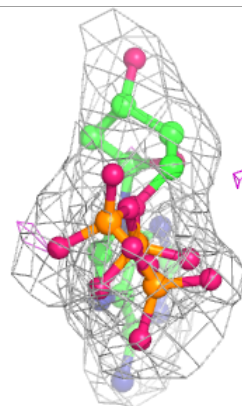
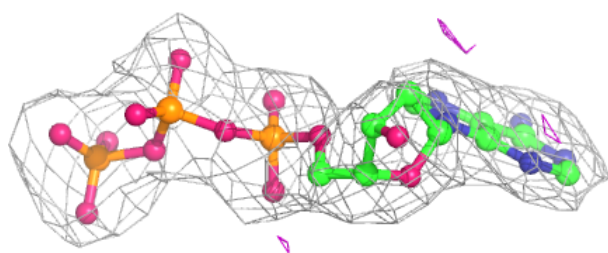
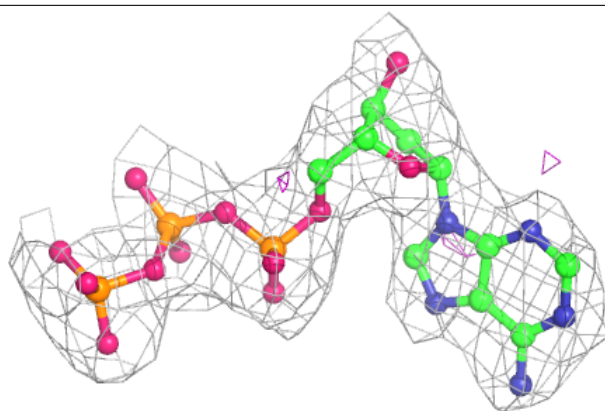
**Electron density around 0KX K 706:**

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

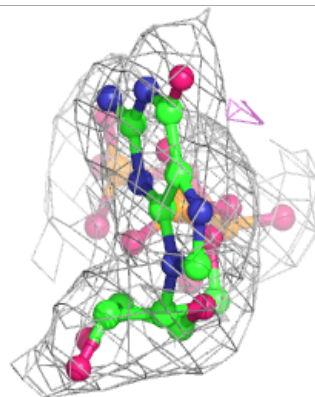
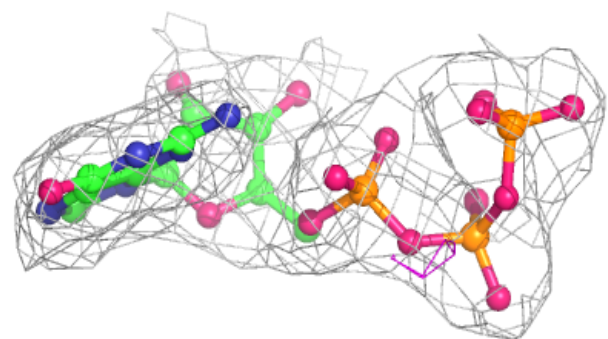
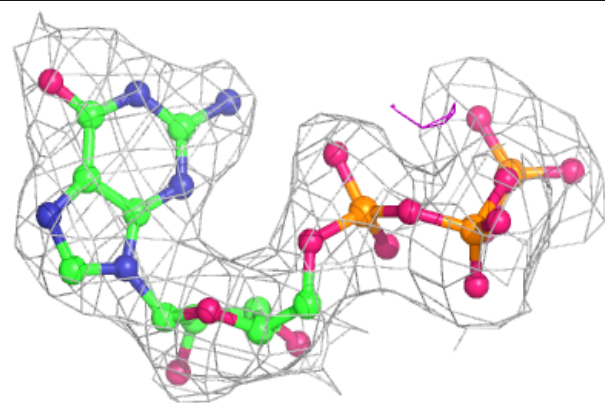


**Electron density around DTP B 708:**

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

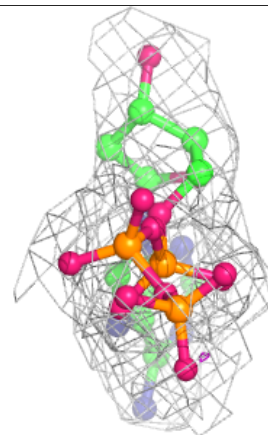
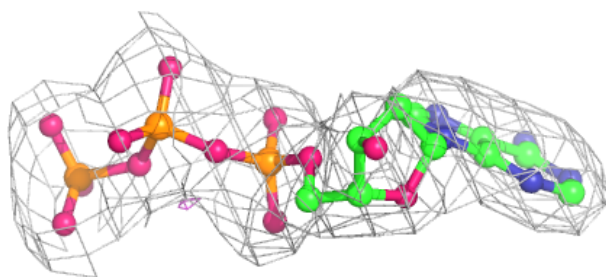
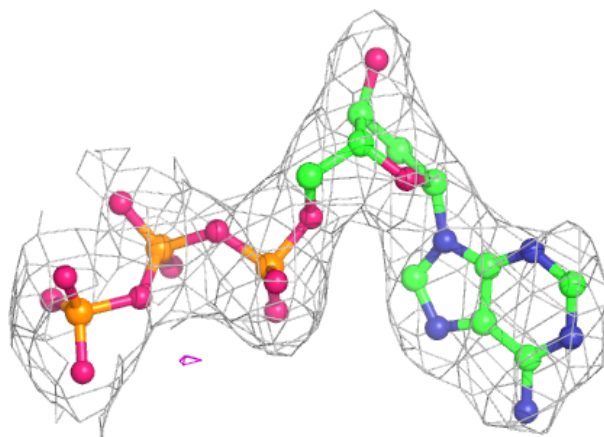
**Electron density around GTP C 707:**

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



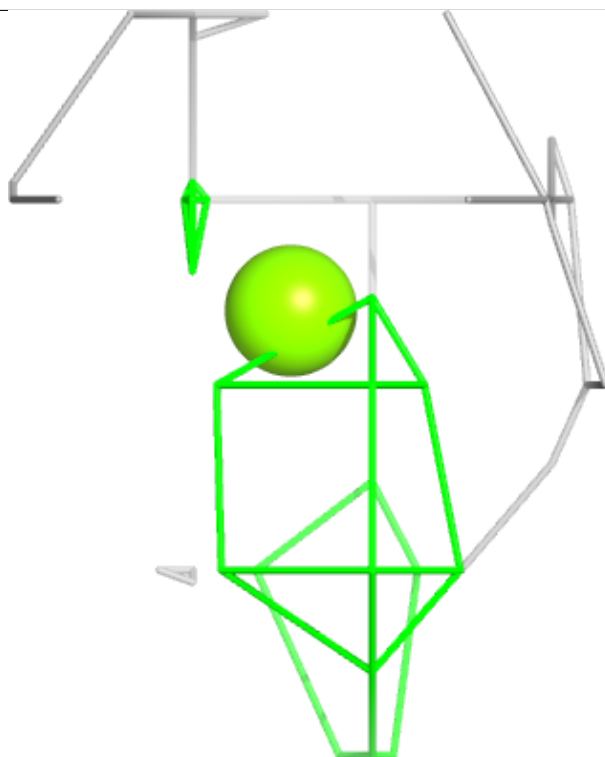
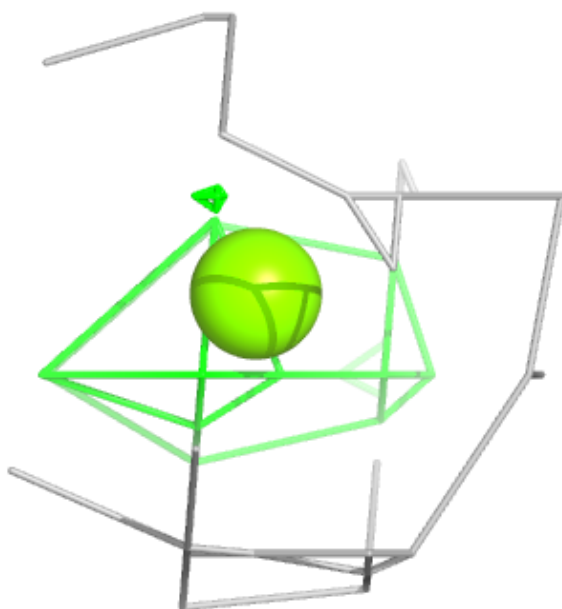
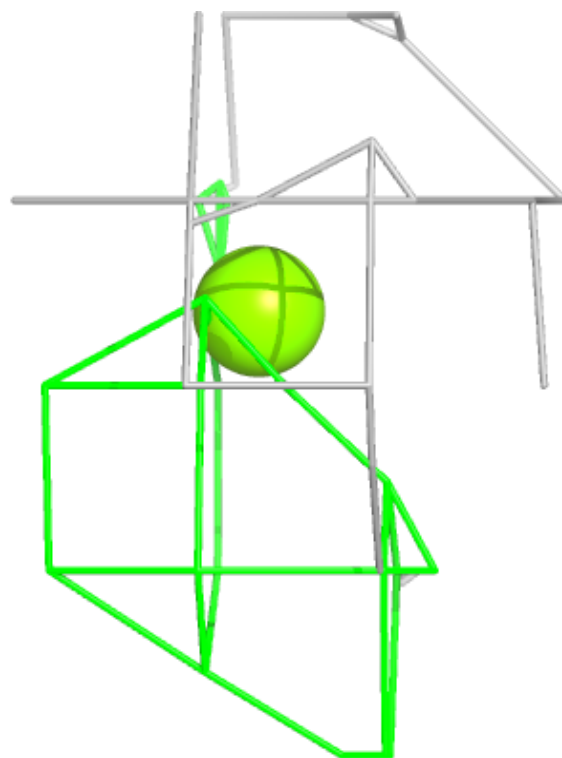
**Electron density around DTP K 701:**

