



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 04:18 AM BST

PDB ID : 6TXA  
Title : Crystal structure of tetrameric human D137N-SAMHD1 (residues 109-626) with XTP, dGMPNPP and Mg  
Authors : Morris, E.R.; Kunzelmann, S.; Caswell, S.J.; Arnold, L.H.; Purkiss, A.; Kelly, G.; Taylor, I.A.  
Deposited on : 2020-01-13  
Resolution : 2.85 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

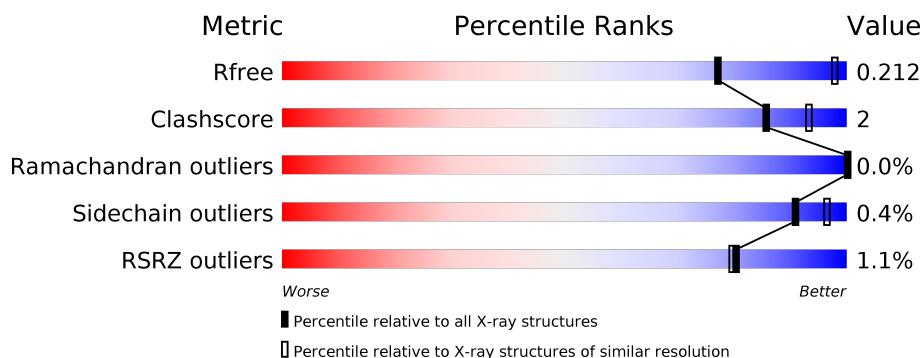
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	
1	B	520	
1	C	520	
1	D	520	
1	E	520	
1	F	520	

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Mol	Chain	Length	Quality of chain
1	G	520	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>87%5%8%</div></div></div>
1	H	520	<div><div><div></div><div></div><div></div></div><div>87%5%8%</div></div>
1	I	520	<div><div><div></div><div></div><div></div></div><div>88%•8%</div></div>
1	J	520	<div><div><div></div><div></div><div></div></div><div>87%5%8%</div></div>
1	K	520	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>87%••8%</div></div></div>
1	L	520	<div><div><div>3%</div><div><div></div><div></div><div></div></div><div>86%6%8%</div></div></div>
1	M	520	<div><div><div>3%</div><div><div></div><div></div><div></div></div><div>87%•8%</div></div></div>
1	N	520	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>88%•8%</div></div></div>
1	O	520	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>88%5%7%</div></div></div>
1	P	520	<div><div><div>3%</div><div><div></div><div></div><div></div></div><div>87%5%8%</div></div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 62976 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	480	Total	C	N	O	S	0	0	0
			3862	2472	667	703	20			
1	B	479	Total	C	N	O	S	0	0	0
			3845	2461	665	699	20			
1	C	480	Total	C	N	O	S	0	0	0
			3853	2467	667	699	20			
1	D	481	Total	C	N	O	S	0	0	0
			3852	2465	667	700	20			
1	E	479	Total	C	N	O	S	0	0	0
			3845	2461	665	699	20			
1	F	478	Total	C	N	O	S	0	0	0
			3831	2452	659	700	20			
1	G	479	Total	C	N	O	S	0	0	0
			3830	2450	660	700	20			
1	H	480	Total	C	N	O	S	0	0	0
			3870	2478	670	702	20			
1	I	479	Total	C	N	O	S	0	0	0
			3843	2460	664	699	20			
1	J	478	Total	C	N	O	S	0	0	0
			3827	2451	662	694	20			
1	K	478	Total	C	N	O	S	0	0	0
			3828	2450	659	699	20			
1	L	478	Total	C	N	O	S	0	0	0
			3789	2425	648	696	20			
1	M	476	Total	C	N	O	S	0	0	0
			3780	2419	648	693	20			
1	N	477	Total	C	N	O	S	0	0	0
			3818	2444	656	698	20			
1	O	486	Total	C	N	O	S	0	0	0
			3867	2472	665	710	20			
1	P	478	Total	C	N	O	S	0	0	0
			3793	2431	651	691	20			



There are 48 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
A	137	ASN	ASP	engineered mutation	UNP Q9Y3Z3
B	107	GLY	-	expression tag	UNP Q9Y3Z3
B	108	SER	-	expression tag	UNP Q9Y3Z3
B	137	ASN	ASP	engineered mutation	UNP Q9Y3Z3
C	107	GLY	-	expression tag	UNP Q9Y3Z3
C	108	SER	-	expression tag	UNP Q9Y3Z3
C	137	ASN	ASP	engineered mutation	UNP Q9Y3Z3
D	107	GLY	-	expression tag	UNP Q9Y3Z3
D	108	SER	-	expression tag	UNP Q9Y3Z3
D	137	ASN	ASP	engineered mutation	UNP Q9Y3Z3
E	107	GLY	-	expression tag	UNP Q9Y3Z3
E	108	SER	-	expression tag	UNP Q9Y3Z3
E	137	ASN	ASP	engineered mutation	UNP Q9Y3Z3
F	107	GLY	-	expression tag	UNP Q9Y3Z3
F	108	SER	-	expression tag	UNP Q9Y3Z3
F	137	ASN	ASP	engineered mutation	UNP Q9Y3Z3
G	107	GLY	-	expression tag	UNP Q9Y3Z3
G	108	SER	-	expression tag	UNP Q9Y3Z3
G	137	ASN	ASP	engineered mutation	UNP Q9Y3Z3
H	107	GLY	-	expression tag	UNP Q9Y3Z3
H	108	SER	-	expression tag	UNP Q9Y3Z3
H	137	ASN	ASP	engineered mutation	UNP Q9Y3Z3
I	107	GLY	-	expression tag	UNP Q9Y3Z3
I	108	SER	-	expression tag	UNP Q9Y3Z3
I	137	ASN	ASP	engineered mutation	UNP Q9Y3Z3
J	107	GLY	-	expression tag	UNP Q9Y3Z3
J	108	SER	-	expression tag	UNP Q9Y3Z3
J	137	ASN	ASP	engineered mutation	UNP Q9Y3Z3
K	107	GLY	-	expression tag	UNP Q9Y3Z3
K	108	SER	-	expression tag	UNP Q9Y3Z3
K	137	ASN	ASP	engineered mutation	UNP Q9Y3Z3
L	107	GLY	-	expression tag	UNP Q9Y3Z3
L	108	SER	-	expression tag	UNP Q9Y3Z3
L	137	ASN	ASP	engineered mutation	UNP Q9Y3Z3
M	107	GLY	-	expression tag	UNP Q9Y3Z3
M	108	SER	-	expression tag	UNP Q9Y3Z3
M	137	ASN	ASP	engineered mutation	UNP Q9Y3Z3
N	107	GLY	-	expression tag	UNP Q9Y3Z3
N	108	SER	-	expression tag	UNP Q9Y3Z3
N	137	ASN	ASP	engineered mutation	UNP Q9Y3Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
O	107	GLY	-	expression tag	UNP Q9Y3Z3
O	108	SER	-	expression tag	UNP Q9Y3Z3
O	137	ASN	ASP	engineered mutation	UNP Q9Y3Z3
P	107	GLY	-	expression tag	UNP Q9Y3Z3
P	108	SER	-	expression tag	UNP Q9Y3Z3
P	137	ASN	ASP	engineered mutation	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
2	J	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0
2	K	1	Total Fe 1 1	0	0
2	E	1	Total Fe 1 1	0	0
2	H	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0
2	I	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0
2	A	1	Total Fe 1 1	0	0
2	N	1	Total Fe 1 1	0	0
2	O	1	Total Fe 1 1	0	0
2	L	1	Total Fe 1 1	0	0
2	F	1	Total Fe 1 1	0	0
2	M	1	Total Fe 1 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	3	Total 3	Mg 3	0	0
3	D	3	Total 3	Mg 3	0	0
3	K	3	Total 3	Mg 3	0	0
3	E	3	Total 3	Mg 3	0	0
3	H	3	Total 3	Mg 3	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	3	Total 3	Mg 3	0	0
3	O	3	Total 3	Mg 3	0	0
3	L	3	Total 3	Mg 3	0	0
3	F	3	Total 3	Mg 3	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]guanosine (three-letter code: XG4) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by author).

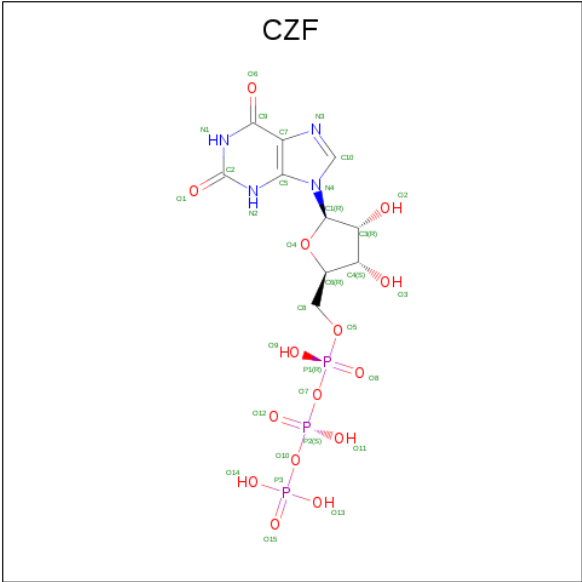


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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	H	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	H	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	I	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	I	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	I	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	J	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	J	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	K	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	K	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	L	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	M	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	M	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	N	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	N	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	O	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	O	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	P	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	P	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 5 is [[[2 {R},3 {S},4 {R},5 {R}]-5-[2,6-bis(oxidanylidene)-3 {H}-purin-9-yl]-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] phosphono hydrogen phosphate (three-letter code: CZF) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>4</sub>O<sub>15</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	4	15	3		
5	B	1	Total	C	N	O	P	0	0
			32	10	4	15	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	4	15	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	4	15	3		
5	E	1	Total	C	N	O	P	0	0
			32	10	4	15	3		
5	F	1	Total	C	N	O	P	0	0
			32	10	4	15	3		
5	G	1	Total	C	N	O	P	0	0
			32	10	4	15	3		
5	H	1	Total	C	N	O	P	0	0
			32	10	4	15	3		
5	J	1	Total	C	N	O	P	0	0
			32	10	4	15	3		
5	J	1	Total	C	N	O	P	0	0
			32	10	4	15	3		
5	K	1	Total	C	N	O	P	0	0
			32	10	4	15	3		
5	L	1	Total	C	N	O	P	0	0
			32	10	4	15	3		
5	M	1	Total	C	N	O	P	0	0
			32	10	4	15	3		
5	N	1	Total	C	N	O	P	0	0
			32	10	4	15	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	O	1	Total	C	N	O	P	0	0
			32	10	4	15	3		
5	P	1	Total	C	N	O	P	0	0
			32	10	4	15	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	E	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	G	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		

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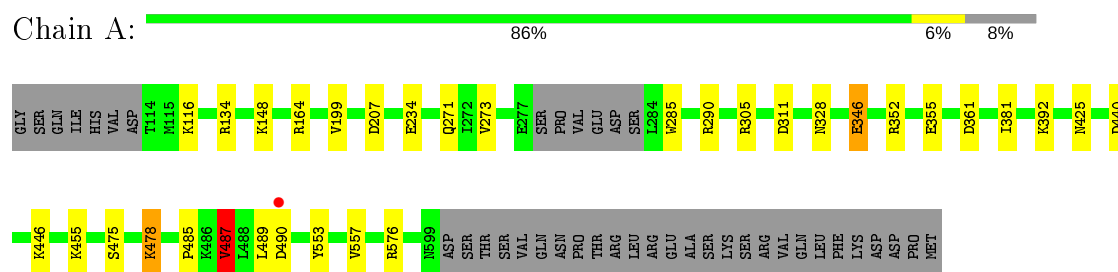
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	J	1	Total	O	S	0	0
			5	4	1		
6	K	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	N	1	Total	O	S	0	0
			5	4	1		
6	O	1	Total	O	S	0	0
			5	4	1		



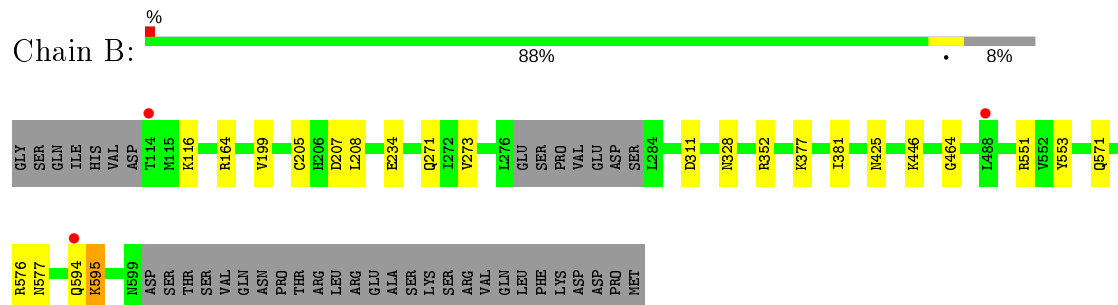
### 3 Residue-property plots [i](#)

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.

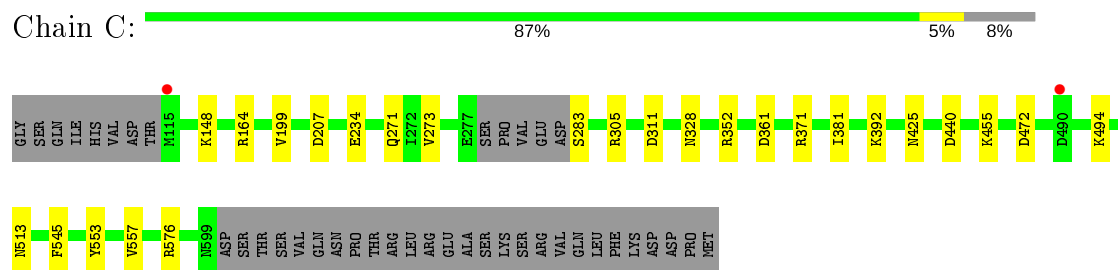
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



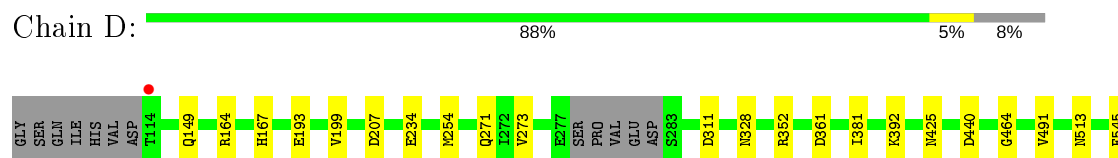
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

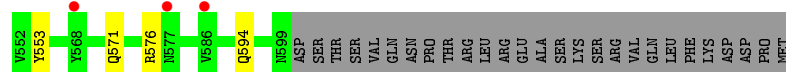
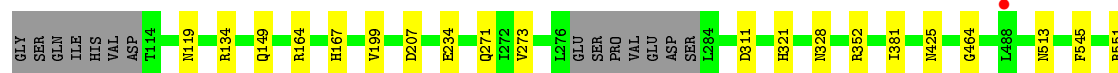
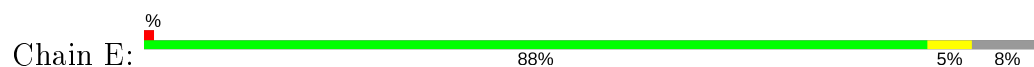


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

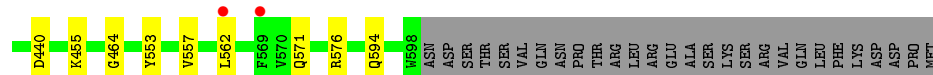
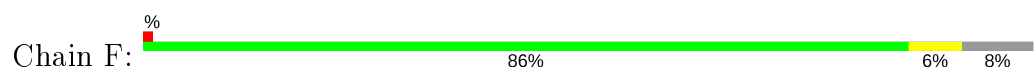




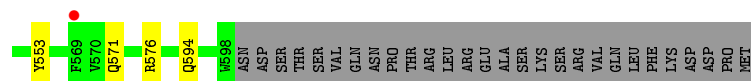
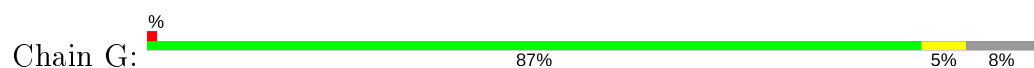
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



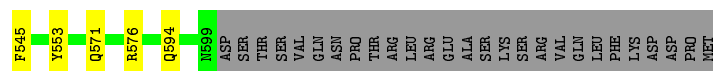
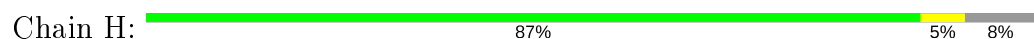
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



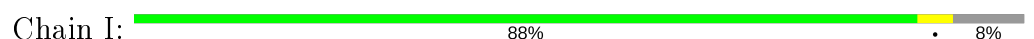
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

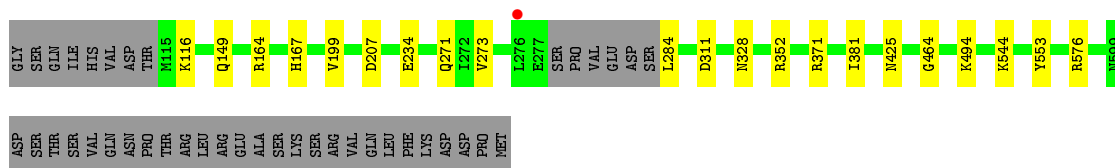


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



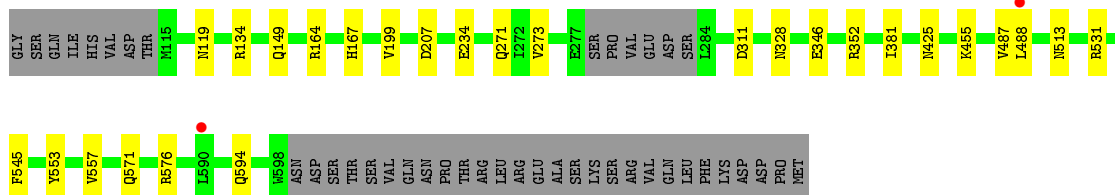
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





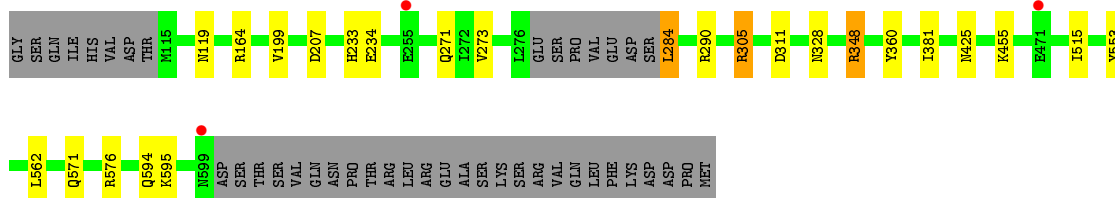
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain J: 87% 5% 8%



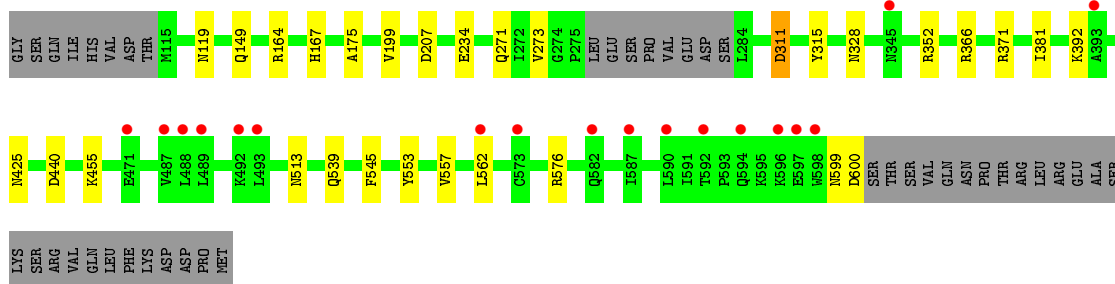
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain K: 87% 8%



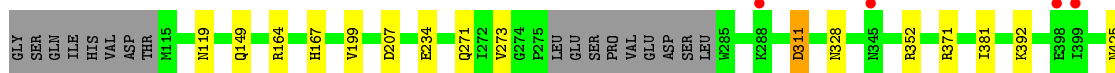
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

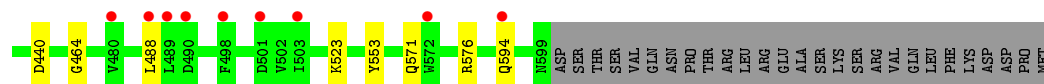
Chain L: 3% 86% 6% 8%



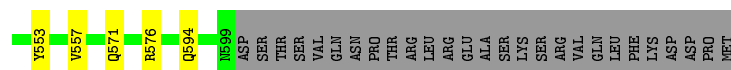
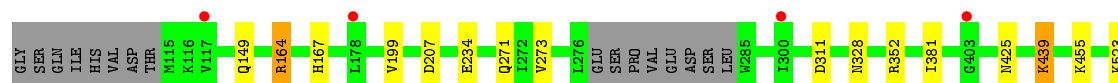
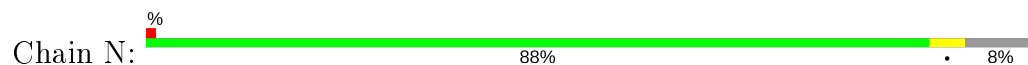
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain M: 3% 87% 8%

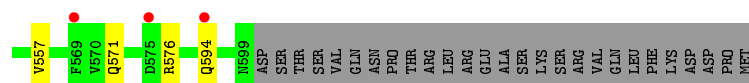
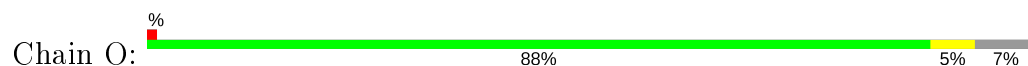




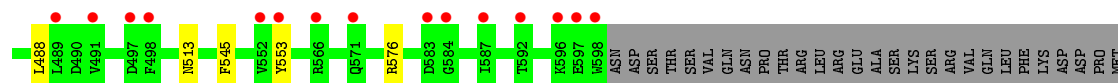
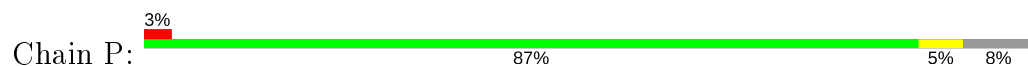
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



- 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, $\alpha$ , $\beta$ , $\gamma$	97.78Å 172.90Å 275.89Å 90.00° 95.20° 90.00°	Depositor
Resolution (Å)	146.24 – 2.85 274.75 – 2.84	Depositor EDS
% Data completeness (in resolution range)	66.4 (146.24-2.85) 65.8 (274.75-2.84)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.194 , 0.212 0.196 , 0.212	Depositor DCC
$R_{free}$ test set	7031 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.5	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 37.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	62976	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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: SO4, MG, CZF, XG4, 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	0.64	1/3955 (0.0%)	0.84	11/5356 (0.2%)
1	B	0.59	0/3938	0.79	6/5336 (0.1%)
1	C	0.60	0/3946	0.80	8/5344 (0.1%)
1	D	0.62	0/3945	0.81	7/5346 (0.1%)
1	E	0.57	0/3938	0.78	7/5336 (0.1%)
1	F	0.58	1/3924 (0.0%)	0.80	6/5320 (0.1%)
1	G	0.57	0/3923	0.79	5/5321 (0.1%)
1	H	0.60	0/3963	0.80	6/5364 (0.1%)
1	I	0.55	0/3936	0.77	5/5333 (0.1%)
1	J	0.57	0/3920	0.80	8/5313 (0.2%)
1	K	0.56	1/3921 (0.0%)	0.83	9/5316 (0.2%)
1	L	0.56	0/3882	0.78	6/5272 (0.1%)
1	M	0.53	0/3873	0.76	6/5258 (0.1%)
1	N	0.57	0/3911	0.78	5/5302 (0.1%)
1	O	0.54	0/3962	0.78	6/5379 (0.1%)
1	P	0.54	0/3886	0.80	8/5275 (0.2%)
All	All	0.57	3/62823 (0.0%)	0.79	109/85171 (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
1	C	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	305	ARG	NE-CZ	-5.57	1.25	1.33
1	F	346	GLU	CD-OE2	-5.17	1.20	1.25
1	A	355	GLU	CD-OE1	5.03	1.31	1.25

The worst 5 of 109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	305	ARG	NE-CZ-NH2	16.28	128.44	120.30
1	D	164	ARG	NE-CZ-NH1	11.82	126.21	120.30
1	J	164	ARG	NE-CZ-NH1	11.38	125.99	120.30
1	L	164	ARG	NE-CZ-NH1	11.24	125.92	120.30
1	H	164	ARG	NE-CZ-NH1	11.13	125.86	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	487	VAL	Mainchain
1	C	283	SER	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3862	0	3768	18	0
1	B	3845	0	3742	16	0
1	C	3853	0	3758	11	1
1	D	3852	0	3745	14	0
1	E	3845	0	3742	17	0
1	F	3831	0	3713	21	0
1	G	3830	0	3698	15	0
1	H	3870	0	3792	16	0
1	I	3843	0	3735	14	0
1	J	3827	0	3716	24	0
1	K	3828	0	3706	23	0
1	L	3789	0	3621	23	0
1	M	3780	0	3621	25	0
1	N	3818	0	3695	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	3867	0	3722	21	0
1	P	3793	0	3650	15	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	3	0	0	0	0
3	F	3	0	0	0	0
3	G	3	0	0	0	0
3	H	3	0	0	0	0
3	I	3	0	0	0	0
3	J	3	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	3	0	0	0	0
3	O	3	0	0	0	0
3	P	3	0	0	0	0
4	A	62	0	26	2	0
4	B	62	0	26	3	0
4	C	62	0	26	5	0
4	D	62	0	26	3	0
4	E	62	0	26	3	0
4	F	62	0	26	3	0
4	G	62	0	26	5	0
4	H	62	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	93	0	39	9	0
4	J	62	0	26	4	0
4	K	62	0	26	4	0
4	L	31	0	13	2	0
4	M	62	0	26	6	0
4	N	62	0	26	6	0
4	O	62	0	26	4	0
4	P	62	0	26	5	0
5	A	32	0	0	2	0
5	B	32	0	0	1	0
5	C	64	0	0	1	0
5	E	32	0	0	1	0
5	F	32	0	0	1	0
5	G	32	0	0	0	0
5	H	32	0	0	2	0
5	J	64	0	0	3	0
5	K	32	0	0	1	0
5	L	32	0	0	0	0
5	M	32	0	0	0	0
5	N	32	0	0	1	0
5	O	32	0	0	2	0
5	P	32	0	0	2	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	0	0
6	E	5	0	0	0	0
6	F	5	0	0	0	0
6	G	5	0	0	1	0
6	H	5	0	0	0	0
6	I	5	0	0	0	0
6	J	5	0	0	0	0
6	K	5	0	0	0	0
6	L	5	0	0	0	0
6	M	5	0	0	0	0
6	N	5	0	0	0	0
6	O	5	0	0	0	0
All	All	62976	0	59840	270	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 270 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:NH2	4:N:708:XG4:O2G	2.08	0.85
1:K:305:ARG:HH11	1:K:348:ARG:CD	1.97	0.78
1:J:488:LEU:N	1:M:488:LEU:HB2	1.99	0.77
1:M:523:LYS:NZ	5:O:707:CZF:O13	2.16	0.77
1:K:305:ARG:NH1	1:K:348:ARG:NE	2.34	0.75

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]	1.78	0.42

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	476/520 (92%)	459 (96%)	16 (3%)	1 (0%)	47	75
1	B	475/520 (91%)	460 (97%)	15 (3%)	0	100	100
1	C	476/520 (92%)	459 (96%)	17 (4%)	0	100	100
1	D	477/520 (92%)	461 (97%)	16 (3%)	0	100	100
1	E	475/520 (91%)	460 (97%)	15 (3%)	0	100	100
1	F	474/520 (91%)	459 (97%)	15 (3%)	0	100	100
1	G	475/520 (91%)	461 (97%)	14 (3%)	0	100	100
1	H	476/520 (92%)	461 (97%)	15 (3%)	0	100	100
1	I	475/520 (91%)	461 (97%)	14 (3%)	0	100	100
1	J	474/520 (91%)	462 (98%)	12 (2%)	0	100	100
1	K	474/520 (91%)	460 (97%)	14 (3%)	0	100	100
1	L	474/520 (91%)	460 (97%)	14 (3%)	0	100	100
1	M	472/520 (91%)	456 (97%)	16 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	473/520 (91%)	460 (97%)	13 (3%)	0	100	100
1	O	484/520 (93%)	466 (96%)	17 (4%)	1 (0%)	47	75
1	P	474/520 (91%)	459 (97%)	15 (3%)	0	100	100
All	All	7604/8320 (91%)	7364 (97%)	238 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	487	VAL
1	O	280	VAL

### 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	411/464 (89%)	408 (99%)	3 (1%)	84	94
1	B	408/464 (88%)	406 (100%)	2 (0%)	88	96
1	C	409/464 (88%)	407 (100%)	2 (0%)	88	96
1	D	408/464 (88%)	407 (100%)	1 (0%)	93	98
1	E	408/464 (88%)	407 (100%)	1 (0%)	93	98
1	F	406/464 (88%)	405 (100%)	1 (0%)	93	98
1	G	404/464 (87%)	401 (99%)	3 (1%)	84	94
1	H	413/464 (89%)	411 (100%)	2 (0%)	88	96
1	I	407/464 (88%)	405 (100%)	2 (0%)	88	96
1	J	404/464 (87%)	403 (100%)	1 (0%)	93	98
1	K	405/464 (87%)	403 (100%)	2 (0%)	88	96
1	L	396/464 (85%)	395 (100%)	1 (0%)	92	97
1	M	396/464 (85%)	395 (100%)	1 (0%)	92	97
1	N	404/464 (87%)	402 (100%)	2 (0%)	88	96
1	O	408/464 (88%)	407 (100%)	1 (0%)	93	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	397/464 (86%)	396 (100%)	1 (0%)	92	97
All	All	6484/7424 (87%)	6458 (100%)	26 (0%)	91	96

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	328	ASN
1	H	576	ARG
1	O	576	ARG
1	G	576	ARG
1	H	494	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 127 ligands modelled in this entry, 64 are monoatomic - leaving 63 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$
6	SO4	B	707	-	4,4,4	0.43	0	6,6,6	0.50	0
5	CZF	B	706	3	25,34,34	0.99	1 (4%)	29,54,54	2.62	5 (17%)
4	XG4	K	706	3,2	29,33,33	1.48	4 (13%)	35,52,52	2.20	6 (17%)
4	XG4	G	706	3,2	29,33,33	1.80	5 (17%)	35,52,52	2.68	12 (34%)
4	XG4	J	706	3,2	29,33,33	1.74	6 (20%)	35,52,52	2.86	11 (31%)
4	XG4	N	705	3,2	29,33,33	1.46	4 (13%)	35,52,52	2.35	10 (28%)
4	XG4	O	701	3	29,33,33	1.52	5 (17%)	35,52,52	2.40	8 (22%)
6	SO4	N	707	-	4,4,4	0.38	0	6,6,6	0.43	0
4	XG4	F	708	3	29,33,33	1.32	4 (13%)	35,52,52	2.44	9 (25%)
4	XG4	F	705	3,2	29,33,33	1.67	3 (10%)	35,52,52	2.57	10 (28%)
4	XG4	E	705	3,2	29,33,33	1.75	5 (17%)	35,52,52	2.75	11 (31%)
4	XG4	D	706	3,2	29,33,33	1.98	5 (17%)	35,52,52	2.88	13 (37%)
6	SO4	K	708	-	4,4,4	0.34	0	6,6,6	0.27	0
5	CZF	E	706	3	25,34,34	1.14	2 (8%)	29,54,54	2.55	3 (10%)
6	SO4	G	708	-	4,4,4	0.50	0	6,6,6	0.60	0
4	XG4	I	705	3,2	29,33,33	1.63	4 (13%)	35,52,52	2.57	9 (25%)
6	SO4	F	707	-	4,4,4	0.57	0	6,6,6	0.71	0
5	CZF	F	706	3	25,34,34	1.10	1 (4%)	29,54,54	2.49	3 (10%)
4	XG4	M	708	3	29,33,33	1.38	5 (17%)	35,52,52	2.30	7 (20%)
5	CZF	C	707	3	25,34,34	1.09	2 (8%)	29,54,54	2.52	3 (10%)
4	XG4	L	705	3,2	29,33,33	1.66	5 (17%)	35,52,52	2.41	11 (31%)
5	CZF	C	709	3	25,34,34	1.07	1 (4%)	29,54,54	2.45	3 (10%)
6	SO4	M	707	-	4,4,4	0.50	0	6,6,6	0.55	0
4	XG4	H	706	3,2	29,33,33	2.08	7 (24%)	35,52,52	2.74	13 (37%)
4	XG4	A	708	3	29,33,33	1.60	5 (17%)	35,52,52	2.43	11 (31%)
6	SO4	J	708	-	4,4,4	0.51	0	6,6,6	0.44	0
5	CZF	N	706	3	25,34,34	1.07	1 (4%)	29,54,54	2.60	2 (6%)
4	XG4	P	701	3	29,33,33	1.46	4 (13%)	35,52,52	2.38	8 (22%)
5	CZF	K	707	3	25,34,34	1.12	2 (8%)	29,54,54	2.59	3 (10%)
4	XG4	E	708	3	29,33,33	1.52	5 (17%)	35,52,52	2.33	10 (28%)
5	CZF	H	707	3	25,34,34	1.07	1 (4%)	29,54,54	2.53	2 (6%)
5	CZF	J	707	3	25,34,34	1.00	2 (8%)	29,54,54	2.39	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	SO4	L	707	-	4,4,4	0.42	0	6,6,6	0.51	0
4	XG4	C	706	3,2	29,33,33	1.89	6 (20%)	35,52,52	2.78	10 (28%)
5	CZF	G	707	3	25,34,34	1.03	1 (4%)	29,54,54	2.57	3 (10%)
4	XG4	G	701	3	29,33,33	1.57	5 (17%)	35,52,52	2.56	10 (28%)
5	CZF	M	706	3	25,34,34	1.14	2 (8%)	29,54,54	2.70	3 (10%)
4	XG4	C	701	3	29,33,33	1.52	5 (17%)	35,52,52	2.54	10 (28%)
5	CZF	A	706	3	25,34,34	1.18	3 (12%)	29,54,54	2.51	3 (10%)
5	CZF	L	706	3	25,34,34	1.04	1 (4%)	29,54,54	2.60	3 (10%)
4	XG4	N	708	3	29,33,33	1.50	5 (17%)	35,52,52	2.53	9 (25%)
5	CZF	J	701	3	25,34,34	1.08	2 (8%)	29,54,54	2.55	2 (6%)
4	XG4	O	706	3,2	29,33,33	1.55	3 (10%)	35,52,52	2.52	10 (28%)
6	SO4	A	707	-	4,4,4	0.64	0	6,6,6	0.64	0
6	SO4	C	708	-	4,4,4	0.41	0	6,6,6	0.58	0
6	SO4	D	707	-	4,4,4	0.47	0	6,6,6	0.40	0
6	SO4	E	707	-	4,4,4	0.48	0	6,6,6	0.76	0
5	CZF	O	707	3	25,34,34	1.10	1 (4%)	29,54,54	2.51	3 (10%)
4	XG4	H	701	3	29,33,33	1.45	4 (13%)	35,52,52	2.73	9 (25%)
4	XG4	A	705	3,2	29,33,33	1.85	4 (13%)	35,52,52	2.79	11 (31%)
5	CZF	P	707	3	25,34,34	1.33	2 (8%)	29,54,54	2.60	2 (6%)
4	XG4	I	708	3	29,33,33	1.38	5 (17%)	35,52,52	2.38	7 (20%)
4	XG4	M	705	3,2	29,33,33	1.48	4 (13%)	35,52,52	2.31	8 (22%)
4	XG4	K	701	3	29,33,33	1.48	4 (13%)	35,52,52	2.61	12 (34%)
4	XG4	J	709	3	29,33,33	1.67	5 (17%)	35,52,52	2.57	9 (25%)
4	XG4	D	701	3	29,33,33	1.58	6 (20%)	35,52,52	2.54	10 (28%)
6	SO4	I	706	-	4,4,4	0.50	0	6,6,6	0.44	0
6	SO4	O	708	-	4,4,4	0.61	0	6,6,6	0.44	0
6	SO4	H	708	-	4,4,4	0.72	0	6,6,6	0.29	0
4	XG4	I	707	3	29,33,33	1.57	7 (24%)	35,52,52	2.33	8 (22%)
4	XG4	P	706	3,2	29,33,33	1.56	4 (13%)	35,52,52	2.75	11 (31%)
4	XG4	B	708	3	29,33,33	1.46	5 (17%)	35,52,52	2.77	9 (25%)
4	XG4	B	705	3,2	29,33,33	1.71	3 (10%)	35,52,52	2.43	11 (31%)

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	CZF	B	706	3	-	5/18/38/38	0/3/3/3
4	XG4	K	706	3,2	-	2/15/34/34	0/3/3/3
4	XG4	G	706	3,2	-	2/15/34/34	0/3/3/3
4	XG4	J	706	3,2	-	5/15/34/34	0/3/3/3
4	XG4	N	705	3,2	-	2/15/34/34	0/3/3/3
4	XG4	O	701	3	-	4/15/34/34	0/3/3/3
4	XG4	F	708	3	-	2/15/34/34	0/3/3/3
4	XG4	F	705	3,2	-	3/15/34/34	0/3/3/3
4	XG4	E	705	3,2	-	2/15/34/34	0/3/3/3
4	XG4	D	706	3,2	-	3/15/34/34	0/3/3/3
5	CZF	E	706	3	-	5/18/38/38	0/3/3/3
4	XG4	I	705	3,2	-	2/15/34/34	0/3/3/3
5	CZF	F	706	3	-	5/18/38/38	0/3/3/3
4	XG4	M	708	3	-	6/15/34/34	0/3/3/3
5	CZF	C	707	3	-	7/18/38/38	0/3/3/3
4	XG4	L	705	3,2	-	4/15/34/34	0/3/3/3
5	CZF	C	709	3	-	3/18/38/38	0/3/3/3
4	XG4	H	706	3,2	-	4/15/34/34	0/3/3/3
4	XG4	A	708	3	-	3/15/34/34	0/3/3/3
4	XG4	N	708	3	-	6/15/34/34	0/3/3/3
5	CZF	N	706	3	-	4/18/38/38	0/3/3/3
4	XG4	P	701	3	-	3/15/34/34	0/3/3/3
5	CZF	K	707	3	-	4/18/38/38	0/3/3/3
4	XG4	E	708	3	-	3/15/34/34	0/3/3/3
5	CZF	H	707	3	-	6/18/38/38	0/3/3/3
5	CZF	J	707	3	-	3/18/38/38	0/3/3/3
4	XG4	C	706	3,2	-	2/15/34/34	0/3/3/3
5	CZF	G	707	3	-	6/18/38/38	0/3/3/3
4	XG4	G	701	3	-	6/15/34/34	0/3/3/3
5	CZF	M	706	3	-	6/18/38/38	0/3/3/3
4	XG4	C	701	3	-	3/15/34/34	0/3/3/3
5	CZF	A	706	3	-	4/18/38/38	0/3/3/3
5	CZF	J	701	3	-	6/18/38/38	0/3/3/3
4	XG4	O	706	3,2	-	4/15/34/34	0/3/3/3
5	CZF	L	706	3	-	5/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CZF	O	707	3	-	2/18/38/38	0/3/3/3
4	XG4	K	701	3	-	1/15/34/34	0/3/3/3
4	XG4	H	701	3	-	2/15/34/34	0/3/3/3
4	XG4	A	705	3,2	-	2/15/34/34	0/3/3/3
5	CZF	P	707	3	-	3/18/38/38	0/3/3/3
4	XG4	I	708	3	-	6/15/34/34	0/3/3/3
4	XG4	M	705	3,2	-	4/15/34/34	0/3/3/3
4	XG4	J	709	3	-	2/15/34/34	0/3/3/3
4	XG4	D	701	3	-	2/15/34/34	0/3/3/3
4	XG4	I	707	3	-	4/15/34/34	0/3/3/3
4	XG4	P	706	3,2	-	3/15/34/34	0/3/3/3
4	XG4	B	708	3	-	4/15/34/34	0/3/3/3
4	XG4	B	705	3,2	-	4/15/34/34	0/3/3/3

The worst 5 of 176 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	706	XG4	PA-O1A	6.61	1.56	1.46
4	D	706	XG4	PA-O1A	6.60	1.56	1.46
4	H	706	XG4	PA-O1A	6.50	1.56	1.46
4	A	705	XG4	PA-O1A	6.49	1.56	1.46
4	F	705	XG4	PA-O1A	5.64	1.55	1.46

The worst 5 of 358 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	707	CZF	C9-N1-C2	11.89	125.18	115.14
5	M	706	CZF	C9-N1-C2	11.79	125.10	115.14
5	K	707	CZF	C9-N1-C2	11.67	124.99	115.14
5	N	706	CZF	C9-N1-C2	11.43	124.80	115.14
5	J	701	CZF	C9-N1-C2	11.31	124.69	115.14

There are no chirality outliers.

5 of 179 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	705	XG4	PB-N3A-PA-O1A
4	D	706	XG4	PB-N3A-PA-O1A
4	D	706	XG4	PG-O3B-PB-O1B

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Mol	Chain	Res	Type	Atoms
5	E	706	CZF	P2-O10-P3-O14
4	I	705	XG4	PB-N3A-PA-O1A

There are no ring outliers.

42 monomers are involved in 77 short contacts:

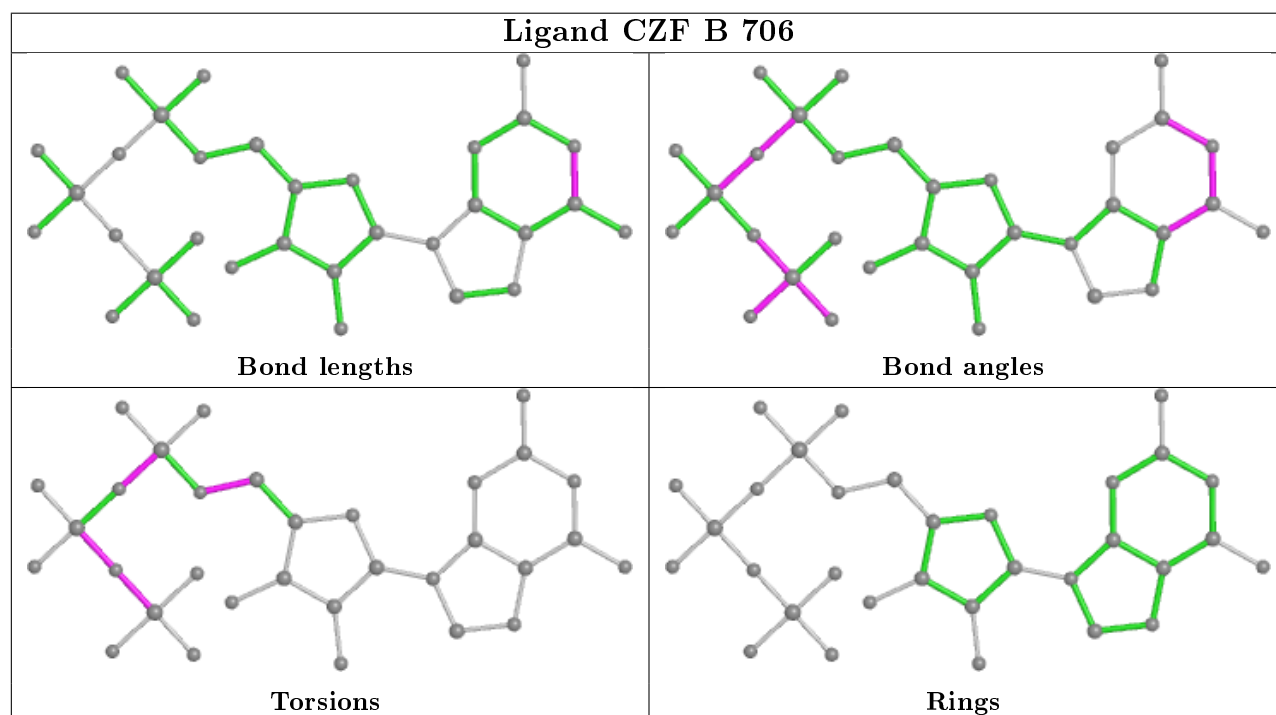
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	706	CZF	1	0
4	K	706	XG4	3	0
4	J	706	XG4	1	0
4	N	705	XG4	2	0
4	O	701	XG4	2	0
4	F	708	XG4	2	0
4	F	705	XG4	1	0
4	E	705	XG4	1	0
4	D	706	XG4	2	0
5	E	706	CZF	1	0
6	G	708	SO4	1	0
4	I	705	XG4	1	0
5	F	706	CZF	1	0
4	M	708	XG4	5	0
4	L	705	XG4	2	0
5	C	709	CZF	1	0
4	H	706	XG4	1	0
4	A	708	XG4	1	0
5	N	706	CZF	1	0
4	P	701	XG4	2	0
5	K	707	CZF	1	0
4	E	708	XG4	2	0
5	H	707	CZF	2	0
4	C	706	XG4	2	0
4	G	701	XG4	5	0
4	C	701	XG4	3	0
5	A	706	CZF	2	0
4	N	708	XG4	4	0
5	J	701	CZF	3	0
4	O	706	XG4	2	0
5	O	707	CZF	2	0
4	A	705	XG4	1	0
5	P	707	CZF	2	0
4	I	708	XG4	3	0
4	M	705	XG4	1	0

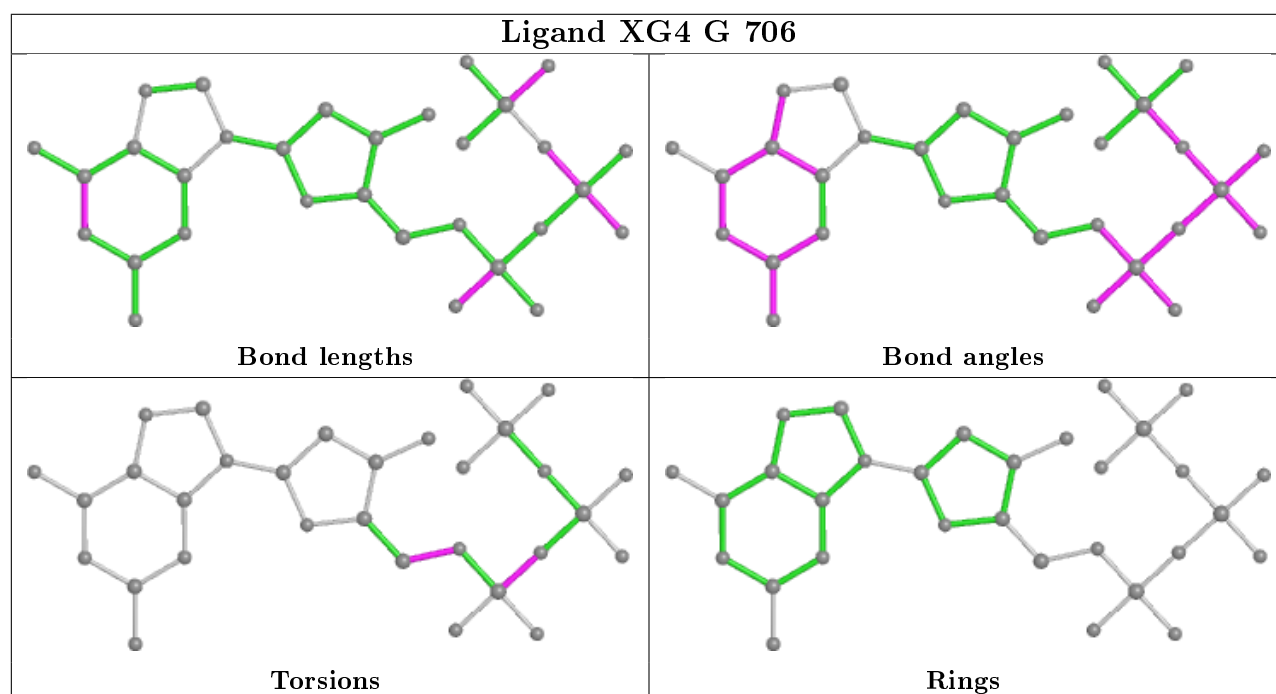
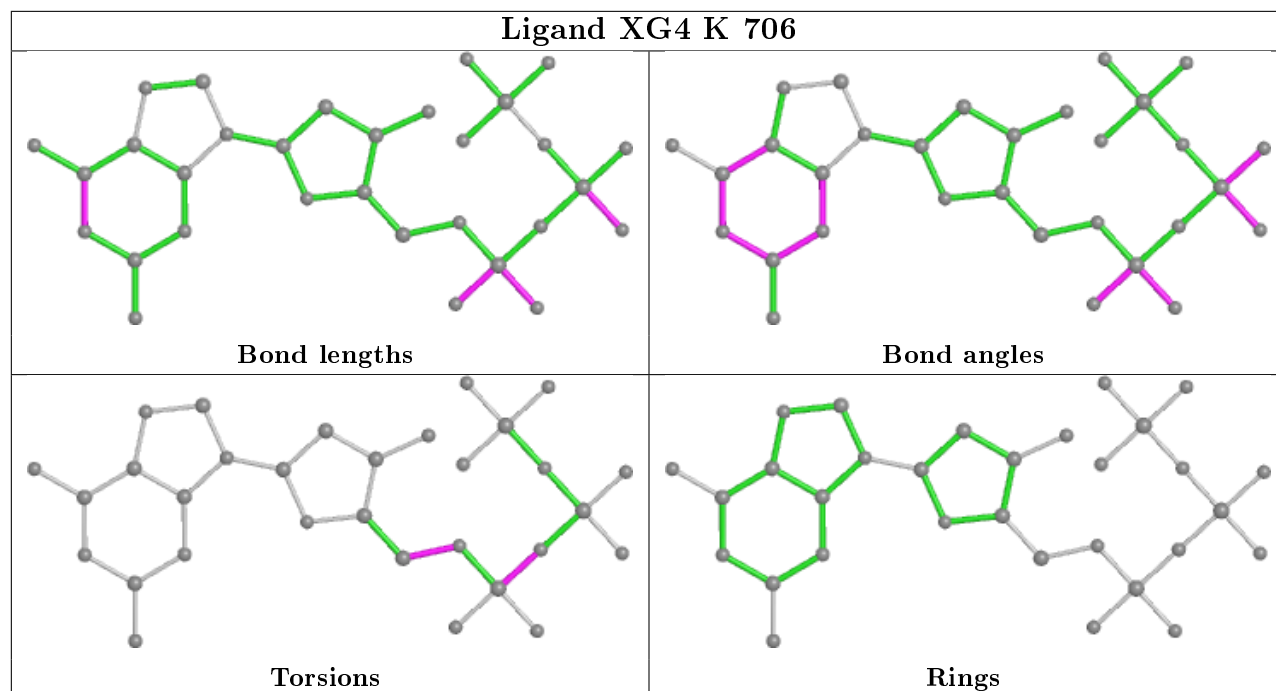
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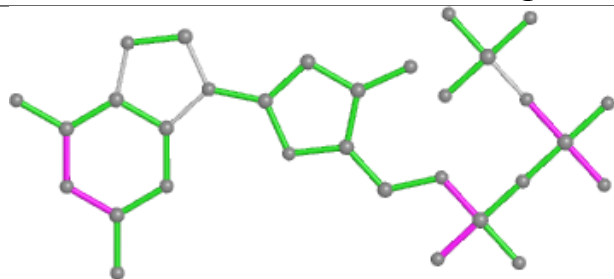
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	701	XG4	1	0
4	J	709	XG4	3	0
4	D	701	XG4	1	0
4	I	707	XG4	5	0
4	P	706	XG4	3	0
4	B	708	XG4	2	0
4	B	705	XG4	1	0

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.

