wwPDB X-ray Structure Validation Summary Report (i)

Jan 15, 2024 – 10:51 pm GMT

PDB ID	:	6TXE
Title	:	Crystal structure of tetrameric human wt-SAMHD1 (residues 109-626) with GTP, dATP, dTMPNPP and Mg
Authors	:	Morris, E.R.; Kunzelmann, S.; Caswell, S.J.; Arnold, L.H.; Purkiss, A.G.; Kelly, G.; Taylor, I.A.
Deposited on	:	2020-01-14
Resolution	:	3.19 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

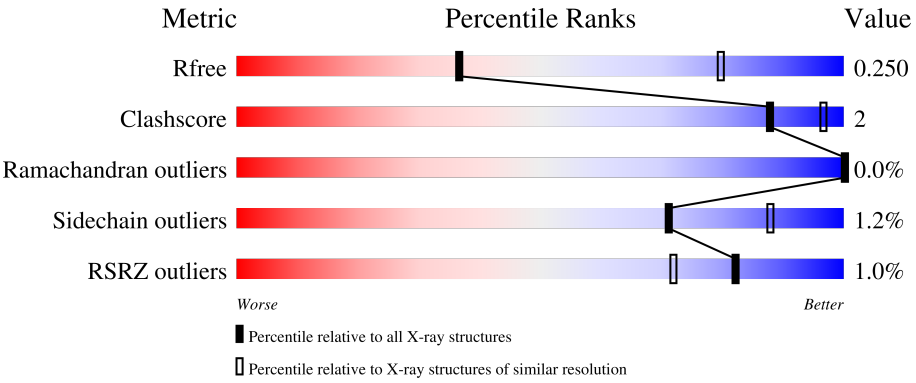
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.19 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	520	86% 6% 8%
1	B	520	87% 5% 8%
1	C	520	87% 5% 8%
1	D	520	87% 5% 8%

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Mol	Chain	Length	Quality of chain
1	E	520	88% 8%
1	F	520	85% 6% 8%
1	G	520	86% 6% 8%
1	H	520	86% 6% 8%
1	I	520	% 86% 5% 8%
1	J	520	87% 5% 8%
1	K	520	87% 5% 8%
1	L	520	% 86% 5% 8%
1	M	520	4% 87% 9%
1	N	520	% 87% 8%
1	O	520	3% 87% 5% 8%
1	P	520	3% 86% 5% 9%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 62675 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	666	704	20			
1	B	479	Total	C	N	O	S	0	0	0
			3841	2458	663	700	20			
1	C	480	Total	C	N	O	S	0	0	0
			3839	2459	662	698	20			
1	D	481	Total	C	N	O	S	0	0	0
			3852	2465	666	701	20			
1	E	479	Total	C	N	O	S	0	0	0
			3845	2461	664	700	20			
1	F	478	Total	C	N	O	S	0	0	0
			3831	2452	658	701	20			
1	G	479	Total	C	N	O	S	0	0	0
			3826	2447	658	701	20			
1	H	480	Total	C	N	O	S	0	0	0
			3862	2473	667	702	20			
1	I	477	Total	C	N	O	S	0	0	0
			3824	2448	658	698	20			
1	J	478	Total	C	N	O	S	0	0	0
			3823	2448	660	695	20			
1	K	478	Total	C	N	O	S	0	0	0
			3824	2448	658	698	20			
1	L	478	Total	C	N	O	S	0	0	0
			3785	2422	646	697	20			
1	M	475	Total	C	N	O	S	0	0	0
			3744	2398	636	690	20			
1	N	477	Total	C	N	O	S	0	0	0
			3812	2442	652	698	20			
1	O	481	Total	C	N	O	S	0	0	0
			3818	2441	654	703	20			
1	P	474	Total	C	N	O	S	0	0	0
			3728	2391	635	682	20			

There are 32 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0
2	E	1	Total Fe 1 1	0	0
2	F	1	Total Fe 1 1	0	0
2	G	1	Total Fe 1 1	0	0
2	H	1	Total Fe 1 1	0	0
2	I	1	Total Fe 1 1	0	0
2	J	1	Total Fe 1 1	0	0
2	K	1	Total Fe 1 1	0	0
2	L	1	Total Fe 1 1	0	0
2	M	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	P	1	Total Fe 1 1	0	0

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

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

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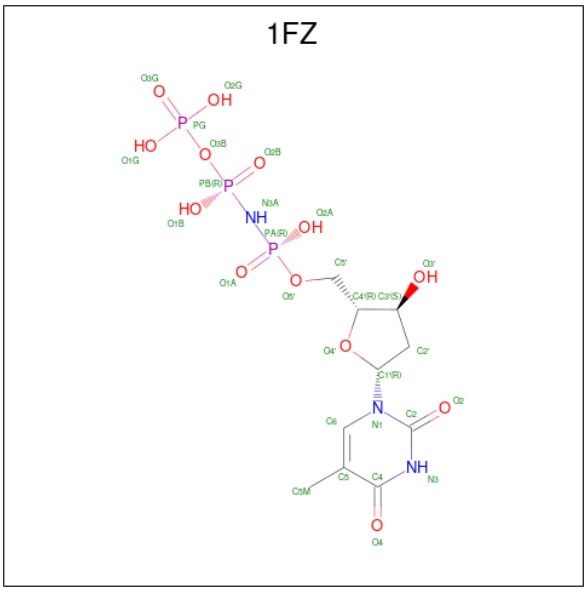
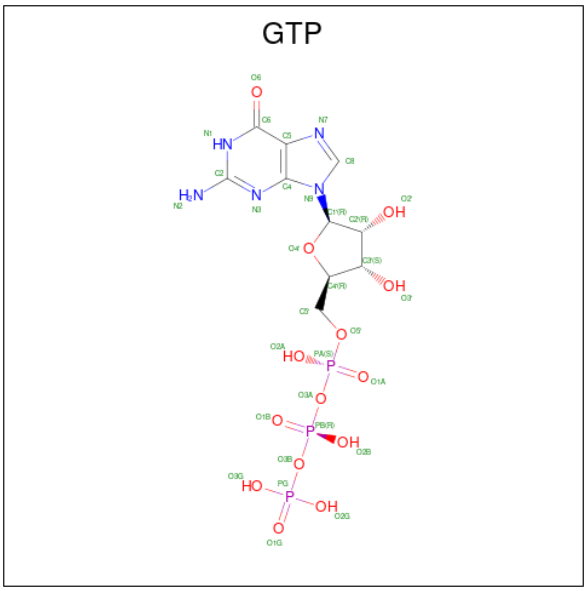
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	2	Total Mg 2 2	0	0
3	G	2	Total Mg 2 2	0	0
3	H	2	Total Mg 2 2	0	0
3	I	2	Total Mg 2 2	0	0
3	J	2	Total Mg 2 2	0	0
3	K	2	Total Mg 2 2	0	0
3	L	2	Total Mg 2 2	0	0
3	M	2	Total Mg 2 2	0	0
3	N	2	Total Mg 2 2	0	0
3	O	2	Total Mg 2 2	0	0
3	P	2	Total Mg 2 2	0	0

- Molecule 4 is 5'-O-[(R)-hydroxy{[(R)-hydroxy(phosphonooxy)phosphoryl]amino}phosphoryl]thymidine (three-letter code: 1FZ) (formula: $C_{10}H_{18}N_3O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			29	10	3	13	3		
4	B	1	Total	C	N	O	P	0	0
			29	10	3	13	3		
4	C	1	Total	C	N	O	P	0	0
			29	10	3	13	3		
4	D	1	Total	C	N	O	P	0	0
			29	10	3	13	3		
4	E	1	Total	C	N	O	P	0	0
			29	10	3	13	3		
4	F	1	Total	C	N	O	P	0	0
			29	10	3	13	3		
4	G	1	Total	C	N	O	P	0	0
			29	10	3	13	3		
4	H	1	Total	C	N	O	P	0	0
			29	10	3	13	3		
4	I	1	Total	C	N	O	P	0	0
			29	10	3	13	3		
4	J	1	Total	C	N	O	P	0	0
			29	10	3	13	3		
4	K	1	Total	C	N	O	P	0	0
			29	10	3	13	3		
4	L	1	Total	C	N	O	P	0	0
			29	10	3	13	3		
4	M	1	Total	C	N	O	P	0	0
			29	10	3	13	3		
4	N	1	Total	C	N	O	P	0	0
			29	10	3	13	3		
4	O	1	Total	C	N	O	P	0	0
			29	10	3	13	3		
4	P	1	Total	C	N	O	P	0	0
			29	10	3	13	3		

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



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

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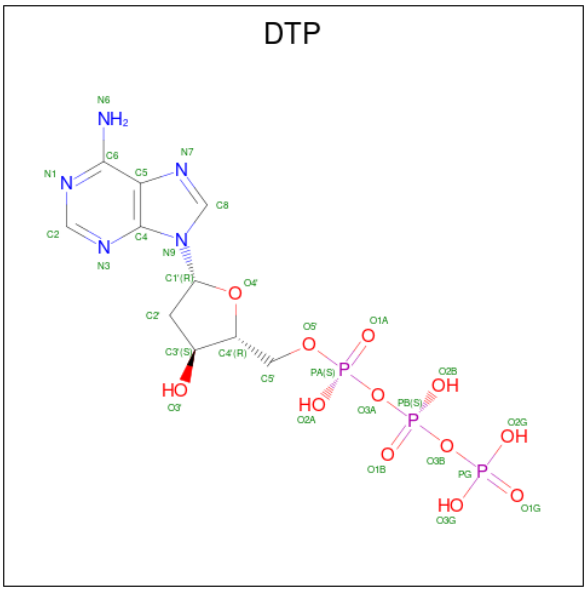
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	O	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	P	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 6 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



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

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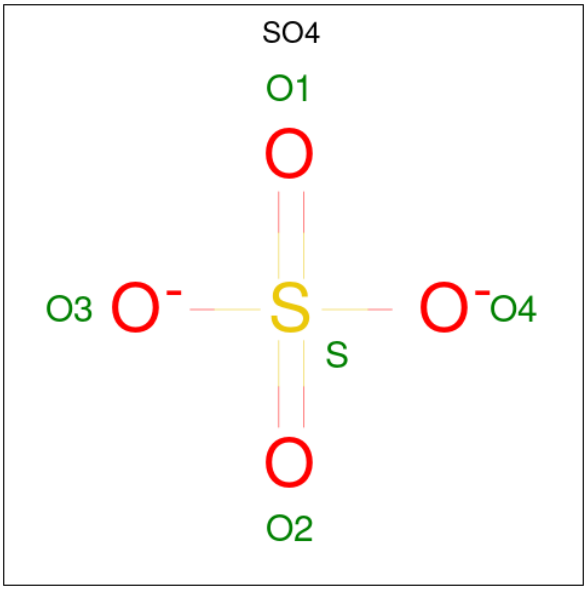
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	J	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
6	K	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
6	L	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
6	M	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
6	M	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
6	N	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
6	N	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		

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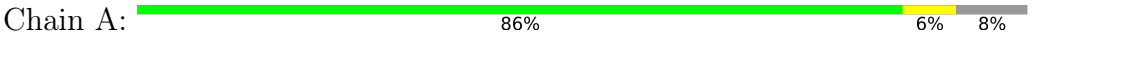
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	1	Total O S 5 4 1	0	0
7	H	1	Total O S 5 4 1	0	0
7	I	1	Total O S 5 4 1	0	0
7	J	1	Total O S 5 4 1	0	0
7	K	1	Total O S 5 4 1	0	0
7	N	1	Total O S 5 4 1	0	0
7	O	1	Total O S 5 4 1	0	0

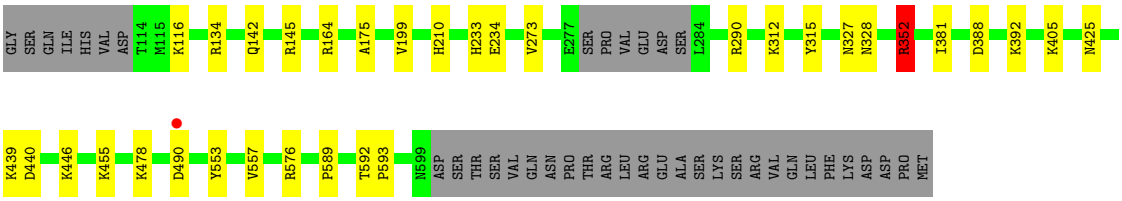
3 Residue-property plots (i)

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

• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

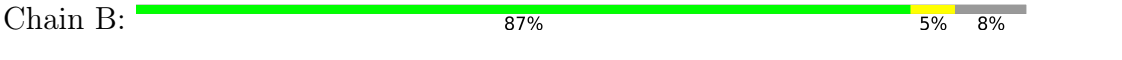
Chain A:

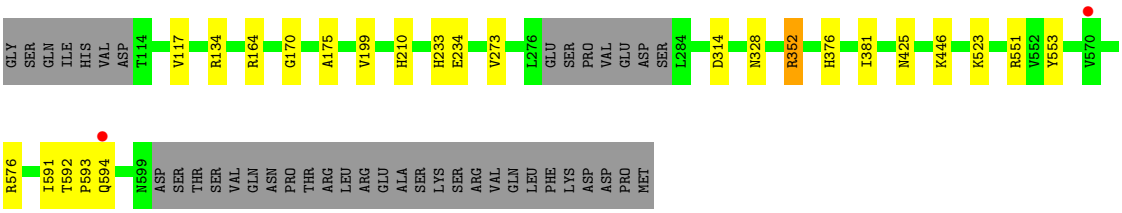




• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

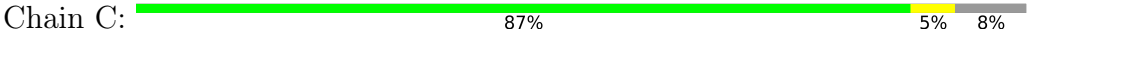
Chain B:

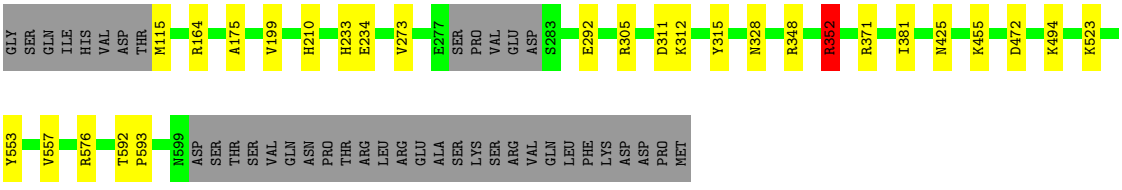




• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

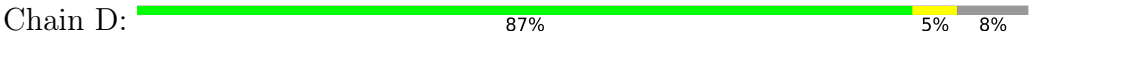
Chain C:

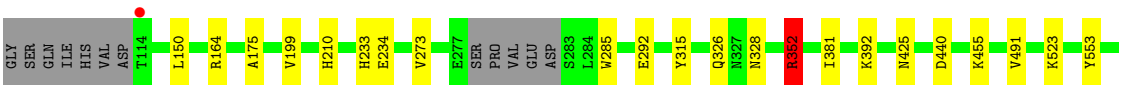


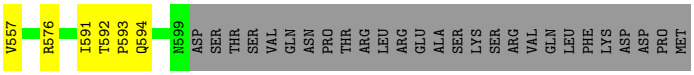


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain D:

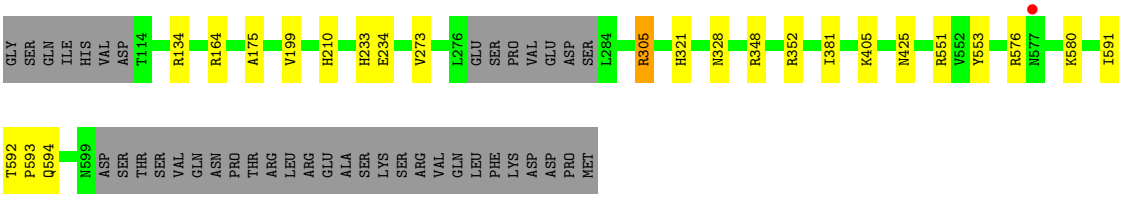






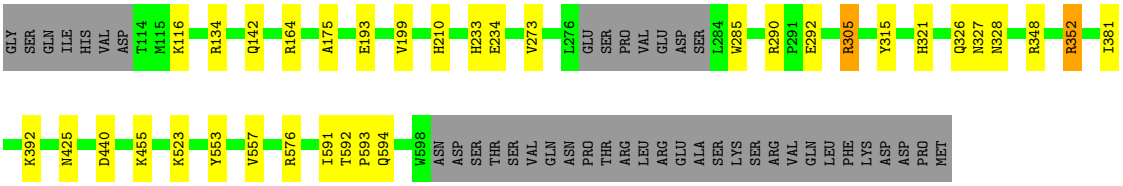
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain E:



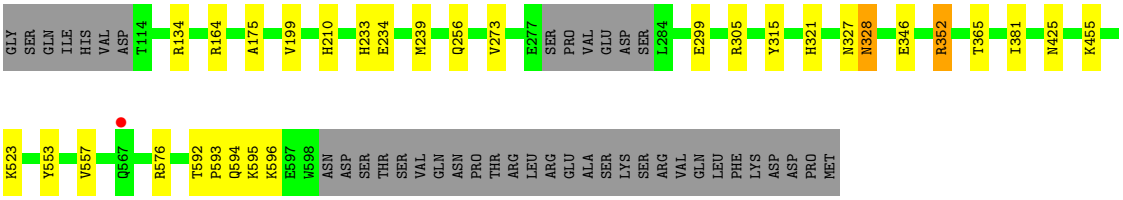
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain F:



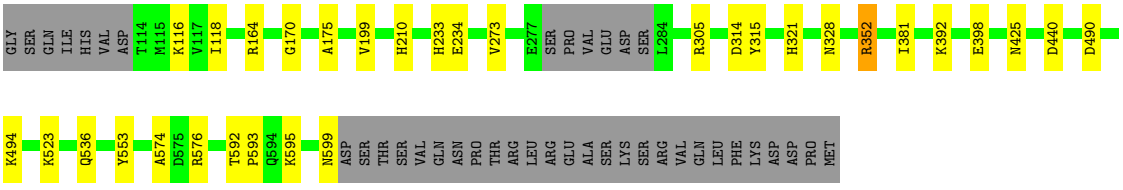
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain G:



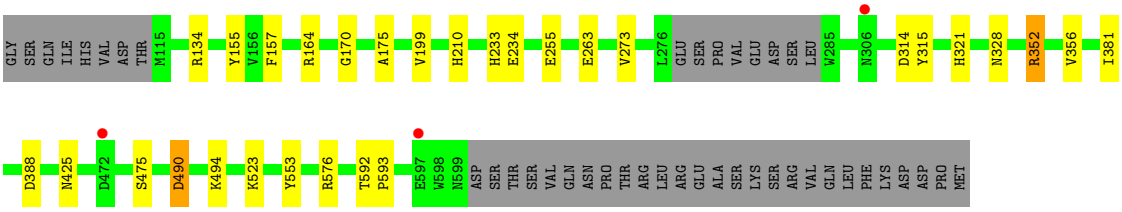
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain H:



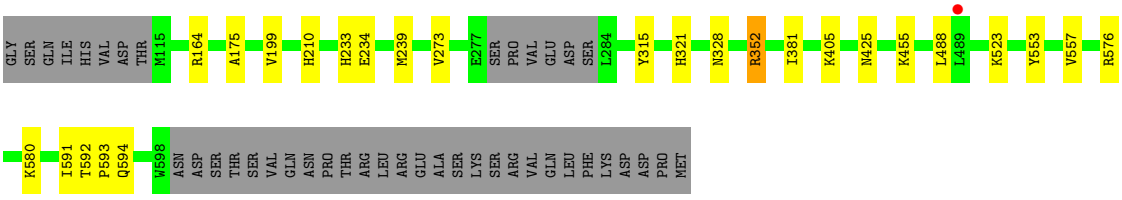
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain I:



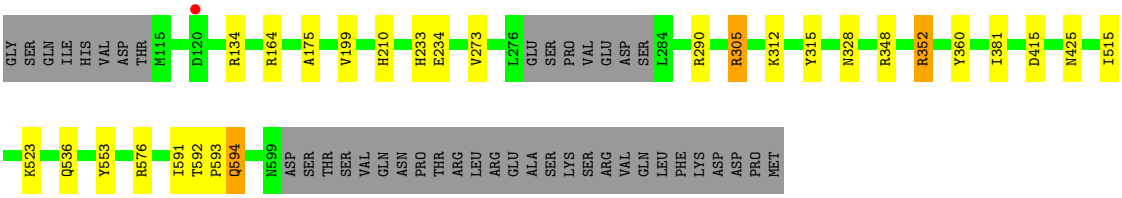
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain J:



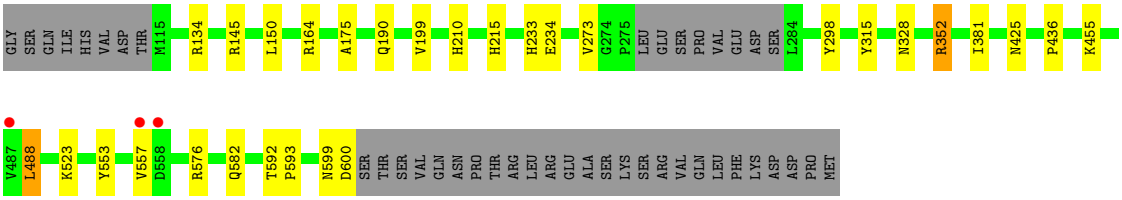
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain K:



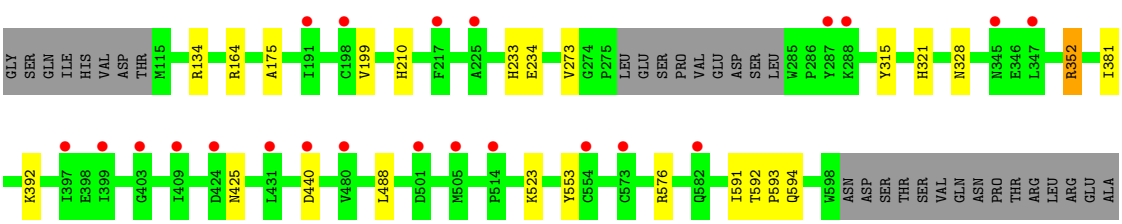
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain L:



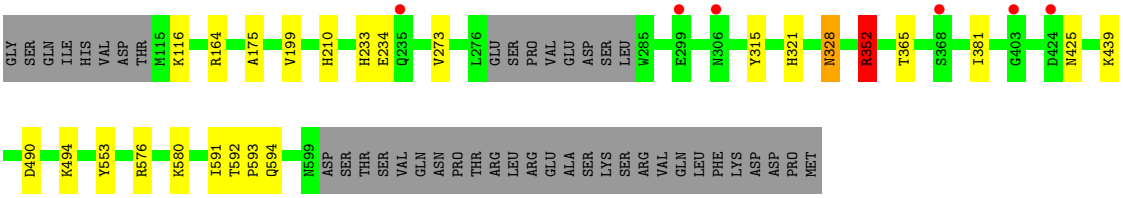
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain M:



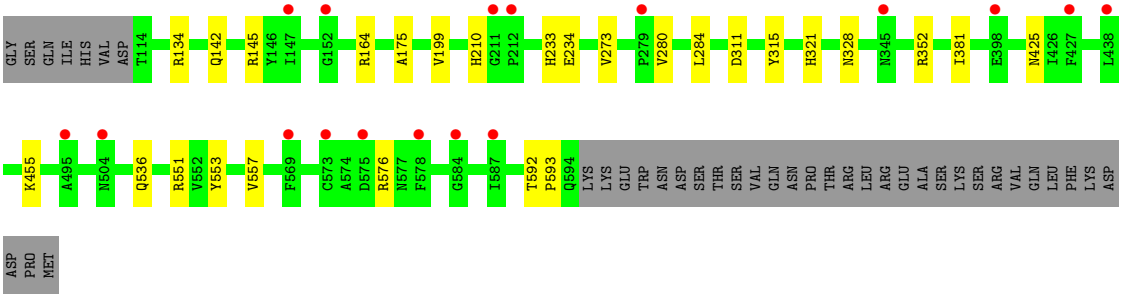
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain N:



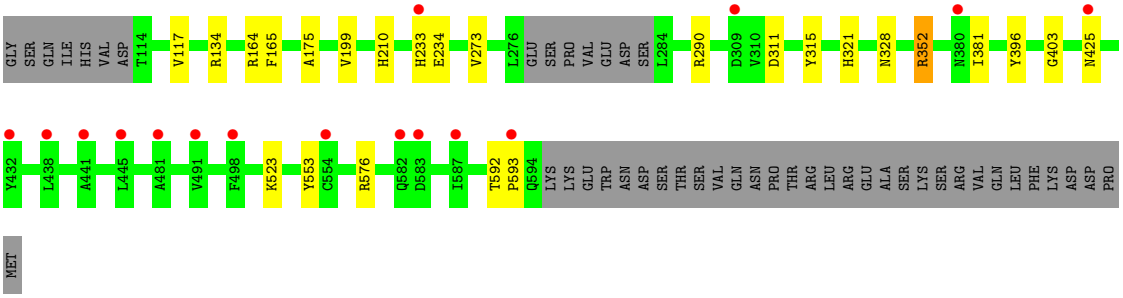
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain O:



• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	97.48Å 172.23Å 275.27Å 90.00° 95.31° 90.00°	Depositor
Resolution (Å)	91.22 – 3.19 274.09 – 3.19	Depositor EDS
% Data completeness (in resolution range)	53.4 (91.22-3.19) 53.2 (274.09-3.19)	Depositor EDS
R_{merge}	0.43	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.218 , 0.252 0.219 , 0.250	Depositor DCC
R_{free} test set	4073 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	50.1	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	62675	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, DTP, MG, 1FZ, GTP, 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	0.53	0/3955	0.75	5/5356 (0.1%)
1	B	0.51	0/3934	0.72	4/5332 (0.1%)
1	C	0.51	1/3932 (0.0%)	0.71	4/5328 (0.1%)
1	D	0.51	0/3945	0.74	3/5346 (0.1%)
1	E	0.49	0/3938	0.71	5/5336 (0.1%)
1	F	0.50	1/3924 (0.0%)	0.72	4/5320 (0.1%)
1	G	0.53	0/3919	0.73	4/5317 (0.1%)
1	H	0.52	1/3955 (0.0%)	0.75	3/5355 (0.1%)
1	I	0.47	0/3917	0.71	4/5308 (0.1%)
1	J	0.48	0/3916	0.74	3/5309 (0.1%)
1	K	0.49	0/3917	0.72	5/5311 (0.1%)
1	L	0.52	1/3878 (0.0%)	0.75	2/5268 (0.0%)
1	M	0.48	0/3837	0.69	2/5216 (0.0%)
1	N	0.50	0/3905	0.74	3/5294 (0.1%)
1	O	0.49	0/3911	0.70	4/5310 (0.1%)
1	P	0.48	0/3819	0.74	3/5189 (0.1%)
All	All	0.50	4/62602 (0.0%)	0.73	58/84895 (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	G	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	298	TYR	CG-CD2	5.96	1.46	1.39
1	F	193	GLU	CD-OE2	5.22	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	292	GLU	CD-OE1	-5.18	1.20	1.25
1	H	398	GLU	CD-OE2	-5.07	1.20	1.25

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	164	ARG	NE-CZ-NH1	14.86	127.73	120.30
1	D	164	ARG	NE-CZ-NH1	14.57	127.58	120.30
1	H	164	ARG	NE-CZ-NH2	-14.55	113.03	120.30
1	P	164	ARG	NE-CZ-NH1	14.51	127.56	120.30
1	N	164	ARG	NE-CZ-NH2	-14.46	113.07	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	595	LYS	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	3766	18	0
1	B	3841	0	3729	14	0
1	C	3839	0	3730	15	1
1	D	3852	0	3743	18	0
1	E	3845	0	3740	13	0
1	F	3831	0	3711	20	0
1	G	3826	0	3685	18	0
1	H	3862	0	3773	17	0
1	I	3824	0	3709	17	2
1	J	3823	0	3703	23	0
1	K	3824	0	3700	18	0
1	L	3785	0	3608	17	3
1	M	3744	0	3554	24	0
1	N	3812	0	3687	14	0
1	O	3818	0	3675	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	3728	0	3568	14	2
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	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
3	M	2	0	0	0	0
3	N	2	0	0	0	0
3	O	2	0	0	0	0
3	P	2	0	0	0	0
4	A	29	0	14	1	0
4	B	29	0	14	0	0
4	C	29	0	14	2	0
4	D	29	0	14	2	0
4	E	29	0	14	0	0
4	F	29	0	14	0	0
4	G	29	0	14	0	0
4	H	29	0	14	0	0
4	I	29	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	29	0	14	1	0
4	K	29	0	14	2	0
4	L	29	0	14	2	0
4	M	29	0	14	0	0
4	N	29	0	14	0	0
4	O	29	0	14	1	0
4	P	29	0	14	1	0
5	A	32	0	12	4	0
5	B	32	0	12	2	0
5	D	64	0	24	1	0
5	E	32	0	12	0	0
5	F	32	0	12	2	0
5	G	32	0	12	2	0
5	H	32	0	12	2	0
5	I	64	0	24	5	0
5	K	32	0	12	1	0
5	L	32	0	12	1	0
5	M	32	0	12	0	0
5	N	32	0	12	1	0
5	O	32	0	12	4	0
5	P	32	0	12	3	0
6	A	30	0	12	1	0
6	B	30	0	12	2	0
6	C	30	0	12	2	0
6	D	30	0	12	2	0
6	E	30	0	12	2	0
6	F	30	0	12	0	0
6	G	30	0	12	1	0
6	H	30	0	12	0	0
6	I	30	0	12	2	0
6	J	30	0	12	0	0
6	K	30	0	12	2	0
6	L	30	0	12	3	0
6	M	60	0	24	4	0
6	N	60	0	24	2	0
7	B	5	0	0	0	0
7	C	5	0	0	0	0
7	D	5	0	0	0	0
7	E	5	0	0	1	0
7	F	5	0	0	0	0
7	H	5	0	0	1	0
7	I	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	J	5	0	0	0	0
7	K	5	0	0	0	0
7	N	5	0	0	0	0
7	O	5	0	0	0	0
All	All	62675	0	59689	245	4

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 245 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:K:305:ARG:NH1	1:K:348:ARG:HD3	1.55	1.22
1:J:488:LEU:HA	1:M:488:LEU:HB2	1.30	1.13
1:J:488:LEU:CA	1:M:488:LEU:HB2	1.90	1.00
1:K:305:ARG:HH11	1:K:348:ARG:HD3	1.22	0.90
1:J:488:LEU:HB2	1:M:488:LEU:N	1.94	0.83

All (4) 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]	1.29	0.91
1:I:475:SER:OG	1:L:436:PRO:CB[2_754]	1.70	0.50
1:I:475:SER:CB	1:L:436:PRO:CB[2_754]	2.11	0.09
1:L:190:GLN:OE1	1:P:403:GLY:N[2_654]	2.12	0.08

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	476/520 (92%)	461 (97%)	15 (3%)	0	100	100
1	B	475/520 (91%)	459 (97%)	16 (3%)	0	100	100
1	C	476/520 (92%)	459 (96%)	17 (4%)	0	100	100
1	D	477/520 (92%)	460 (96%)	17 (4%)	0	100	100
1	E	475/520 (91%)	459 (97%)	16 (3%)	0	100	100
1	F	474/520 (91%)	458 (97%)	16 (3%)	0	100	100
1	G	475/520 (91%)	458 (96%)	17 (4%)	0	100	100
1	H	476/520 (92%)	459 (96%)	17 (4%)	0	100	100
1	I	473/520 (91%)	458 (97%)	15 (3%)	0	100	100
1	J	474/520 (91%)	459 (97%)	15 (3%)	0	100	100
1	K	474/520 (91%)	458 (97%)	16 (3%)	0	100	100
1	L	474/520 (91%)	457 (96%)	17 (4%)	0	100	100
1	M	471/520 (91%)	455 (97%)	16 (3%)	0	100	100
1	N	473/520 (91%)	457 (97%)	16 (3%)	0	100	100
1	O	479/520 (92%)	460 (96%)	18 (4%)	1 (0%)	47	79
1	P	470/520 (90%)	454 (97%)	16 (3%)	0	100	100
All	All	7592/8320 (91%)	7331 (97%)	260 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	280	VAL

5.3.2 Protein sidechains (i)

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%)	403 (98%)	8 (2%)	57	81
1	B	407/464 (88%)	403 (99%)	4 (1%)	76	90
1	C	406/464 (88%)	401 (99%)	5 (1%)	71	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	408/464 (88%)	405 (99%)	3 (1%)	84 94
1	E	408/464 (88%)	404 (99%)	4 (1%)	76 90
1	F	406/464 (88%)	402 (99%)	4 (1%)	76 90
1	G	403/464 (87%)	397 (98%)	6 (2%)	65 85
1	H	411/464 (89%)	406 (99%)	5 (1%)	71 88
1	I	405/464 (87%)	399 (98%)	6 (2%)	65 85
1	J	403/464 (87%)	399 (99%)	4 (1%)	76 90
1	K	404/464 (87%)	399 (99%)	5 (1%)	71 88
1	L	395/464 (85%)	390 (99%)	5 (1%)	69 87
1	M	389/464 (84%)	385 (99%)	4 (1%)	76 90
1	N	403/464 (87%)	396 (98%)	7 (2%)	60 83
1	O	403/464 (87%)	399 (99%)	4 (1%)	76 90
1	P	388/464 (84%)	384 (99%)	4 (1%)	76 90
All	All	6450/7424 (87%)	6372 (99%)	78 (1%)	71 88

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	488	LEU
1	O	315	TYR
1	M	134	ARG
1	N	352	ARG
1	P	315	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	594	GLN
1	M	210	HIS
1	K	271	GLN
1	L	210	HIS
1	M	425	ASN

5.3.3 RNA

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 107 ligands modelled in this entry, 48 are monoatomic - leaving 59 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	DTP	K	701	3	26,32,32	1.13	2 (7%)	30,50,50	1.62	5 (16%)
5	GTP	I	705	3	26,34,34	0.93	1 (3%)	32,54,54	1.67	8 (25%)
6	DTP	D	701	3	26,32,32	1.01	2 (7%)	30,50,50	1.77	6 (20%)
6	DTP	G	701	3	26,32,32	0.94	2 (7%)	30,50,50	1.60	5 (16%)
7	SO4	I	706	-	4,4,4	0.40	0	6,6,6	0.23	0
4	1FZ	P	704	3,2	29,30,30	1.10	4 (13%)	42,47,47	1.22	3 (7%)
4	1FZ	E	704	3,2	29,30,30	1.14	4 (13%)	42,47,47	1.12	3 (7%)
4	1FZ	B	704	3,2	29,30,30	1.12	4 (13%)	42,47,47	1.49	6 (14%)
6	DTP	L	701	3	26,32,32	0.91	0	30,50,50	1.54	7 (23%)
5	GTP	P	705	3	26,34,34	0.96	1 (3%)	32,54,54	1.18	3 (9%)
7	SO4	N	707	-	4,4,4	0.27	0	6,6,6	0.37	0
4	1FZ	J	704	3,2	29,30,30	1.25	5 (17%)	42,47,47	1.37	5 (11%)
5	GTP	D	702	3	26,34,34	0.97	1 (3%)	32,54,54	1.21	1 (3%)
5	GTP	D	707	3	26,34,34	1.02	1 (3%)	32,54,54	1.28	6 (18%)
5	GTP	H	706	3	26,34,34	0.88	1 (3%)	32,54,54	1.43	3 (9%)
5	GTP	F	705	3	26,34,34	1.11	1 (3%)	32,54,54	1.43	4 (12%)
6	DTP	I	708	3	26,32,32	0.97	2 (7%)	30,50,50	1.49	6 (20%)
6	DTP	M	707	3	26,32,32	0.96	2 (7%)	30,50,50	1.47	4 (13%)
7	SO4	E	706	-	4,4,4	0.49	0	6,6,6	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	DTP	E	707	3	26,32,32	1.00	2 (7%)	30,50,50	1.84	7 (23%)
4	1FZ	L	705	3	29,30,30	1.09	4 (13%)	42,47,47	1.37	4 (9%)
4	1FZ	O	704	3,2	29,30,30	1.14	4 (13%)	42,47,47	1.39	3 (7%)
5	GTP	G	706	3	26,34,34	1.06	1 (3%)	32,54,54	1.41	3 (9%)
5	GTP	B	705	3	26,34,34	1.08	1 (3%)	32,54,54	1.31	4 (12%)
5	GTP	A	705	3	26,34,34	1.04	1 (3%)	32,54,54	1.32	6 (18%)
5	GTP	K	706	3	26,34,34	0.86	0	32,54,54	1.30	4 (12%)
6	DTP	C	701	3	26,32,32	1.04	2 (7%)	30,50,50	1.54	7 (23%)
5	GTP	L	706	3	26,34,34	1.02	1 (3%)	32,54,54	1.20	3 (9%)
4	1FZ	M	704	3,2	29,30,30	1.04	4 (13%)	42,47,47	1.34	5 (11%)
6	DTP	J	706	3	26,32,32	0.90	1 (3%)	30,50,50	1.77	5 (16%)
6	DTP	N	701	3	26,32,32	1.06	3 (11%)	30,50,50	1.60	4 (13%)
7	SO4	C	706	-	4,4,4	0.35	0	6,6,6	0.33	0
4	1FZ	C	705	3,2	29,30,30	1.17	2 (6%)	42,47,47	1.29	4 (9%)
4	1FZ	N	705	3,2	29,30,30	1.05	4 (13%)	42,47,47	1.45	5 (11%)
7	SO4	K	707	-	4,4,4	0.30	0	6,6,6	0.38	0
5	GTP	O	705	3	26,34,34	1.10	3 (11%)	32,54,54	1.26	2 (6%)
4	1FZ	G	705	3,2	29,30,30	1.20	5 (17%)	42,47,47	1.31	3 (7%)
6	DTP	N	708	3	26,32,32	0.96	1 (3%)	30,50,50	1.76	7 (23%)
5	GTP	I	707	3	26,34,34	1.22	2 (7%)	32,54,54	1.62	8 (25%)
7	SO4	O	706	-	4,4,4	0.40	0	6,6,6	0.33	0
6	DTP	F	707	3	26,32,32	0.82	0	30,50,50	1.55	7 (23%)
6	DTP	B	707	3	26,32,32	1.02	2 (7%)	30,50,50	1.38	4 (13%)
4	1FZ	K	705	3,2	29,30,30	1.06	4 (13%)	42,47,47	1.27	3 (7%)
7	SO4	H	707	-	4,4,4	0.44	0	6,6,6	0.30	0
7	SO4	D	708	-	4,4,4	0.47	0	6,6,6	0.55	0
7	SO4	J	705	-	4,4,4	0.31	0	6,6,6	0.36	0
5	GTP	E	705	3	26,34,34	0.97	1 (3%)	32,54,54	1.77	7 (21%)
6	DTP	H	701	3	26,32,32	0.98	2 (7%)	30,50,50	1.46	4 (13%)
4	1FZ	H	705	3,2	29,30,30	1.17	4 (13%)	42,47,47	1.38	5 (11%)
6	DTP	M	706	3	26,32,32	1.08	2 (7%)	30,50,50	1.54	7 (23%)
5	GTP	N	706	3	26,34,34	1.14	1 (3%)	32,54,54	1.37	6 (18%)
6	DTP	A	706	3	26,32,32	0.96	1 (3%)	30,50,50	1.85	8 (26%)
7	SO4	B	706	-	4,4,4	0.39	0	6,6,6	0.29	0
5	GTP	M	705	3	26,34,34	0.86	1 (3%)	32,54,54	1.52	4 (12%)
4	1FZ	F	704	3,2	29,30,30	1.15	4 (13%)	42,47,47	1.24	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	1FZ	I	704	3,2	29,30,30	1.17	4 (13%)	42,47,47	1.27	4 (9%)
4	1FZ	A	704	3,2	29,30,30	1.20	3 (10%)	42,47,47	1.28	5 (11%)
4	1FZ	D	706	3,2	29,30,30	1.30	4 (13%)	42,47,47	1.23	4 (9%)
7	SO4	F	706	-	4,4,4	0.41	0	6,6,6	0.21	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	DTP	K	701	3	-	2/18/34/34	0/3/3/3
5	GTP	I	705	3	-	4/18/38/38	0/3/3/3
6	DTP	D	701	3	-	1/18/34/34	0/3/3/3
6	DTP	G	701	3	-	2/18/34/34	0/3/3/3
4	1FZ	P	704	3,2	-	7/19/34/34	0/2/2/2
4	1FZ	E	704	3,2	-	6/19/34/34	0/2/2/2
4	1FZ	B	704	3,2	-	6/19/34/34	0/2/2/2
6	DTP	L	701	3	-	2/18/34/34	0/3/3/3
5	GTP	P	705	3	-	4/18/38/38	0/3/3/3
4	1FZ	J	704	3,2	-	10/19/34/34	0/2/2/2
5	GTP	D	702	3	-	5/18/38/38	0/3/3/3
5	GTP	D	707	3	-	5/18/38/38	0/3/3/3
5	GTP	H	706	3	-	0/18/38/38	0/3/3/3
5	GTP	F	705	3	-	2/18/38/38	0/3/3/3
6	DTP	I	708	3	-	3/18/34/34	0/3/3/3
6	DTP	M	707	3	-	6/18/34/34	0/3/3/3
6	DTP	E	707	3	-	2/18/34/34	0/3/3/3
4	1FZ	L	705	3	-	12/19/34/34	0/2/2/2
4	1FZ	O	704	3,2	-	9/19/34/34	0/2/2/2
5	GTP	G	706	3	-	1/18/38/38	0/3/3/3
5	GTP	B	705	3	-	2/18/38/38	0/3/3/3
5	GTP	A	705	3	-	7/18/38/38	0/3/3/3
5	GTP	K	706	3	-	1/18/38/38	0/3/3/3
6	DTP	C	701	3	-	2/18/34/34	0/3/3/3
5	GTP	L	706	3	-	7/18/38/38	0/3/3/3
4	1FZ	M	704	3,2	-	5/19/34/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	DTP	J	706	3	-	3/18/34/34	0/3/3/3
6	DTP	N	701	3	-	4/18/34/34	0/3/3/3
4	1FZ	C	705	3,2	-	6/19/34/34	0/2/2/2
4	1FZ	N	705	3,2	-	8/19/34/34	0/2/2/2
5	GTP	O	705	3	-	6/18/38/38	0/3/3/3
4	1FZ	G	705	3,2	-	11/19/34/34	0/2/2/2
6	DTP	N	708	3	-	4/18/34/34	0/3/3/3
5	GTP	I	707	3	-	5/18/38/38	0/3/3/3
6	DTP	F	707	3	-	4/18/34/34	0/3/3/3
6	DTP	B	707	3	-	3/18/34/34	0/3/3/3
4	1FZ	K	705	3,2	-	8/19/34/34	0/2/2/2
5	GTP	E	705	3	-	0/18/38/38	0/3/3/3
6	DTP	H	701	3	-	4/18/34/34	0/3/3/3
4	1FZ	H	705	3,2	-	9/19/34/34	0/2/2/2
6	DTP	M	706	3	-	2/18/34/34	0/3/3/3
5	GTP	N	706	3	-	2/18/38/38	0/3/3/3
6	DTP	A	706	3	-	3/18/34/34	0/3/3/3
5	GTP	M	705	3	-	1/18/38/38	0/3/3/3
4	1FZ	F	704	3,2	-	6/19/34/34	0/2/2/2
4	1FZ	I	704	3,2	-	8/19/34/34	0/2/2/2
4	1FZ	A	704	3,2	-	6/19/34/34	0/2/2/2
4	1FZ	D	706	3,2	-	8/19/34/34	0/2/2/2

The worst 5 of 107 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	707	GTP	C6-N1	-4.43	1.31	1.37
4	H	705	1FZ	PB-O2B	4.06	1.52	1.46
4	I	704	1FZ	PB-O2B	4.02	1.52	1.46
4	D	706	1FZ	PB-O2B	3.99	1.52	1.46
4	A	704	1FZ	PB-O2B	3.95	1.52	1.46

The worst 5 of 231 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	705	GTP	PA-O3A-PB	-5.40	114.29	132.83
4	K	705	1FZ	O1B-PB-O2B	5.06	120.54	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	N	708	DTP	N3-C2-N1	-5.02	120.84	128.68
5	F	705	GTP	PA-O3A-PB	-5.00	115.66	132.83
6	K	701	DTP	N3-C2-N1	-4.96	120.93	128.68

There are no chirality outliers.