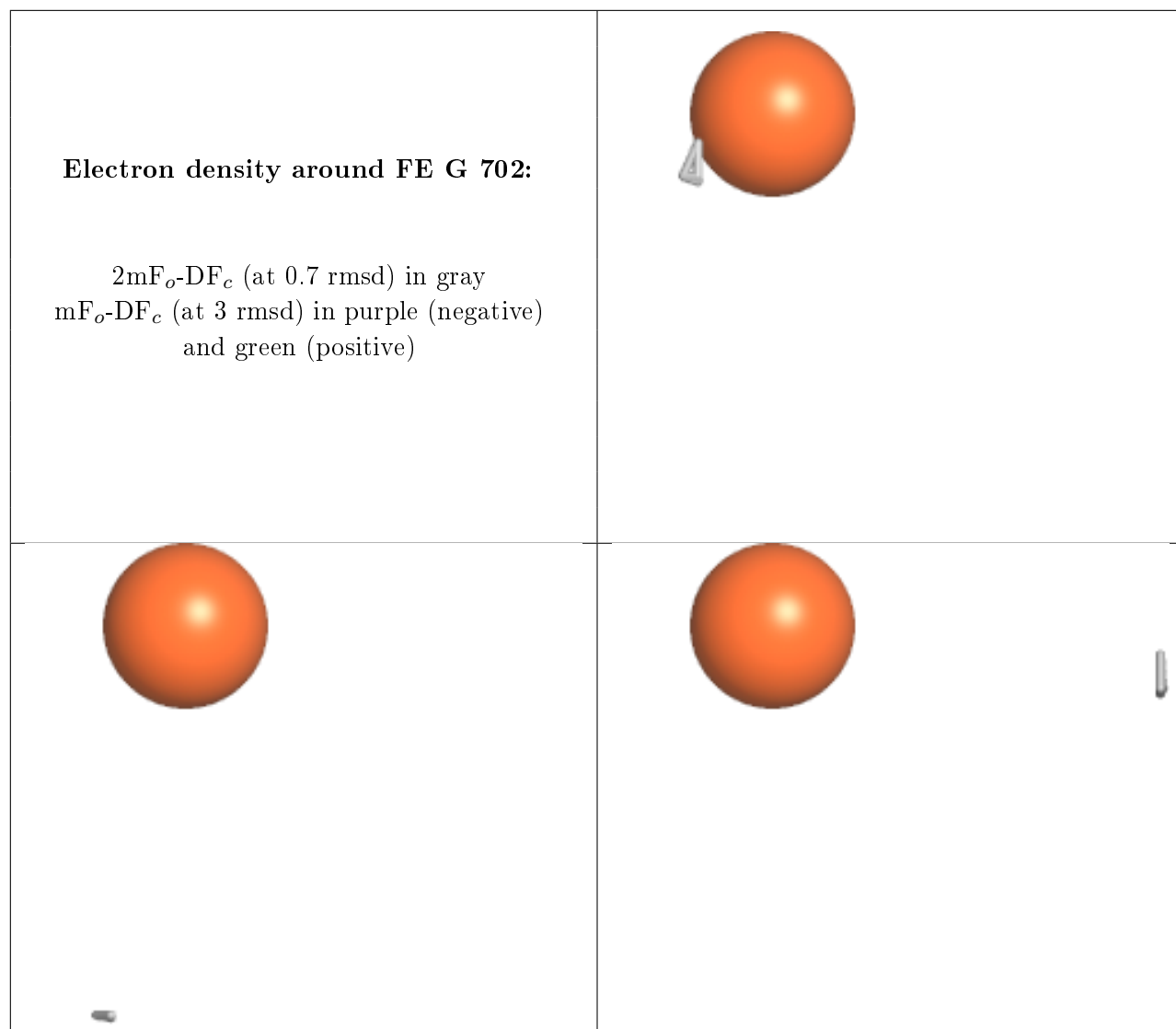
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around MG C 704:**

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

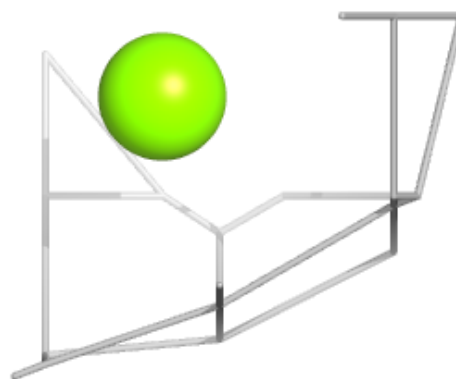
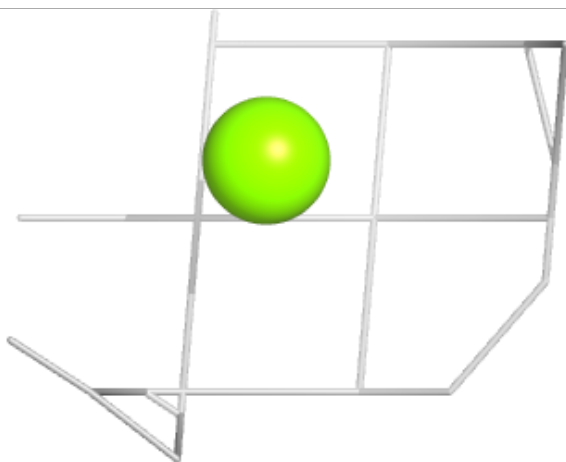
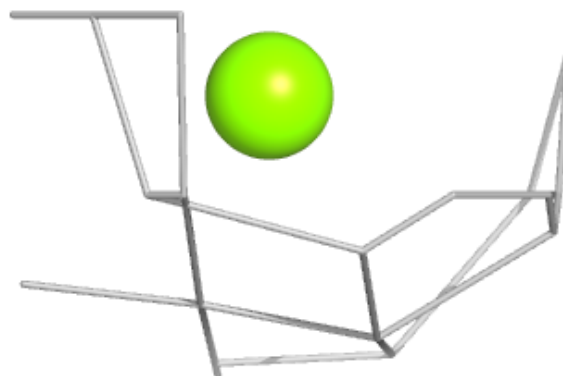






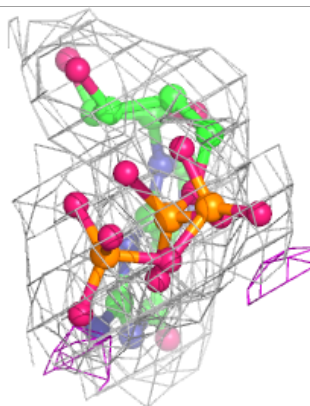
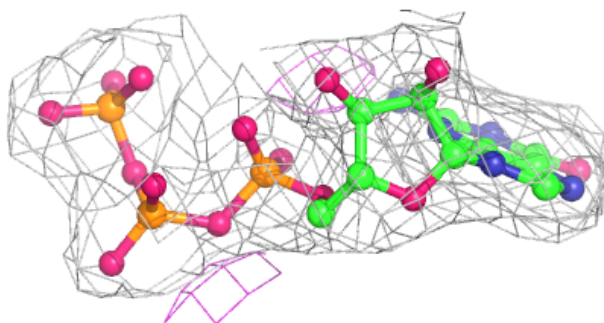
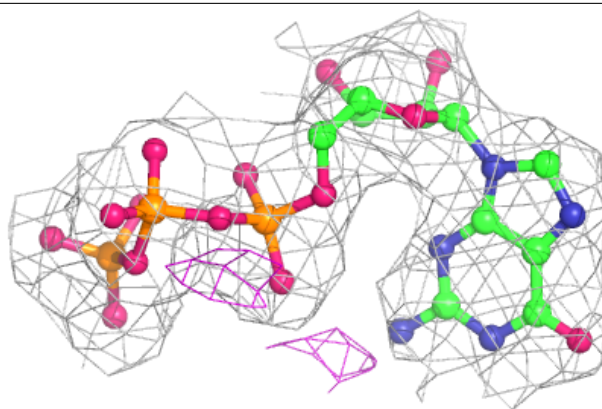
**Electron density around MG J 703:**

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

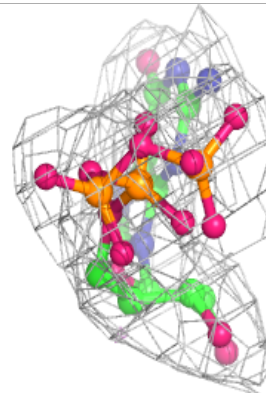
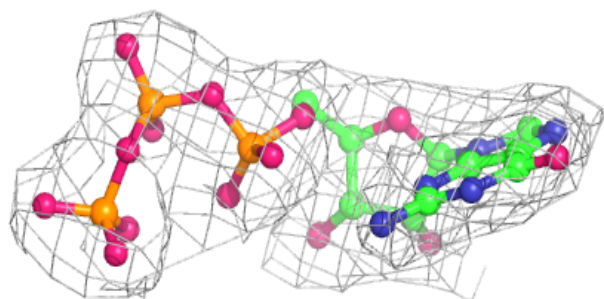
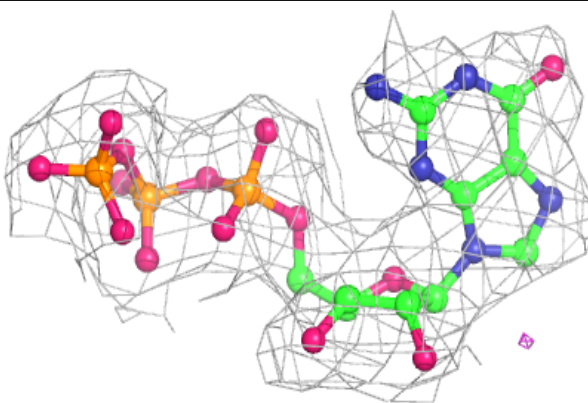