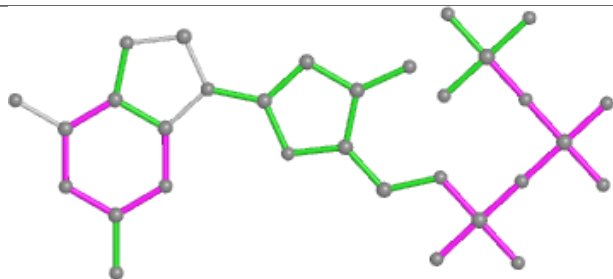




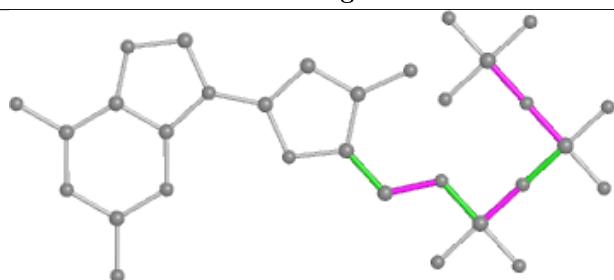
## Ligand XG4 J 706



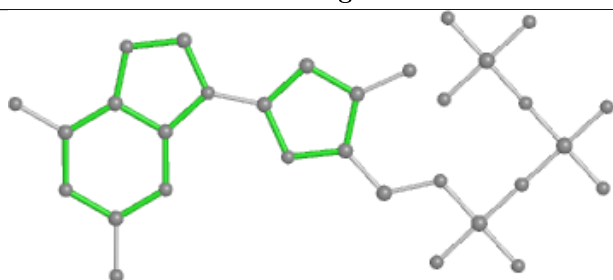
Bond lengths



Bond angles

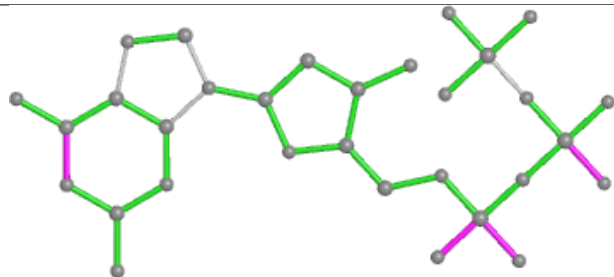


Torsions

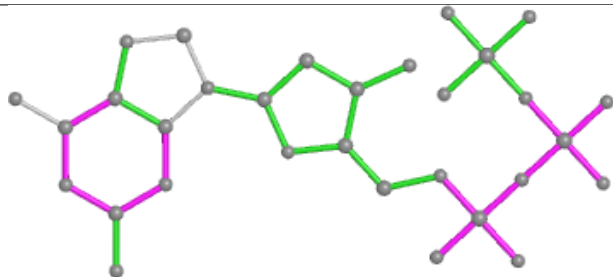


Rings

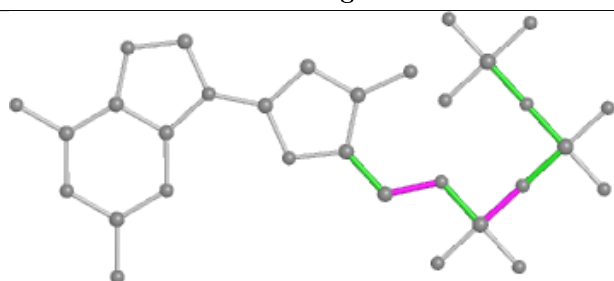
## Ligand XG4 N 705



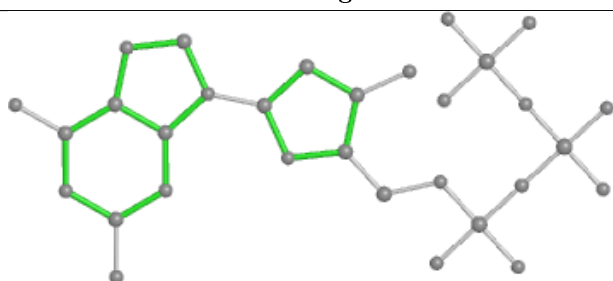
Bond lengths



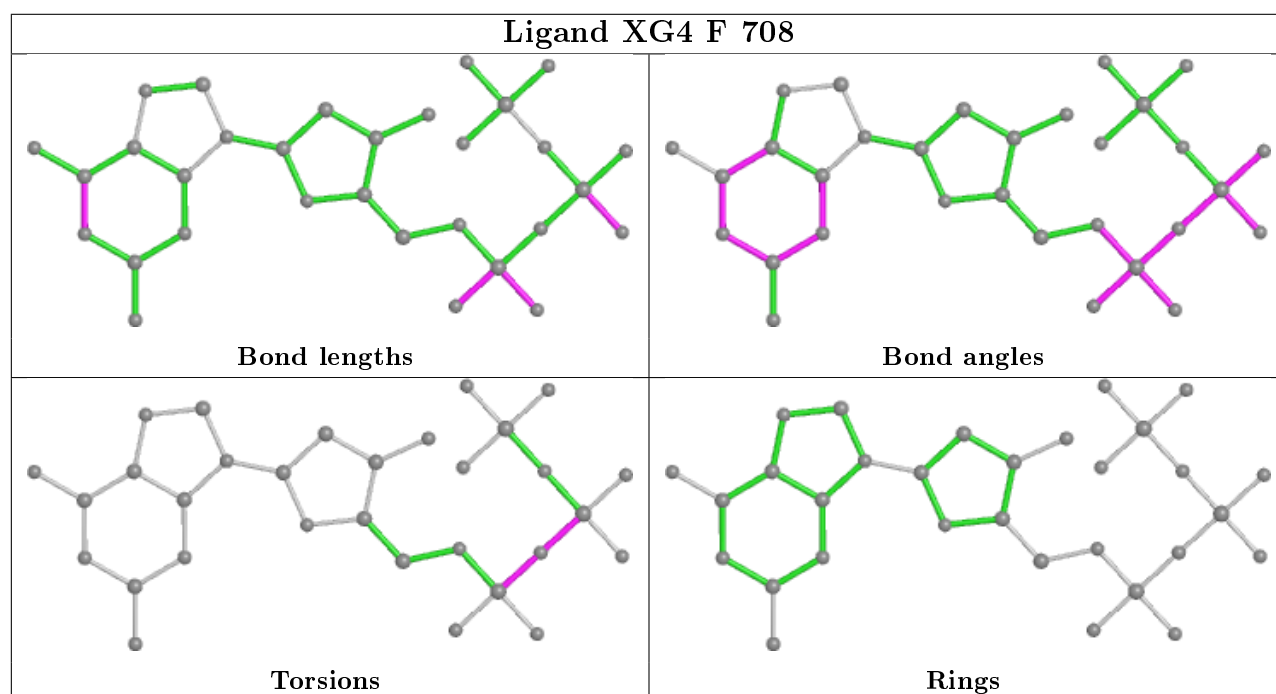
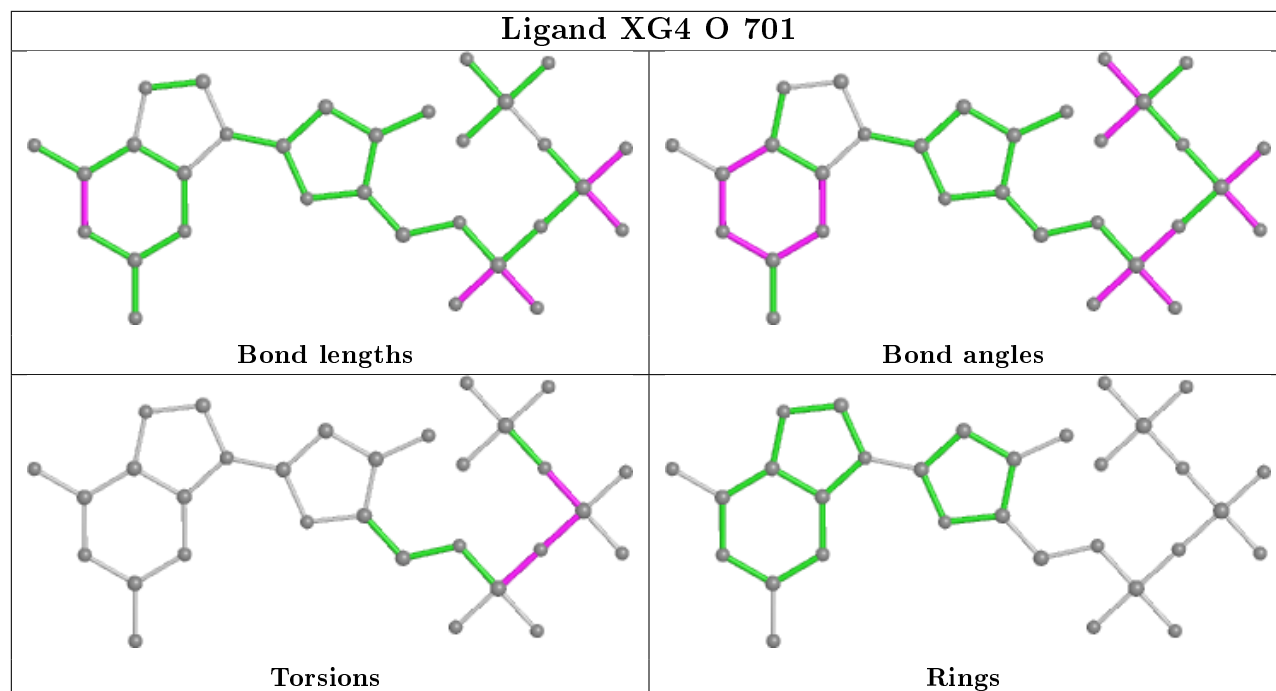
Bond angles

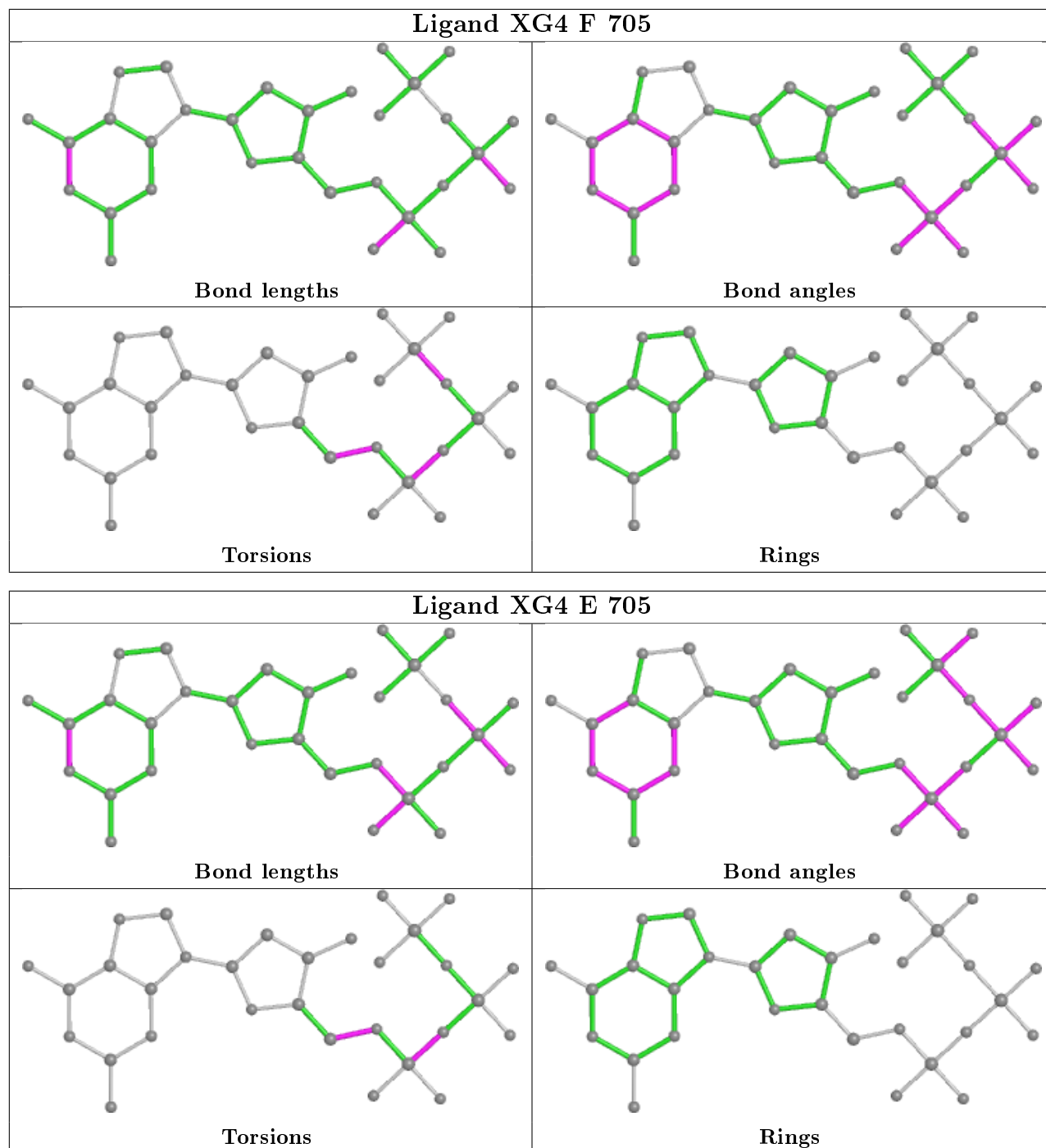


Torsions

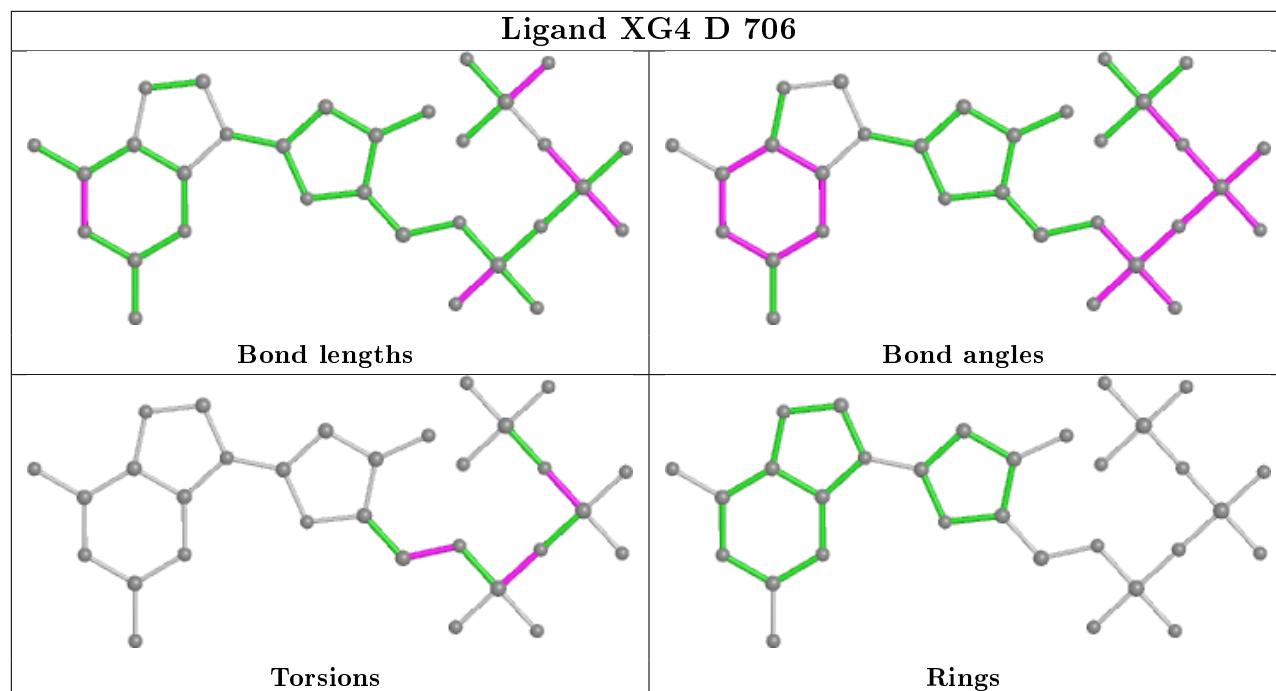


Rings

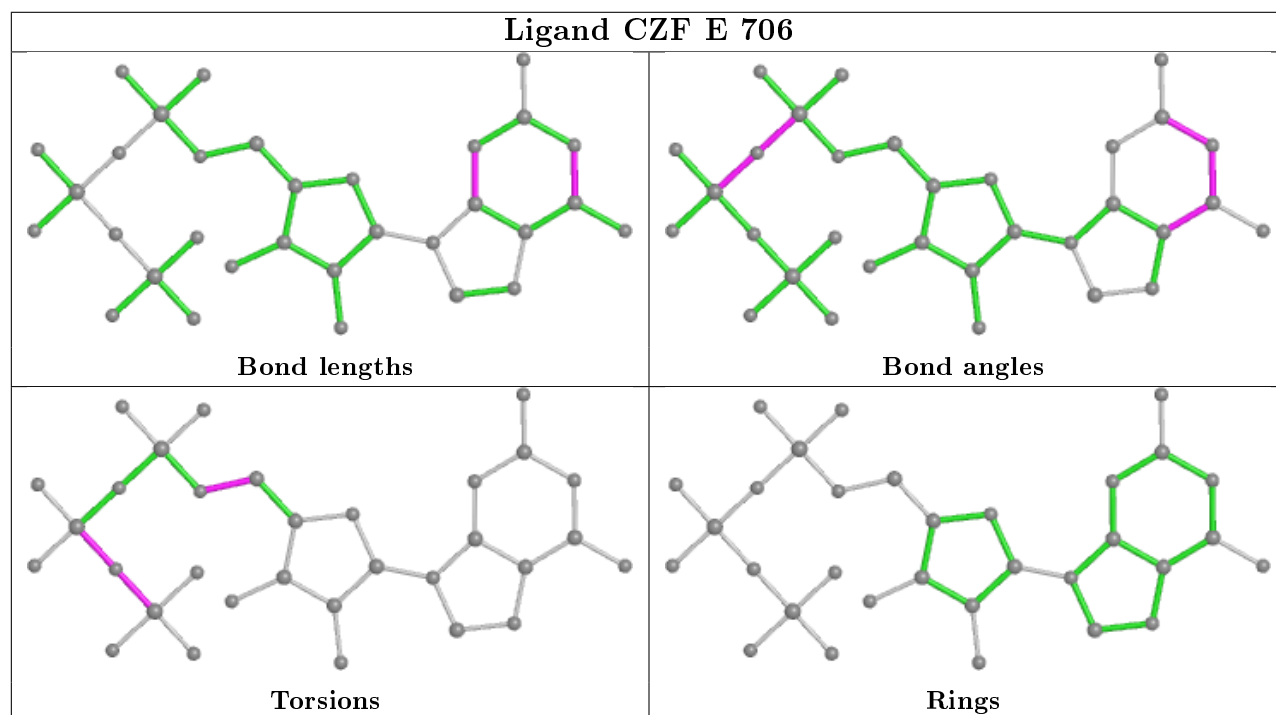




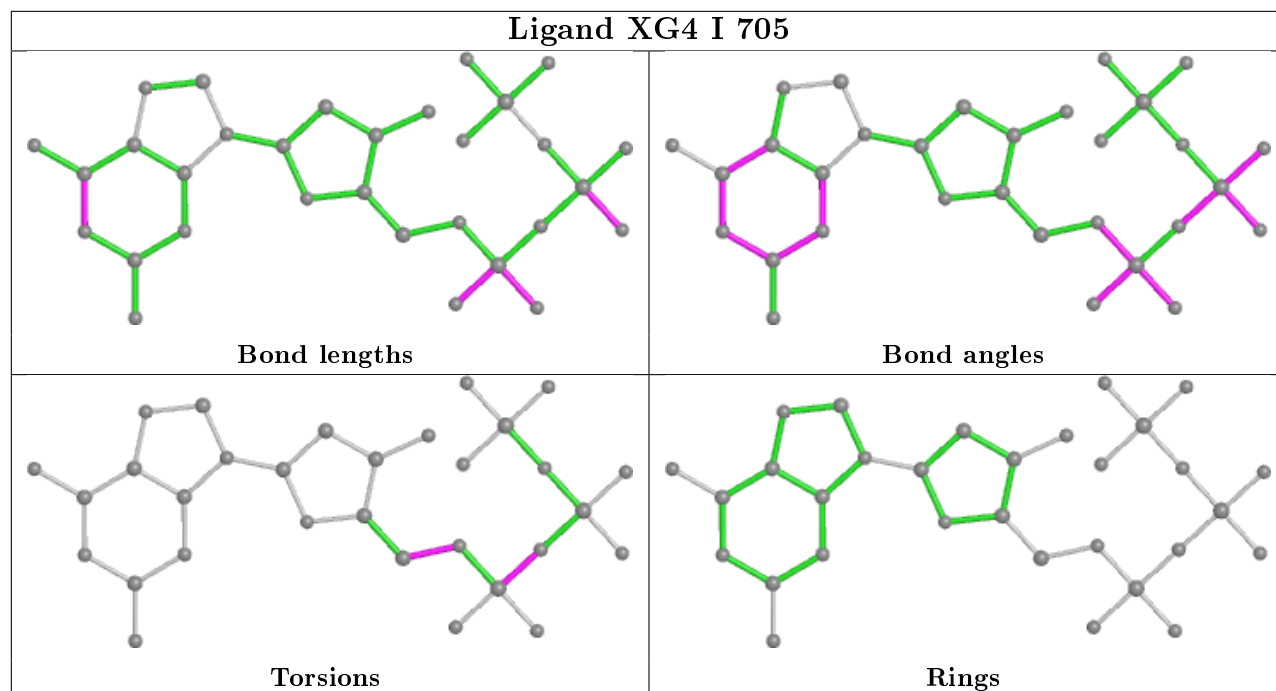
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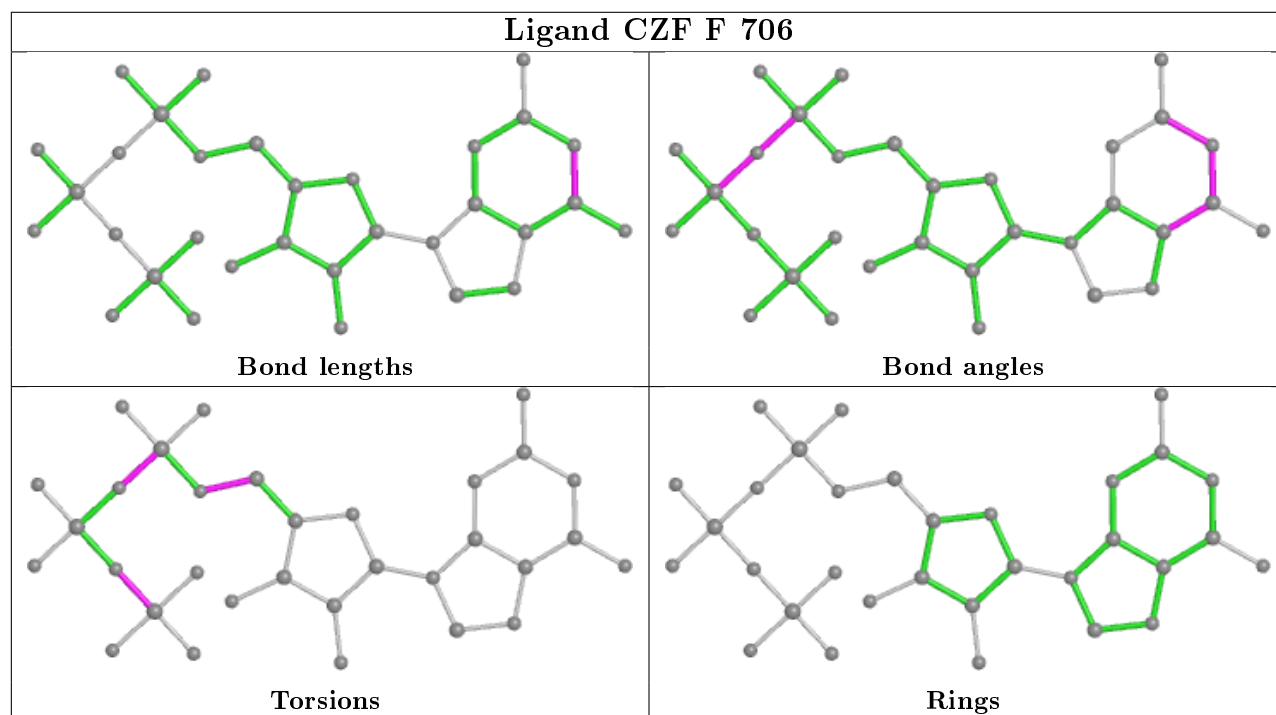
## Ligand CZF E 706



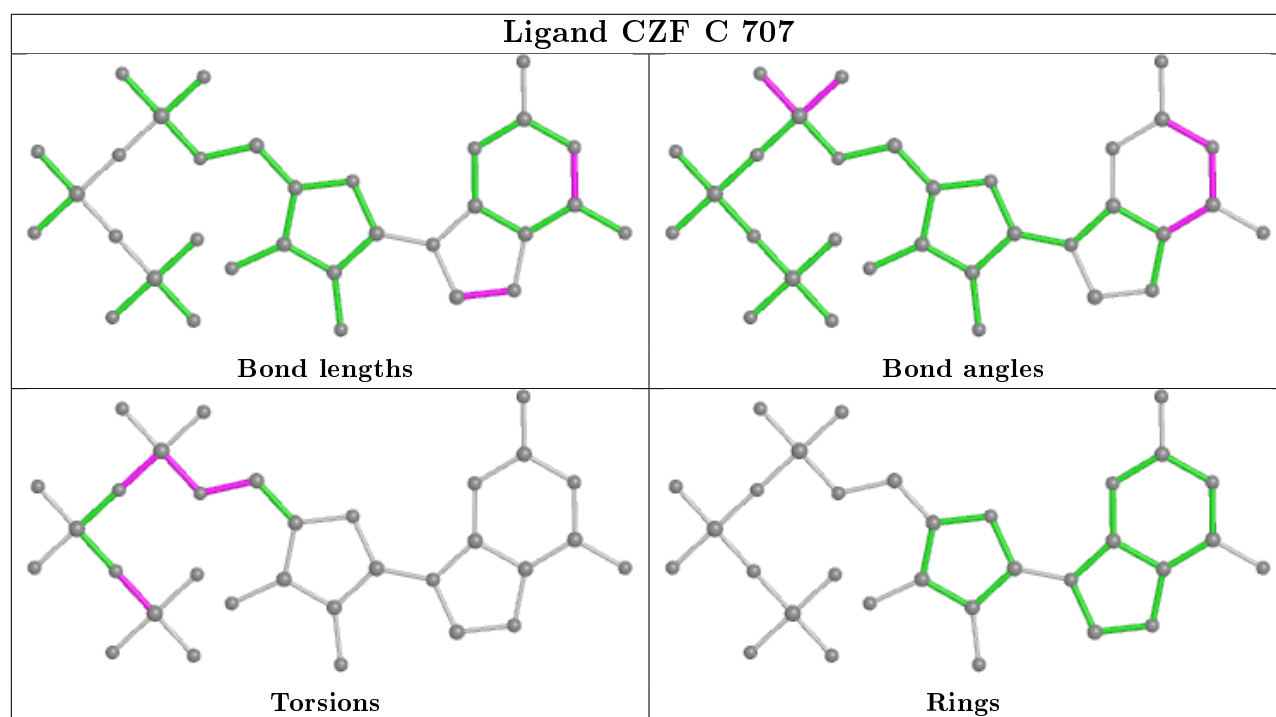
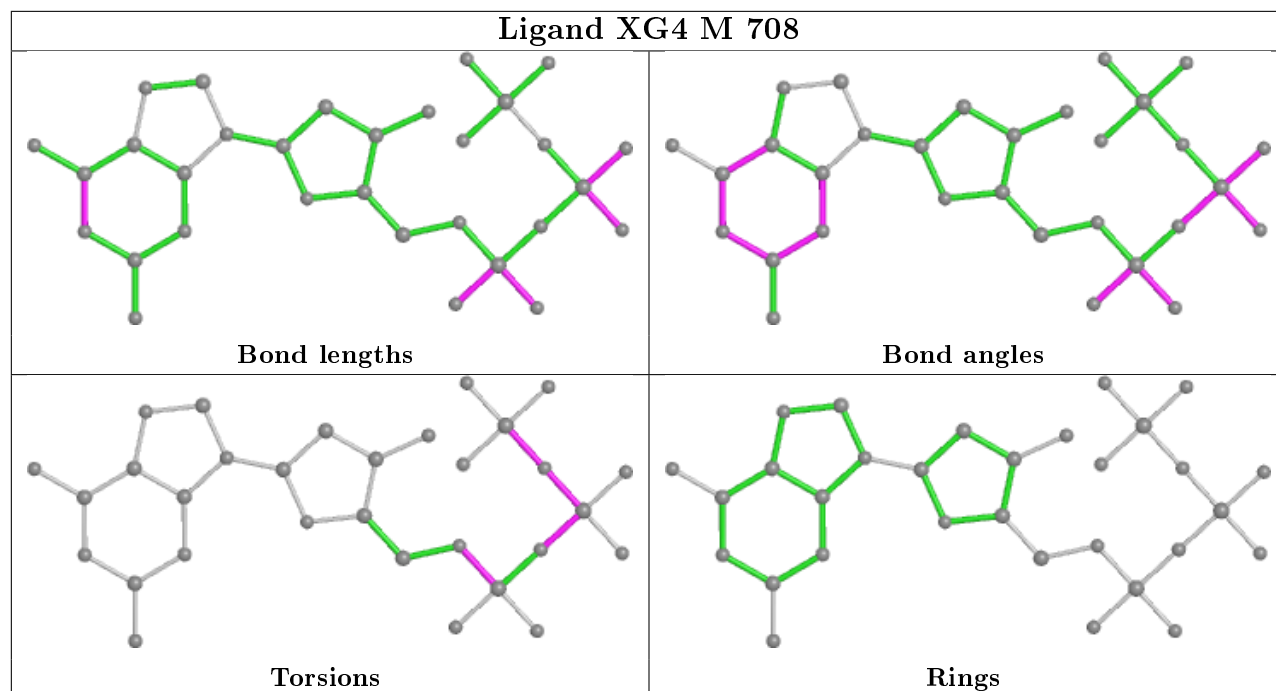
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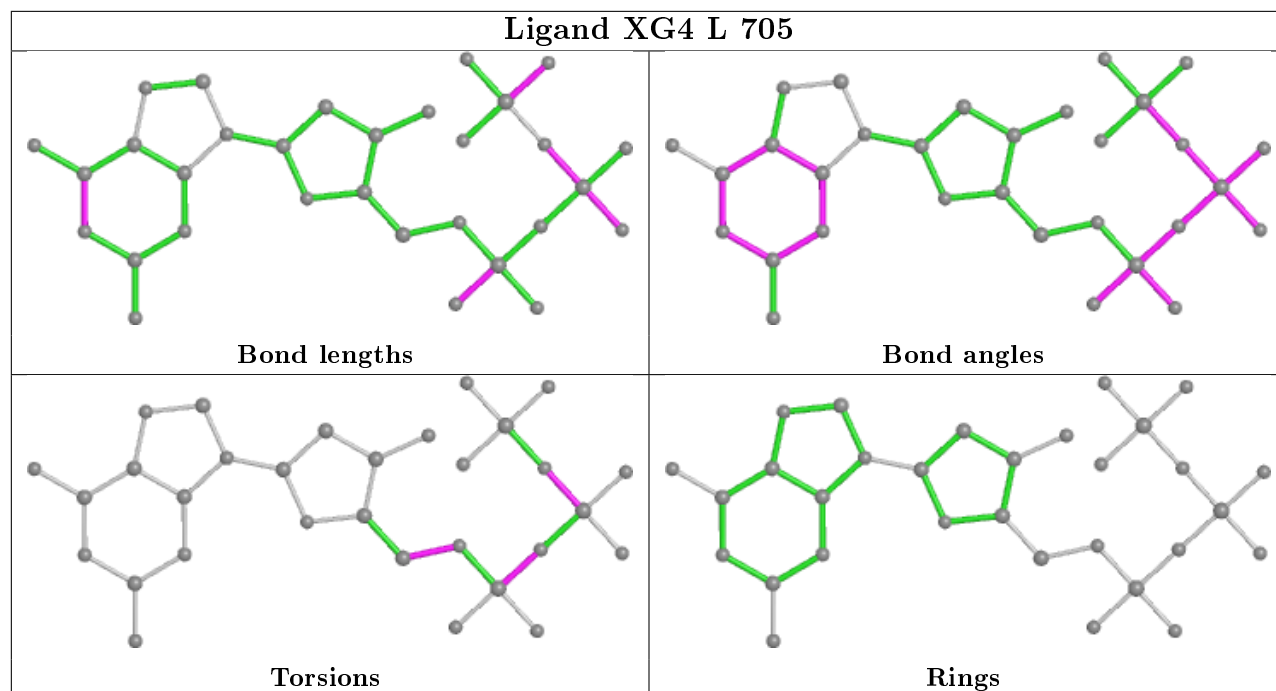
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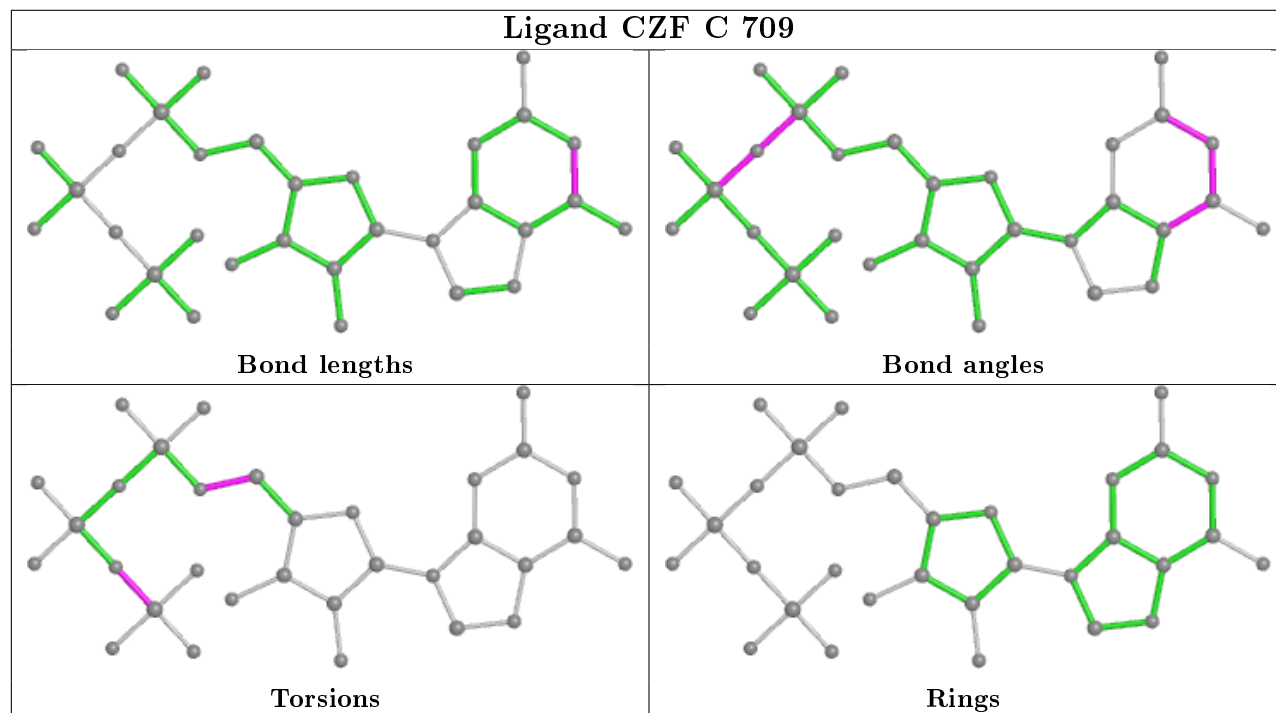




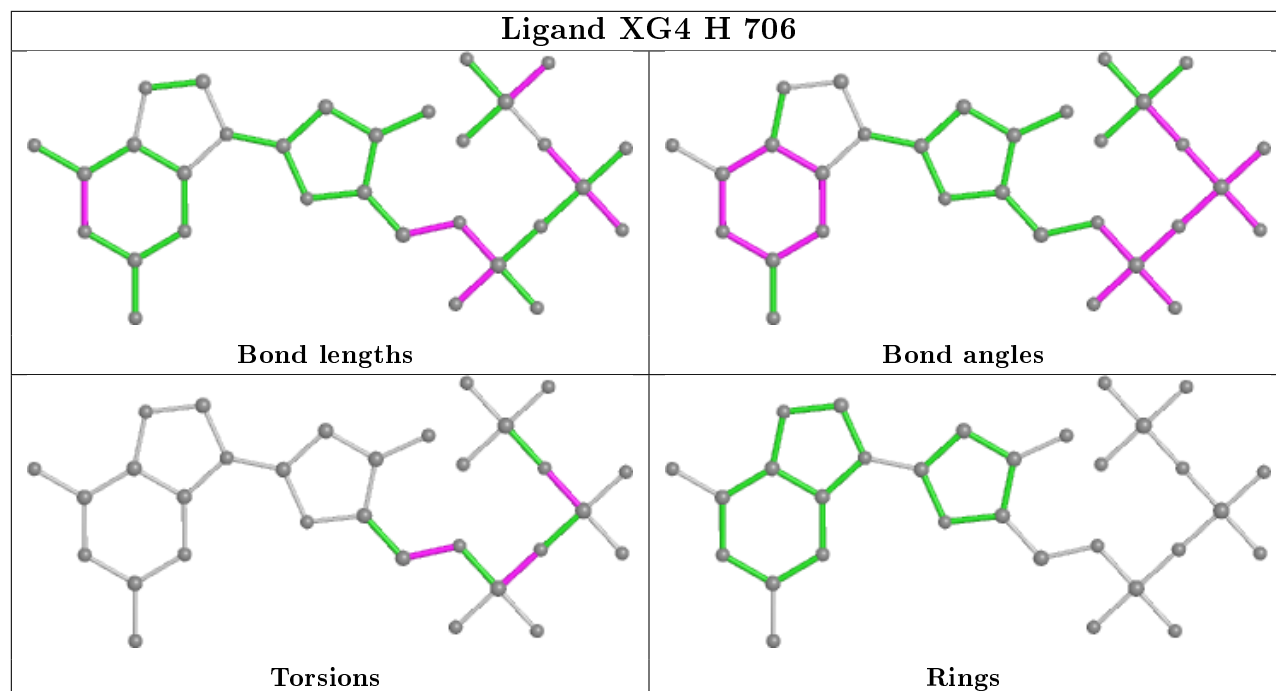
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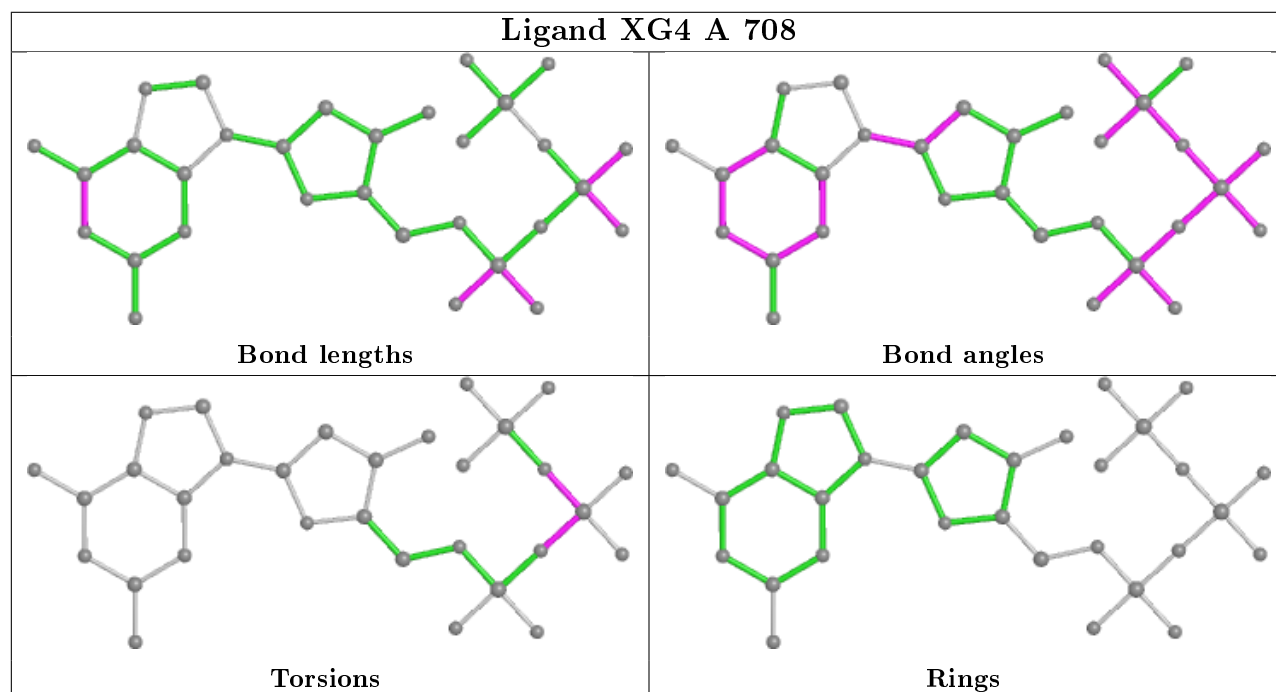
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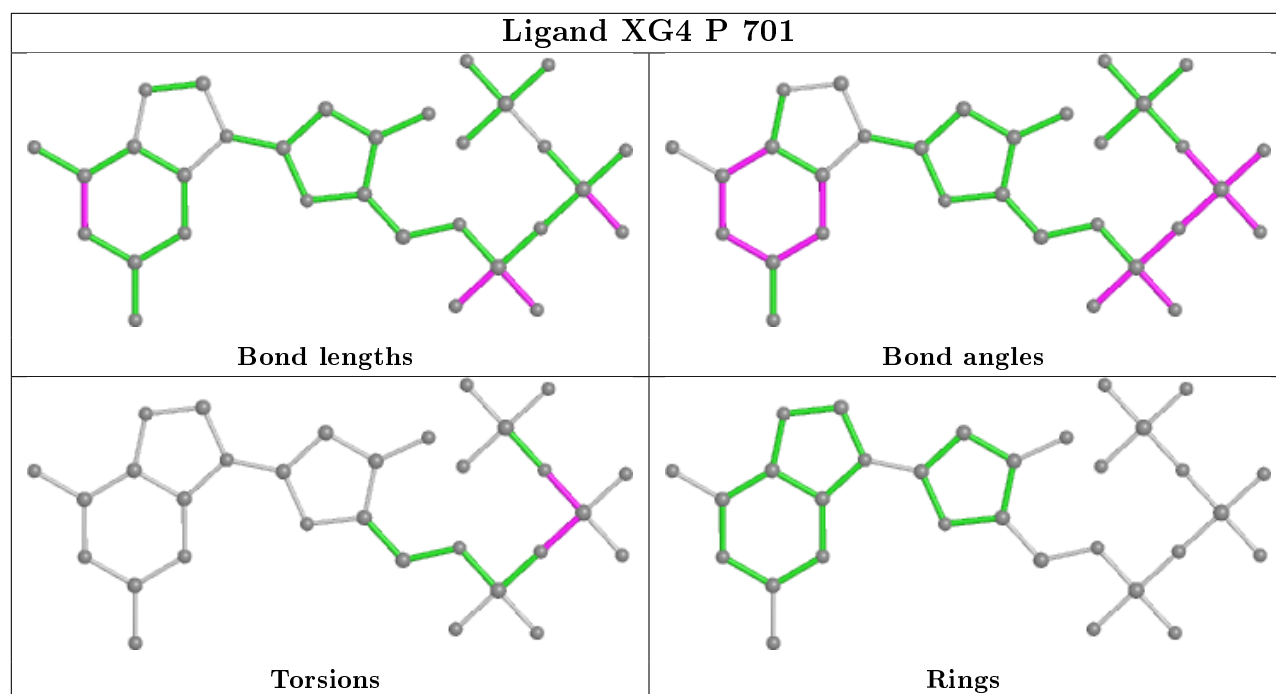
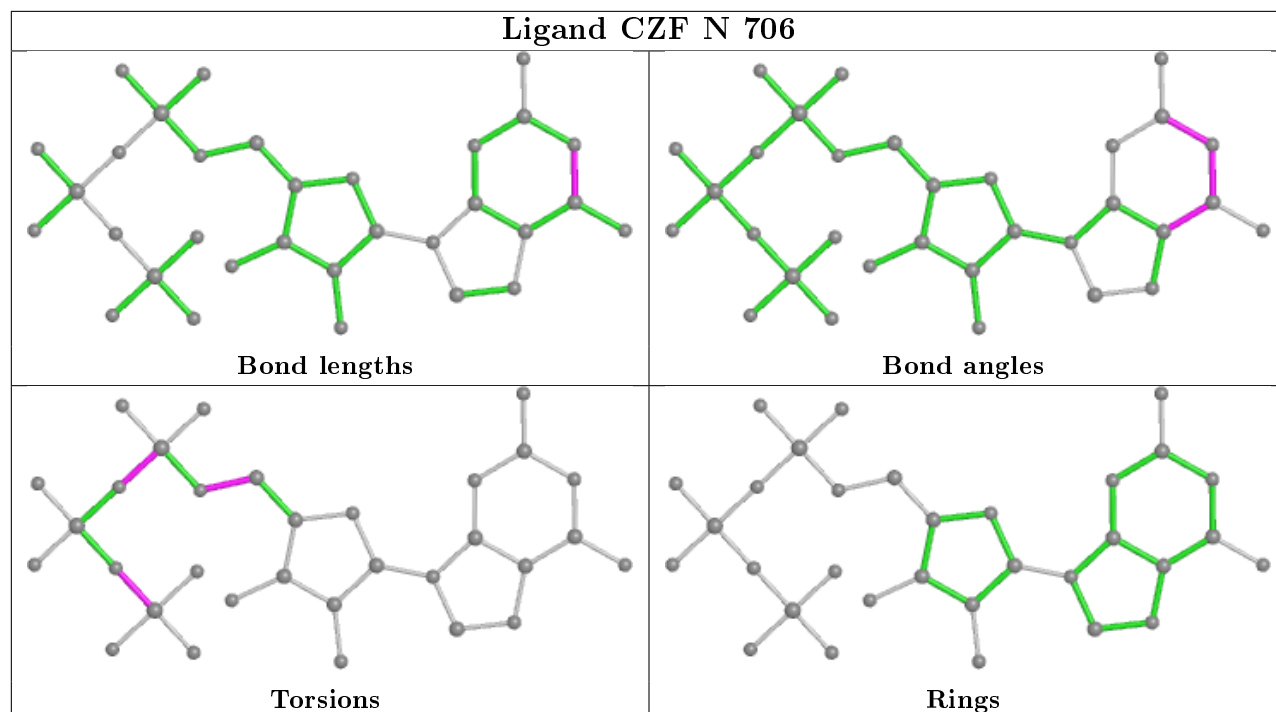


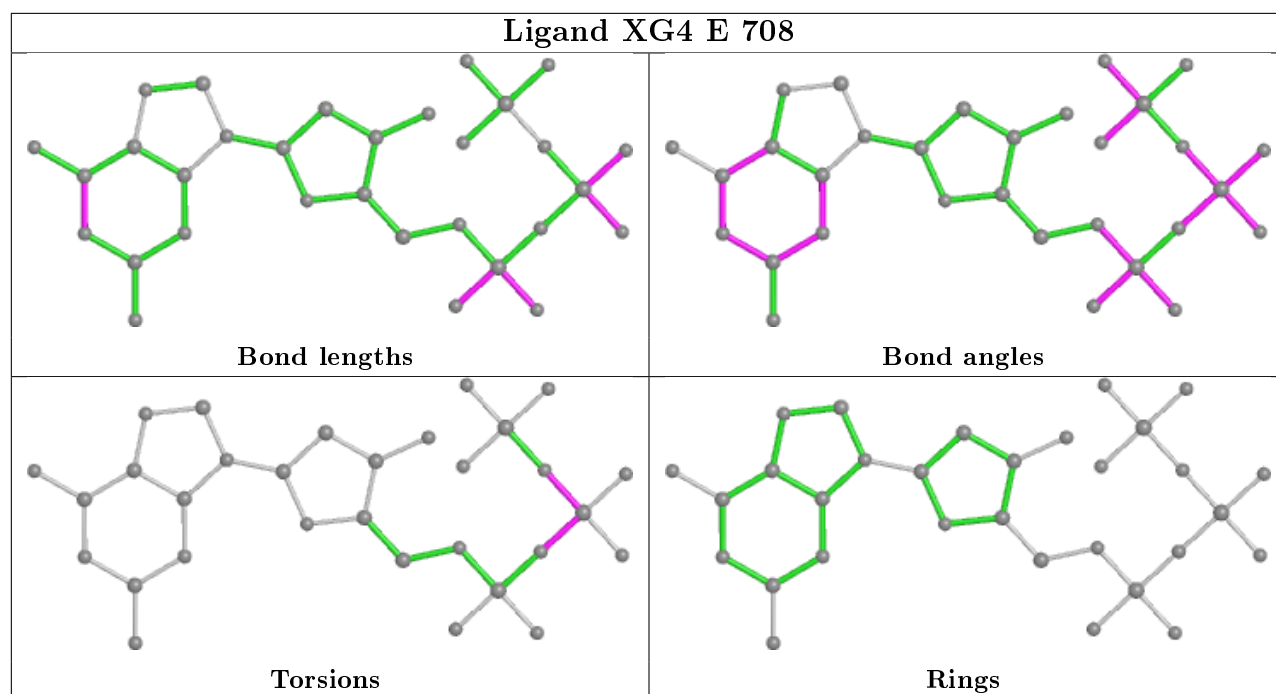
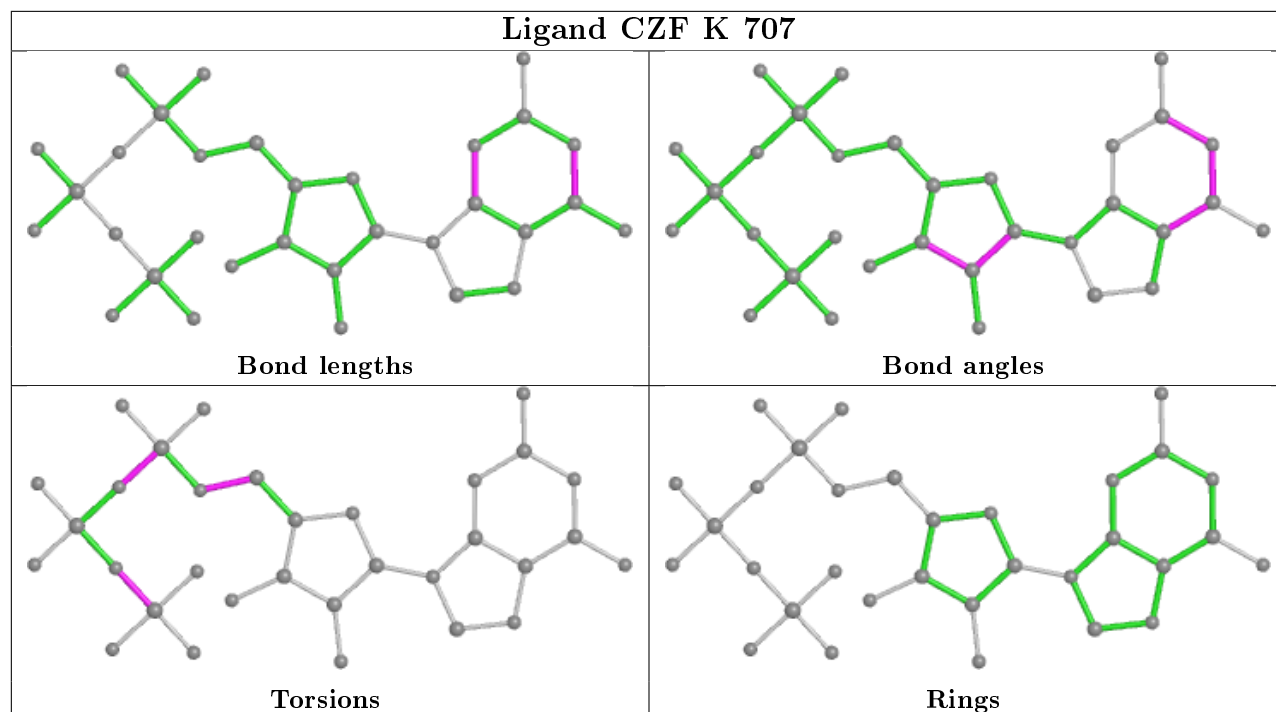
## Ligand XG4 H 706



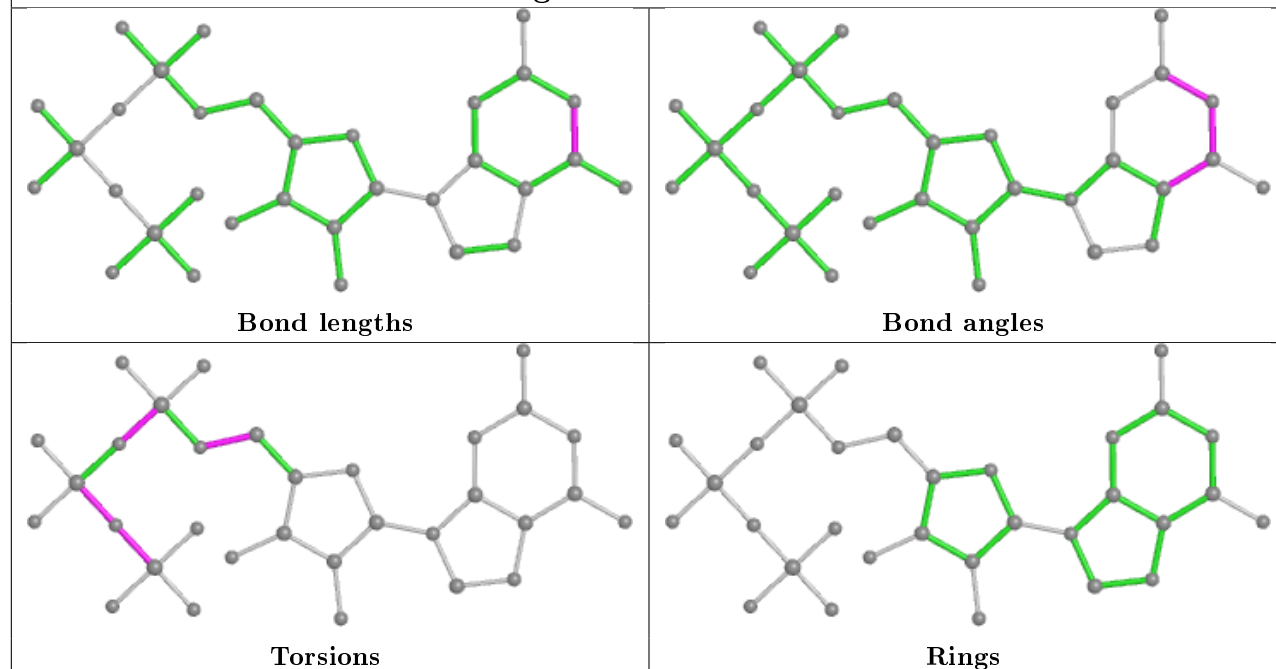
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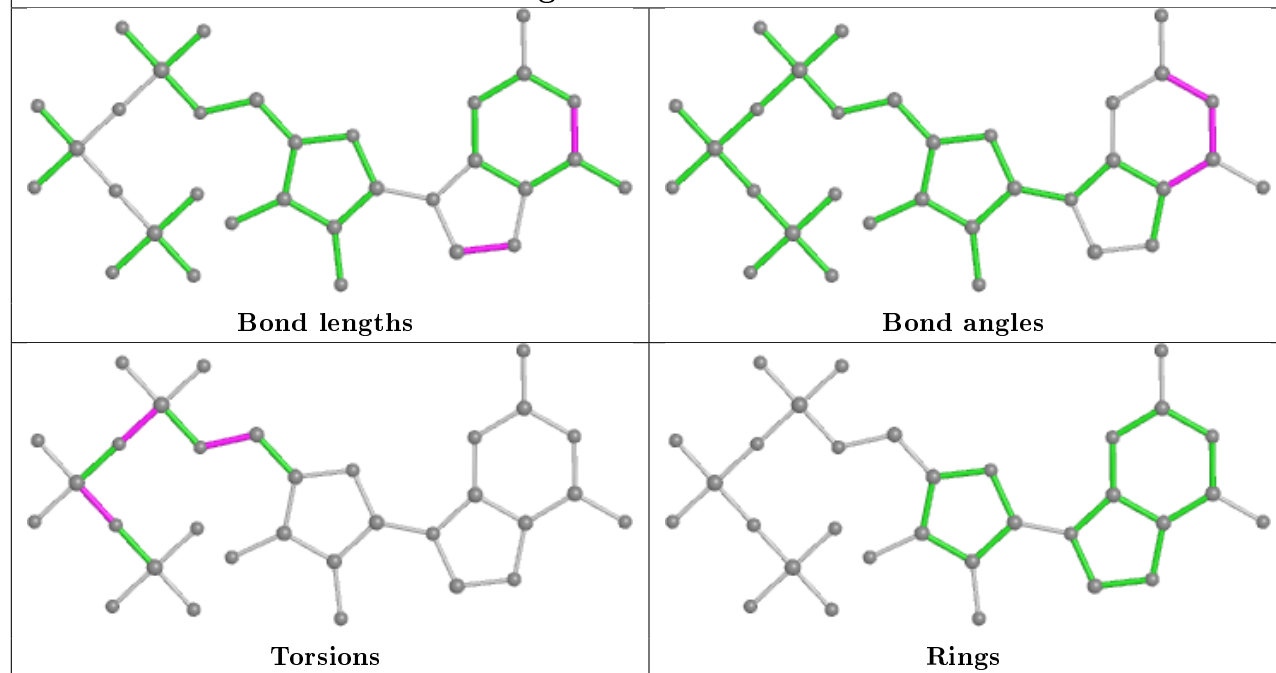