5 of 224 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	704	1FZ	O4'-C1'-N1-C2
4	A	704	1FZ	PA-N3A-PB-O2B
4	A	704	1FZ	PG-O3B-PB-O2B
4	B	704	1FZ	O4'-C1'-N1-C2
4	B	704	1FZ	PA-N3A-PB-O2B

There are no ring outliers.

35 monomers are involved in 55 short contacts:

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

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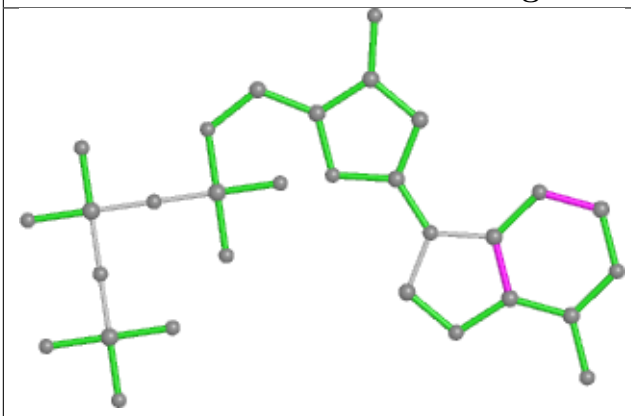
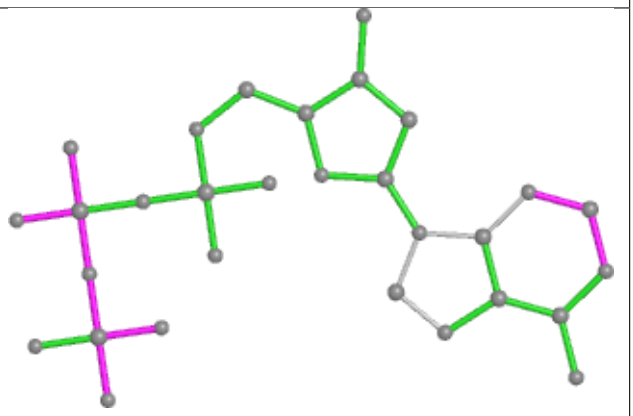
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	705	1FZ	2	0
5	O	705	GTP	4	0
6	N	708	DTP	2	0
5	I	707	GTP	4	0
6	B	707	DTP	2	0
4	K	705	1FZ	2	0
7	H	707	SO4	1	0
6	M	706	DTP	1	0
5	N	706	GTP	1	0
6	A	706	DTP	1	0
4	A	704	1FZ	1	0
4	D	706	1FZ	2	0

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

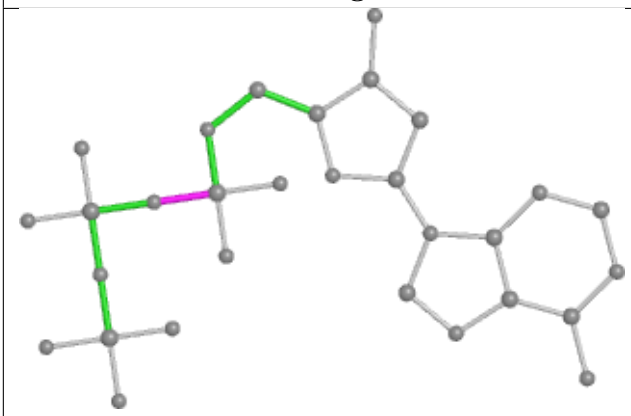
Ligand DTP K 701



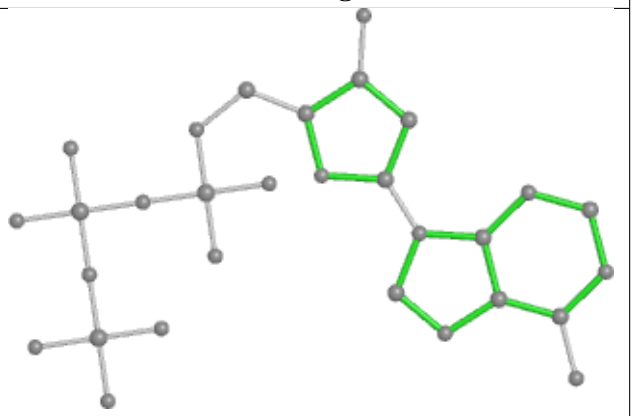
Bond lengths



Bond angles

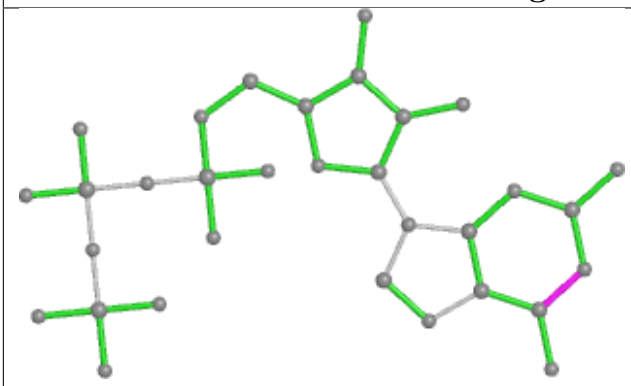


Torsions

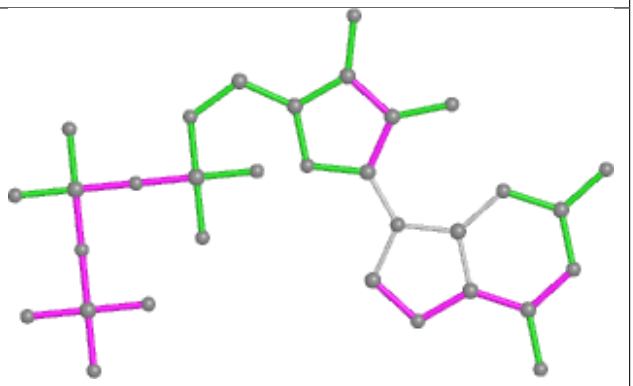


Rings

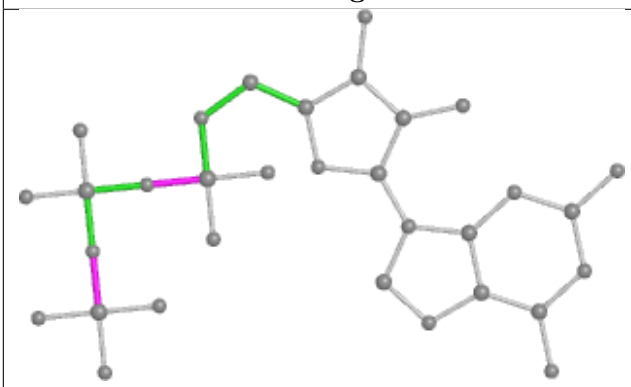
Ligand GTP I 705



Bond lengths



Bond angles



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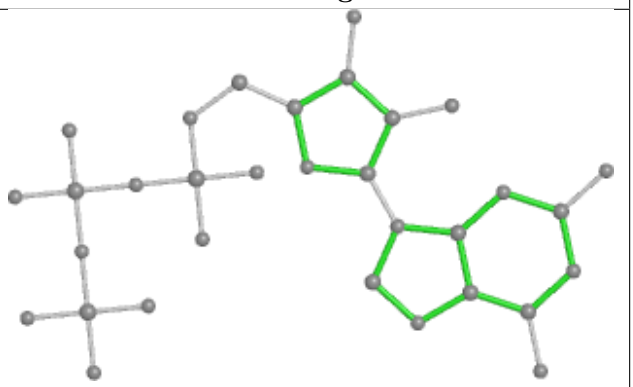
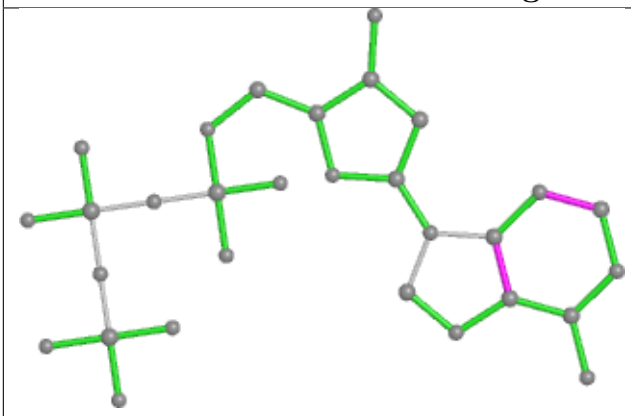


Rings

Ligand DTP D 701



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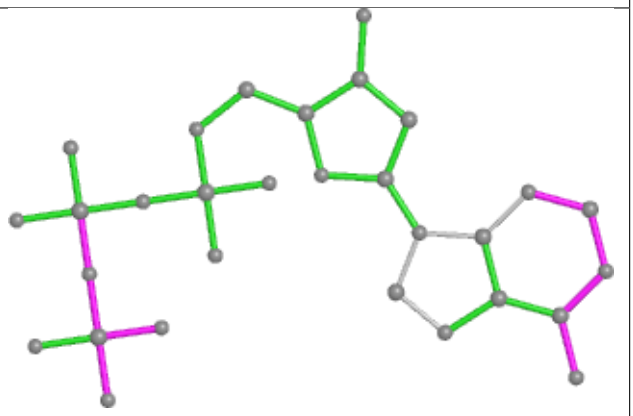
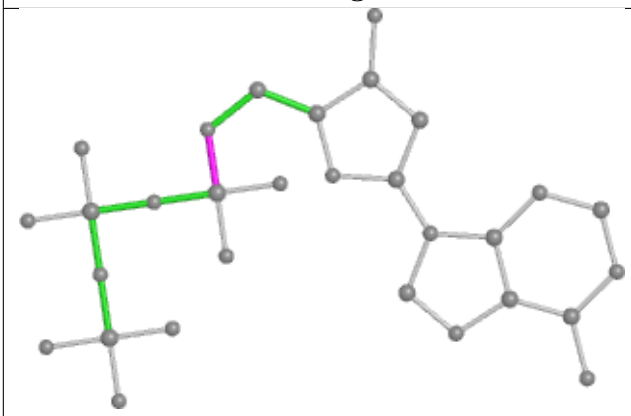
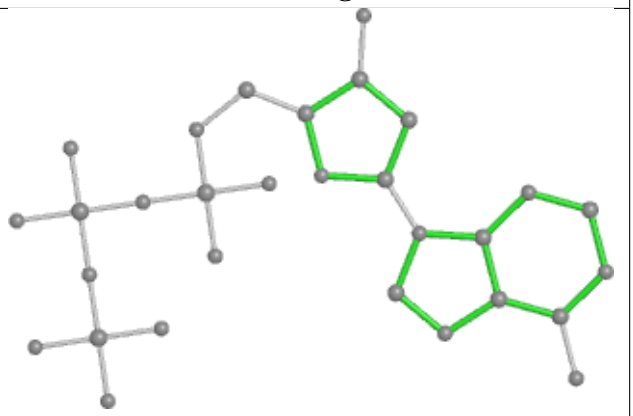


Bond angles

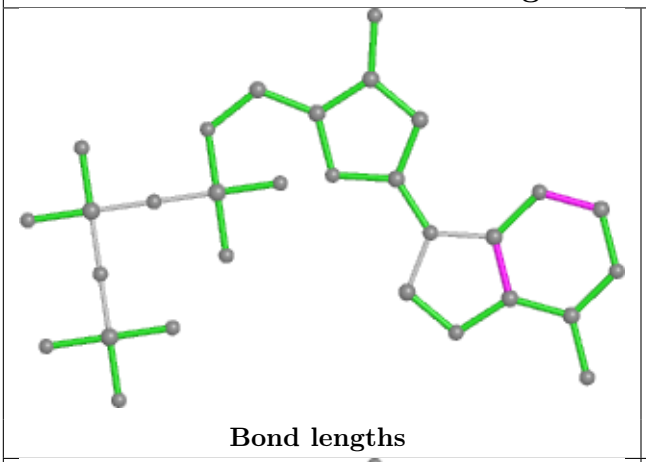


Torsions

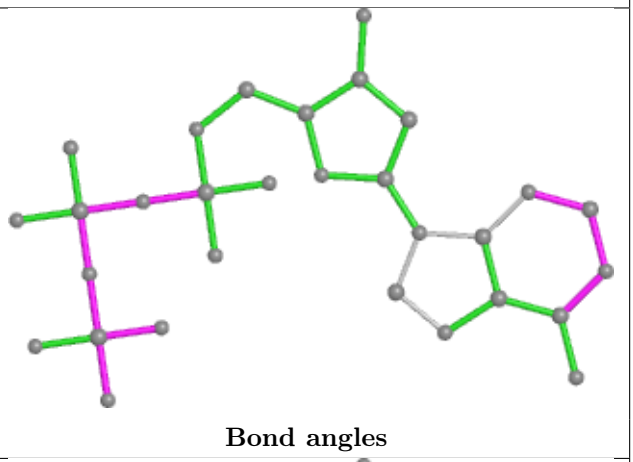


Rings

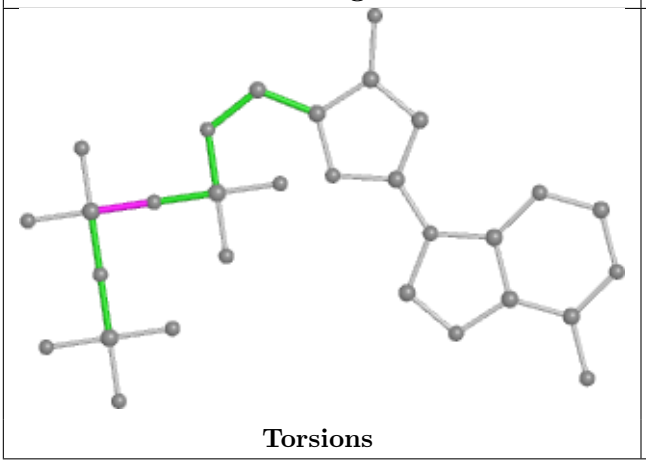
Ligand DTP G 701



Bond lengths



Bond angles



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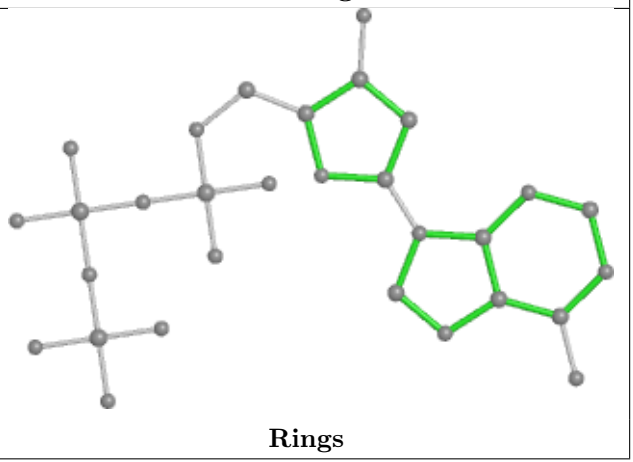
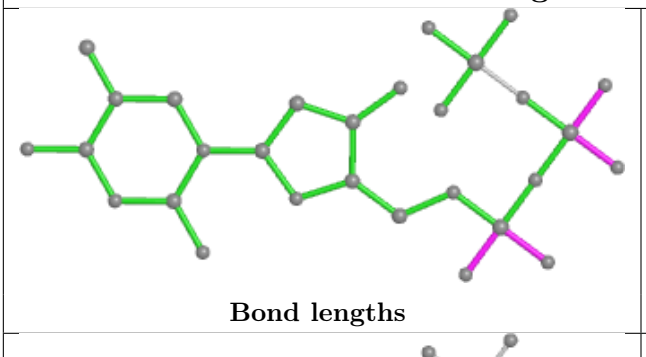
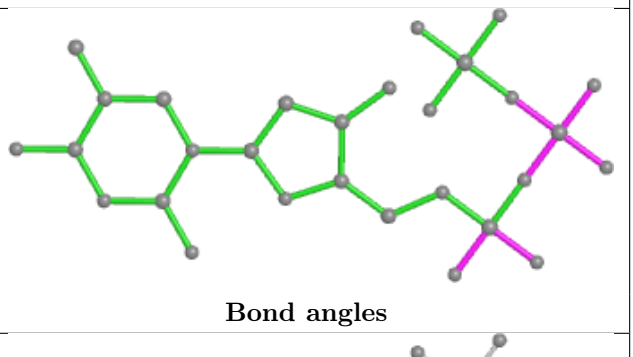


Rings

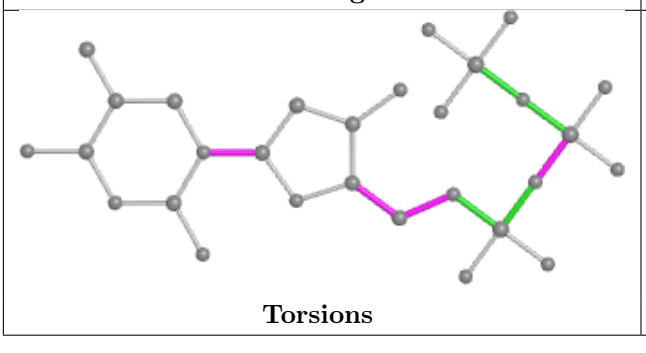
Ligand 1FZ P 704



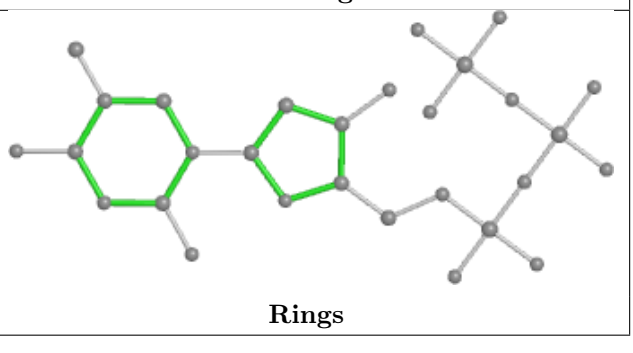
Bond lengths



Bond angles

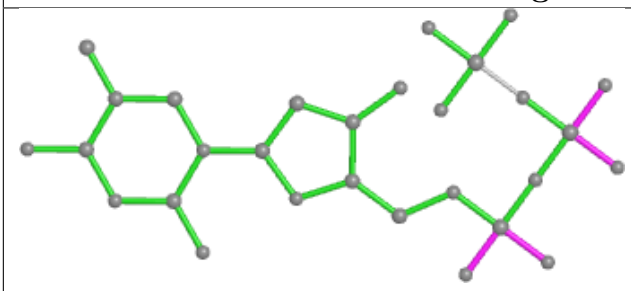


Torsions

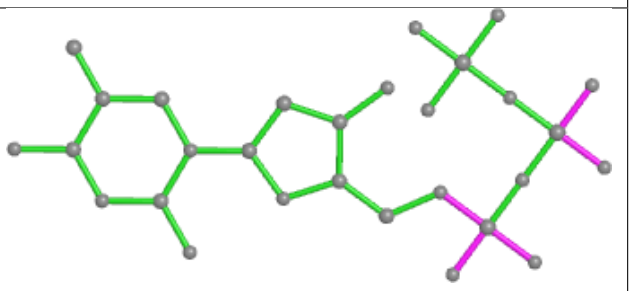


Rings

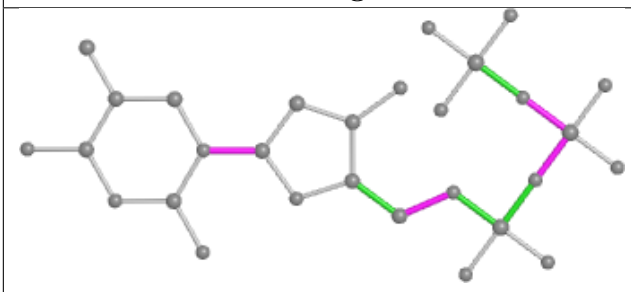
Ligand 1FZ E 704



Bond lengths



Bond angles



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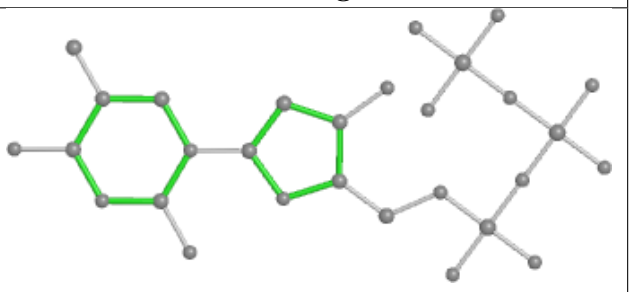
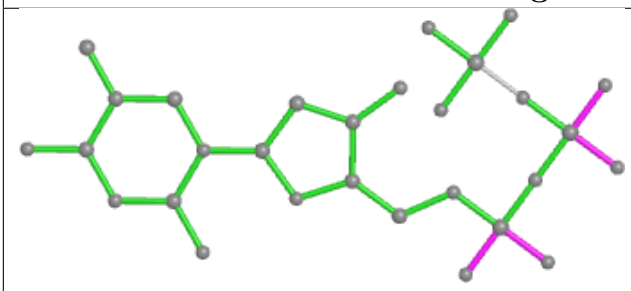
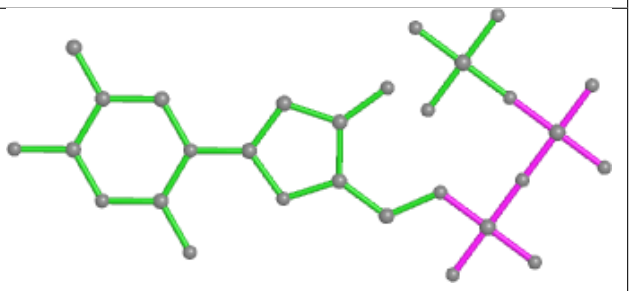


Rings

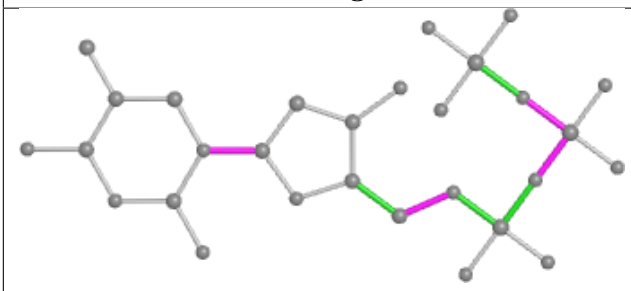
Ligand 1FZ B 704



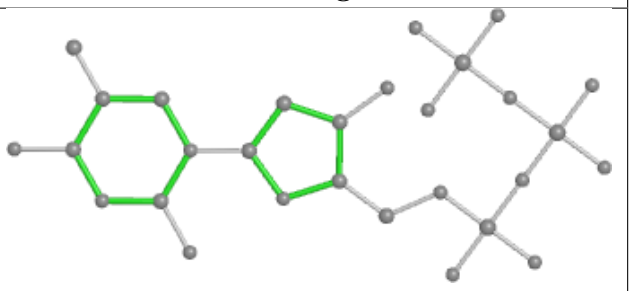
Bond lengths



Bond angles

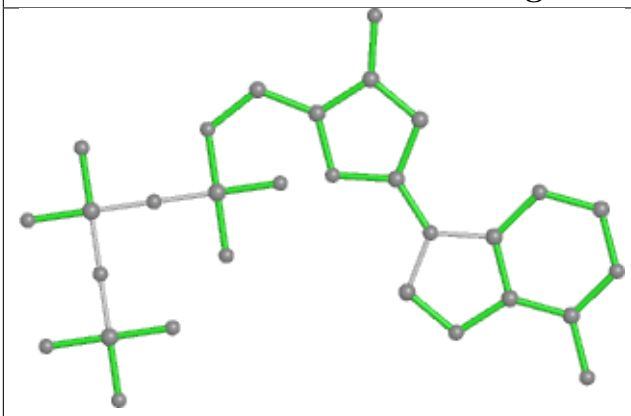


Torsions



Rings

Ligand DTP L 701



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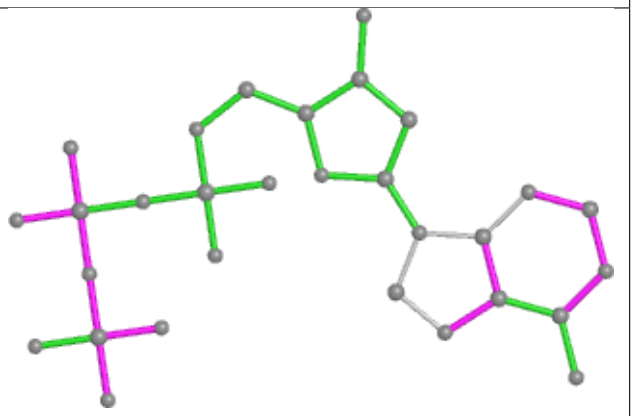

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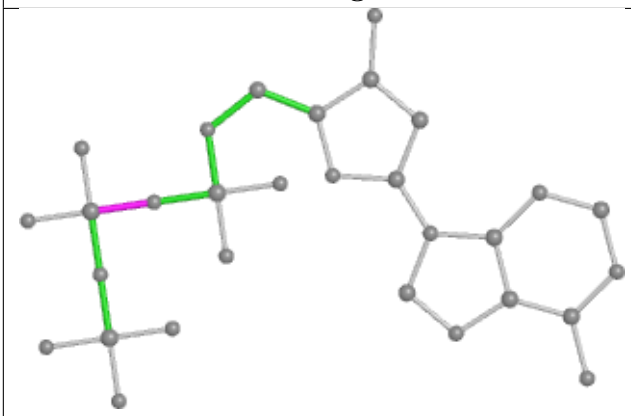

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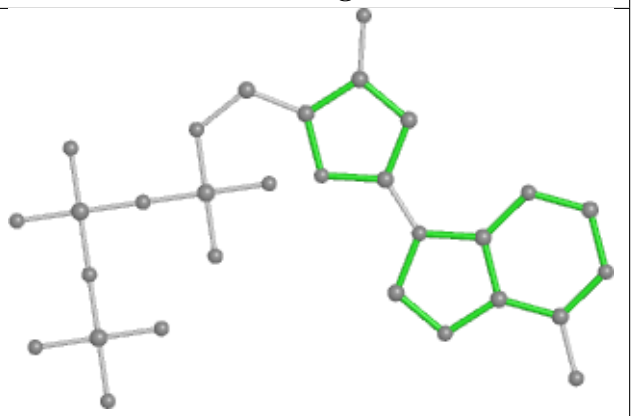
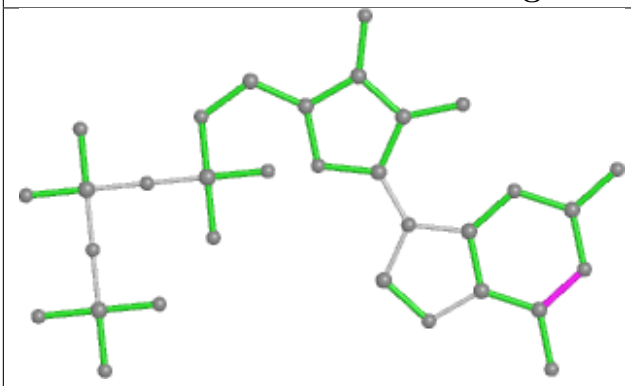


Rings

Ligand GTP P 705



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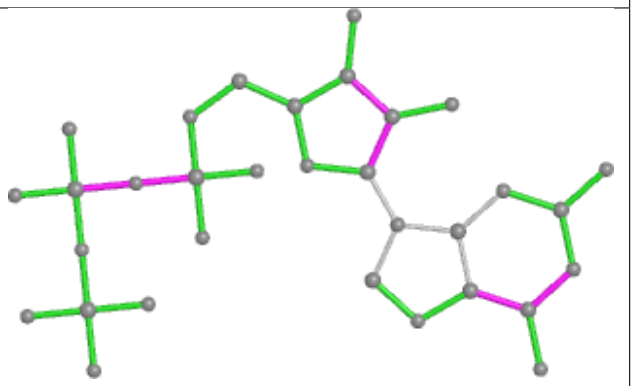

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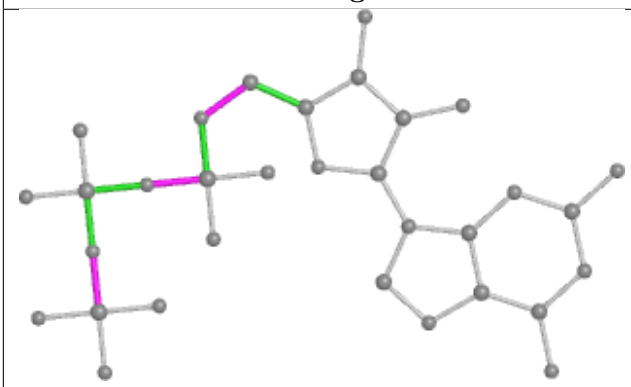

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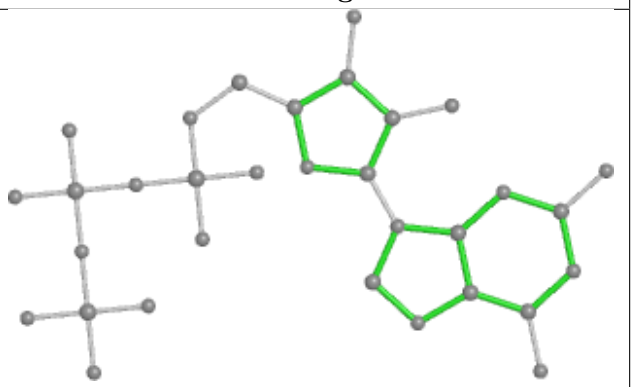
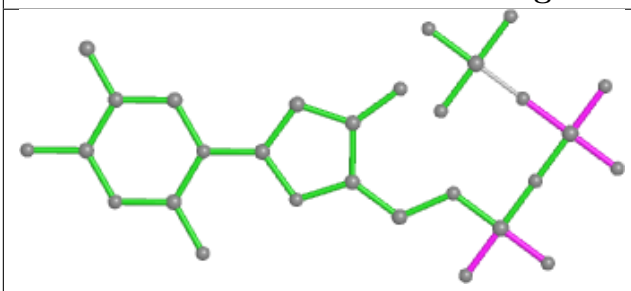


Rings

Ligand 1FZ J 704



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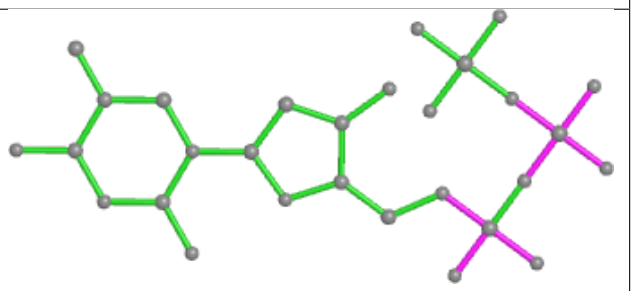
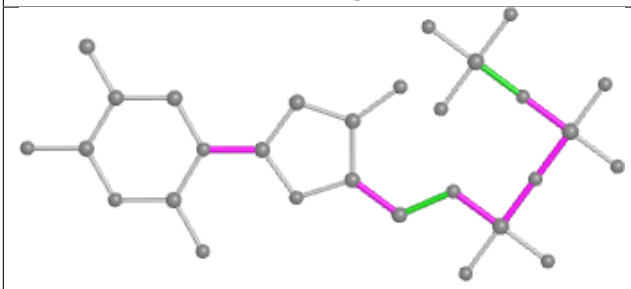


Bond angles



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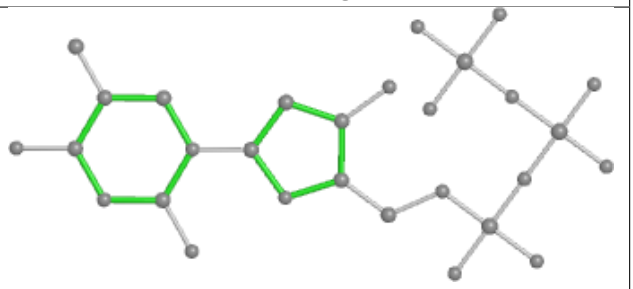
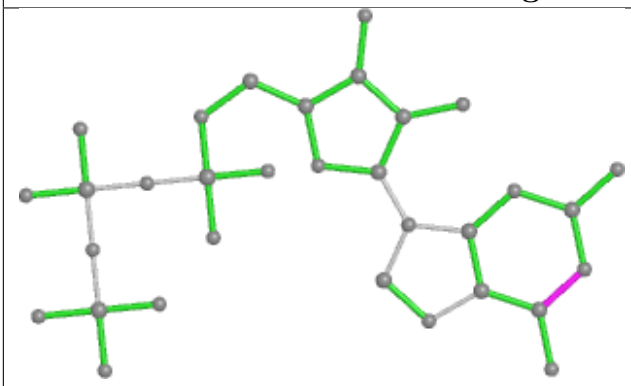


Rings

Ligand GTP D 702



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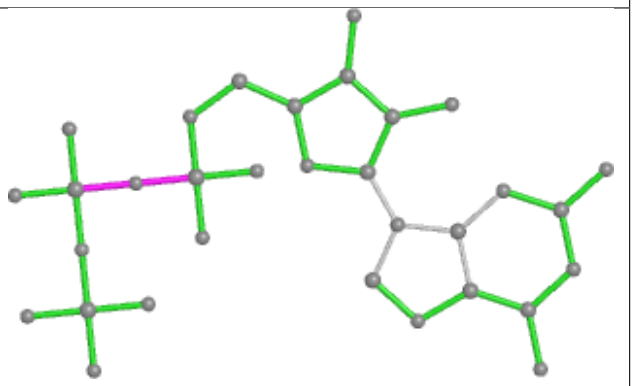

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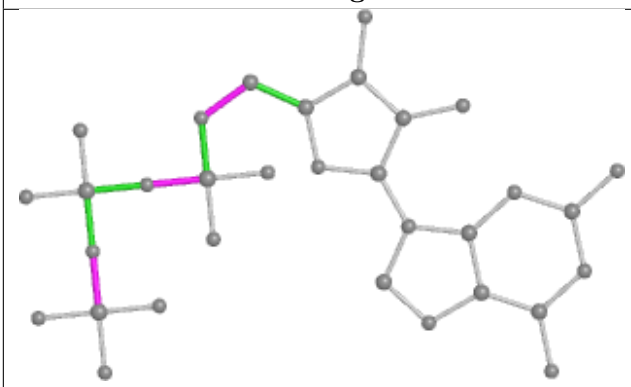

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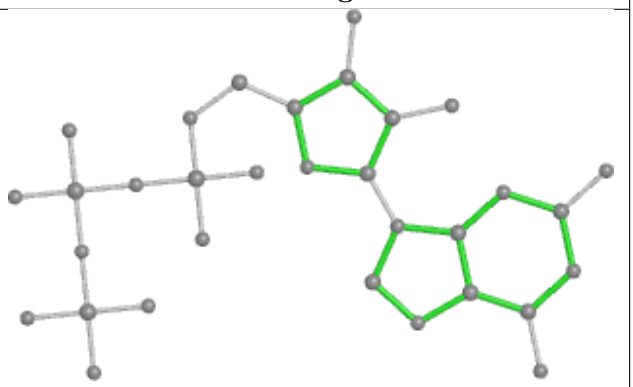
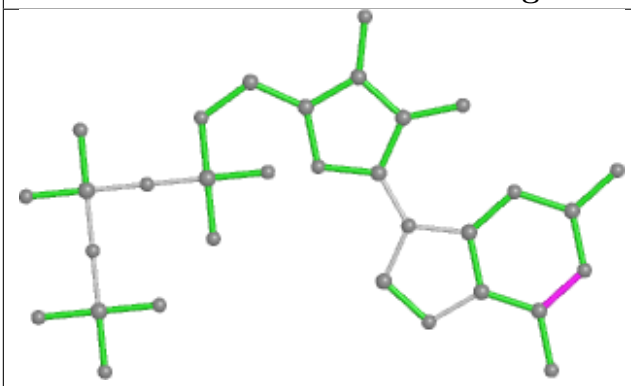


Rings

Ligand GTP D 707



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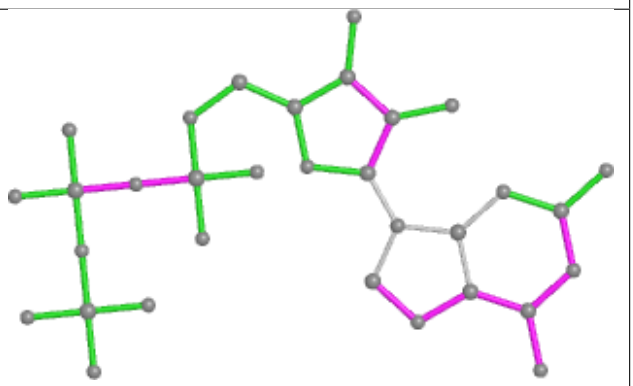

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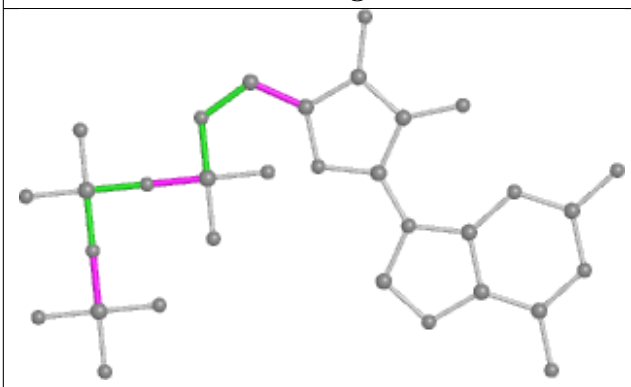

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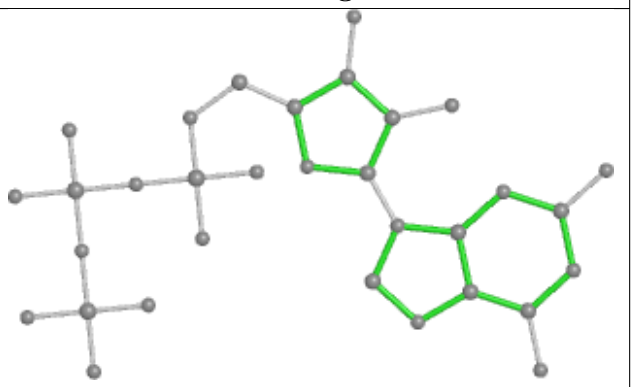
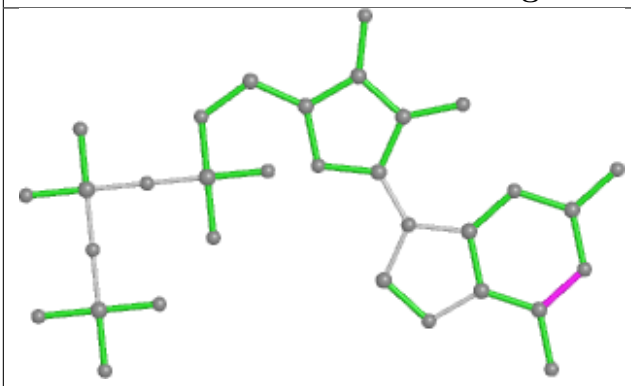


Rings

Ligand GTP H 706



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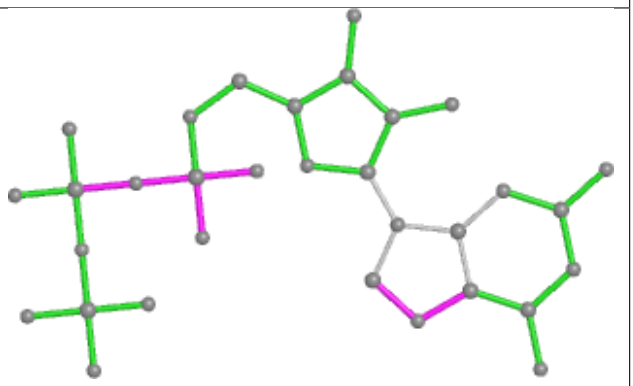
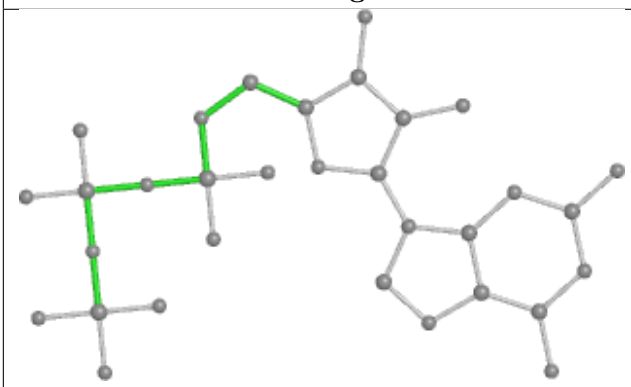


Bond angles



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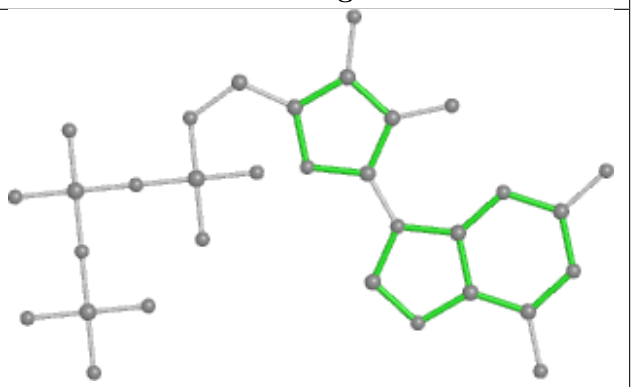
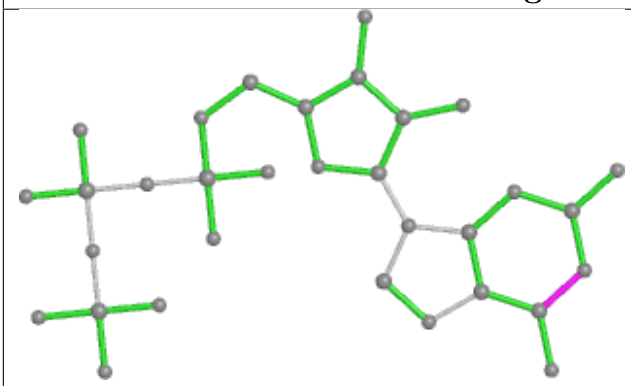


Rings

Ligand GTP F 705



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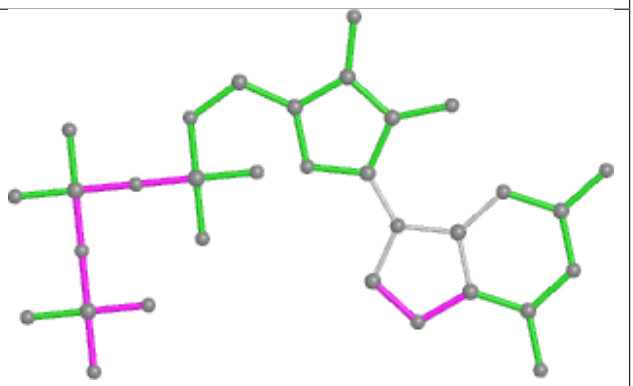

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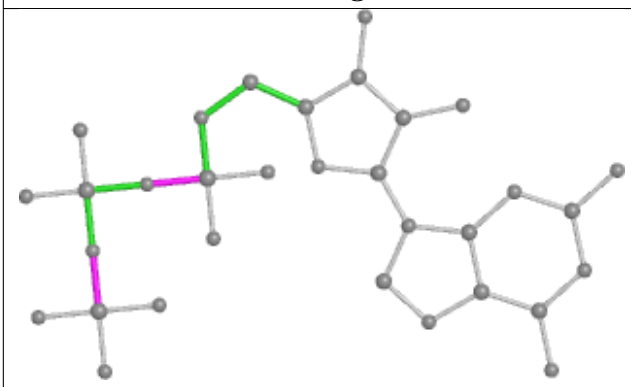