**Electron density around GTP D 707:**

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

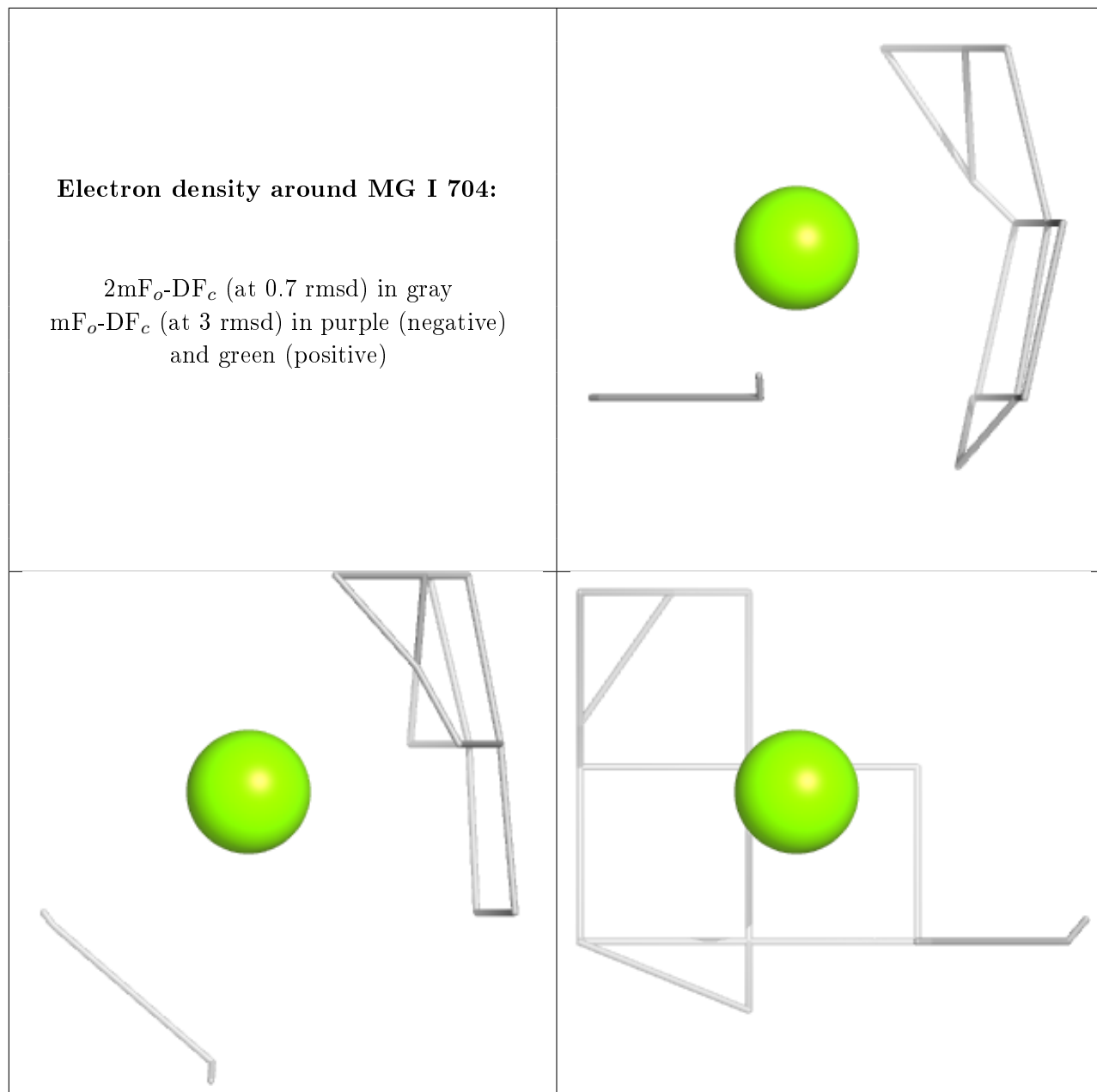
**Electron density around GTP B 706:**

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



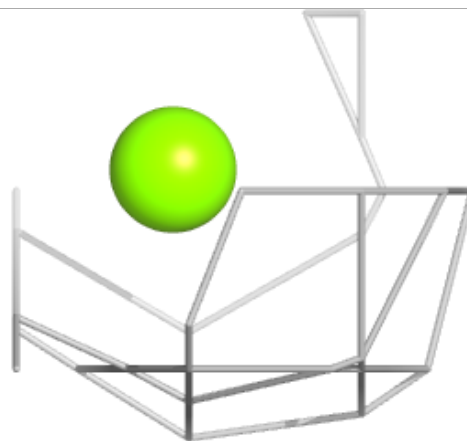
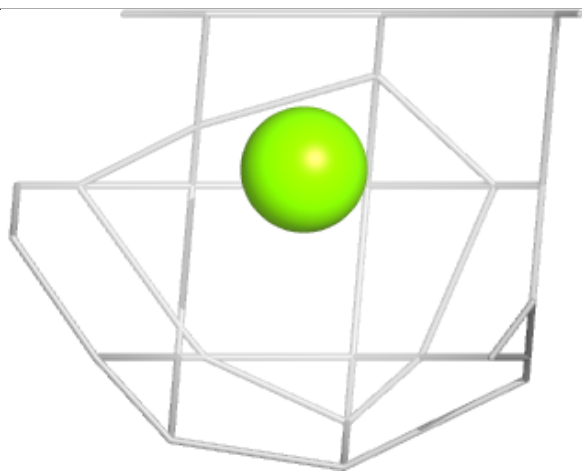
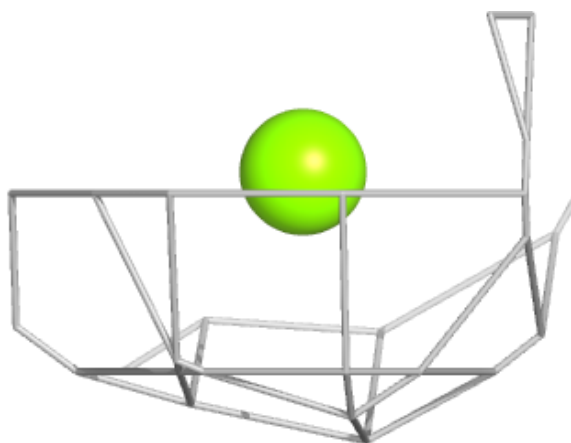
**Electron density around MG I 704:**

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



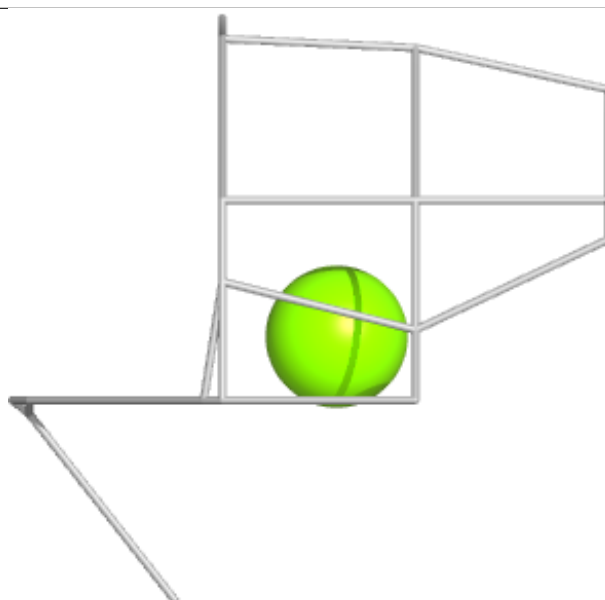
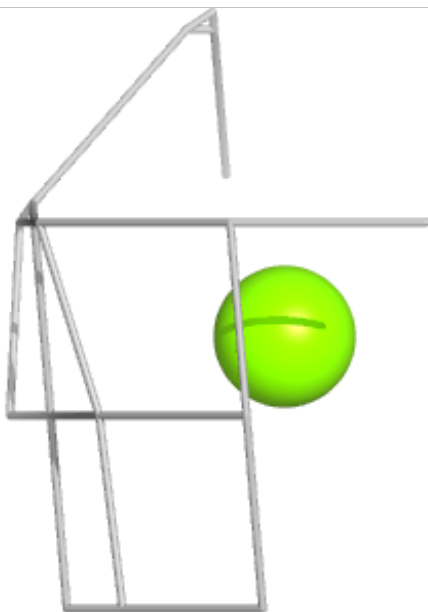
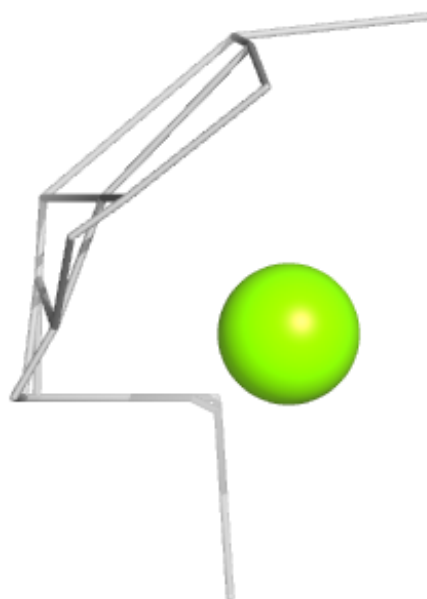
**Electron density around MG G 705:**

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



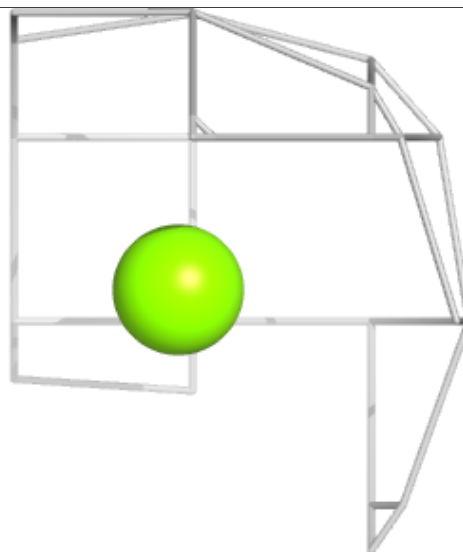
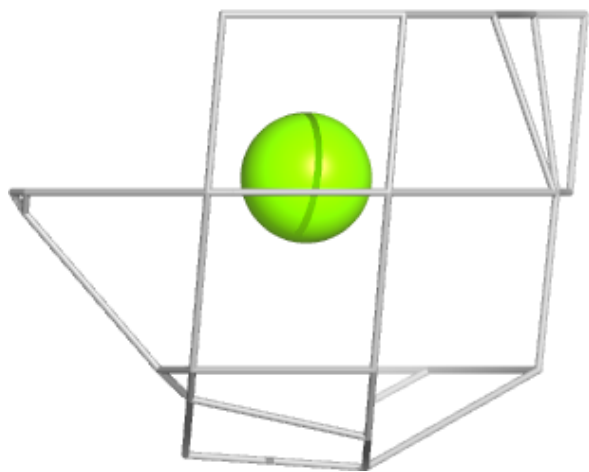
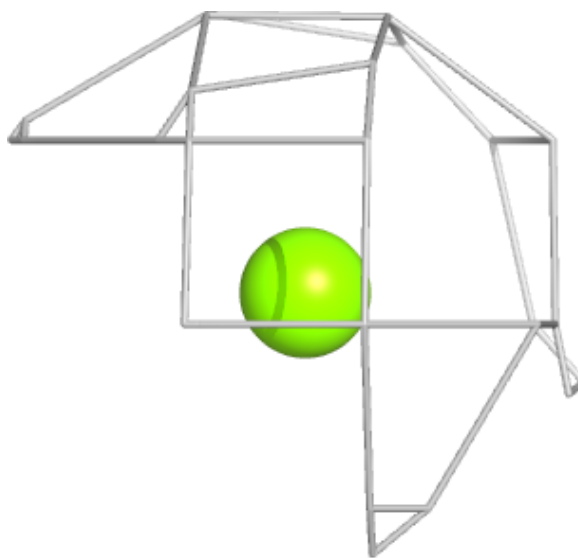
**Electron density around MG A 704:**