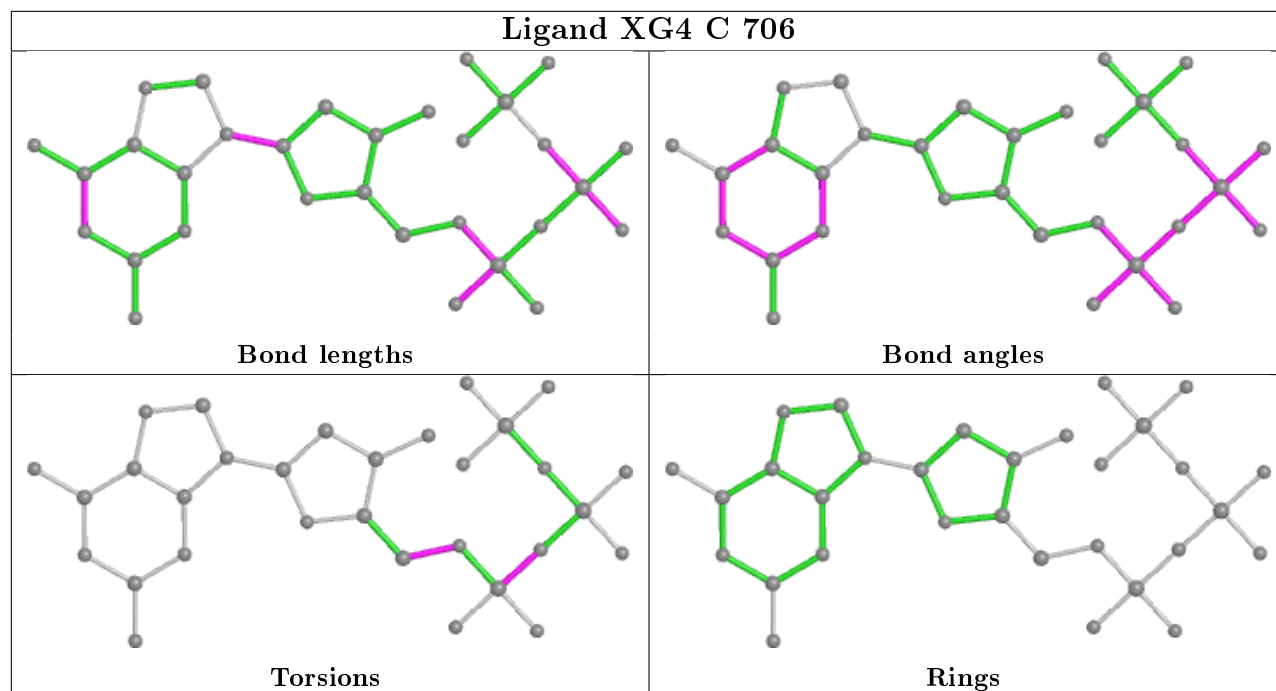
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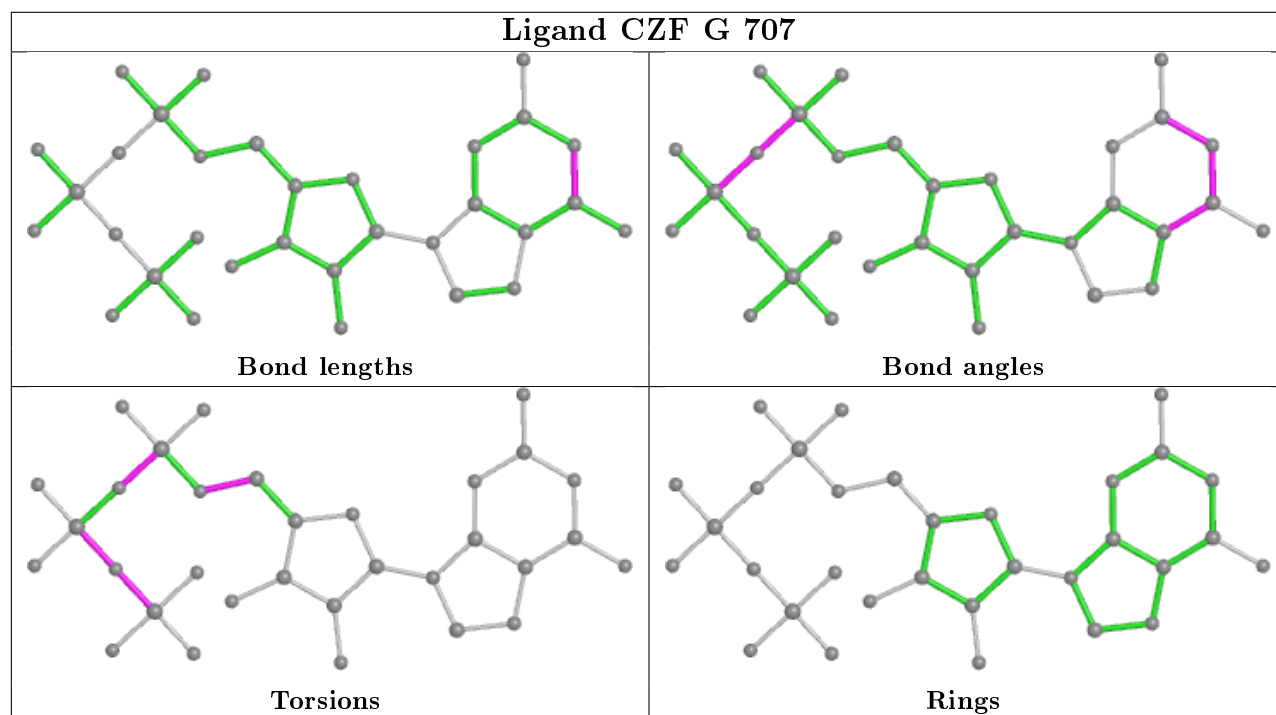
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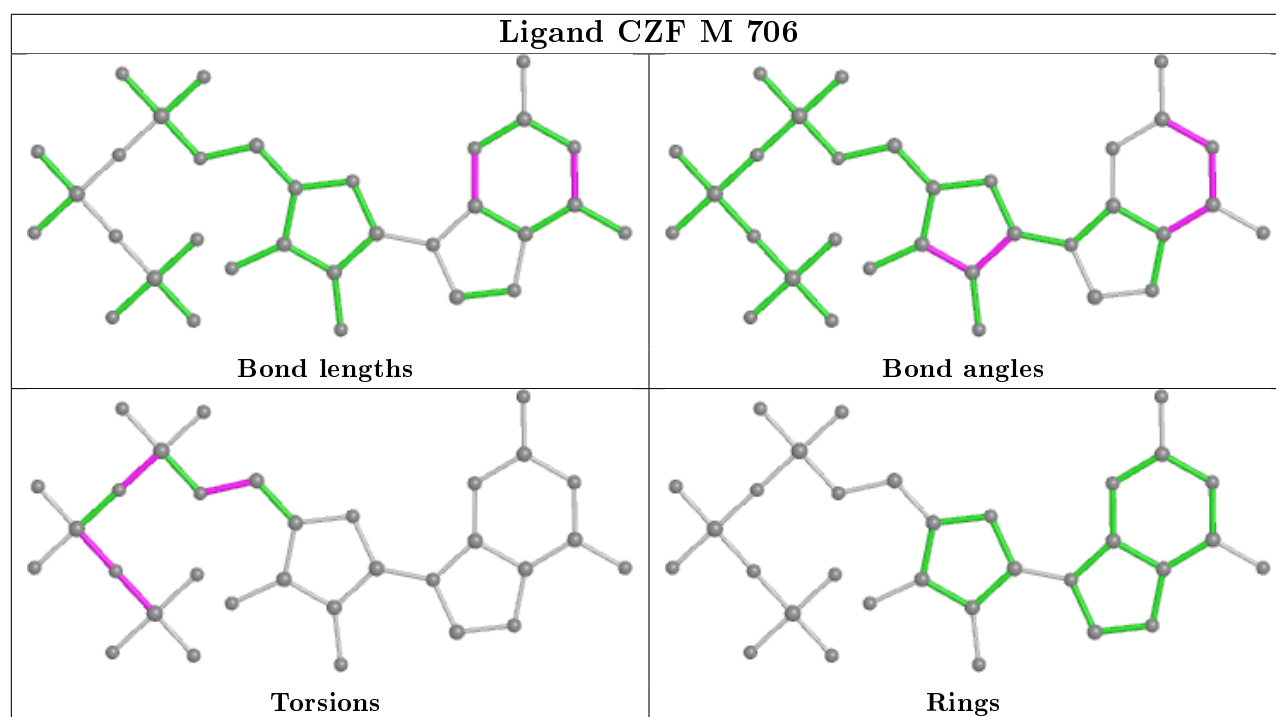
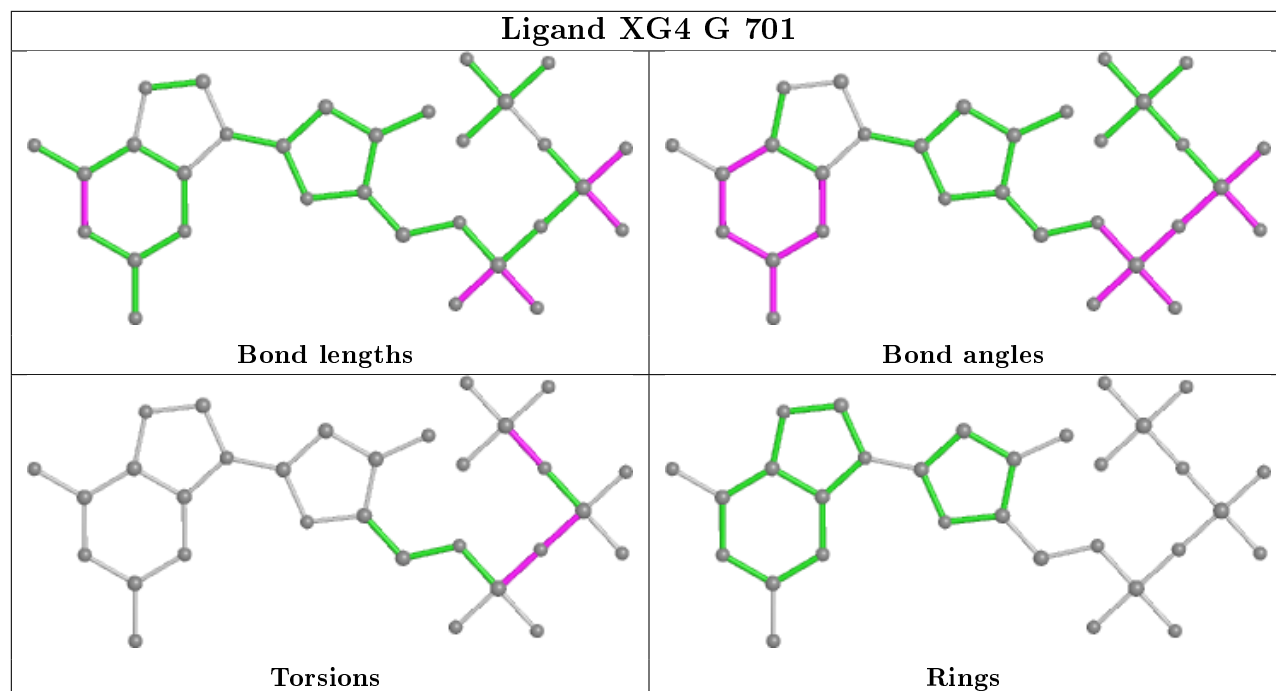


## Ligand XG4 C 706



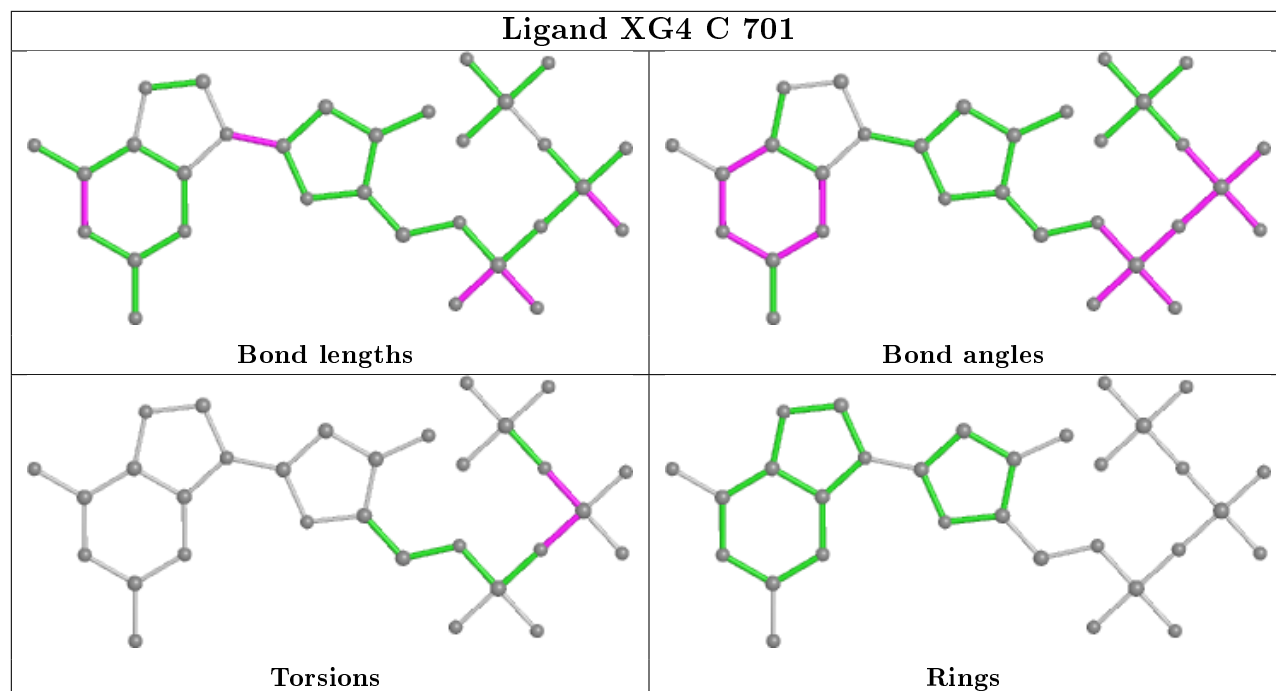
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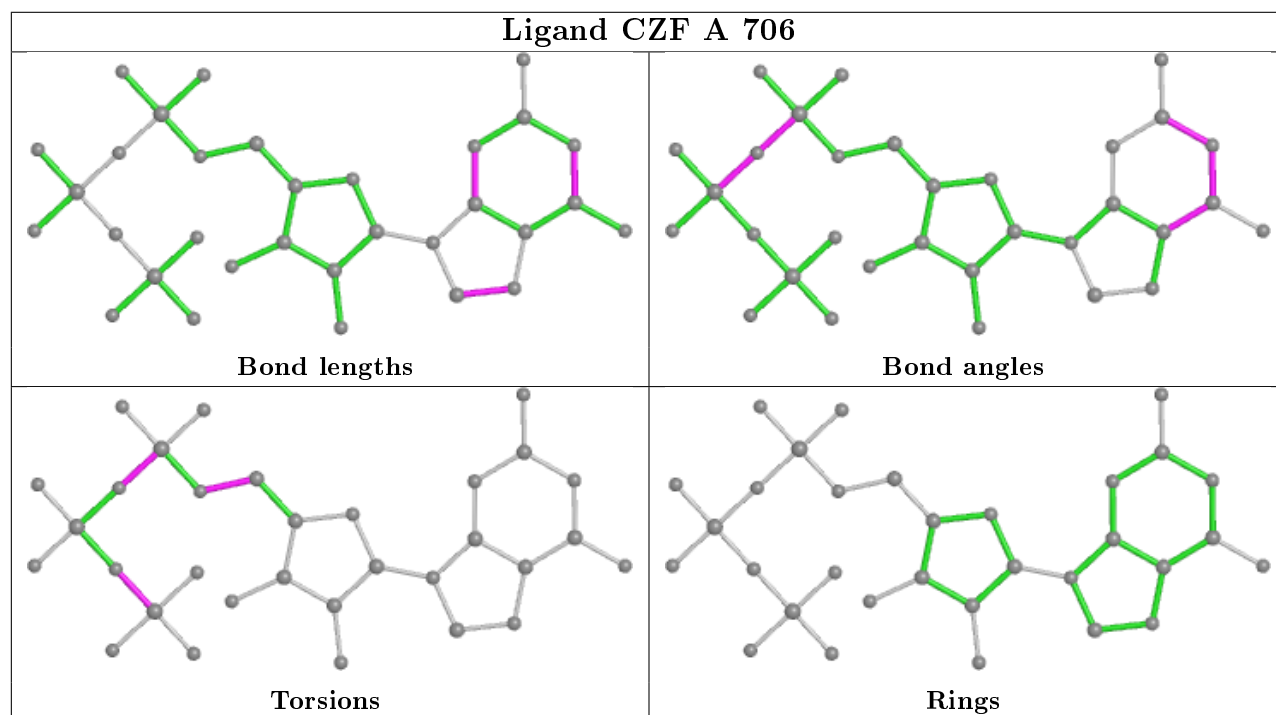


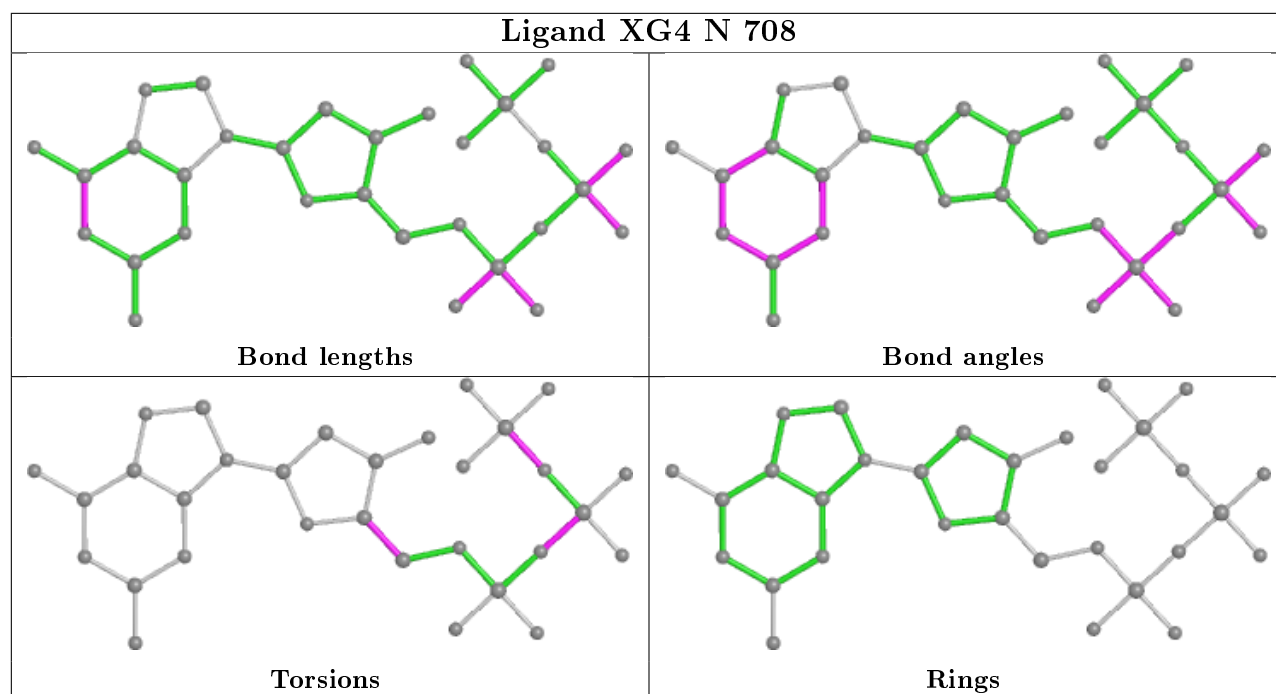
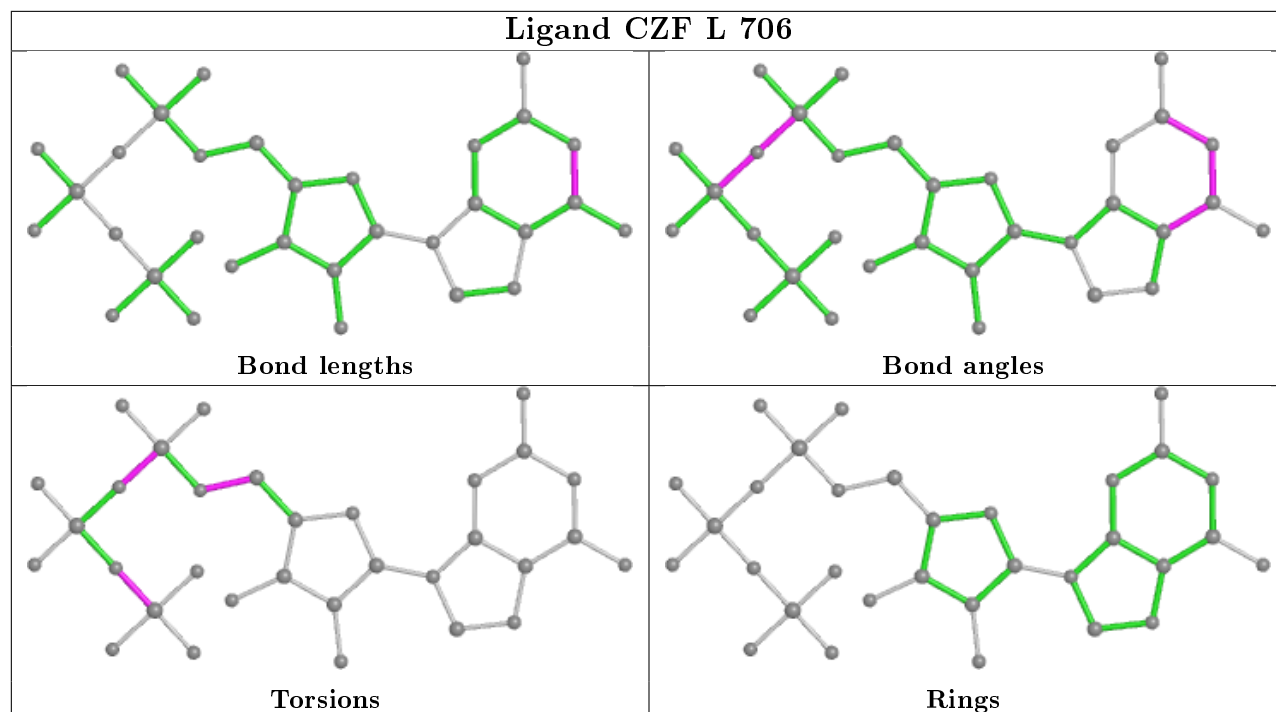


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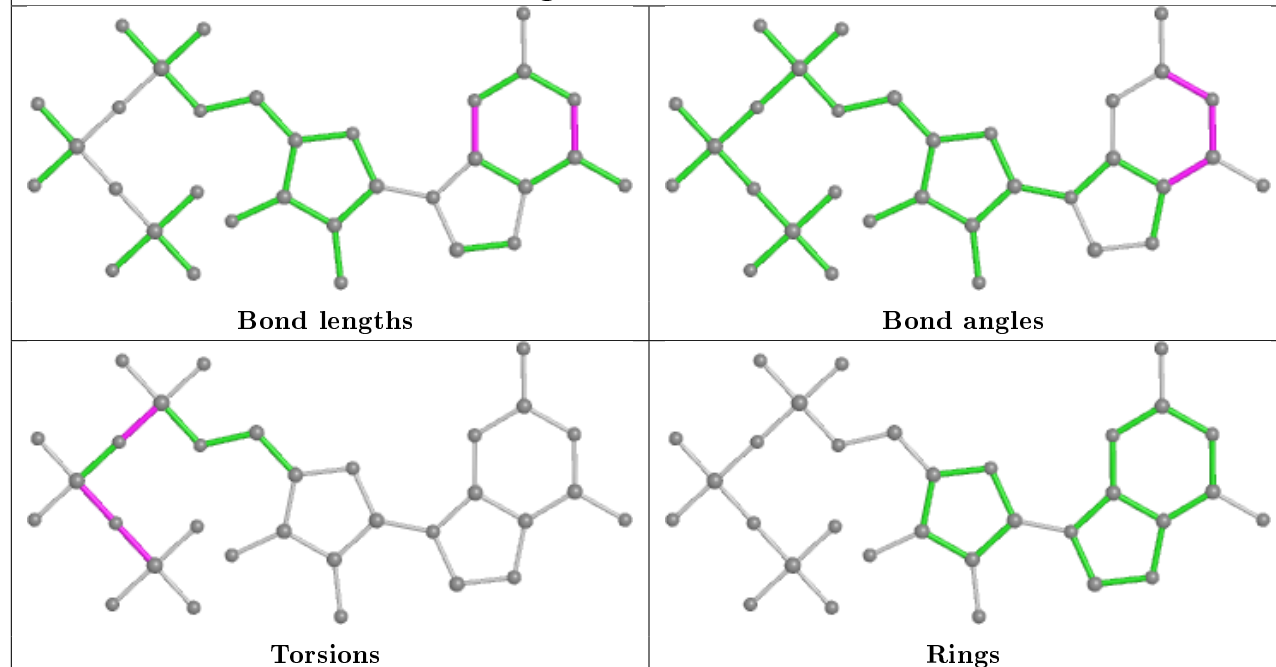


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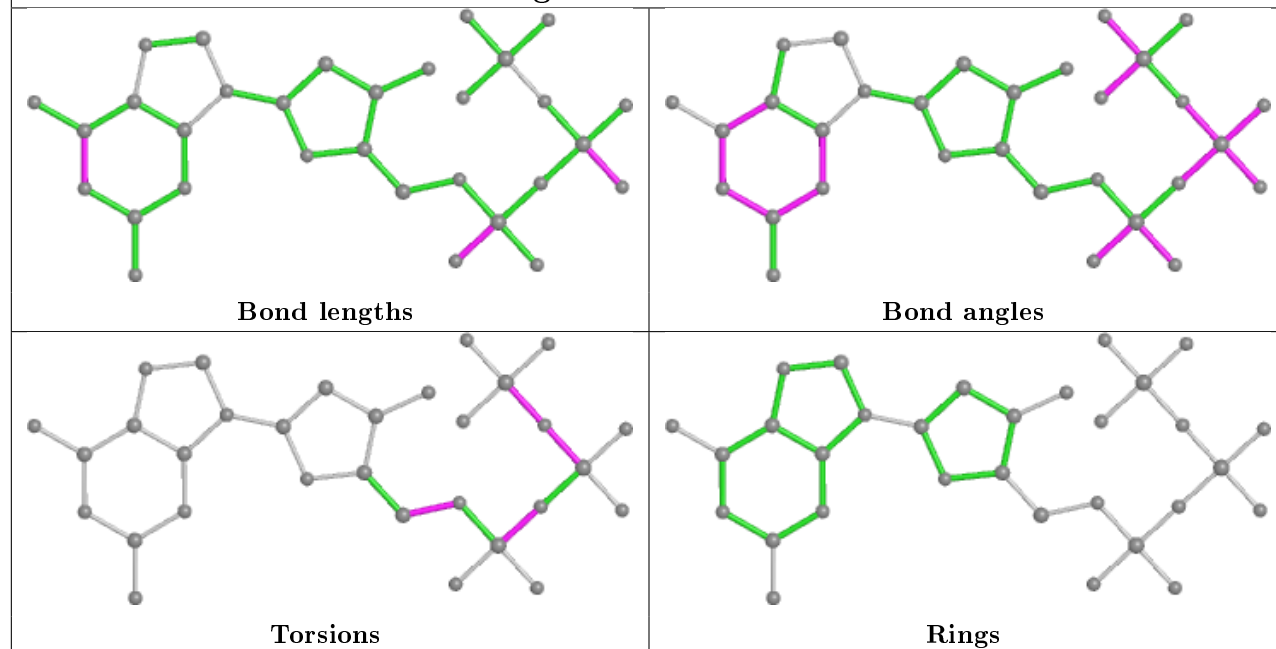


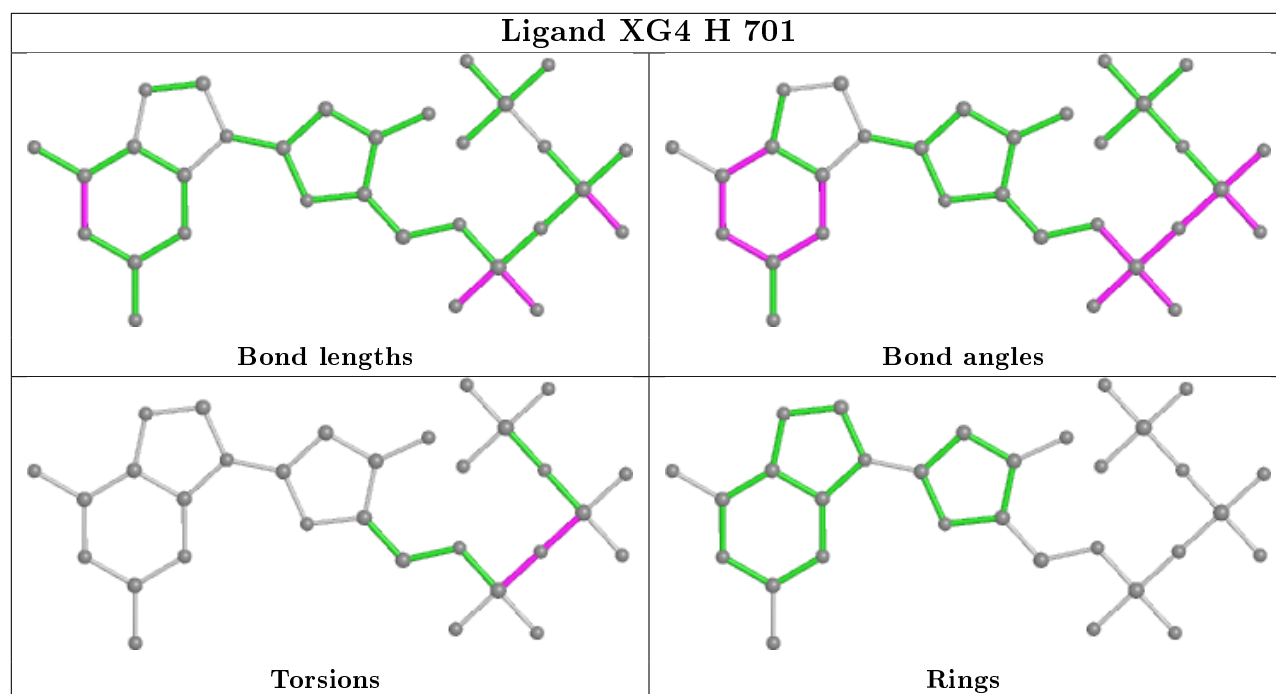
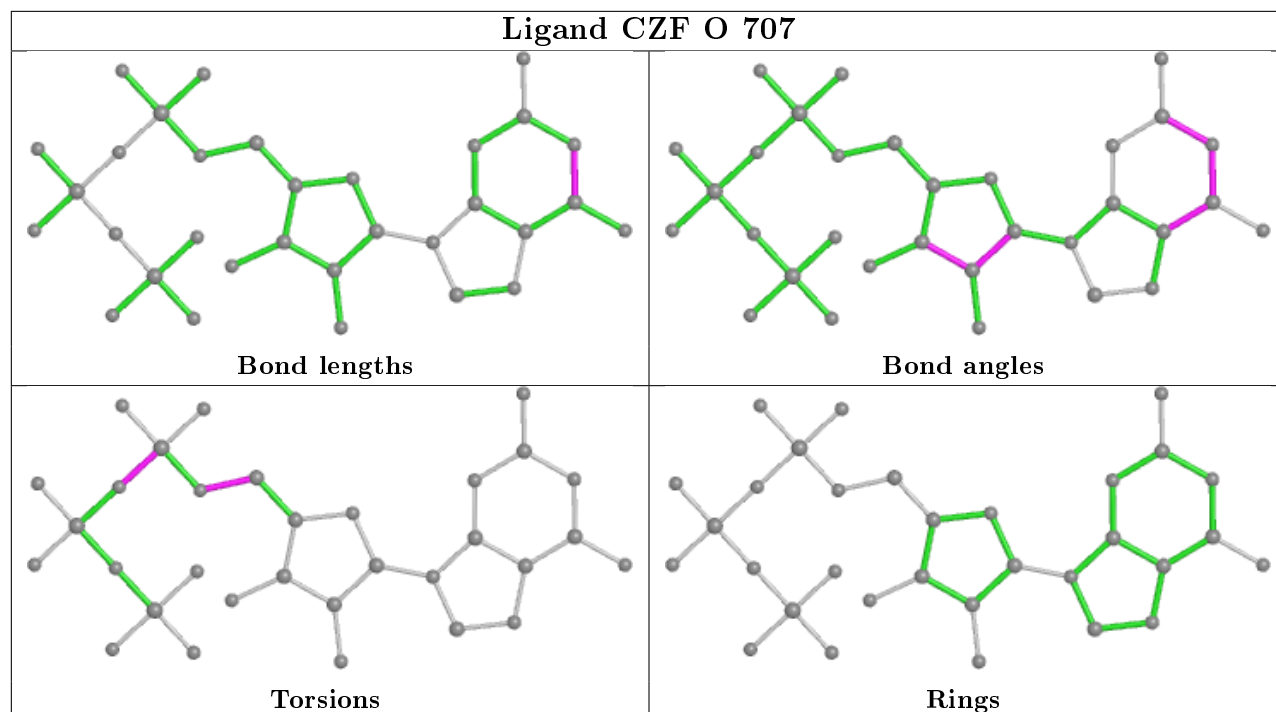


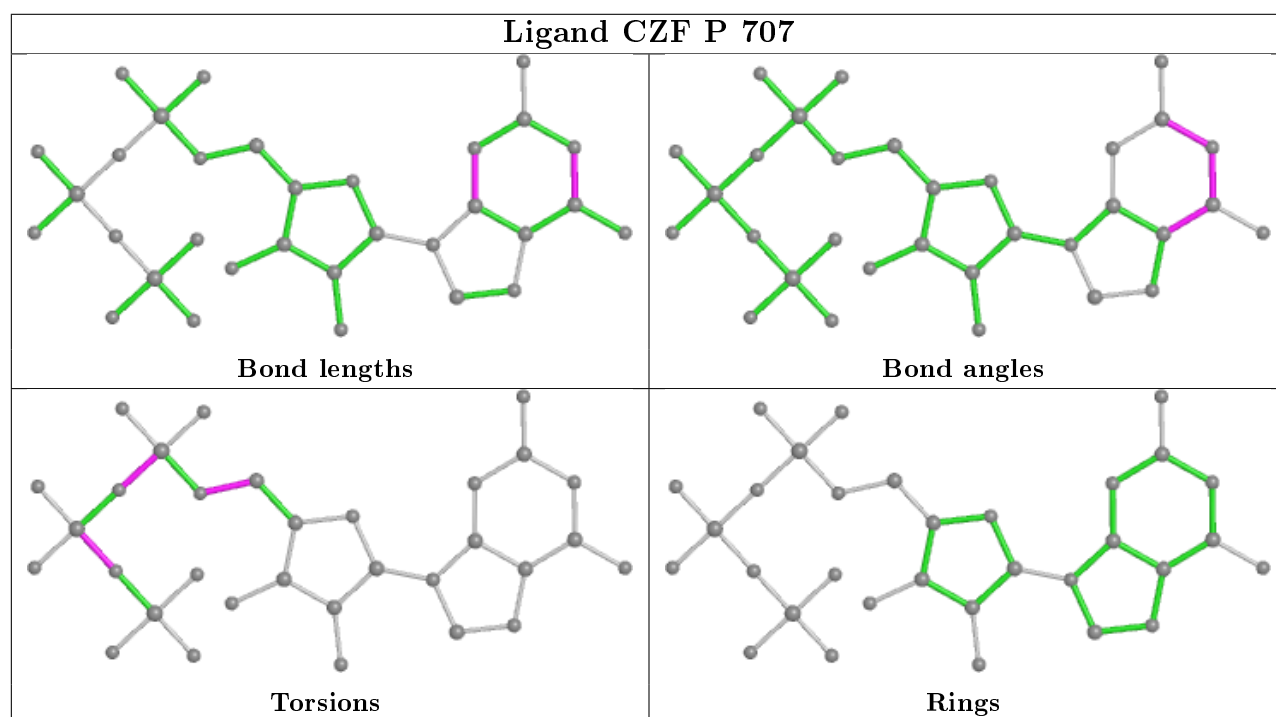
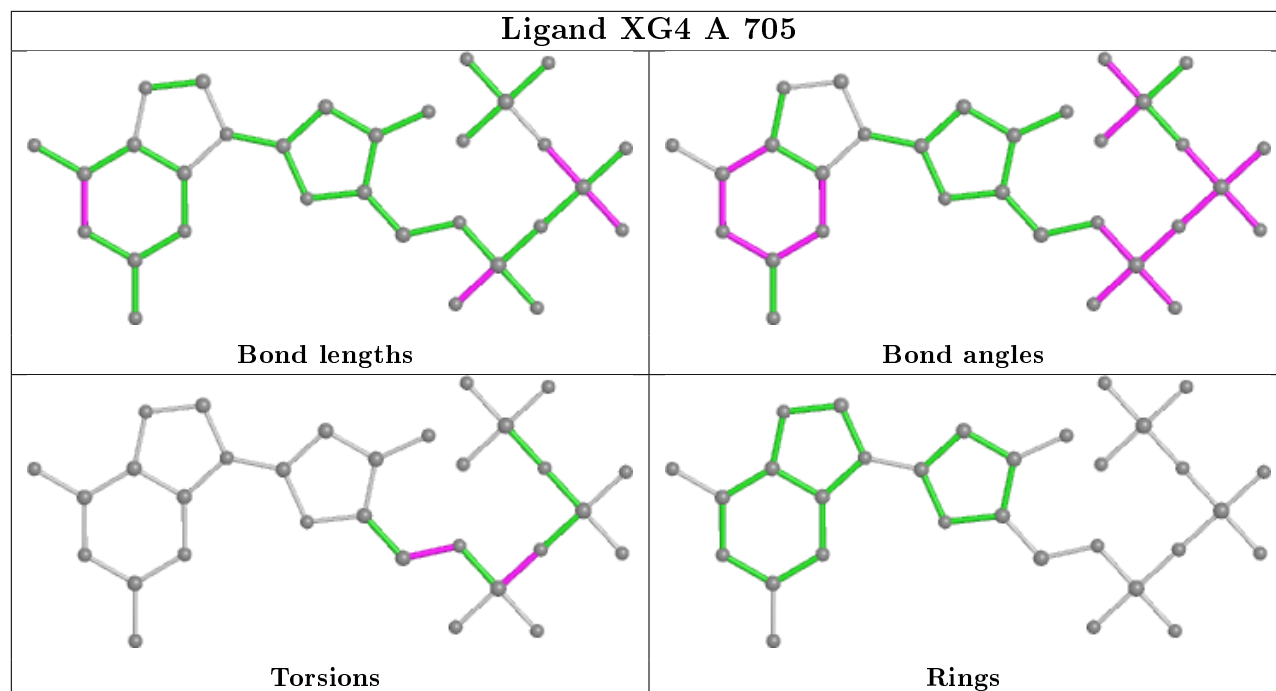
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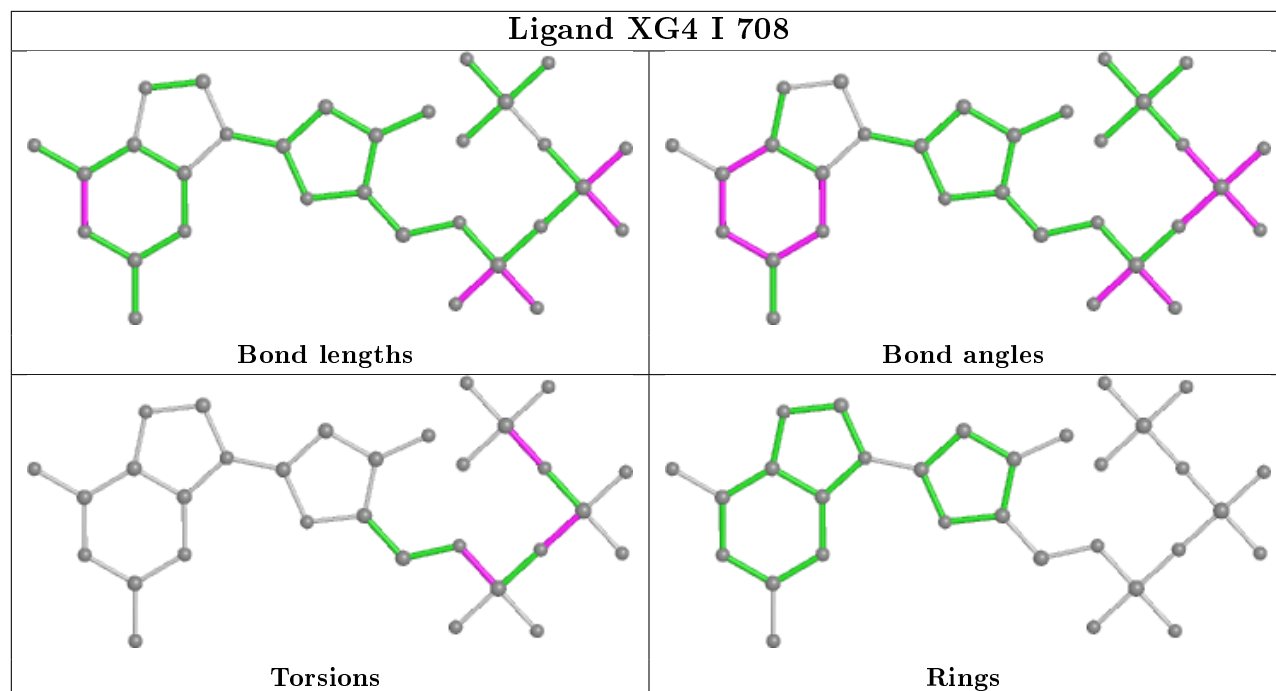
## Ligand XG4 O 706



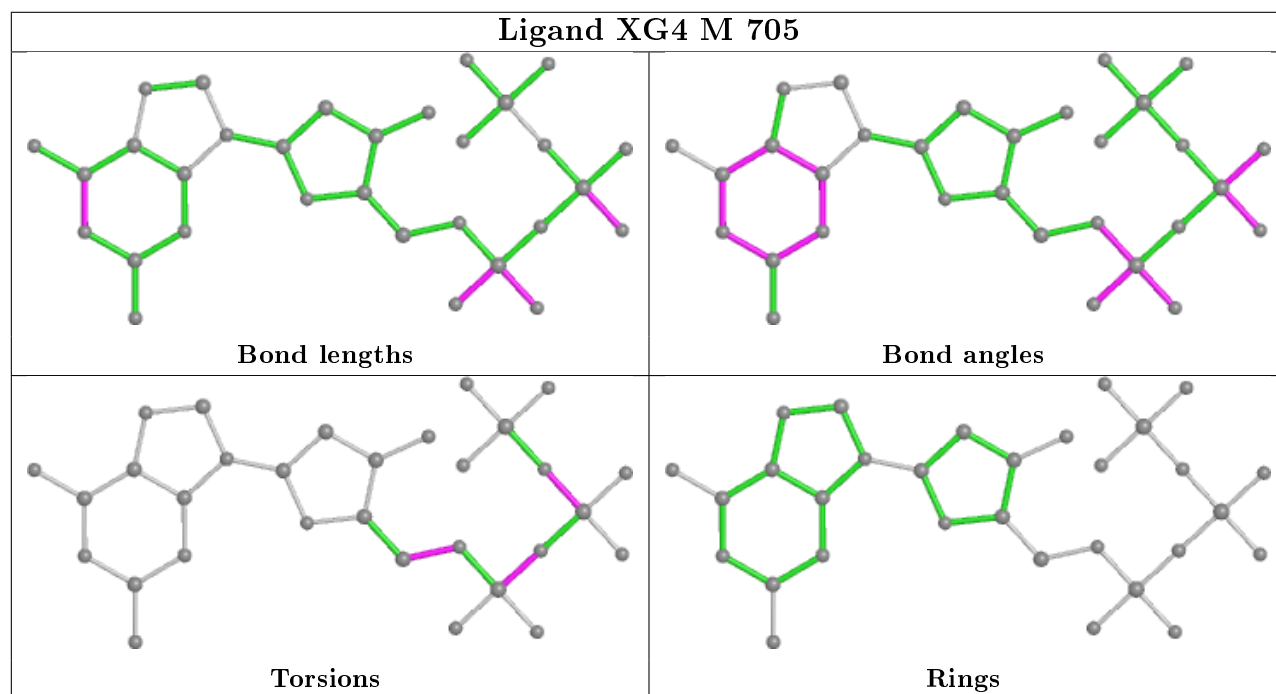




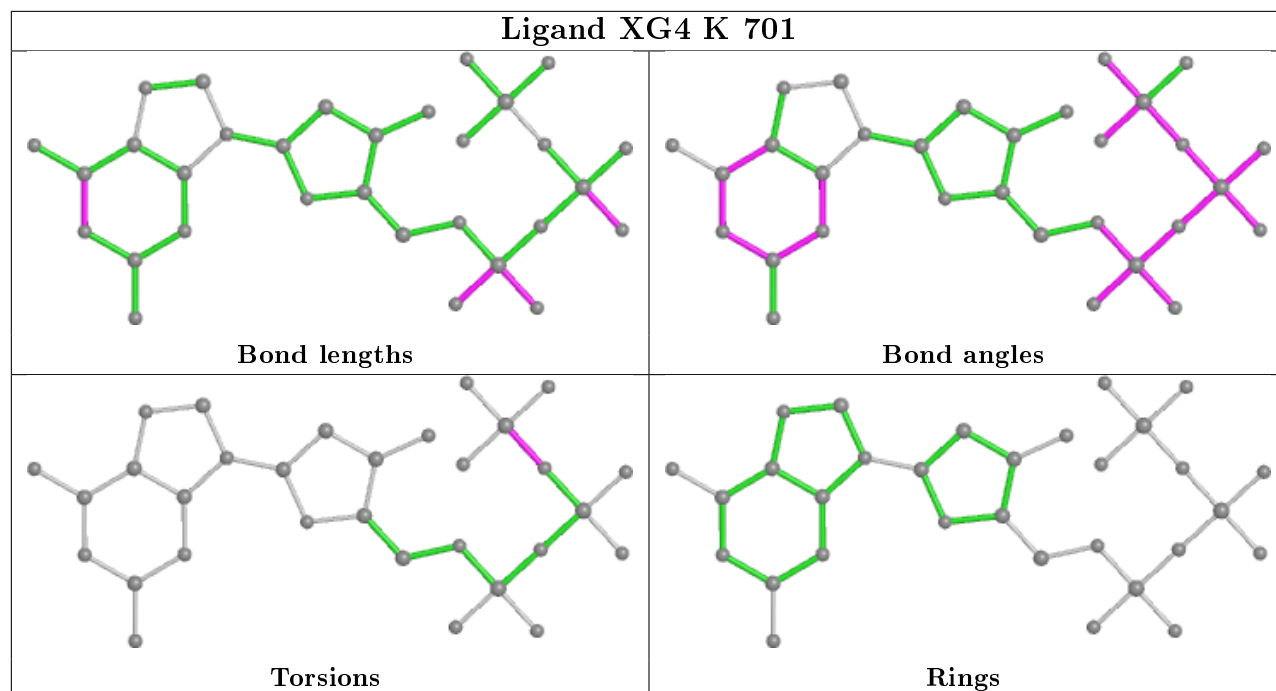
## Ligand XG4 I 708



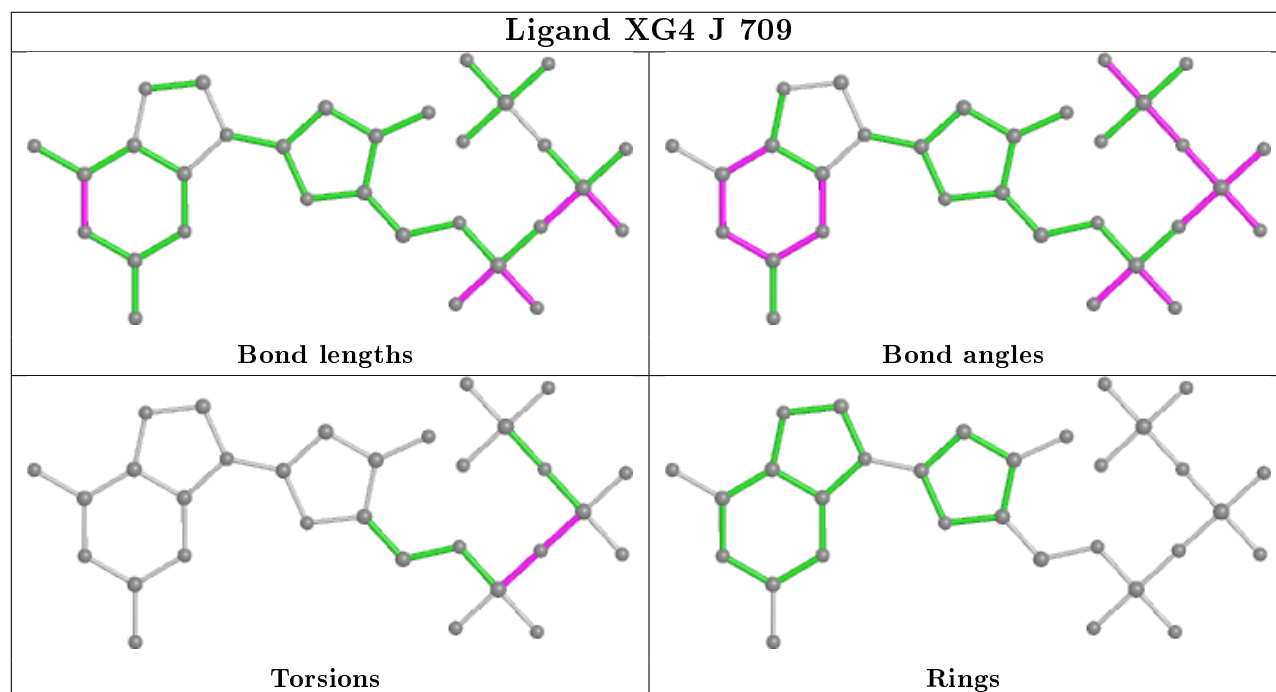
## Ligand XG4 M 705

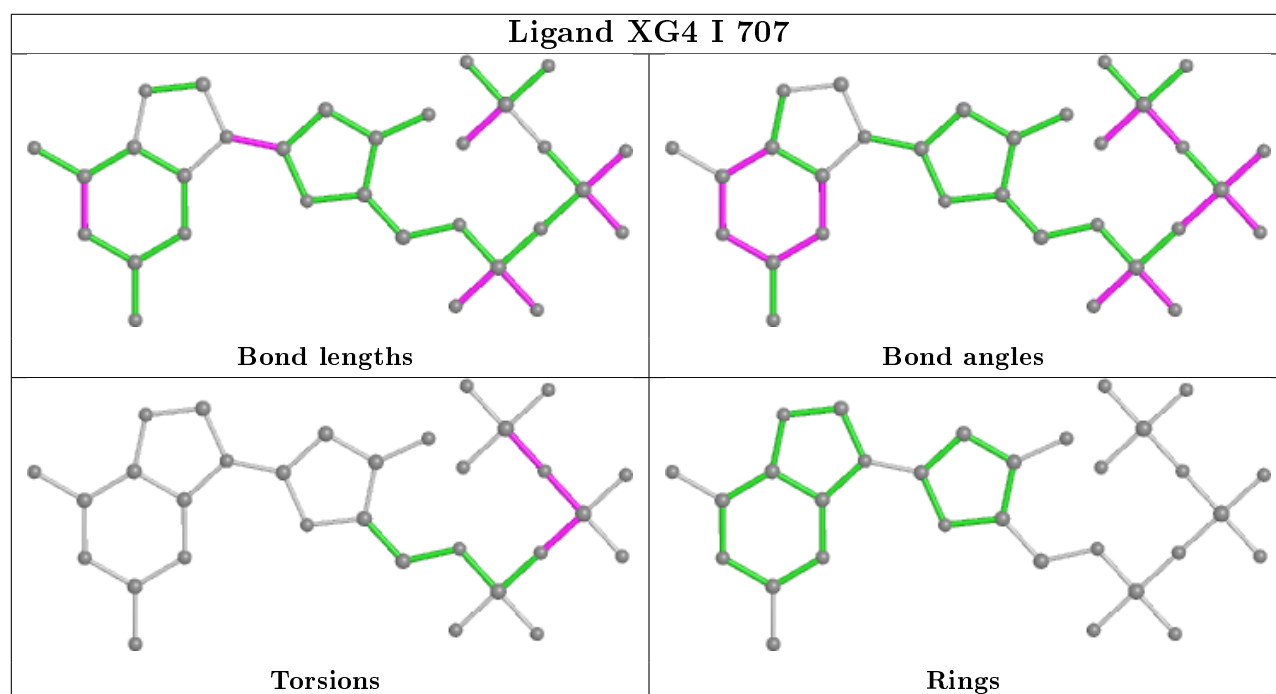
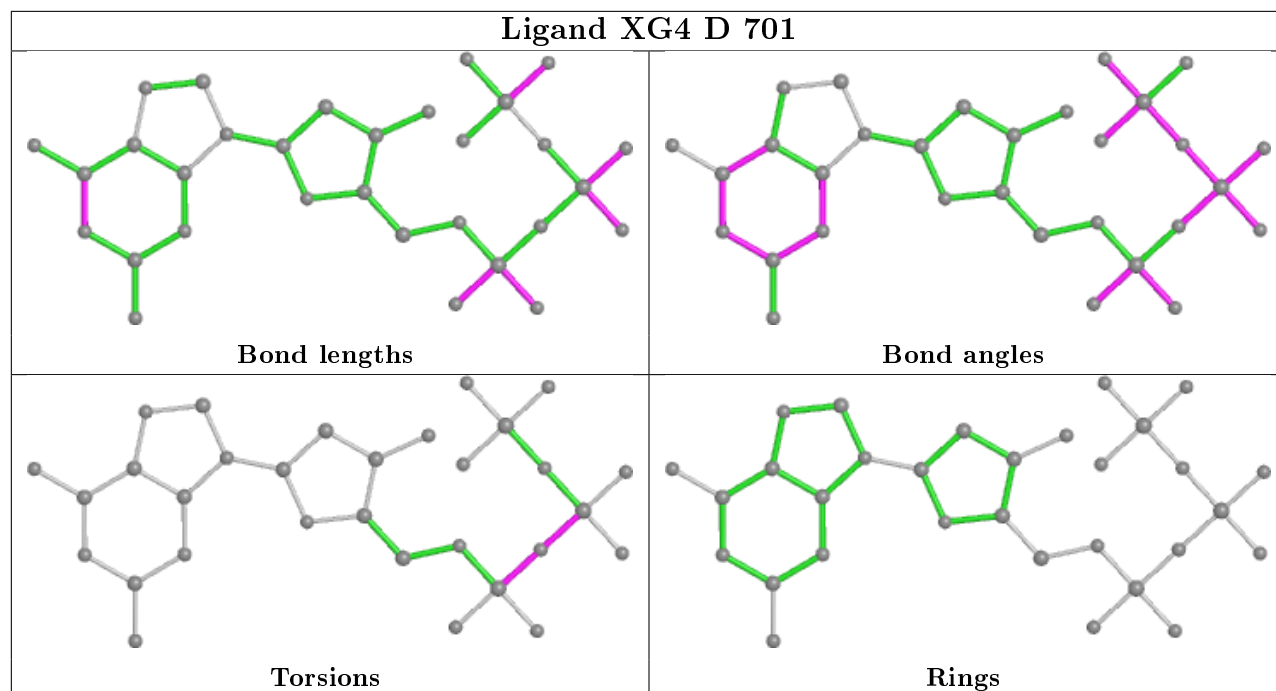


## Ligand XG4 K 701



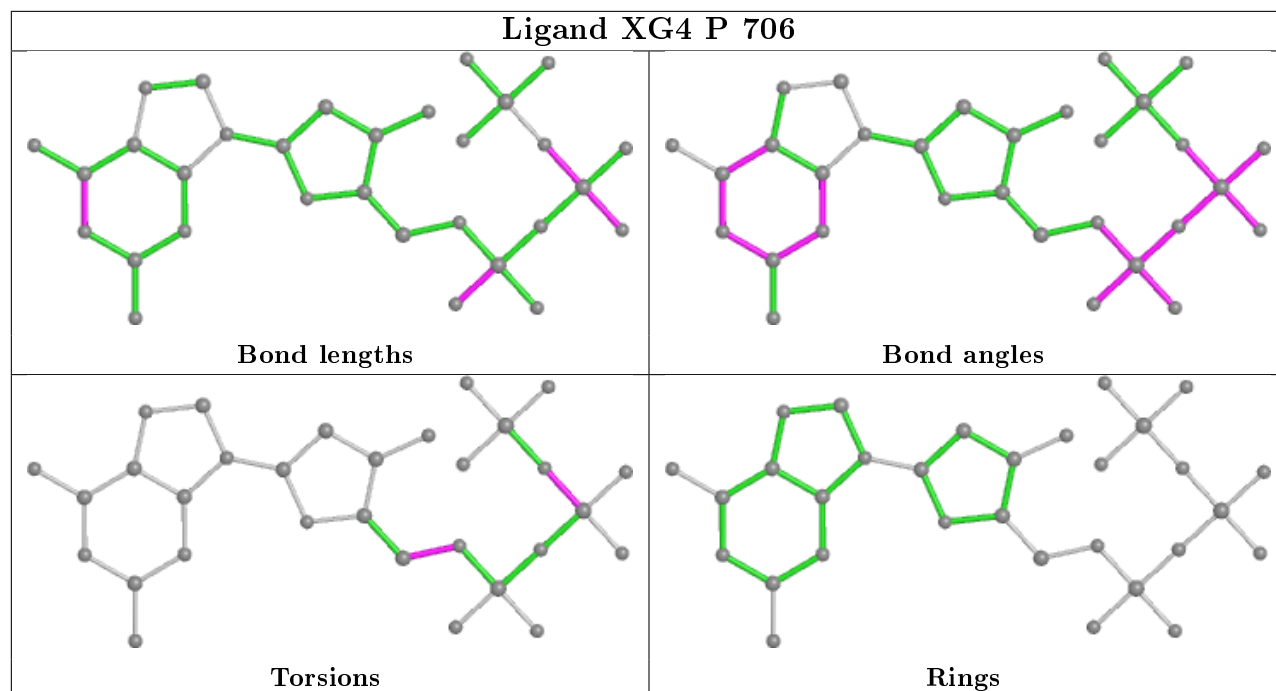
## Ligand XG4 J 709



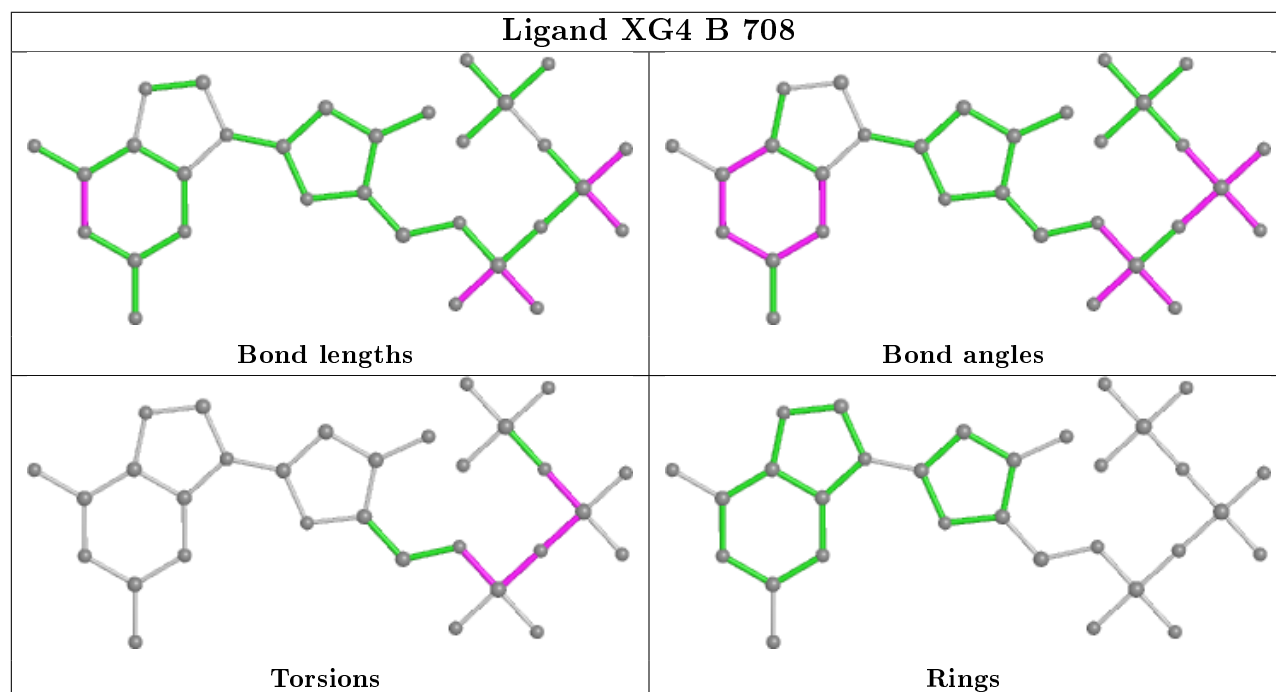


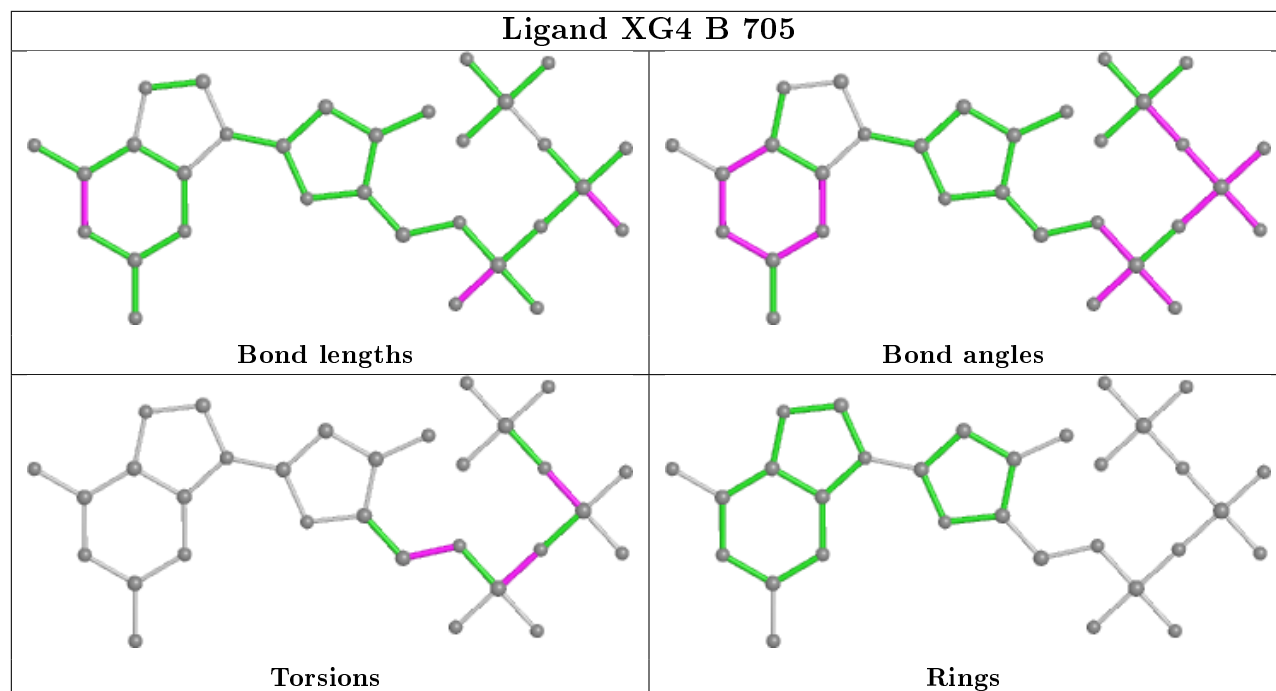


## Ligand XG4 P 706



## Ligand XG4 B 708





## 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	480/520 (92%)	-0.21	1 (0%) 95 95	11, 37, 68, 117	0
1	B	479/520 (92%)	-0.09	3 (0%) 89 89	17, 45, 87, 118	0
1	C	480/520 (92%)	-0.13	2 (0%) 92 92	17, 44, 80, 105	0
1	D	481/520 (92%)	-0.16	1 (0%) 95 95	12, 40, 70, 105	0
1	E	479/520 (92%)	-0.06	4 (0%) 86 85	19, 50, 90, 118	0
1	F	478/520 (91%)	0.01	5 (1%) 82 81	22, 53, 103, 133	0
1	G	479/520 (92%)	-0.08	3 (0%) 89 89	18, 47, 93, 118	0
1	H	480/520 (92%)	-0.25	1 (0%) 95 95	13, 38, 69, 99	0
1	I	479/520 (92%)	0.08	1 (0%) 95 95	23, 63, 97, 109	0
1	J	478/520 (91%)	-0.07	2 (0%) 92 92	19, 49, 87, 101	0
1	K	478/520 (91%)	0.07	3 (0%) 89 89	26, 63, 96, 114	0
1	L	478/520 (91%)	0.20	18 (3%) 40 35	23, 67, 121, 140	0
1	M	476/520 (91%)	0.31	13 (2%) 54 50	36, 77, 110, 126	0
1	N	477/520 (91%)	0.11	4 (0%) 86 85	33, 63, 93, 108	0
1	O	486/520 (93%)	0.22	7 (1%) 75 74	30, 67, 119, 140	0
1	P	478/520 (91%)	0.36	16 (3%) 46 41	37, 74, 140, 166	0
All	All	7666/8320 (92%)	0.02	84 (1%) 80 80	11, 54, 103, 166	0