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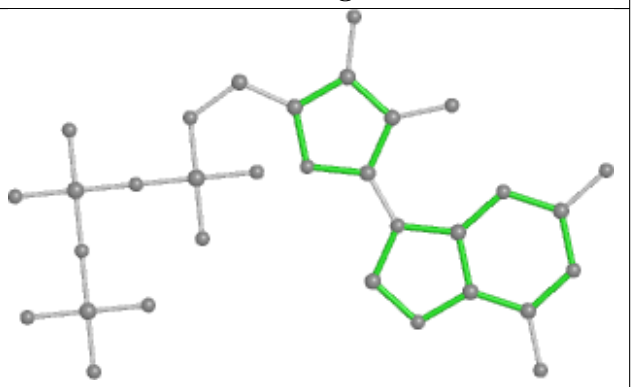
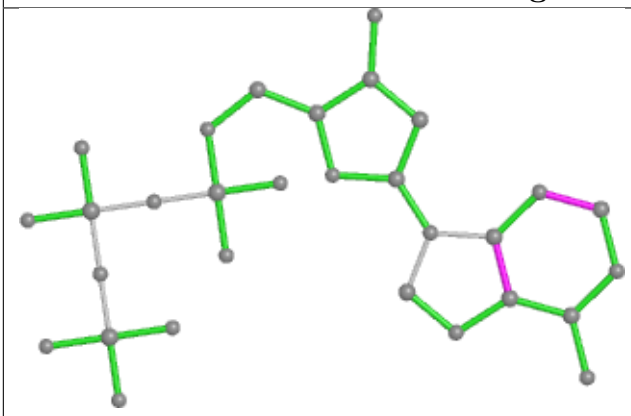


Rings

Ligand DTP I 708



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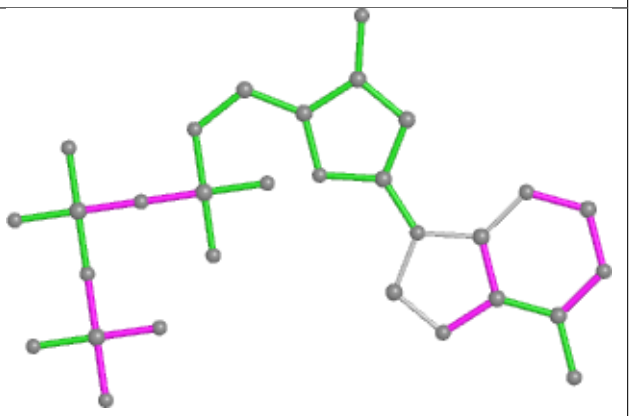
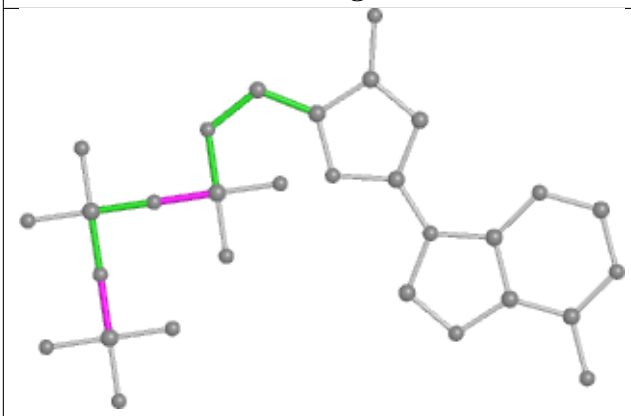


Bond angles



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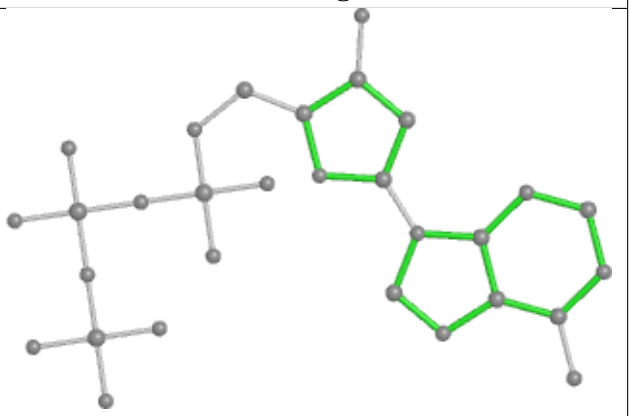
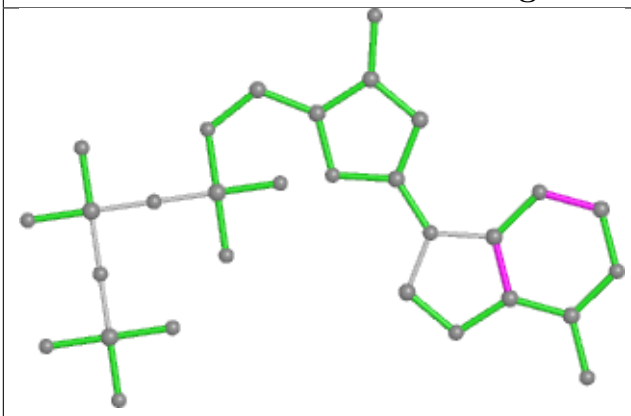


Rings

Ligand DTP M 707



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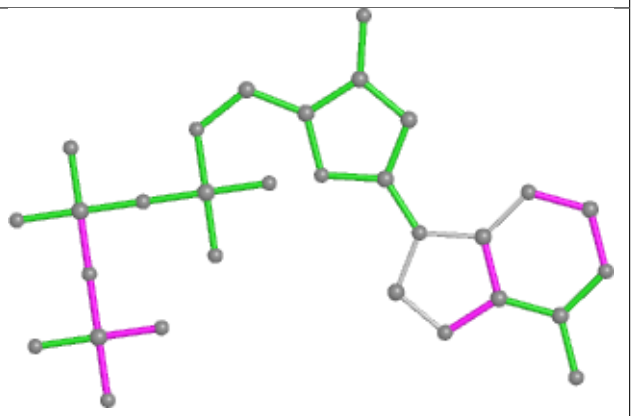
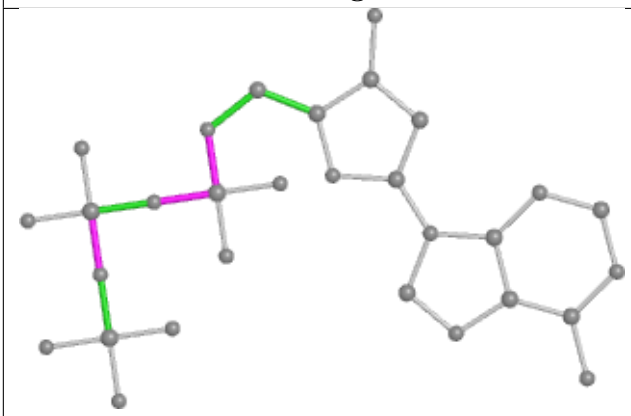


Bond angles



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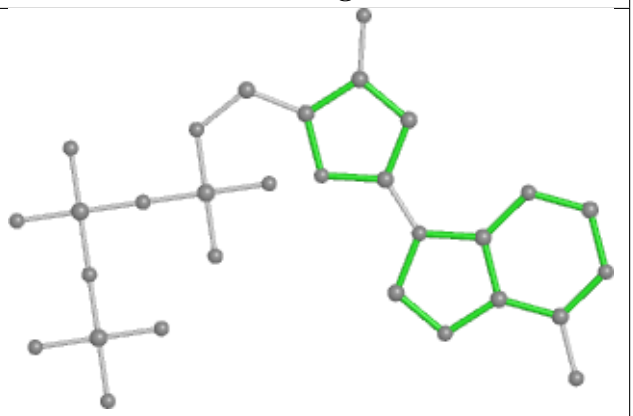
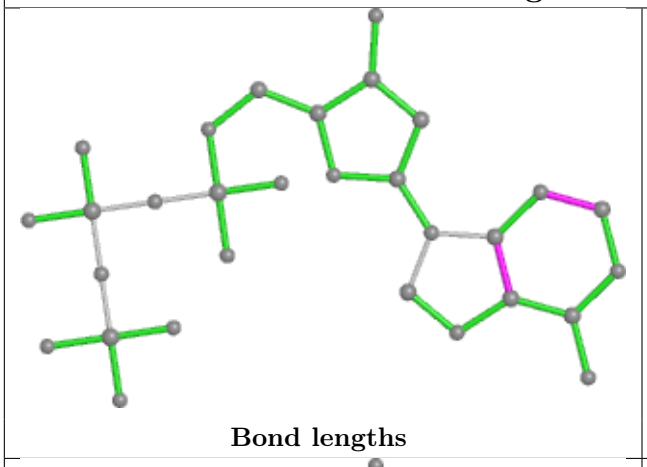


Rings

Ligand DTP E 707



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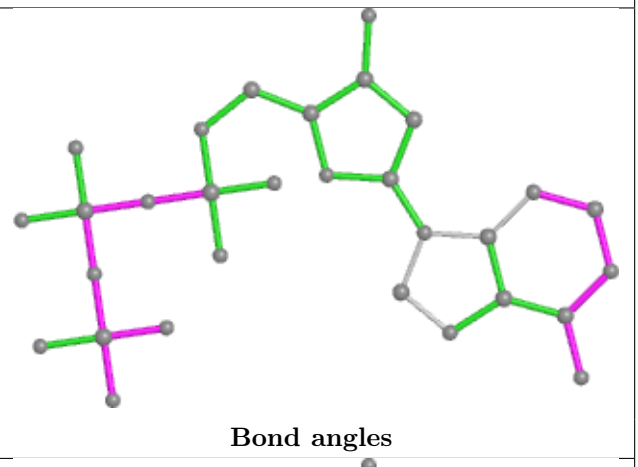

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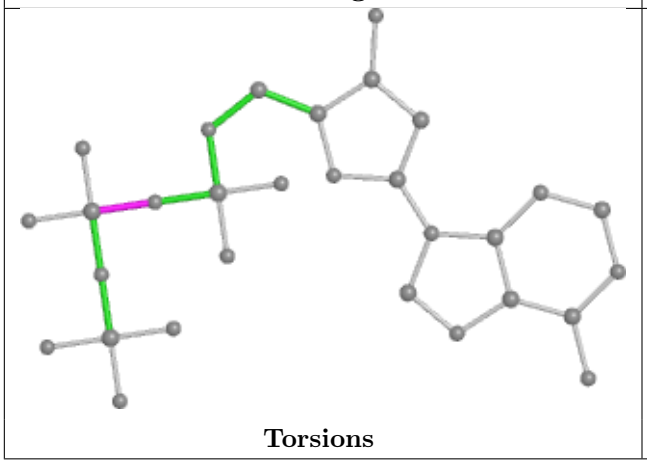

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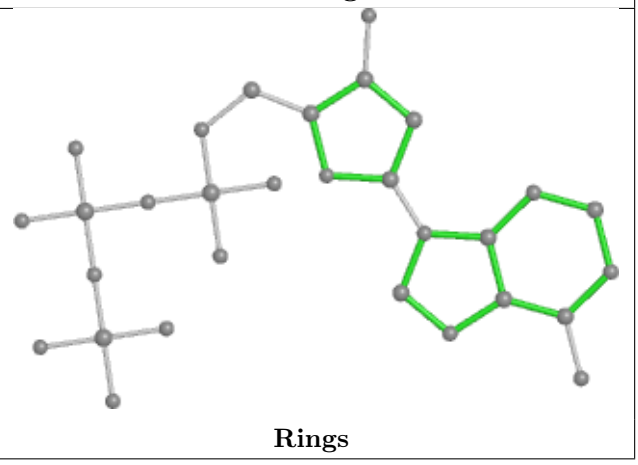
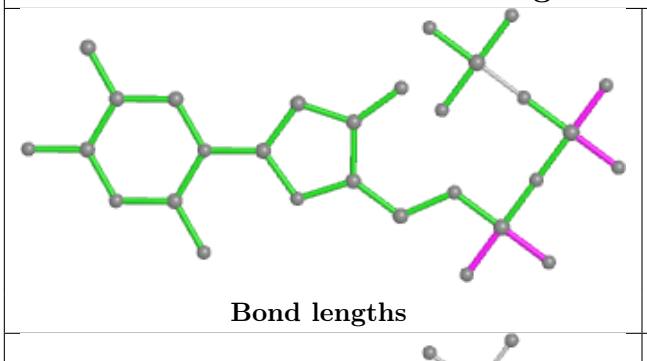


Rings

Ligand 1FZ L 705



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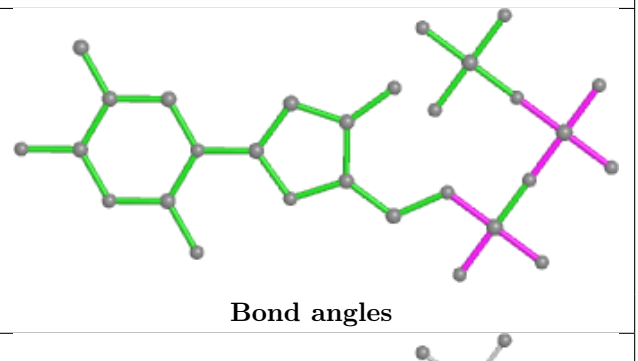

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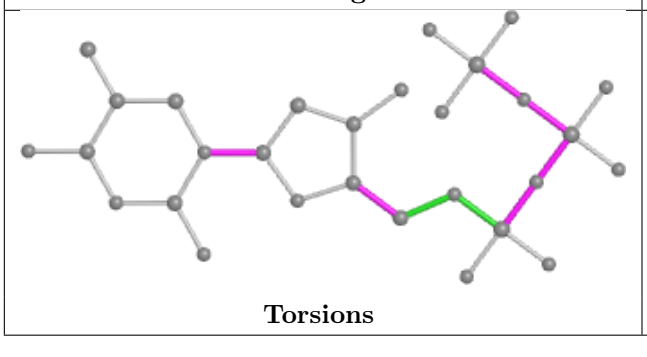

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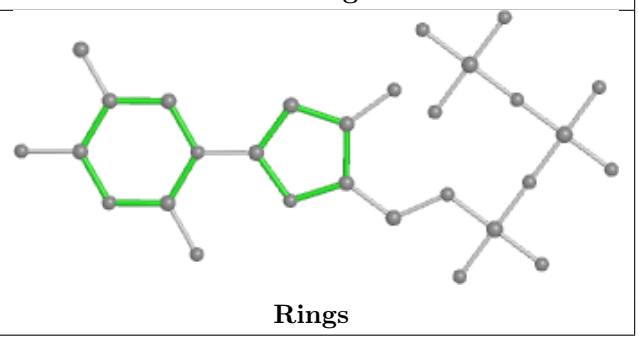
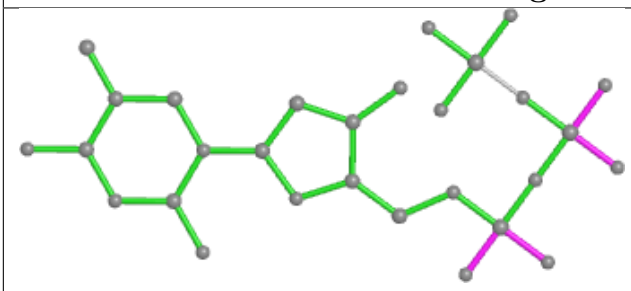


Rings

Ligand 1FZ O 704



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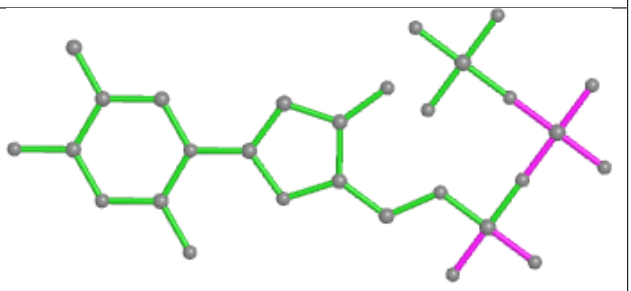

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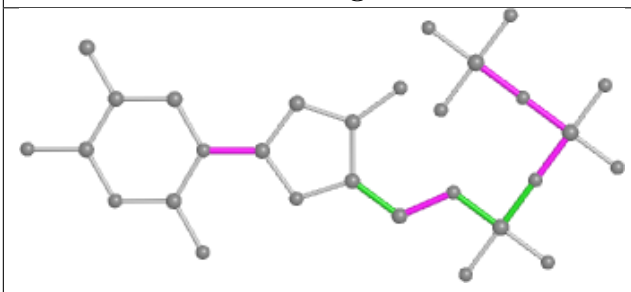

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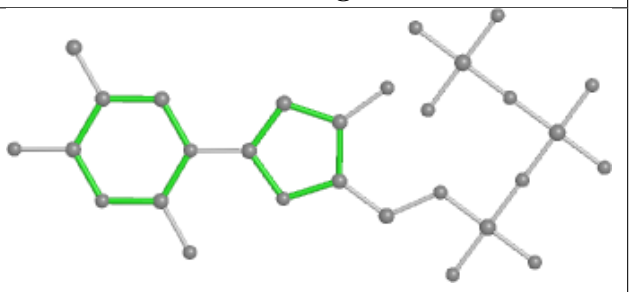
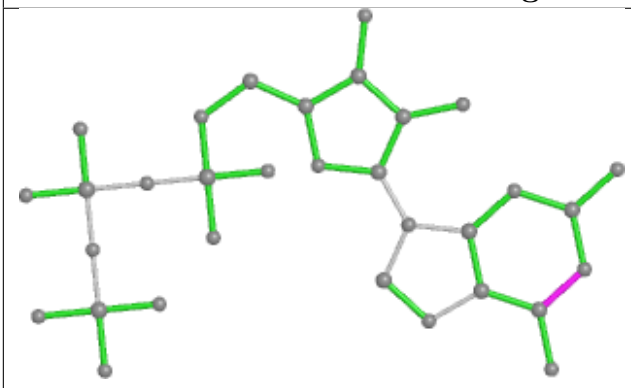


Rings

Ligand GTP G 706



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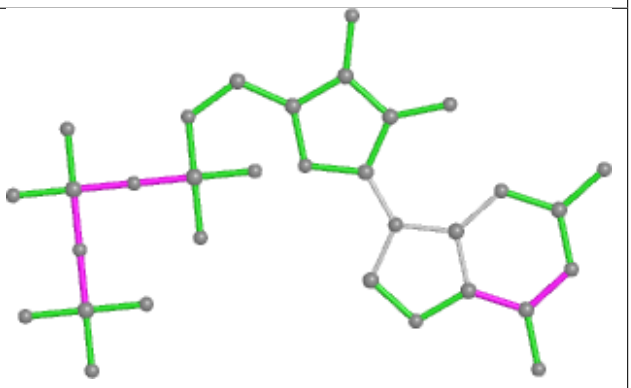

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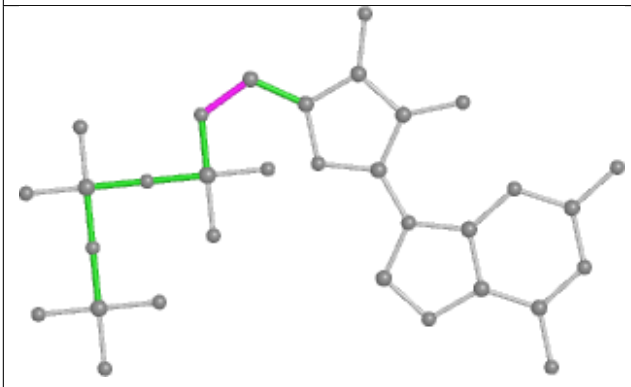

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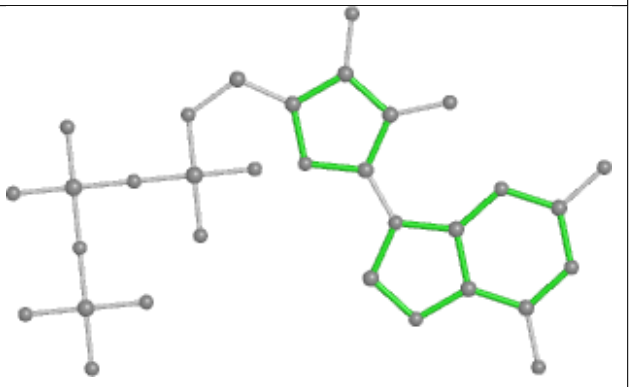
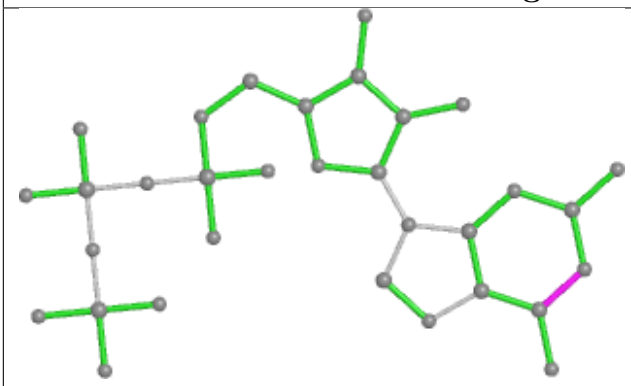


Rings

Ligand GTP B 705



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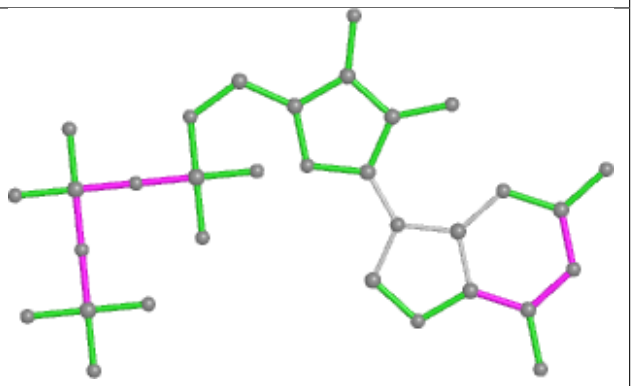
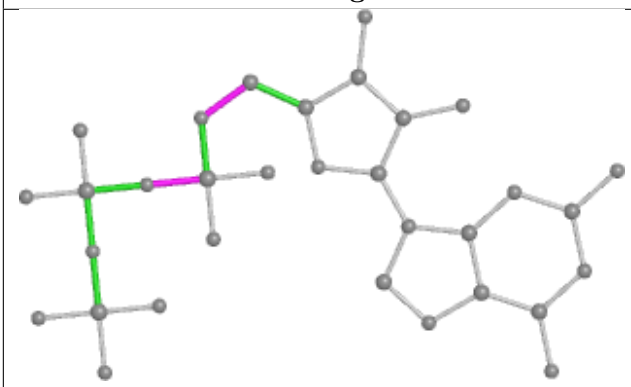


Bond angles



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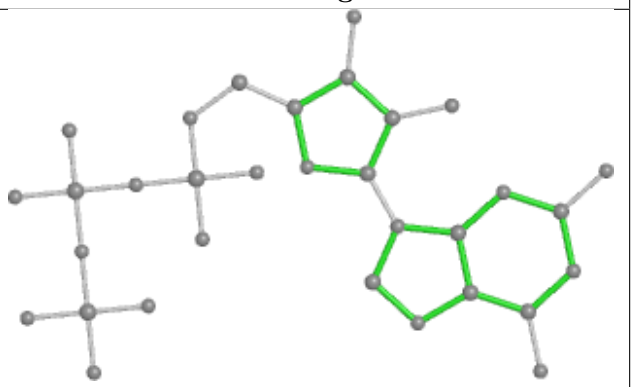
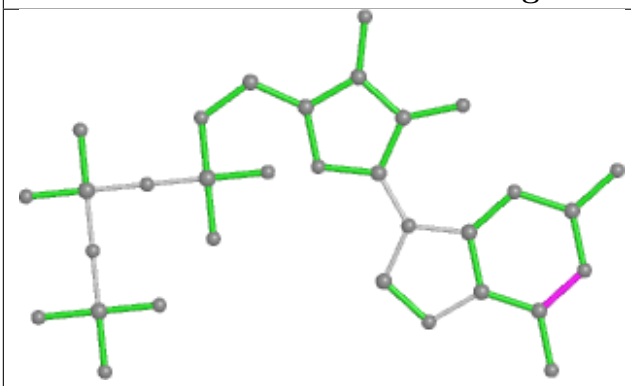
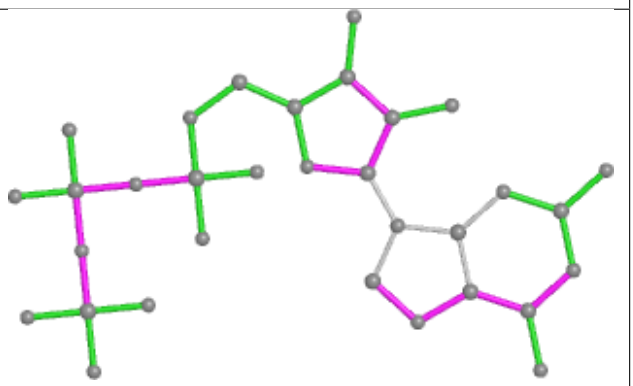


Rings

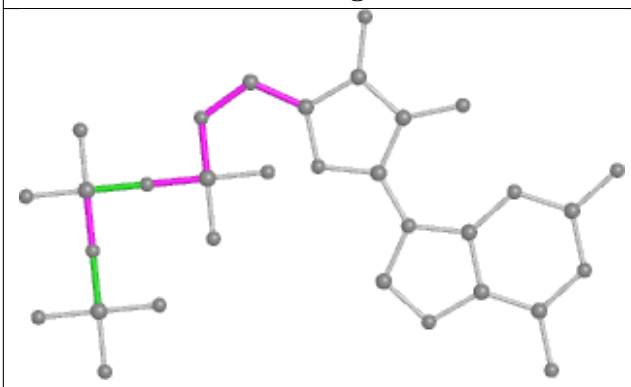
Ligand GTP A 705



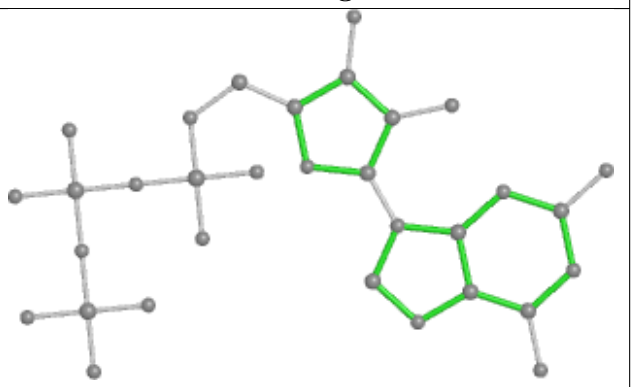
Bond lengths



Bond angles

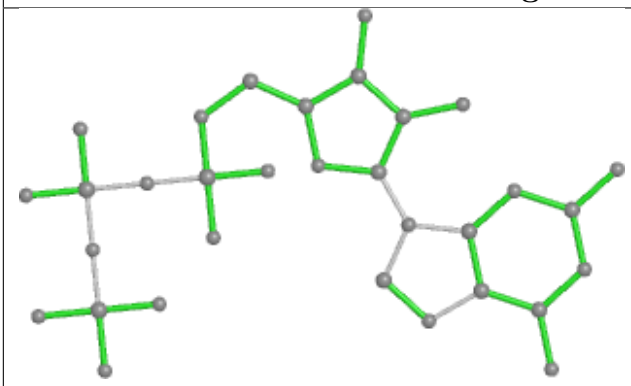


Torsions



Rings

Ligand GTP K 706



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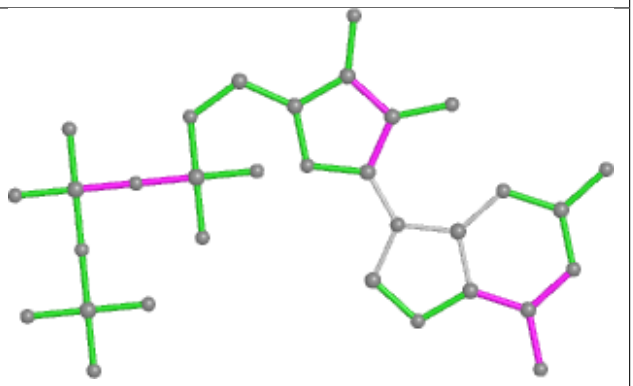

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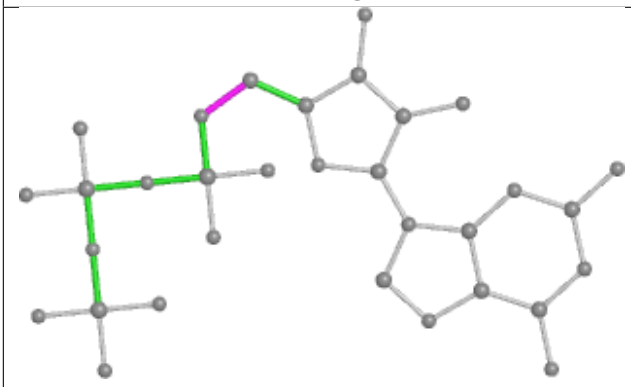

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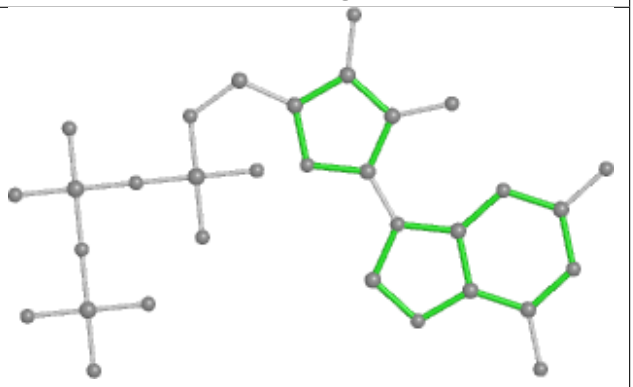
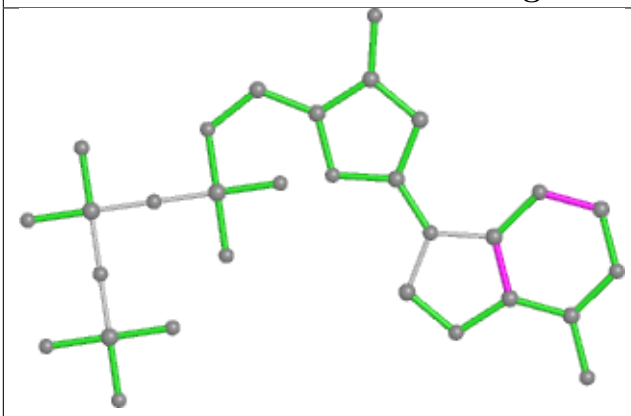


Rings

Ligand DTP C 701



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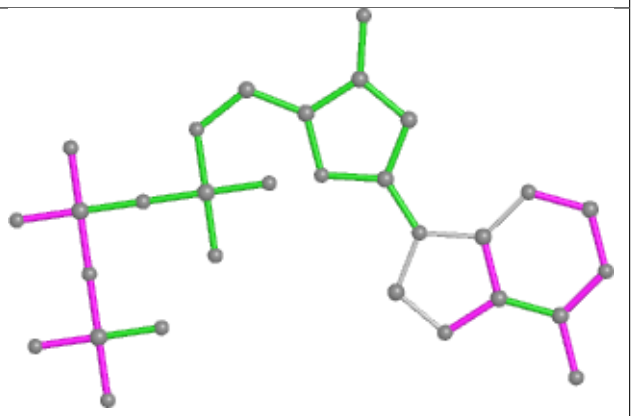

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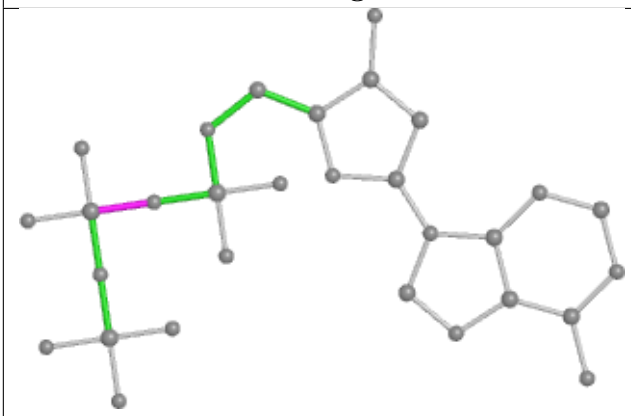

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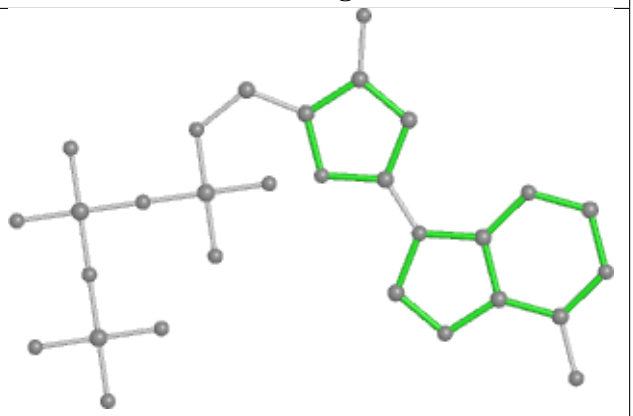
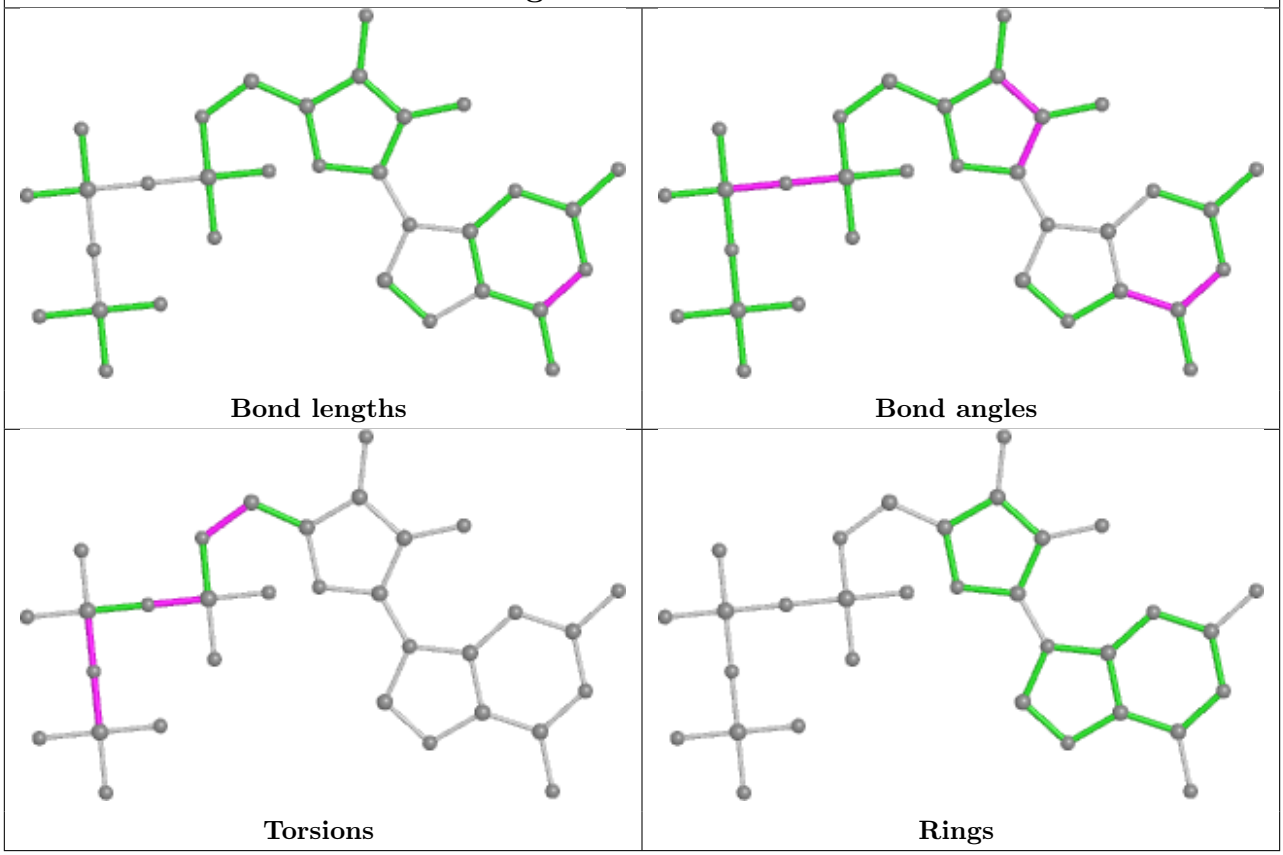
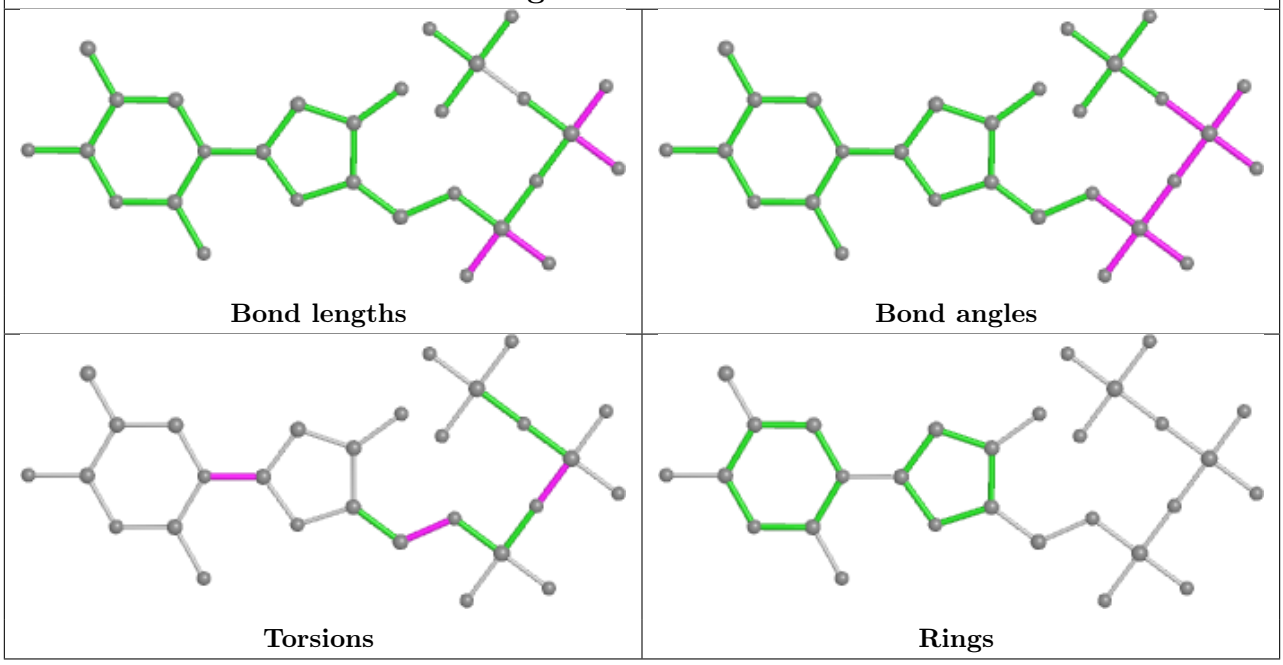


Rings

Ligand GTP L 706



Ligand 1FZ M 704



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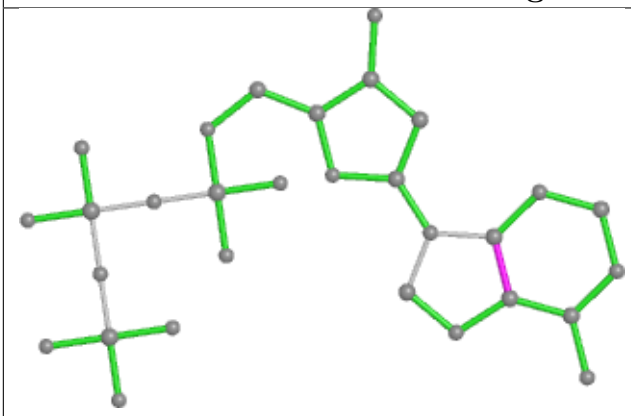

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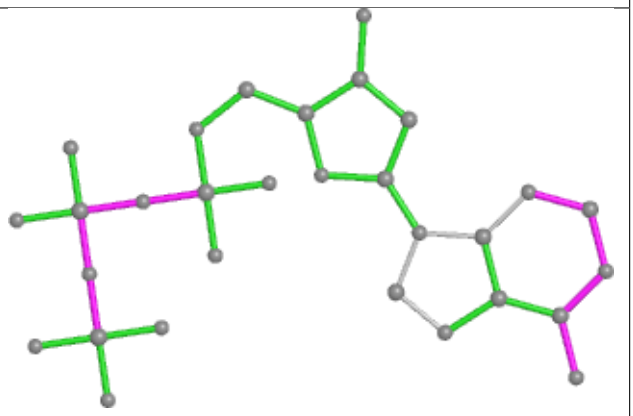

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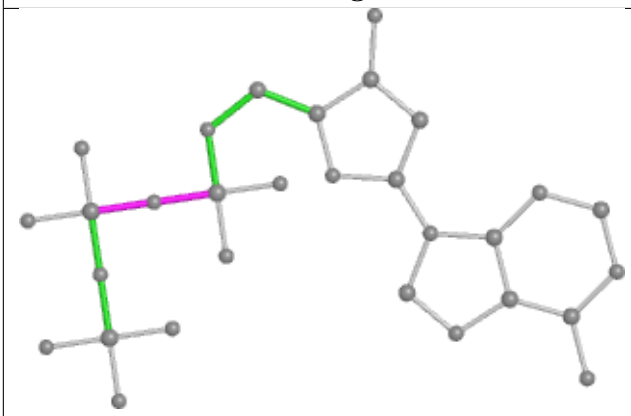

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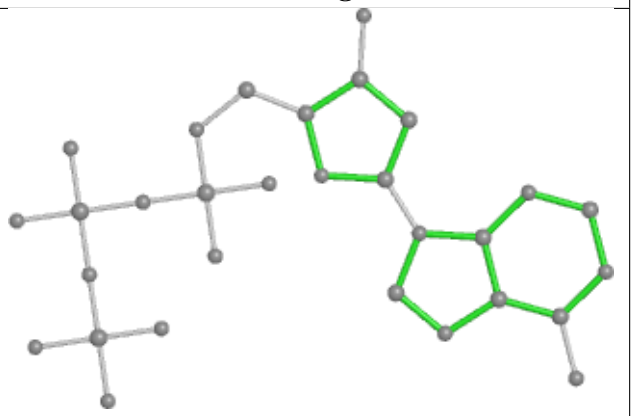

Rings

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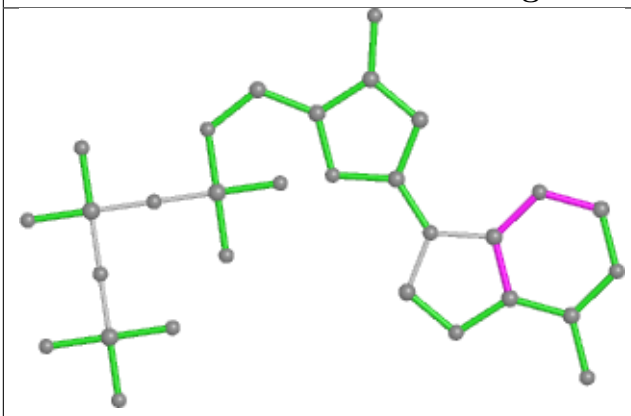