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



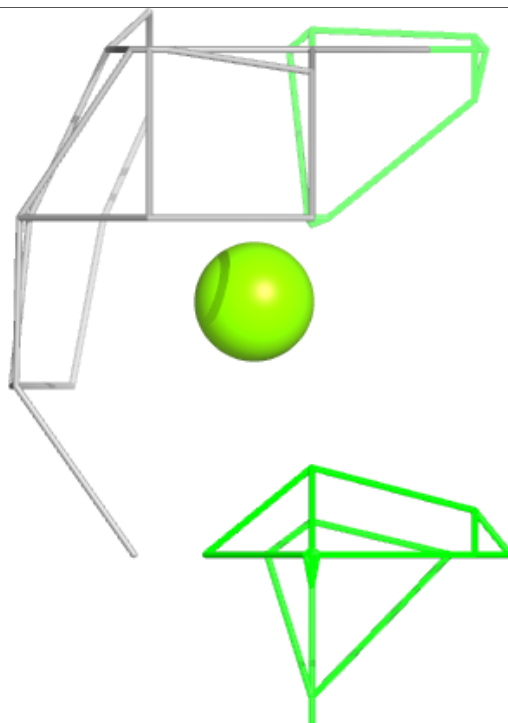
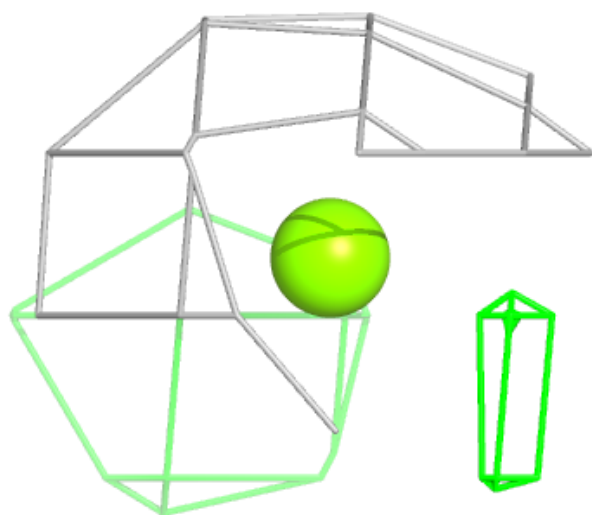
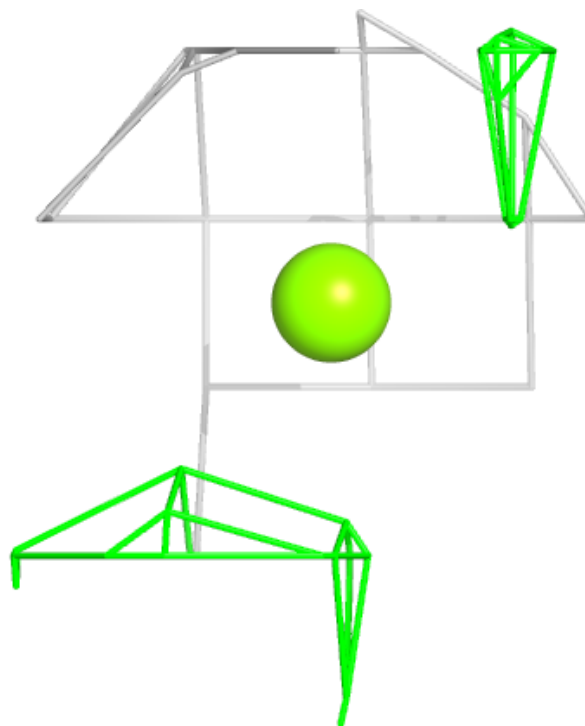
**Electron density around MG B 704:**

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



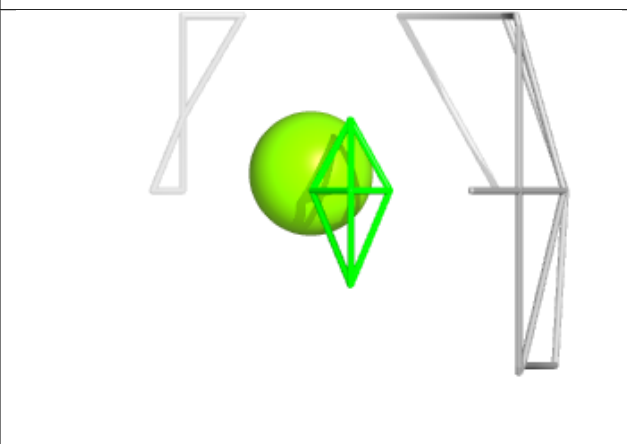
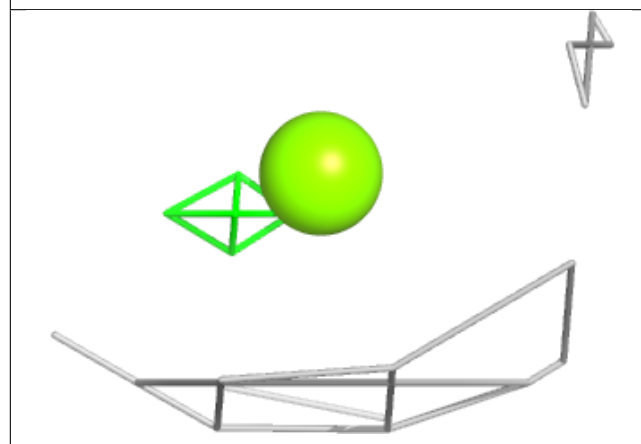
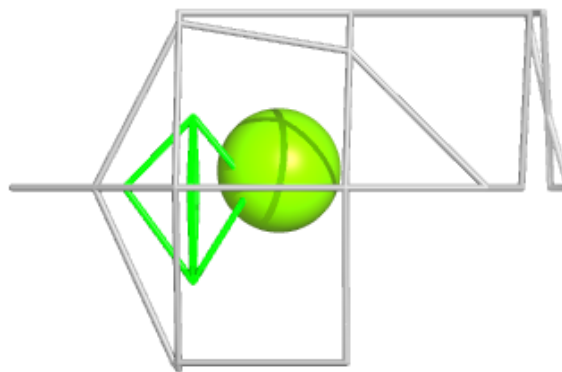
**Electron density around MG B 703:**

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



**Electron density around MG P 704:**

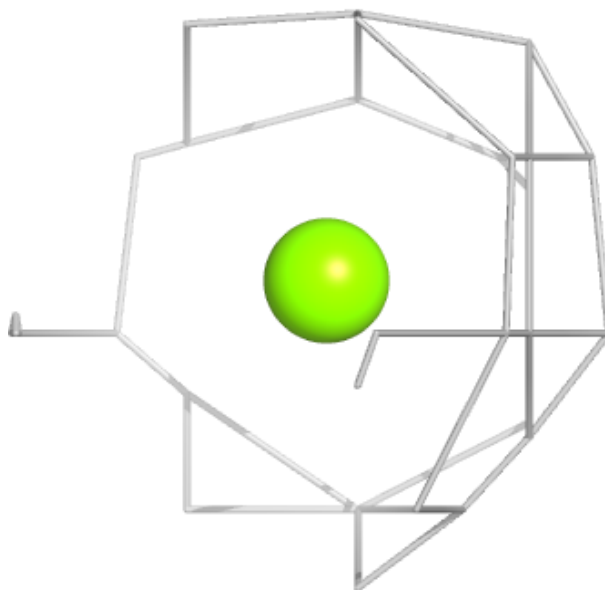
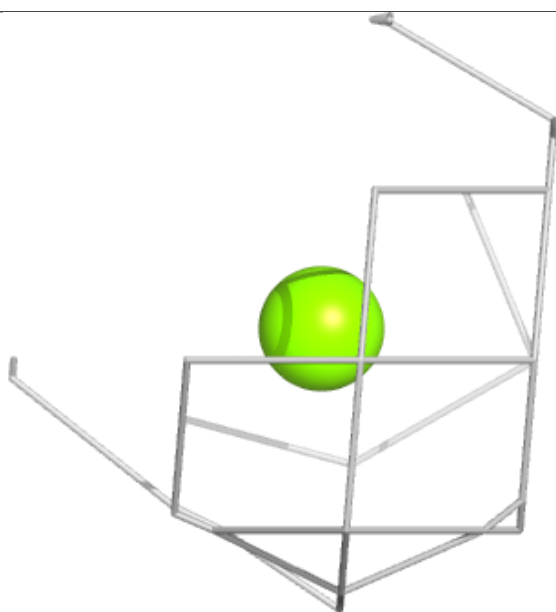
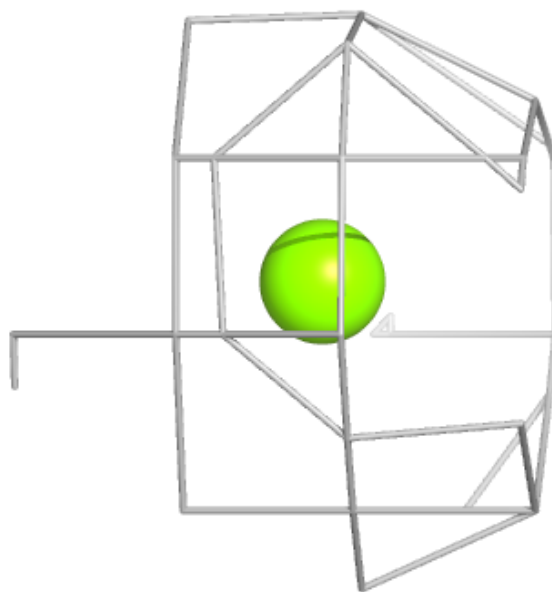
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