The worst 5 of 84 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	480	VAL	4.0
1	B	594	GLN	4.0
1	M	572	TRP	3.8
1	P	583	ASP	3.6
1	M	345	ASN	3.4

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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( $\text{\AA}^2$ )	Q<0.9
6	SO4	I	706	5/5	0.68	0.25	125,130,132,137	0
6	SO4	M	707	5/5	0.79	0.33	140,145,151,154	0
6	SO4	N	707	5/5	0.79	0.31	112,119,120,126	0
6	SO4	G	708	5/5	0.84	0.28	107,109,114,114	0
6	SO4	K	708	5/5	0.89	0.17	88,90,91,93	0
6	SO4	F	707	5/5	0.89	0.26	102,103,107,111	0
6	SO4	L	707	5/5	0.89	0.30	96,99,104,108	0
6	SO4	O	708	5/5	0.92	0.18	96,97,98,100	0
6	SO4	C	708	5/5	0.92	0.14	88,90,92,95	0
3	MG	O	704	1/1	0.93	0.08	13,13,13,13	0
6	SO4	E	707	5/5	0.93	0.18	76,79,81,86	0
3	MG	K	704	1/1	0.94	0.08	21,21,21,21	0
3	MG	N	703	1/1	0.94	0.12	26,26,26,26	0
6	SO4	H	708	5/5	0.95	0.17	79,81,83,83	0
6	SO4	D	707	5/5	0.95	0.19	72,73,74,75	0
6	SO4	J	708	5/5	0.95	0.16	77,78,80,81	0
5	CZF	N	706	32/32	0.95	0.15	49,53,56,57	0
6	SO4	B	707	5/5	0.95	0.13	84,85,86,88	0
6	SO4	A	707	5/5	0.96	0.19	76,78,80,81	0
3	MG	D	704	1/1	0.96	0.18	11,11,11,11	0
4	XG4	P	706	31/31	0.96	0.15	49,58,72,75	0
4	XG4	M	708	31/31	0.96	0.15	45,53,70,74	0
4	XG4	M	705	31/31	0.96	0.13	49,54,61,66	0
3	MG	N	704	1/1	0.96	0.08	22,22,22,22	0
4	XG4	P	701	31/31	0.96	0.16	45,49,57,58	0
5	CZF	O	707	32/32	0.96	0.13	50,59,66,67	0
4	XG4	L	705	31/31	0.96	0.15	38,47,57,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	XG4	C	706	31/31	0.97	0.13	18,20,21,21	0
4	XG4	O	706	31/31	0.97	0.15	34,42,45,49	0
5	CZF	J	701	32/32	0.97	0.14	34,38,50,52	0
5	CZF	K	707	32/32	0.97	0.13	58,63,67,70	0
4	XG4	I	705	31/31	0.97	0.14	34,38,48,48	0
4	XG4	I	708	31/31	0.97	0.14	37,45,67,70	0
4	XG4	A	705	31/31	0.97	0.13	10,10,10,10	0
4	XG4	F	705	31/31	0.97	0.14	19,23,25,27	0
4	XG4	K	706	31/31	0.97	0.13	32,35,41,42	0
4	XG4	G	706	31/31	0.97	0.14	16,18,20,21	0
5	CZF	P	707	32/32	0.97	0.14	39,46,59,61	0
3	MG	H	703	1/1	0.97	0.25	11,11,11,11	0
4	XG4	H	706	31/31	0.97	0.13	11,13,14,14	0
4	XG4	J	706	31/31	0.97	0.13	15,16,19,19	0
3	MG	C	704	1/1	0.97	0.14	12,12,12,12	0
3	MG	F	703	1/1	0.97	0.14	12,12,12,12	0
4	XG4	D	706	31/31	0.97	0.13	11,11,11,12	0
3	MG	J	704	1/1	0.98	0.18	10,10,10,10	0
4	XG4	D	701	31/31	0.98	0.11	13,14,18,18	0
4	XG4	B	708	31/31	0.98	0.14	26,27,35,35	0
3	MG	A	704	1/1	0.98	0.12	13,13,13,13	0
4	XG4	F	708	31/31	0.98	0.12	20,22,30,30	0
2	FE	M	701	1/1	0.98	0.07	61,61,61,61	0
3	MG	M	704	1/1	0.98	0.07	14,14,14,14	0
4	XG4	N	705	31/31	0.98	0.12	37,41,46,47	0
4	XG4	N	708	31/31	0.98	0.13	38,41,54,55	0
3	MG	B	704	1/1	0.98	0.10	13,13,13,13	0
3	MG	P	703	1/1	0.98	0.19	15,15,15,15	0
3	MG	M	703	1/1	0.98	0.07	21,21,21,21	0
4	XG4	I	707	31/31	0.98	0.14	26,27,43,44	0
5	CZF	E	706	32/32	0.98	0.13	27,30,40,41	0
4	XG4	B	705	31/31	0.98	0.12	13,15,19,20	0
5	CZF	A	706	32/32	0.98	0.13	21,24,32,33	0
5	CZF	B	706	32/32	0.98	0.13	14,15,23,24	0
4	XG4	O	701	31/31	0.98	0.13	28,31,35,37	0
4	XG4	E	705	31/31	0.98	0.13	15,19,28,29	0
3	MG	A	703	1/1	0.98	0.16	10,10,10,10	0
3	MG	J	705	1/1	0.98	0.08	16,16,16,16	0
5	CZF	C	709	32/32	0.98	0.13	27,31,38,39	0
3	MG	E	703	1/1	0.98	0.14	11,11,11,11	0
4	XG4	E	708	31/31	0.98	0.12	15,16,23,23	0
5	CZF	C	707	32/32	0.98	0.12	14,14,17,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CZF	J	707	32/32	0.98	0.13	22,27,34,35	0
2	FE	O	702	1/1	0.98	0.10	50,50,50,50	0
3	MG	O	705	1/1	0.98	0.07	40,40,40,40	0
3	MG	H	704	1/1	0.98	0.20	11,11,11,11	0
5	CZF	F	706	32/32	0.98	0.13	26,30,39,40	0
4	XG4	G	701	31/31	0.98	0.13	28,33,36,36	0
5	CZF	L	706	32/32	0.98	0.12	19,23,34,35	0
3	MG	D	705	1/1	0.98	0.10	15,15,15,15	0
3	MG	E	702	1/1	0.98	0.22	11,11,11,11	0
4	XG4	K	701	31/31	0.98	0.12	26,27,37,38	0
5	CZF	H	707	32/32	0.98	0.12	16,17,22,22	0
3	MG	P	704	1/1	0.98	0.09	22,22,22,22	0
3	MG	K	705	1/1	0.98	0.05	39,39,39,39	0
5	CZF	M	706	32/32	0.98	0.11	30,32,44,45	0
5	CZF	G	707	32/32	0.98	0.12	13,15,24,24	0
3	MG	I	703	1/1	0.98	0.14	19,19,19,19	0
4	XG4	A	708	31/31	0.98	0.12	12,13,19,19	0
4	XG4	H	701	31/31	0.98	0.13	22,24,29,29	0
4	XG4	J	709	31/31	0.98	0.13	14,15,21,21	0
4	XG4	C	701	31/31	0.99	0.13	21,22,33,33	0
3	MG	H	705	1/1	0.99	0.08	14,14,14,14	0
3	MG	I	702	1/1	0.99	0.25	13,13,13,13	0
3	MG	L	703	1/1	0.99	0.10	12,12,12,12	0
3	MG	I	704	1/1	0.99	0.06	13,13,13,13	0
3	MG	G	705	1/1	0.99	0.09	13,13,13,13	0
3	MG	L	704	1/1	0.99	0.09	11,11,11,11	0
3	MG	G	704	1/1	0.99	0.13	11,11,11,11	0
3	MG	L	702	1/1	0.99	0.18	12,12,12,12	0
3	MG	F	704	1/1	0.99	0.12	15,15,15,15	0
2	FE	H	702	1/1	0.99	0.10	13,13,13,13	0
2	FE	L	701	1/1	0.99	0.11	40,40,40,40	0
3	MG	D	703	1/1	0.99	0.26	12,12,12,12	0
2	FE	J	702	1/1	0.99	0.10	18,18,18,18	0
3	MG	B	702	1/1	0.99	0.28	12,12,12,12	0
3	MG	C	705	1/1	0.99	0.15	13,13,13,13	0
2	FE	N	701	1/1	0.99	0.08	41,41,41,41	0
3	MG	P	705	1/1	0.99	0.06	16,16,16,16	0
2	FE	F	701	1/1	0.99	0.12	28,28,28,28	0
3	MG	E	704	1/1	0.99	0.13	15,15,15,15	0
3	MG	A	702	1/1	0.99	0.30	10,10,10,10	0
3	MG	G	703	1/1	0.99	0.28	11,11,11,11	0
2	FE	G	702	1/1	0.99	0.11	19,19,19,19	0

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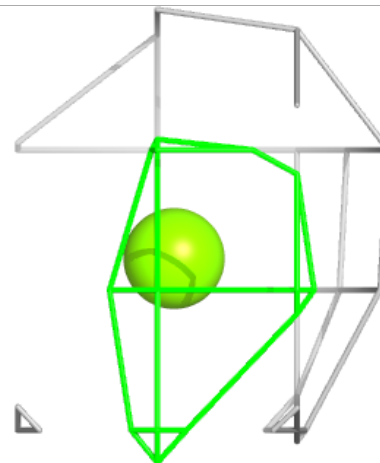
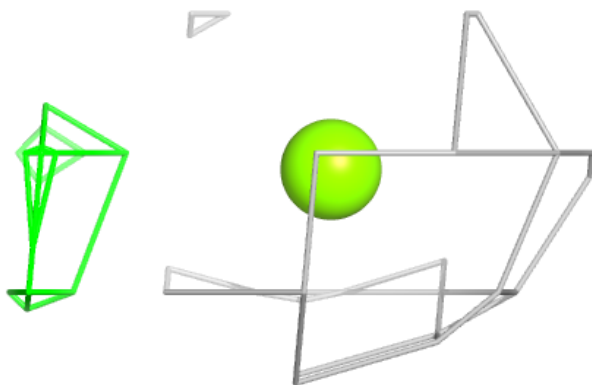
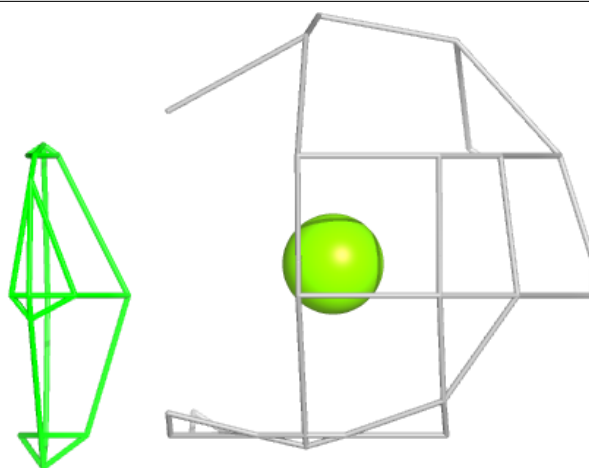
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FE	E	701	1/1	0.99	0.11	24,24,24,24	0
3	MG	C	703	1/1	0.99	0.29	12,12,12,12	0
3	MG	K	703	1/1	0.99	0.22	13,13,13,13	0
3	MG	F	702	1/1	0.99	0.28	12,12,12,12	0
2	FE	K	702	1/1	0.99	0.12	50,50,50,50	0
2	FE	I	701	1/1	0.99	0.09	37,37,37,37	0
3	MG	M	702	1/1	0.99	0.17	14,14,14,14	0
3	MG	N	702	1/1	0.99	0.20	14,14,14,14	0
2	FE	D	702	1/1	0.99	0.12	17,17,17,17	0
3	MG	B	703	1/1	0.99	0.15	12,12,12,12	0
3	MG	J	703	1/1	1.00	0.22	11,11,11,11	0
3	MG	O	703	1/1	1.00	0.25	13,13,13,13	0
2	FE	P	702	1/1	1.00	0.13	48,48,48,48	0
2	FE	C	702	1/1	1.00	0.11	15,15,15,15	0
2	FE	A	701	1/1	1.00	0.09	11,11,11,11	0
2	FE	B	701	1/1	1.00	0.12	20,20,20,20	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 O 704:**

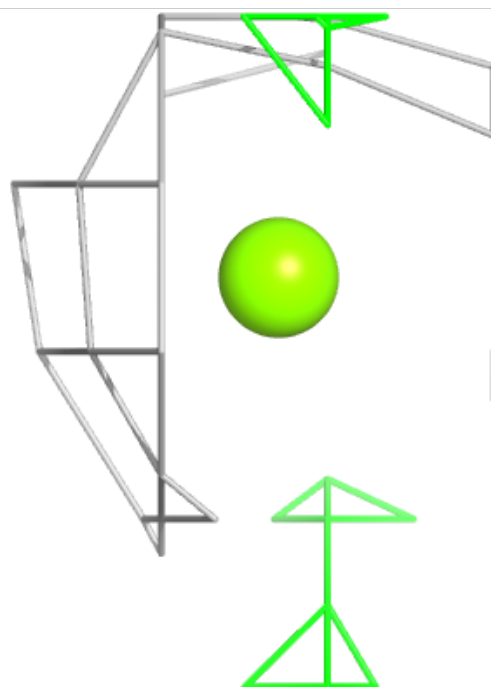
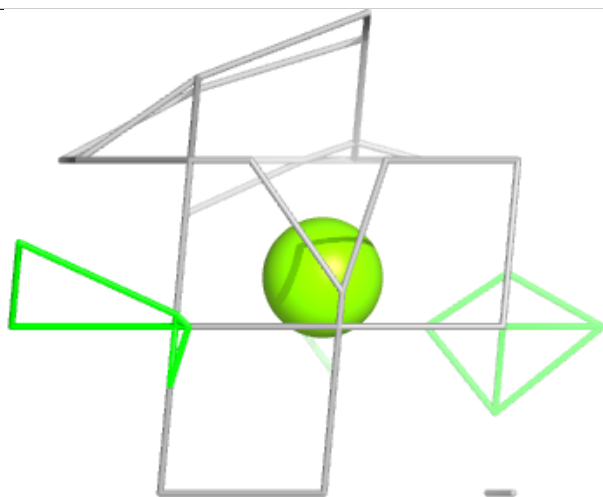
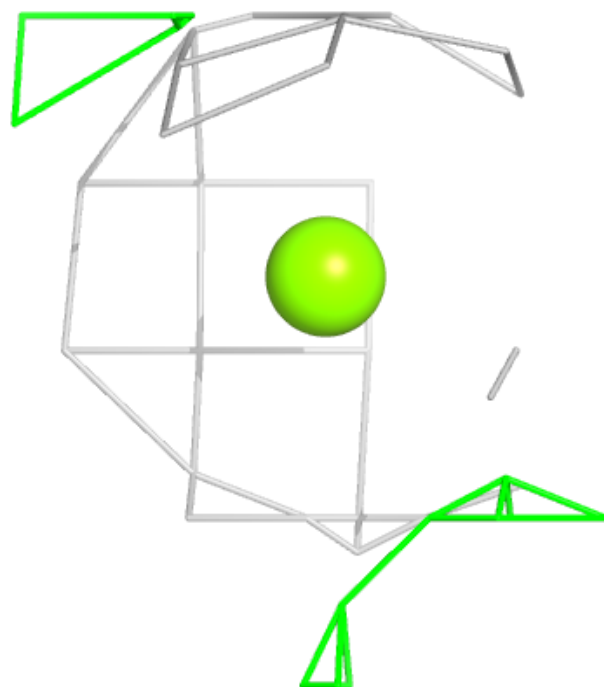
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





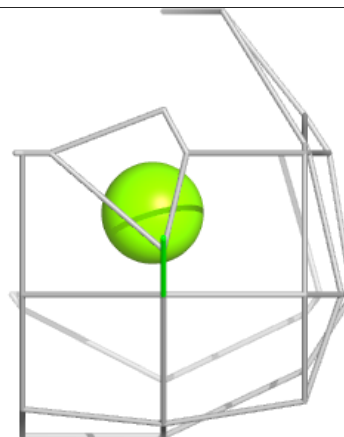
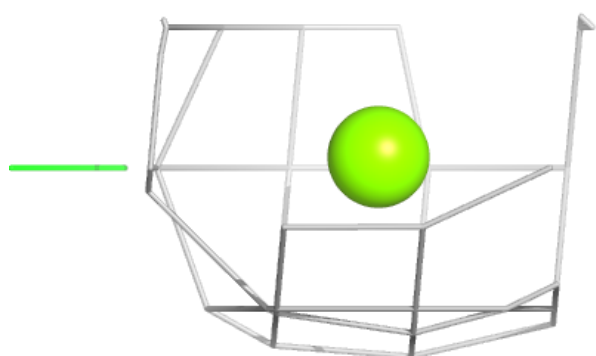
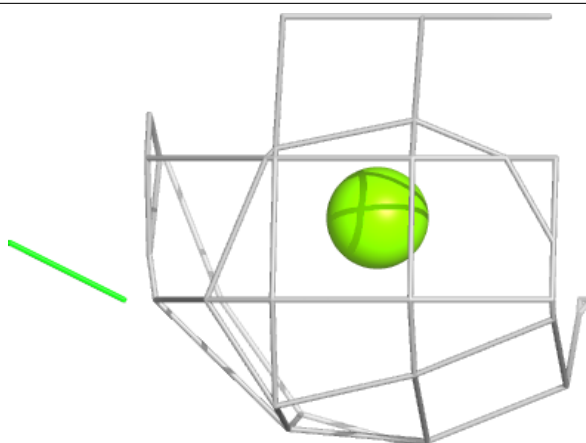
**Electron density around MG K 704:**

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

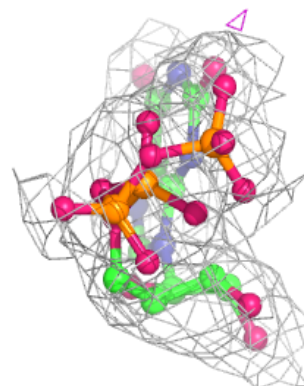
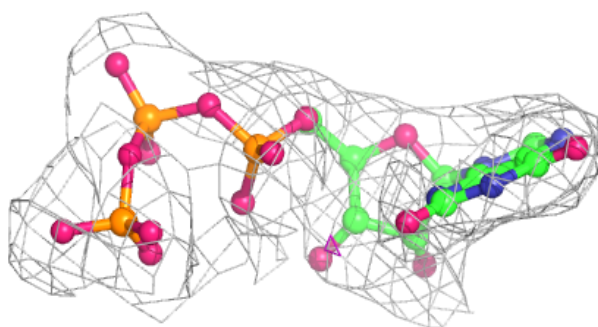
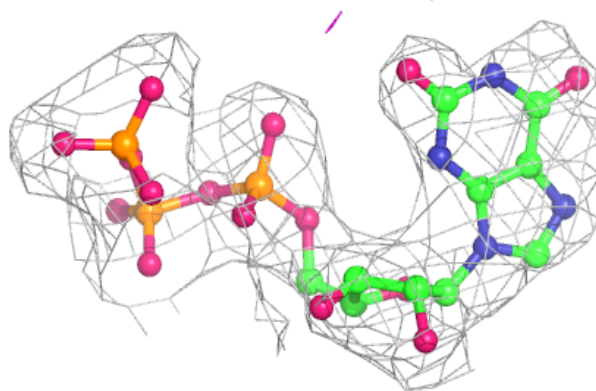


**Electron density around MG N 703:**

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

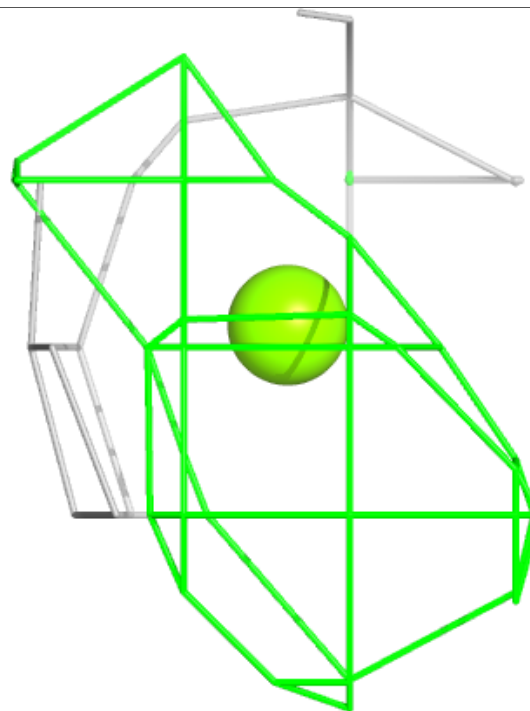
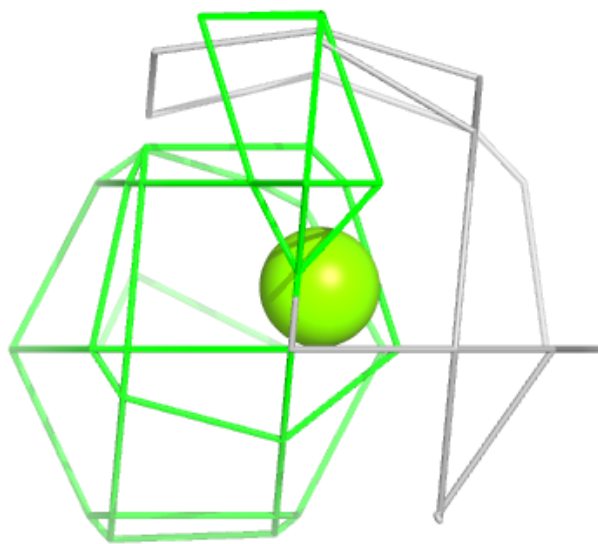
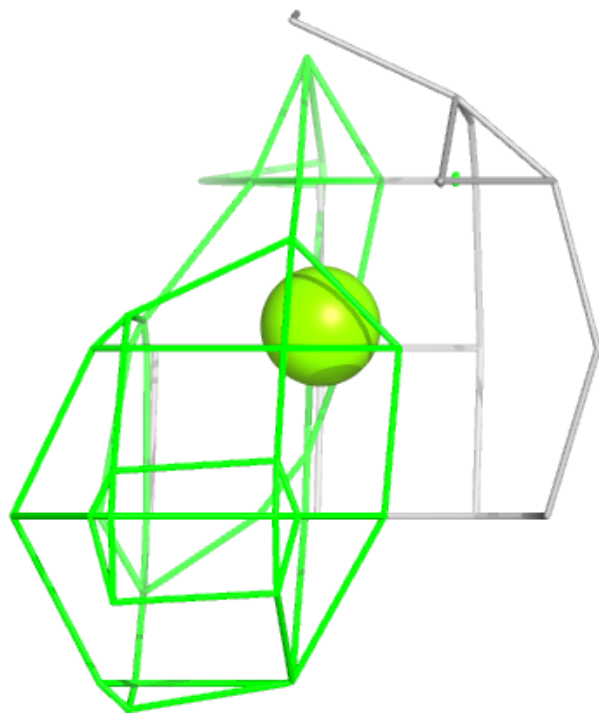
**Electron density around CZF N 706:**

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



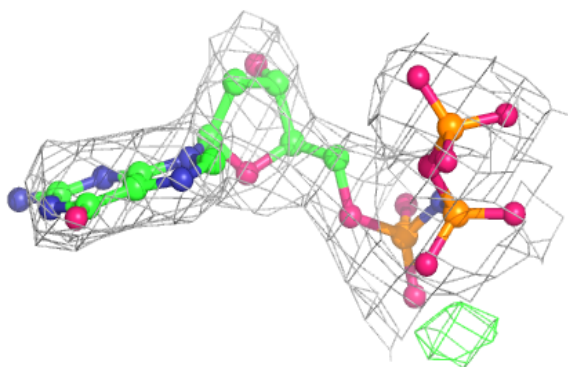
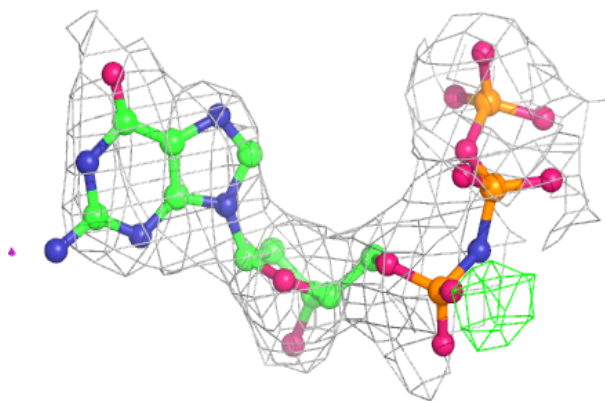
**Electron density around MG D 704:**

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

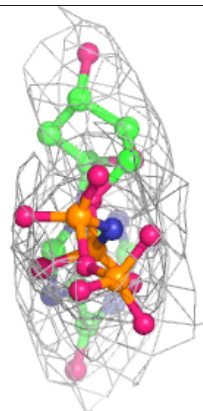
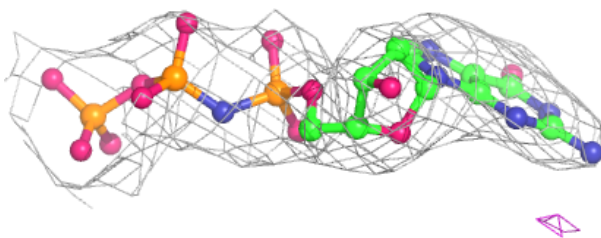
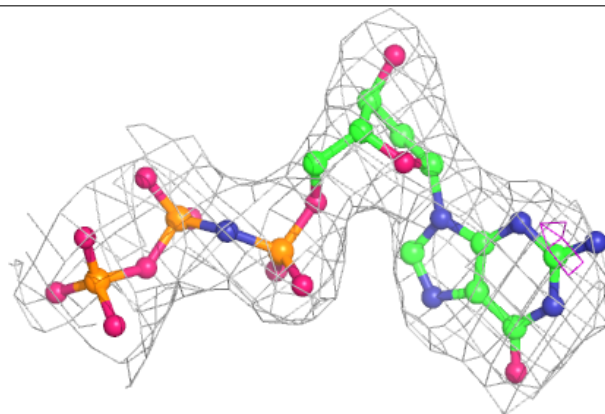


**Electron density around XG4 P 706:**

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

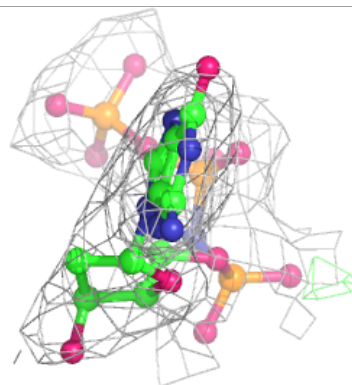
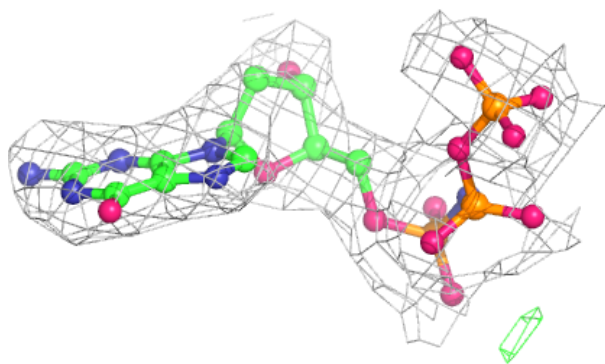
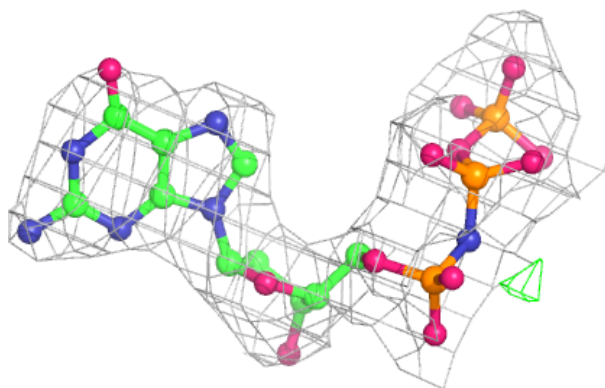
**Electron density around XG4 M 708:**

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



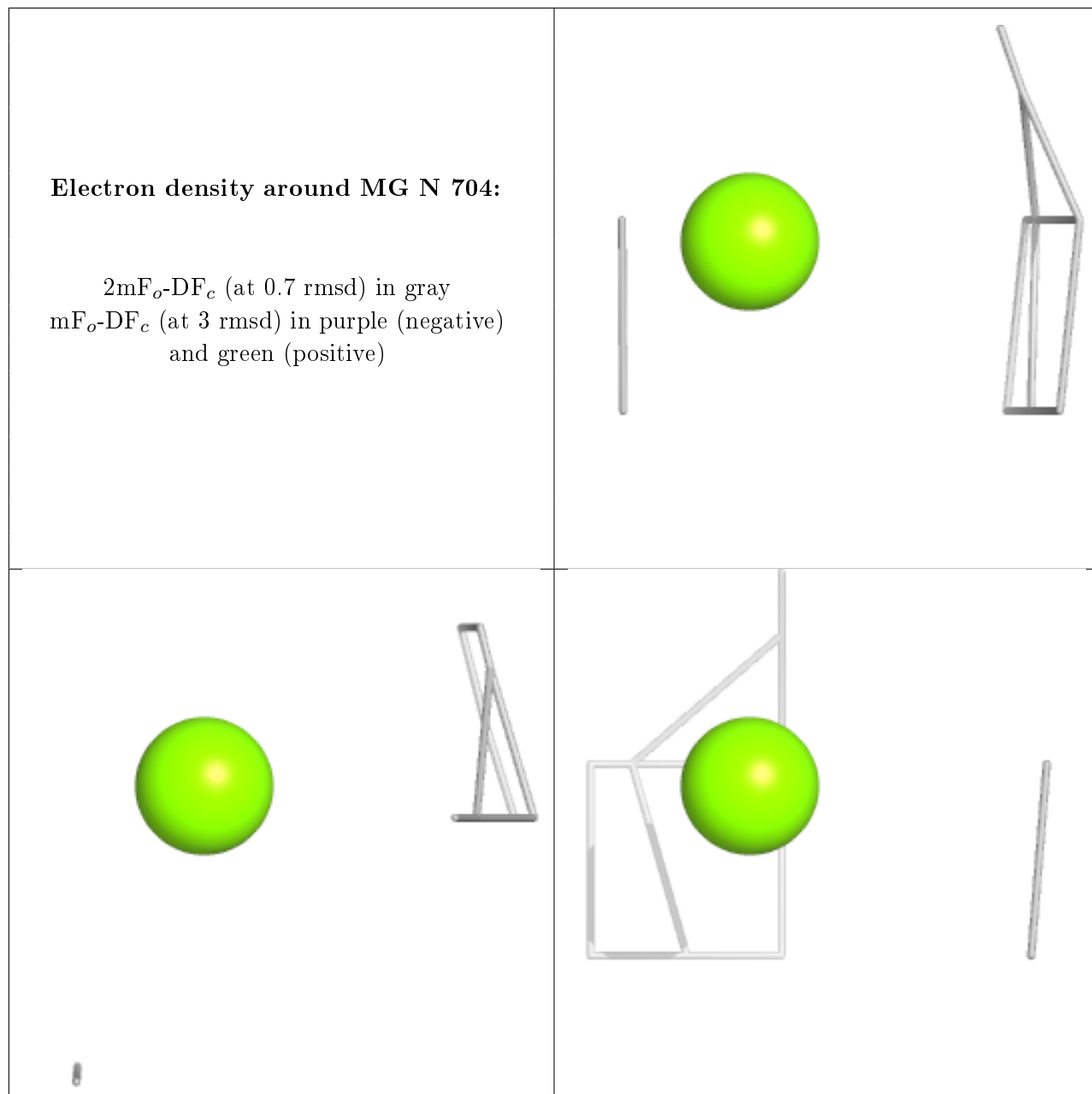
**Electron density around XG4 M 705:**

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



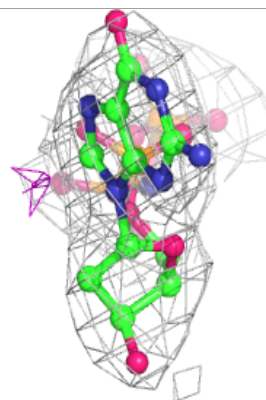
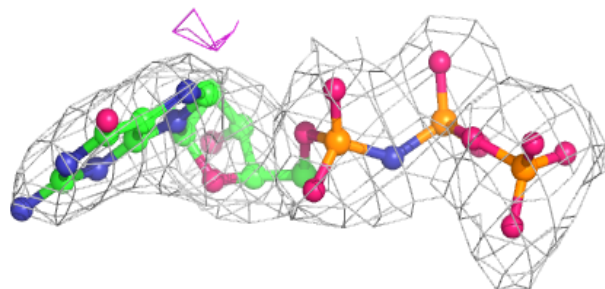
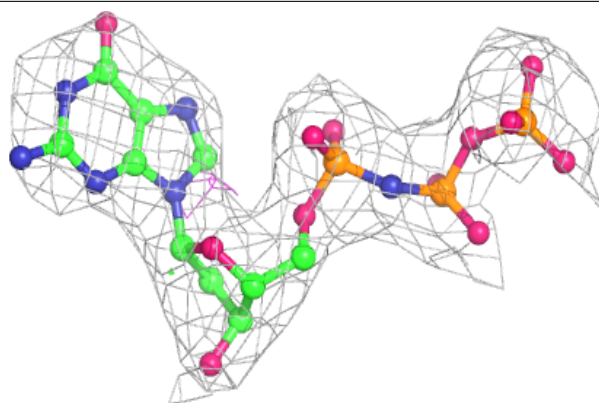
**Electron density around MG N 704:**

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

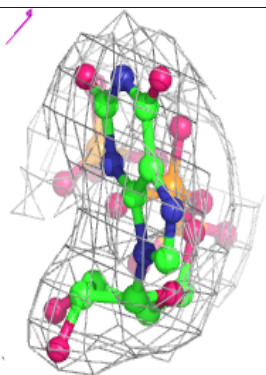
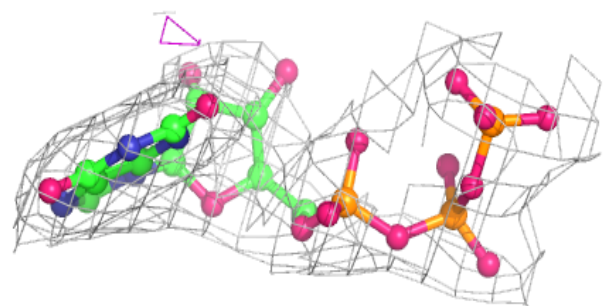
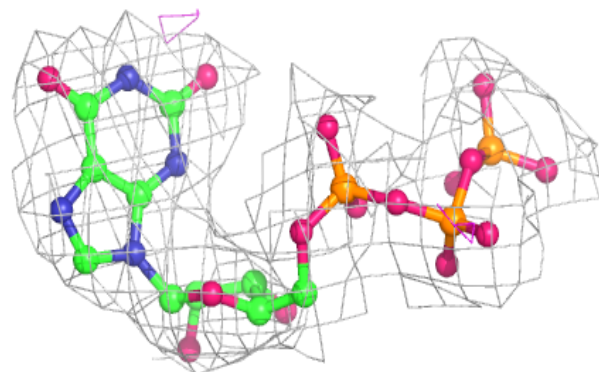


**Electron density around XG4 P 701:**

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

**Electron density around CZF O 707:**

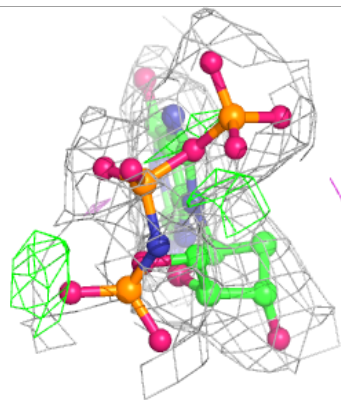
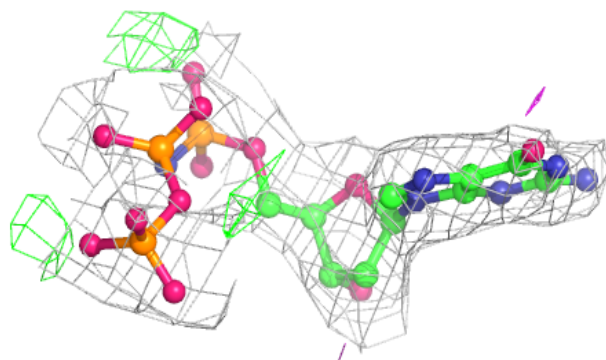
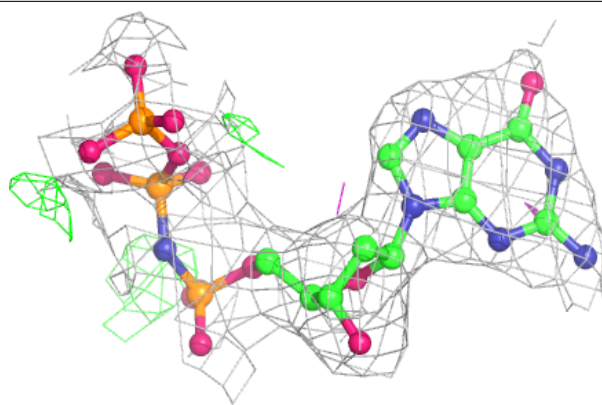
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



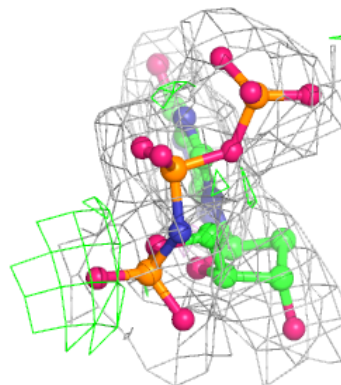
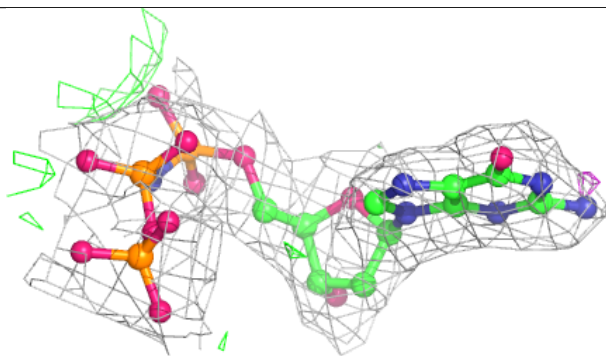
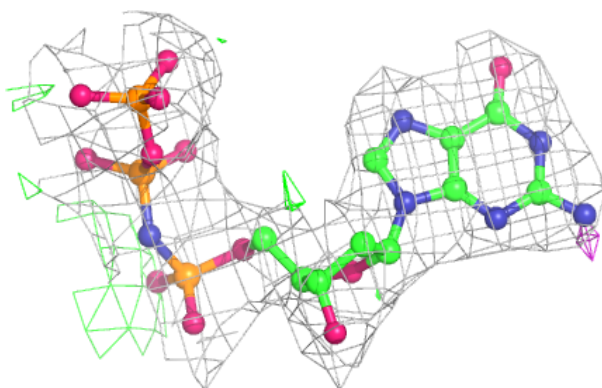


**Electron density around XG4 L 705:**

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

**Electron density around XG4 C 706:**

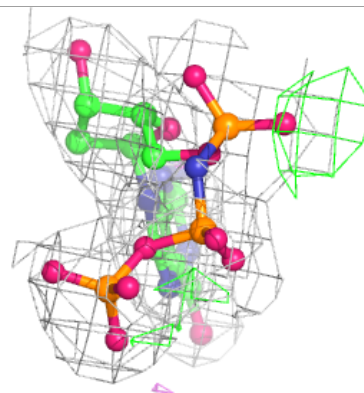
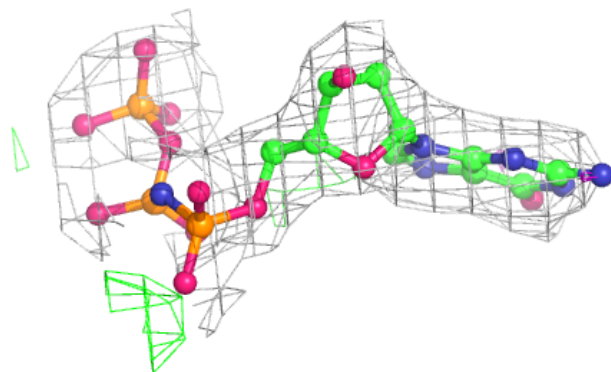
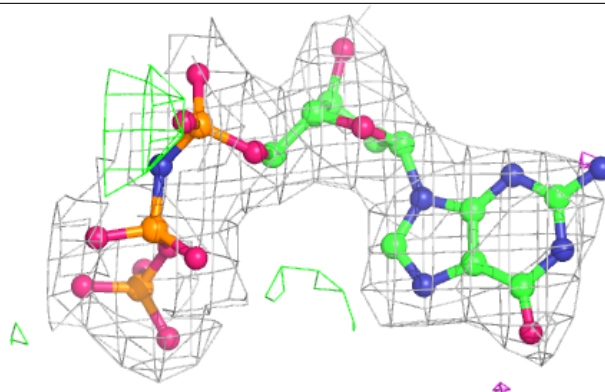
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



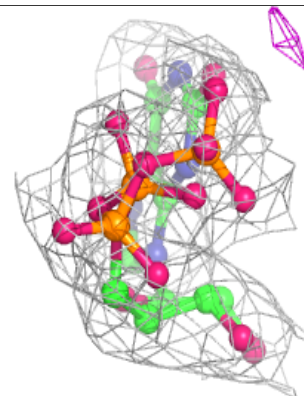
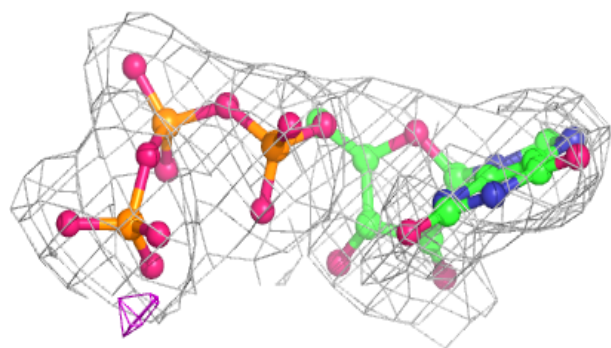
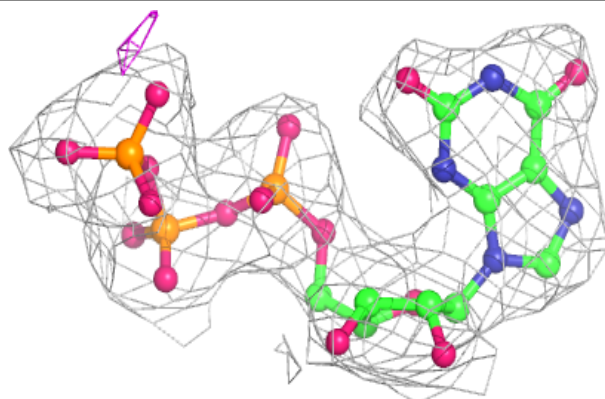


**Electron density around XG4 O 706:**

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

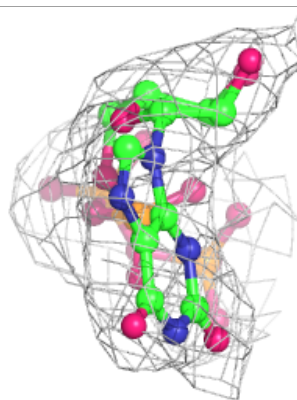
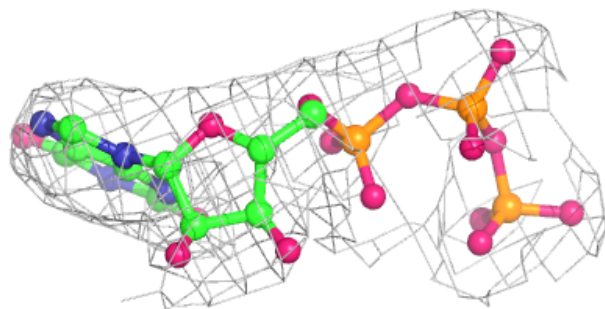
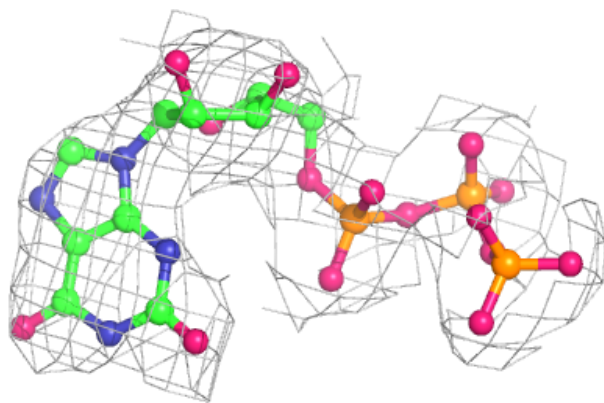
**Electron density around CZF J 701:**

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

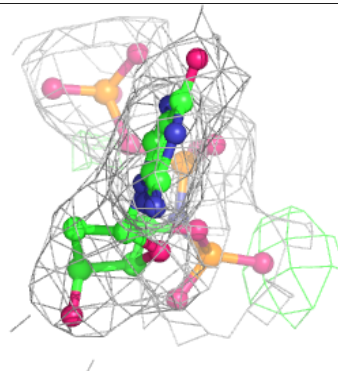
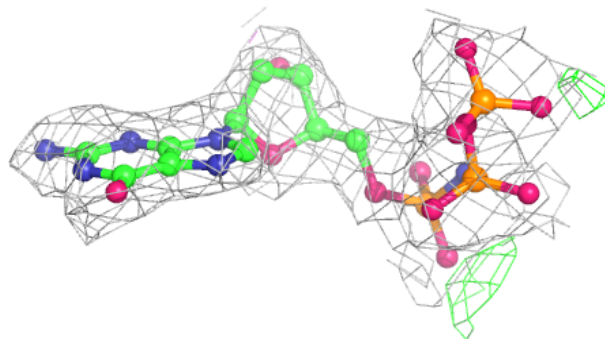
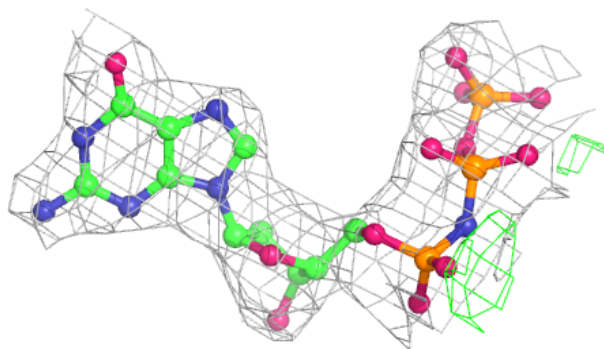


**Electron density around CZF K 707:**

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

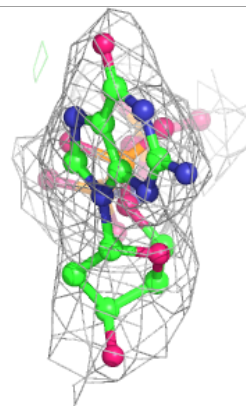
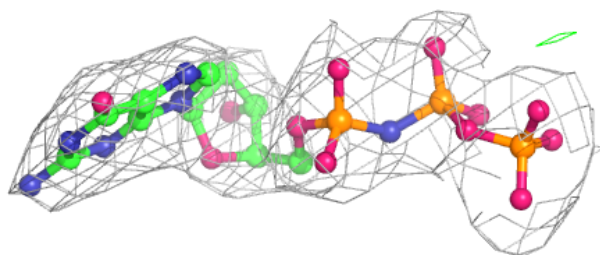
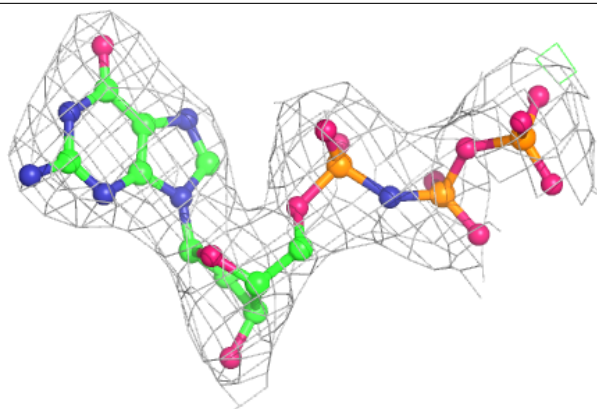
**Electron density around XG4 I 705:**

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

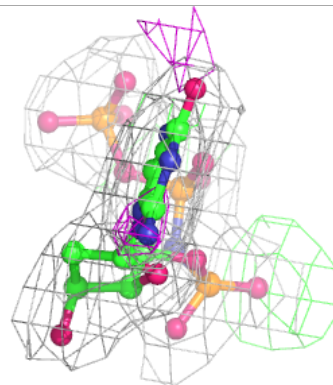
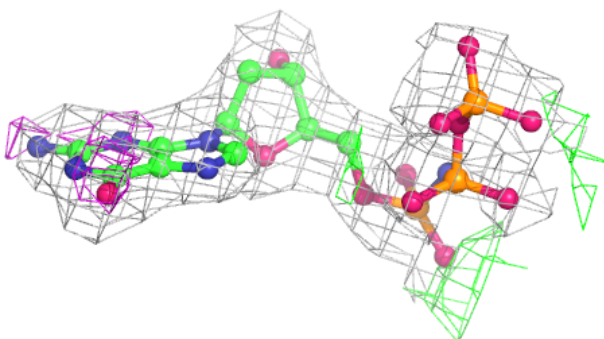
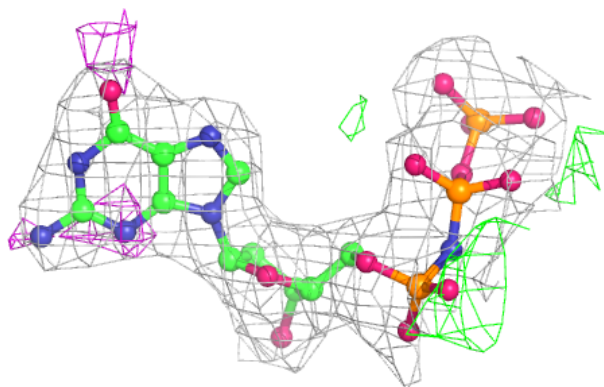


**Electron density around XG4 I 708:**

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

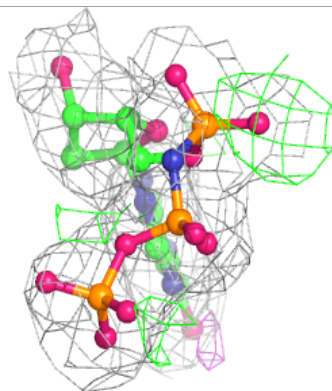
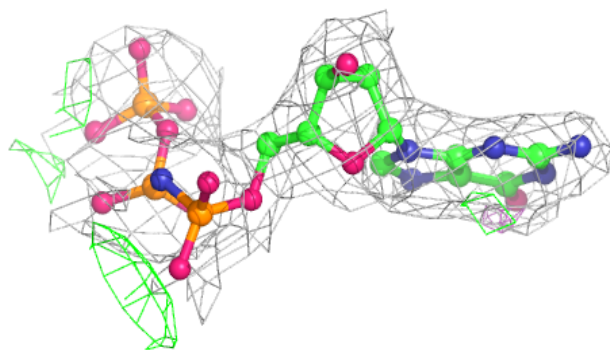
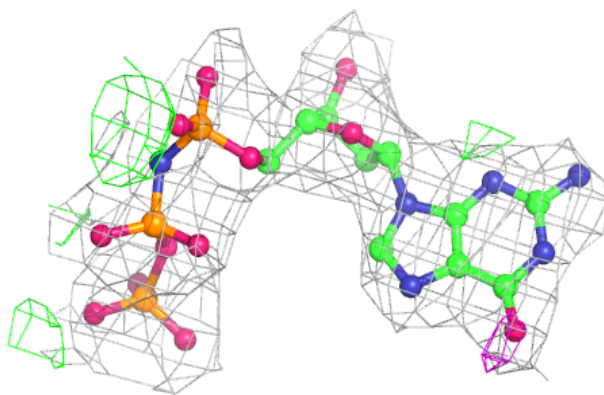
**Electron density around XG4 A 705:**