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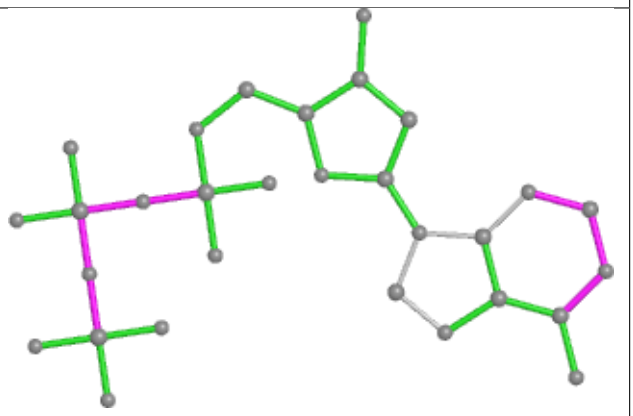

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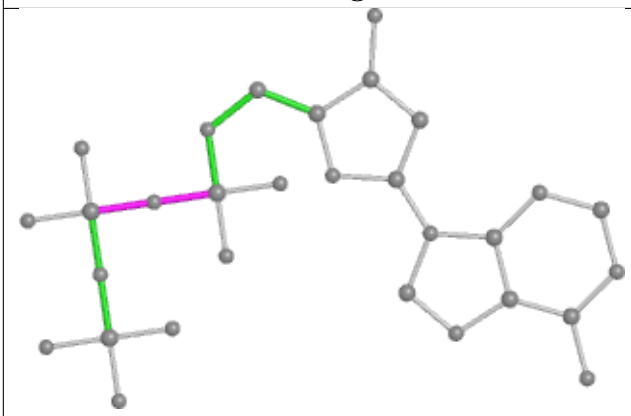

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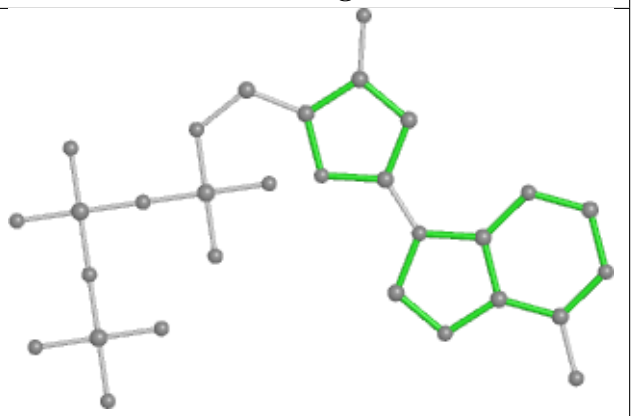
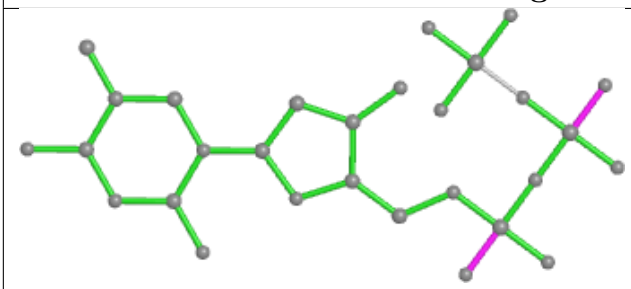


Rings

Ligand 1FZ C 705



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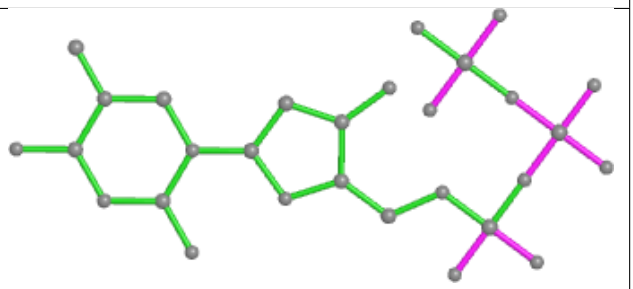
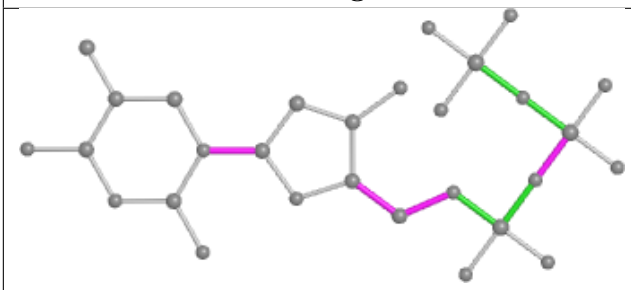


Bond angles



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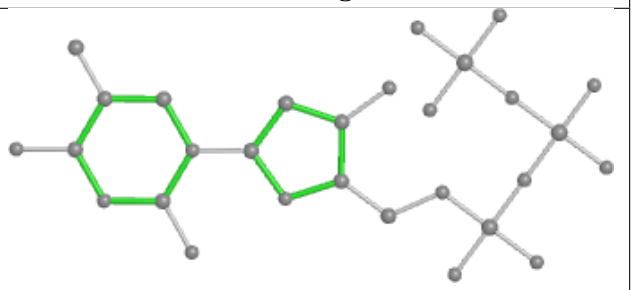
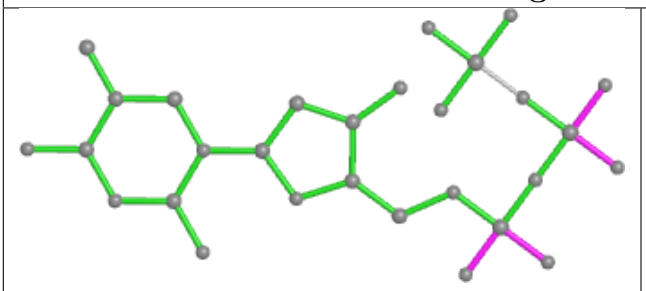


Rings

Ligand 1FZ N 705



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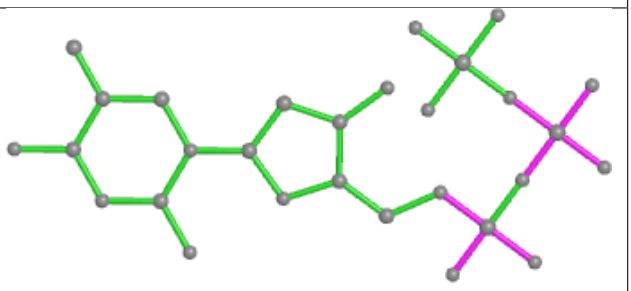

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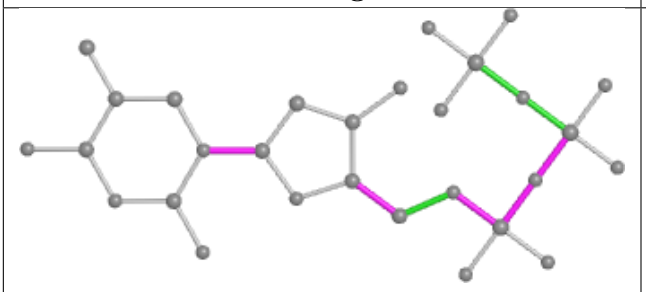

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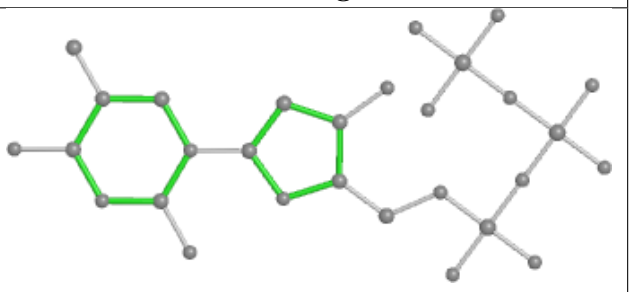
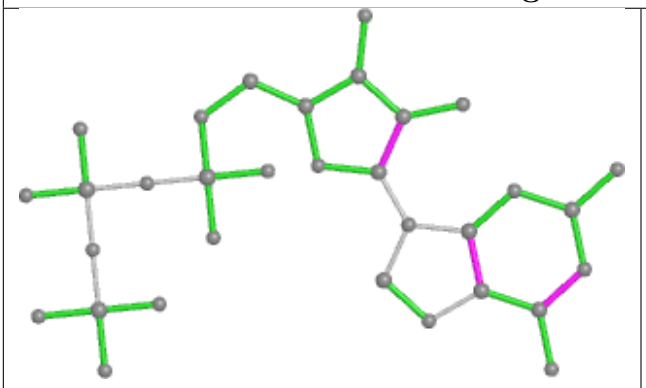


Rings

Ligand GTP O 705



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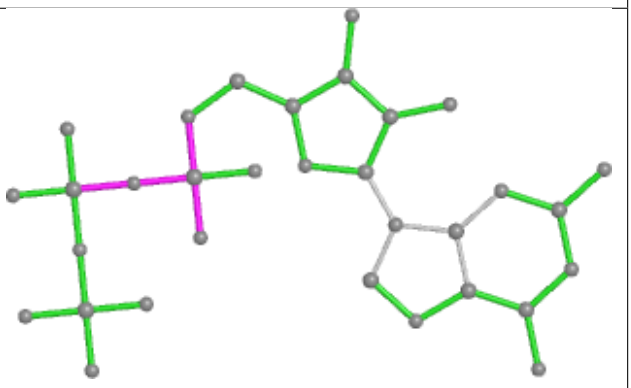

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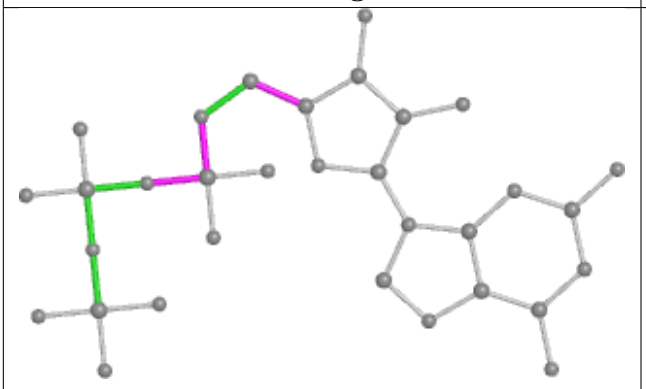

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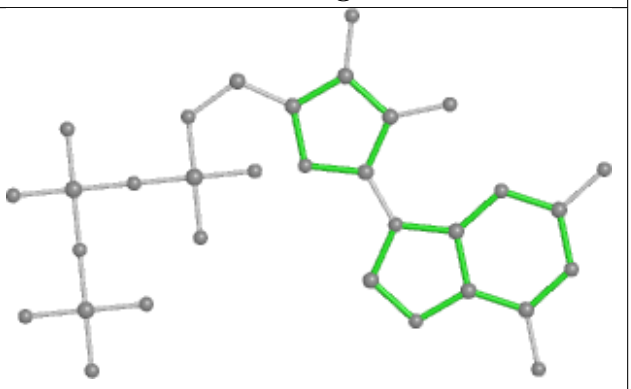
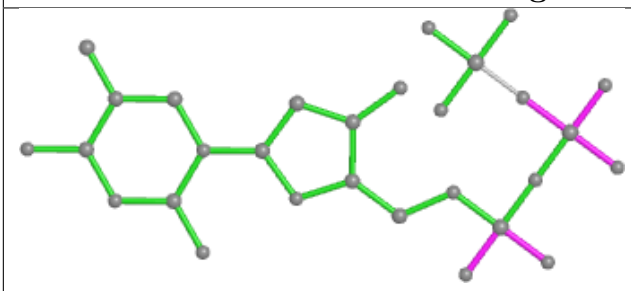


Rings

Ligand 1FZ G 705



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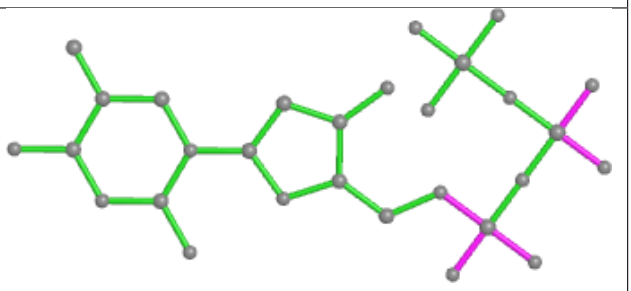
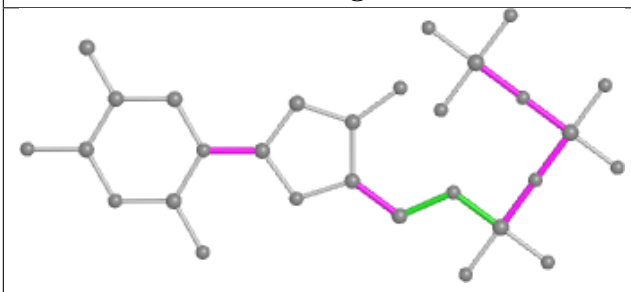


Bond angles



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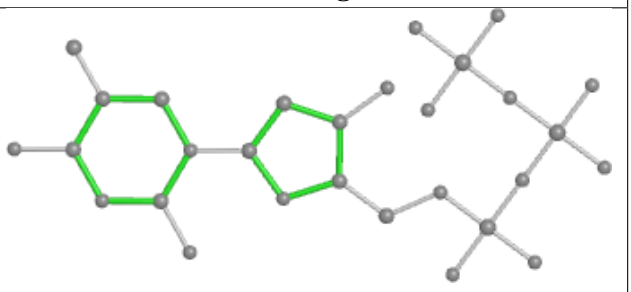
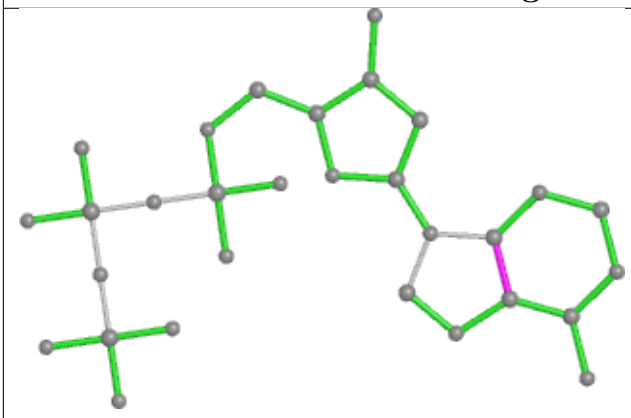


Rings

Ligand DTP N 708



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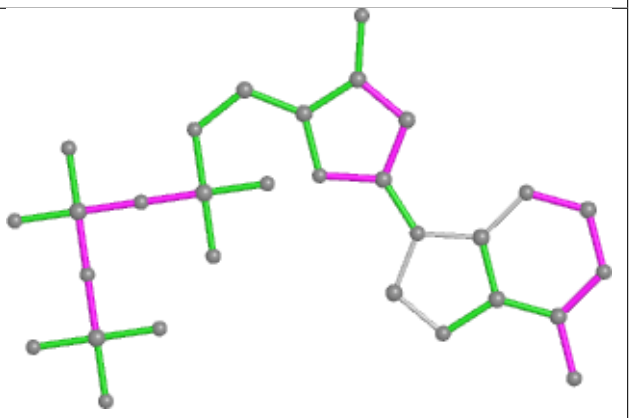
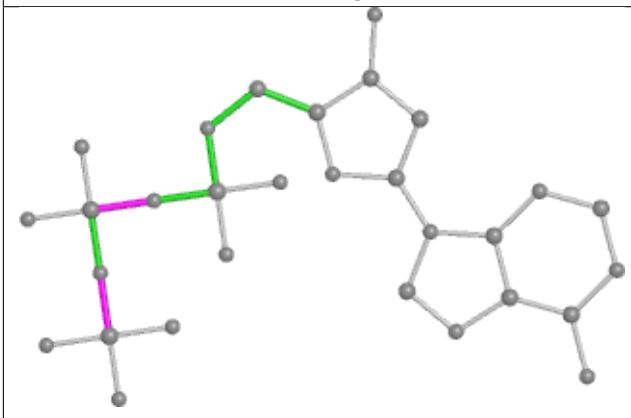


Bond angles



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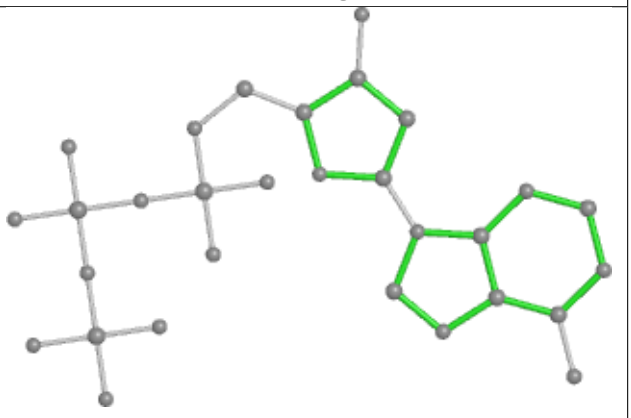
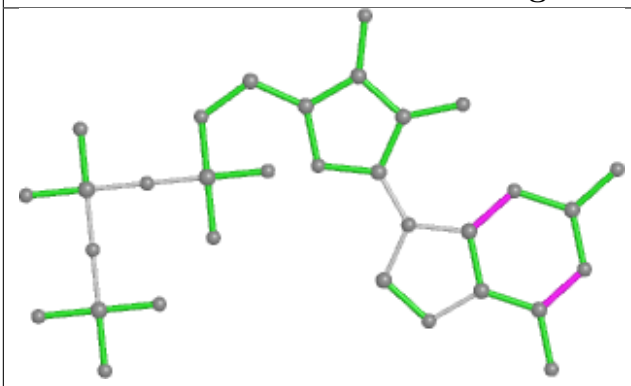


Rings

Ligand GTP I 707



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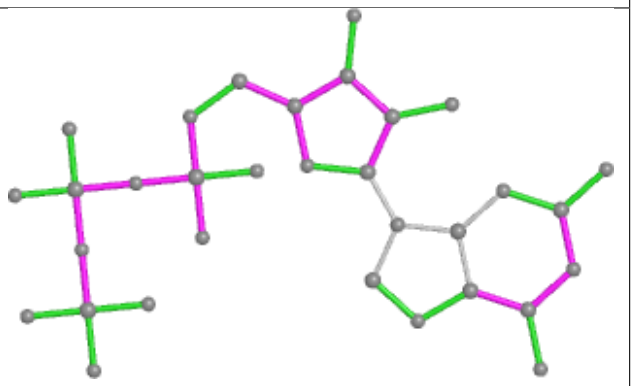

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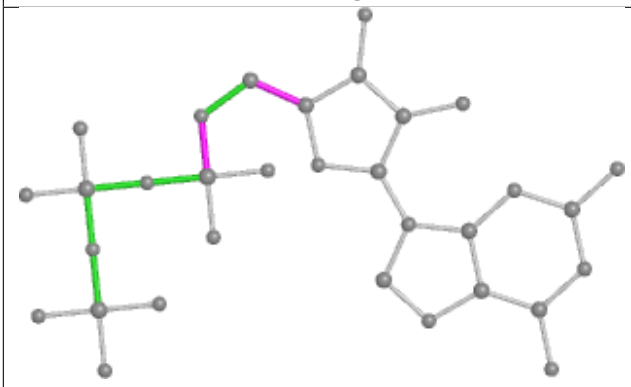

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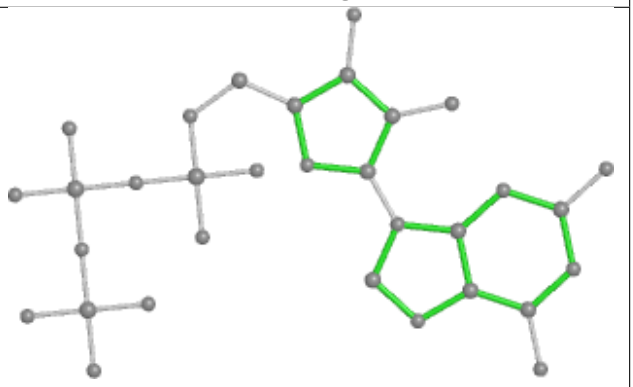
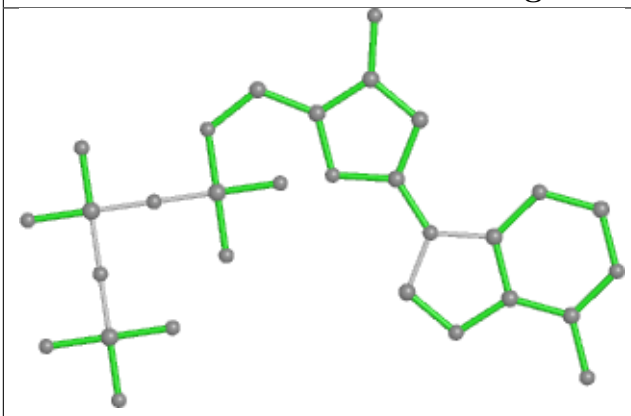


Rings

Ligand DTP F 707



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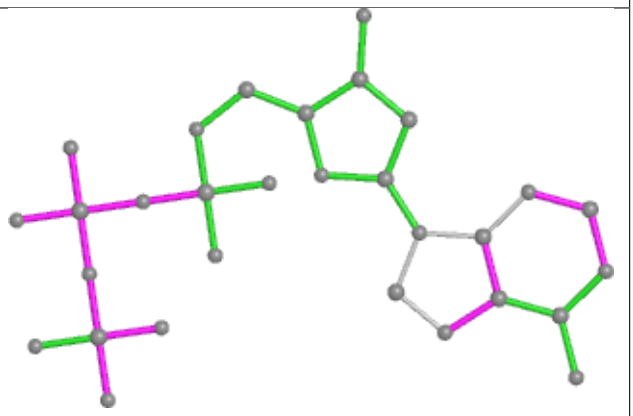
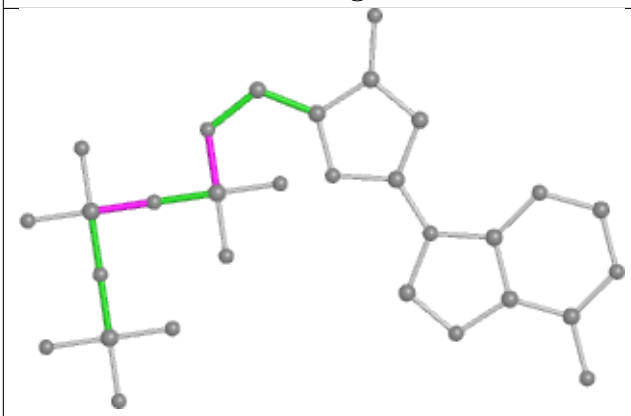


Bond angles



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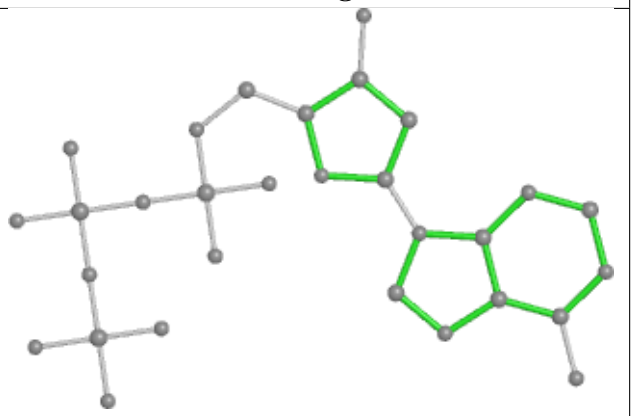
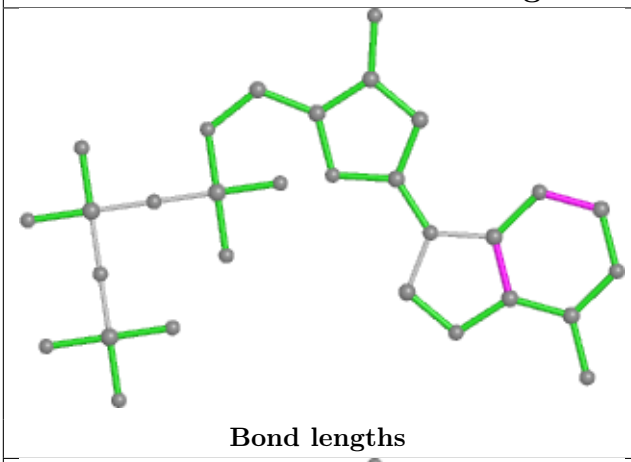


Rings

Ligand DTP B 707



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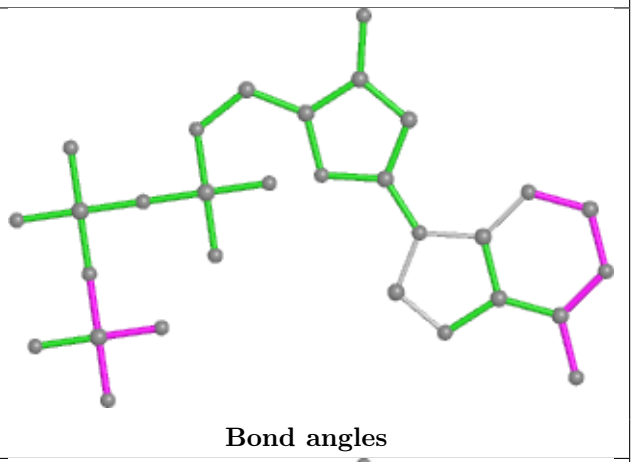

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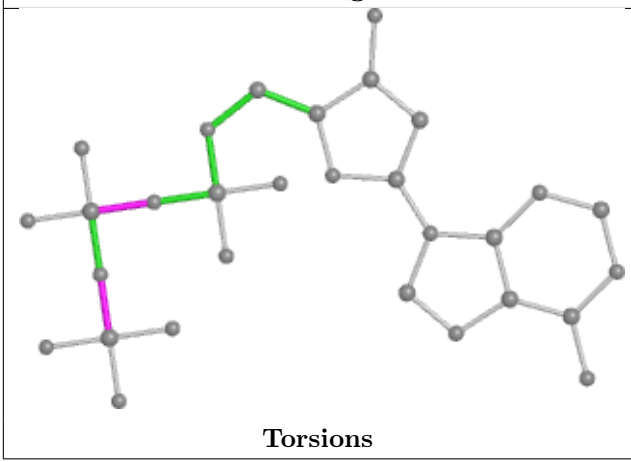

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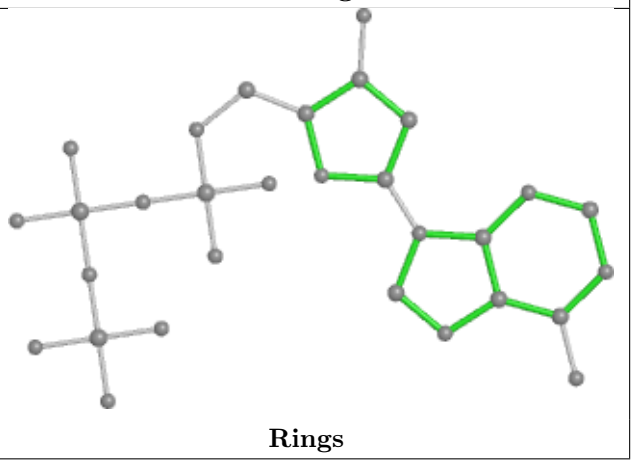
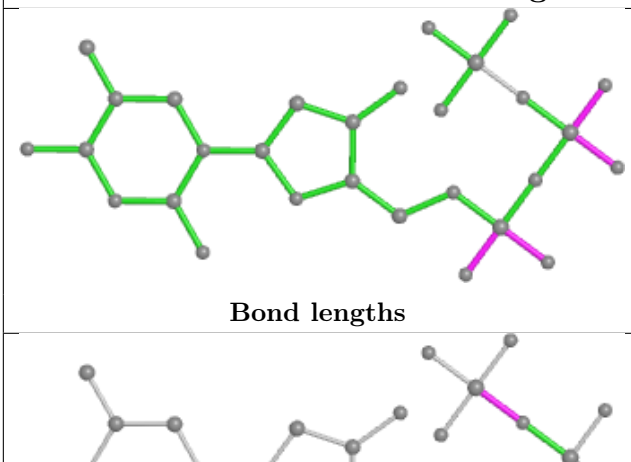


Rings

Ligand 1FZ K 705



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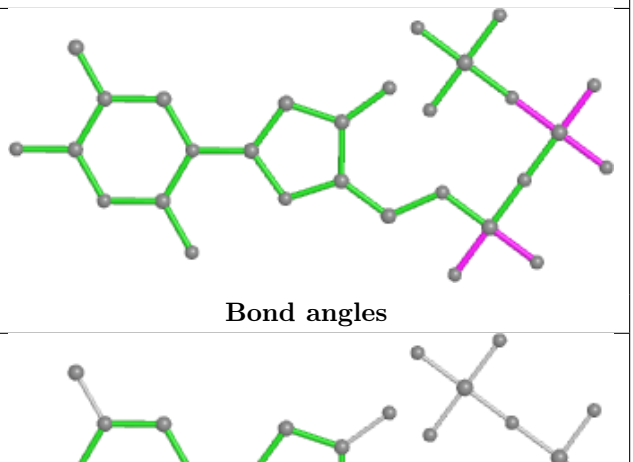
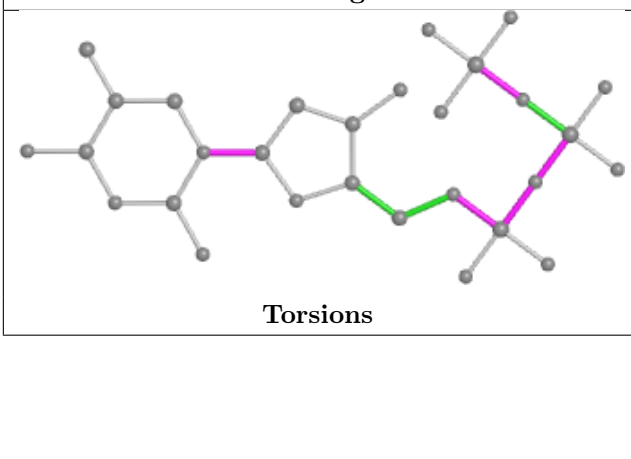
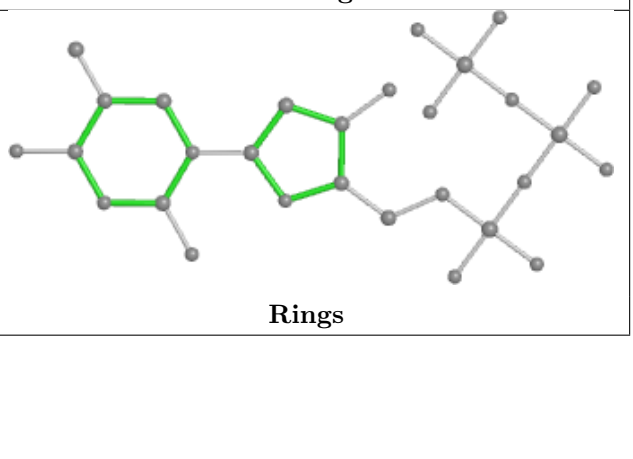


Bond angles

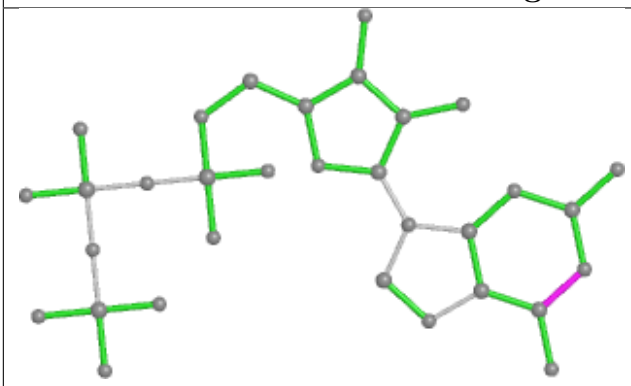


Torsions



Rings

Ligand GTP E 705



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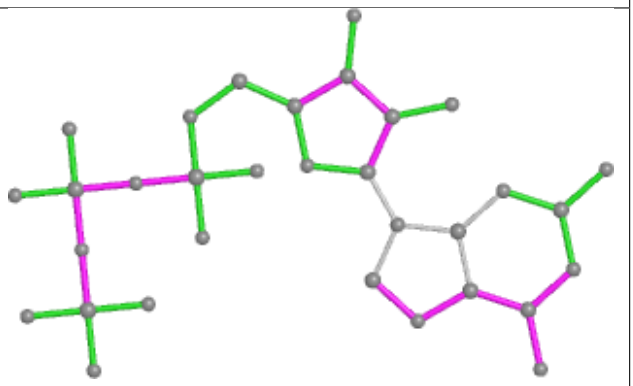
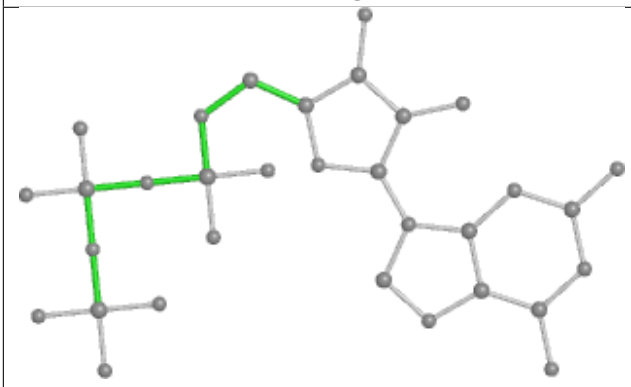
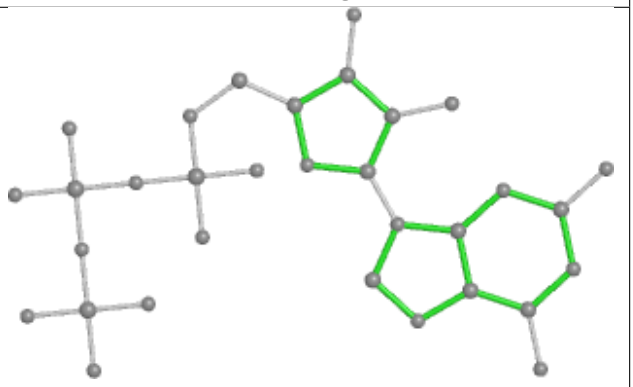