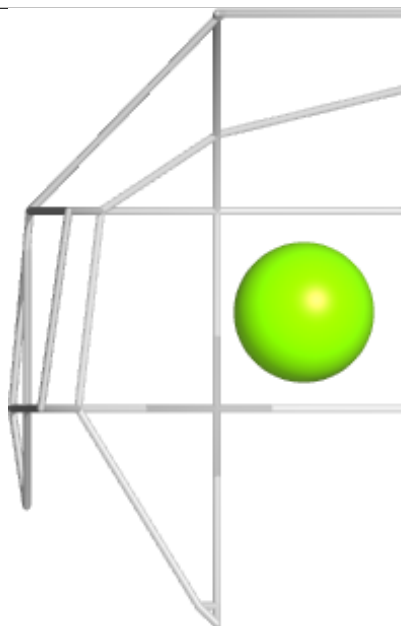
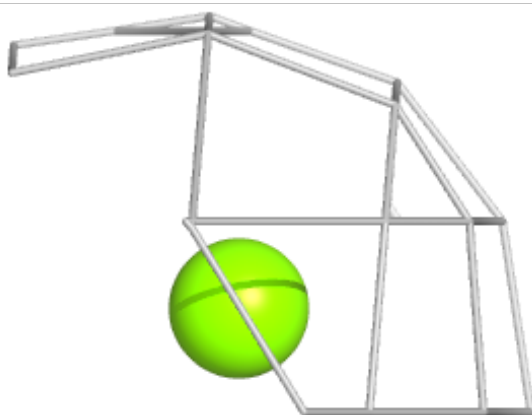
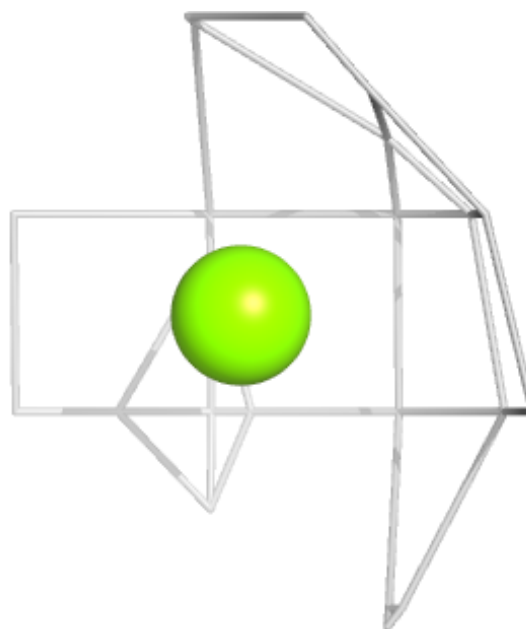
**Electron density around MG O 703:**

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



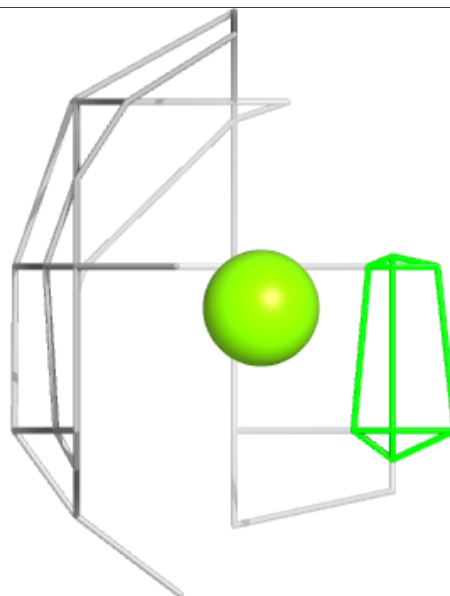
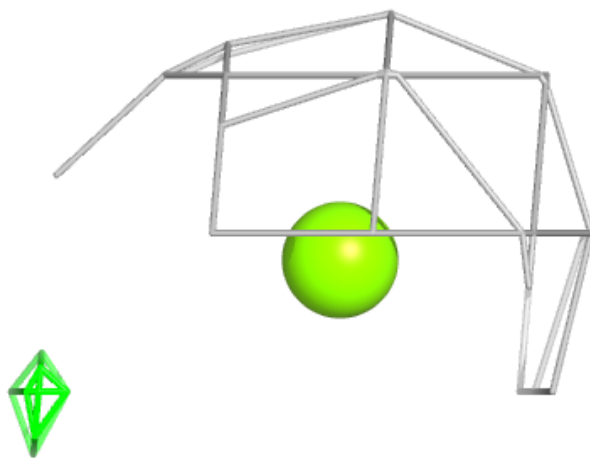
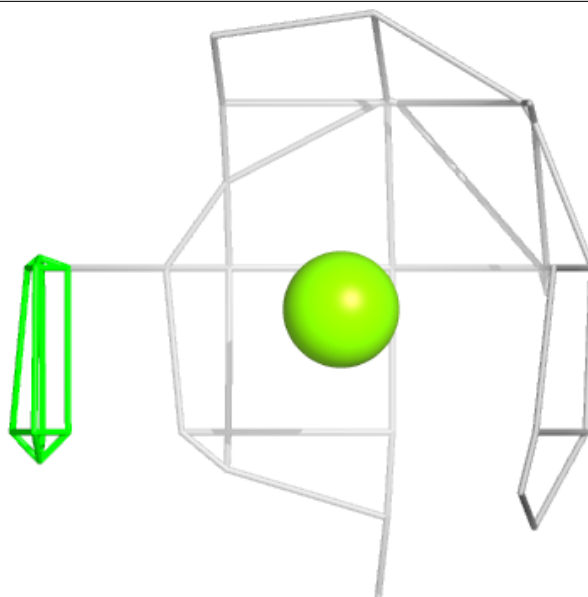
**Electron density around MG O 704:**

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



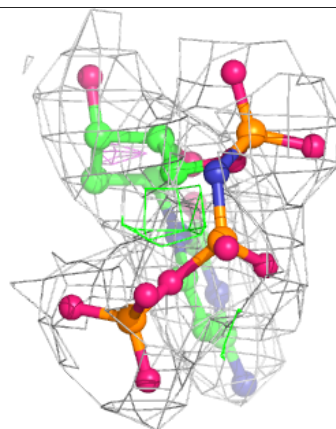
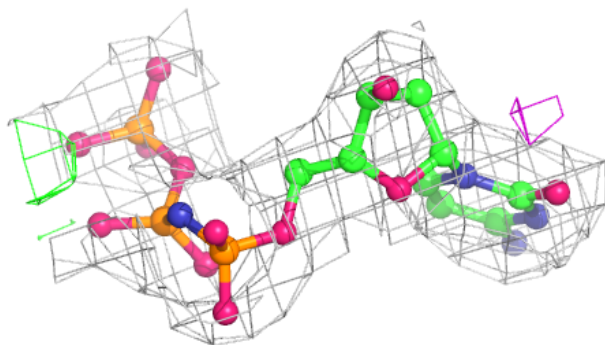
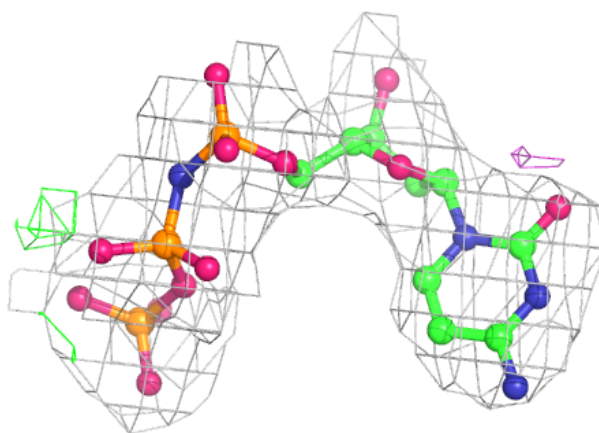
**Electron density around MG J 702:**

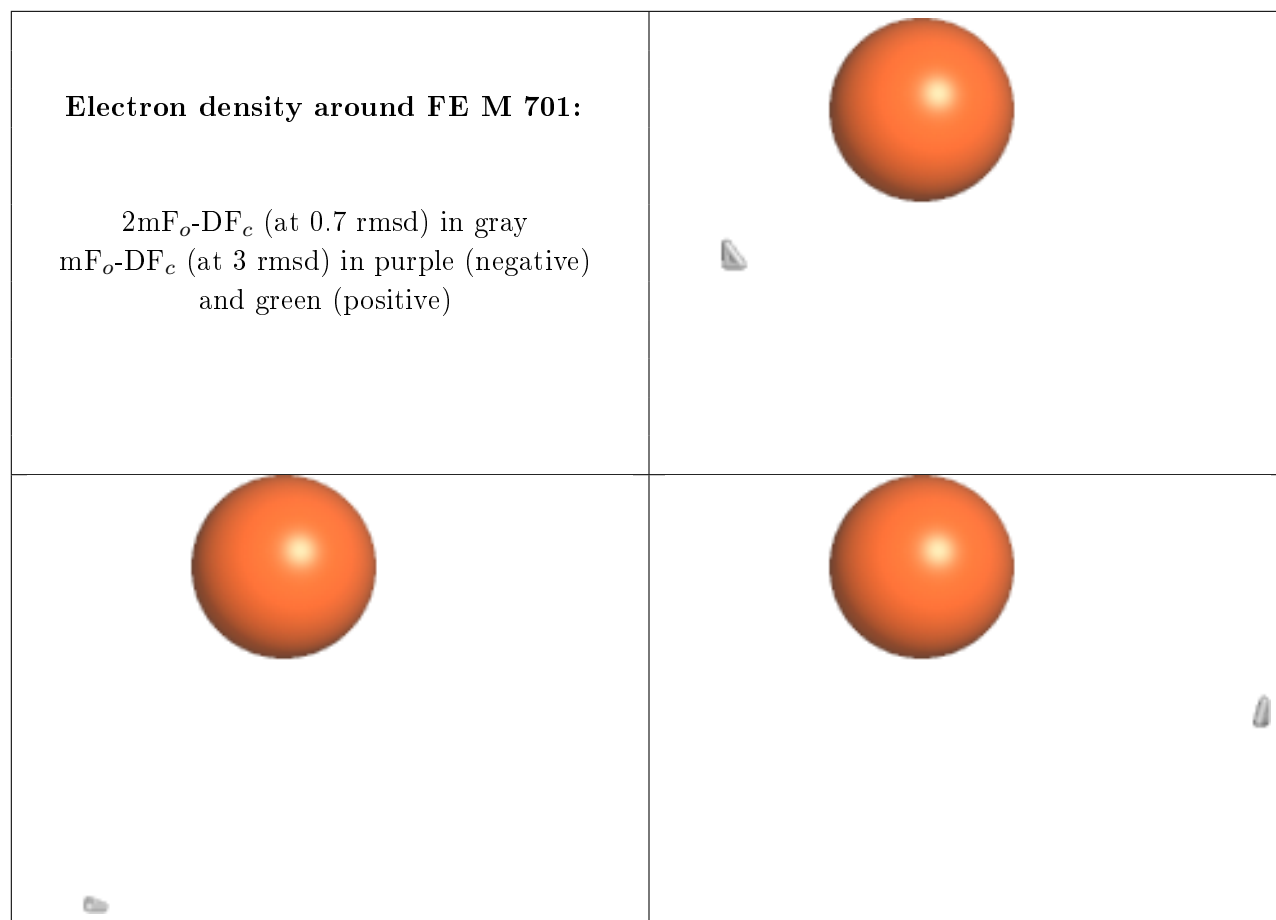
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 0KX B 705:**