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

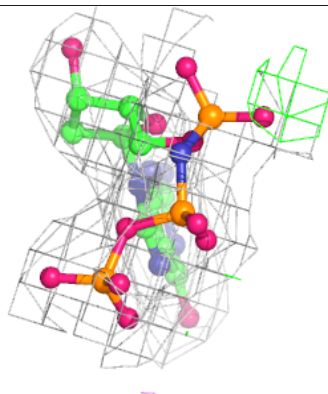
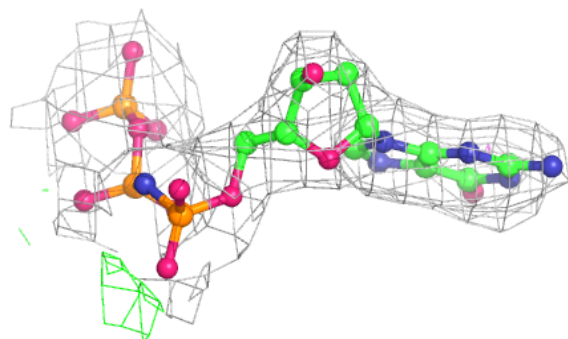
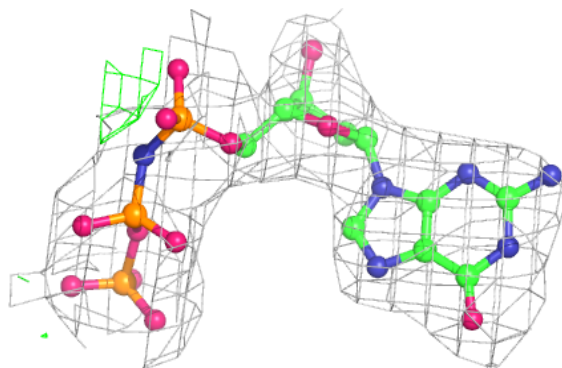


**Electron density around XG4 F 705:**

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

**Electron density around XG4 K 706:**

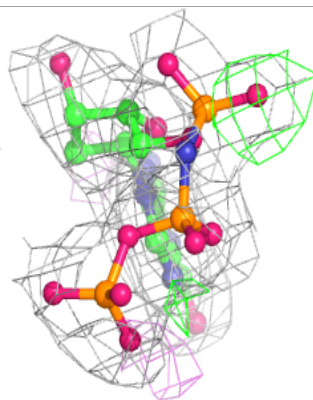
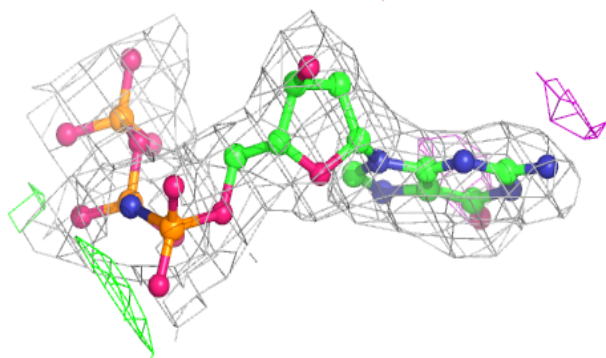
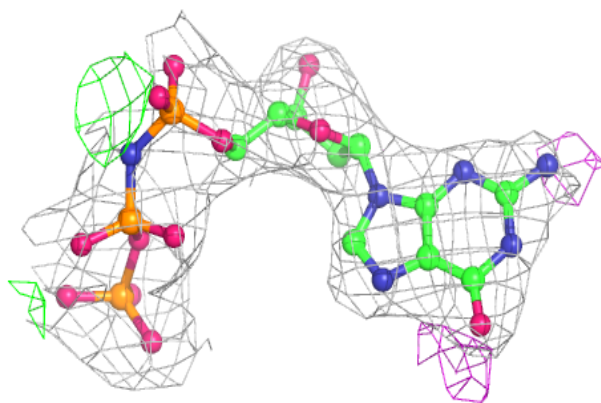
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



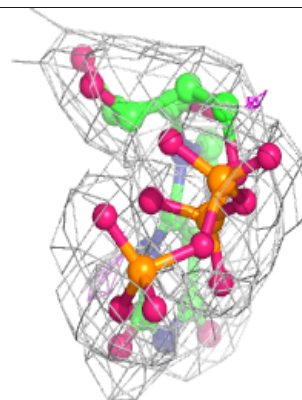
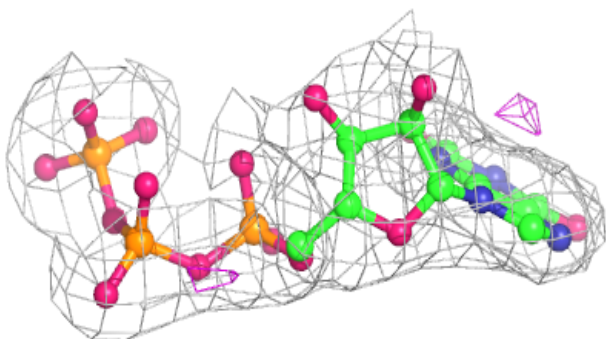
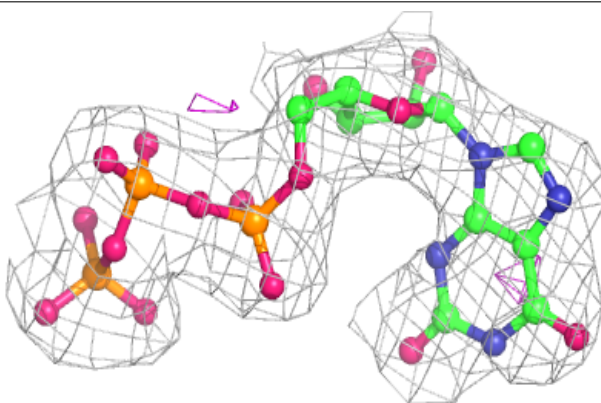


**Electron density around XG4 G 706:**

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

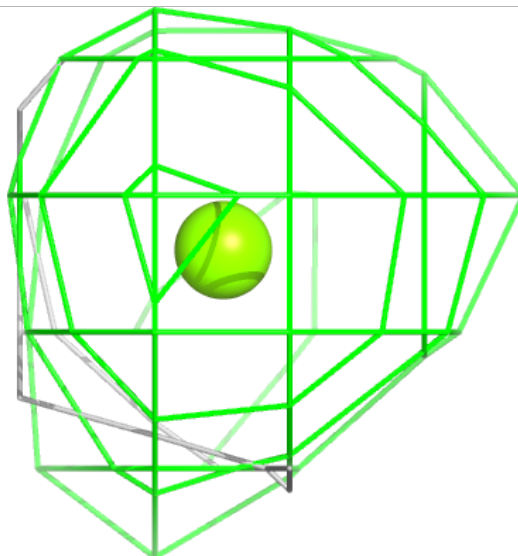
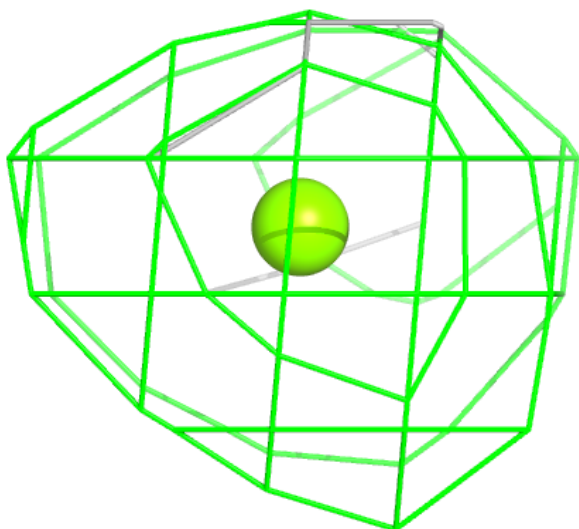
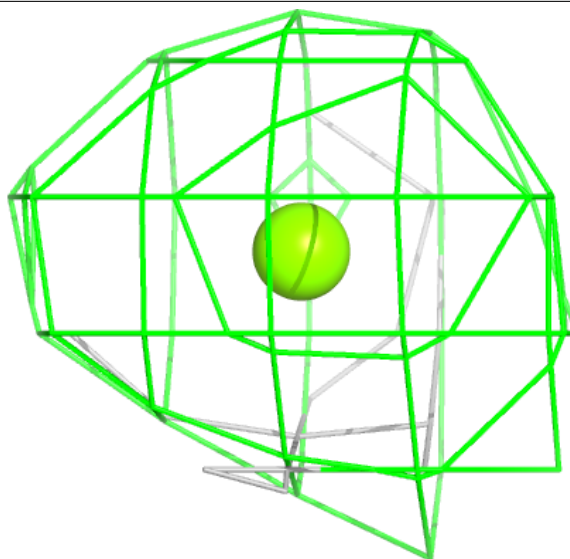
**Electron density around CZF P 707:**

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



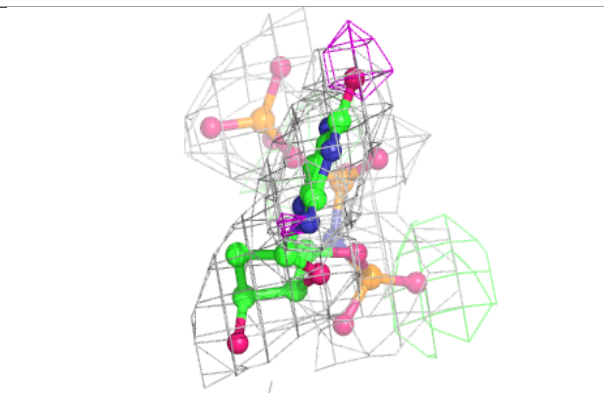
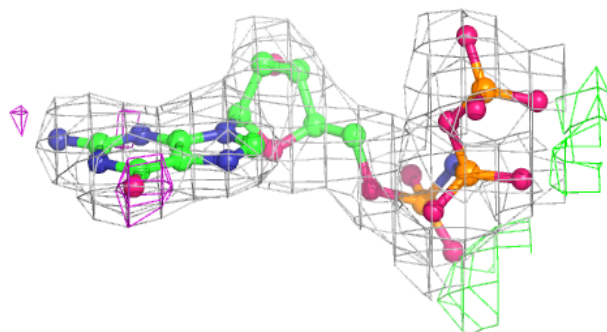
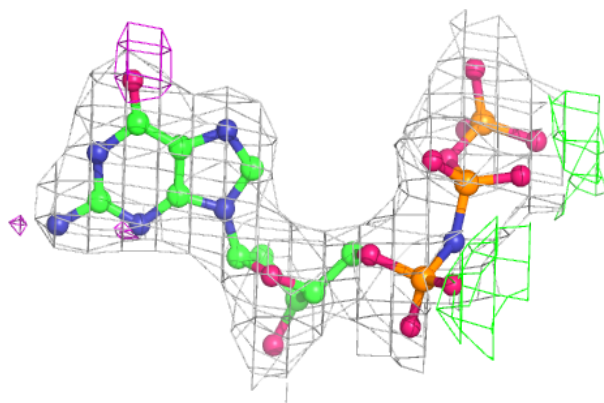
**Electron density around MG H 703:**

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

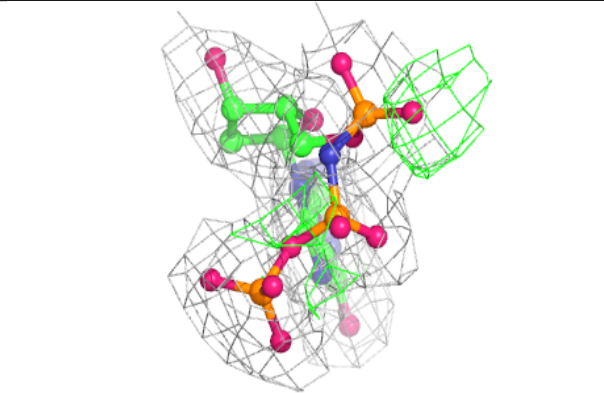
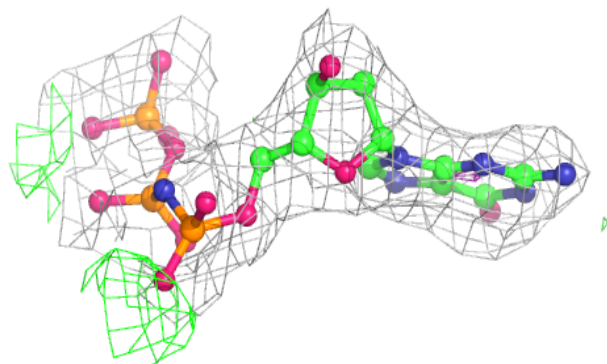
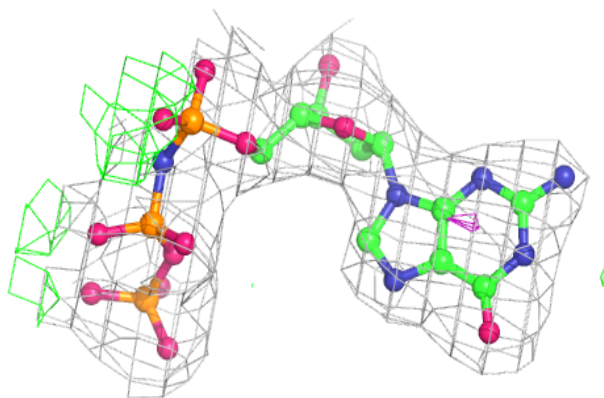


**Electron density around XG4 H 706:**

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

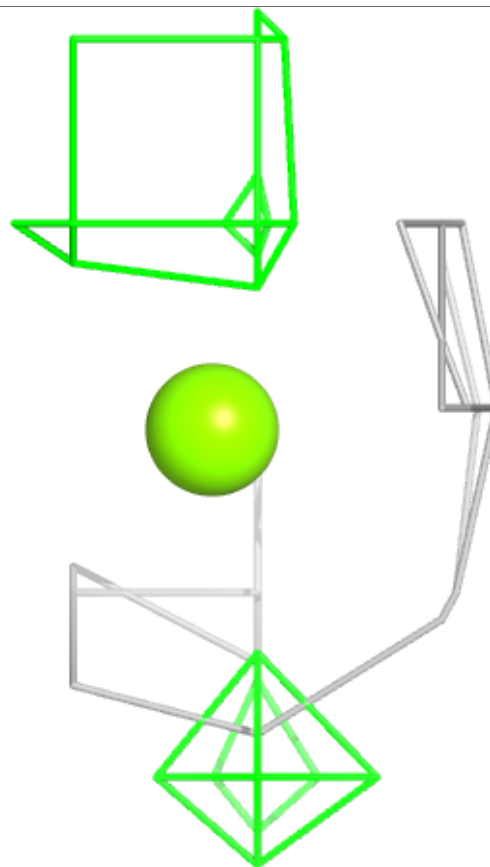
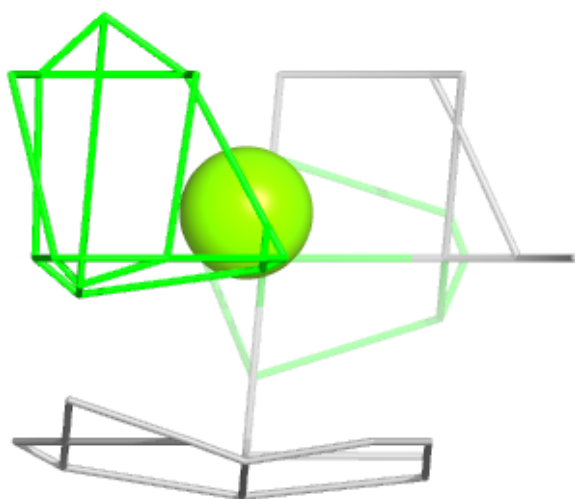
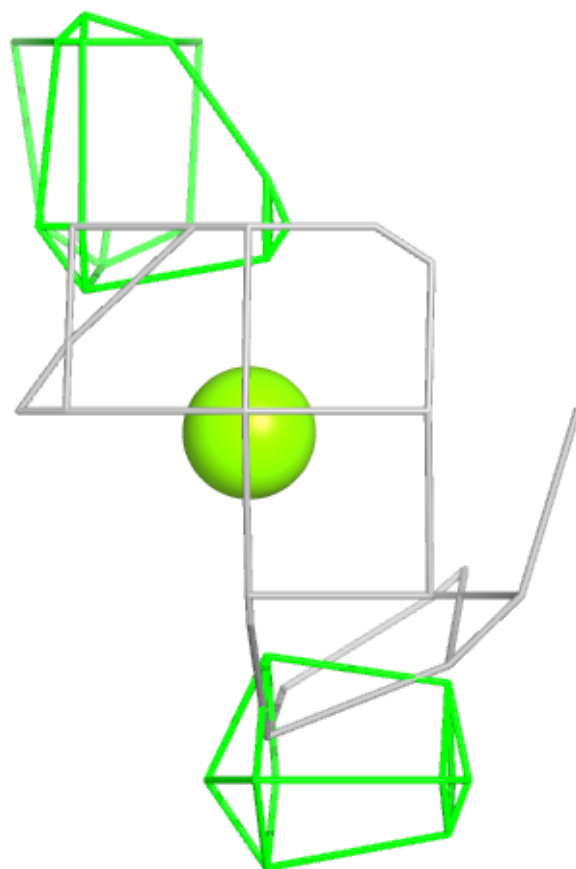
**Electron density around XG4 J 706:**

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



**Electron density around MG C 704:**

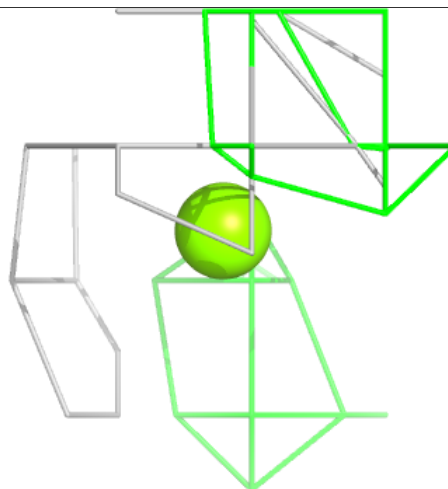
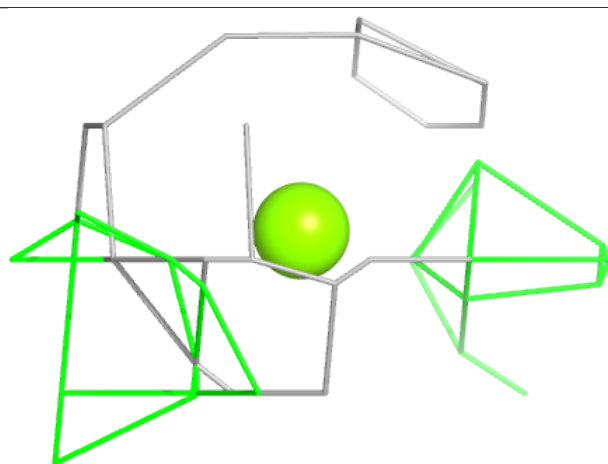
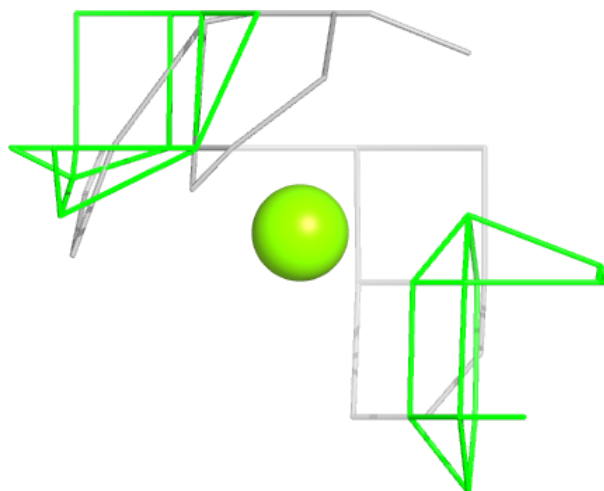
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





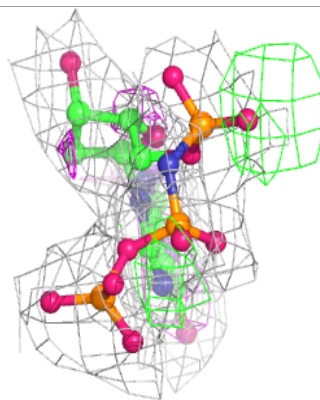
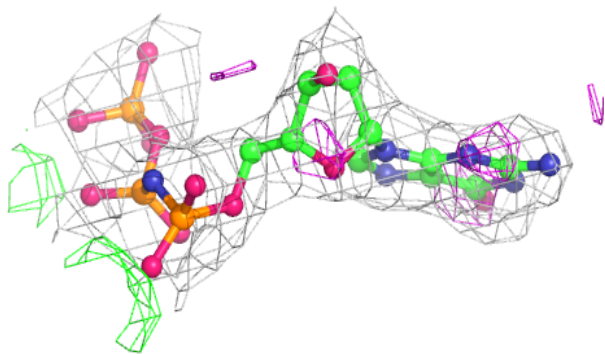
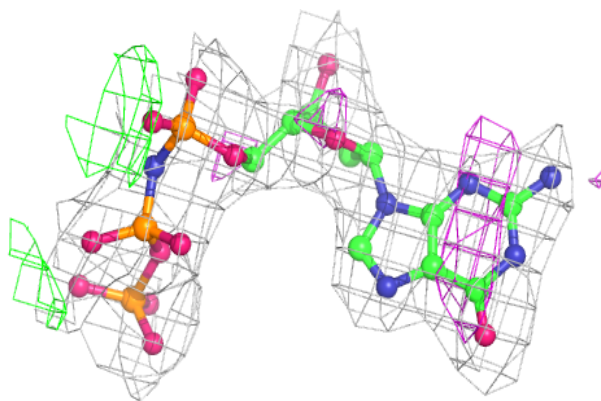
**Electron density around MG F 703:**

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



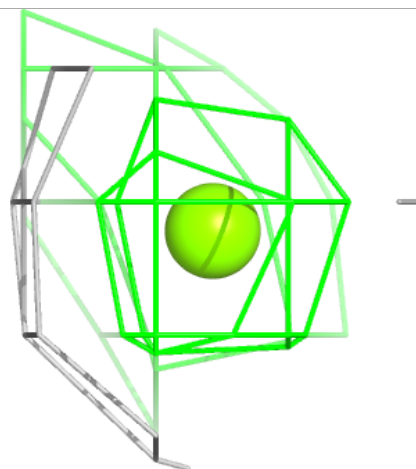
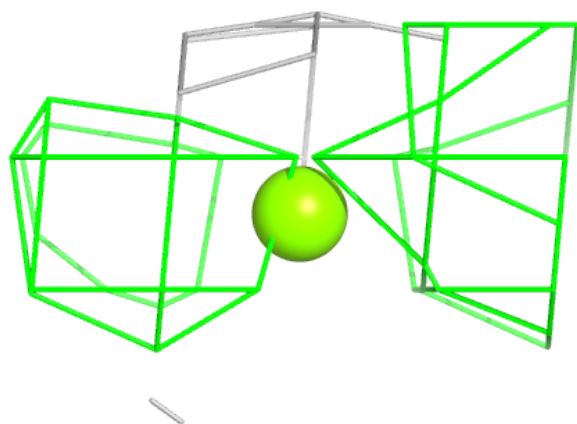
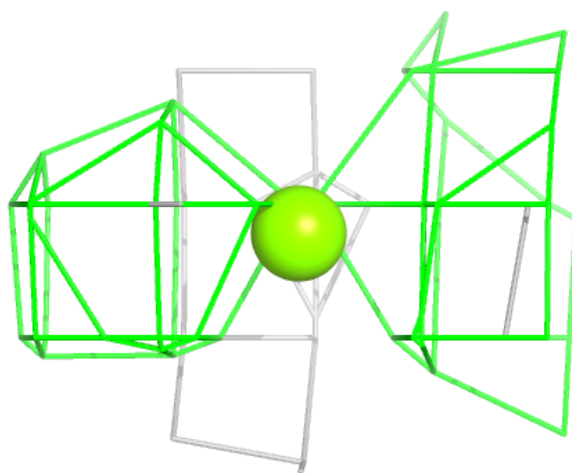
**Electron density around XG4 D 706:**

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



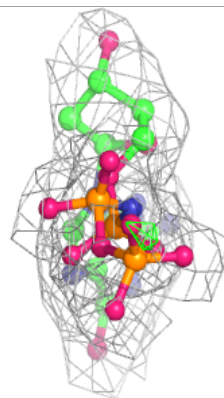
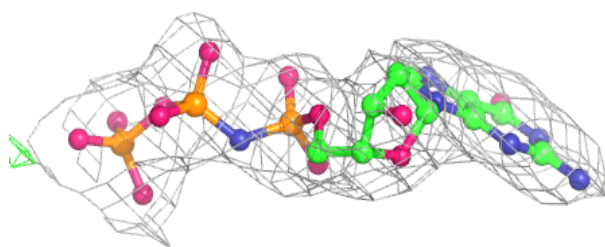
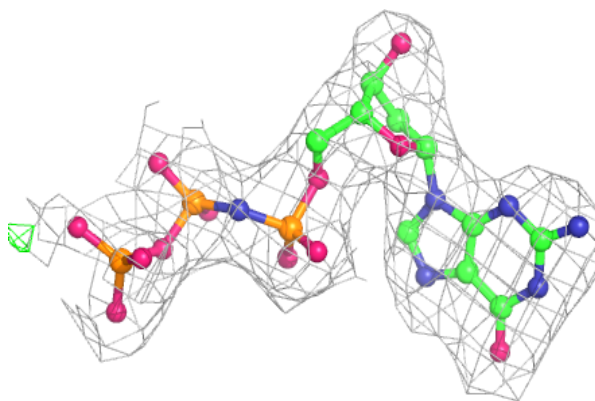
**Electron density around MG J 704:**

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

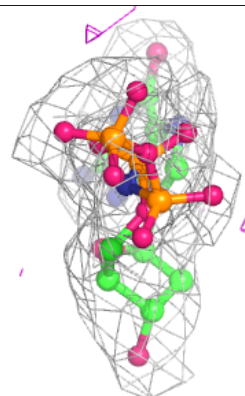
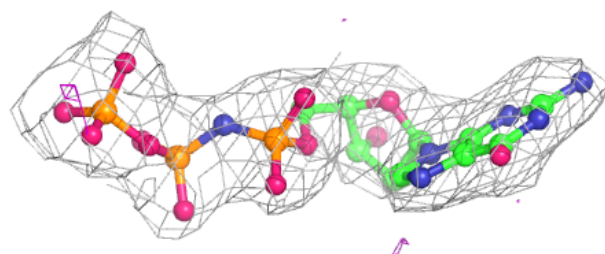
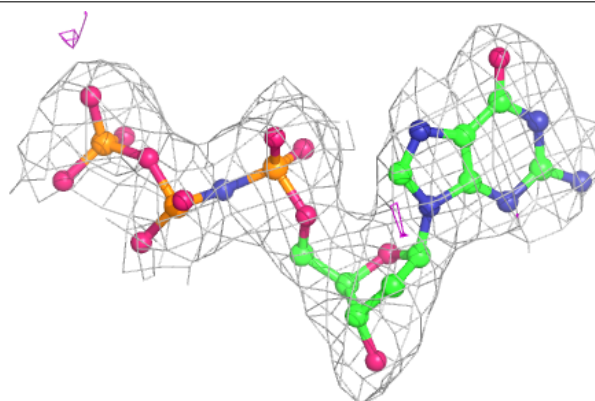


**Electron density around XG4 D 701:**

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

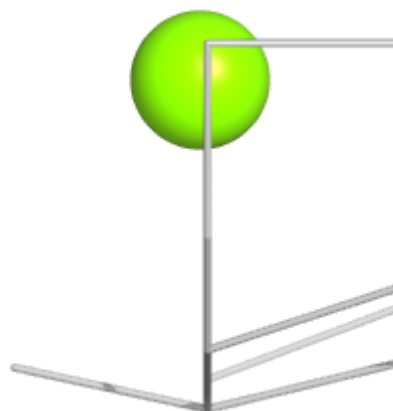
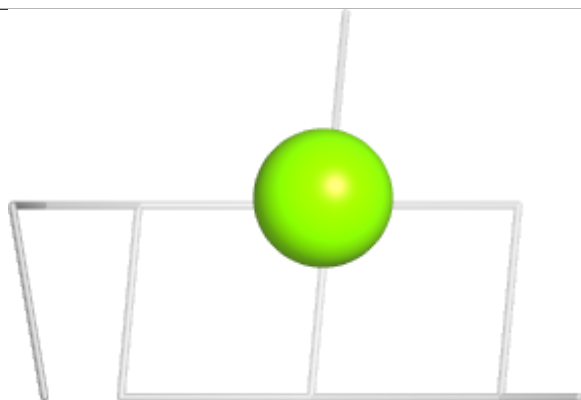
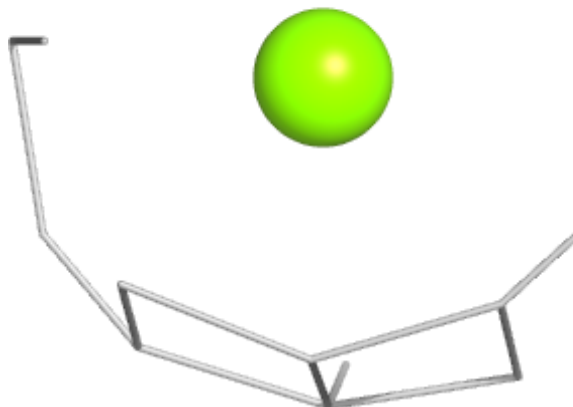
**Electron density around XG4 B 708:**

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



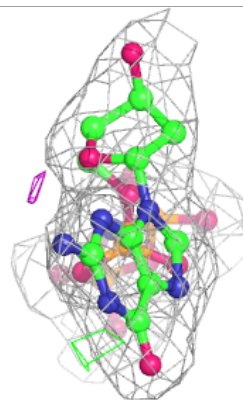
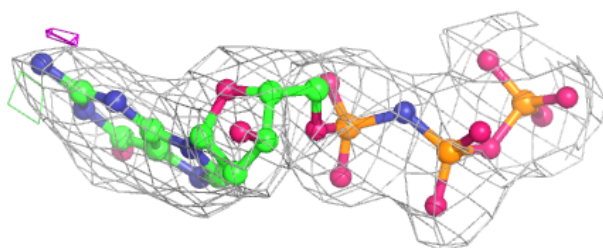
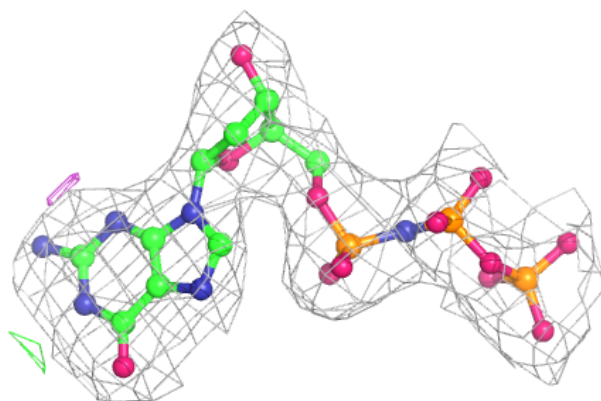
**Electron density around MG A 704:**

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



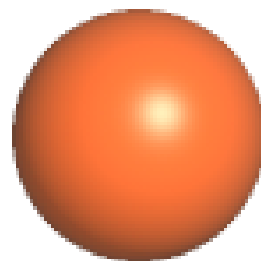
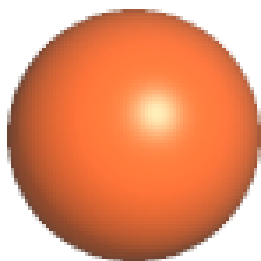
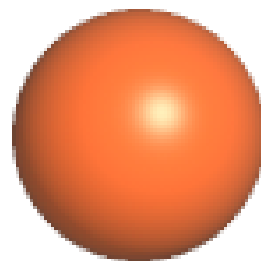
**Electron density around XG4 F 708:**

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



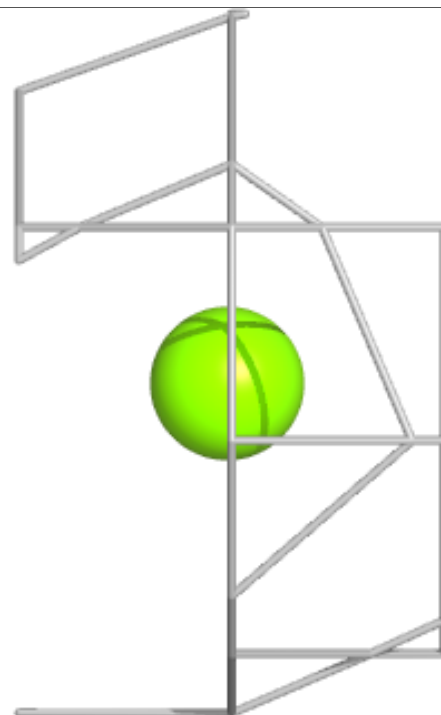
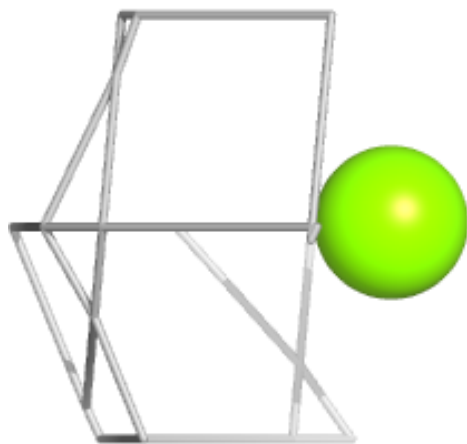
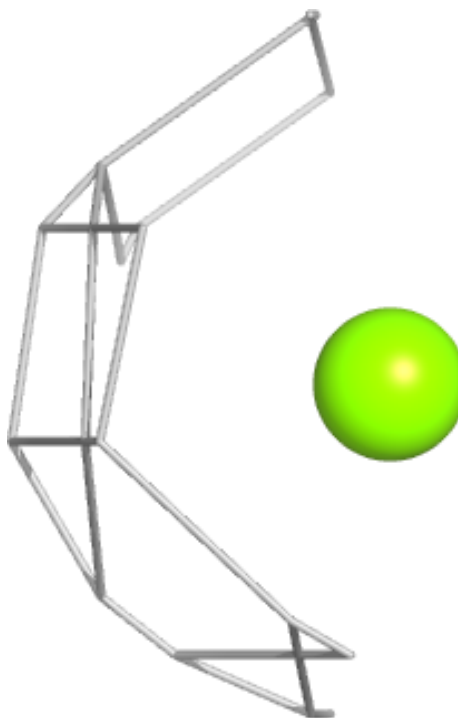
**Electron density around FE M 701:**

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



**Electron density around MG M 704:**

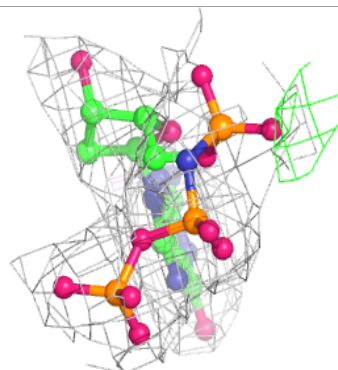
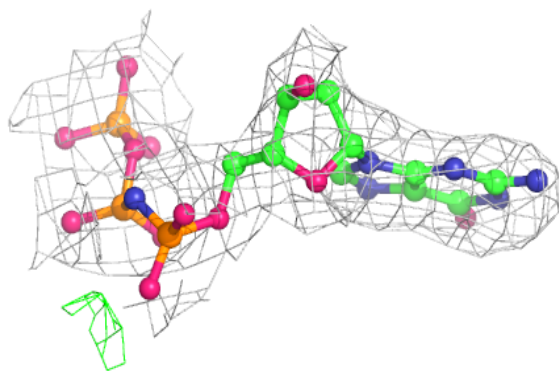
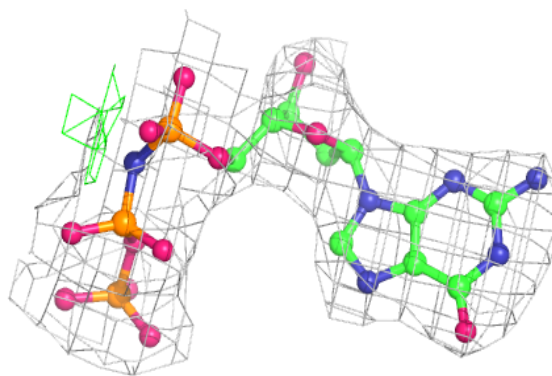
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



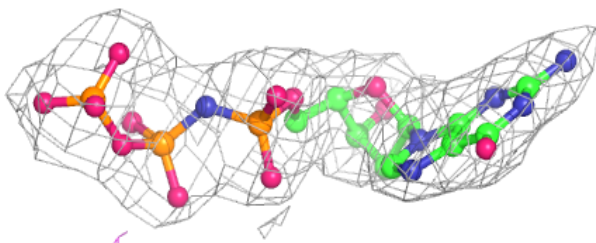
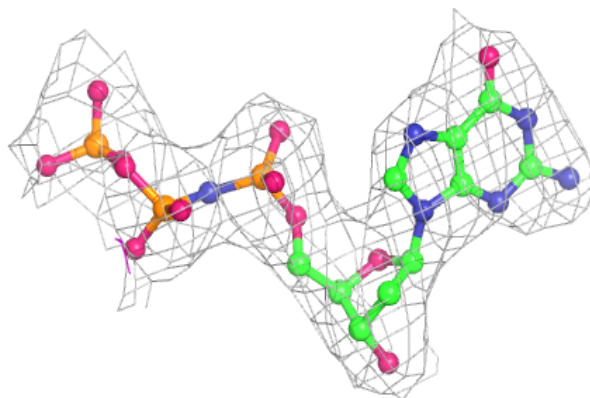


**Electron density around XG4 N 705:**

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

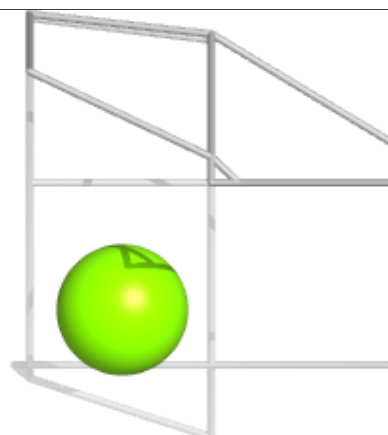
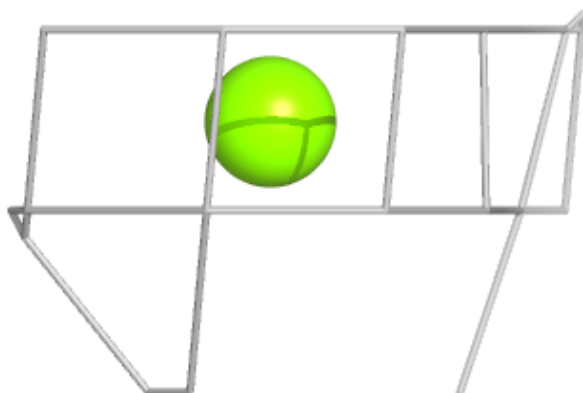
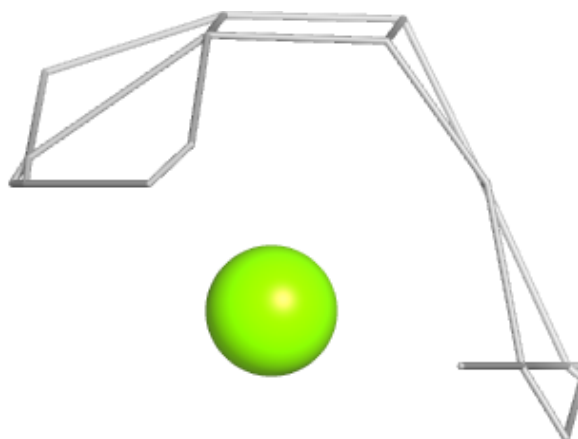
**Electron density around XG4 N 708:**

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



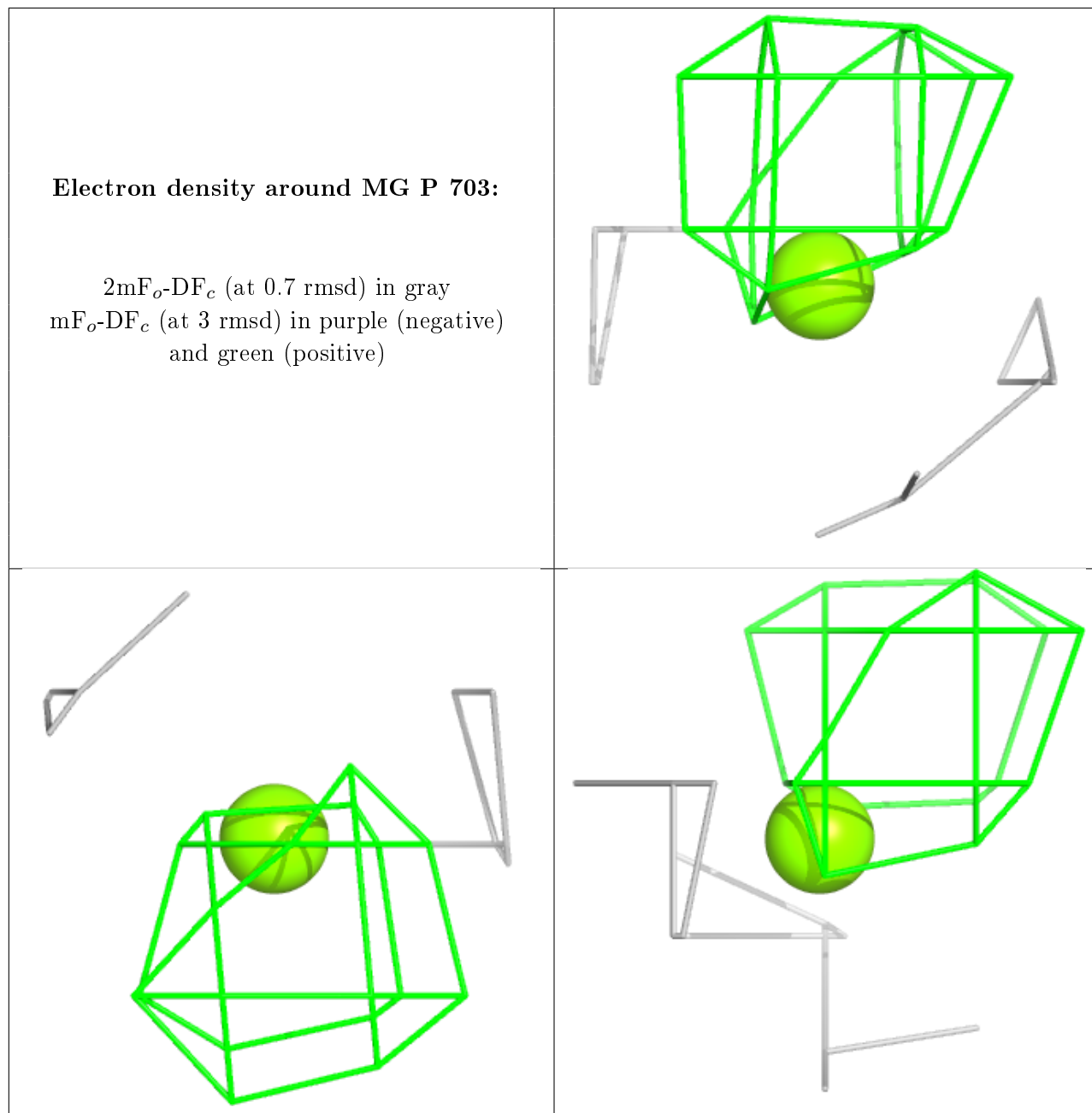
**Electron density around MG B 704:**

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



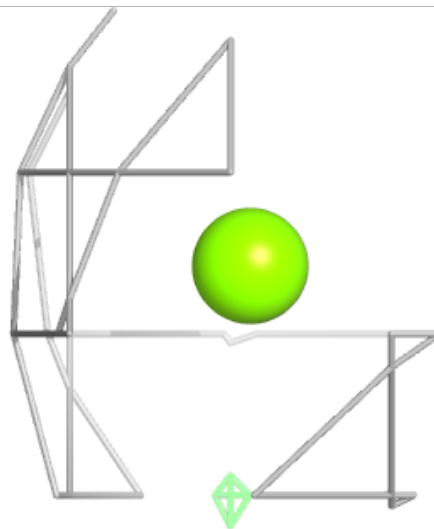
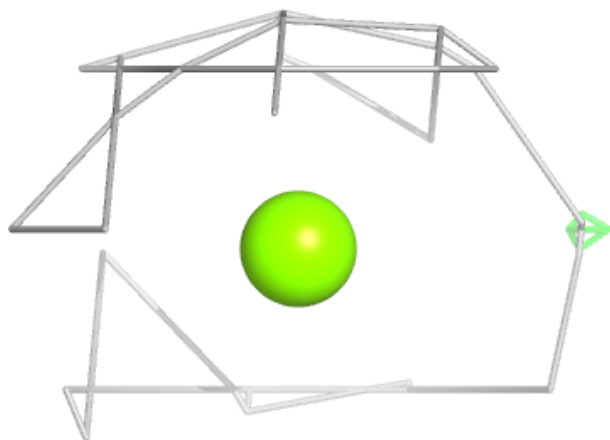
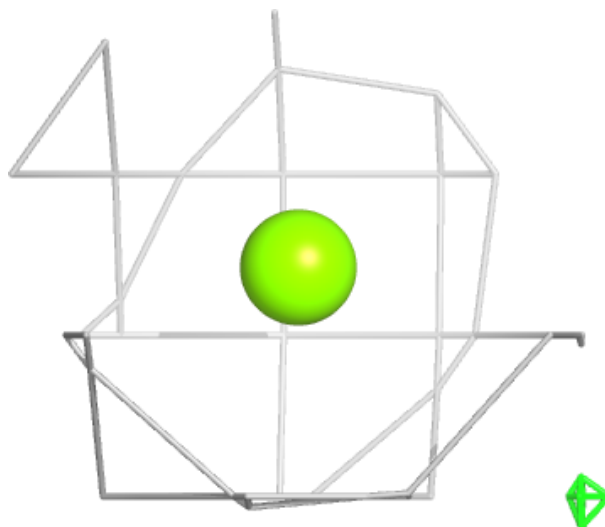
**Electron density around MG P 703:**

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



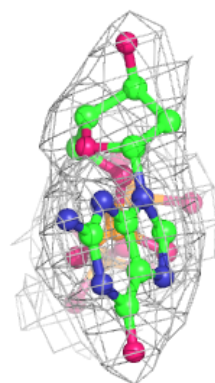
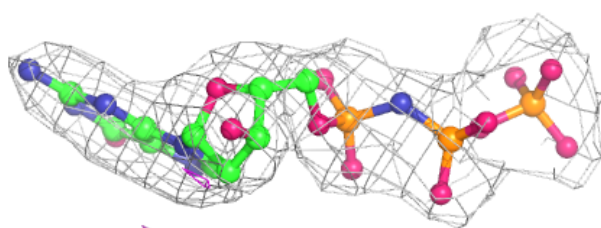
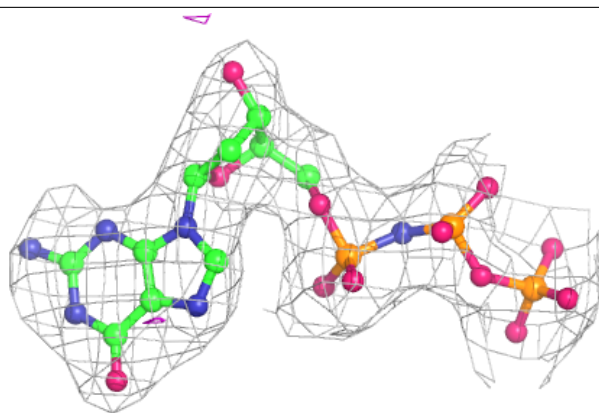
**Electron density around MG M 703:**

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

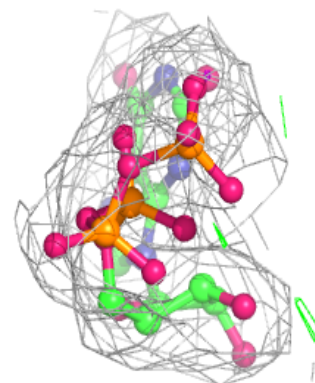
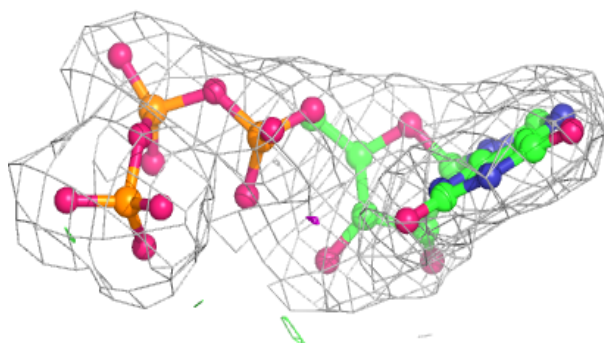
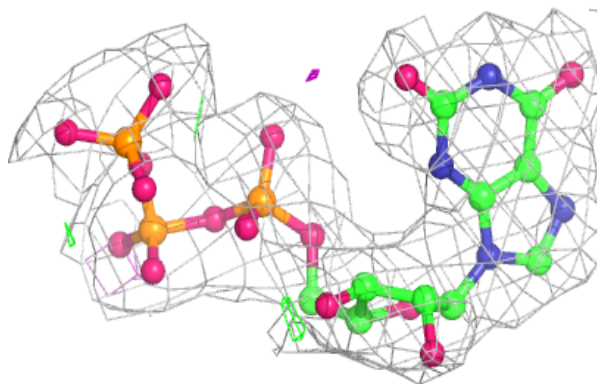


**Electron density around XG4 I 707:**

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

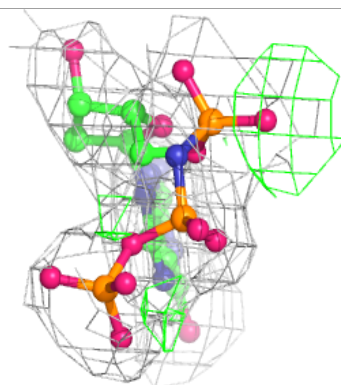
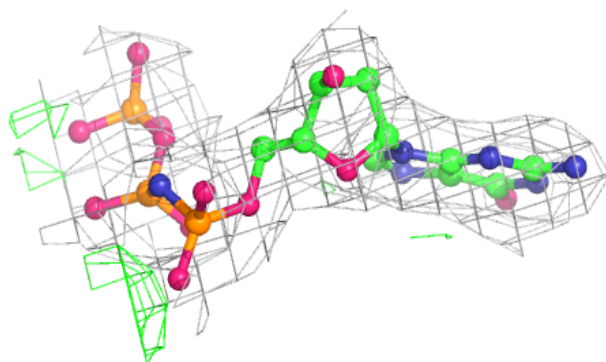
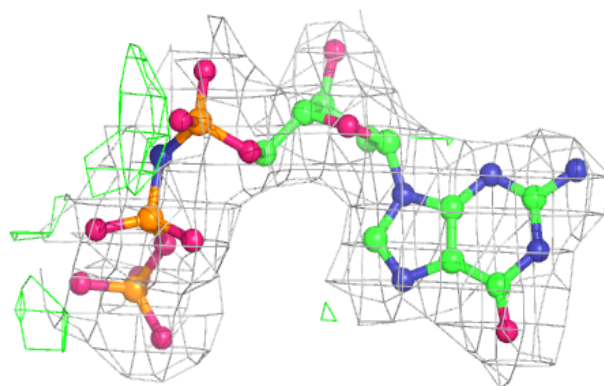
**Electron density around CZF E 706:**

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

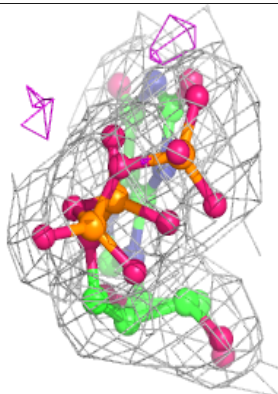
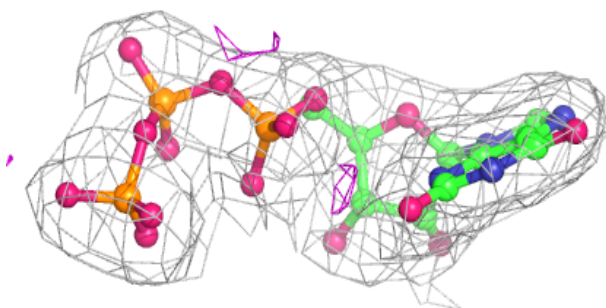
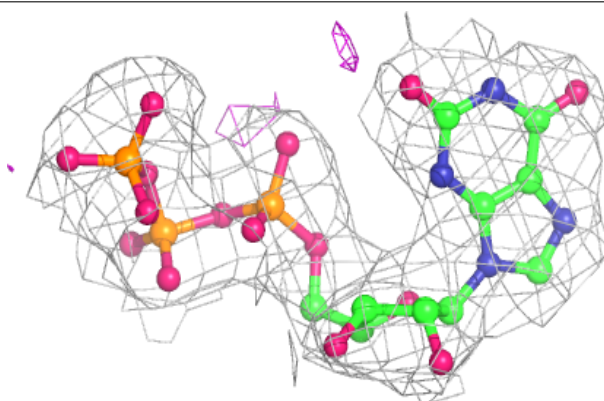


**Electron density around XG4 B 705:**

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

**Electron density around CZF A 706:**

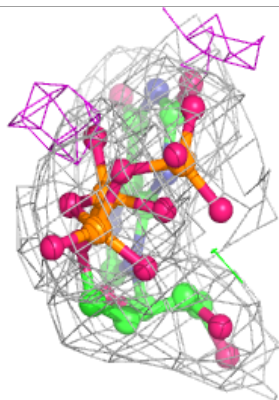
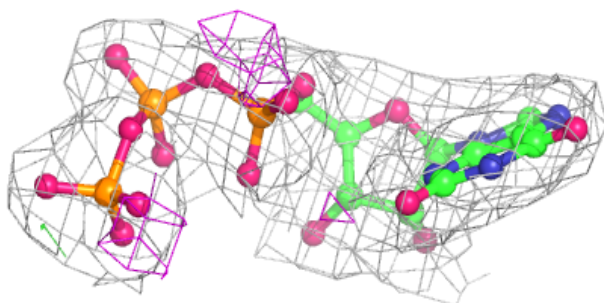
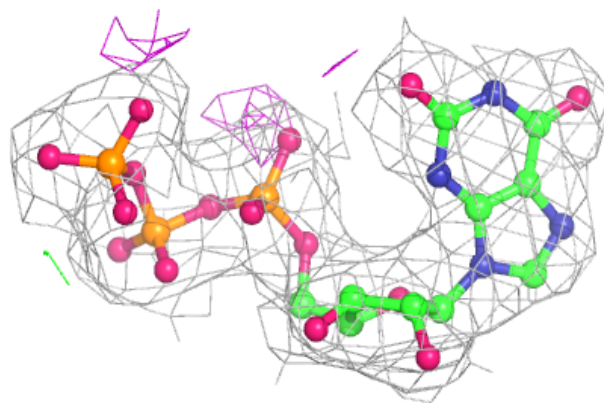
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



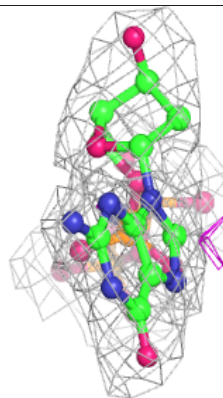
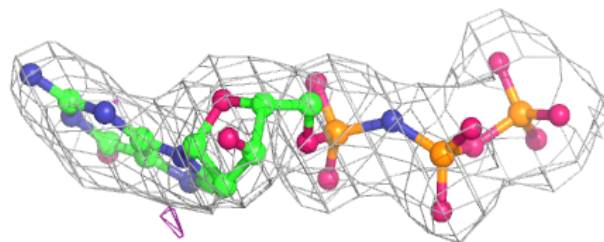
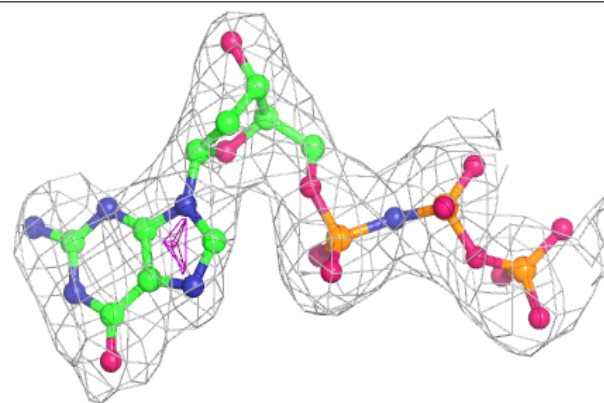


**Electron density around CZF B 706:**

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

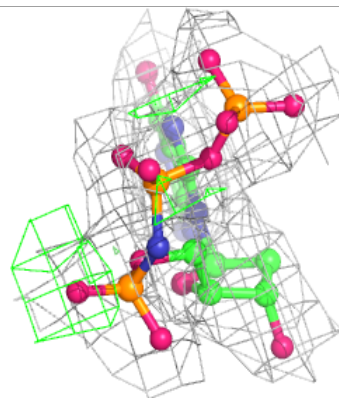
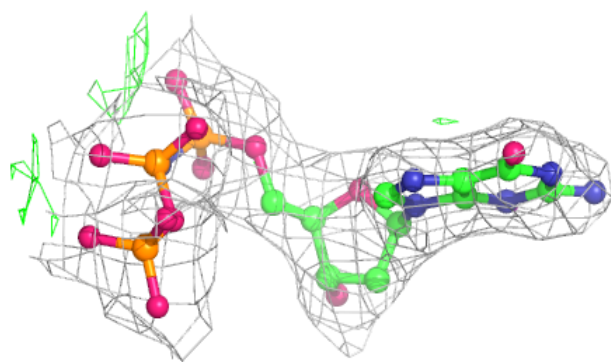
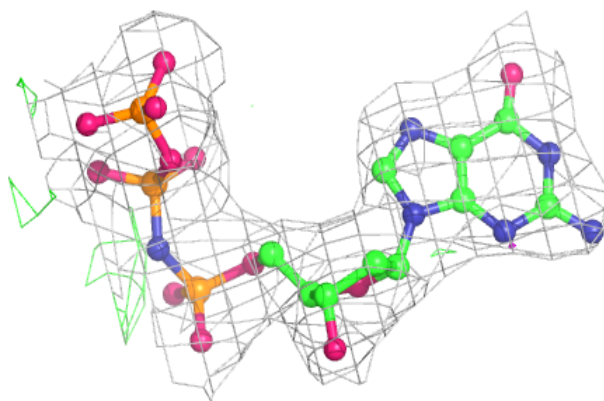
**Electron density around XG4 O 701:**

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



**Electron density around XG4 E 705:**

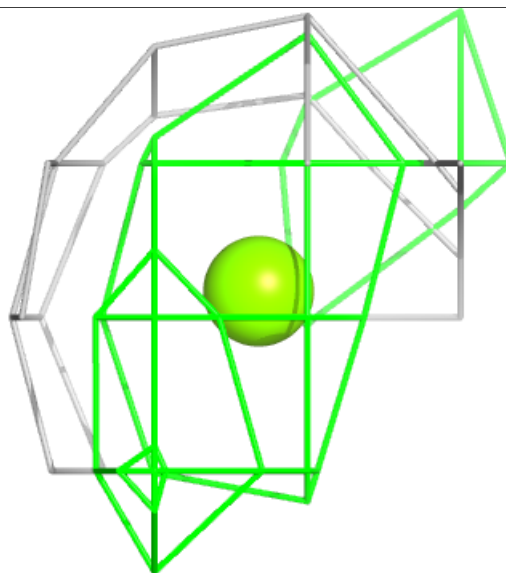
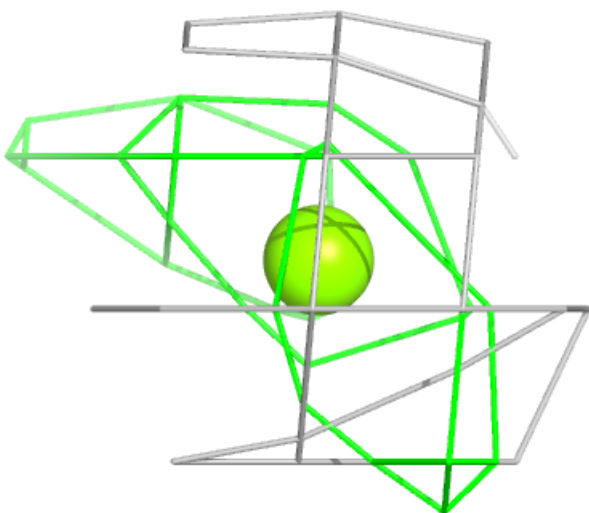
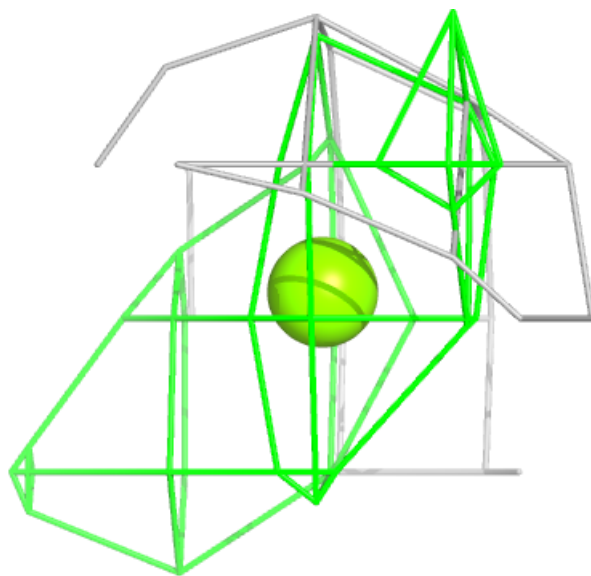
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





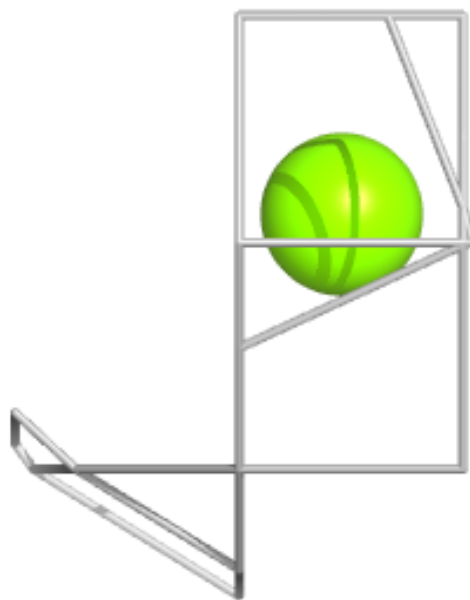
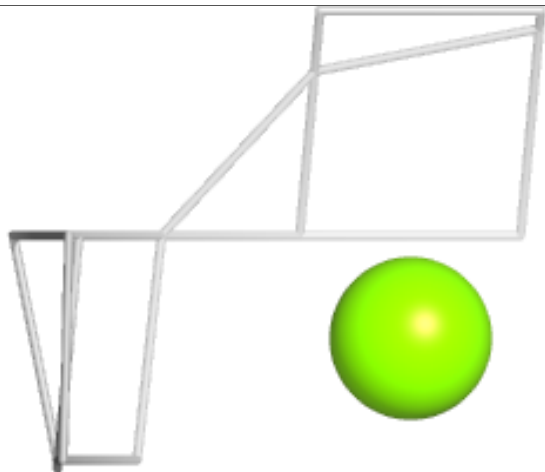
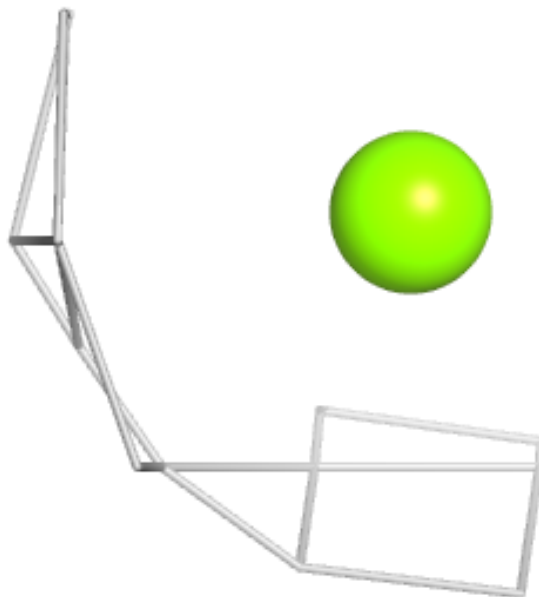
**Electron density around MG A 703:**

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



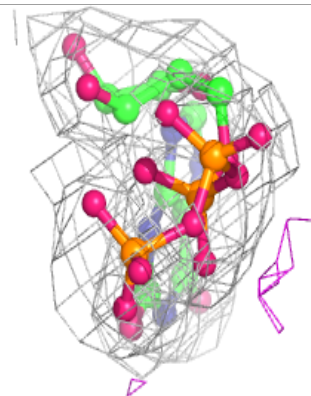
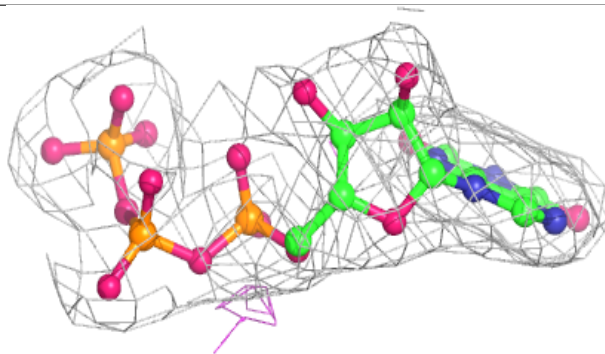
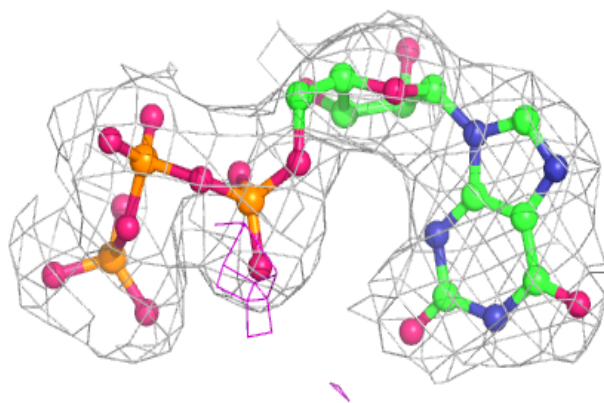
**Electron density around MG J 705:**

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



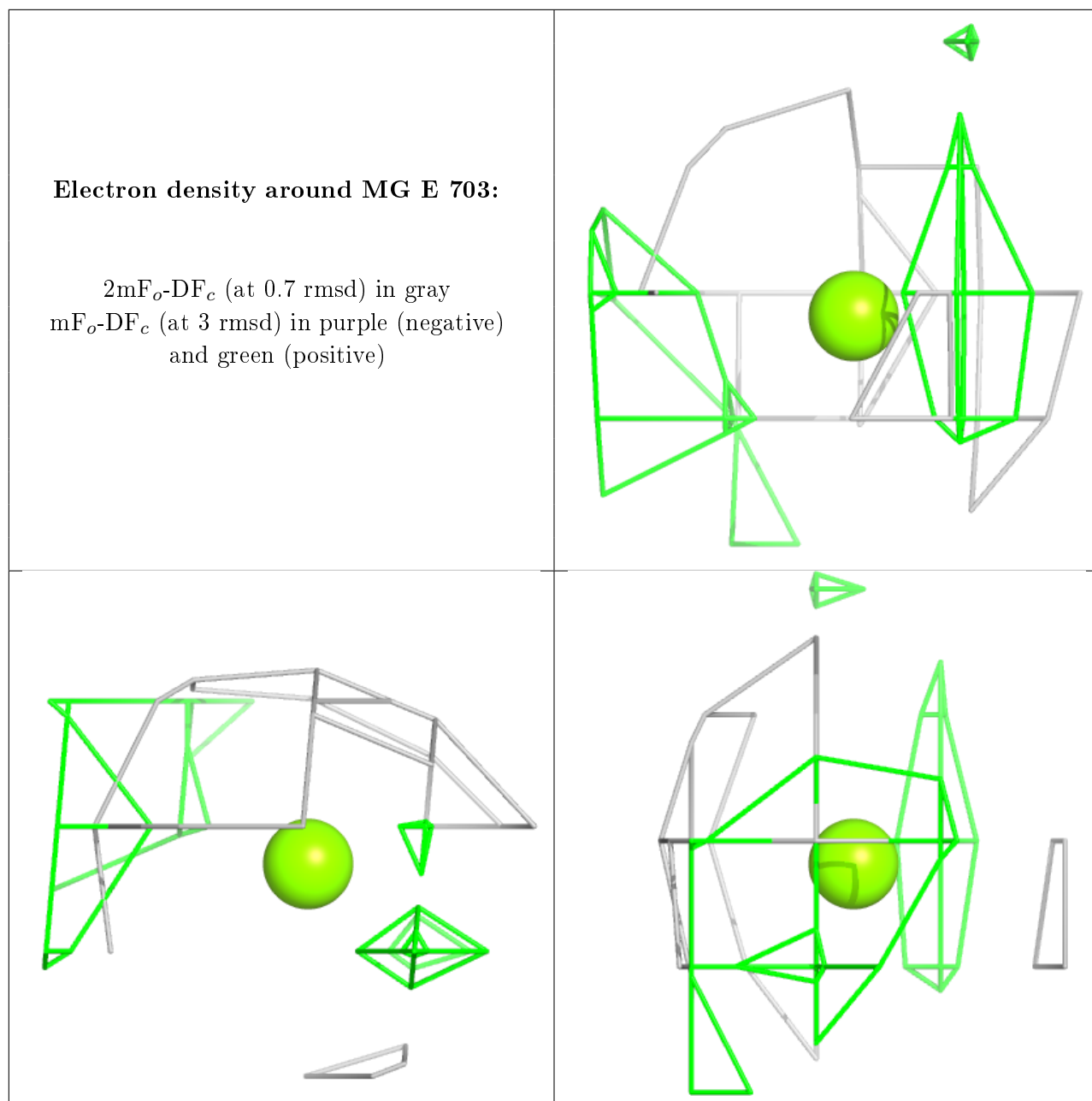
**Electron density around CZF C 709:**

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



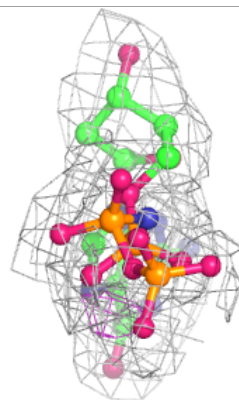
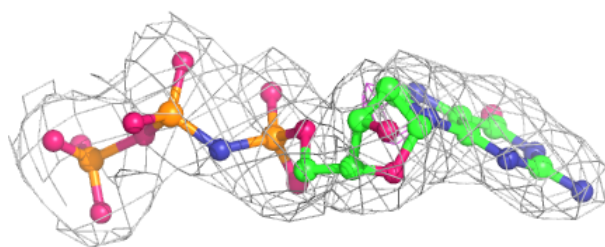
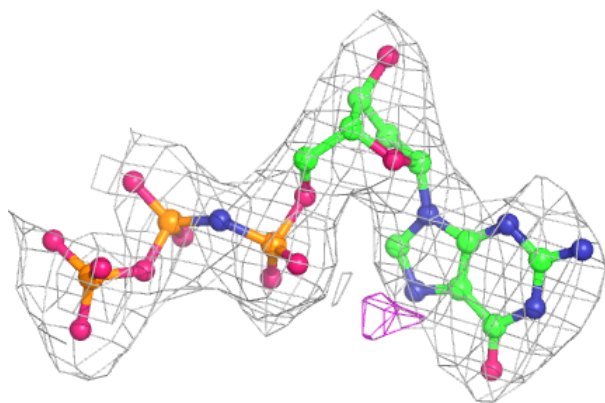
**Electron density around MG E 703:**

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

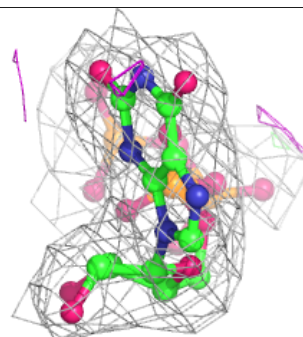
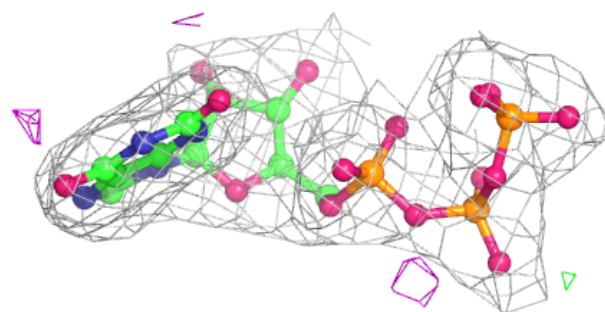
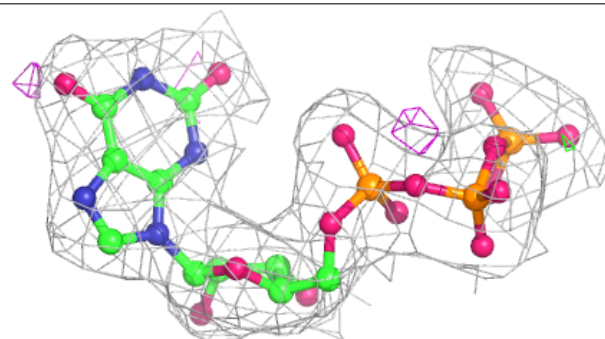


**Electron density around XG4 E 708:**

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

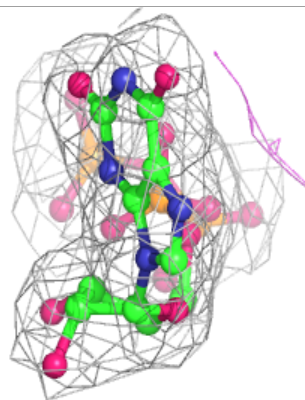
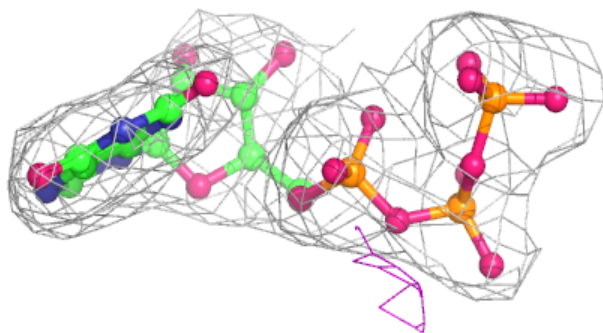
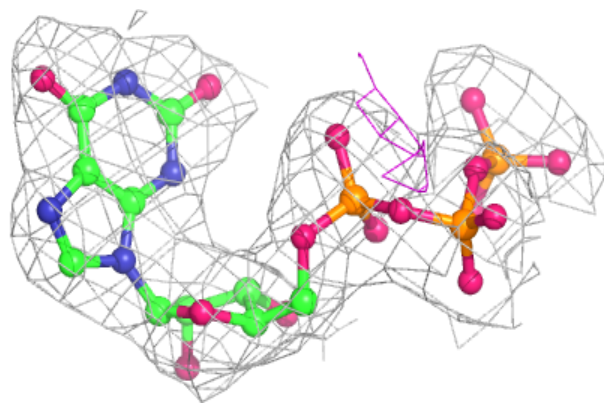
**Electron density around CZF C 707:**

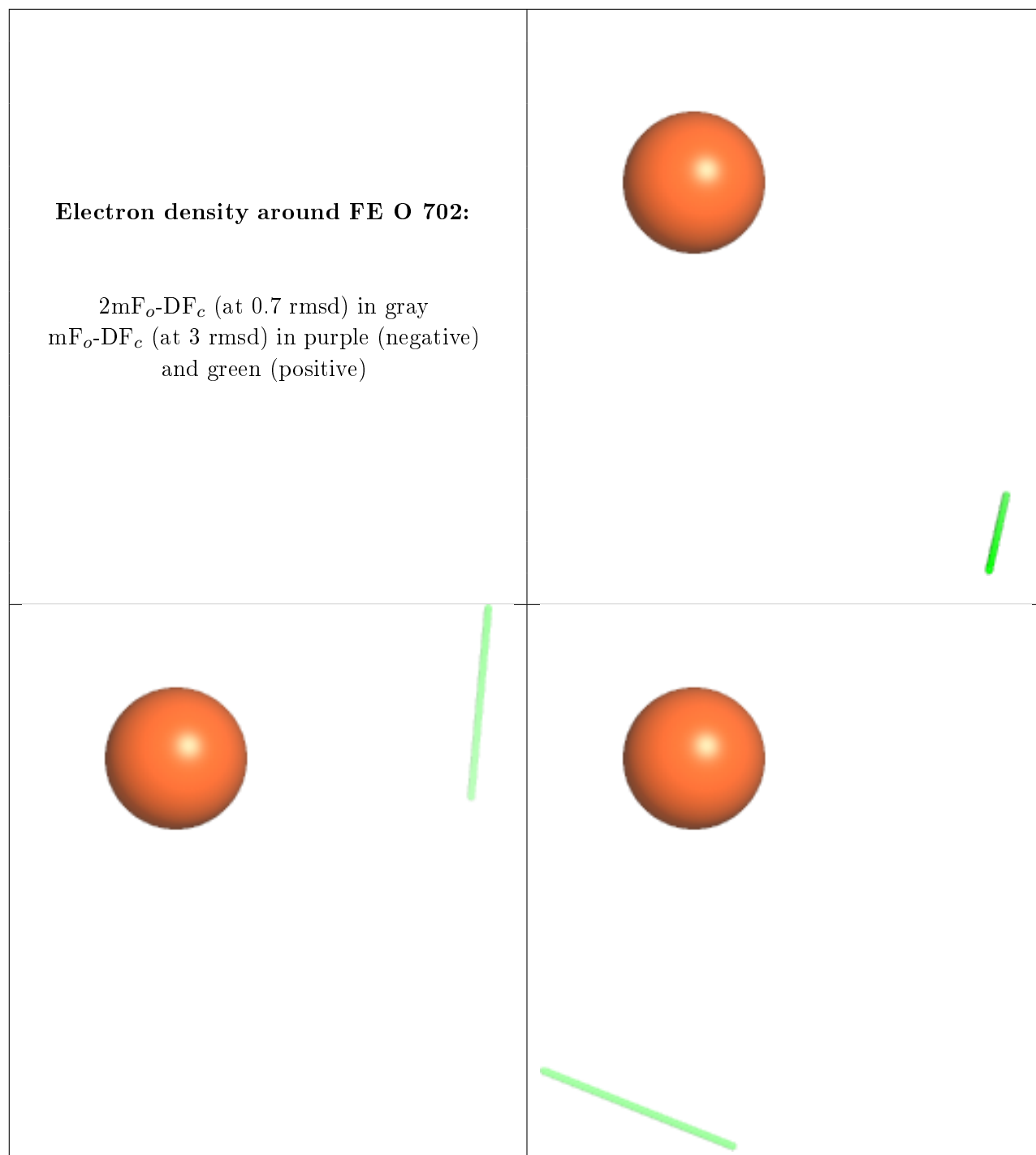
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CZF J 707:**

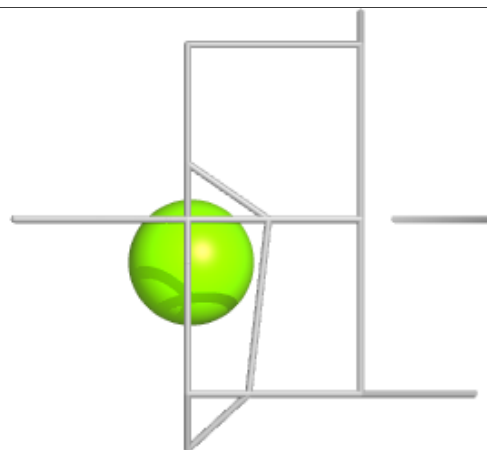
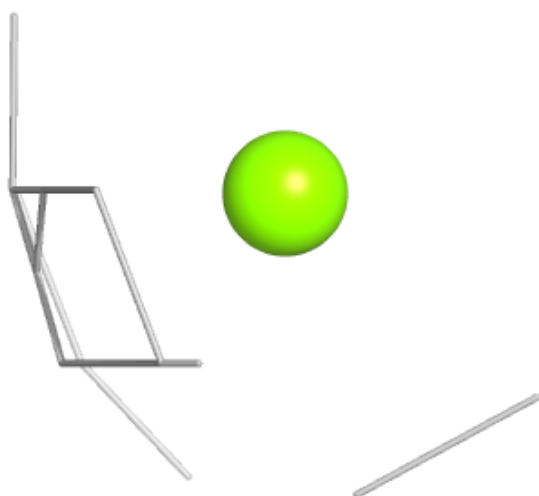
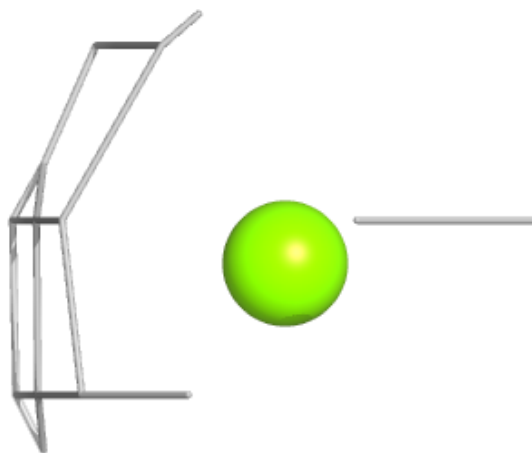
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around MG O 705:**

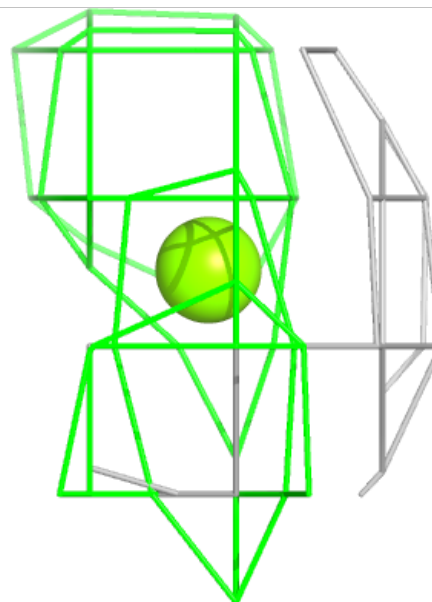
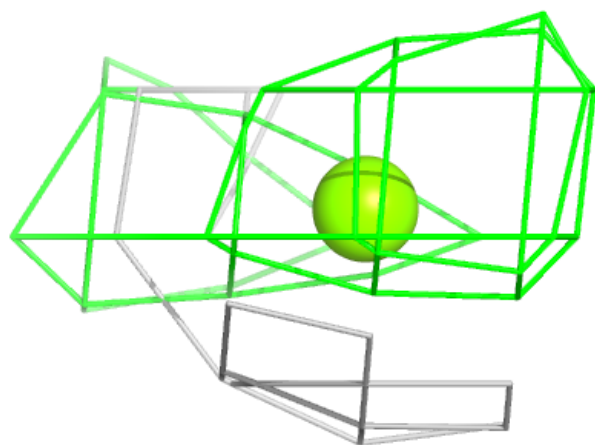
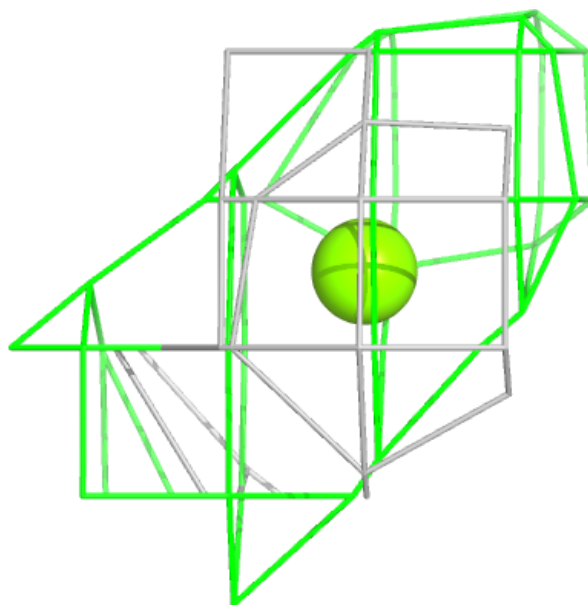
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





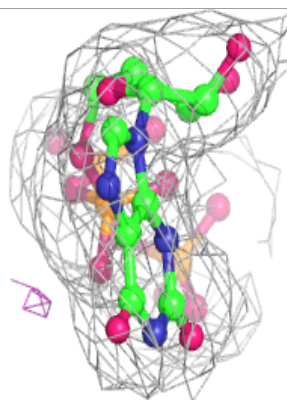
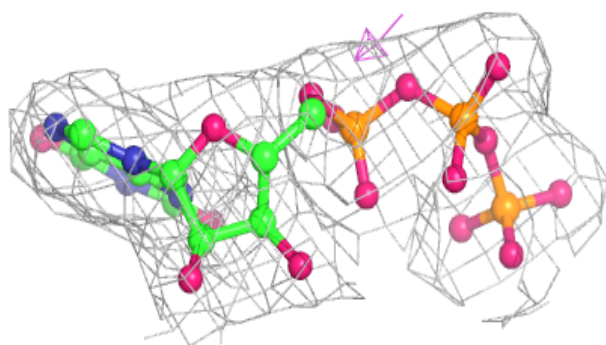
**Electron density around MG H 704:**

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

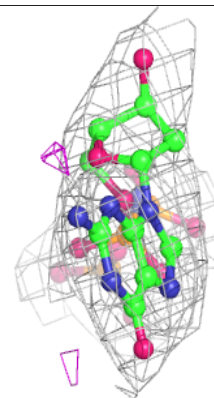
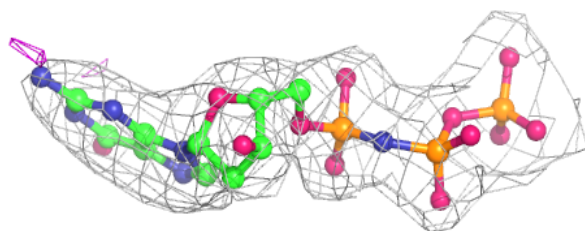
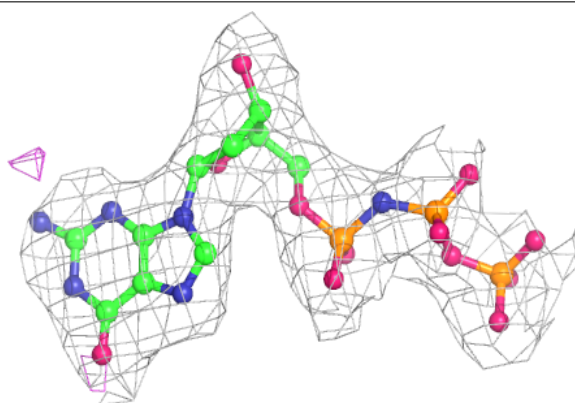


**Electron density around CZF F 706:**

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

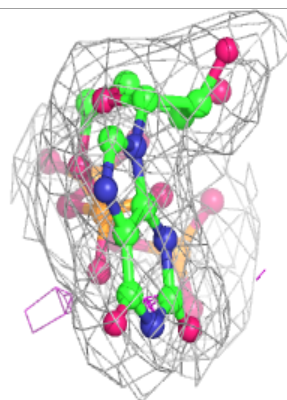
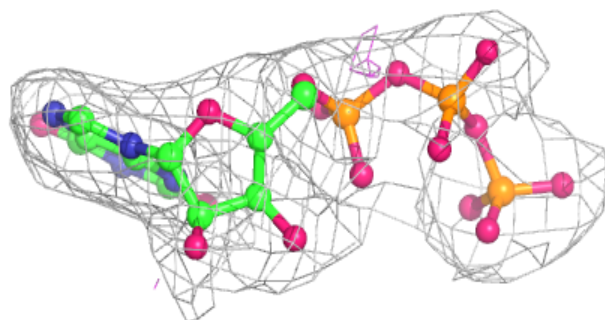
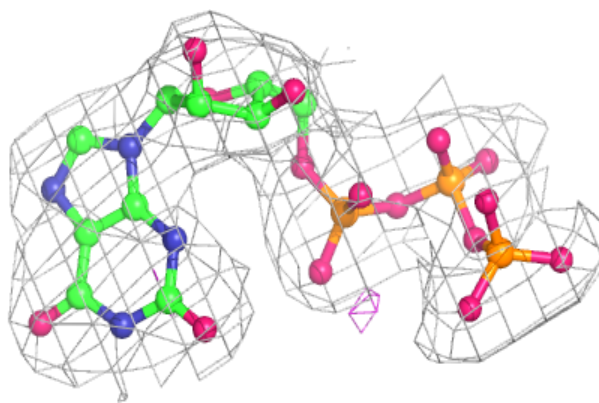
**Electron density around XG4 G 701:**

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



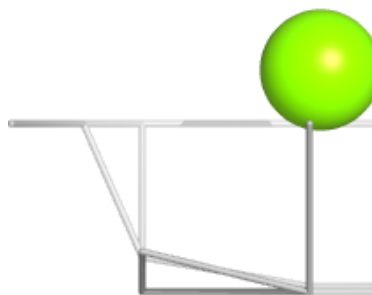
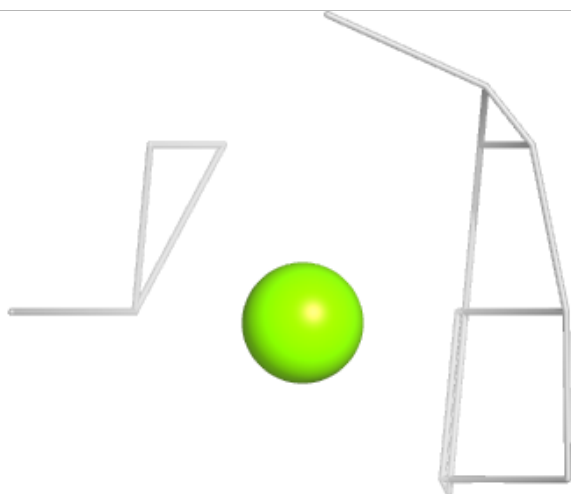
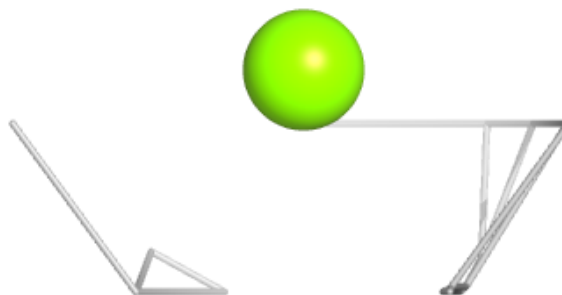
**Electron density around CZF L 706:**

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



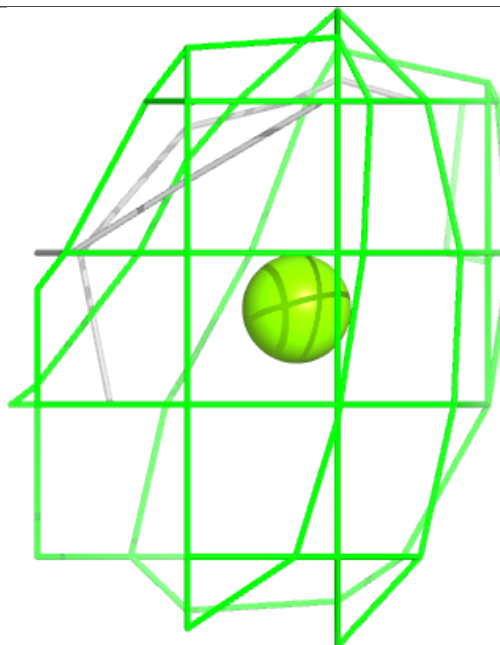
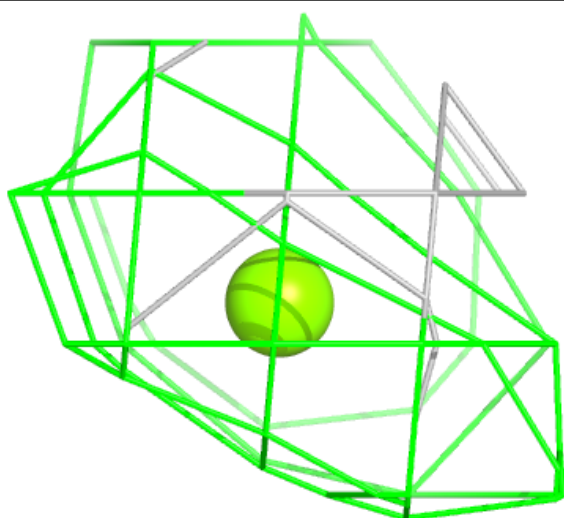
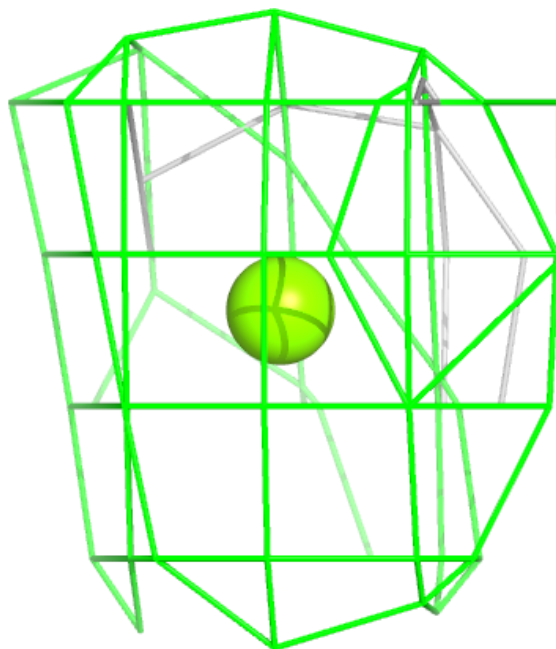
**Electron density around MG D 705:**

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



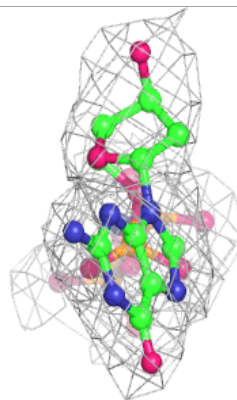
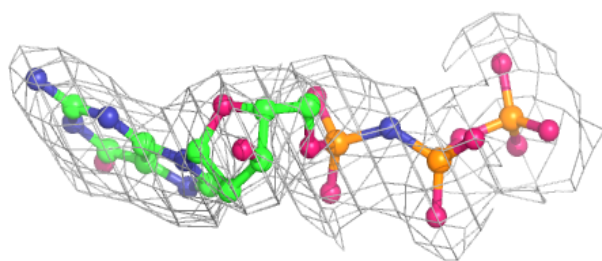
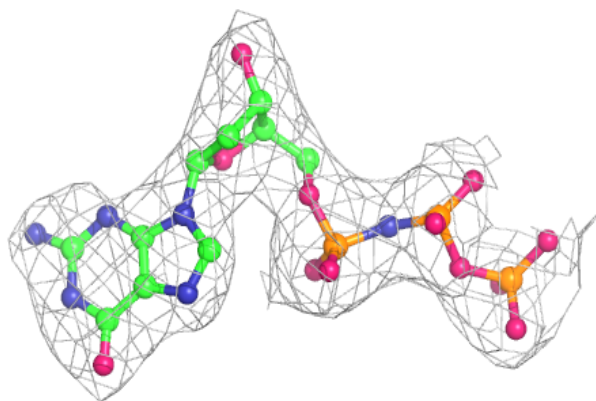
**Electron density around MG E 702:**

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

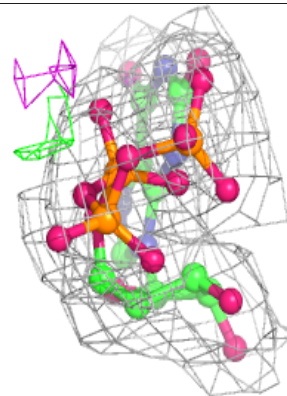
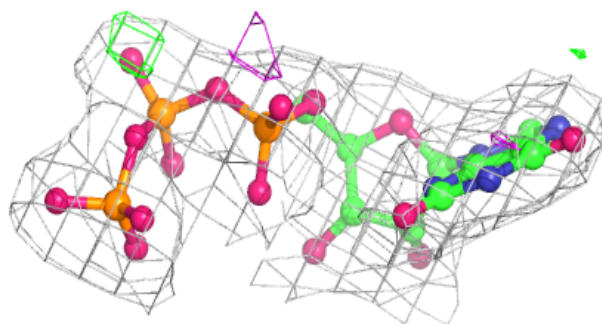
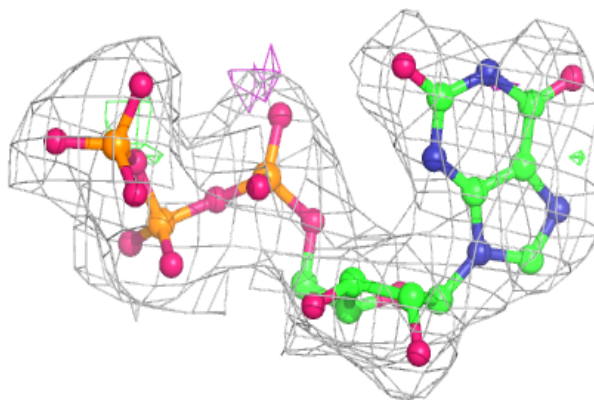


**Electron density around XG4 K 701:**

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

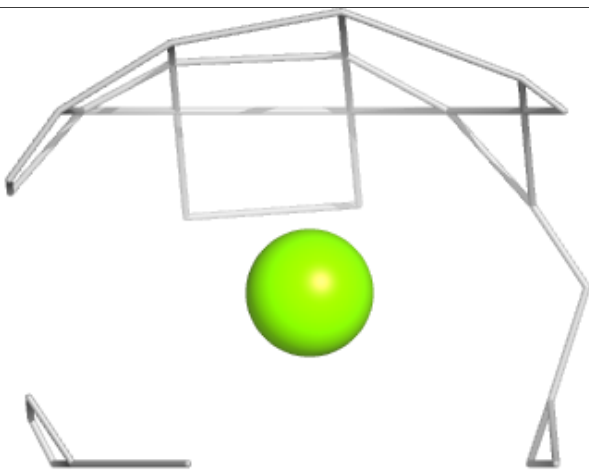
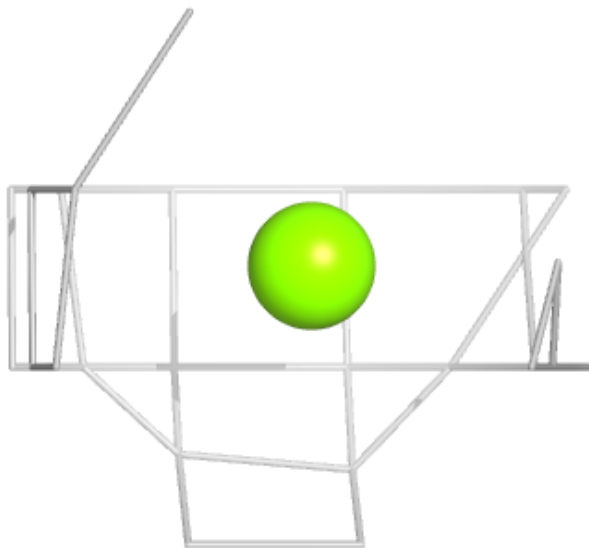
**Electron density around CZF H 707:**

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



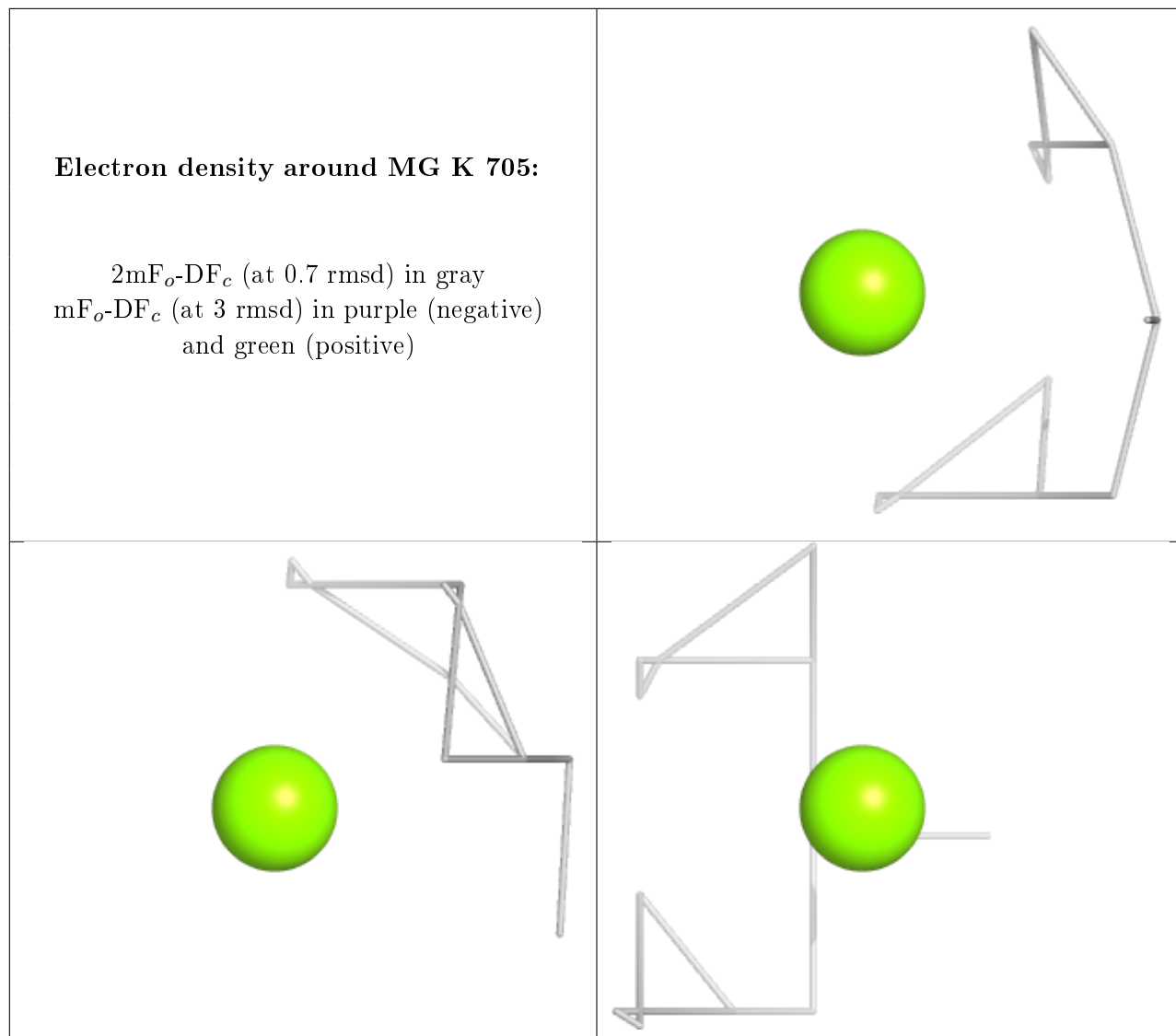
**Electron density around MG P 704:**

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



**Electron density around MG K 705:**

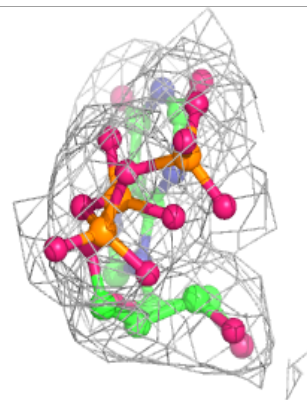
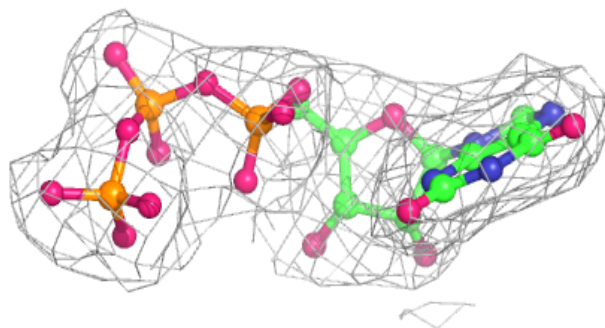
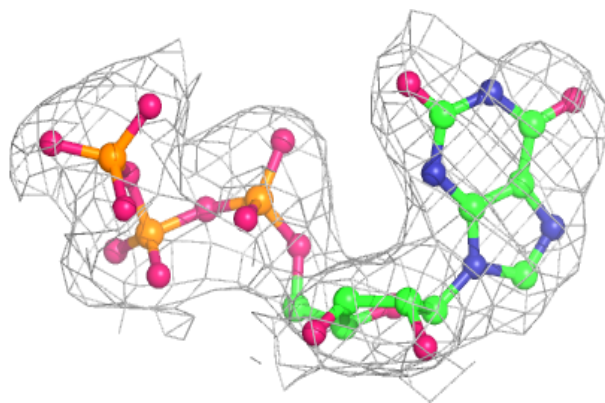
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



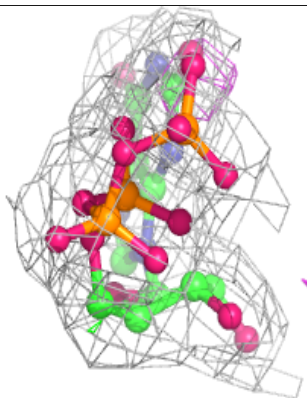
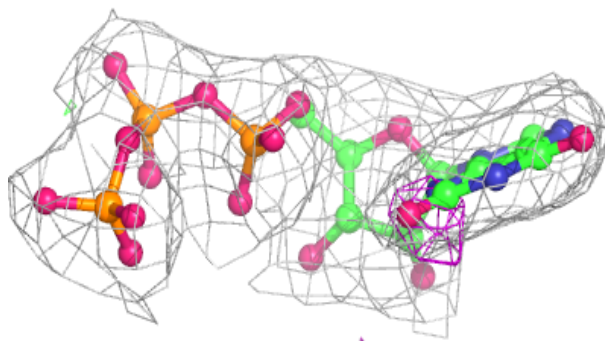
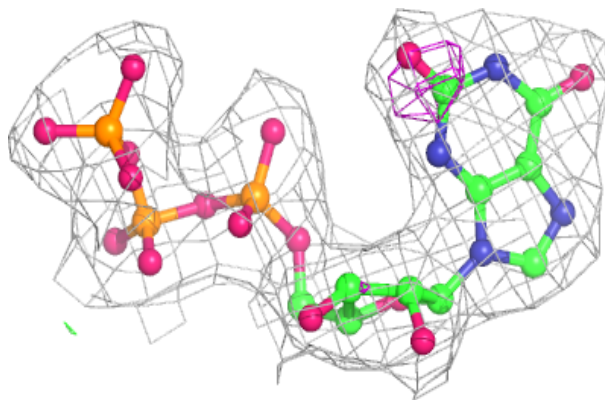


**Electron density around CZF M 706:**

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

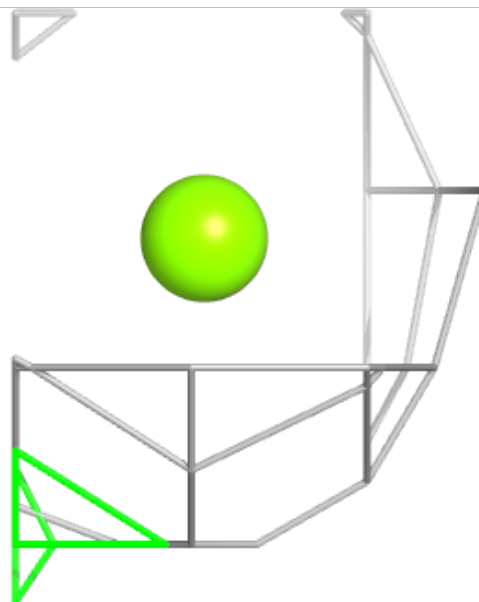
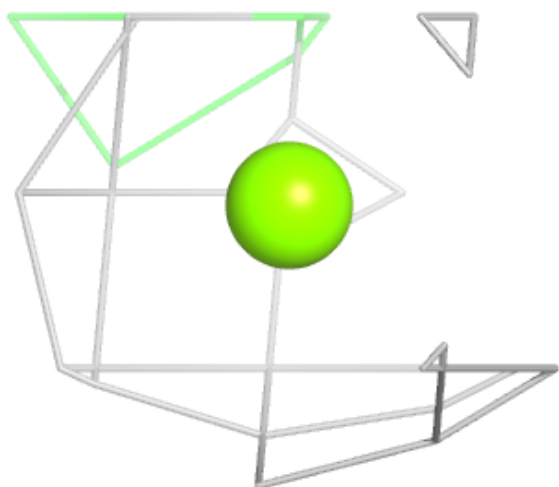
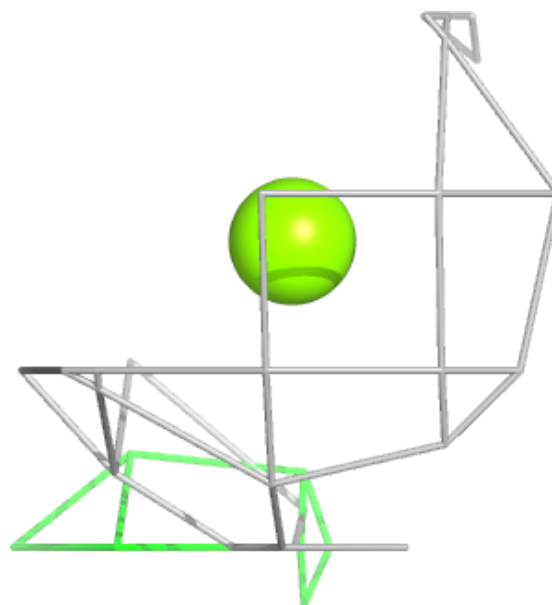
**Electron density around CZF G 707:**

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



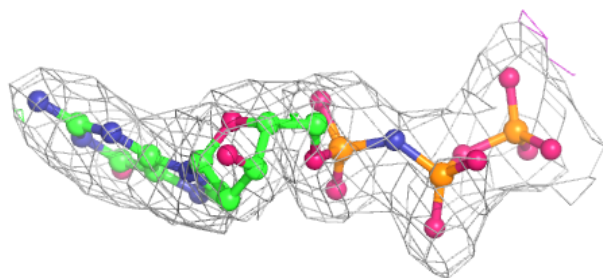
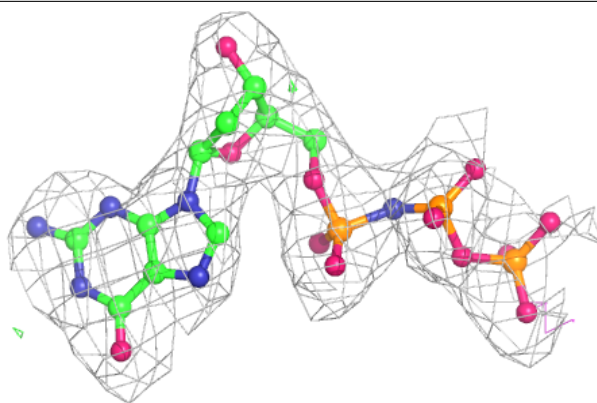
**Electron density around MG I 703:**

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

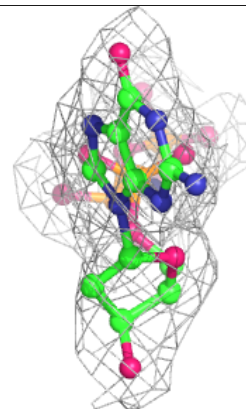
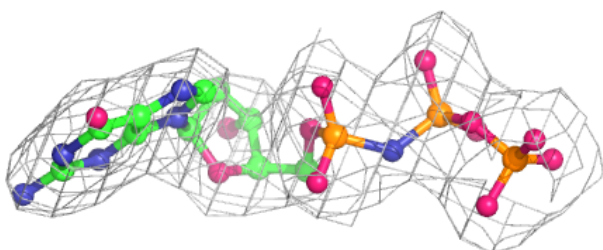
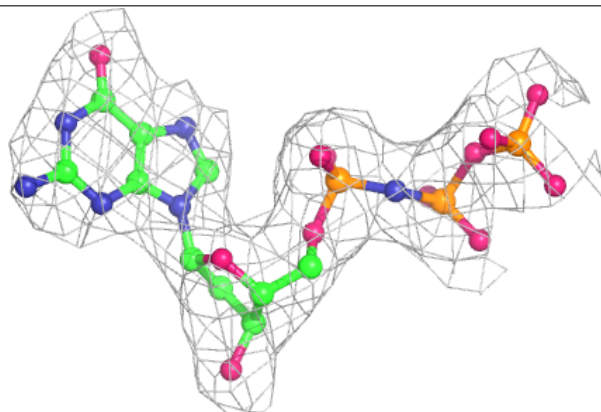