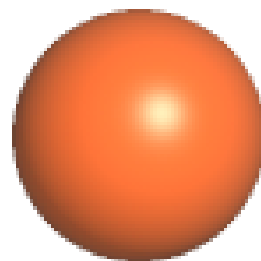
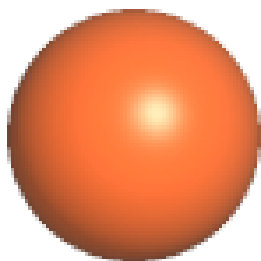
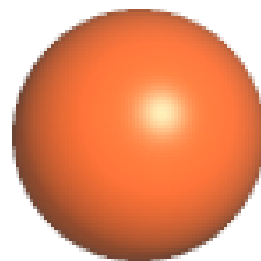
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

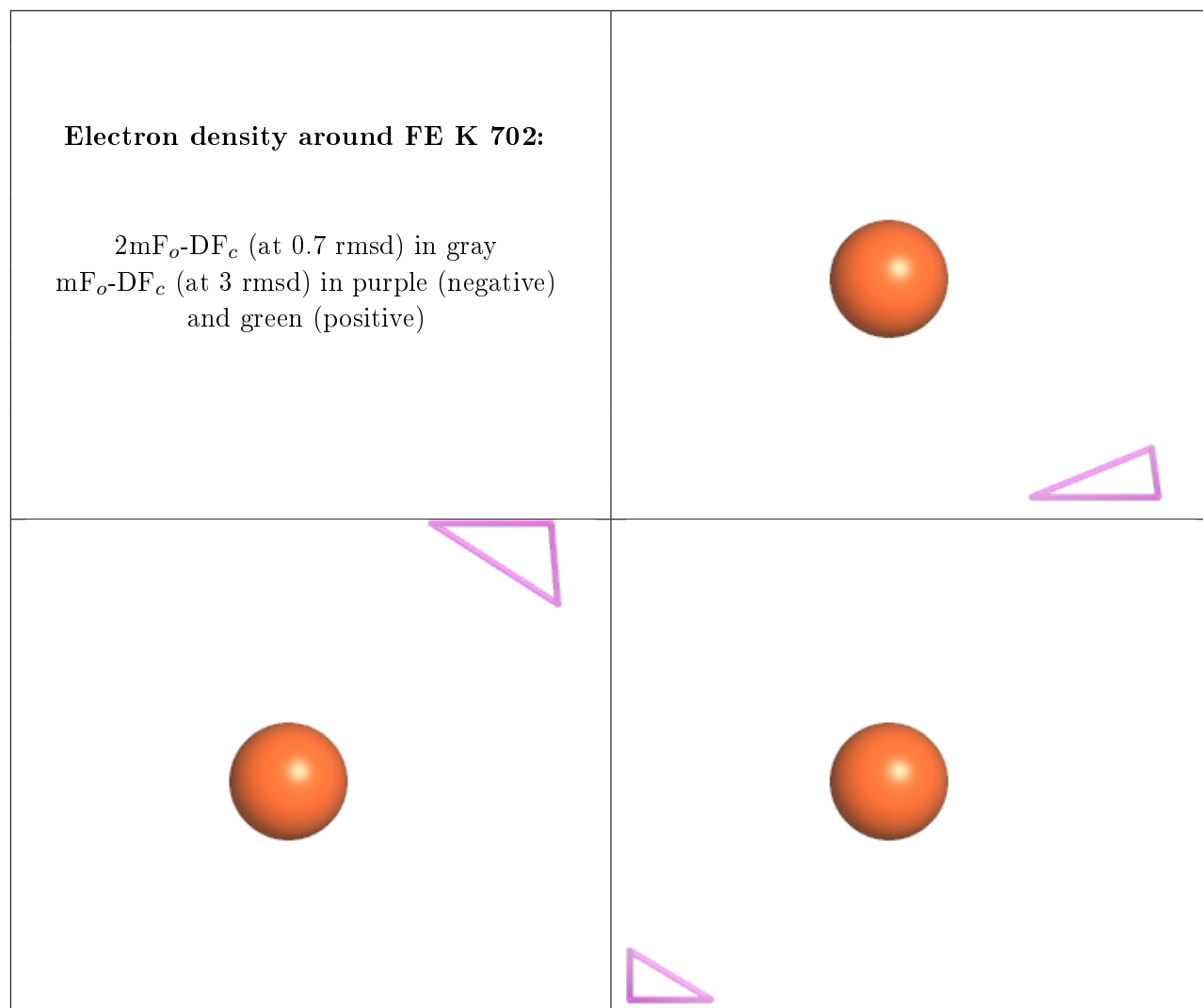




**Electron density around FE A 701:**

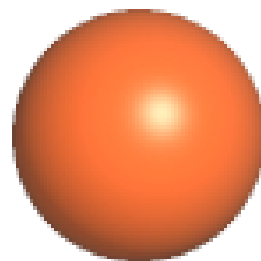
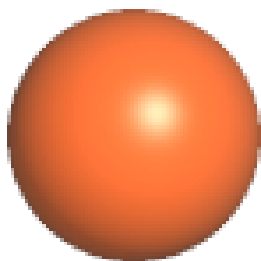
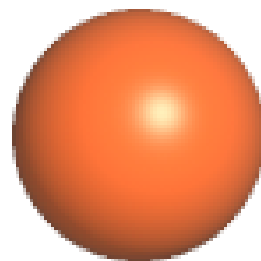
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around FE D 702:**

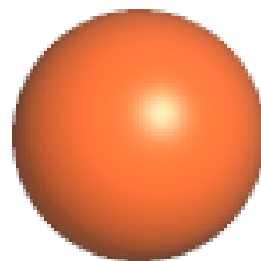
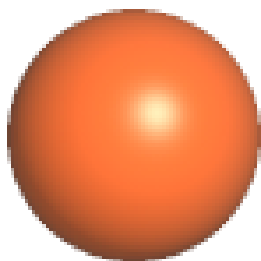
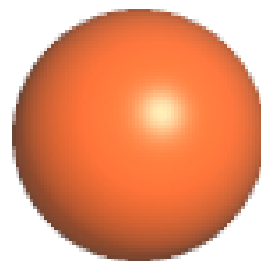
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





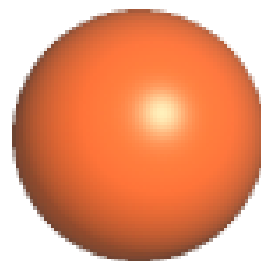
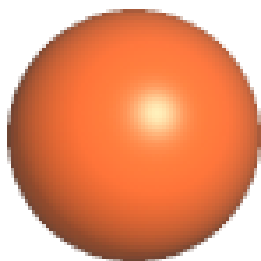
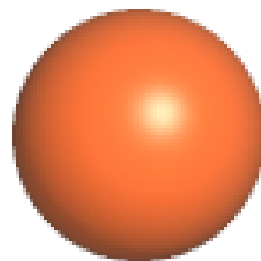
**Electron density around FE B 701:**

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



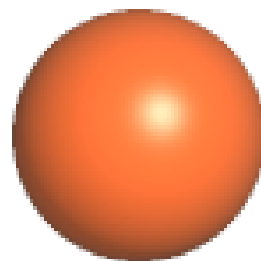
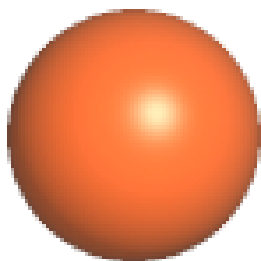
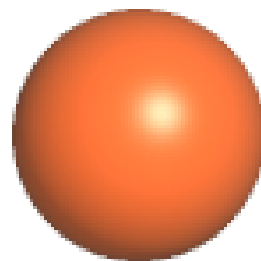
**Electron density around FE E 701:**

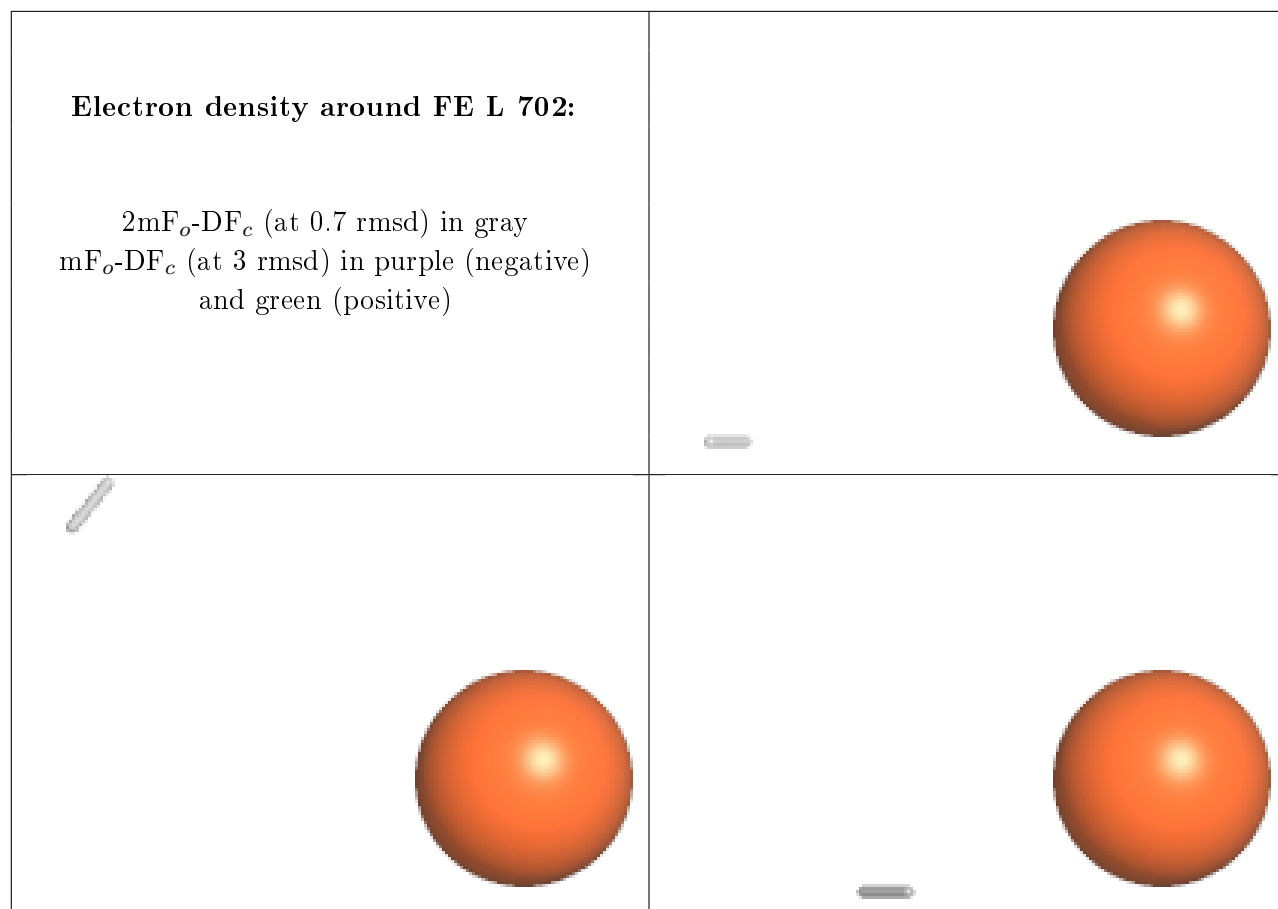
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