**Electron density around XG4 A 708:**

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

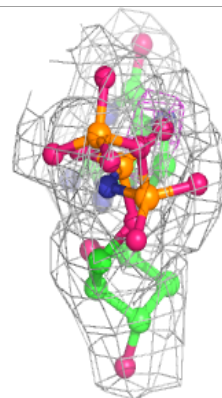
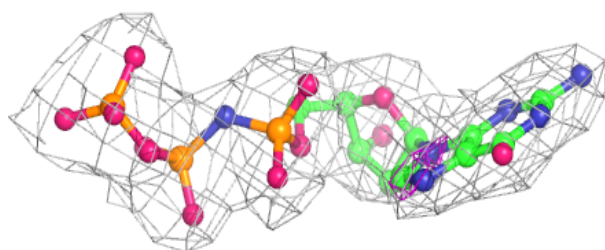
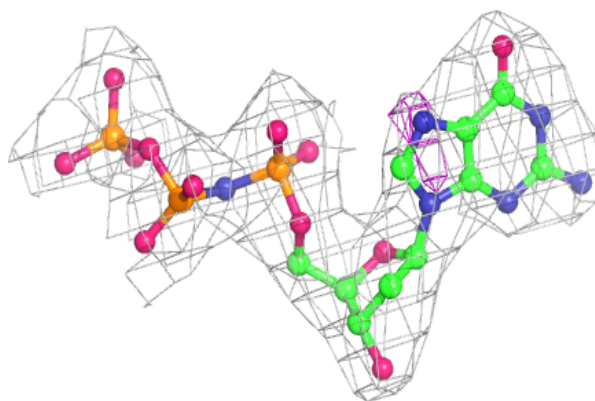
**Electron density around XG4 H 701:**

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

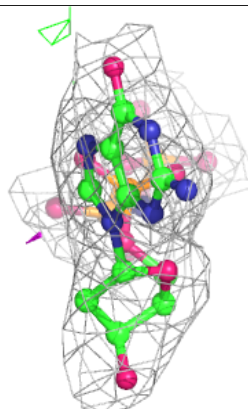
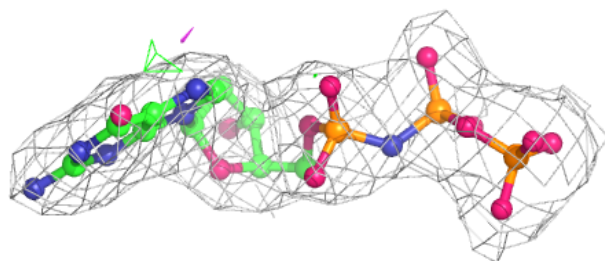
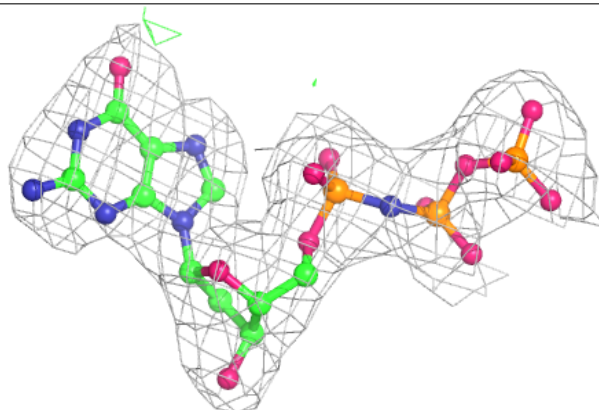


**Electron density around XG4 J 709:**

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

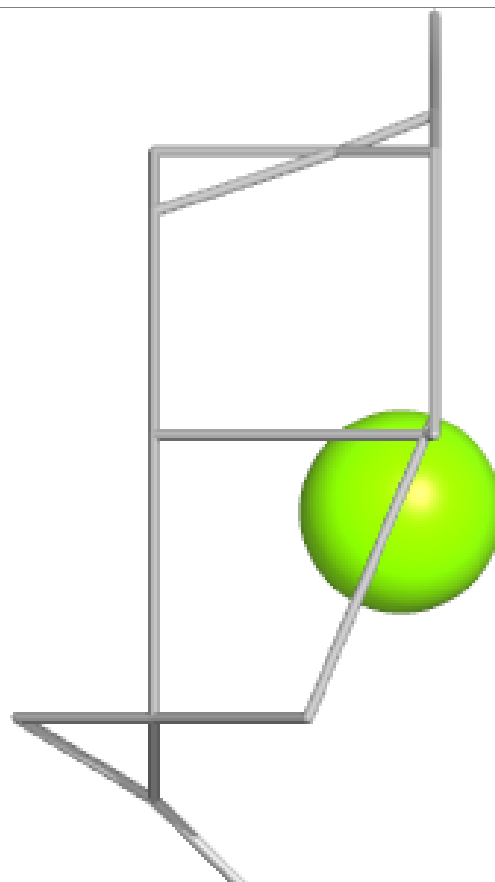
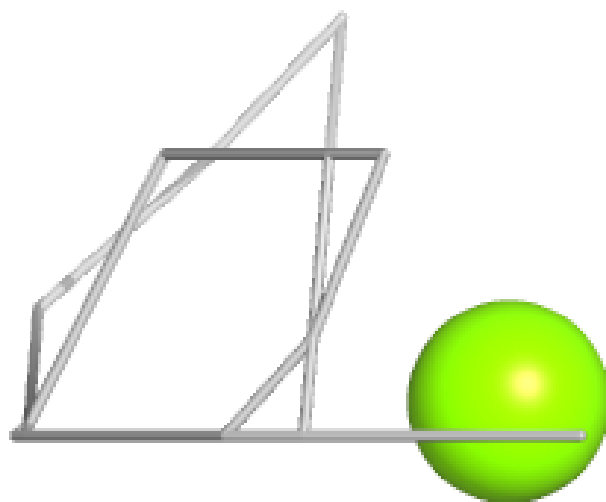
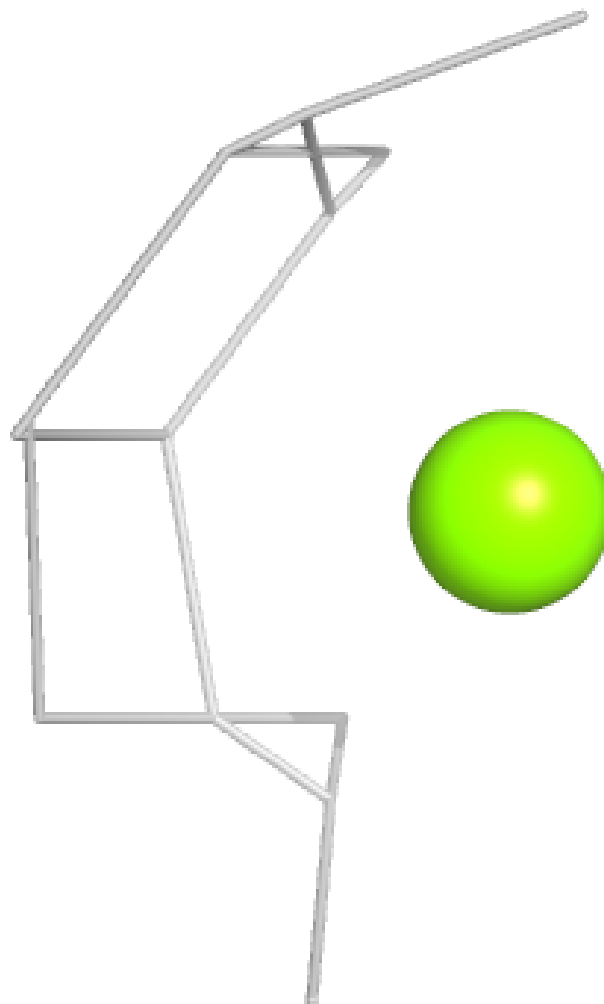
**Electron density around XG4 C 701:**

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



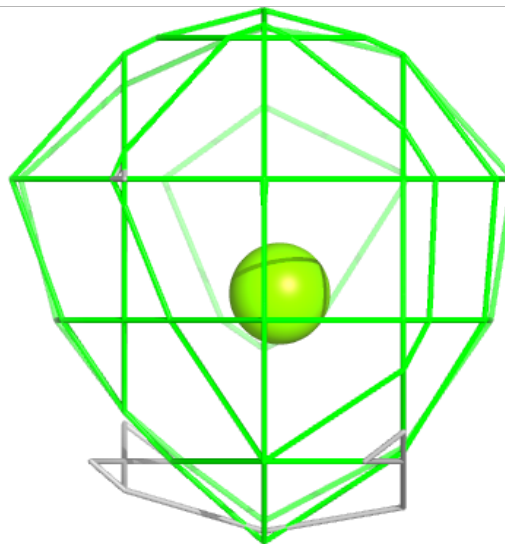
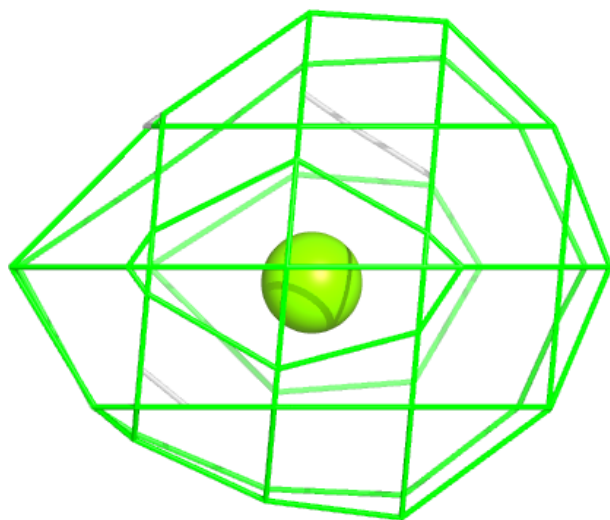
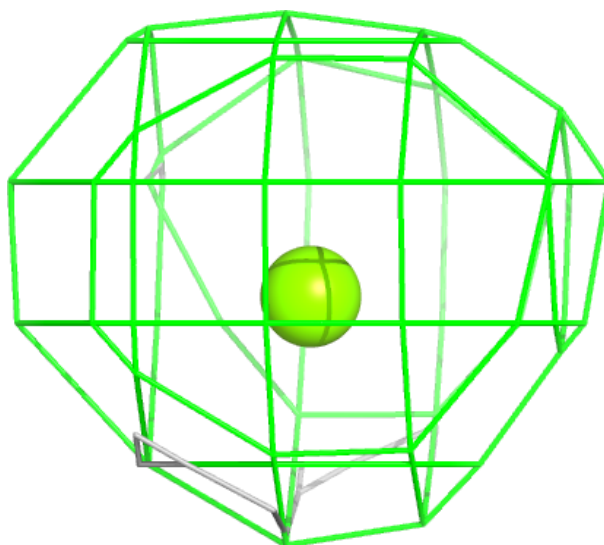
**Electron density around MG H 705:**

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



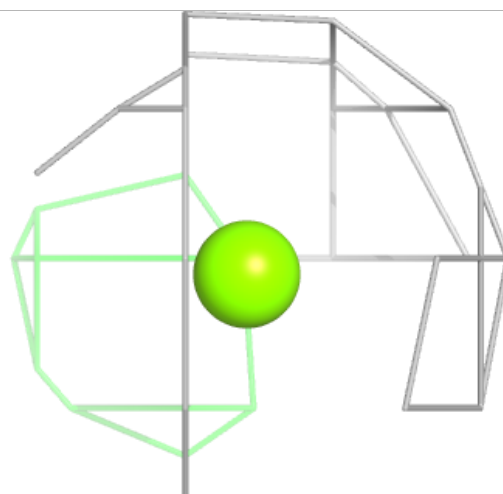
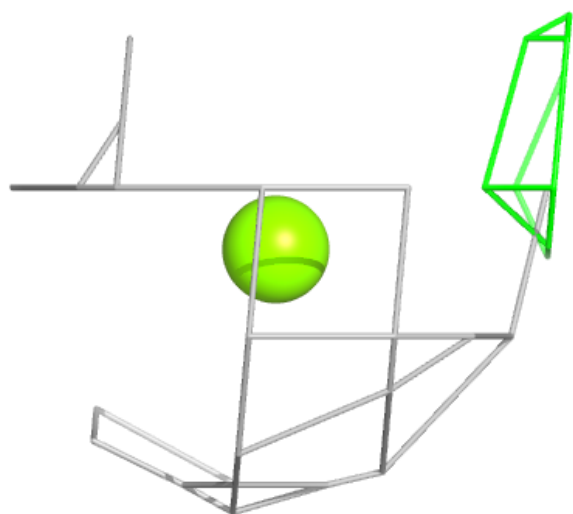
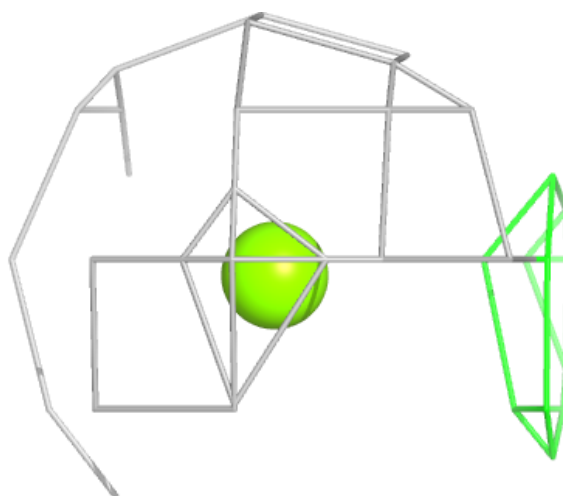
**Electron density around MG I 702:**

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



**Electron density around MG L 703:**

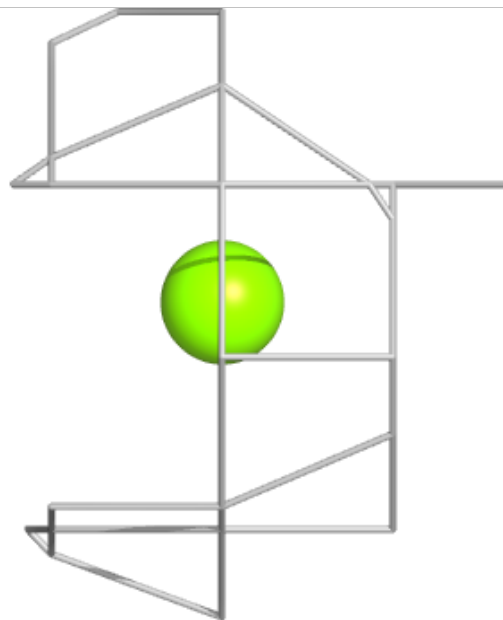
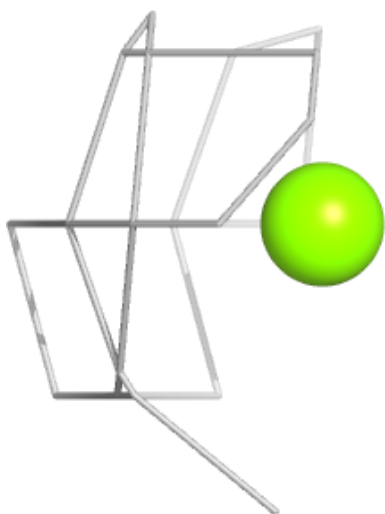
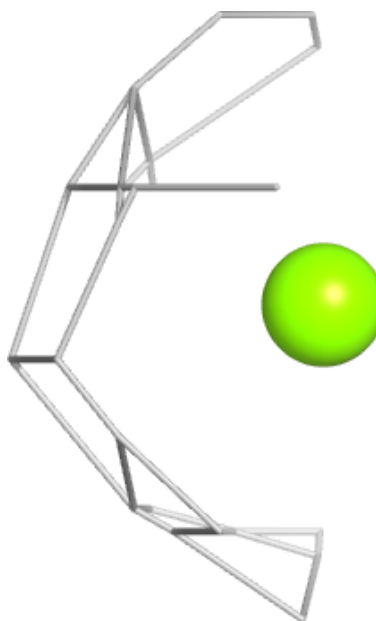
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around MG I 704:**

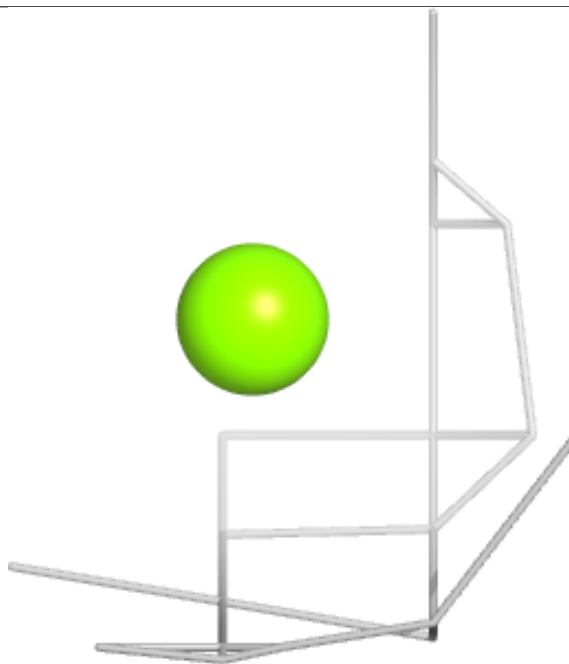
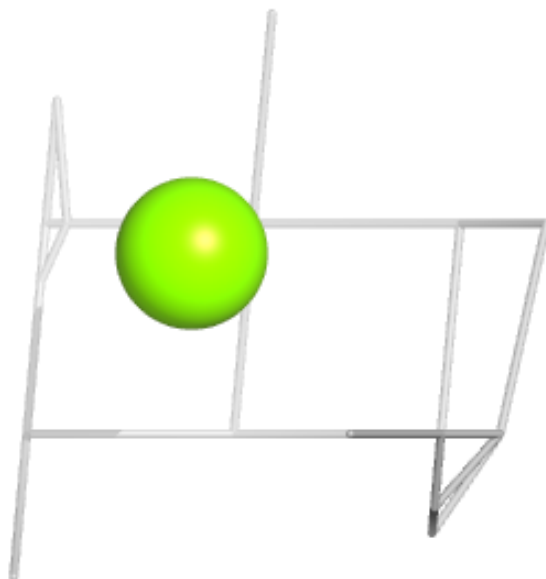
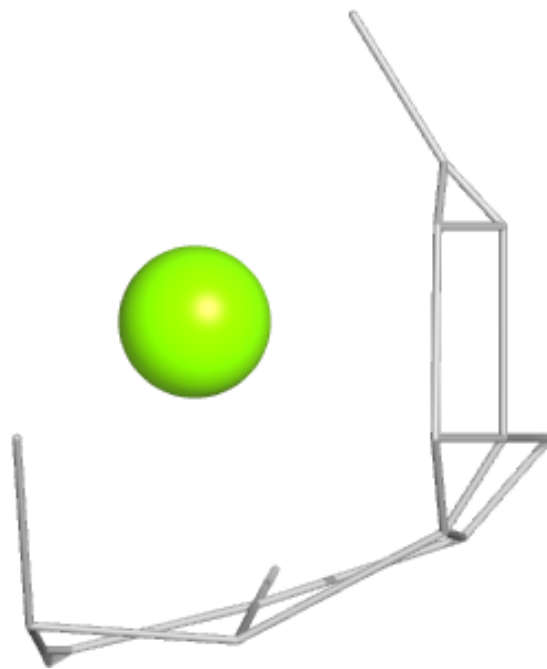
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





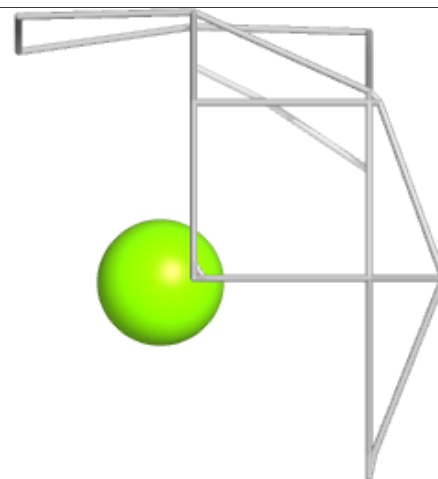
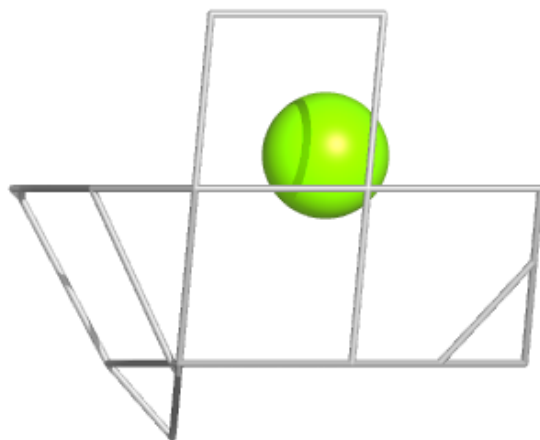
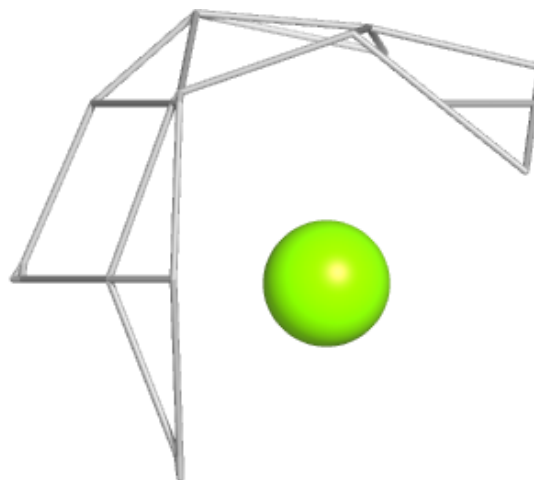
**Electron density around MG G 705:**

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



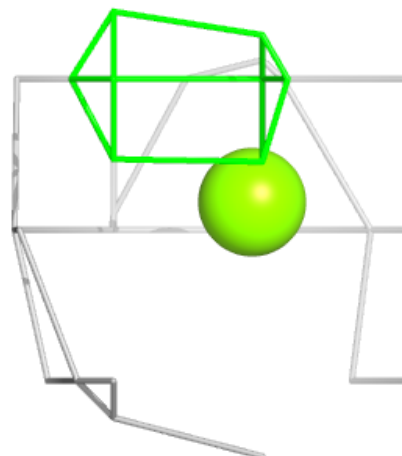
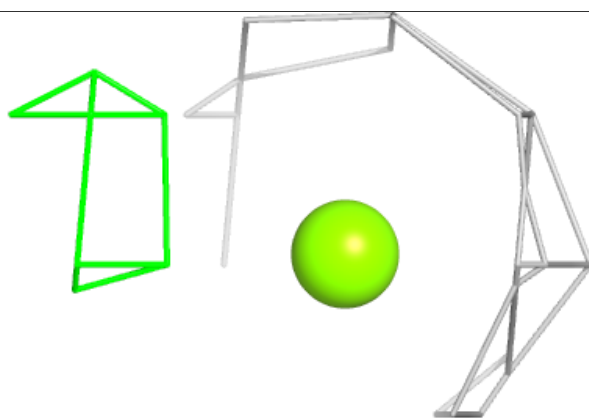
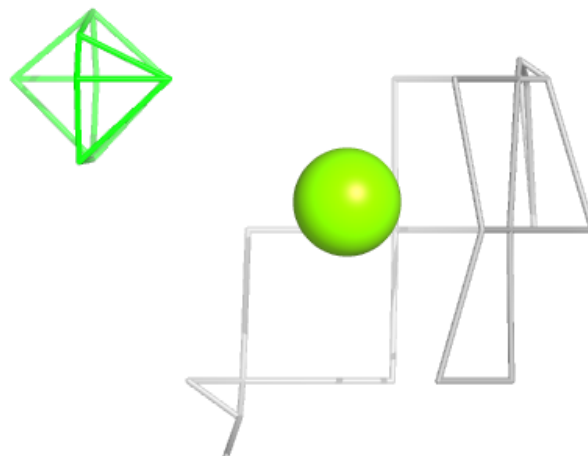
**Electron density around MG L 704:**

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



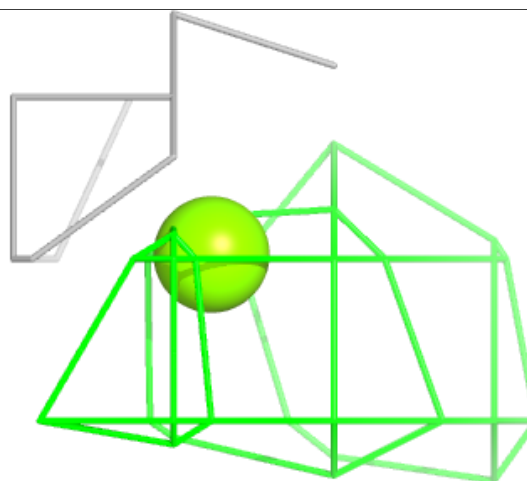
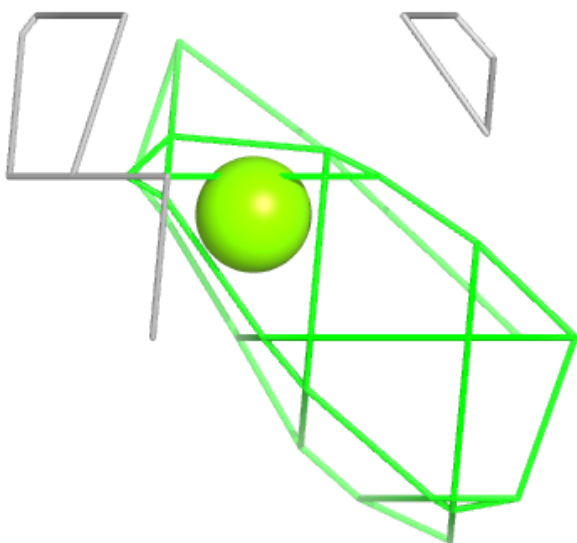
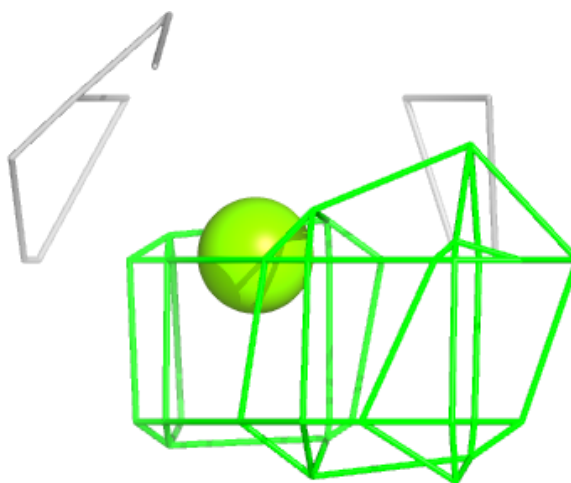
**Electron density around MG G 704:**

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



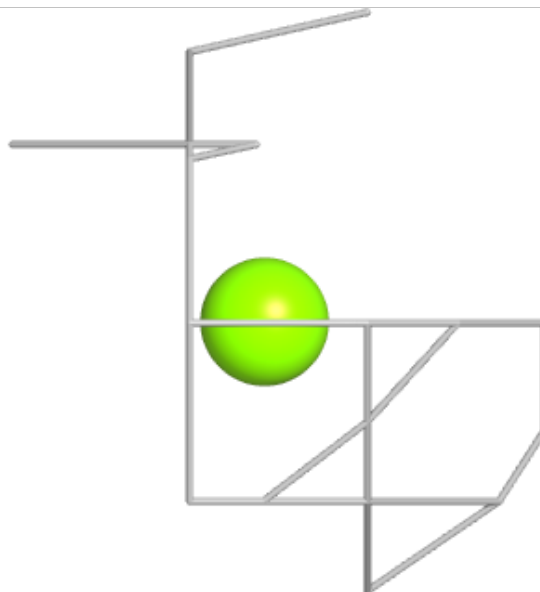
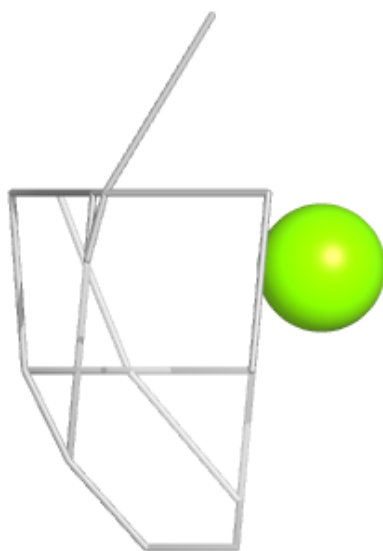
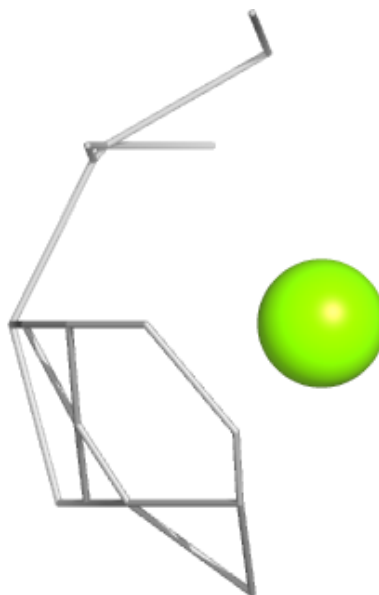
**Electron density around MG L 702:**

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



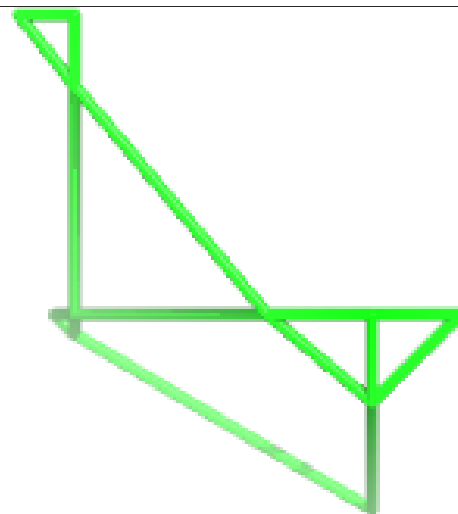
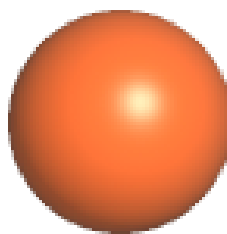
**Electron density around MG F 704:**

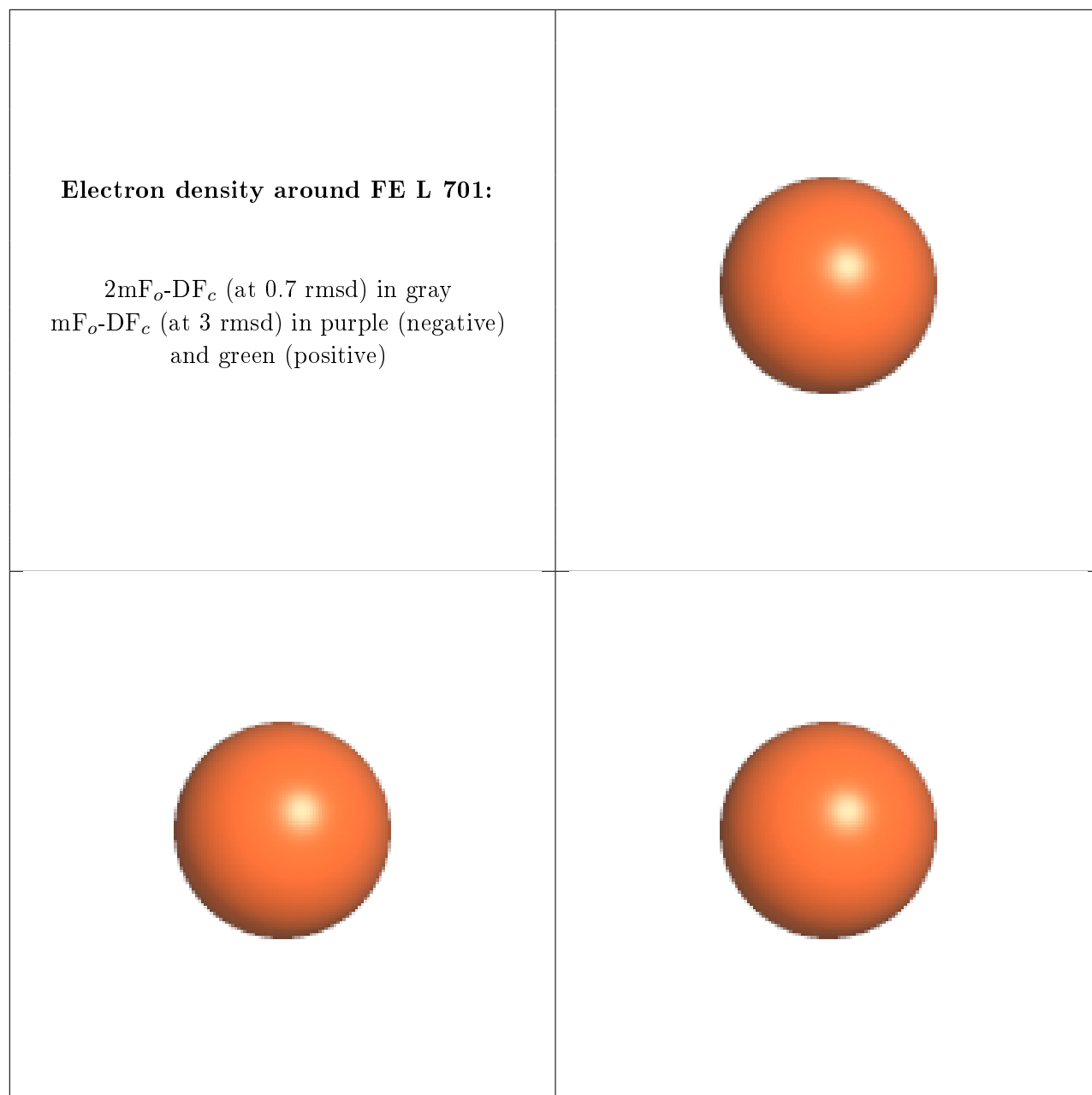
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FE H 702:**

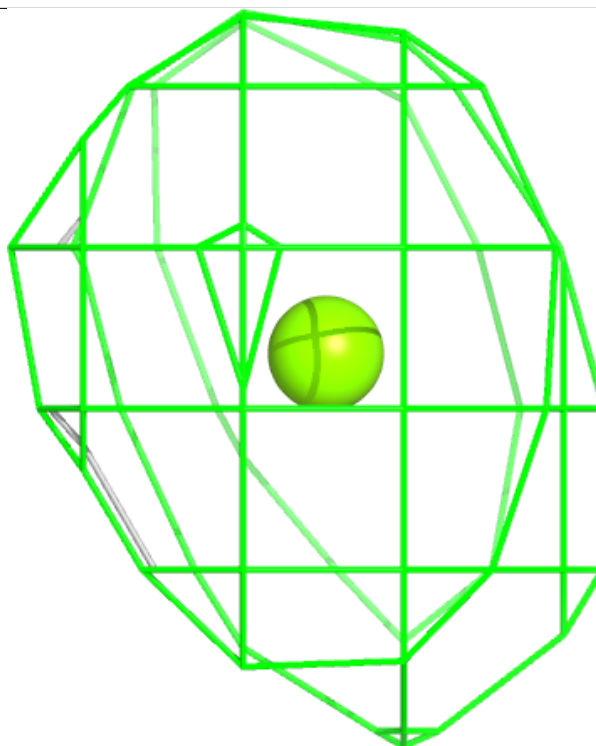
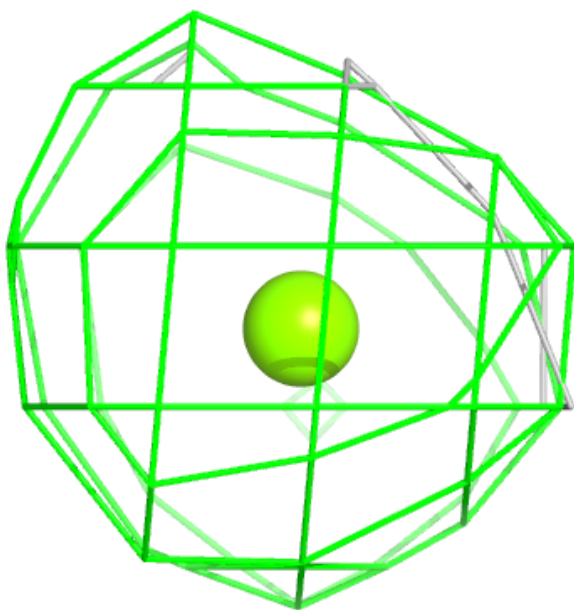
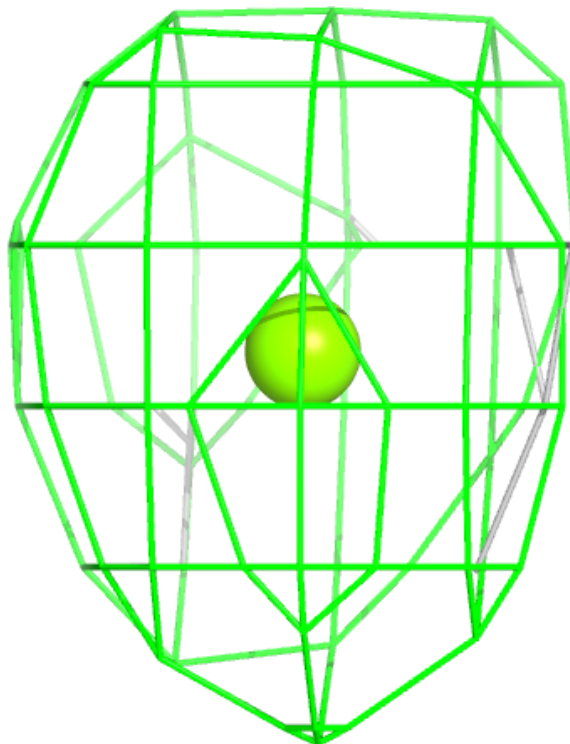
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



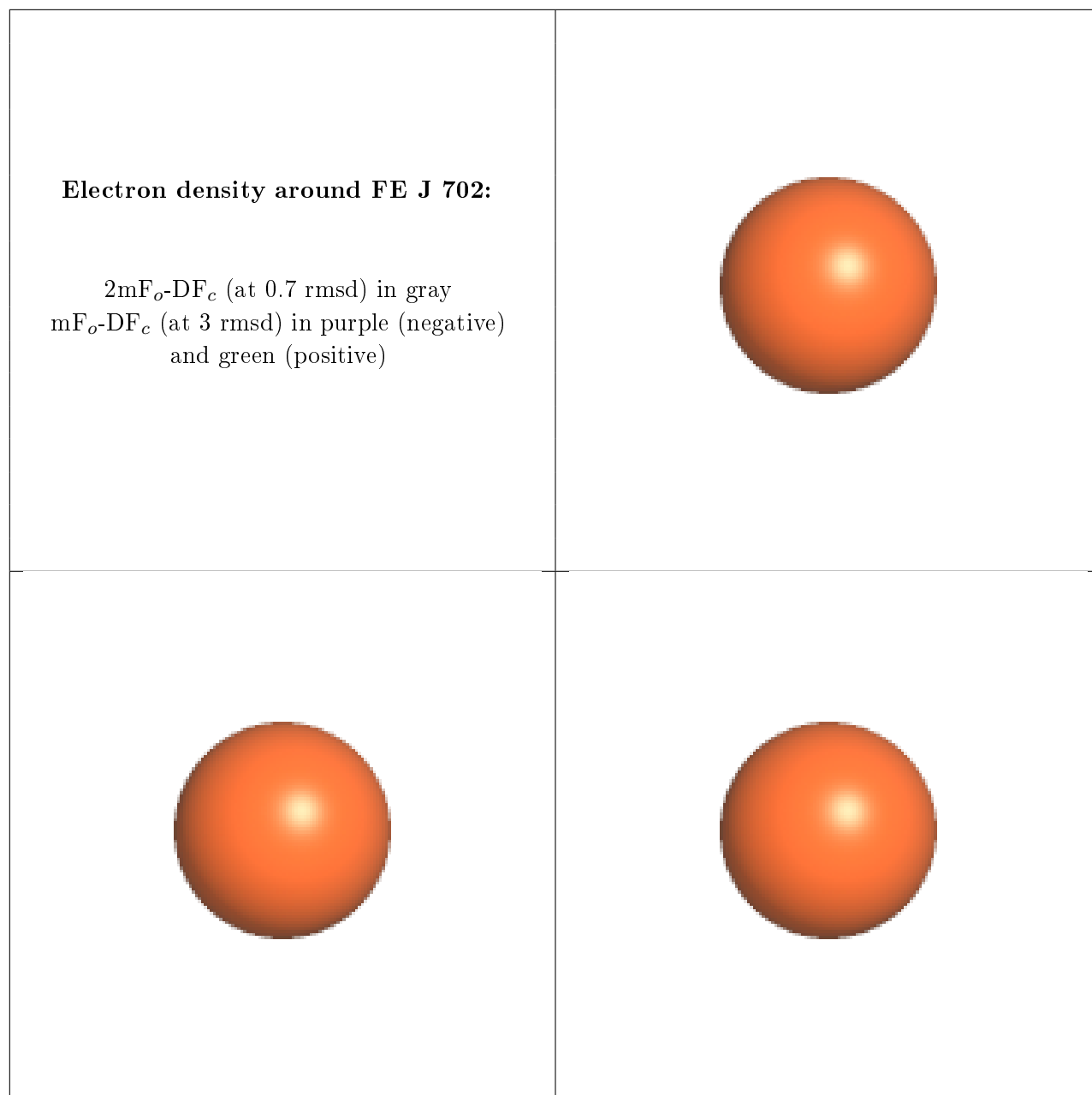


**Electron density around MG D 703:**

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

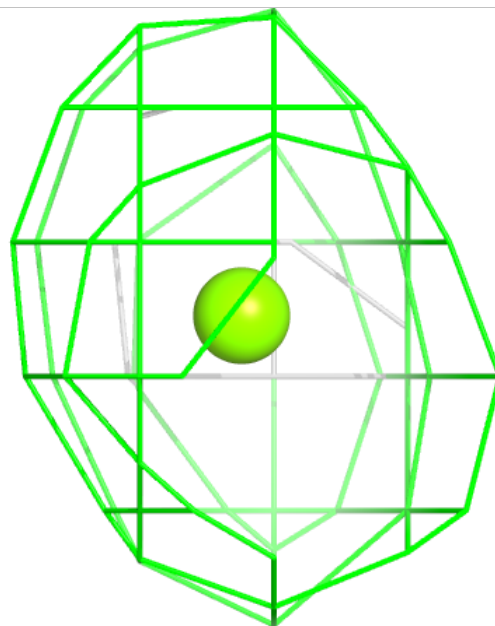
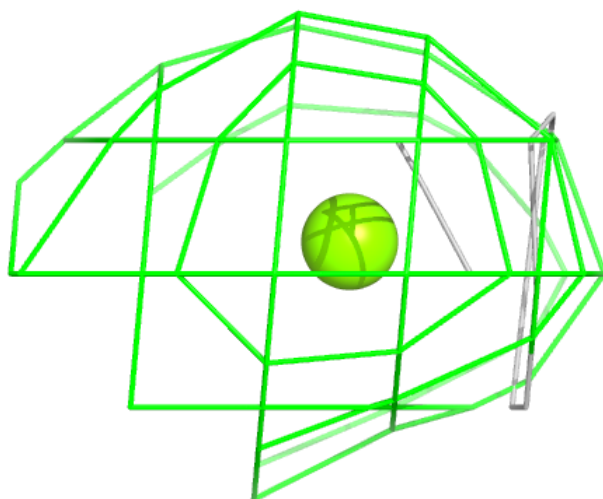
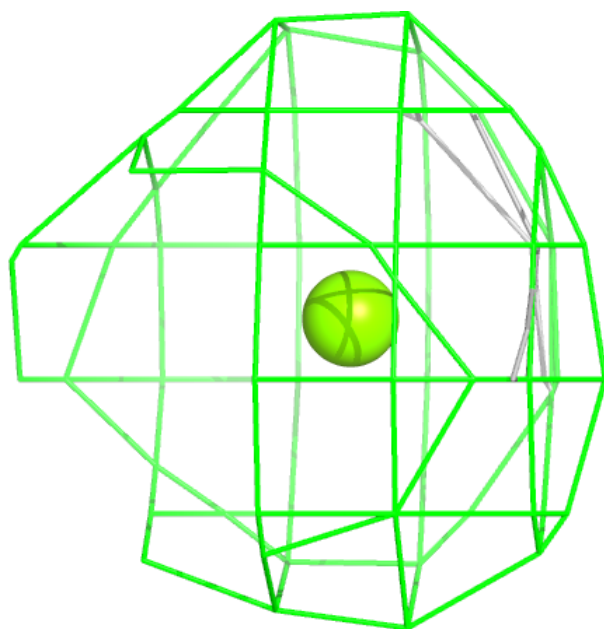






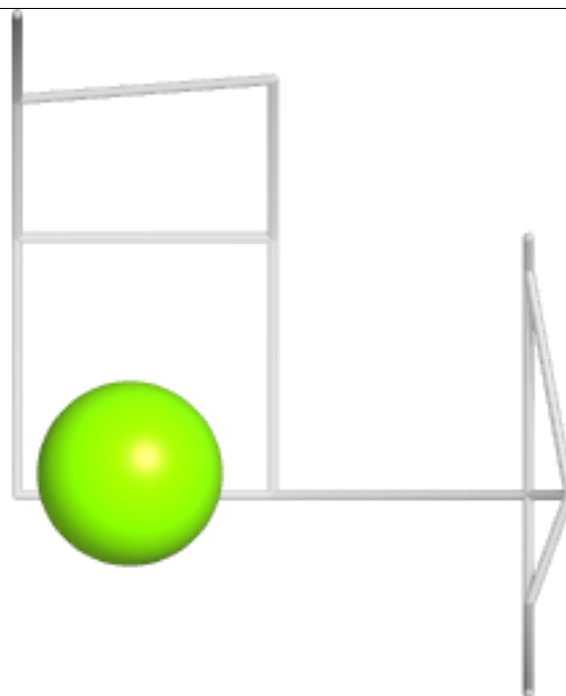
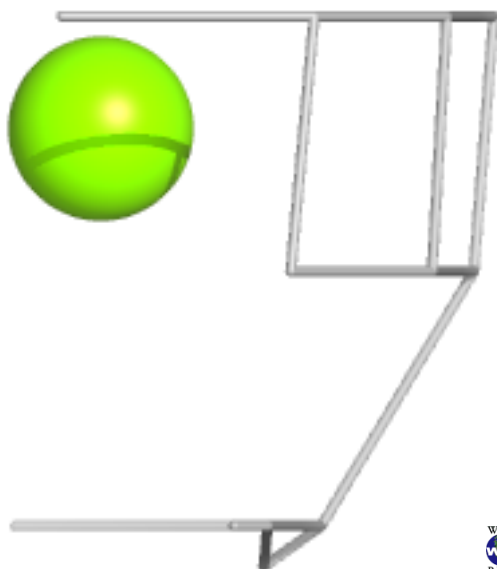
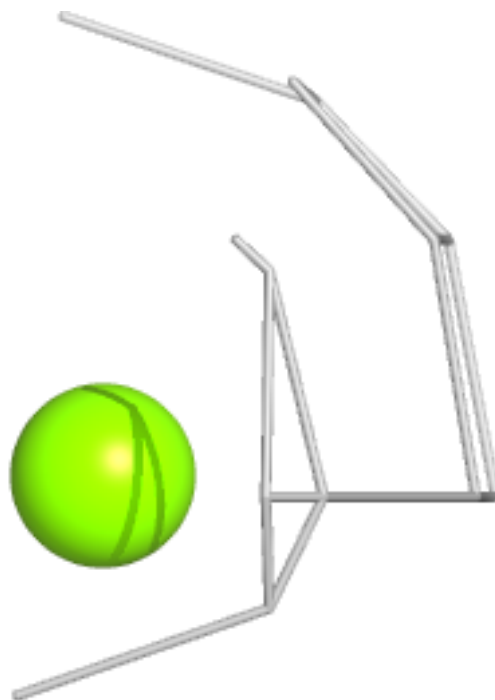
**Electron density around MG B 702:**

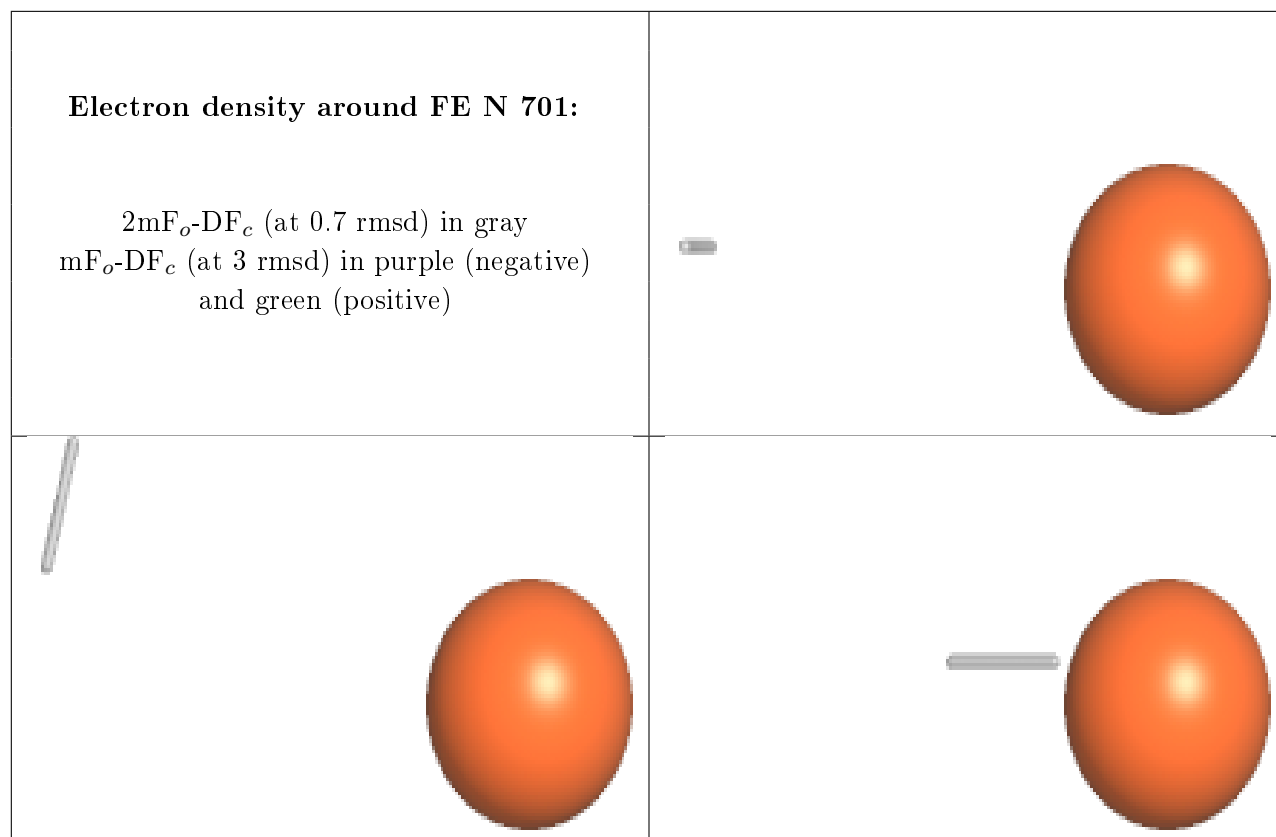
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around MG C 705:**

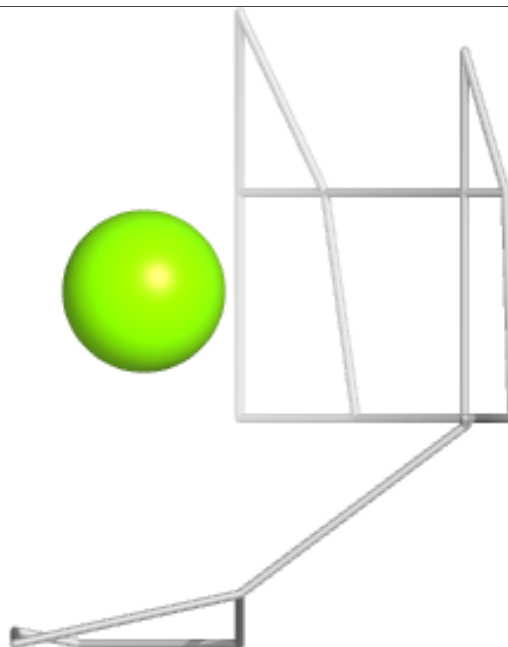
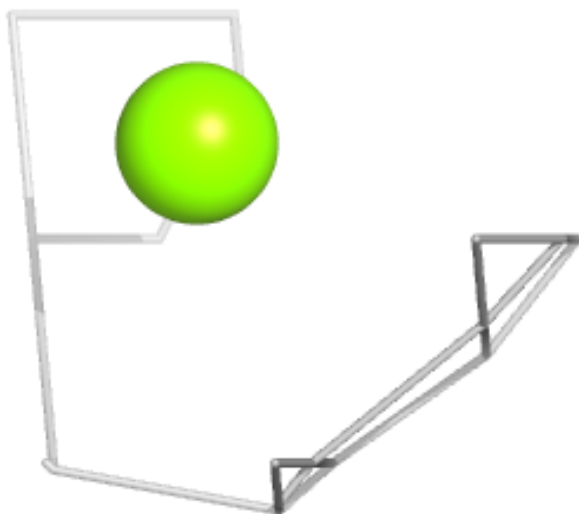
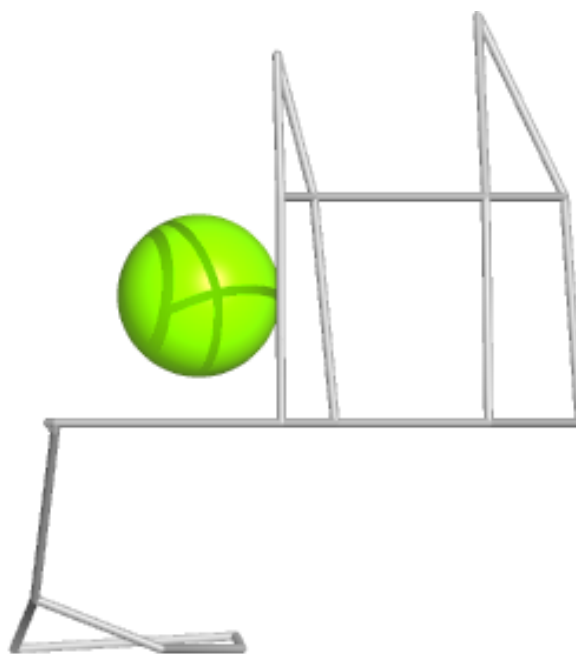
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

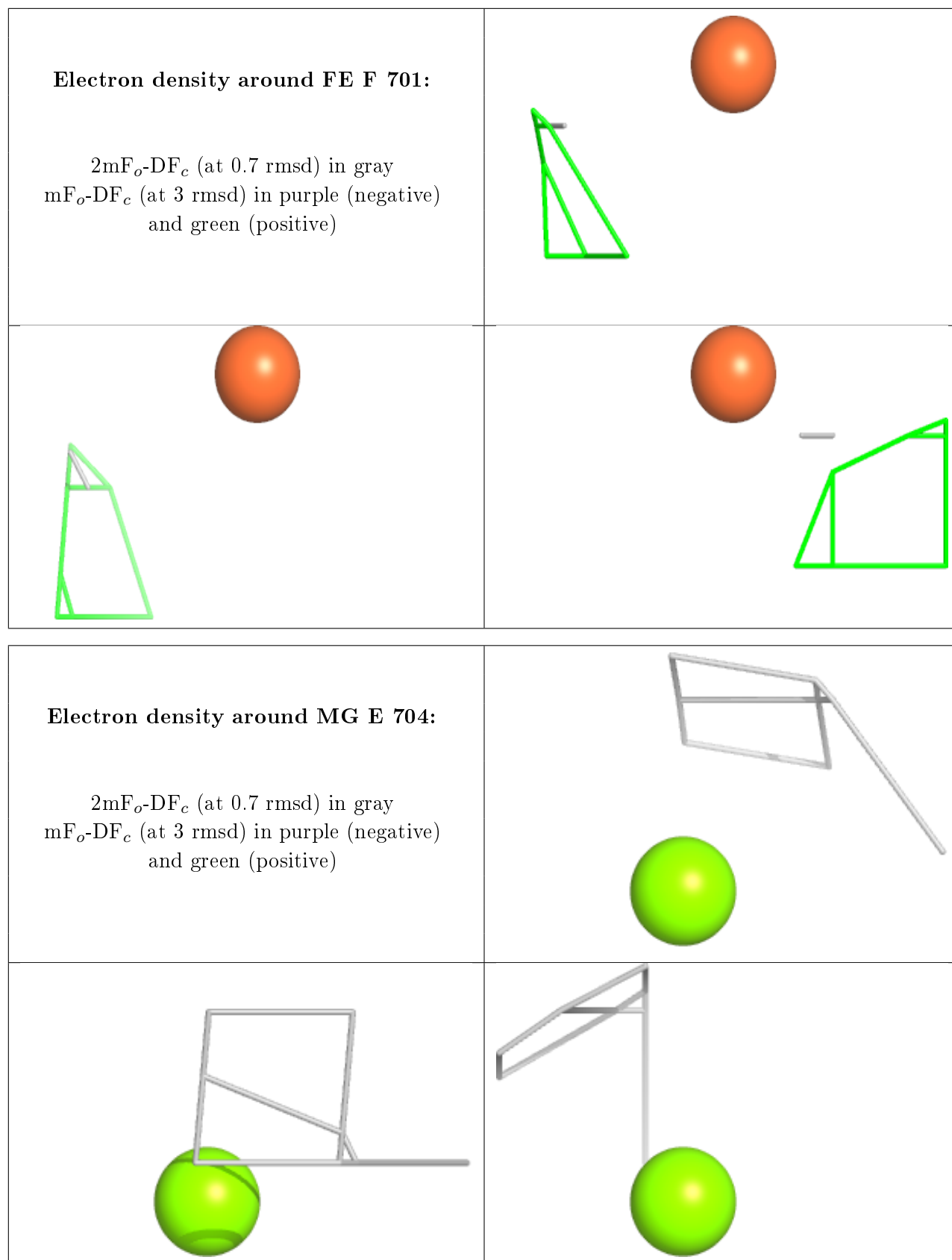




**Electron density around MG P 705:**

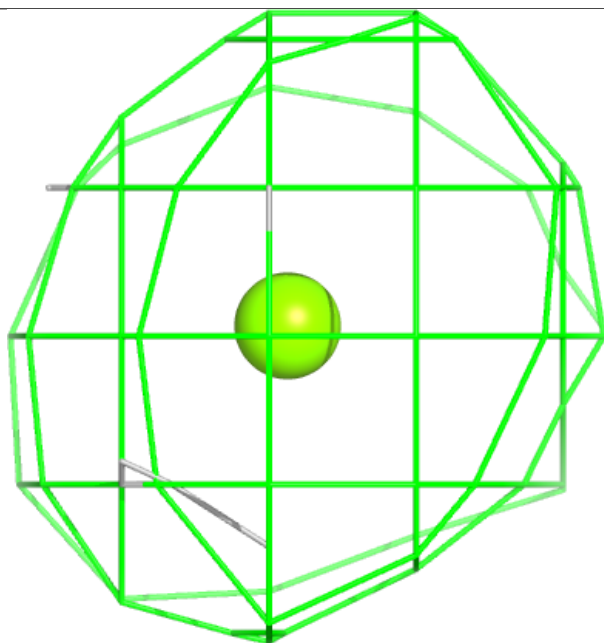
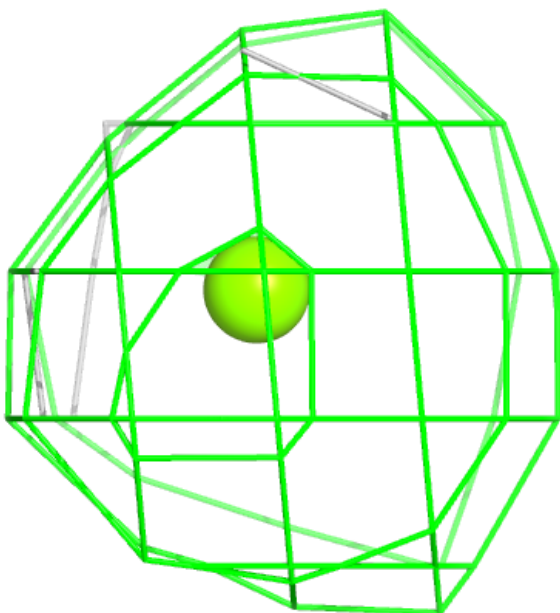
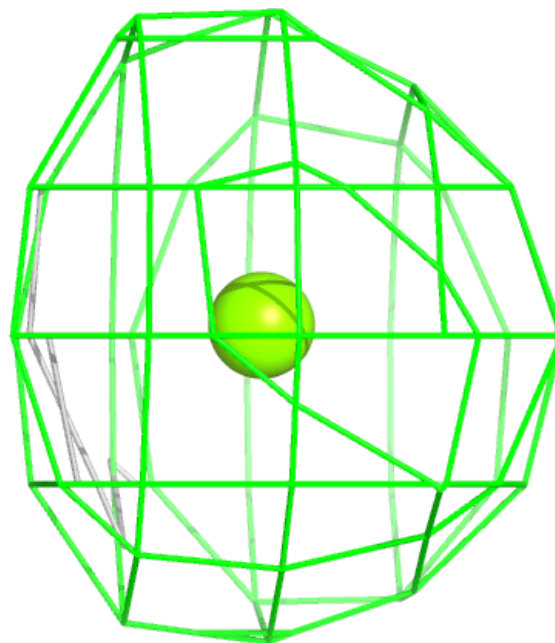
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





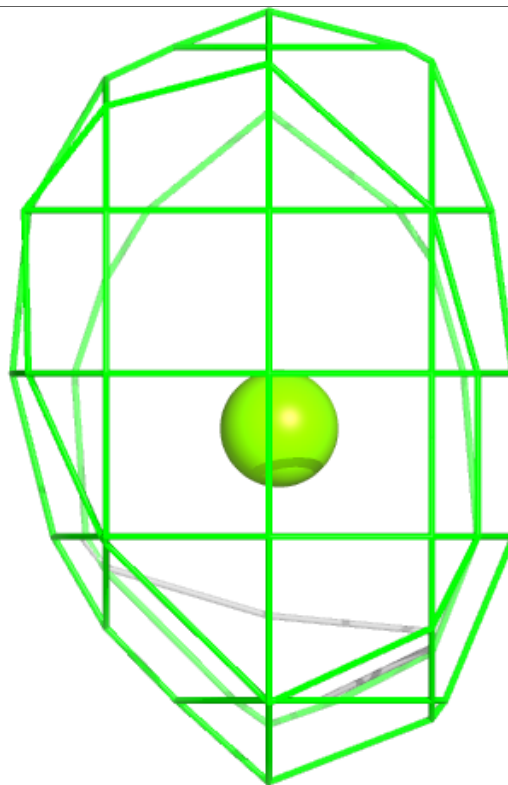
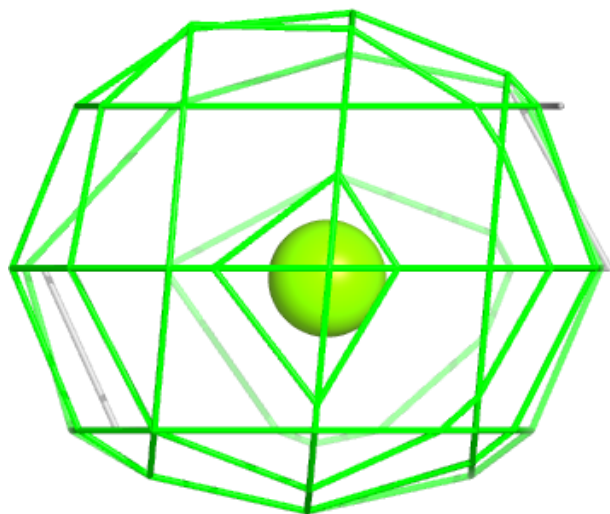
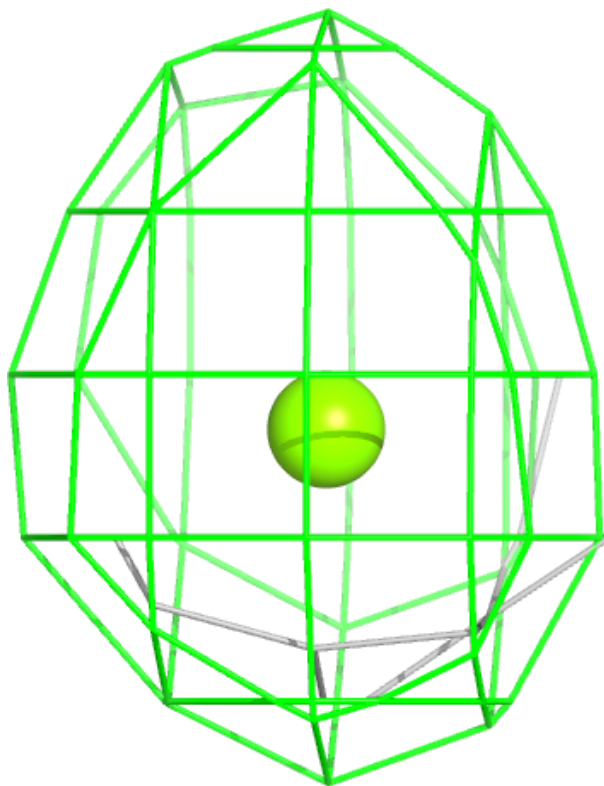
**Electron density around MG A 702:**

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



**Electron density around MG G 703:**

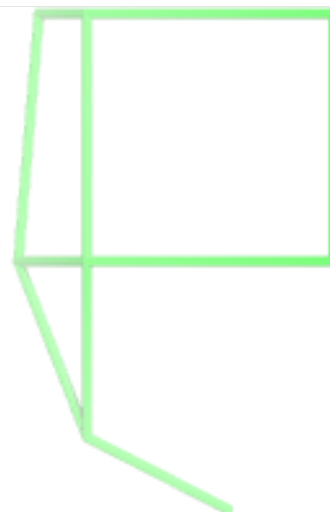
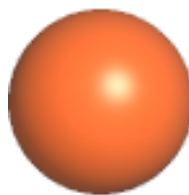
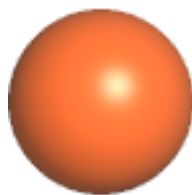
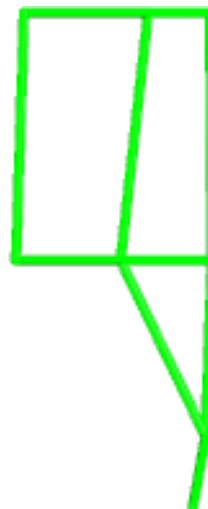
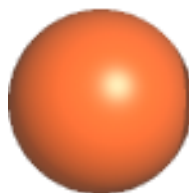
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

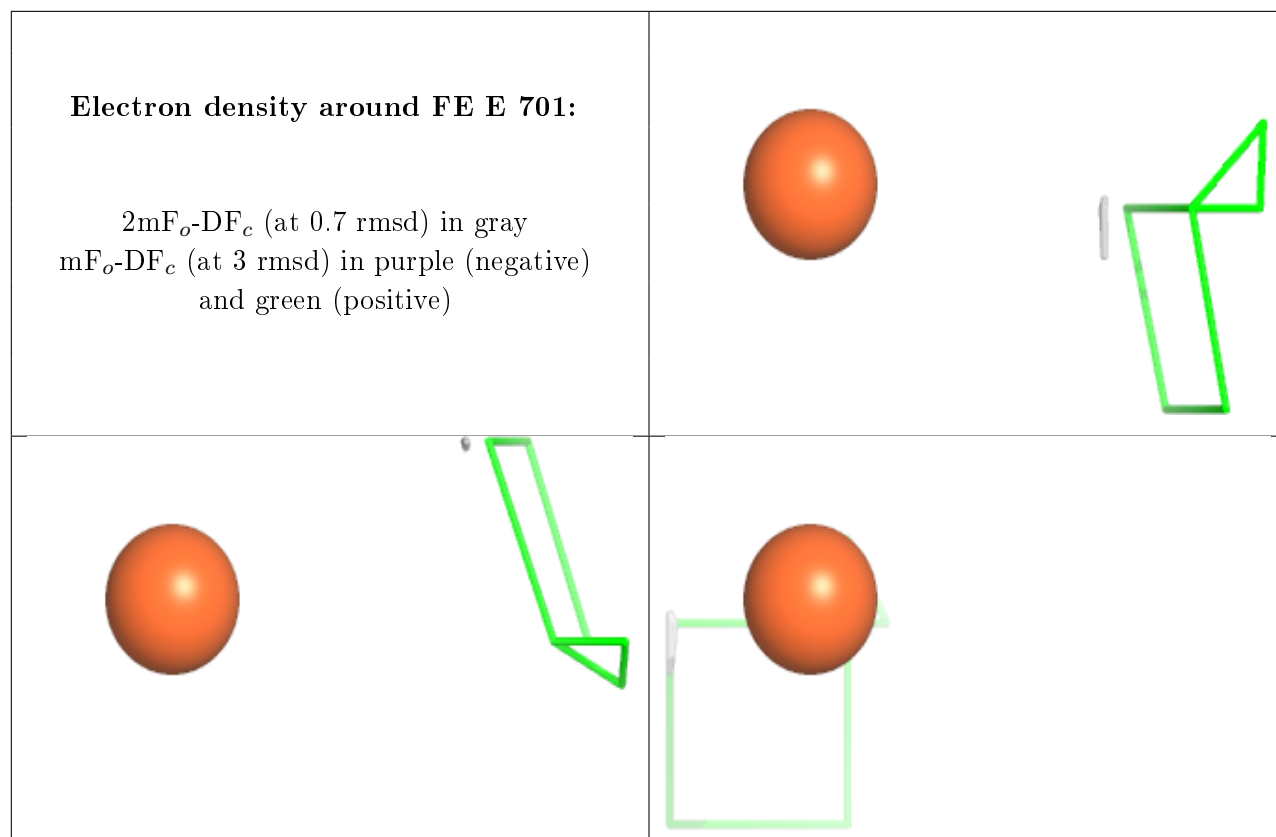




**Electron density around FE G 702:**

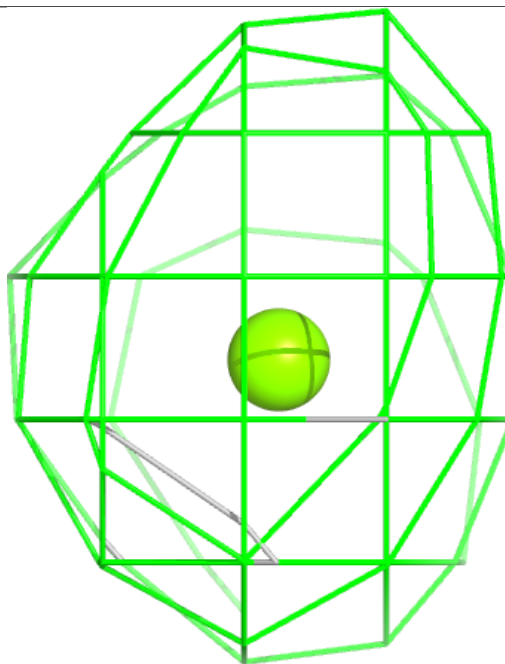
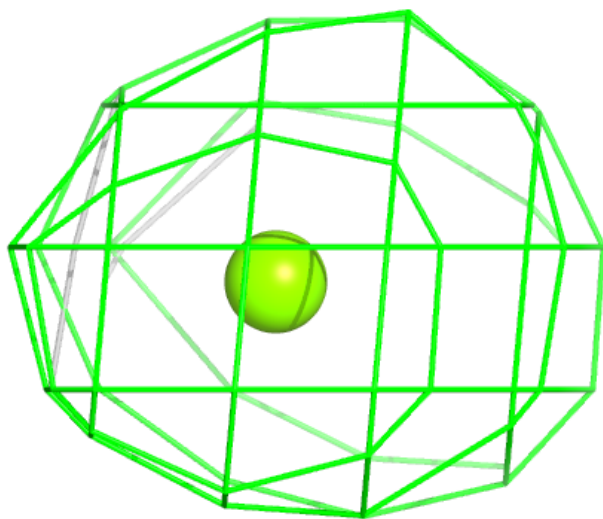
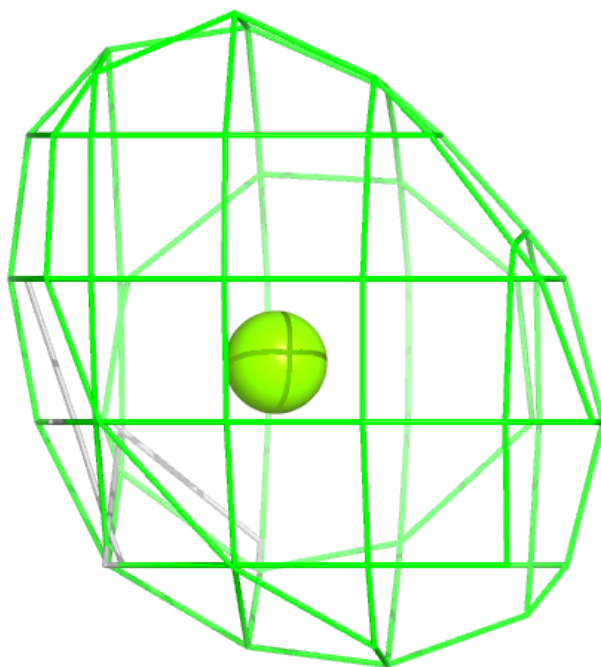
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





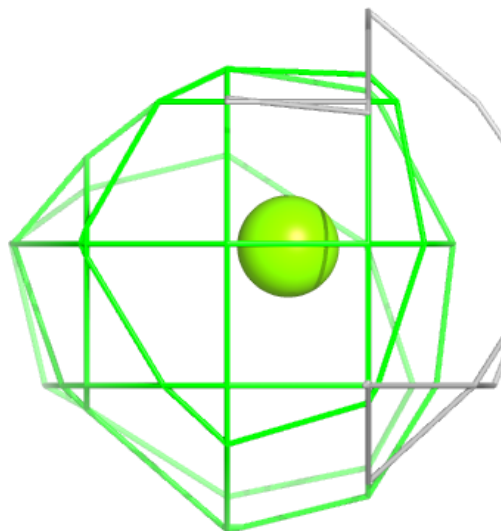
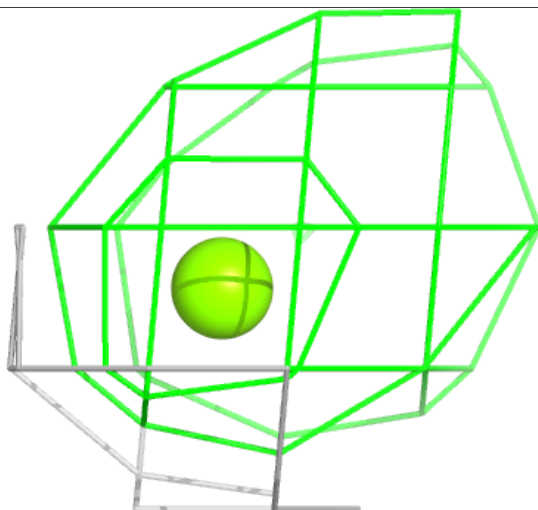
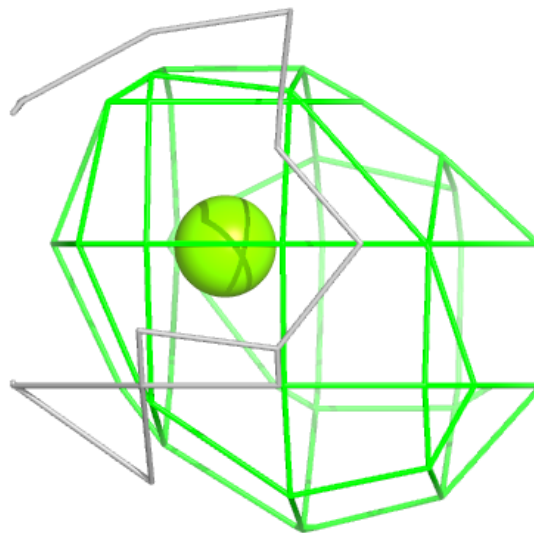
**Electron density around MG C 703:**

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



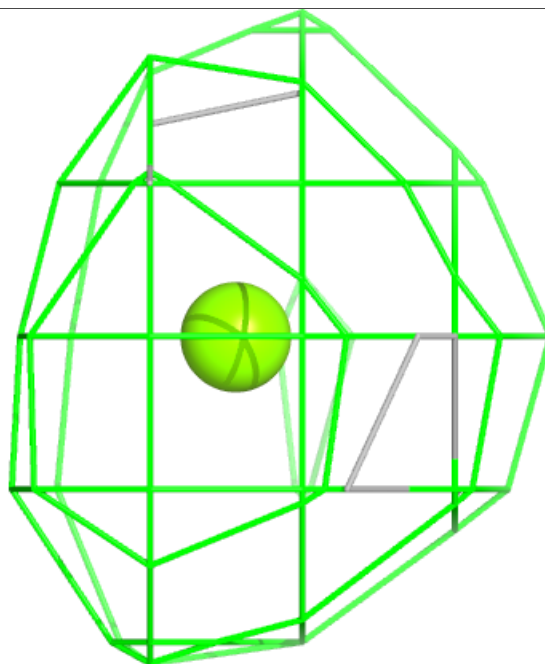
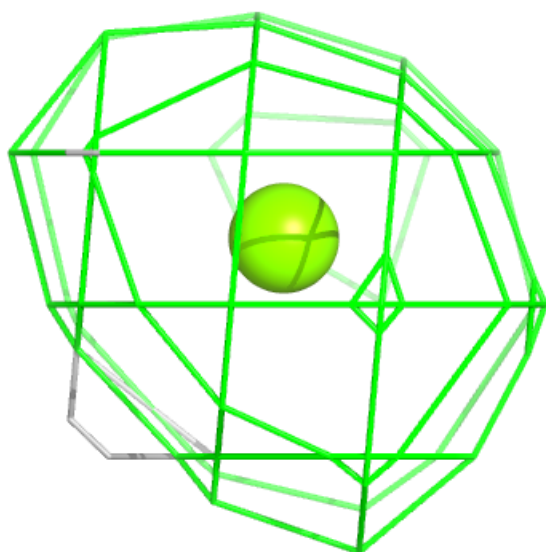
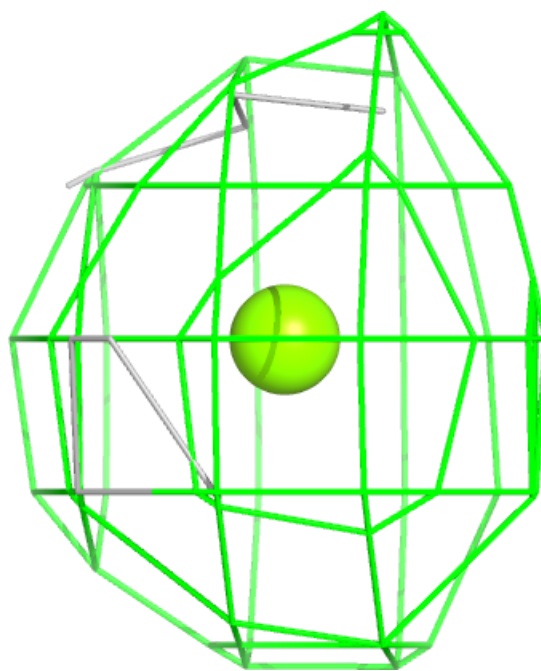
**Electron density around MG K 703:**

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



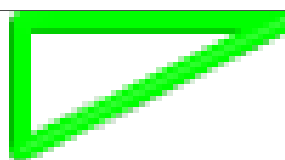
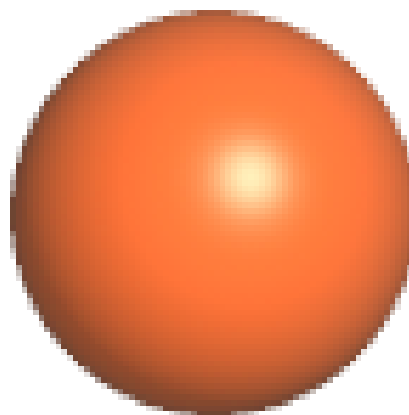
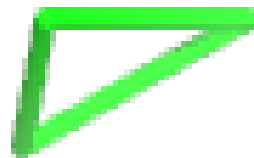
**Electron density around MG F 702:**

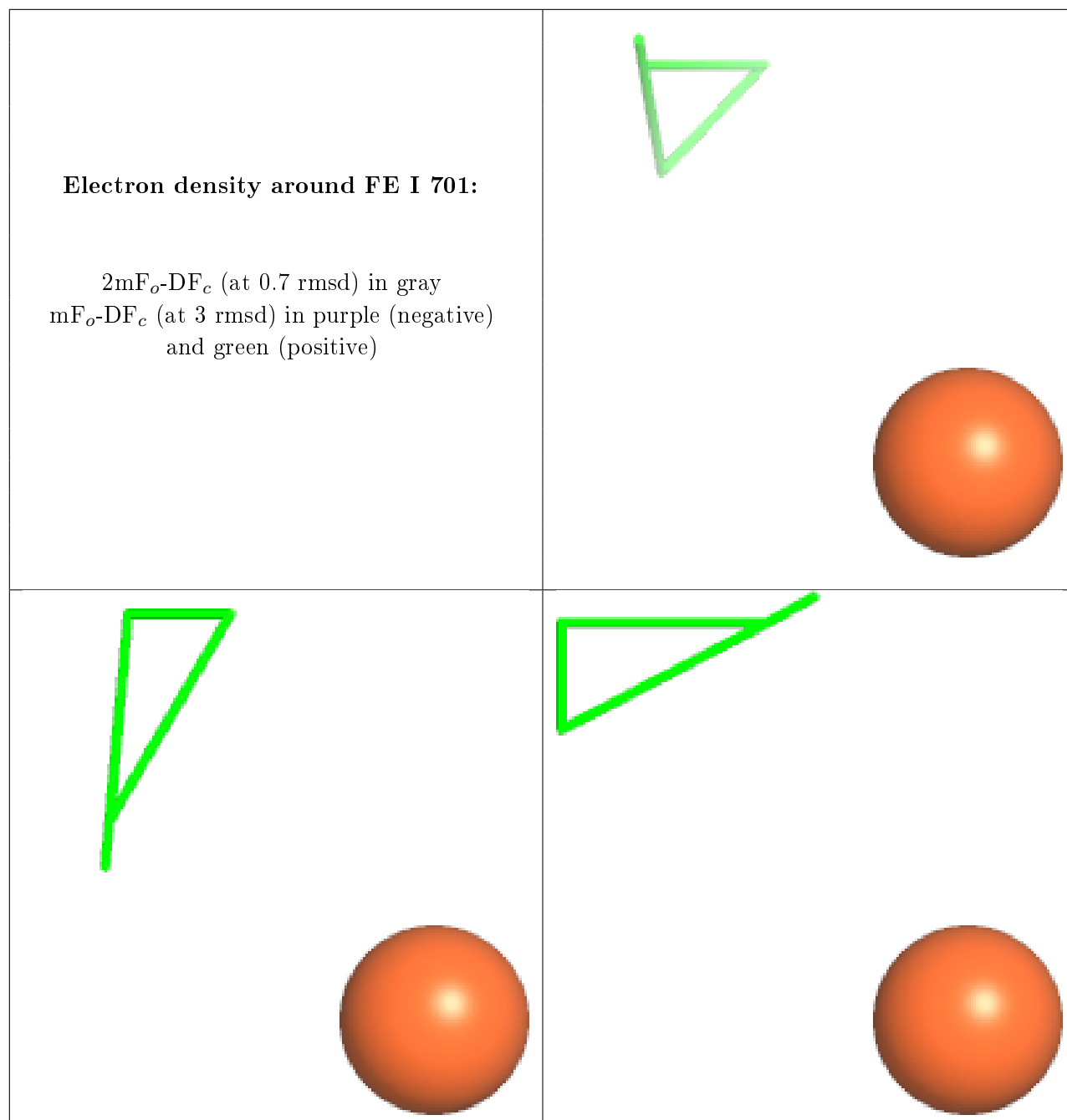
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FE K 702:**

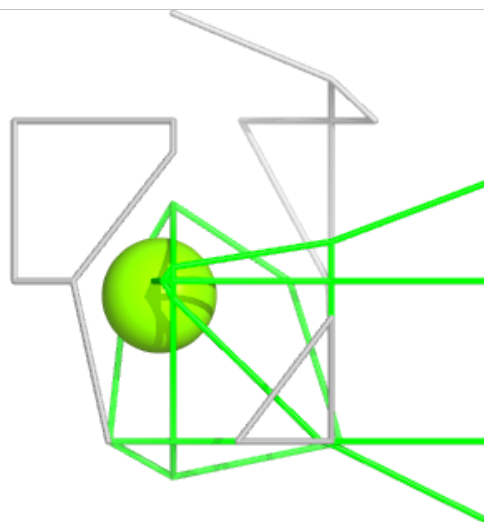
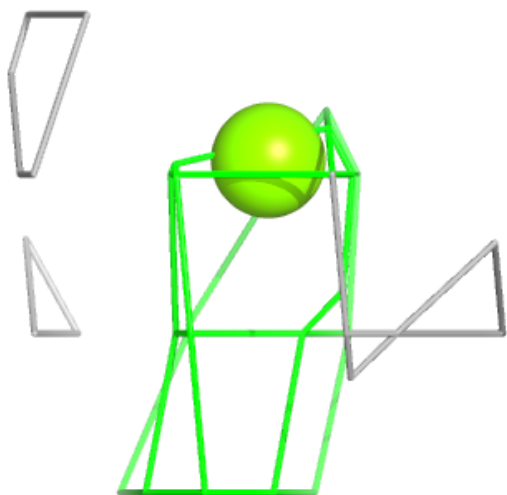
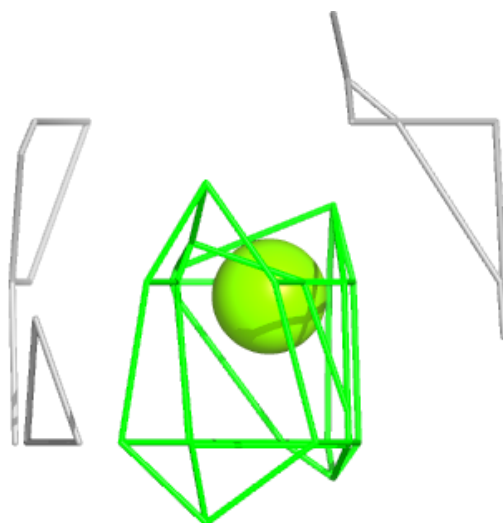
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around MG M 702:**

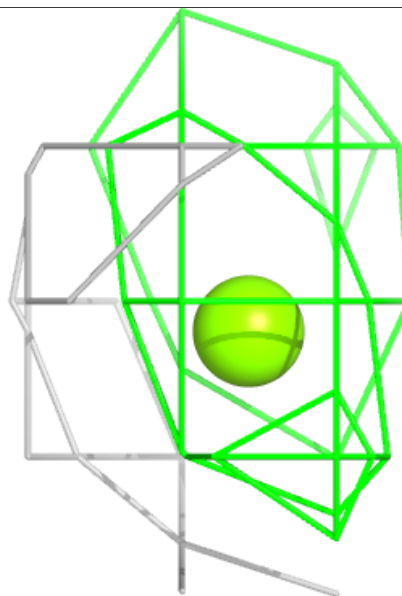
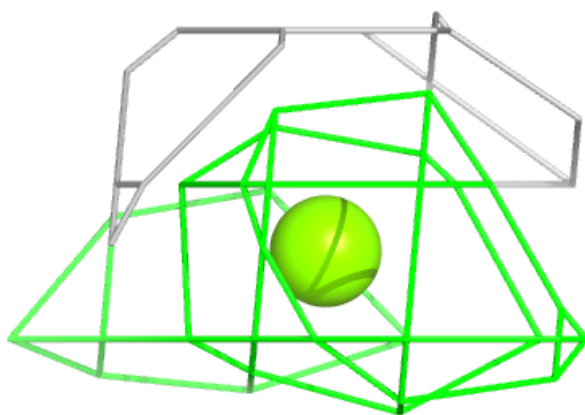
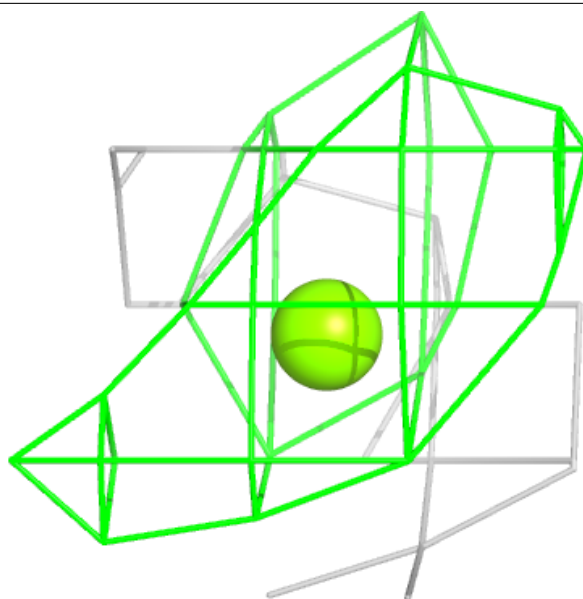
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





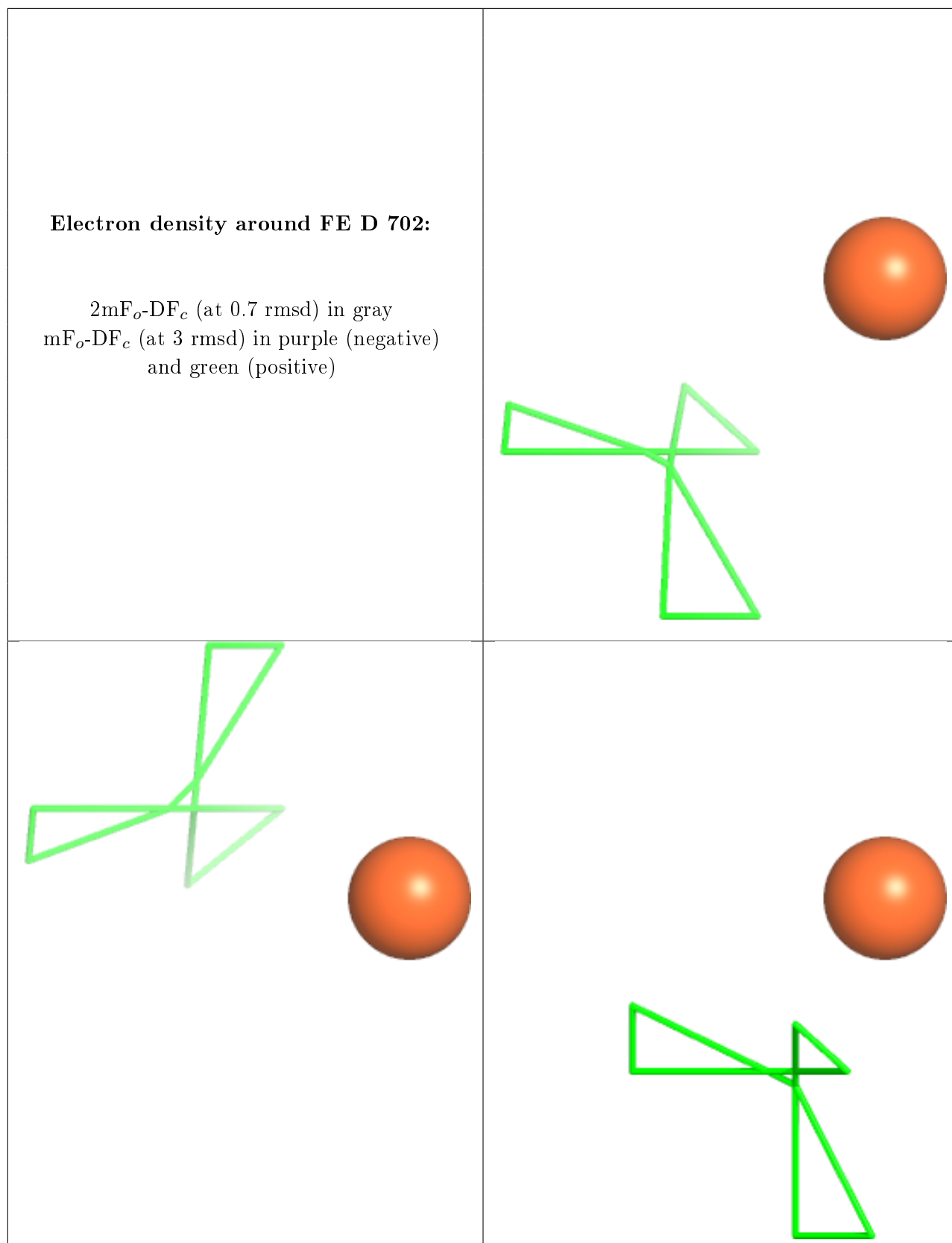
**Electron density around MG N 702:**

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



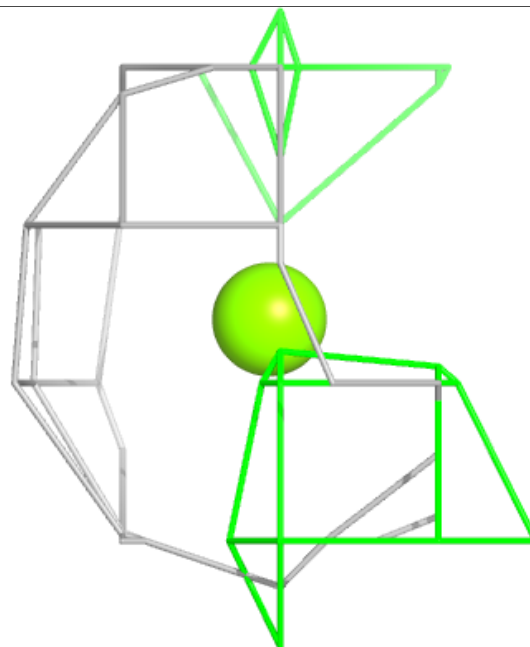
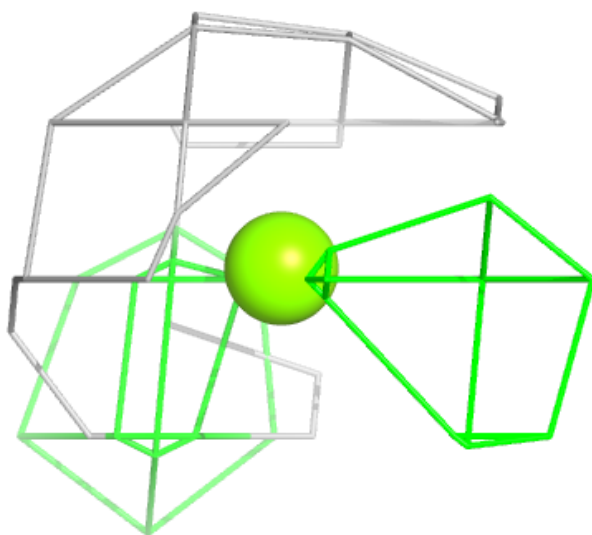
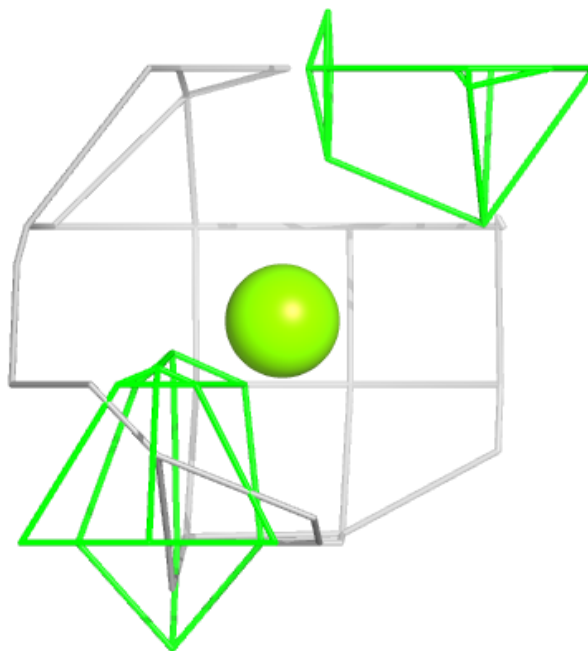
**Electron density around FE D 702:**

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



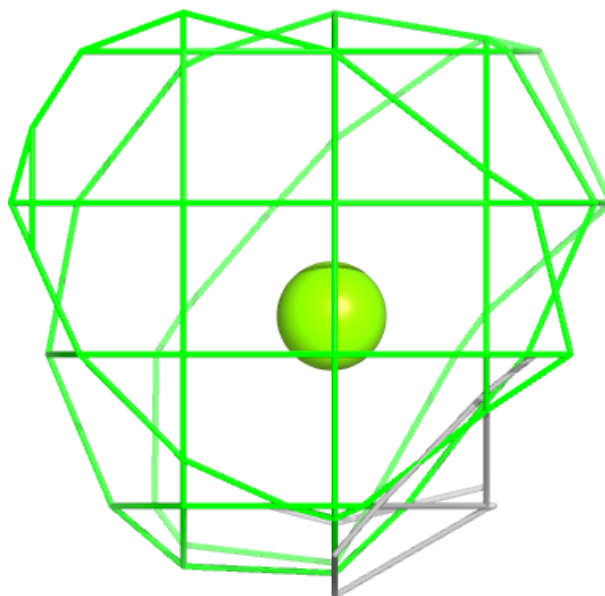
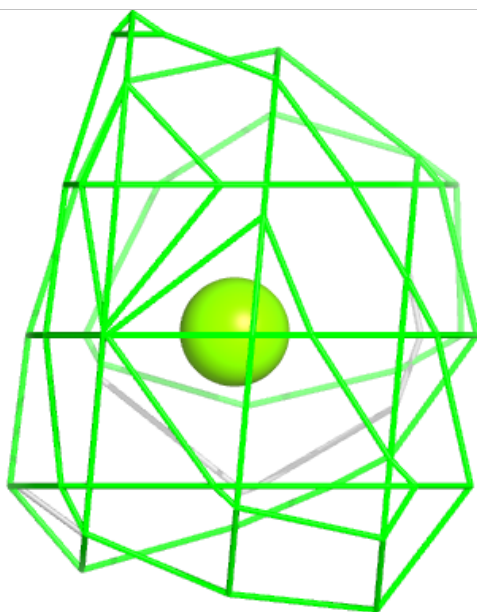
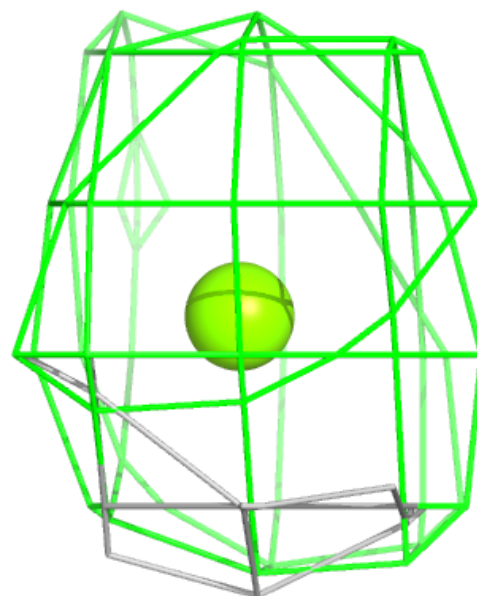
**Electron density around MG B 703:**

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



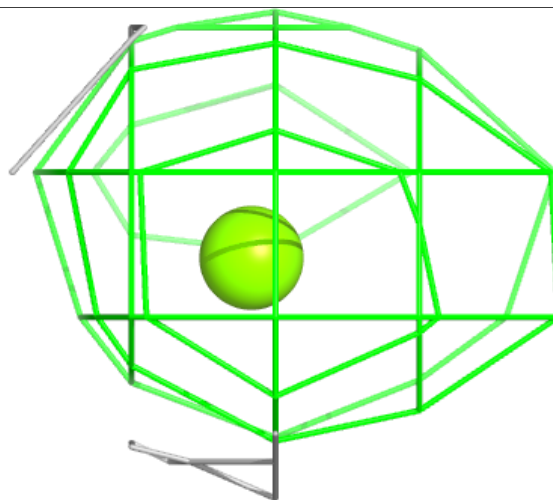
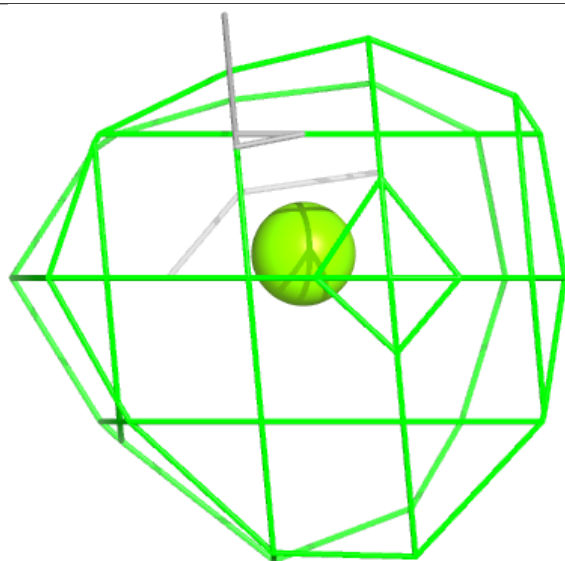
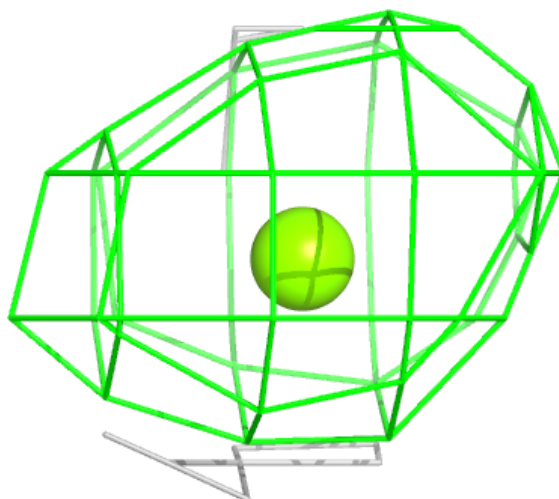
**Electron density around MG J 703:**

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



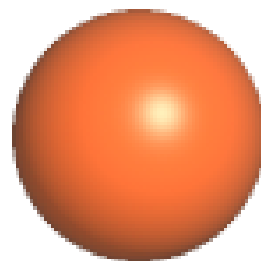
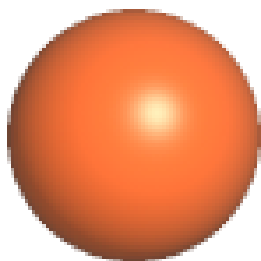
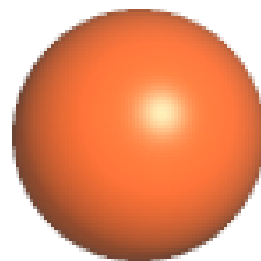
**Electron density around MG O 703:**

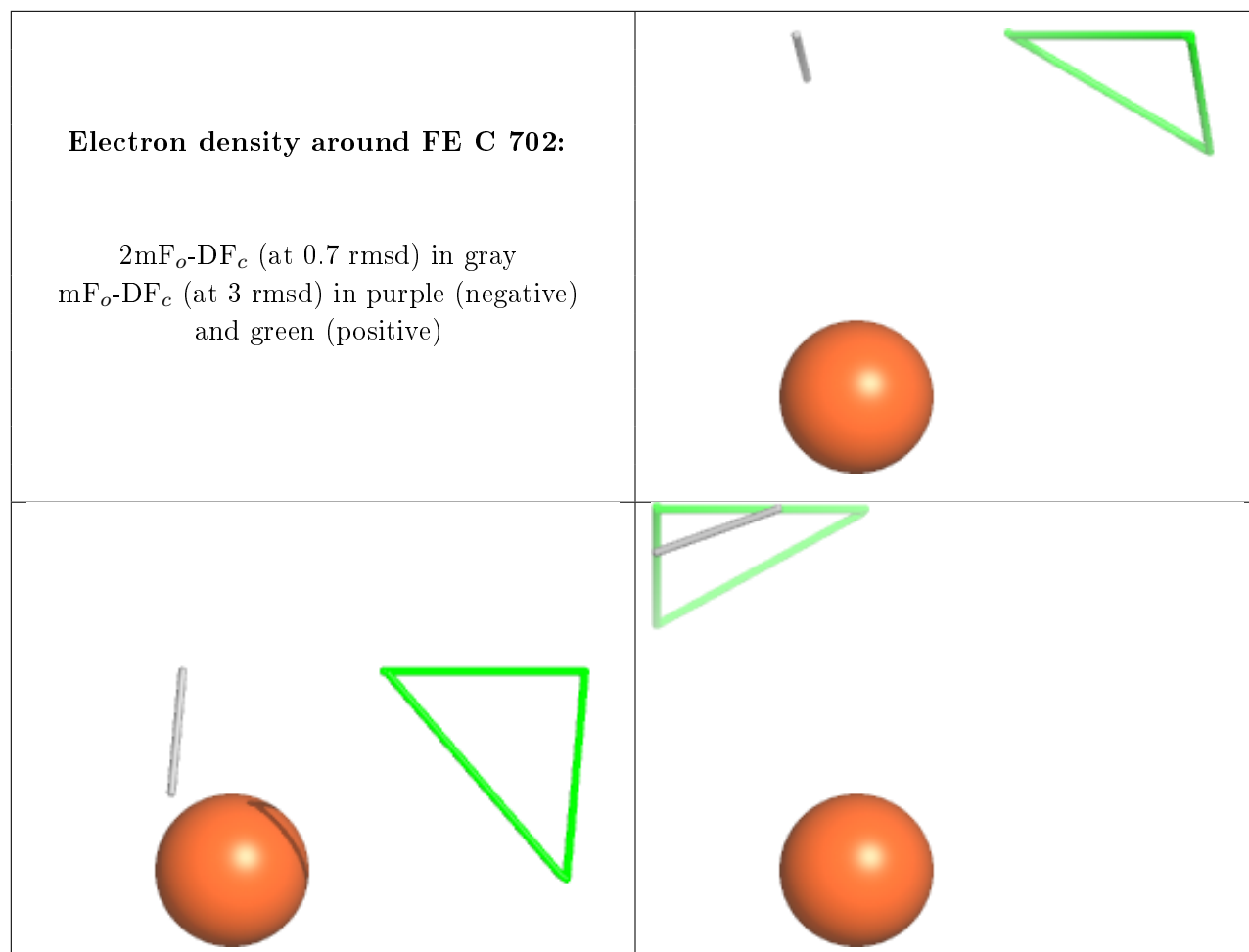
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

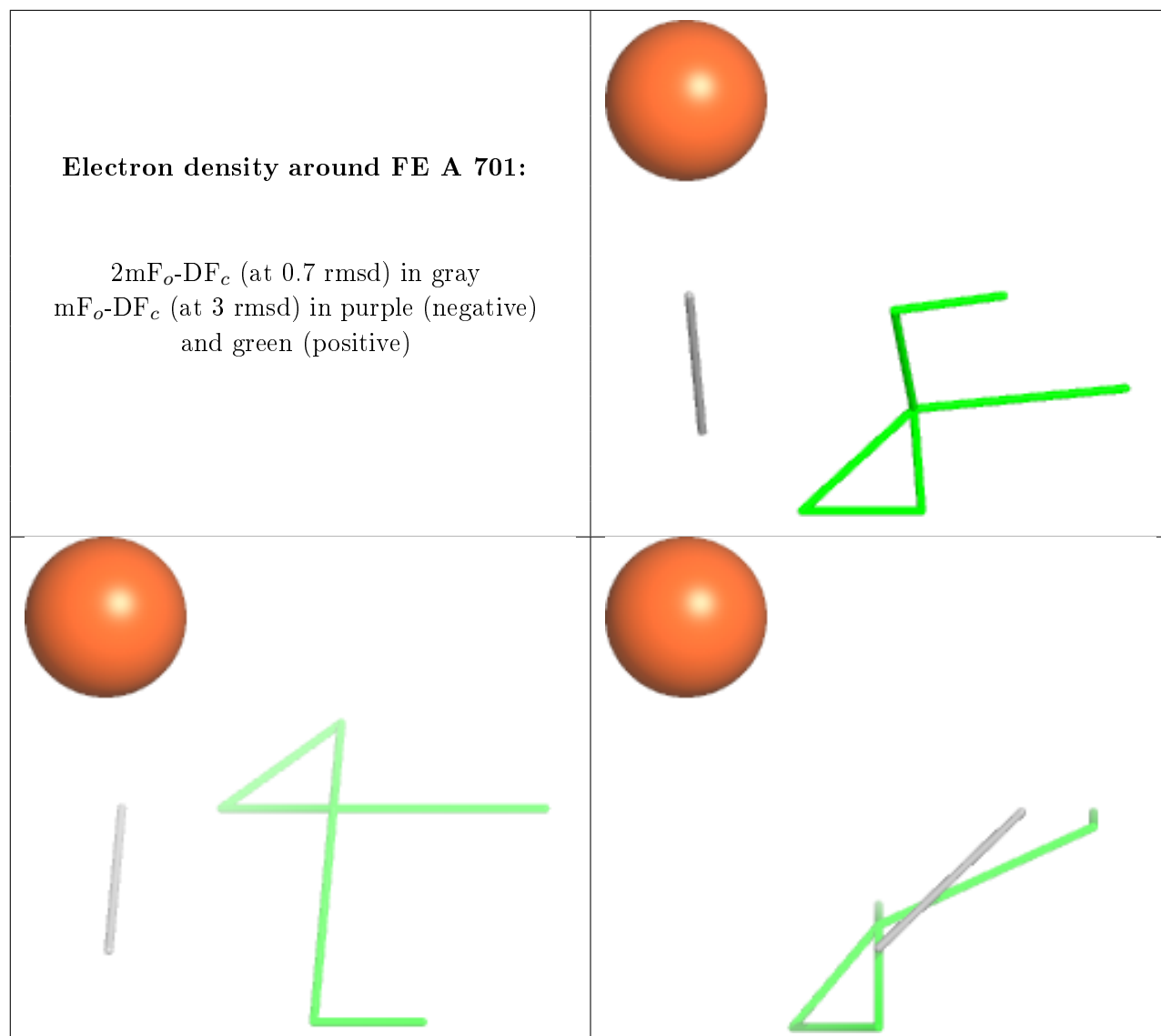


**Electron density around FE P 702:**

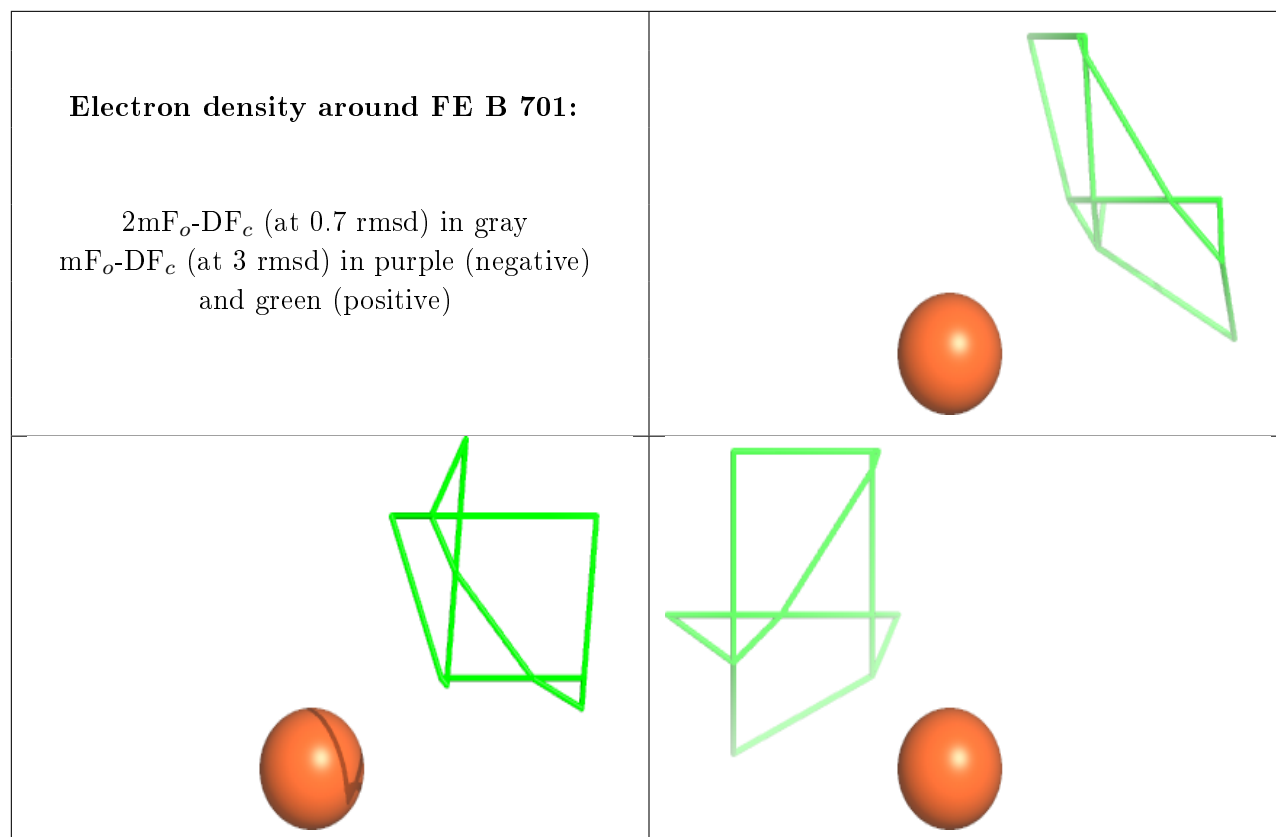
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)











## 6.5 Other polymers [i](#)

There are no such residues in this entry.