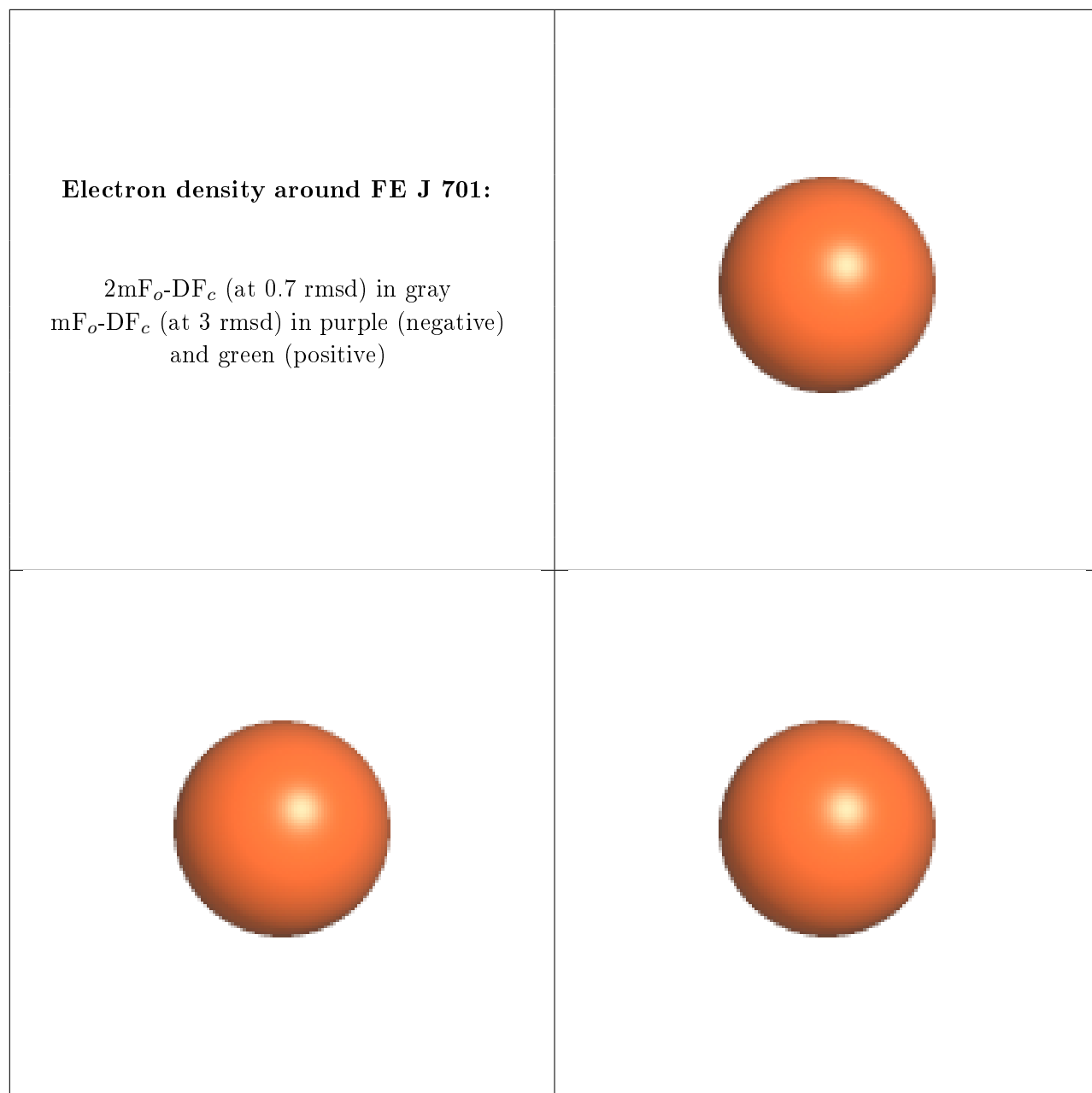


**Electron density around FE H 702:**

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

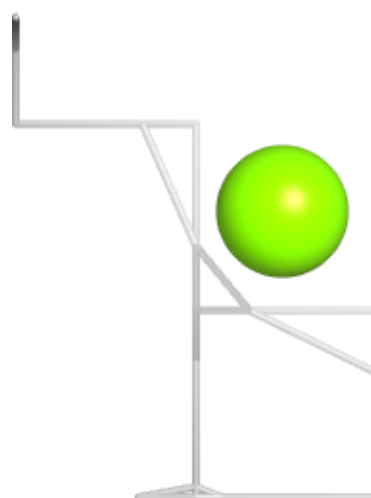
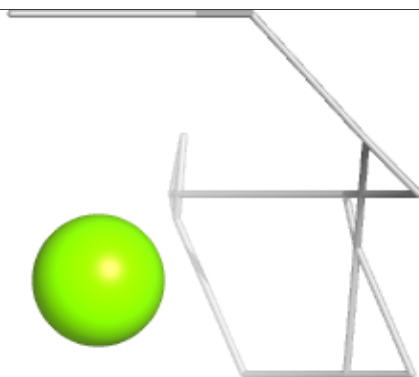
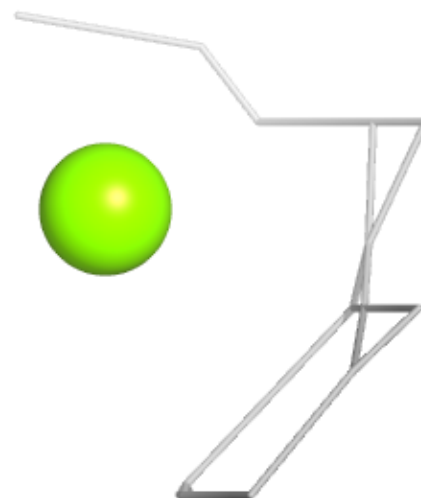






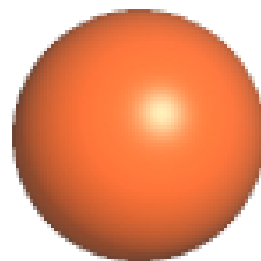
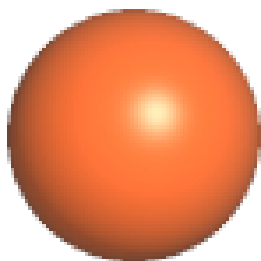
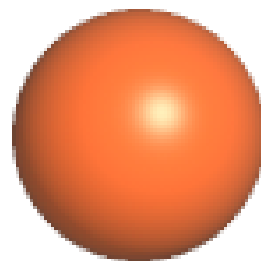
**Electron density around MG M 704:**

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



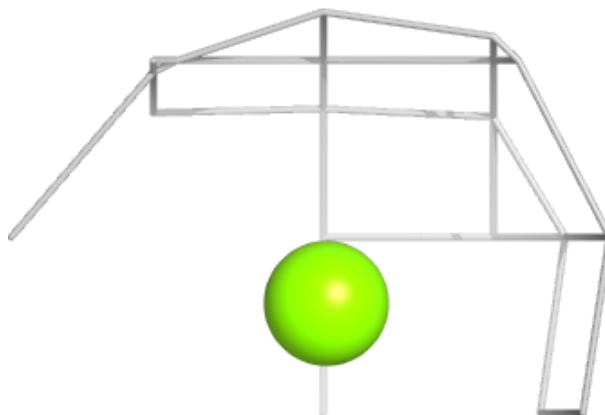
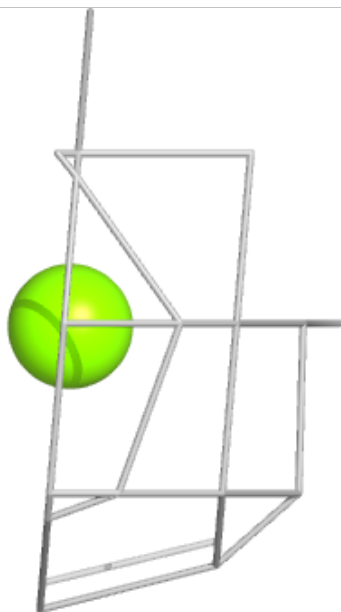
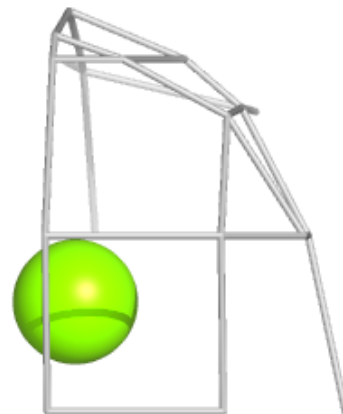
**Electron density around FE O 702:**

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



**Electron density around MG C 705:**

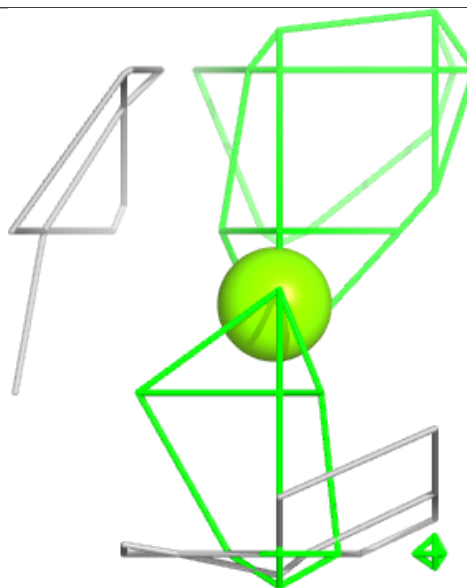
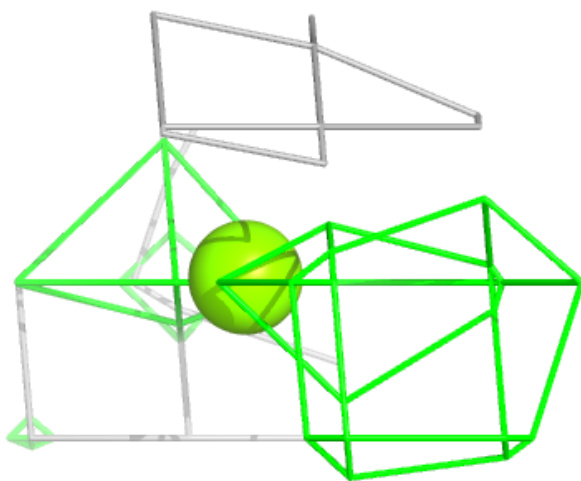
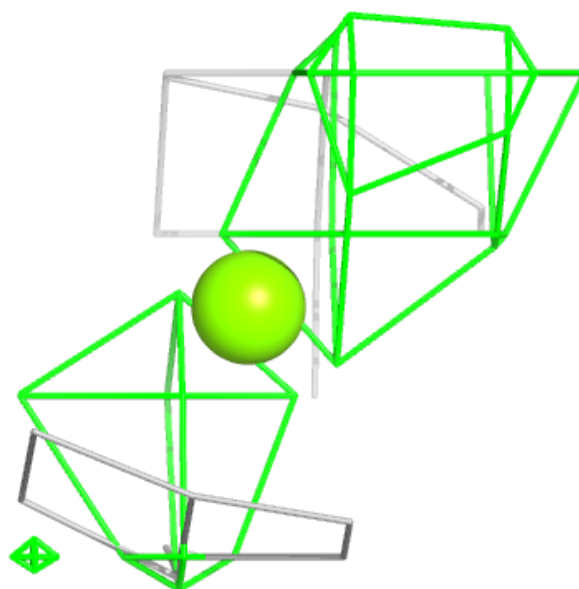
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

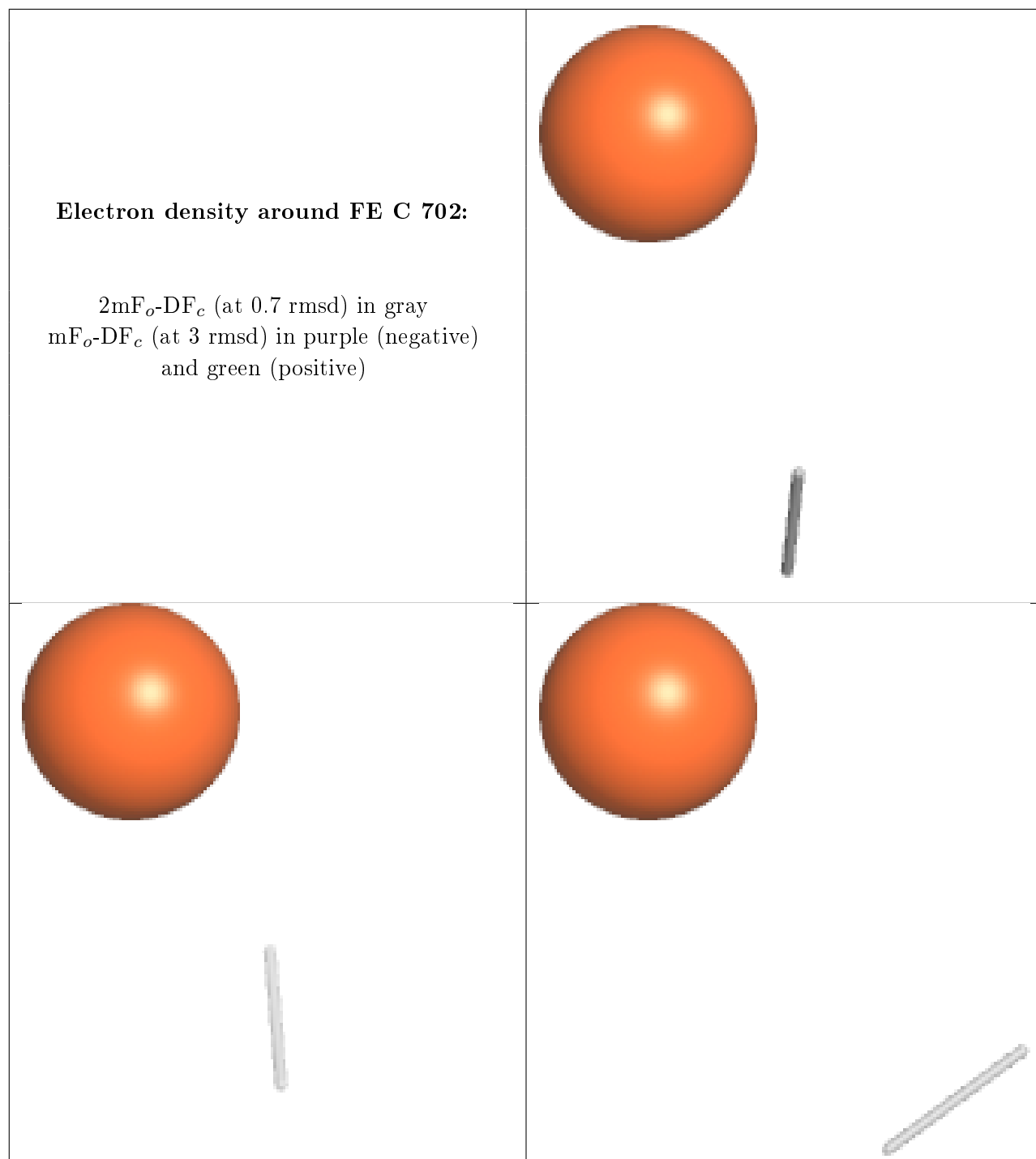


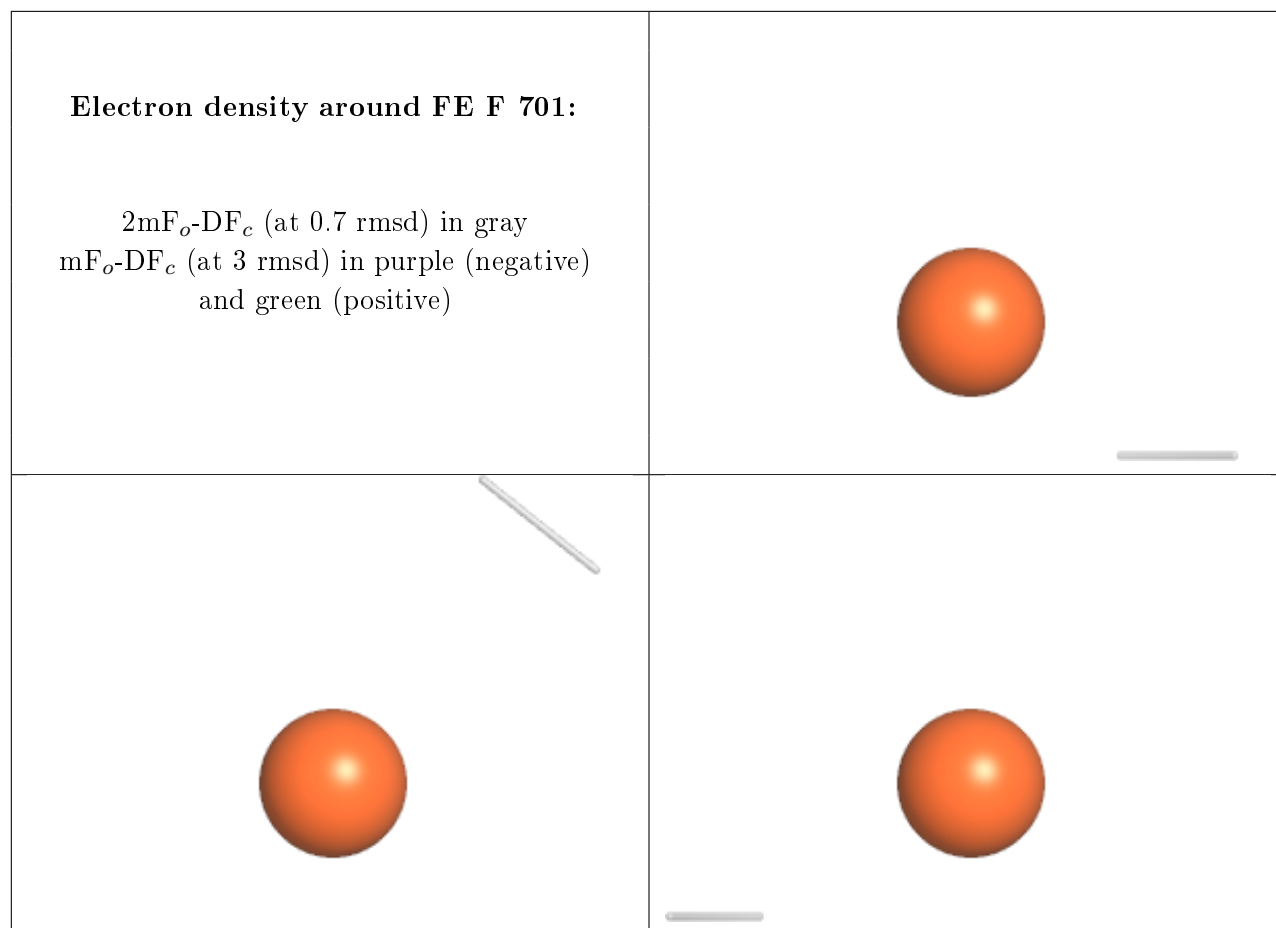


**Electron density around MG A 703:**

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







## 6.5 Other polymers [i](#)

There are no such residues in this entry.