Bond angles

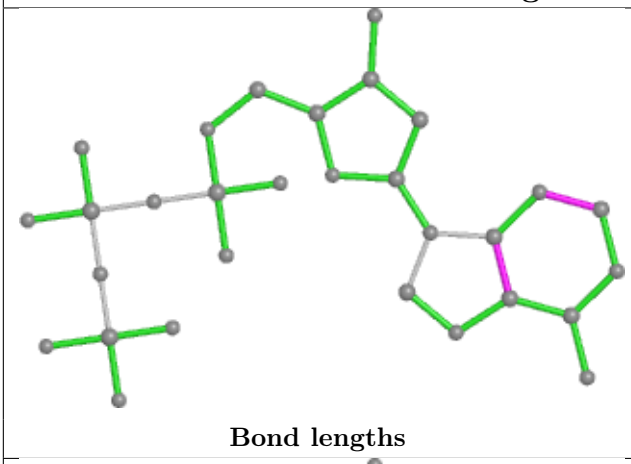


Torsions

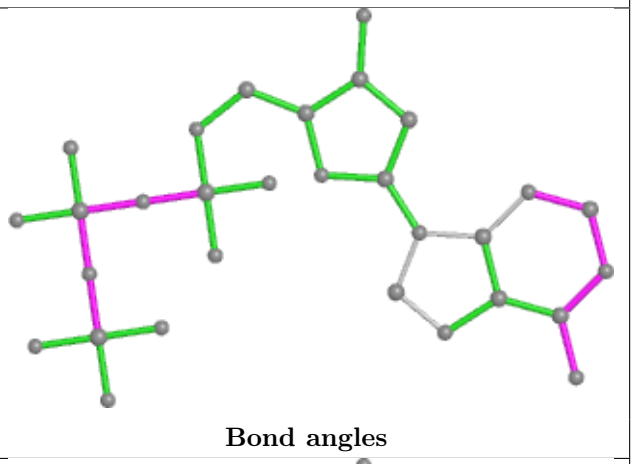


Rings

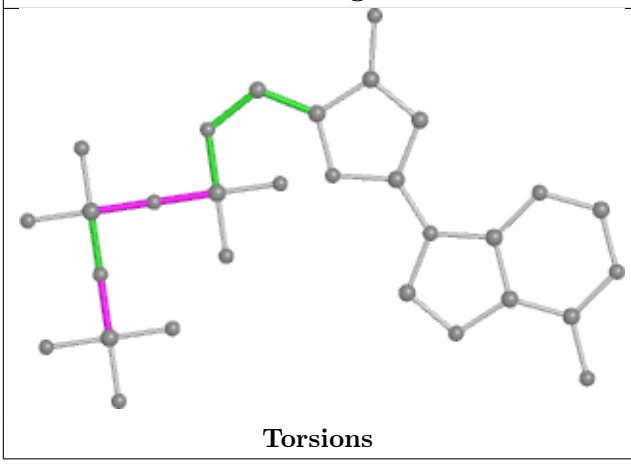
Ligand DTP H 701



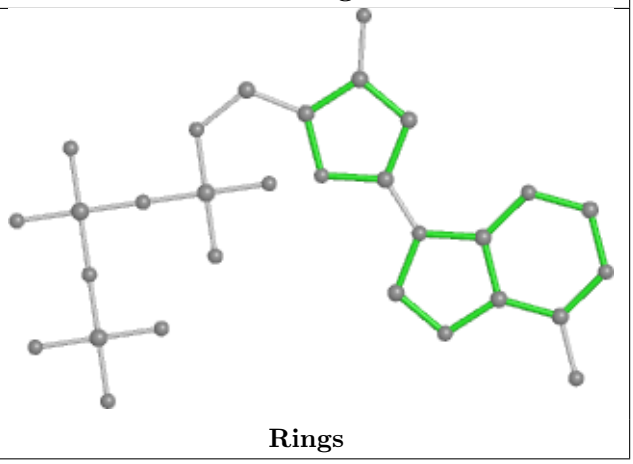
Bond lengths



Bond angles

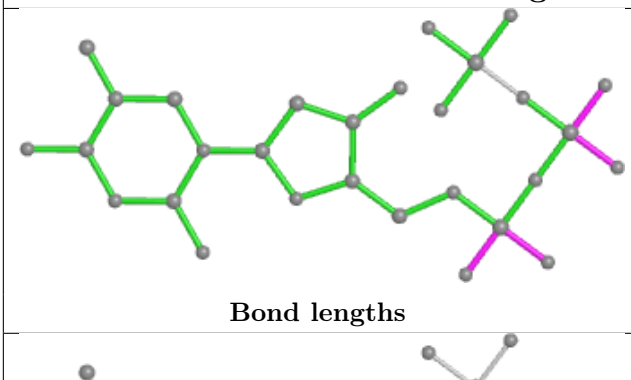


Torsions

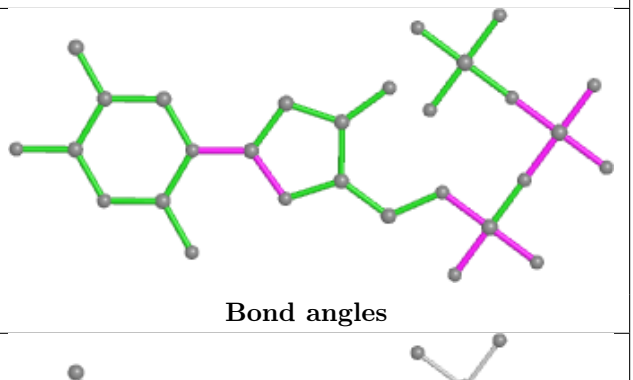


Rings

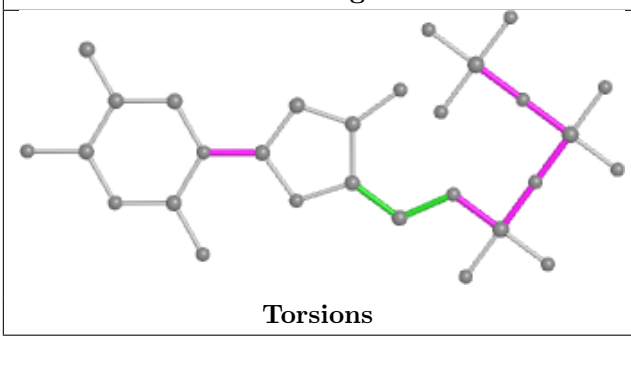
Ligand 1FZ H 705



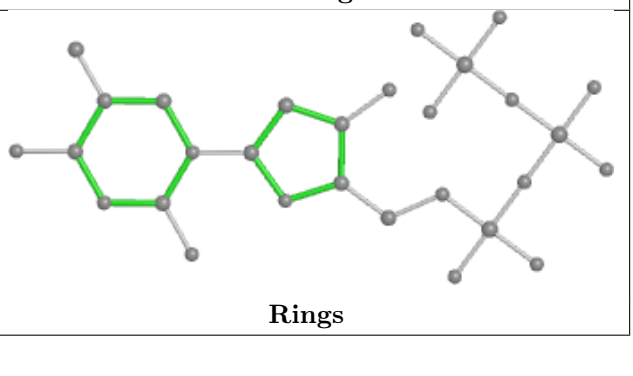
Bond lengths



Bond angles

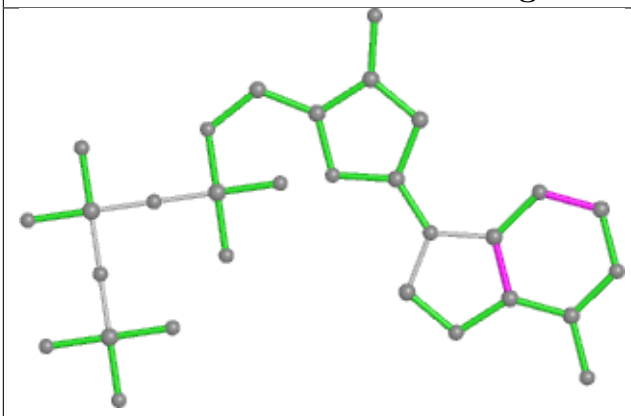


Torsions

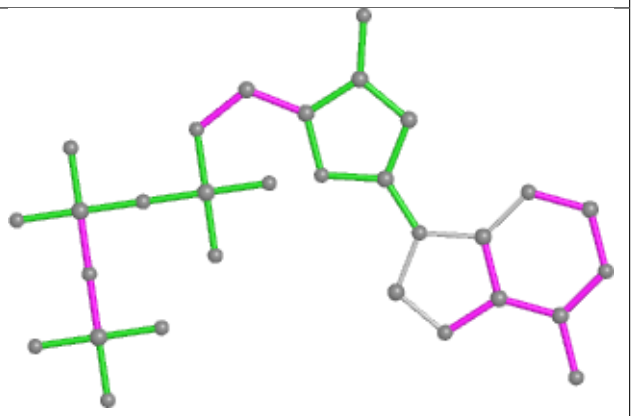


Rings

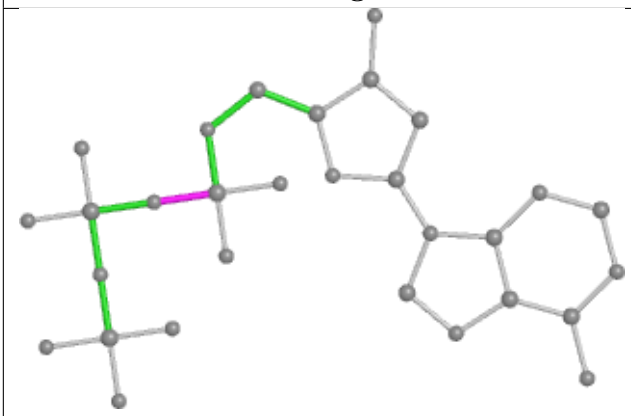
Ligand DTP M 706



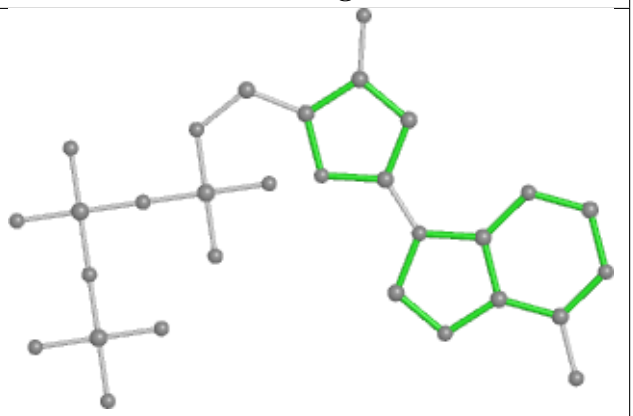
Bond lengths



Bond angles

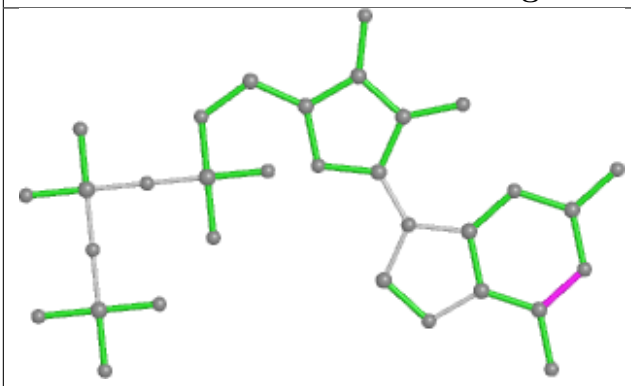


Torsions

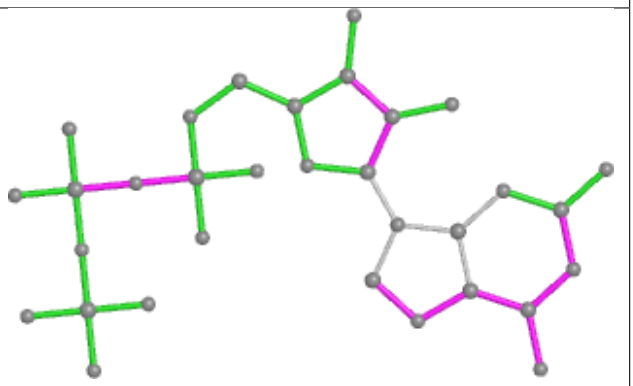


Rings

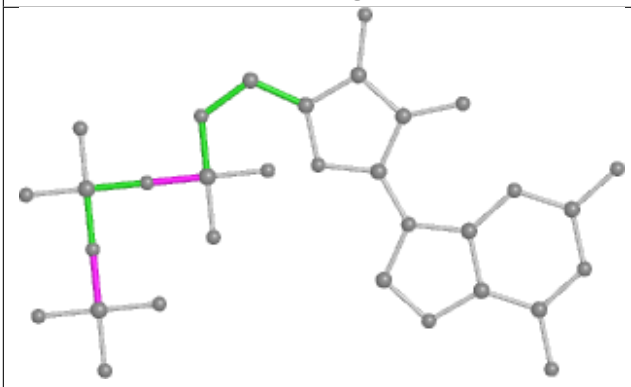
Ligand GTP N 706



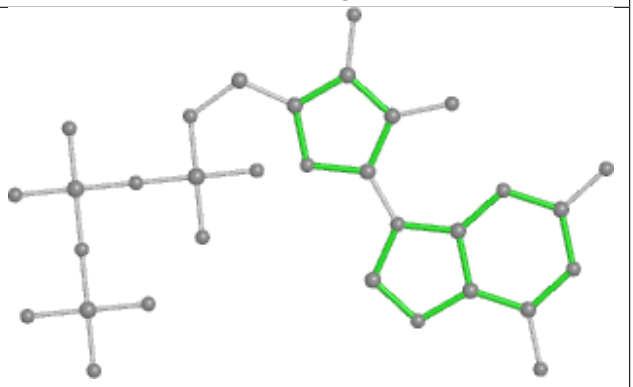
Bond lengths



Bond angles

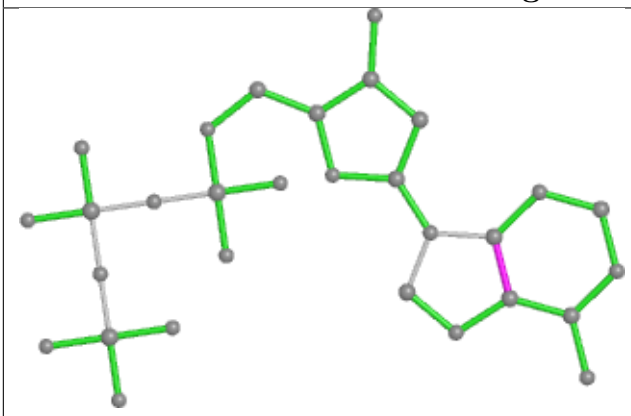


Torsions

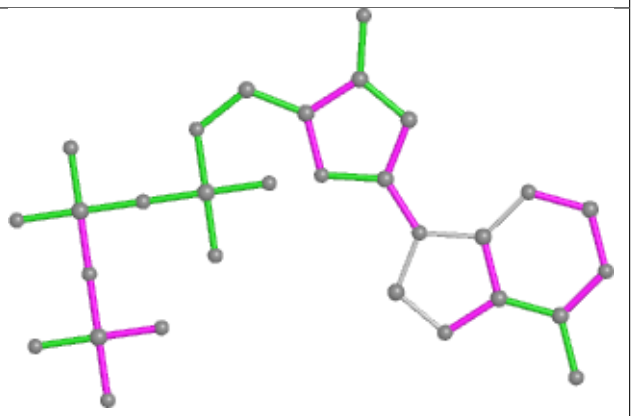


Rings

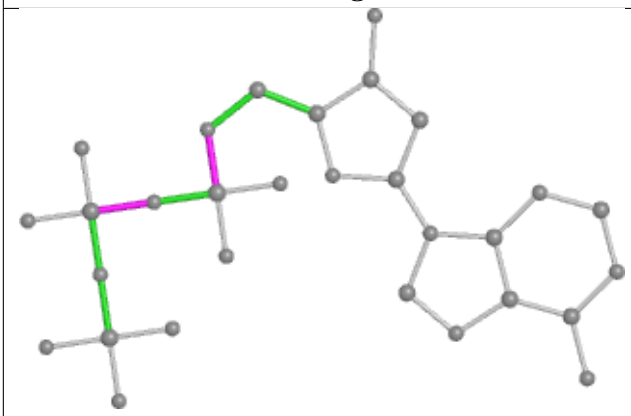
Ligand DTP A 706



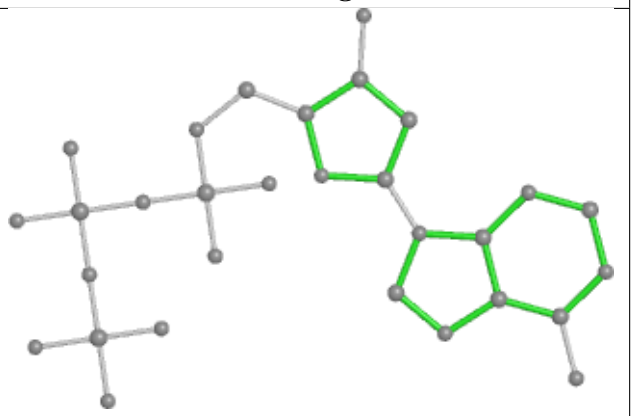
Bond lengths



Bond angles

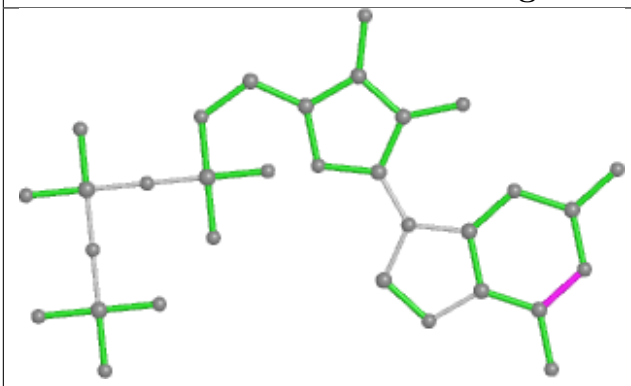


Torsions

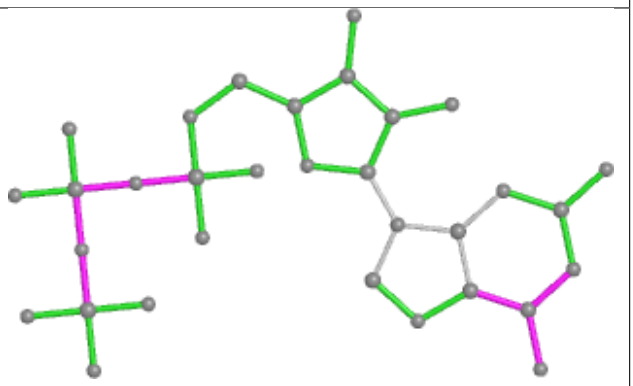


Rings

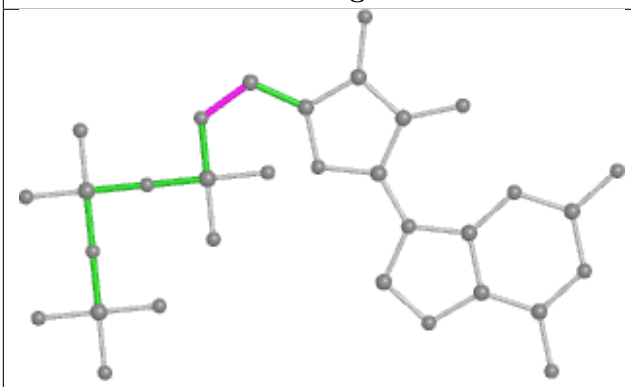
Ligand GTP M 705



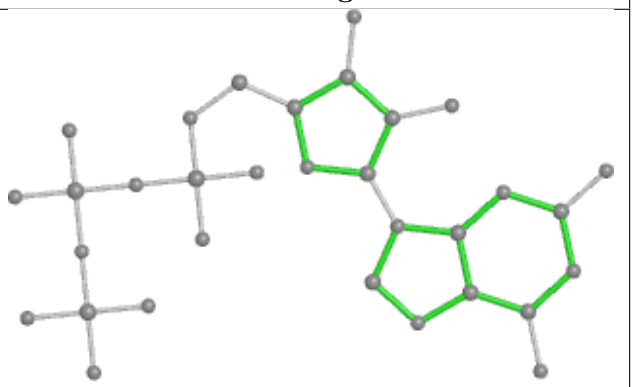
Bond lengths



Bond angles

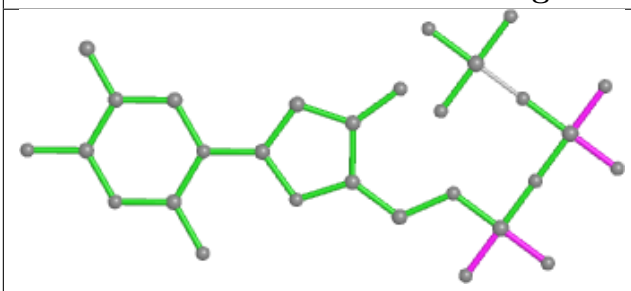


Torsions

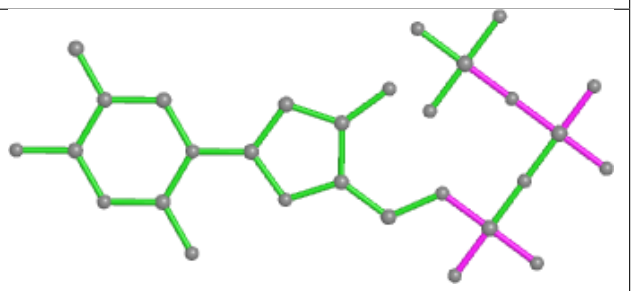


Rings

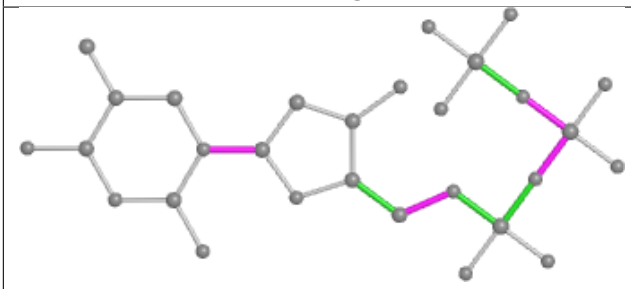
Ligand 1FZ F 704



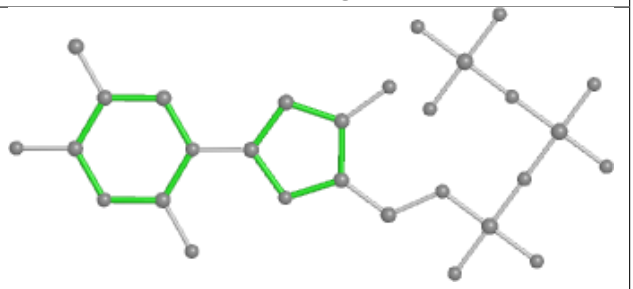
Bond lengths



Bond angles

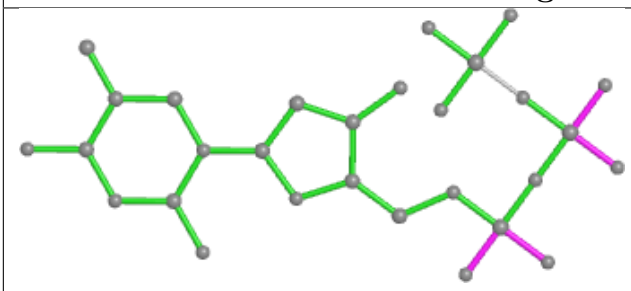


Torsions

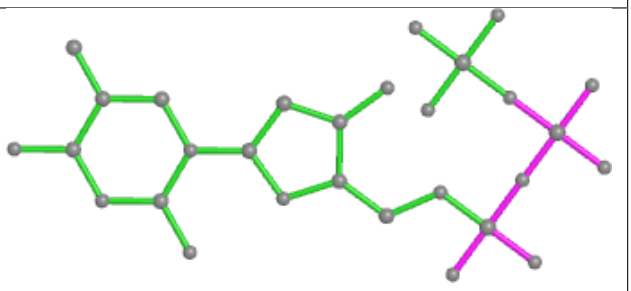


Rings

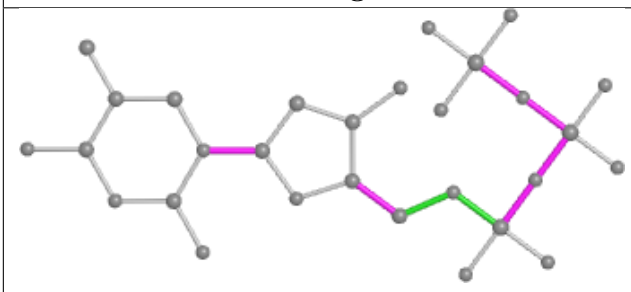
Ligand 1FZ I 704



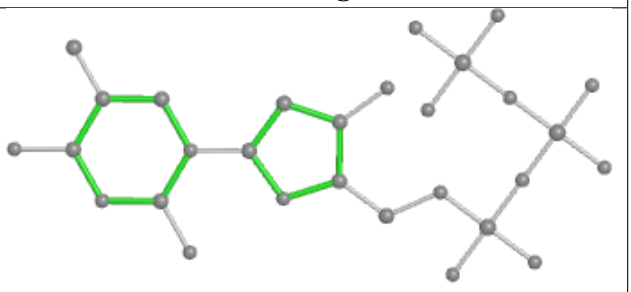
Bond lengths



Bond angles

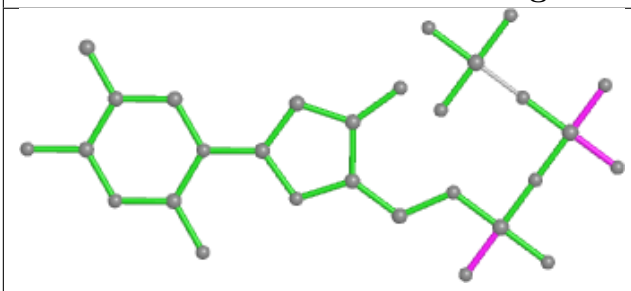


Torsions

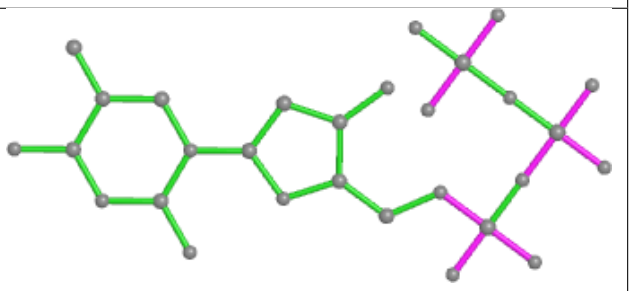


Rings

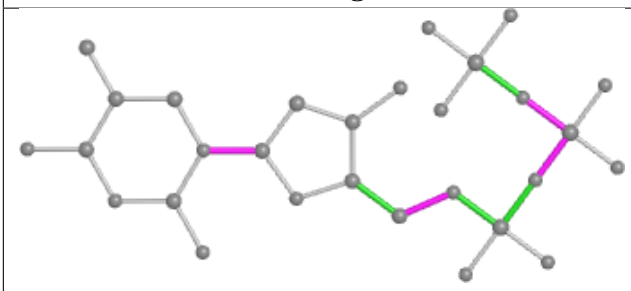
Ligand 1FZ A 704



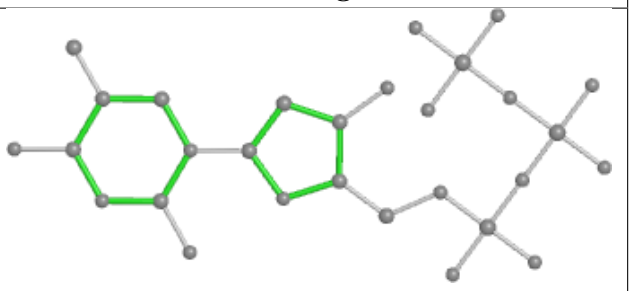
Bond lengths



Bond angles

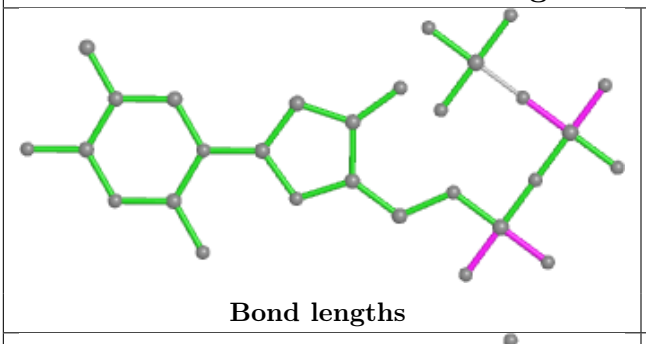


Torsions

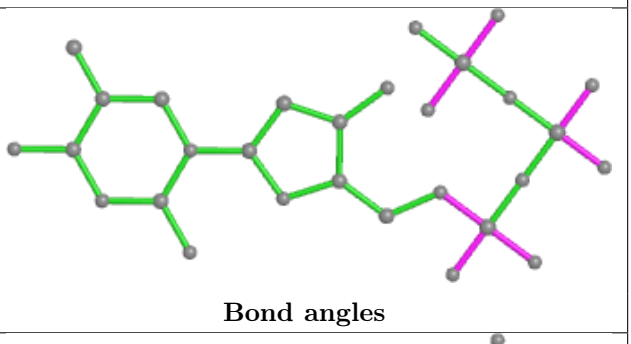


Rings

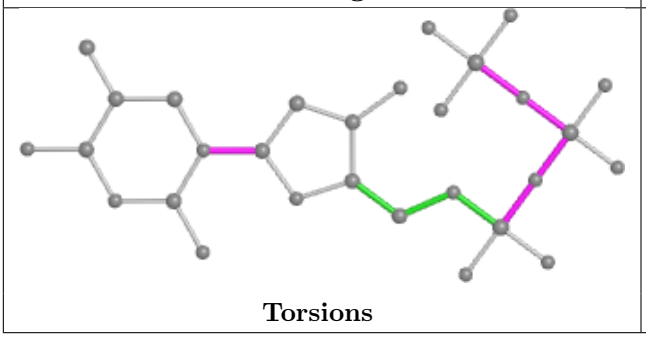
Ligand 1FZ D 706



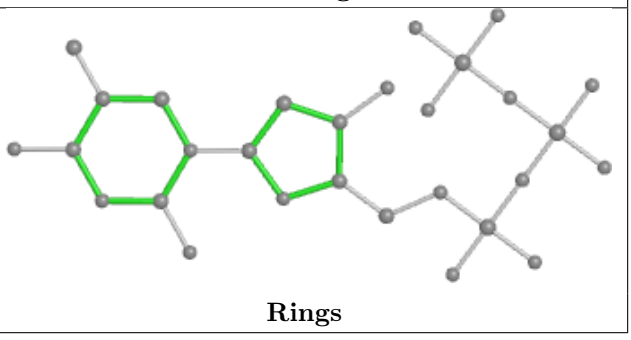
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	480/520 (92%)	-0.20	1 (0%) 95 94	22, 47, 77, 131	0
1	B	479/520 (92%)	-0.14	2 (0%) 92 89	24, 57, 96, 125	0
1	C	480/520 (92%)	-0.12	0 100 100	27, 55, 85, 111	0
1	D	481/520 (92%)	-0.18	1 (0%) 95 94	23, 50, 77, 105	0
1	E	479/520 (92%)	-0.07	1 (0%) 95 94	32, 60, 96, 122	0
1	F	478/520 (91%)	0.04	0 100 100	36, 67, 108, 124	0
1	G	479/520 (92%)	-0.04	1 (0%) 95 94	27, 57, 104, 127	0
1	H	480/520 (92%)	-0.15	0 100 100	27, 50, 77, 94	0
1	I	477/520 (91%)	0.07	3 (0%) 89 83	31, 69, 104, 134	0
1	J	478/520 (91%)	-0.08	1 (0%) 95 94	30, 57, 89, 104	0
1	K	478/520 (91%)	0.03	1 (0%) 95 94	32, 66, 96, 118	0
1	L	478/520 (91%)	0.17	3 (0%) 89 83	27, 73, 118, 138	0
1	M	475/520 (91%)	0.49	22 (4%) 32 20	47, 93, 121, 139	0
1	N	477/520 (91%)	0.27	6 (1%) 77 65	43, 79, 105, 126	0
1	O	481/520 (92%)	0.43	17 (3%) 44 28	43, 83, 122, 154	0
1	P	474/520 (91%)	0.50	16 (3%) 45 29	45, 89, 145, 194	0
All	All	7654/8320 (91%)	0.06	75 (0%) 82 72	22, 65, 110, 194	0

The worst 5 of 75 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	491	VAL	3.8
1	M	217	PHE	3.2
1	P	587	ILE	3.2
1	O	569	PHE	3.2
1	M	573	CYS	3.2

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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	SO4	I	706	5/5	0.77	0.23	125,126,129,131	0
7	SO4	N	707	5/5	0.81	0.30	128,128,132,134	0
7	SO4	O	706	5/5	0.84	0.22	117,121,125,126	0
3	MG	E	702	1/1	0.86	0.16	16,16,16,16	0
7	SO4	C	706	5/5	0.90	0.19	105,105,109,110	0
7	SO4	B	706	5/5	0.90	0.16	93,96,97,99	0
7	SO4	F	706	5/5	0.91	0.18	103,104,105,106	0
3	MG	O	702	1/1	0.92	0.14	19,19,19,19	0
7	SO4	K	707	5/5	0.93	0.16	89,90,91,92	0
5	GTP	N	706	32/32	0.94	0.19	66,68,76,79	0
4	1FZ	L	705	29/29	0.94	0.20	60,75,85,87	0
4	1FZ	M	704	29/29	0.95	0.21	66,74,83,90	0
4	1FZ	P	704	29/29	0.95	0.19	79,85,90,91	0
7	SO4	H	707	5/5	0.95	0.16	78,79,80,81	0
3	MG	H	704	1/1	0.95	0.09	44,44,44,44	0
7	SO4	J	705	5/5	0.95	0.14	102,103,104,105	0
5	GTP	O	705	32/32	0.95	0.17	72,76,80,81	0
6	DTP	M	707	30/30	0.95	0.18	72,74,82,83	0
3	MG	N	703	1/1	0.95	0.13	29,29,29,29	0
3	MG	M	702	1/1	0.96	0.09	20,20,20,20	0
6	DTP	N	708	30/30	0.96	0.18	54,57,80,81	0
3	MG	H	703	1/1	0.96	0.14	15,15,15,15	0
4	1FZ	N	705	29/29	0.96	0.17	54,60,66,67	0
7	SO4	D	708	5/5	0.96	0.12	77,77,79,81	0
4	1FZ	O	704	29/29	0.96	0.18	54,62,65,65	0
3	MG	G	704	1/1	0.96	0.08	18,18,18,18	0
5	GTP	E	705	32/32	0.96	0.16	46,49,54,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GTP	K	706	32/32	0.96	0.18	55,58,65,66	0
4	1FZ	G	705	29/29	0.96	0.17	37,40,53,56	0
4	1FZ	K	705	29/29	0.96	0.18	45,47,49,49	0
6	DTP	M	706	30/30	0.96	0.17	65,71,76,77	0
5	GTP	F	705	32/32	0.97	0.16	46,47,50,52	0
5	GTP	H	706	32/32	0.97	0.18	39,42,46,47	0
5	GTP	I	705	32/32	0.97	0.16	46,48,52,52	0
5	GTP	I	707	32/32	0.97	0.15	37,42,48,49	0
4	1FZ	B	704	29/29	0.97	0.17	41,47,54,59	0
5	GTP	L	706	32/32	0.97	0.15	35,38,41,42	0
5	GTP	M	705	32/32	0.97	0.14	51,56,65,67	0
4	1FZ	D	706	29/29	0.97	0.17	27,31,40,41	0
4	1FZ	E	704	29/29	0.97	0.18	37,45,63,69	0
5	GTP	P	705	32/32	0.97	0.17	62,68,72,73	0
6	DTP	F	707	30/30	0.97	0.16	48,50,53,54	0
6	DTP	G	701	30/30	0.97	0.17	49,52,56,57	0
6	DTP	H	701	30/30	0.97	0.17	49,51,54,54	0
6	DTP	L	701	30/30	0.97	0.17	39,45,49,50	0
4	1FZ	F	704	29/29	0.97	0.16	44,50,65,67	0
3	MG	D	704	1/1	0.97	0.18	15,15,15,15	0
4	1FZ	H	705	29/29	0.97	0.18	32,39,48,53	0
4	1FZ	I	704	29/29	0.97	0.17	39,45,62,62	0
3	MG	I	702	1/1	0.97	0.18	17,17,17,17	0
3	MG	B	703	1/1	0.97	0.08	16,16,16,16	0
7	SO4	E	706	5/5	0.97	0.12	68,68,69,70	0
3	MG	C	703	1/1	0.97	0.15	16,16,16,16	0
3	MG	C	704	1/1	0.97	0.12	16,16,16,16	0
3	MG	O	703	1/1	0.97	0.15	61,61,61,61	0
3	MG	P	702	1/1	0.97	0.08	19,19,19,19	0
5	GTP	B	705	32/32	0.97	0.16	31,33,35,36	0
5	GTP	D	707	32/32	0.97	0.16	40,44,48,48	0
4	1FZ	A	704	29/29	0.97	0.15	31,35,39,41	0
6	DTP	B	707	30/30	0.98	0.16	29,31,34,35	0
6	DTP	D	701	30/30	0.98	0.15	26,27,32,33	0
6	DTP	E	707	30/30	0.98	0.17	32,33,35,35	0
3	MG	K	703	1/1	0.98	0.10	17,17,17,17	0
5	GTP	A	705	32/32	0.98	0.15	35,38,40,41	0
4	1FZ	C	705	29/29	0.98	0.16	34,37,44,46	0
6	DTP	I	708	30/30	0.98	0.17	36,41,50,50	0
6	DTP	J	706	30/30	0.98	0.17	25,26,30,31	0
6	DTP	K	701	30/30	0.98	0.15	41,42,50,51	0
5	GTP	D	702	32/32	0.98	0.16	27,31,33,34	0

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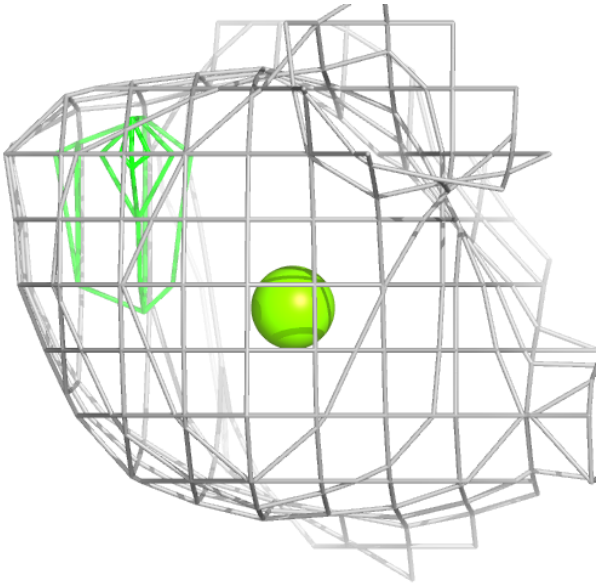
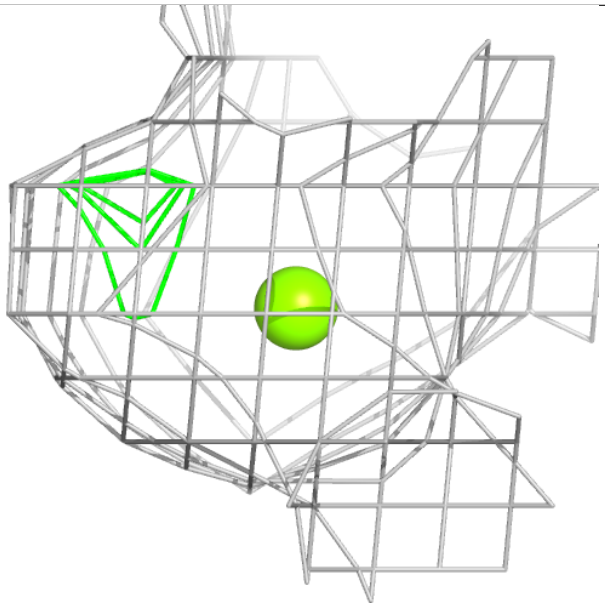
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	K	704	1/1	0.98	0.13	54,54,54,54	0
3	MG	L	703	1/1	0.98	0.16	17,17,17,17	0
6	DTP	N	701	30/30	0.98	0.17	53,56,60,61	0
3	MG	B	702	1/1	0.98	0.16	16,16,16,16	0
5	GTP	G	706	32/32	0.98	0.15	33,38,52,54	0
3	MG	M	703	1/1	0.98	0.09	50,50,50,50	0
3	MG	A	702	1/1	0.98	0.11	15,15,15,15	0
3	MG	N	704	1/1	0.98	0.06	73,73,73,73	0
4	1FZ	J	704	29/29	0.98	0.15	34,37,41,41	0
3	MG	A	703	1/1	0.98	0.07	22,22,22,22	0
3	MG	G	703	1/1	0.98	0.12	16,16,16,16	0
3	MG	J	702	1/1	0.98	0.18	15,15,15,15	0
3	MG	P	703	1/1	0.98	0.05	30,30,30,30	0
3	MG	J	703	1/1	0.98	0.08	30,30,30,30	0
6	DTP	A	706	30/30	0.98	0.16	30,32,38,39	0
2	FE	O	701	1/1	0.99	0.09	45,45,45,45	0
3	MG	D	705	1/1	0.99	0.08	24,24,24,24	0
2	FE	P	701	1/1	0.99	0.11	44,44,44,44	0
3	MG	E	703	1/1	0.99	0.08	24,24,24,24	0
3	MG	L	704	1/1	0.99	0.05	18,18,18,18	0
6	DTP	C	701	30/30	0.99	0.15	26,28,33,34	0
3	MG	F	702	1/1	0.99	0.12	16,16,16,16	0
3	MG	F	703	1/1	0.99	0.10	28,28,28,28	0
2	FE	C	702	1/1	0.99	0.12	20,20,20,20	0
2	FE	E	701	1/1	0.99	0.10	32,32,32,32	0
2	FE	I	701	1/1	0.99	0.10	42,42,42,42	0
2	FE	K	702	1/1	0.99	0.09	38,38,38,38	0
2	FE	L	702	1/1	0.99	0.09	42,42,42,42	0
3	MG	I	703	1/1	0.99	0.07	23,23,23,23	0
2	FE	N	702	1/1	0.99	0.06	50,50,50,50	0
2	FE	B	701	1/1	1.00	0.13	23,23,23,23	0
2	FE	M	701	1/1	1.00	0.06	48,48,48,48	0
2	FE	F	701	1/1	1.00	0.11	33,33,33,33	0
2	FE	G	702	1/1	1.00	0.11	16,16,16,16	0
2	FE	H	702	1/1	1.00	0.09	26,26,26,26	0
2	FE	A	701	1/1	1.00	0.11	26,26,26,26	0
2	FE	J	701	1/1	1.00	0.11	17,17,17,17	0
2	FE	D	703	1/1	1.00	0.12	15,15,15,15	0

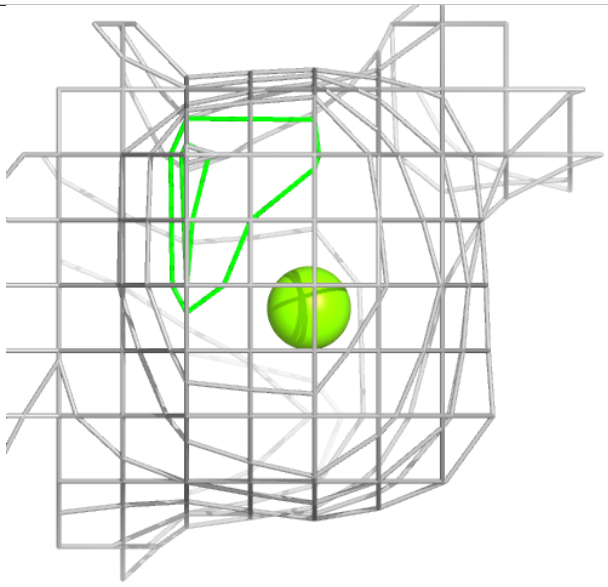
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MG 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)

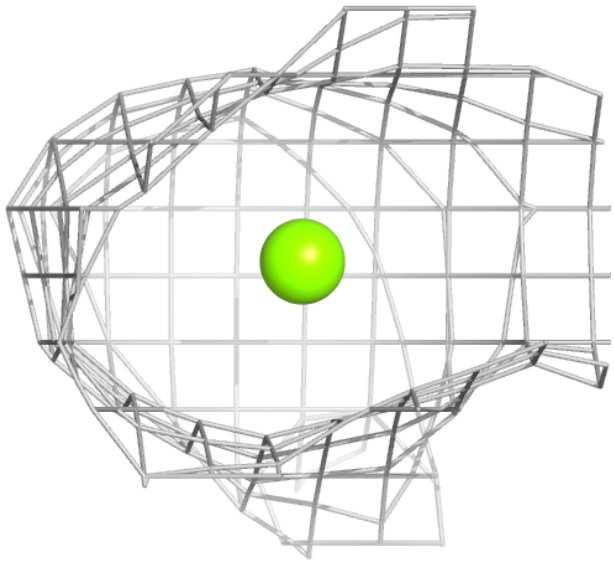


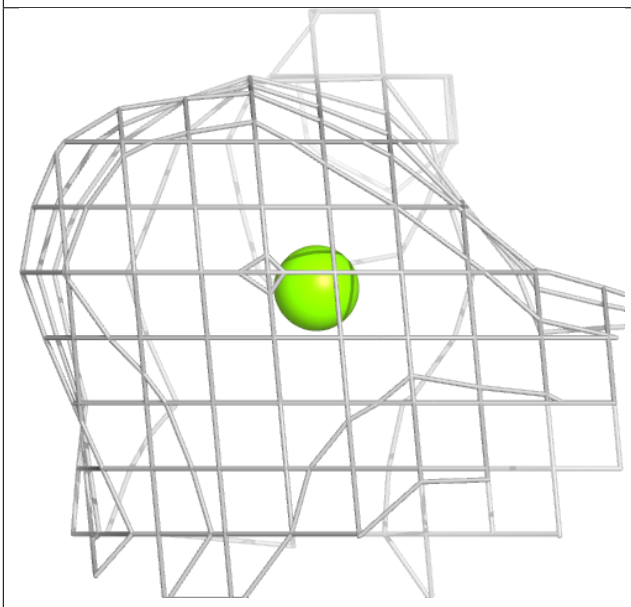


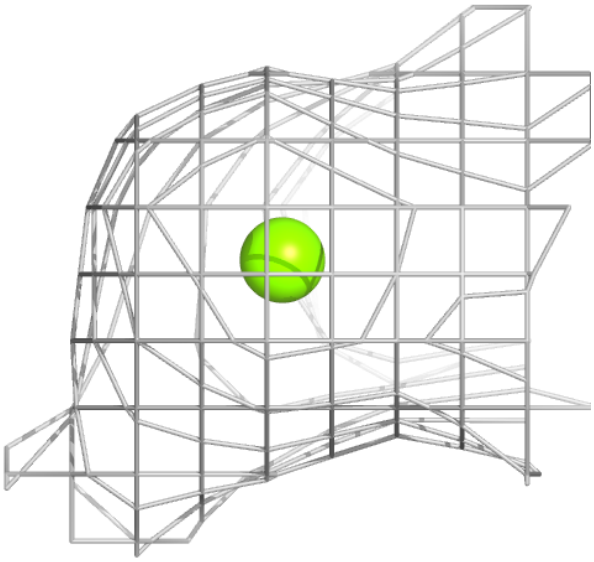


Electron density around MG O 702:

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

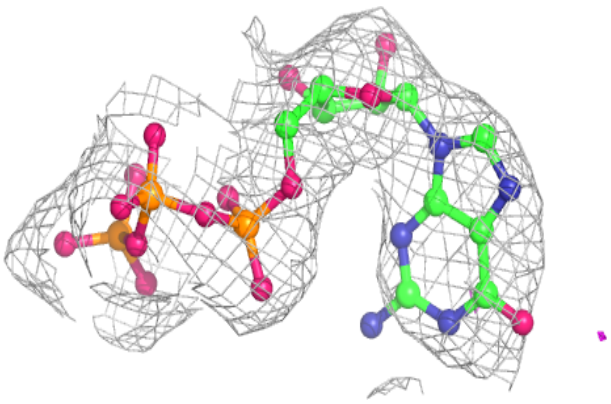


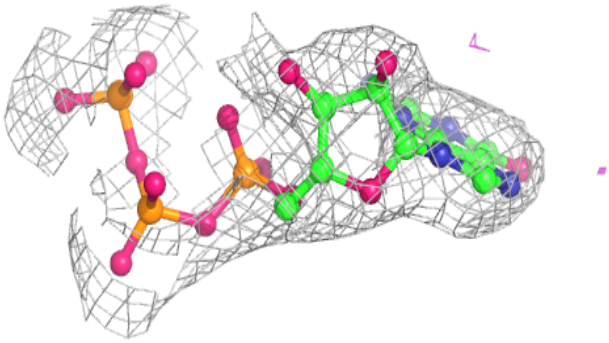


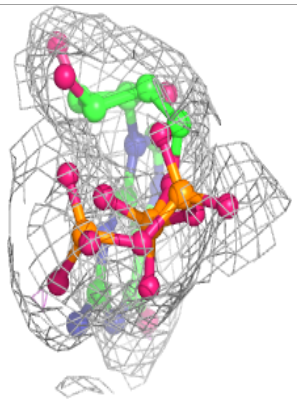


Electron density around GTP N 706:

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

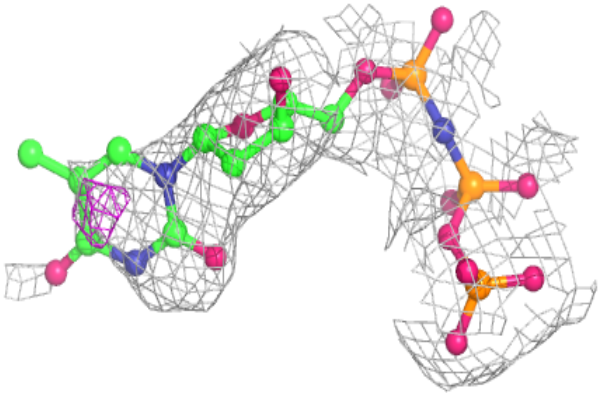


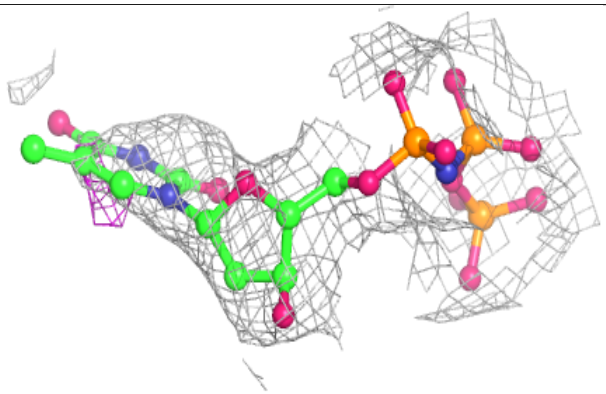


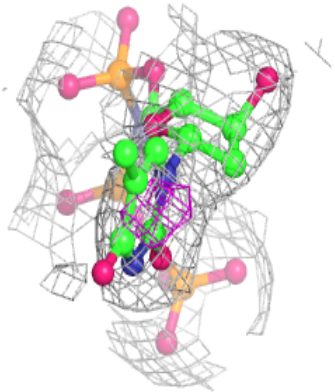


Electron density around 1FZ L 705:

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

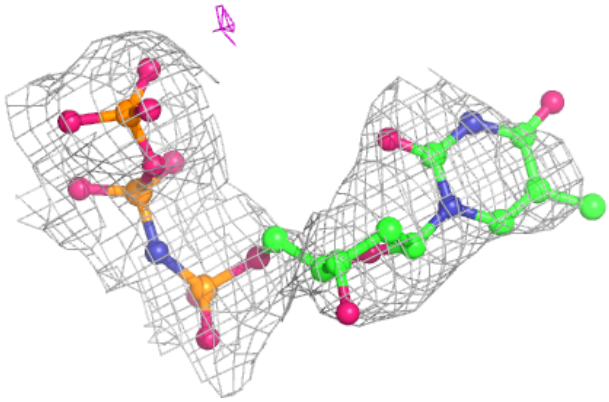


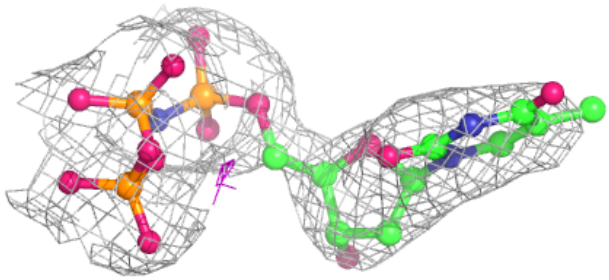


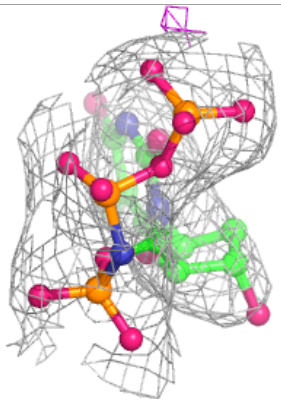


Electron density around 1FZ M 704:

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

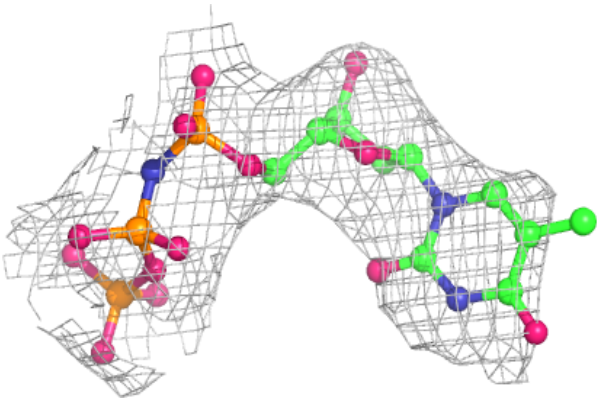


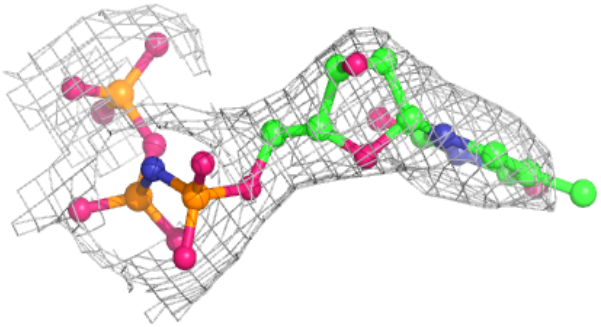


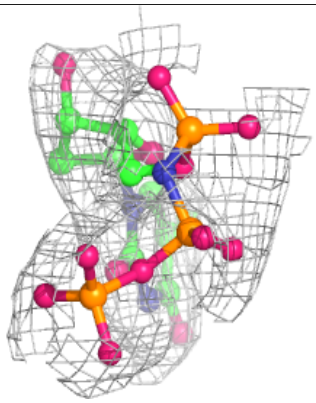


Electron density around 1FZ P 704:

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

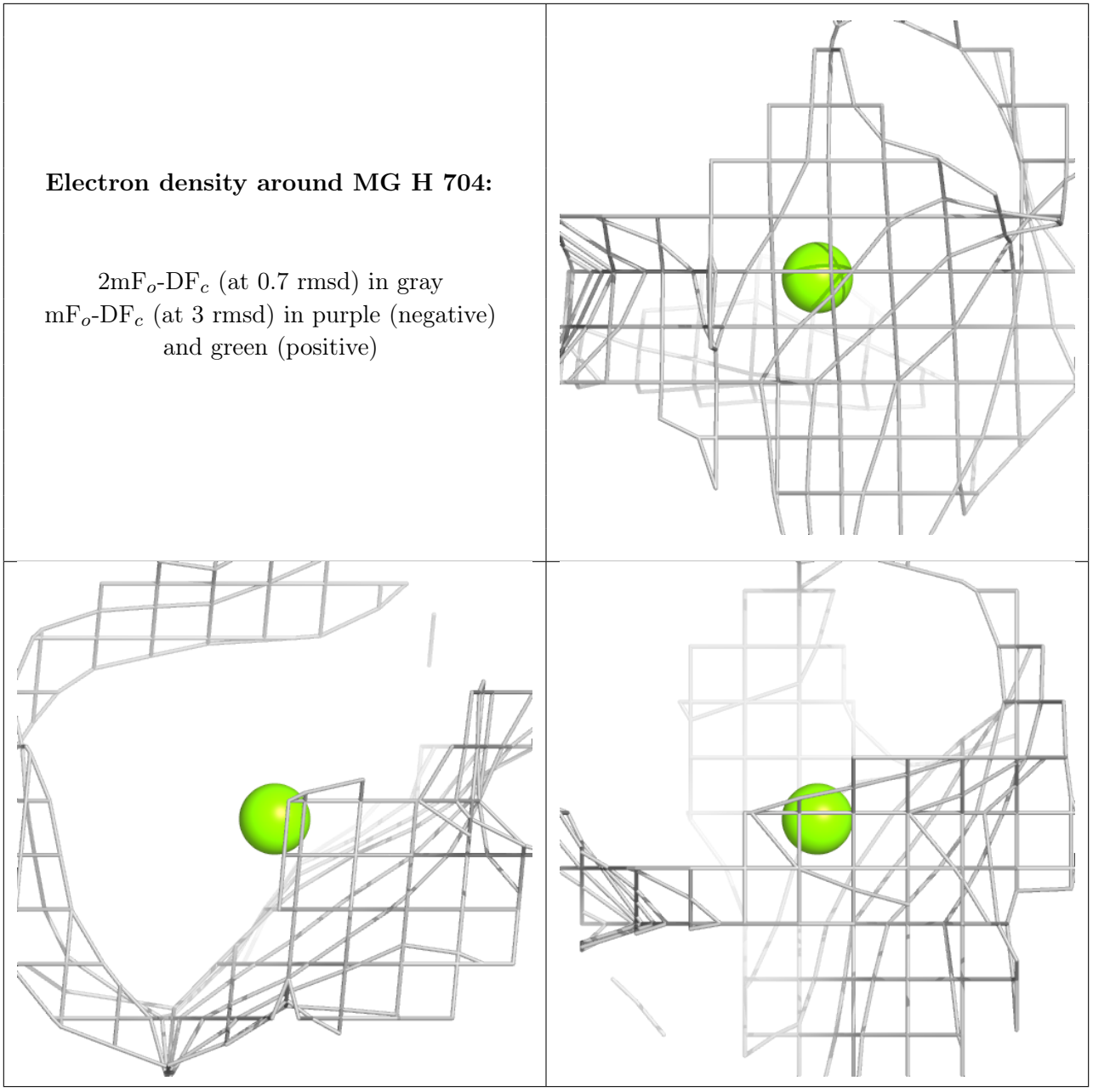






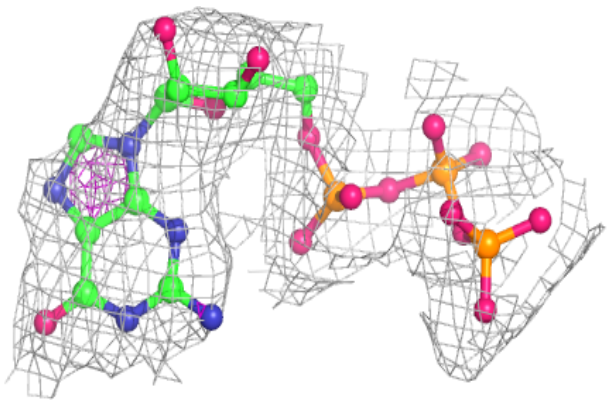
Electron density around MG H 704:

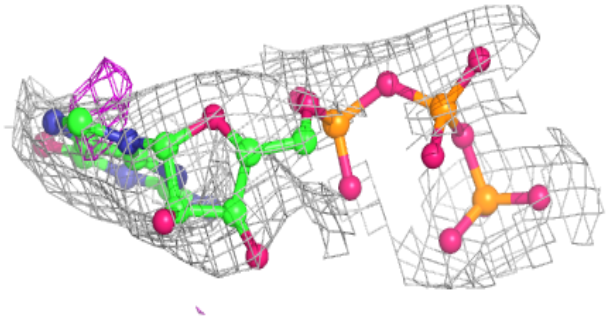
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around GTP O 705:

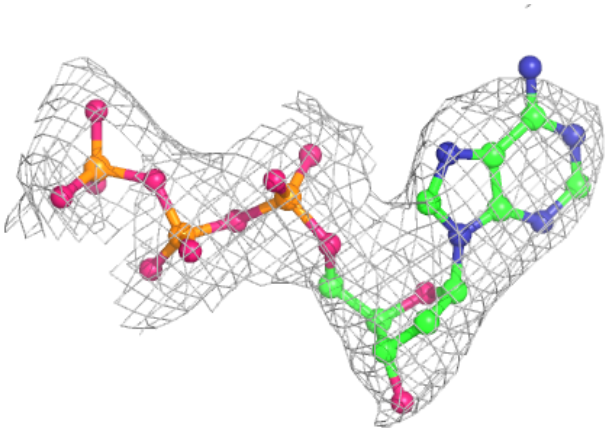
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

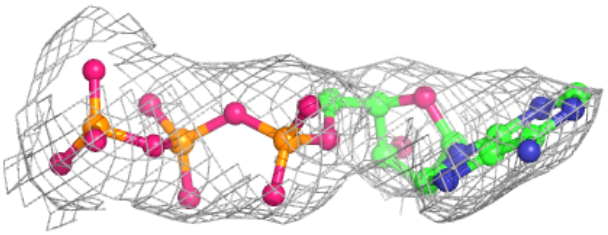


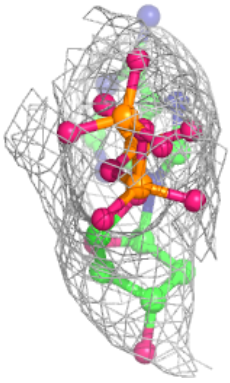


Electron density around DTP M 707:

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

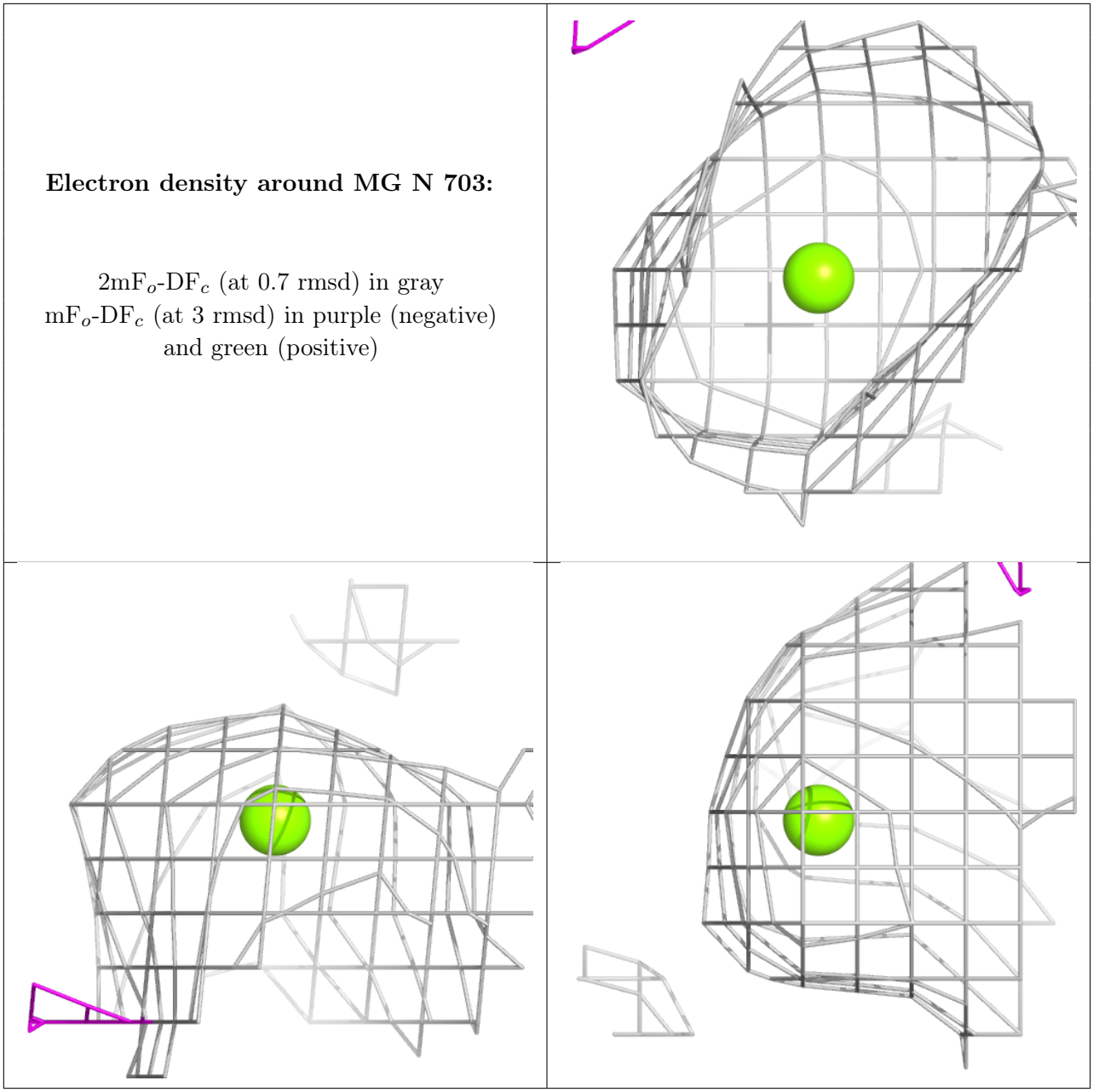






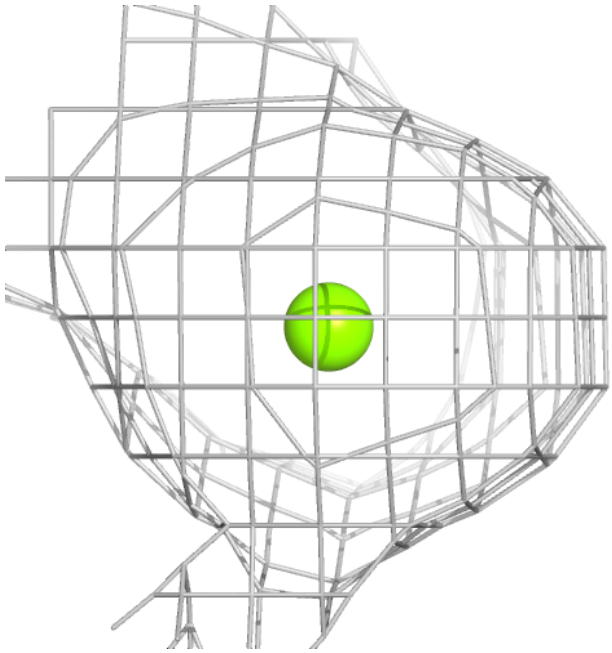
Electron density around MG N 703:

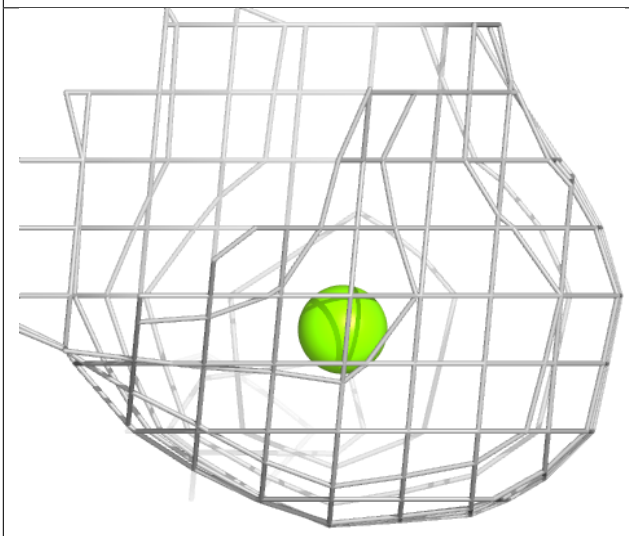
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

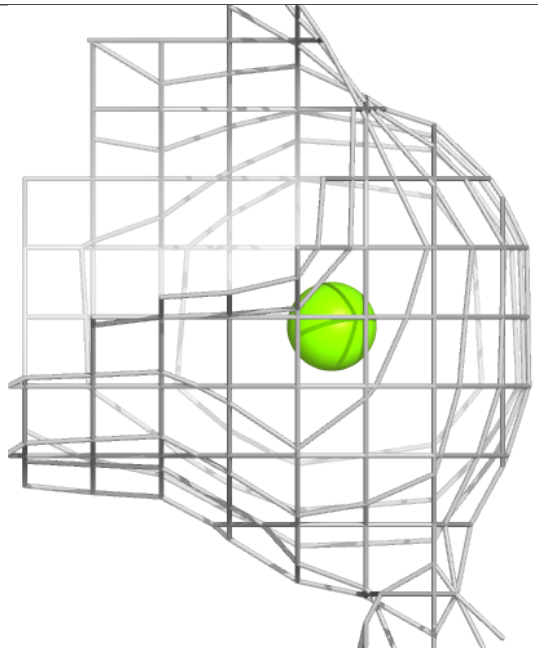


Electron density around MG M 702:

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

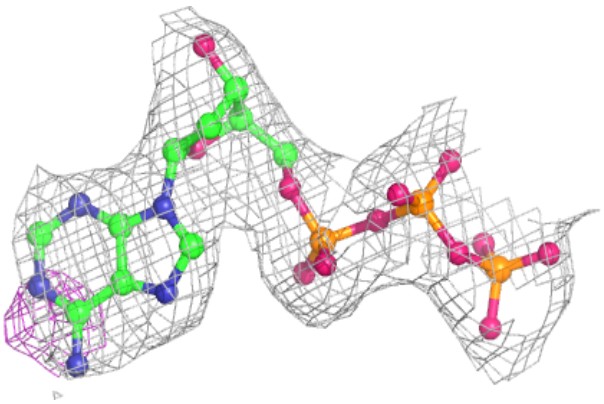


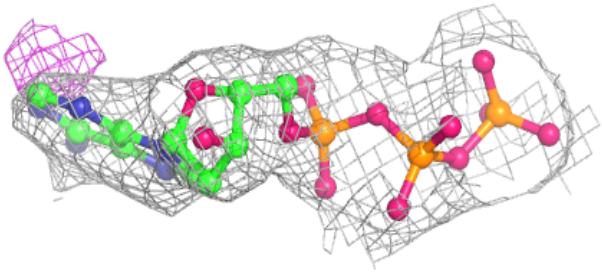


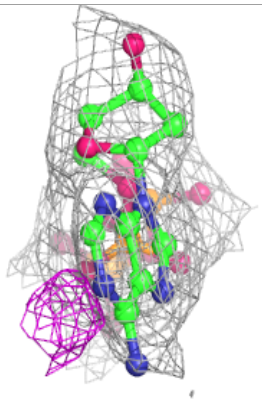


Electron density around DTP N 708:

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

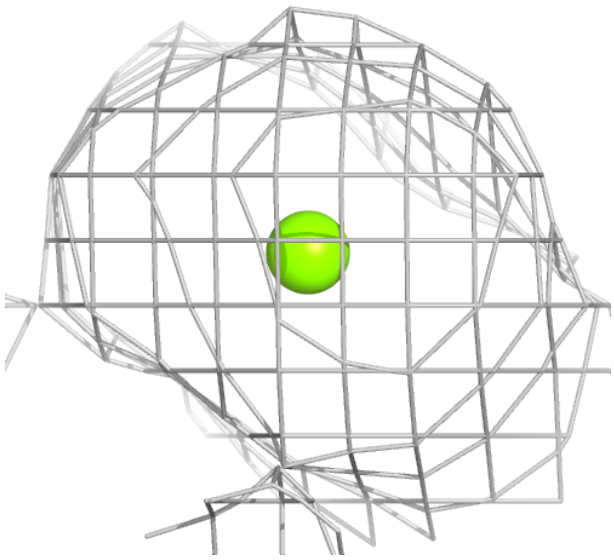


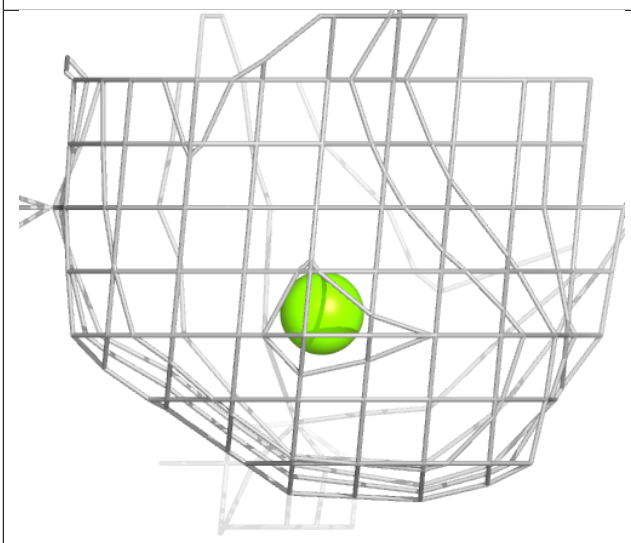


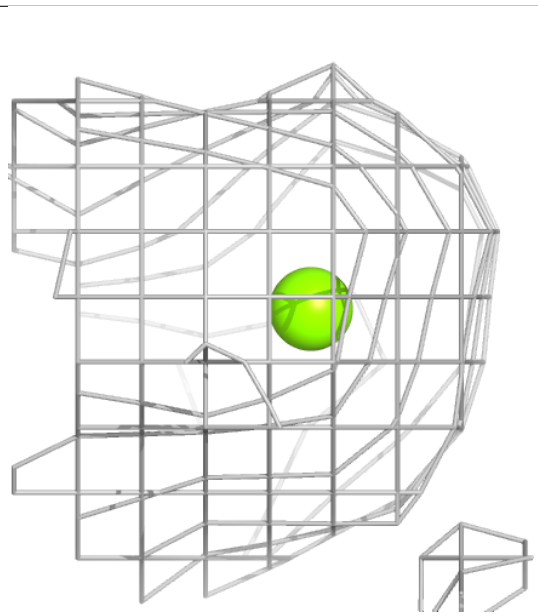


Electron density around MG H 703:

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

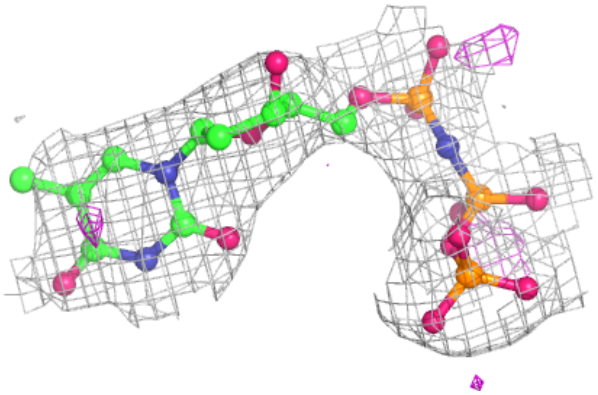


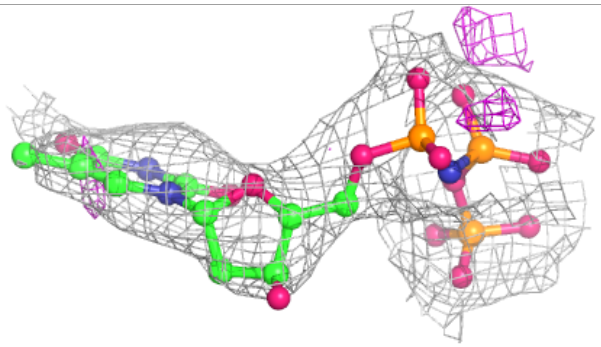


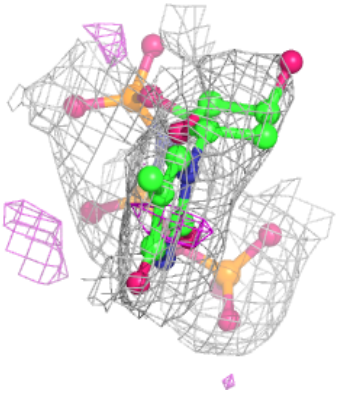


Electron density around 1FZ N 705:

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

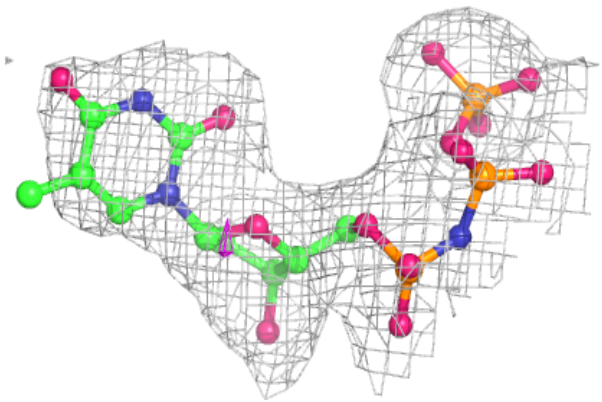


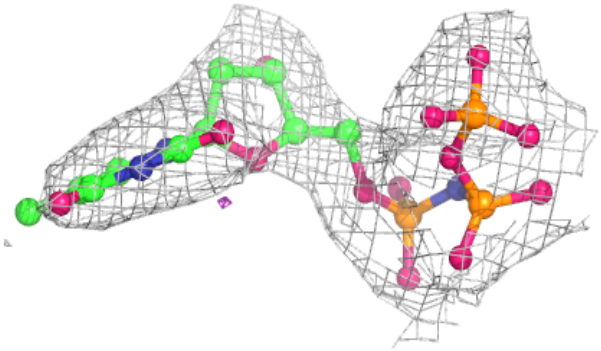


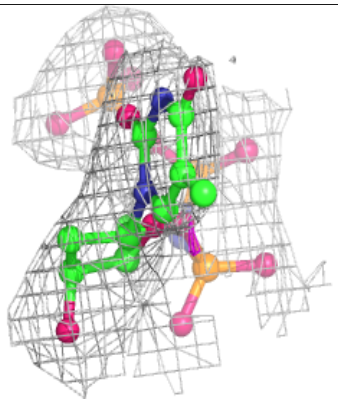


Electron density around 1FZ O 704:

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

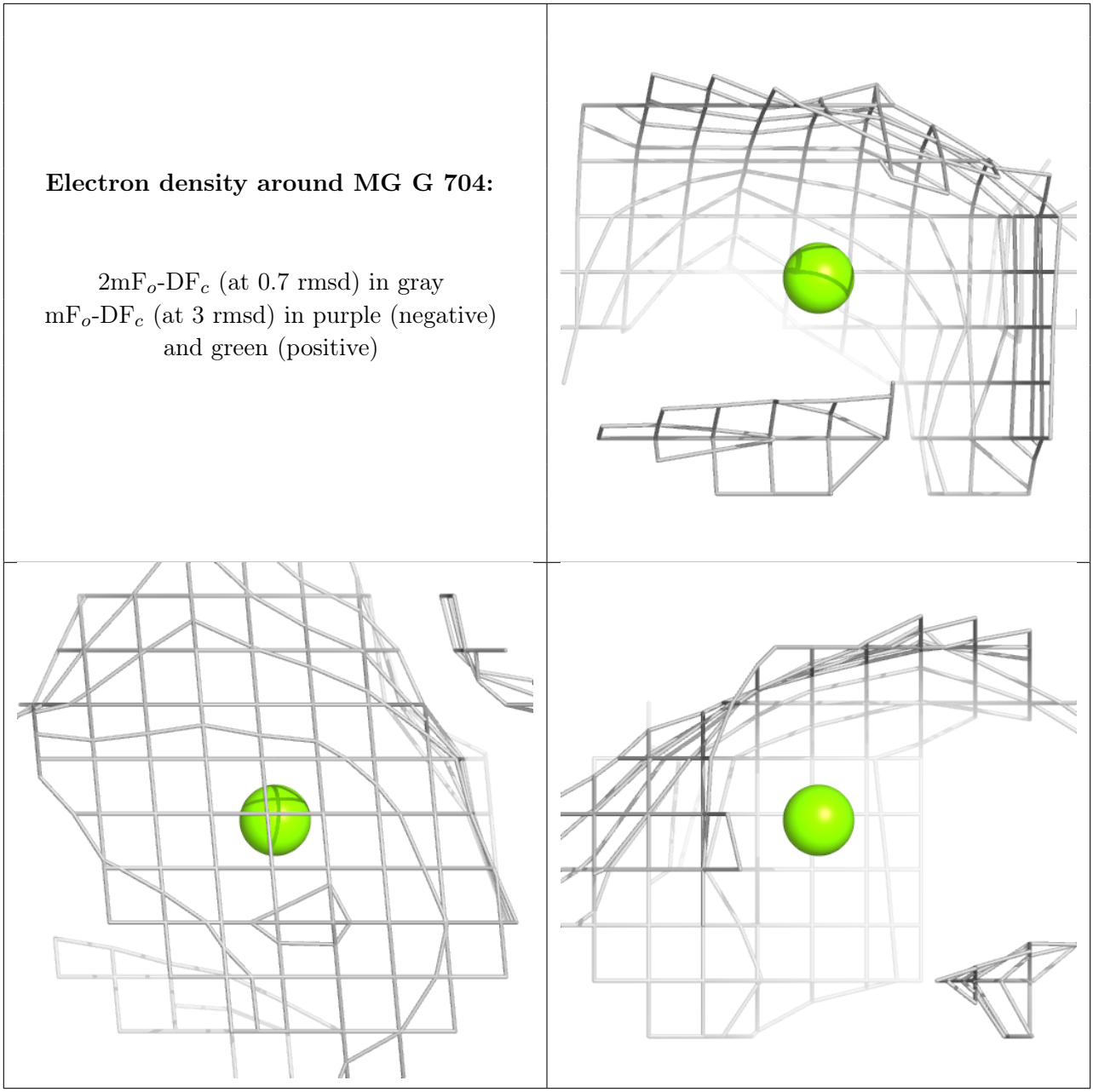






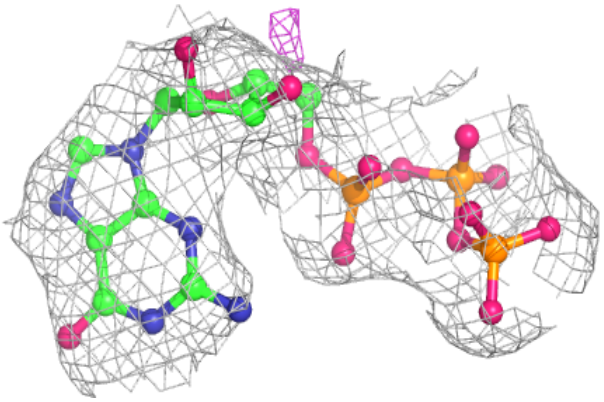
Electron density around MG G 704:

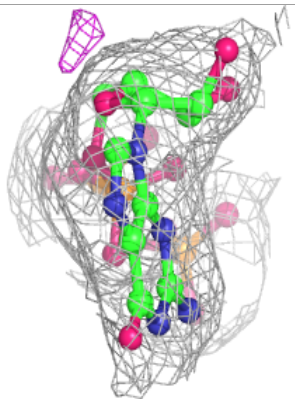
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around GTP E 705:

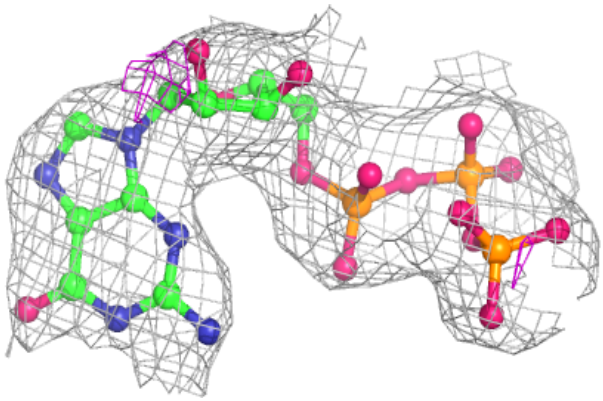
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

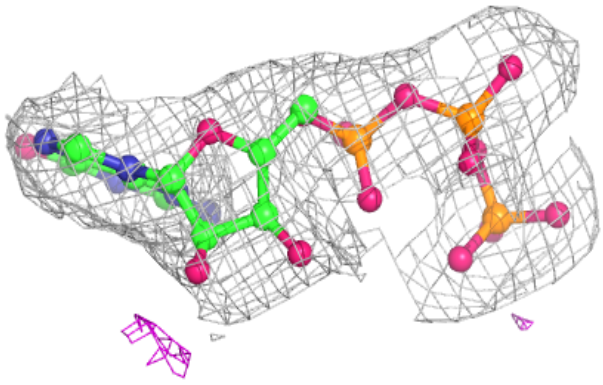


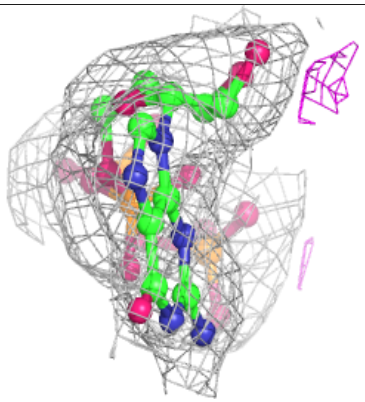


Electron density around GTP K 706:

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

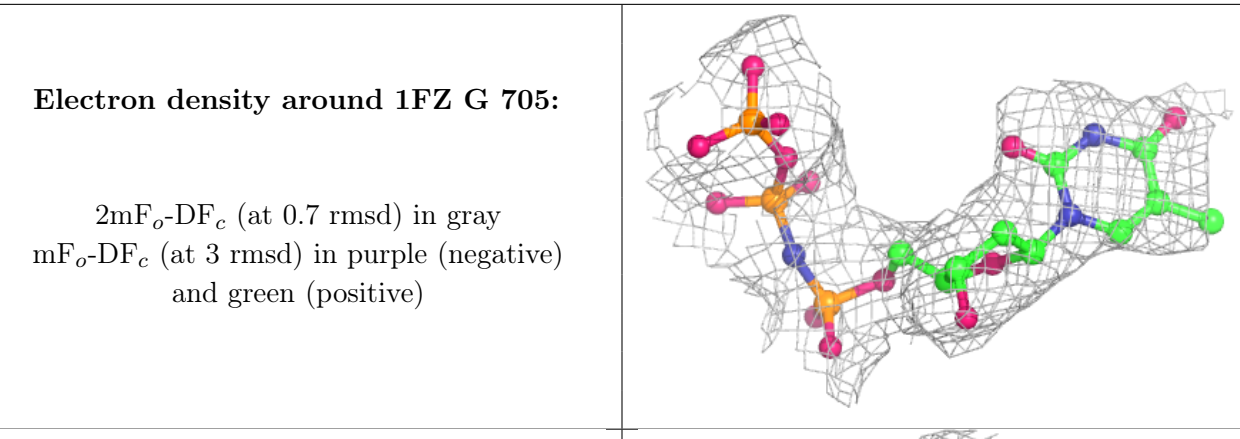






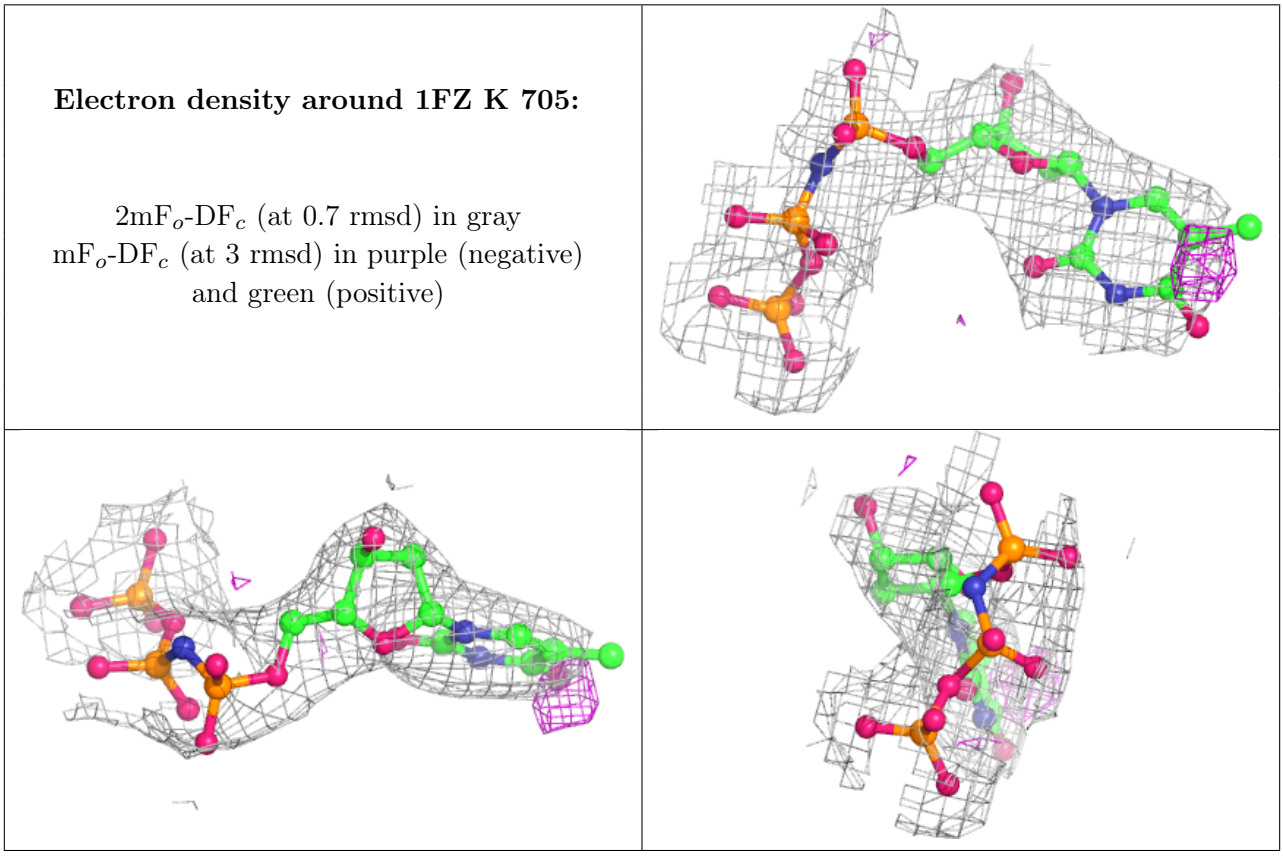
Electron density around 1FZ G 705:

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



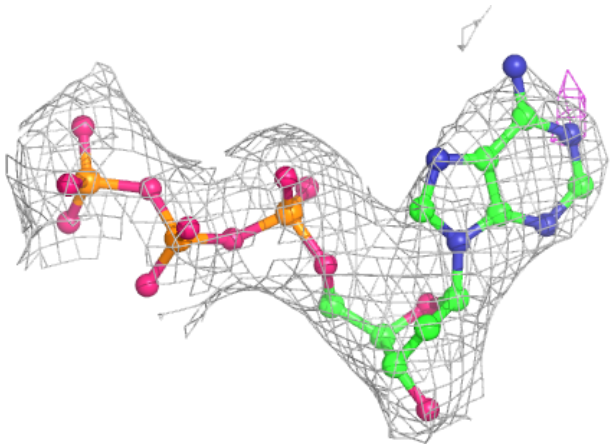
Electron density around 1FZ K 705:

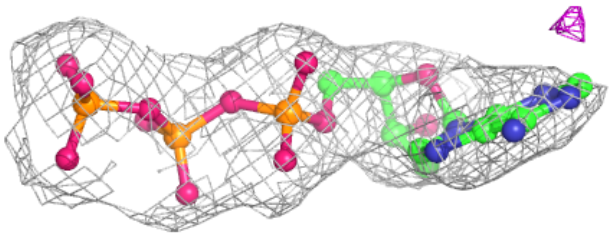
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

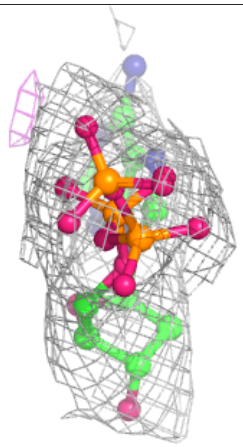


Electron density around DTP M 706:

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

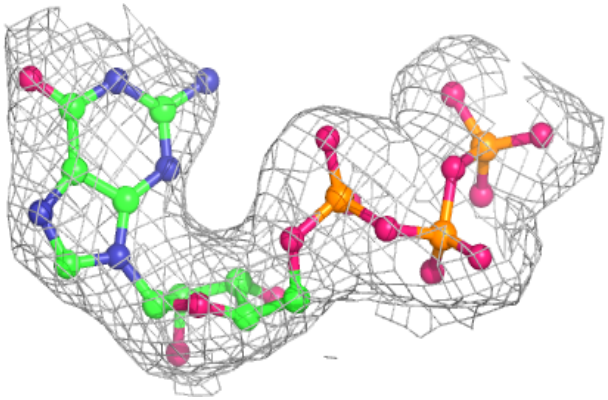


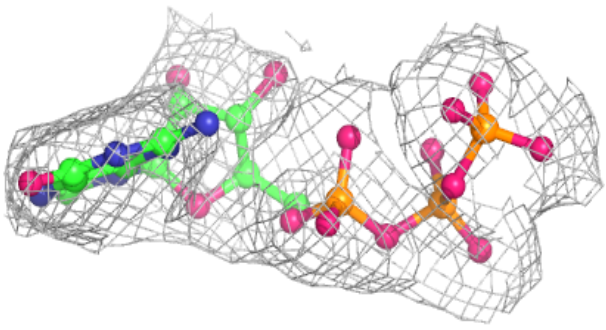


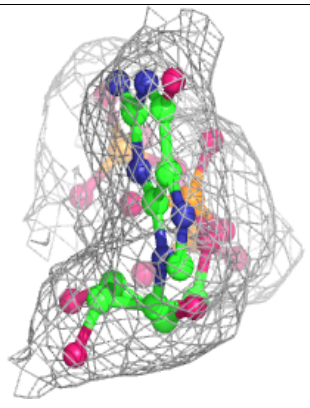


Electron density around GTP F 705:

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

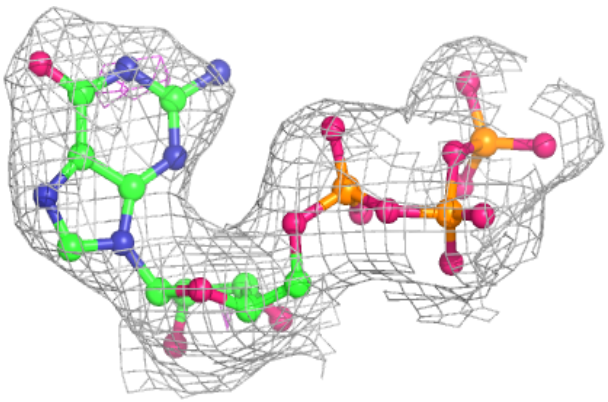


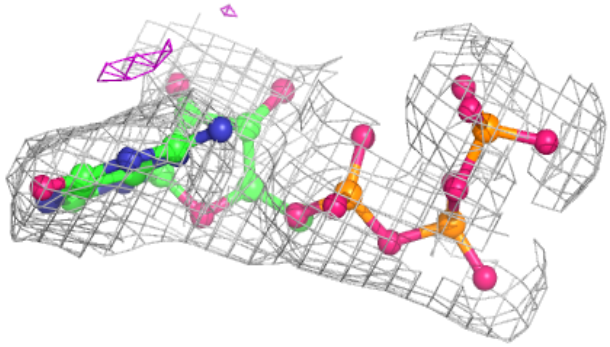


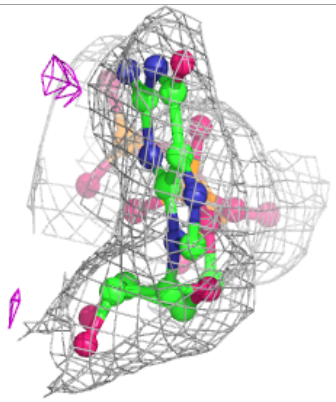


Electron density around GTP H 706:

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

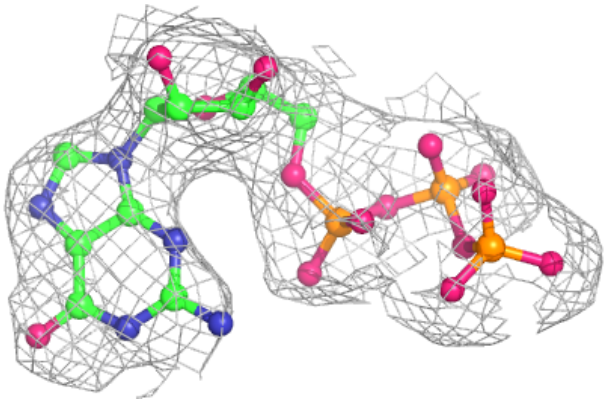


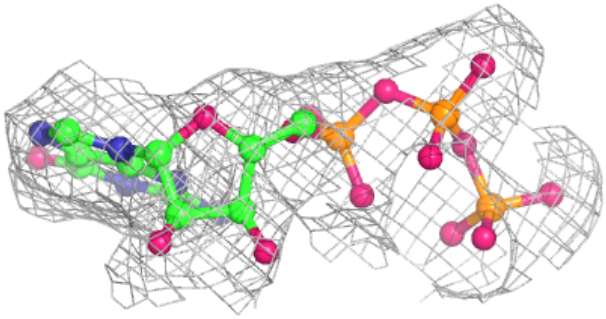


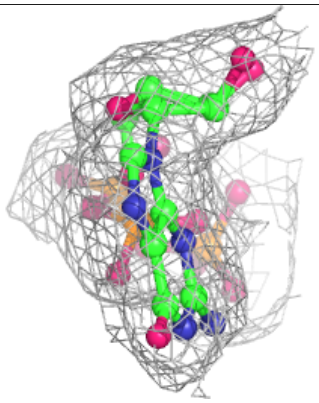


Electron density around GTP I 705:

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

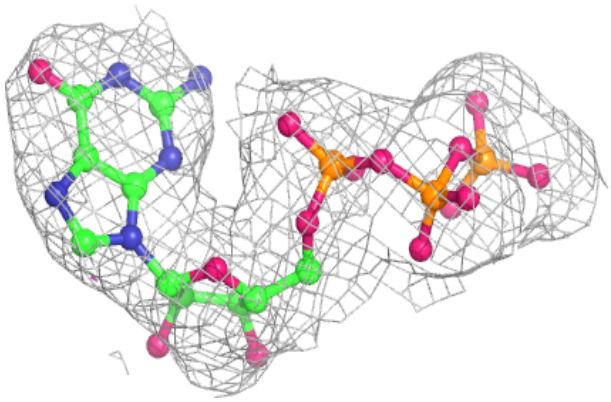


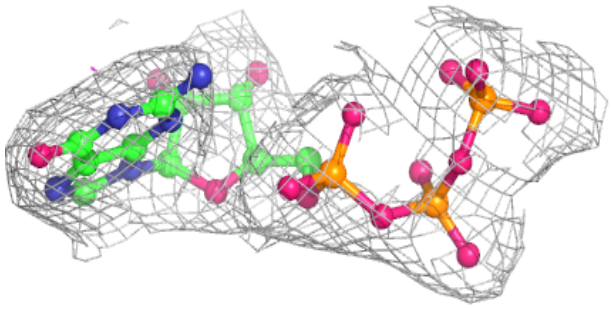


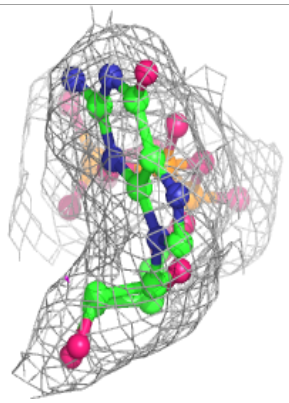


Electron density around GTP I 707:

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

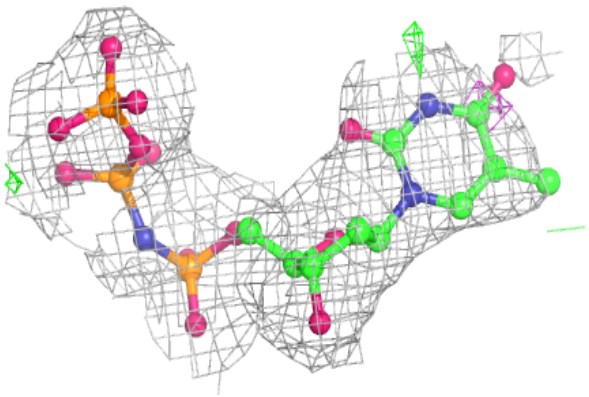


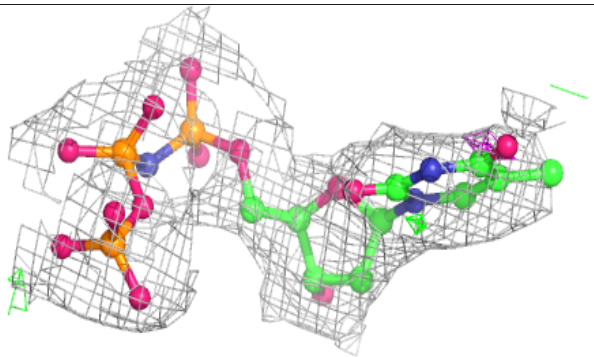


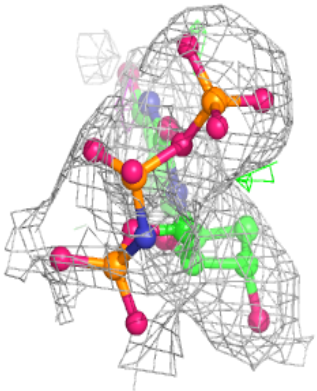


Electron density around 1FZ B 704:

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

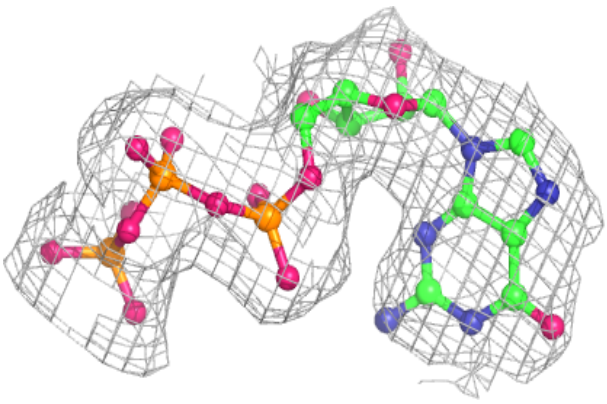


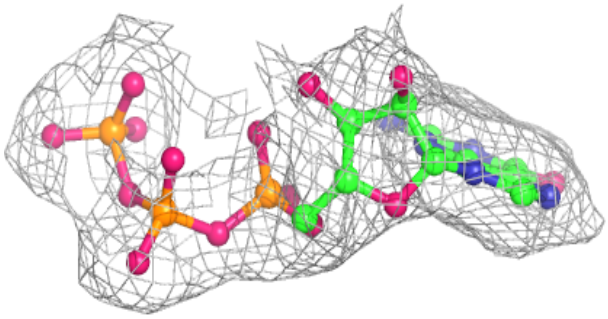


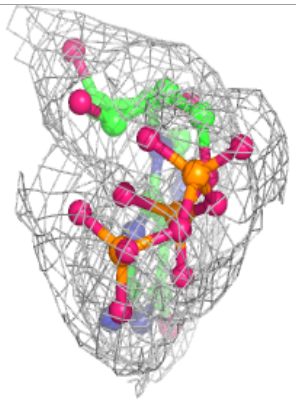


Electron density around GTP L 706:

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

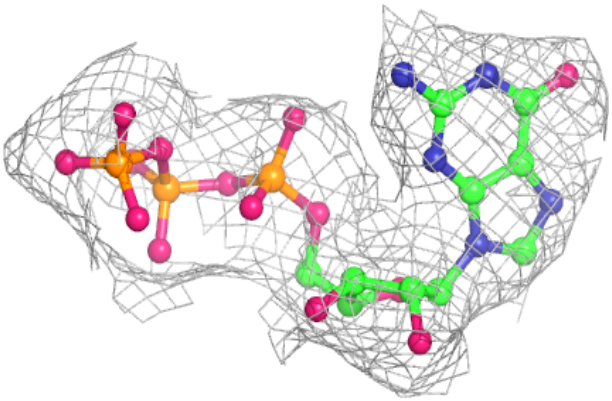


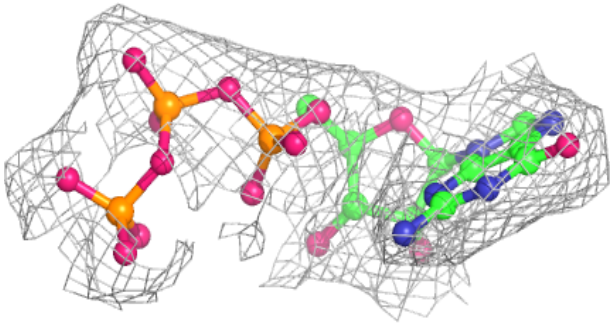


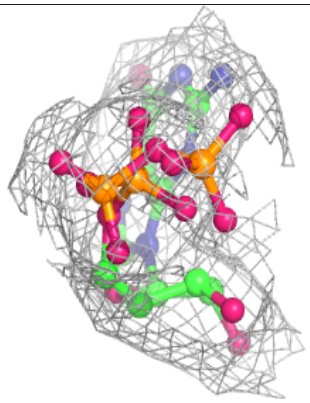


Electron density around GTP M 705:

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

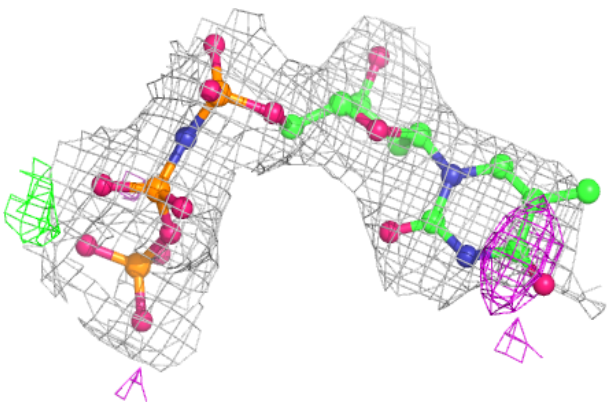


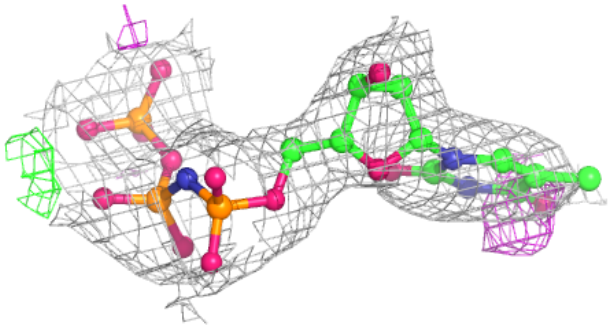




Electron density around 1FZ D 706:

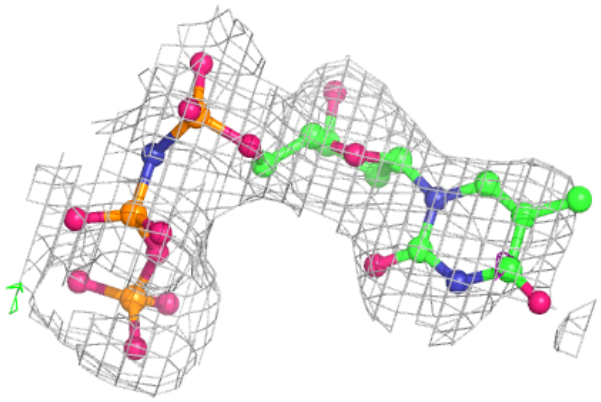
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

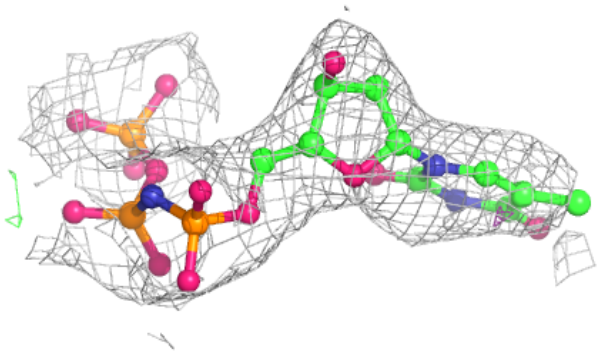


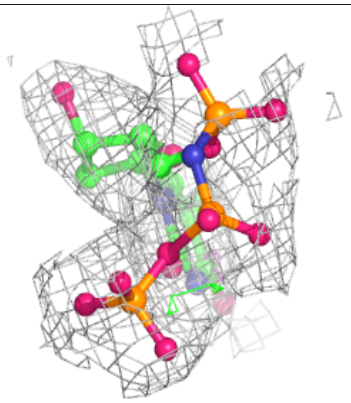


Electron density around 1FZ E 704:

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

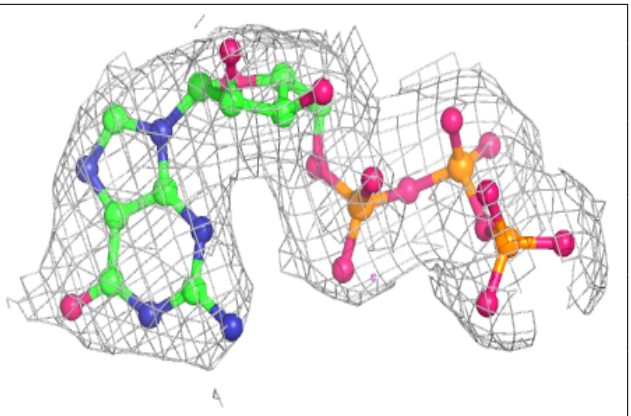


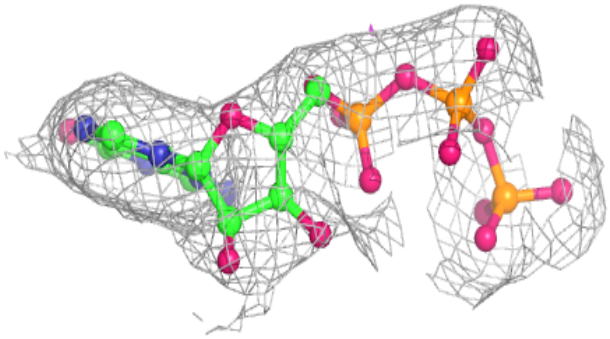


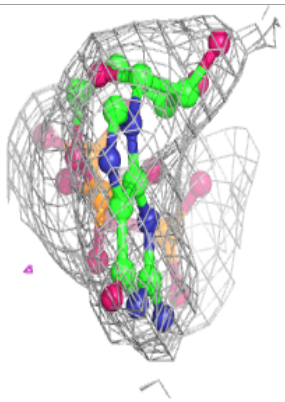


Electron density around GTP P 705:

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

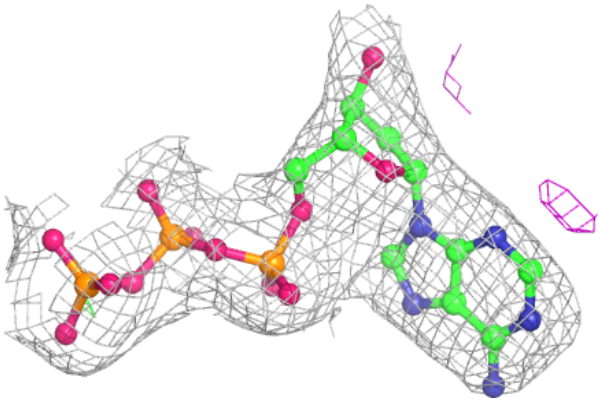


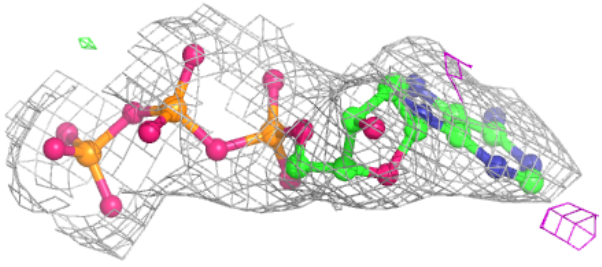


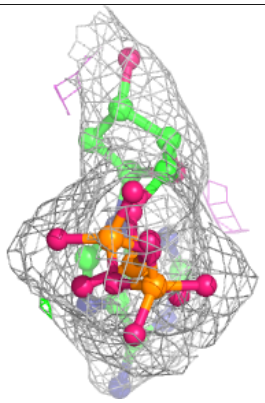


Electron density around DTP F 707:

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

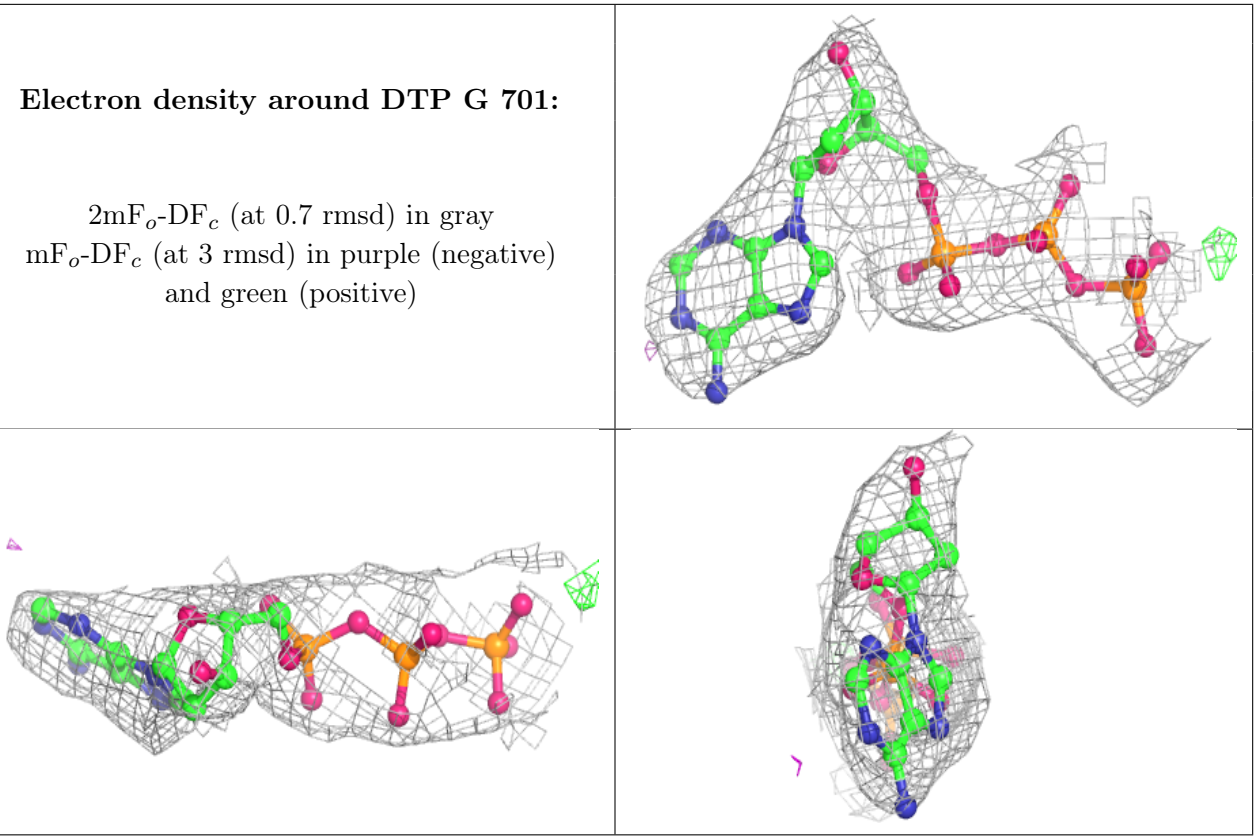






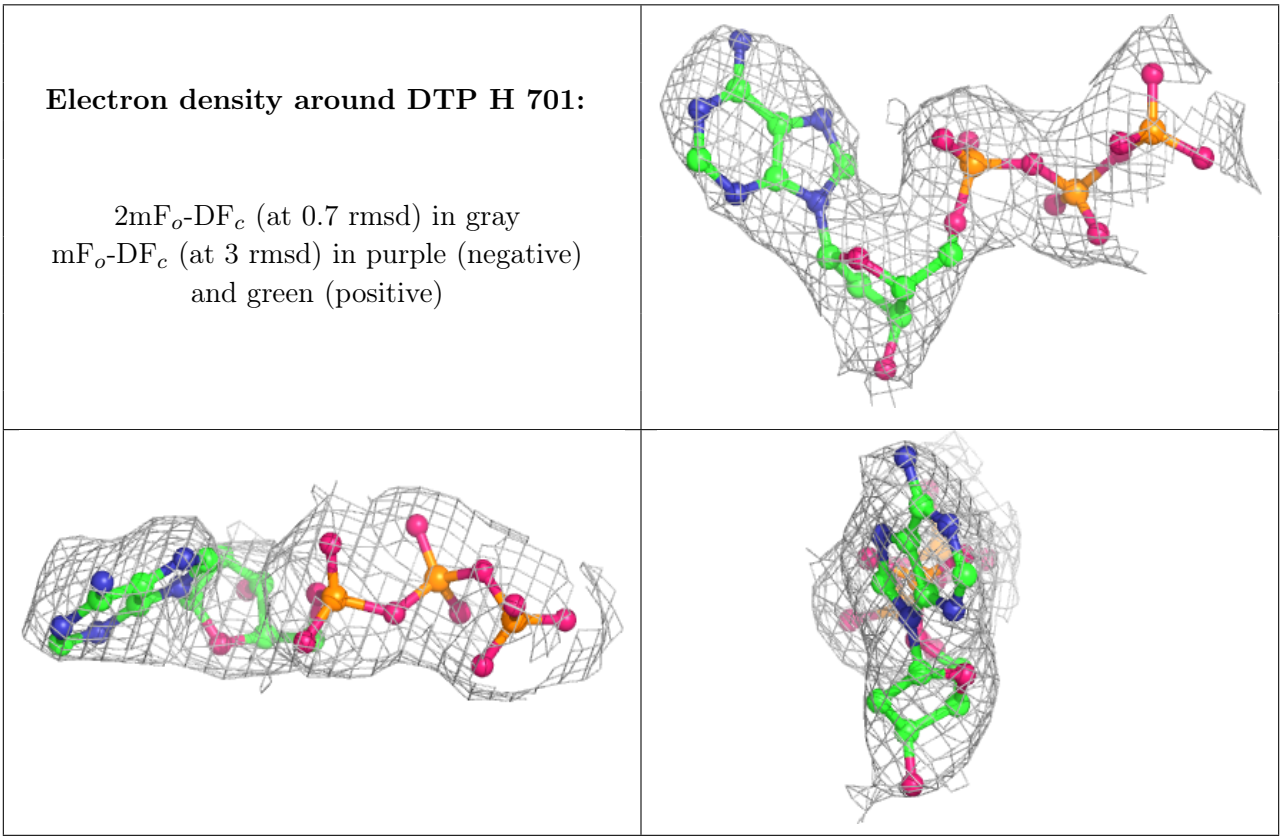
Electron density around DTP G 701:

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



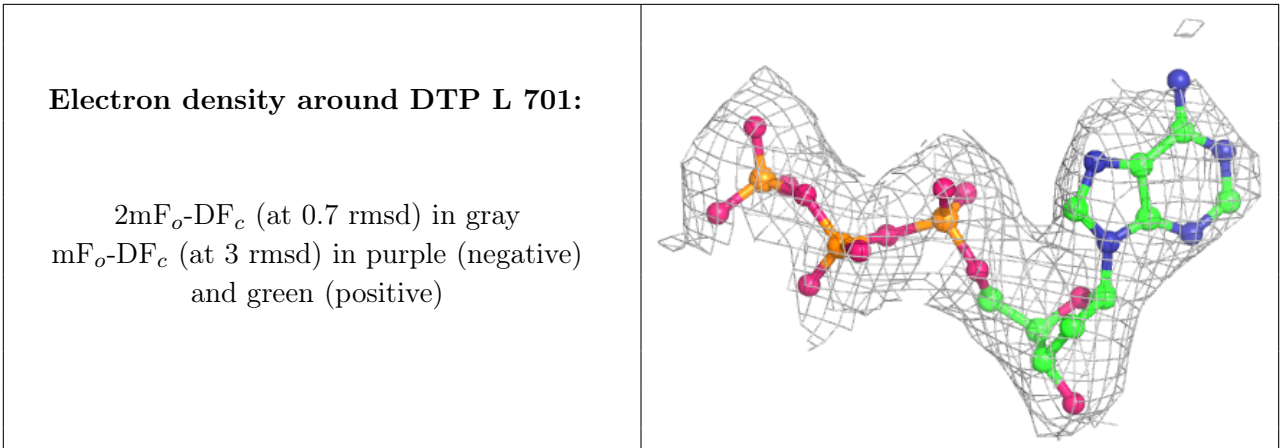
Electron density around DTP H 701:

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



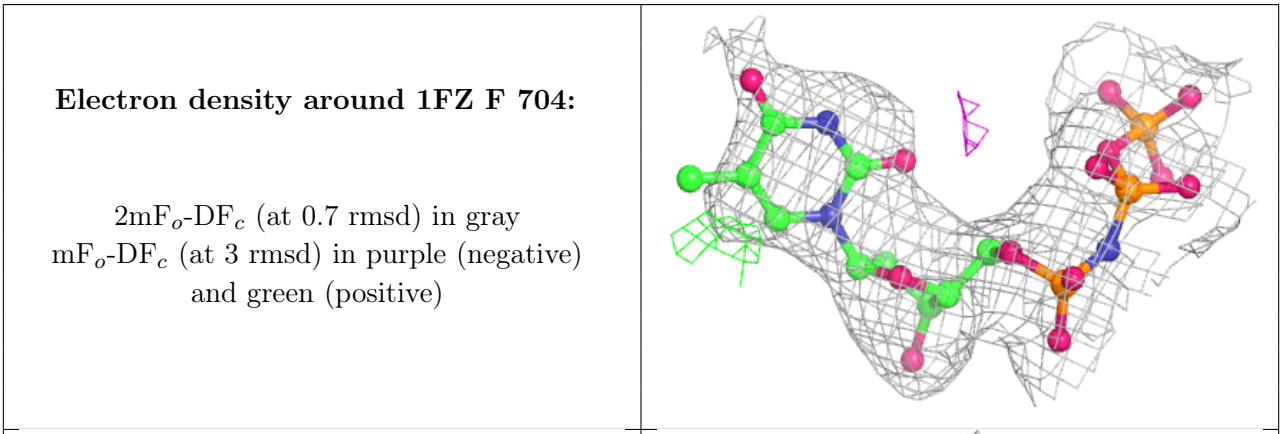
Electron density around DTP L 701:

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



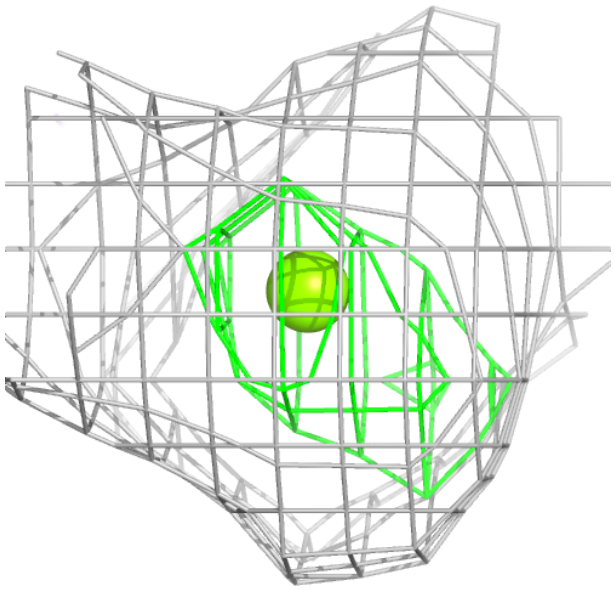
Electron density around 1FZ F 704:

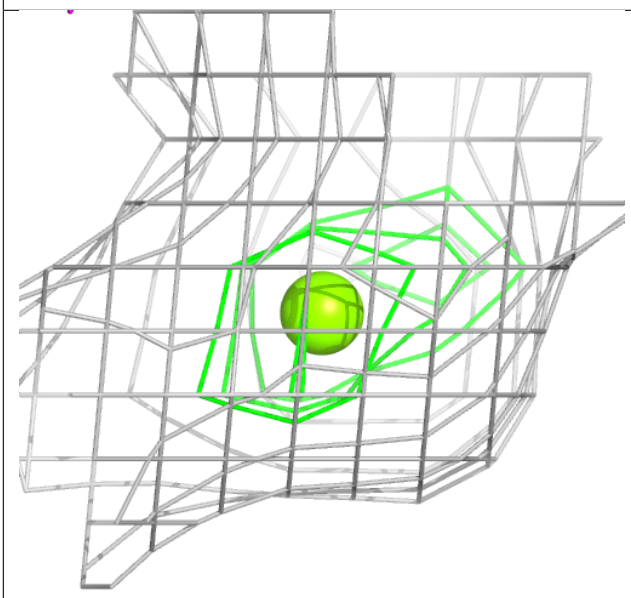
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

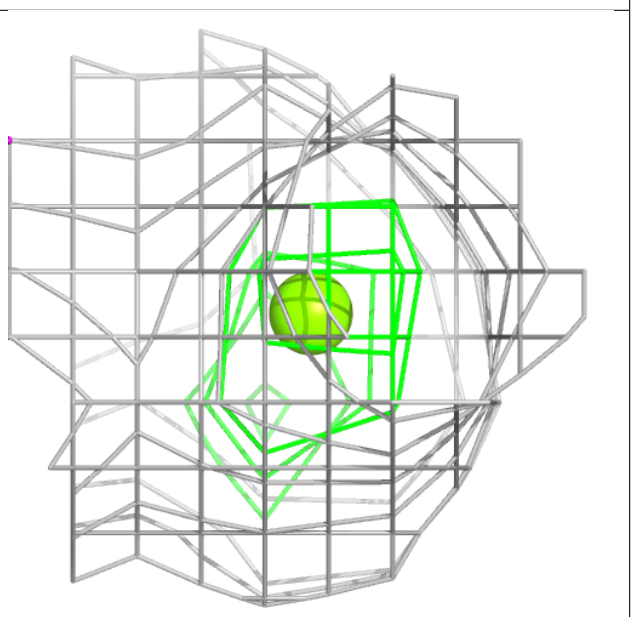


Electron density around MG D 704:

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

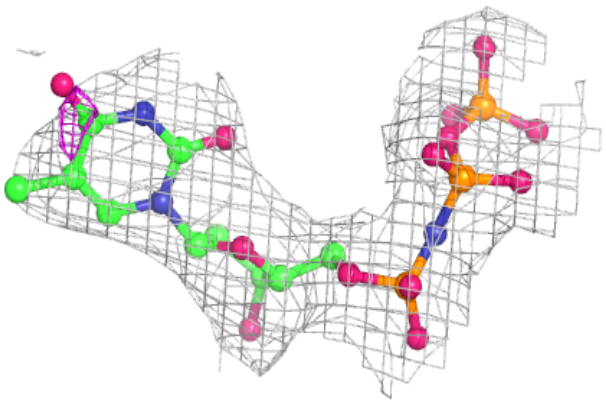


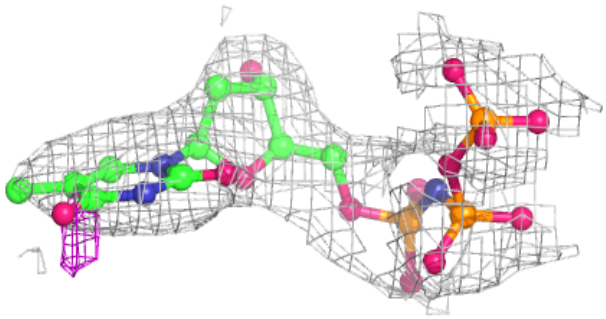


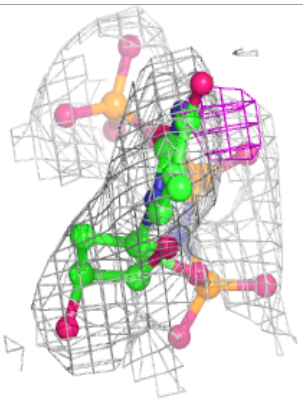


Electron density around 1FZ H 705:

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

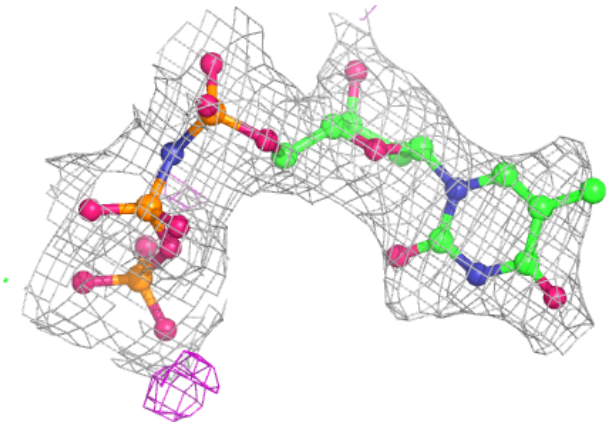


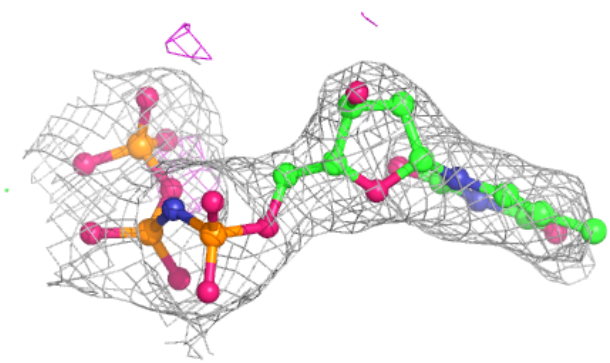


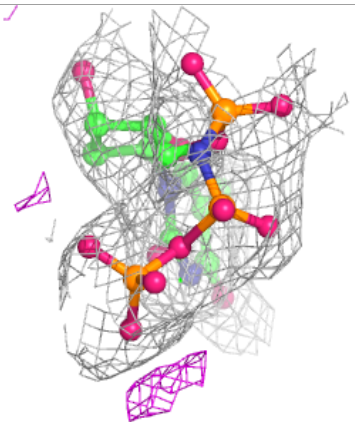


Electron density around 1FZ I 704:

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

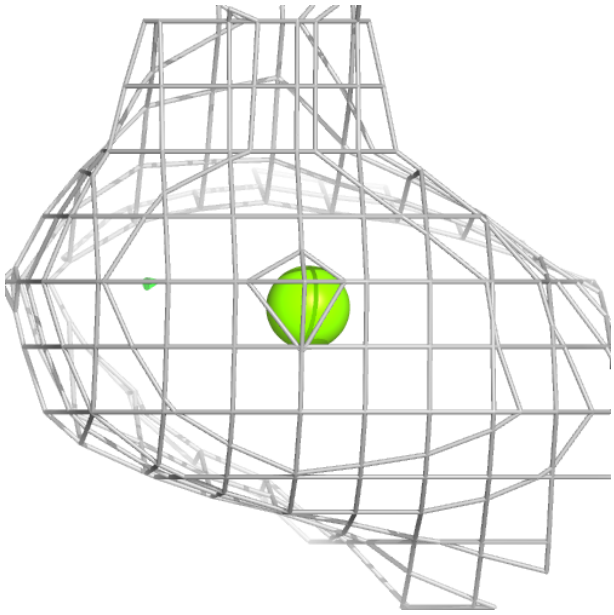


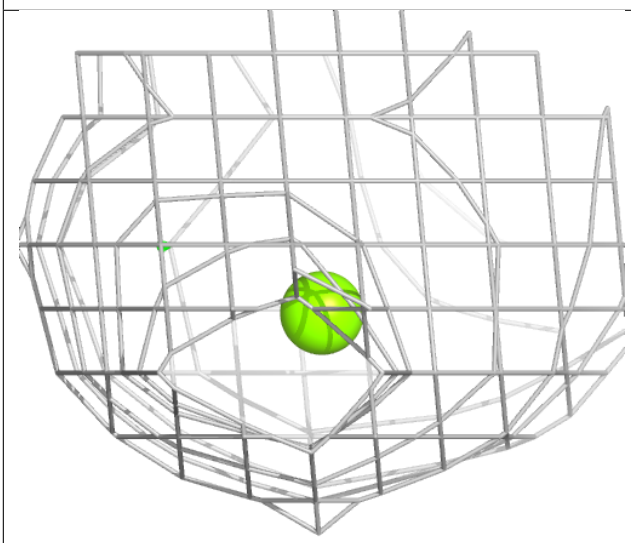


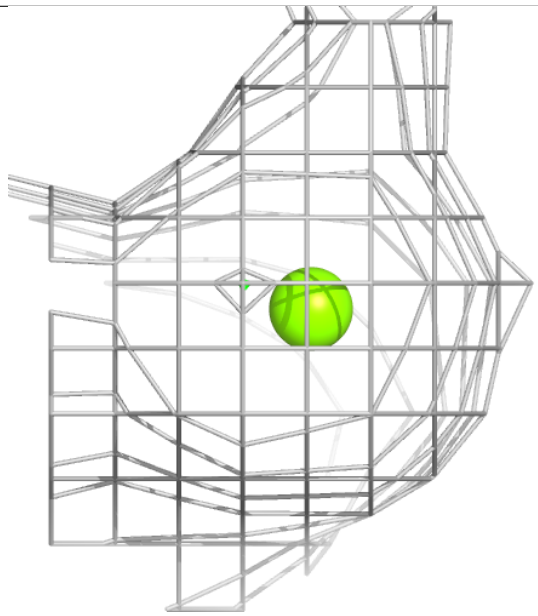


Electron density around MG I 702:

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

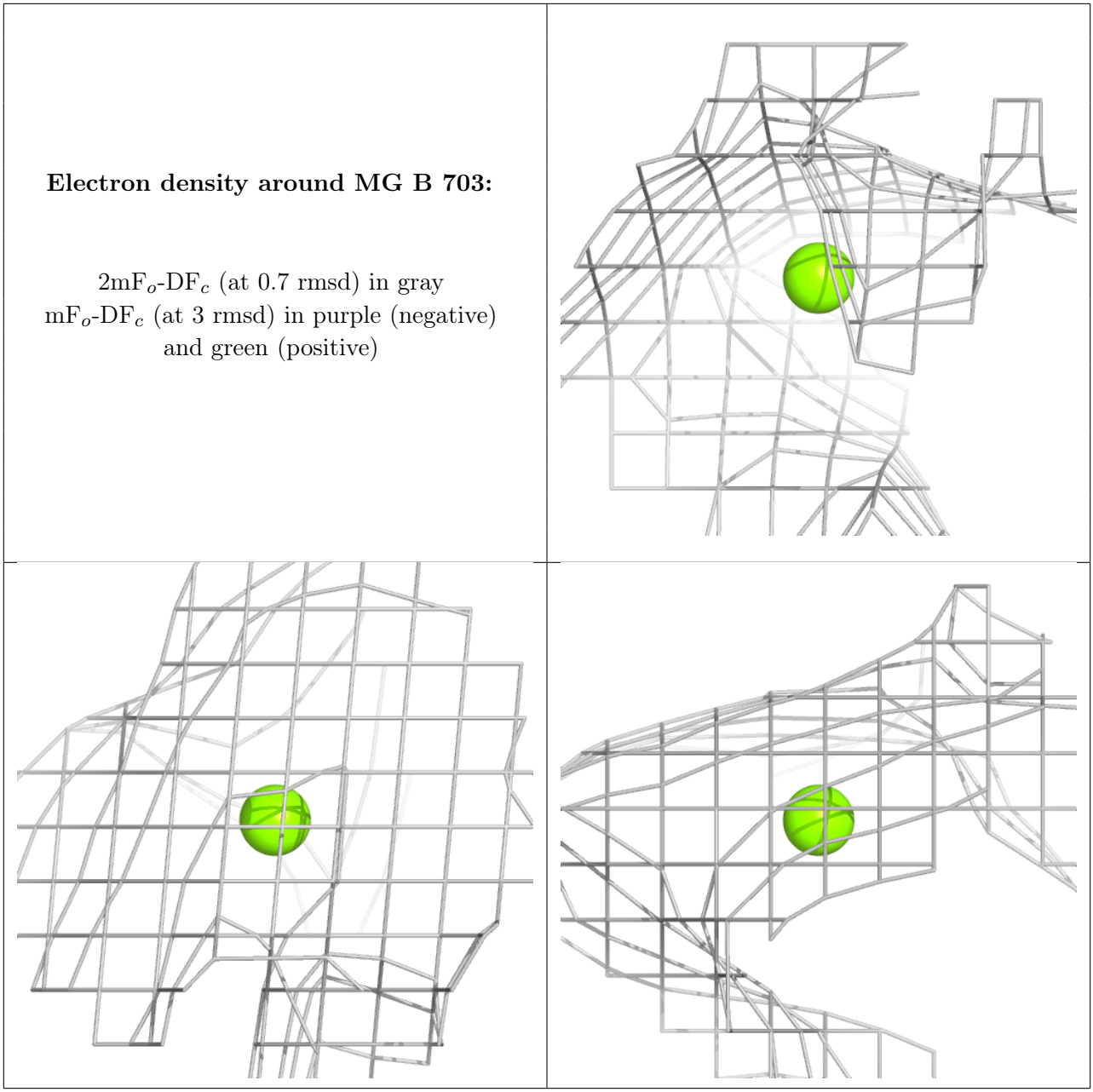






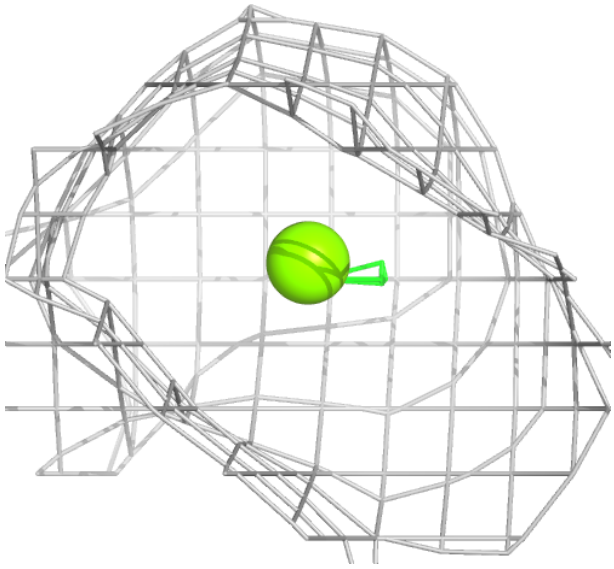
Electron density around MG B 703:

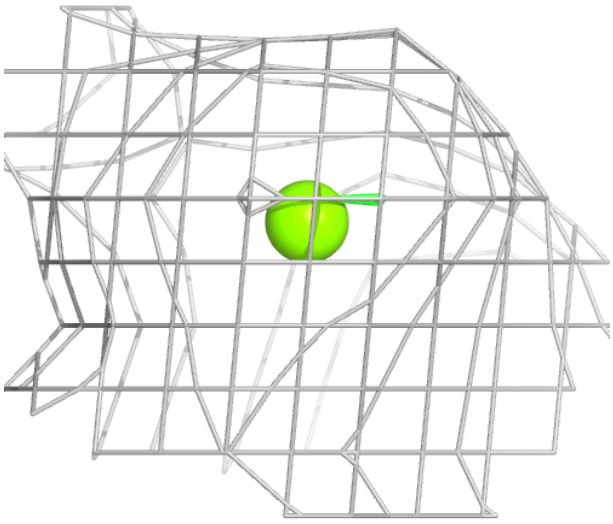
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

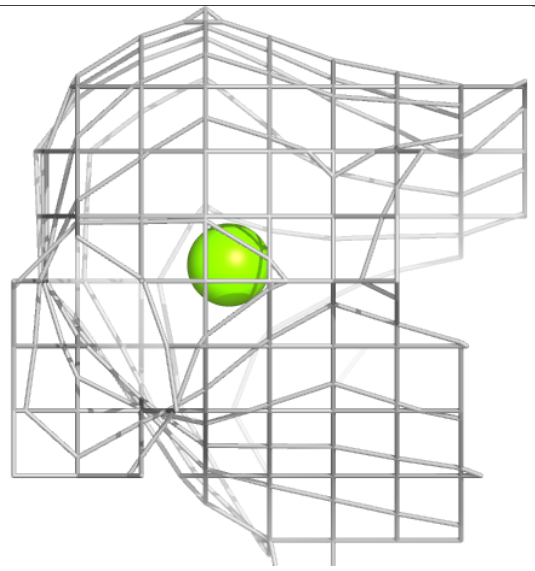


Electron density around MG C 703:

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

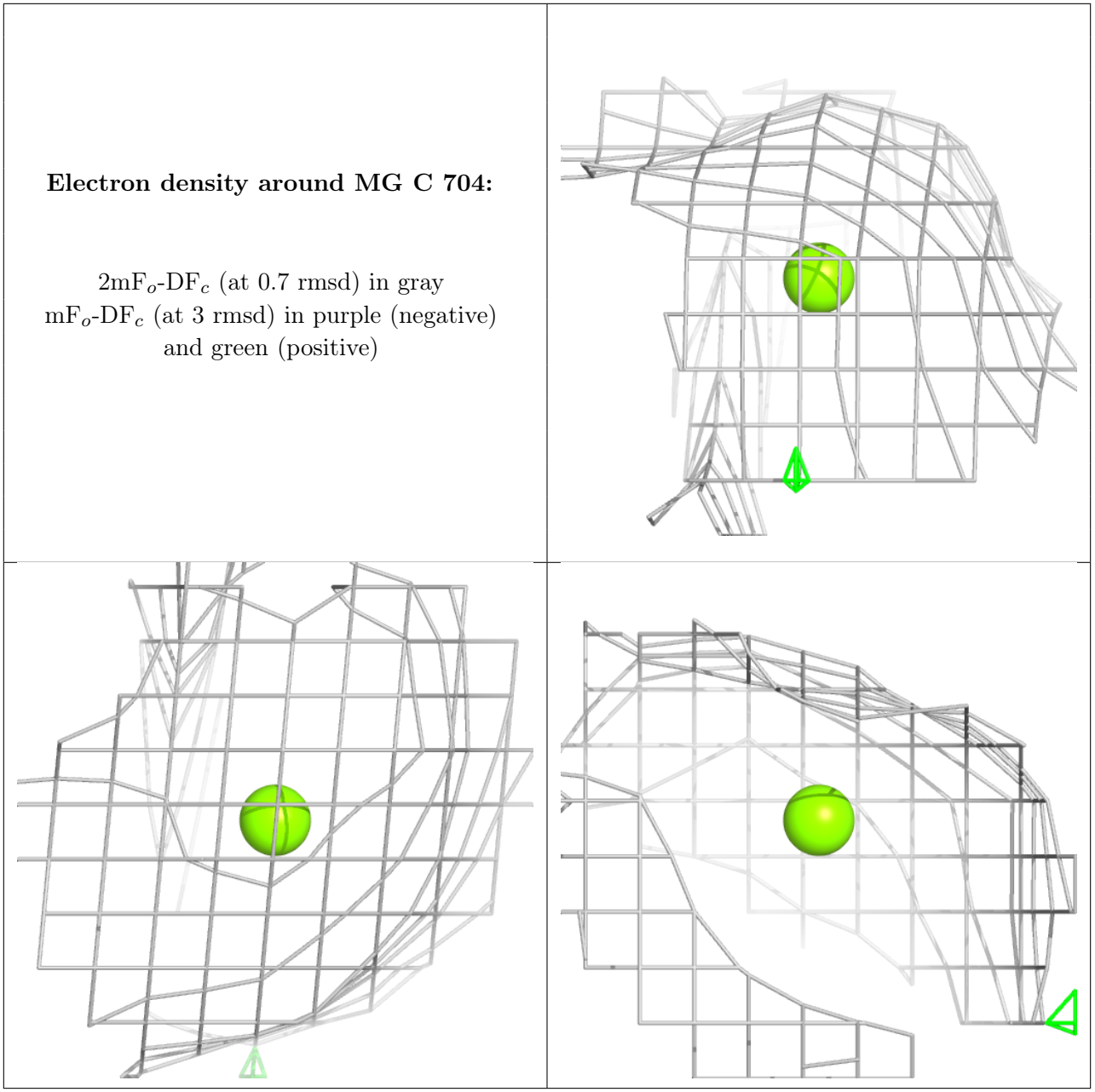






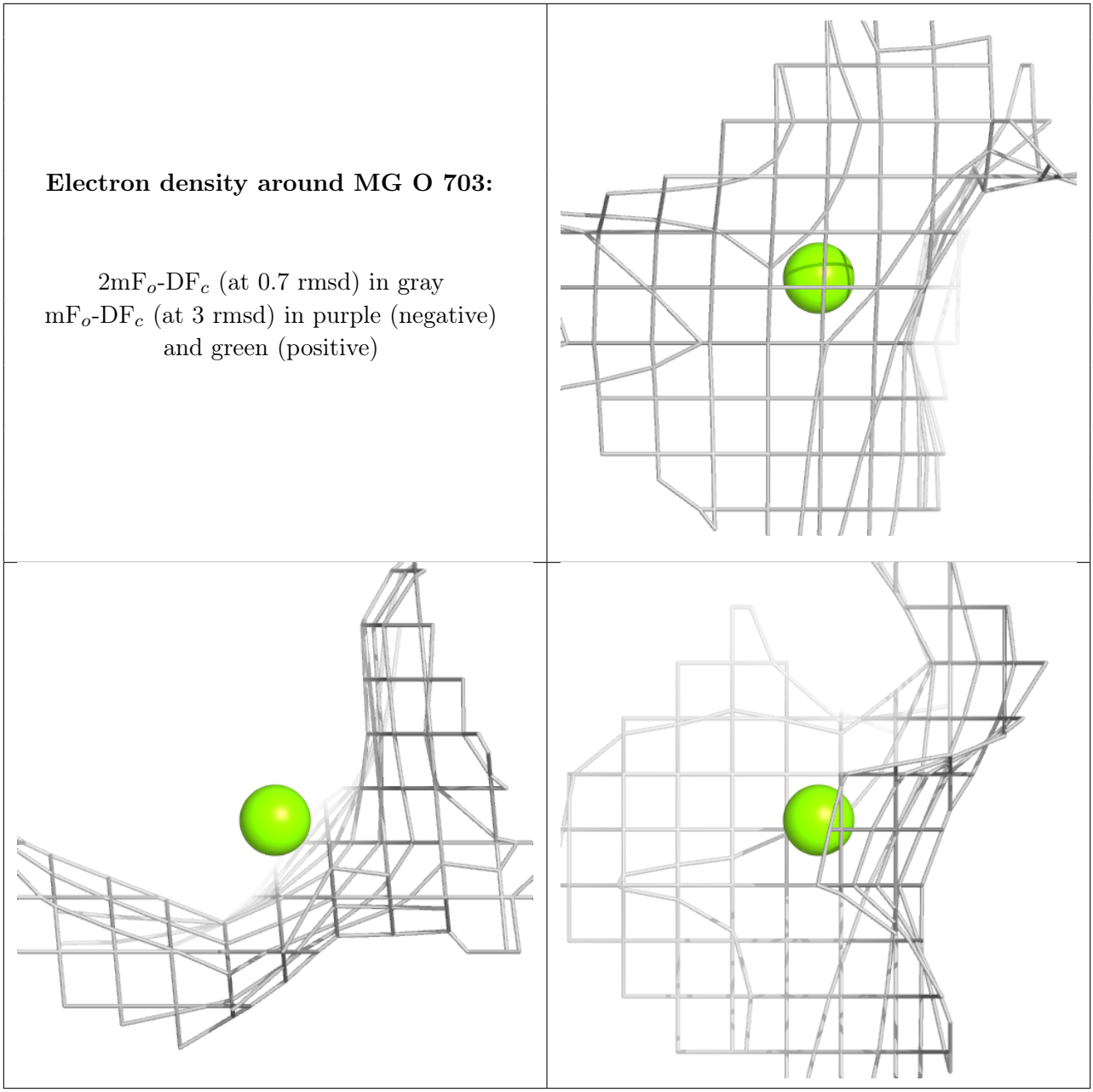
Electron density around MG C 704:

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



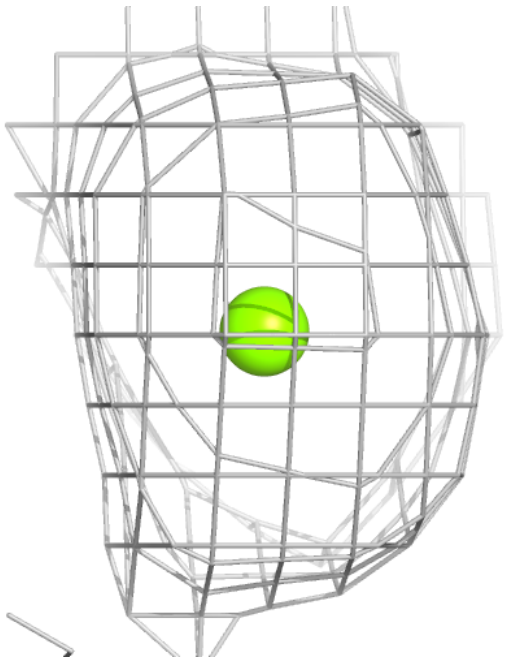
Electron density around MG O 703:

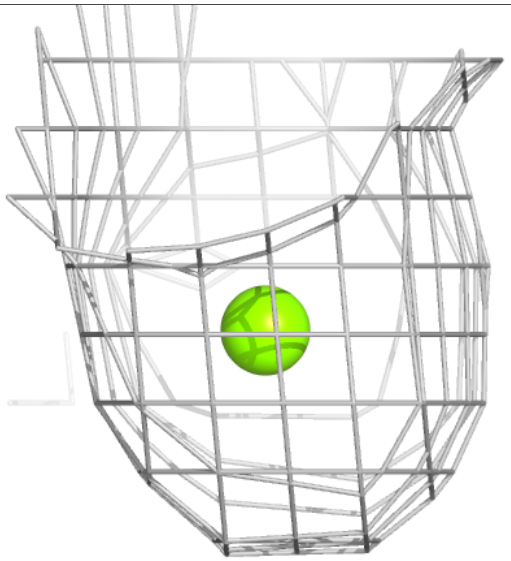
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

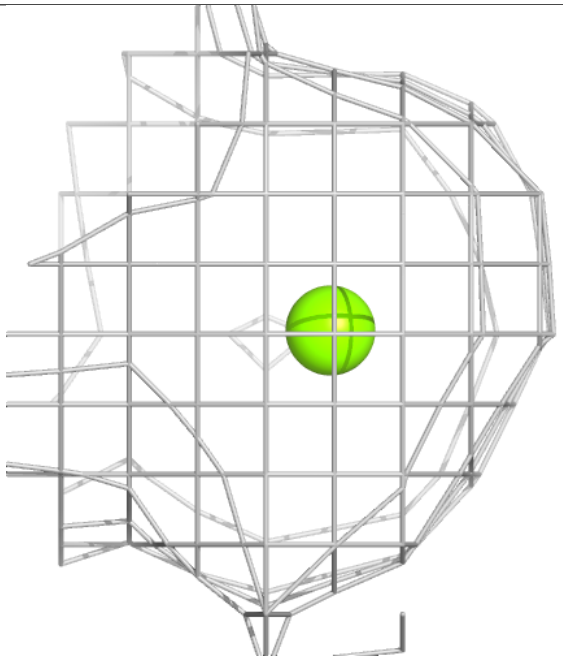


Electron density around MG P 702:

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

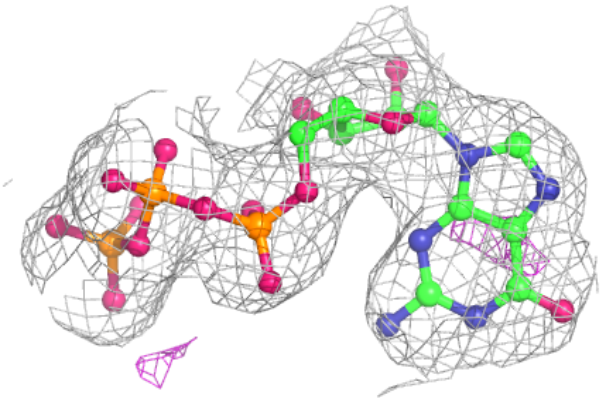


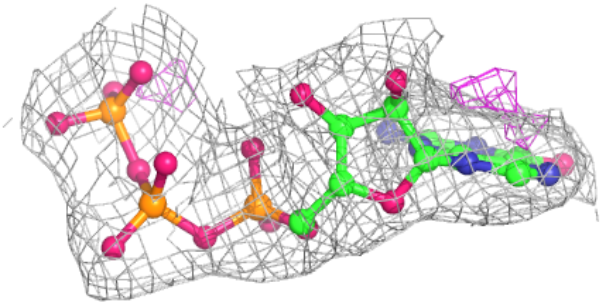


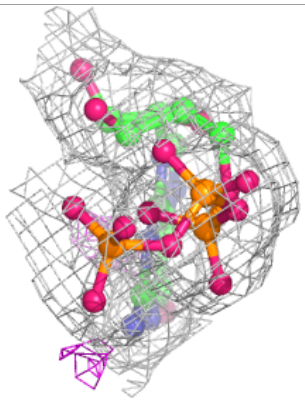


Electron density around GTP B 705:

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

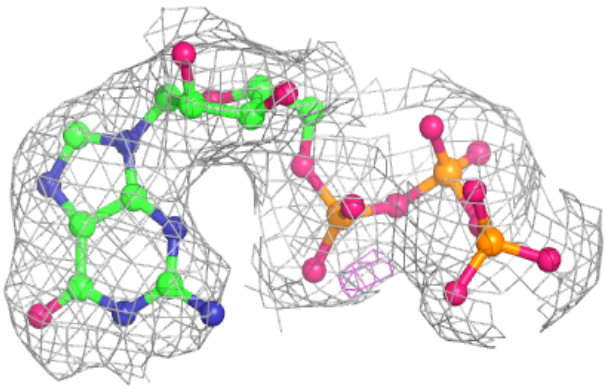


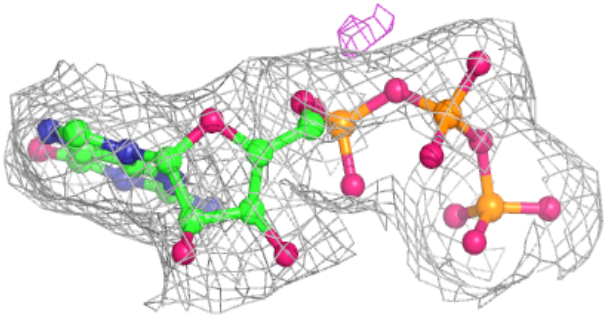


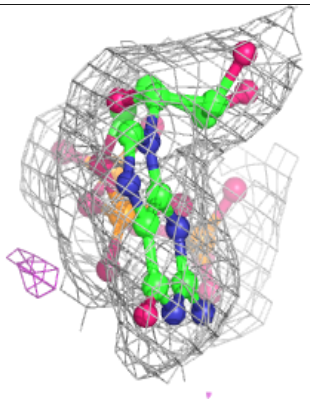


Electron density around GTP D 707:

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

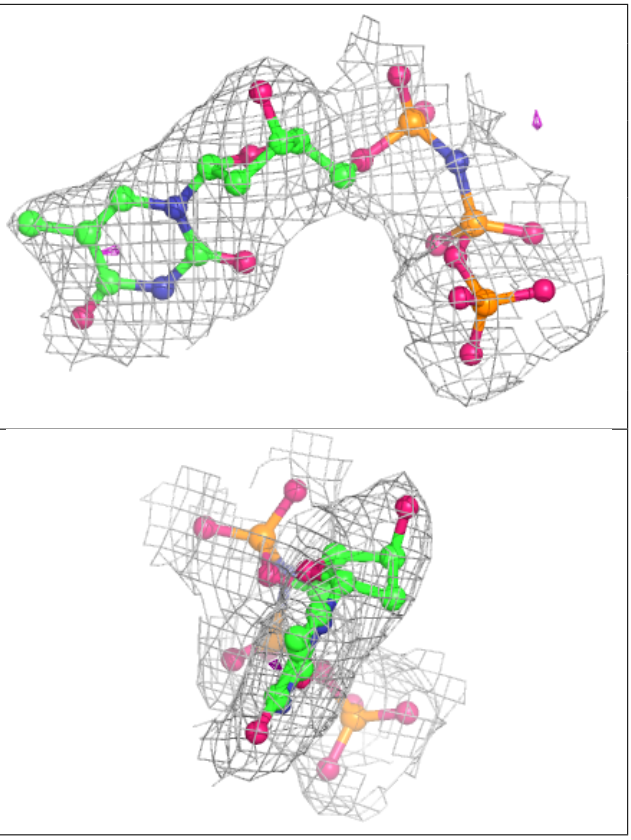






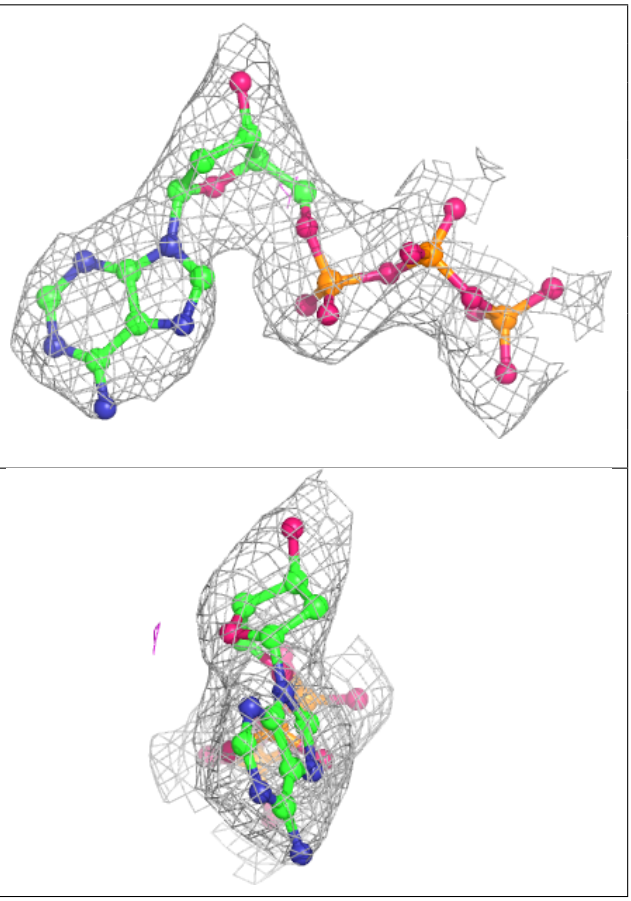
Electron density around 1FZ A 704:

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



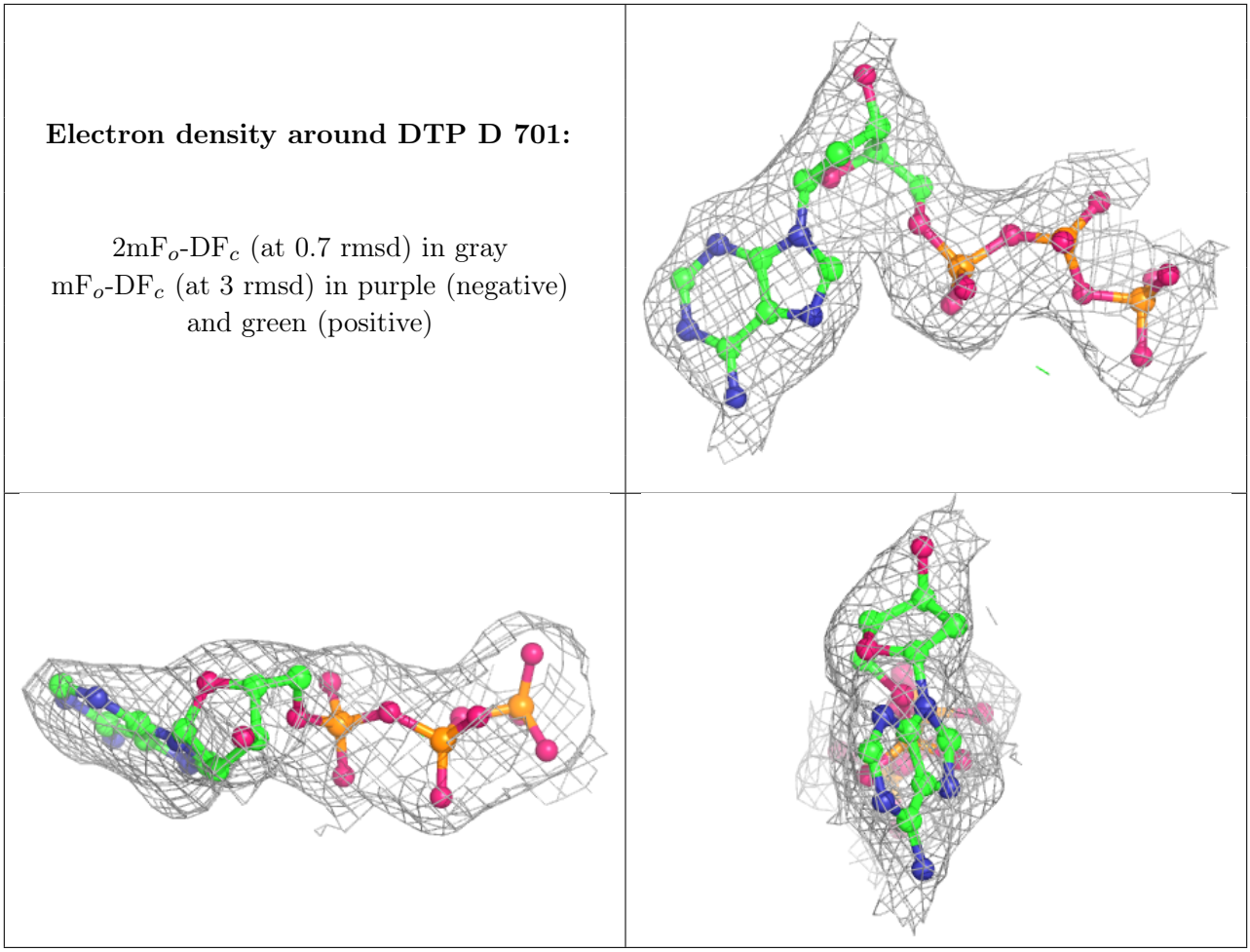
Electron density around DTP B 707:

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



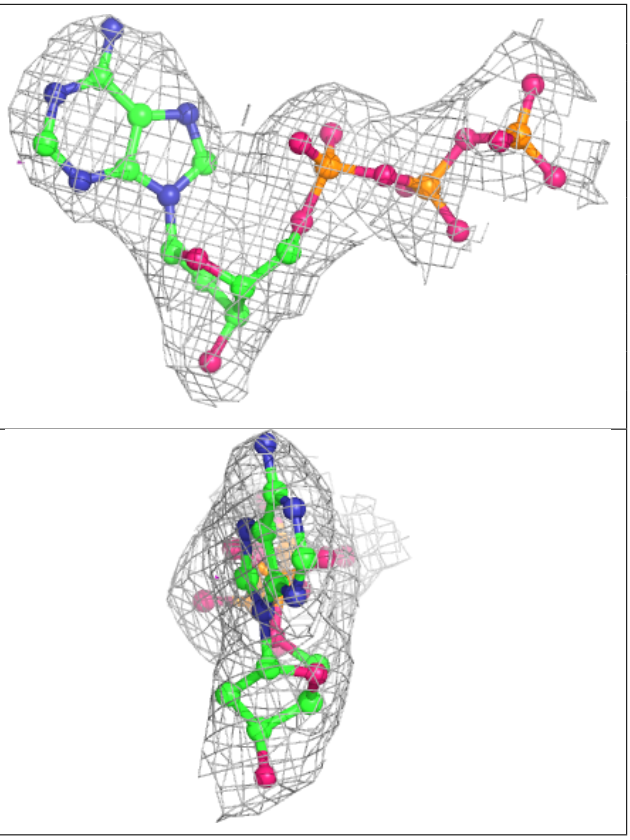
Electron density around DTP D 701:

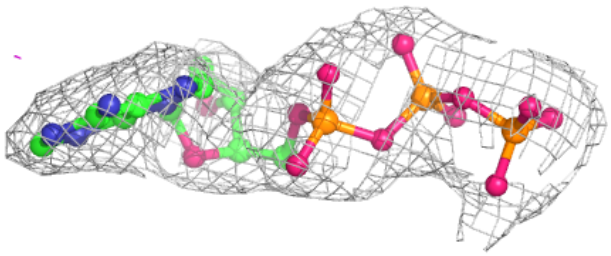
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around DTP E 707:

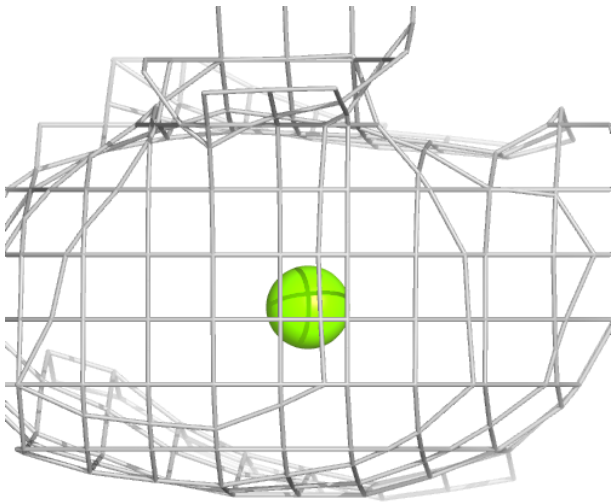
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

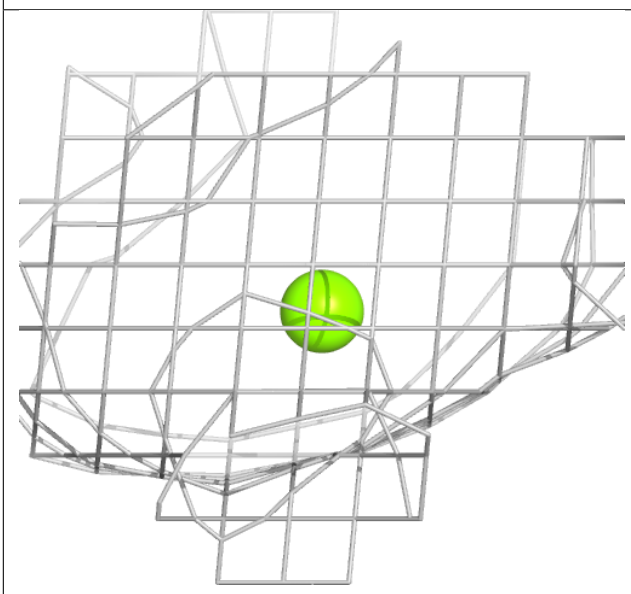


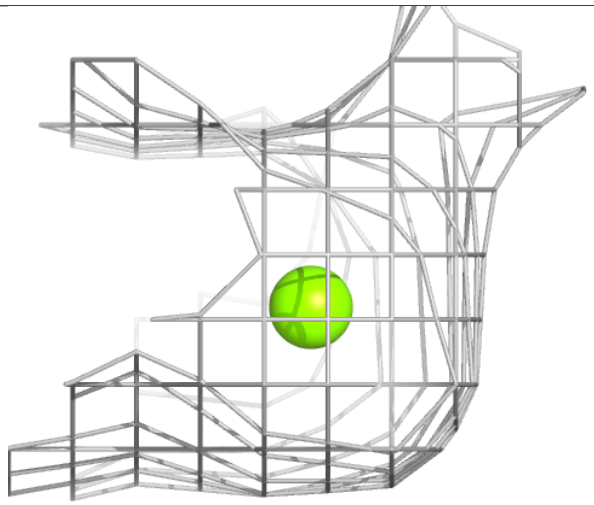


Electron density around MG K 703:

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

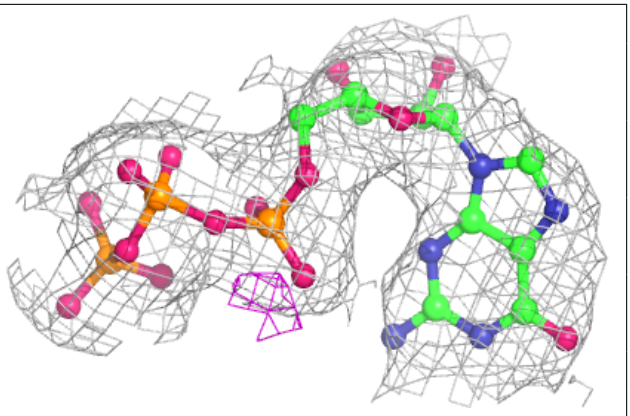


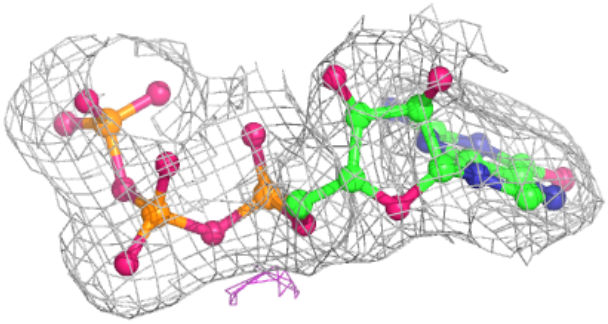


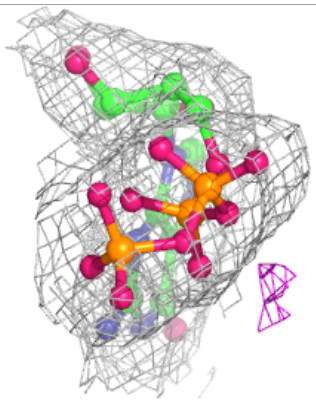


Electron density around GTP A 705:

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

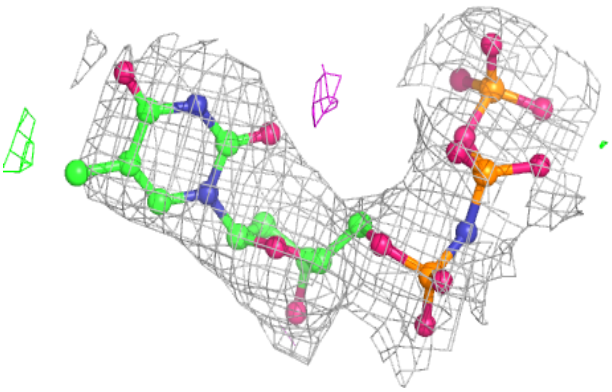


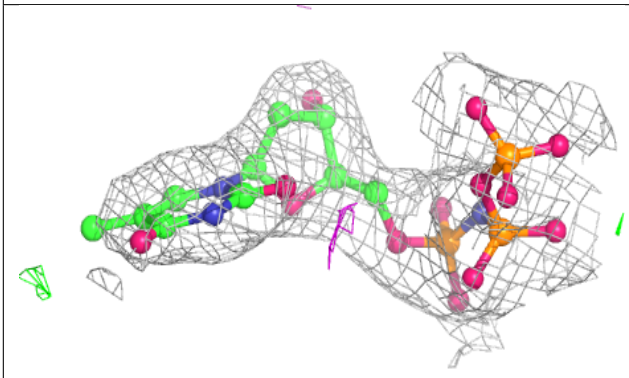


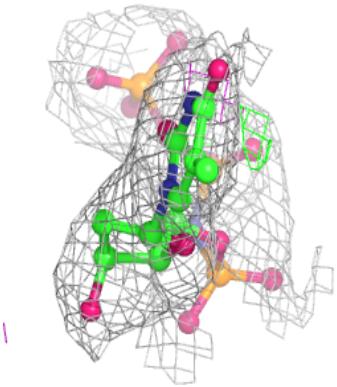


Electron density around 1FZ C 705:

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

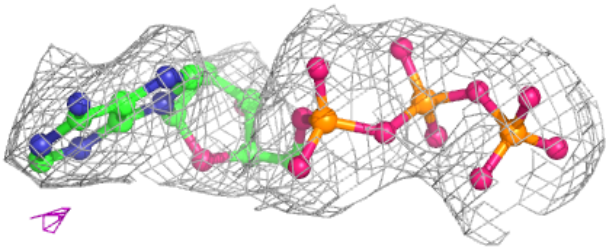


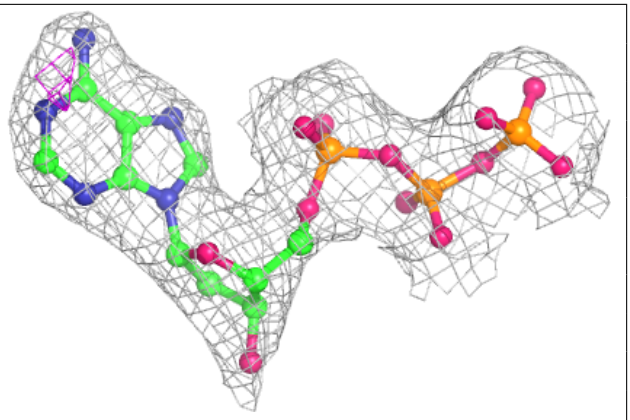


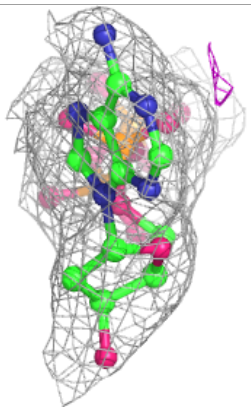


Electron density around DTP I 708:

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

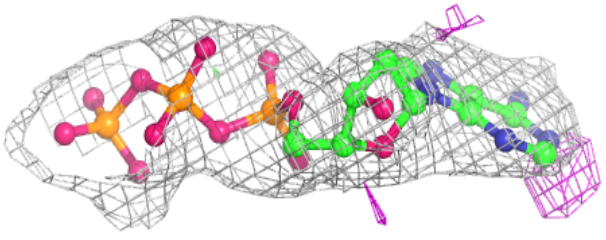


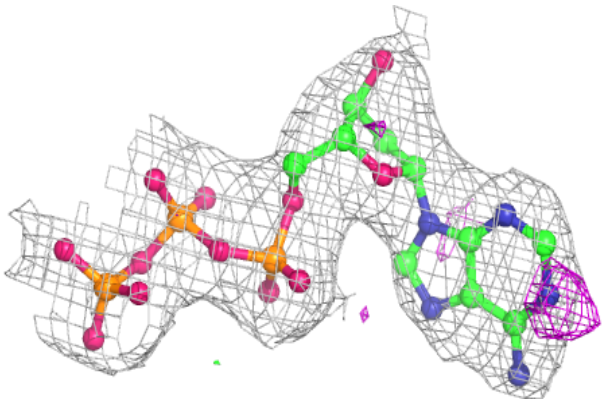


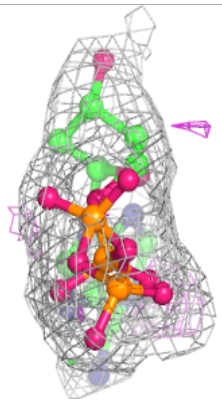


Electron density around DTP J 706:

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

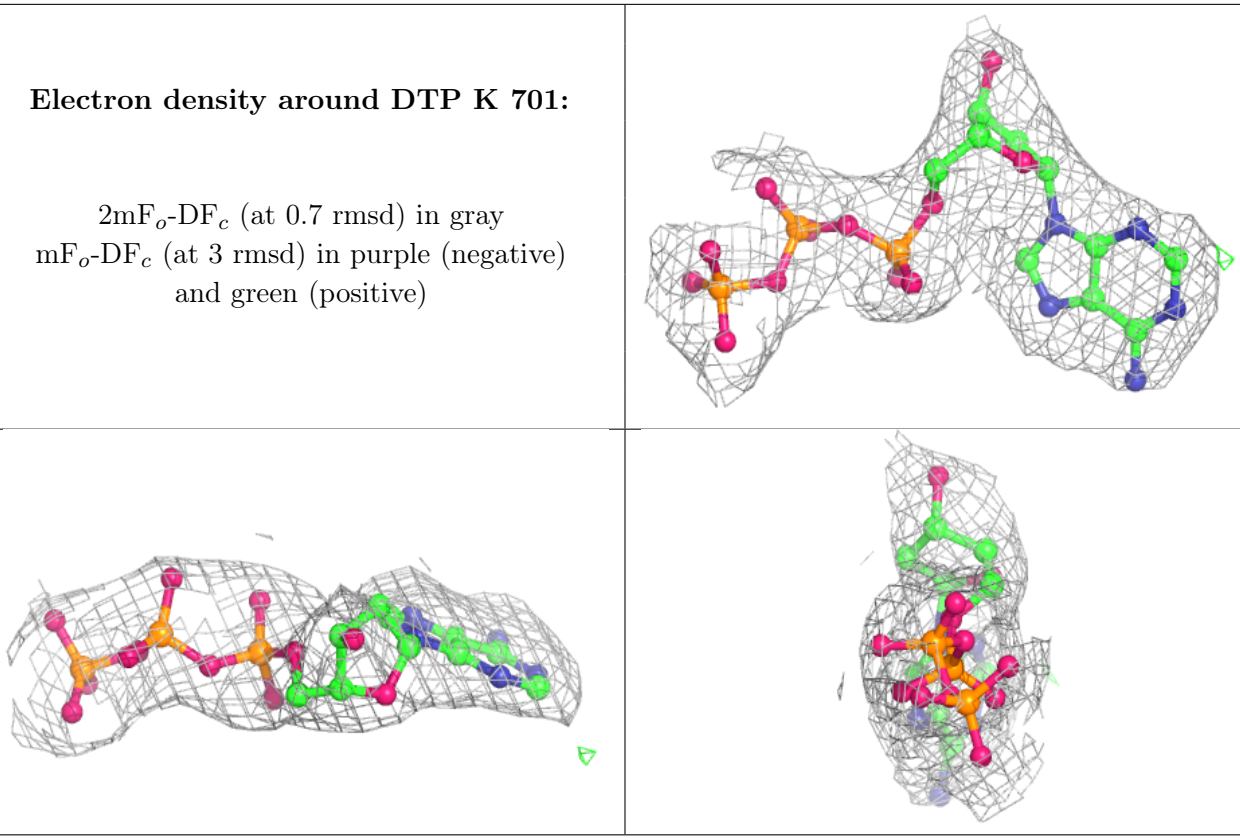






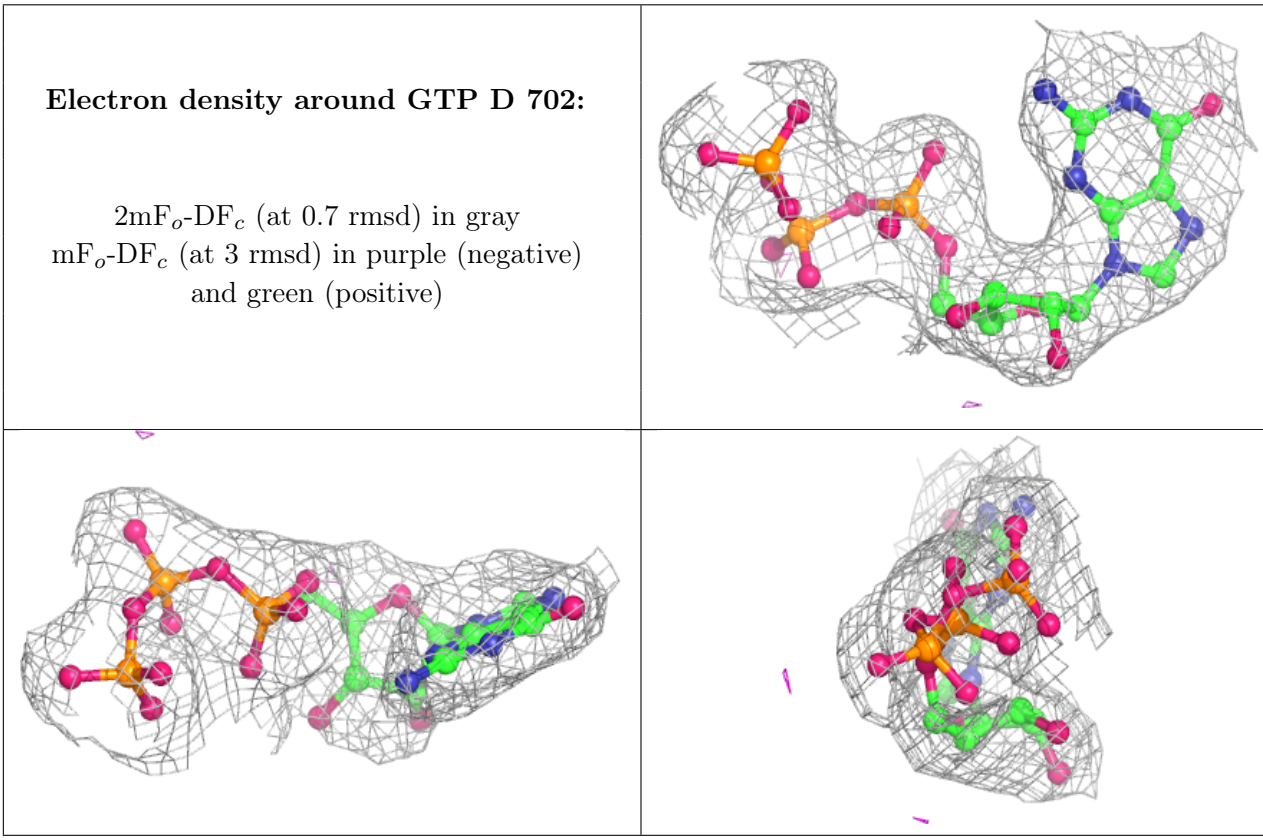
Electron density around DTP K 701:

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



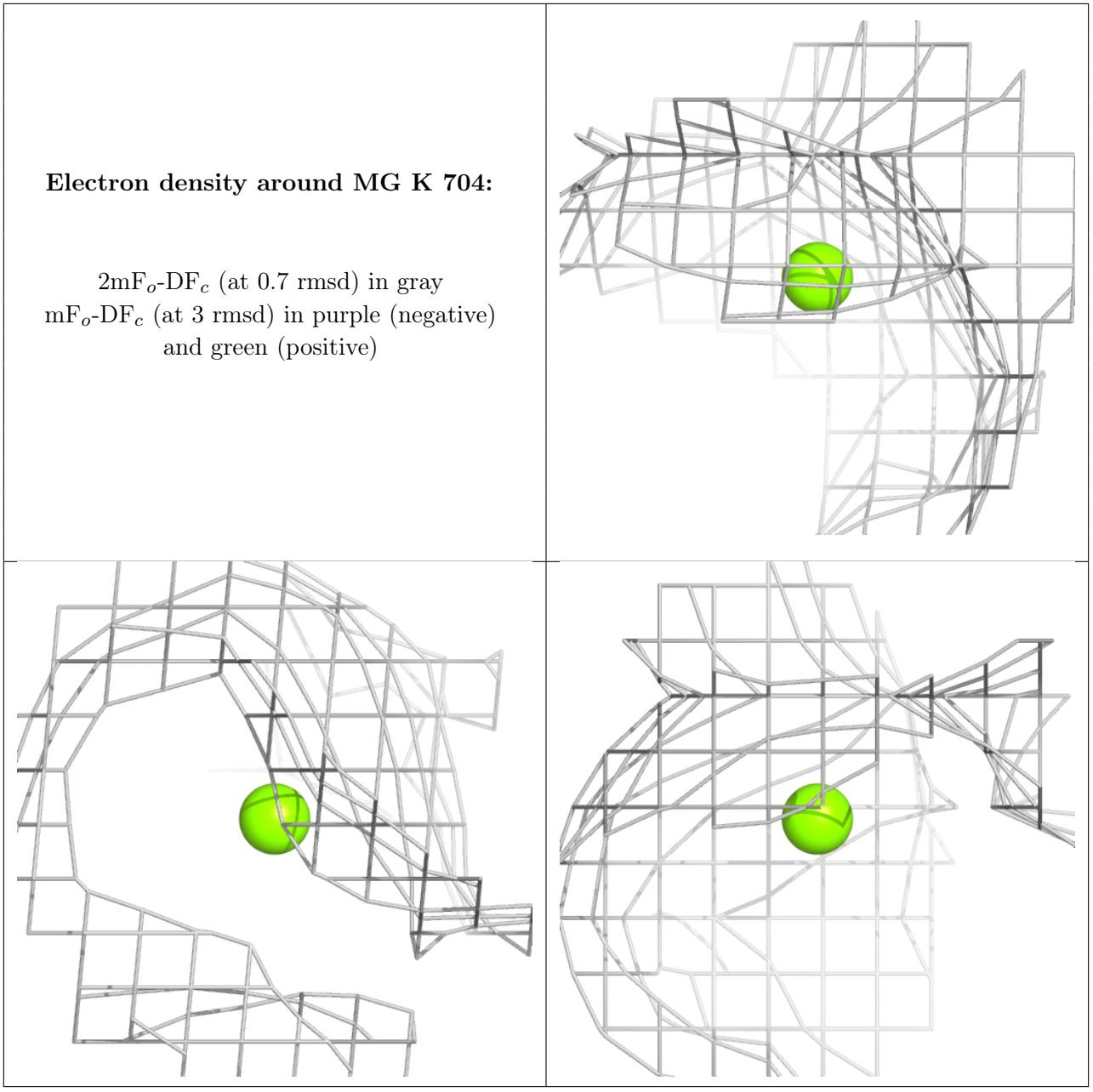
Electron density around GTP D 702:

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



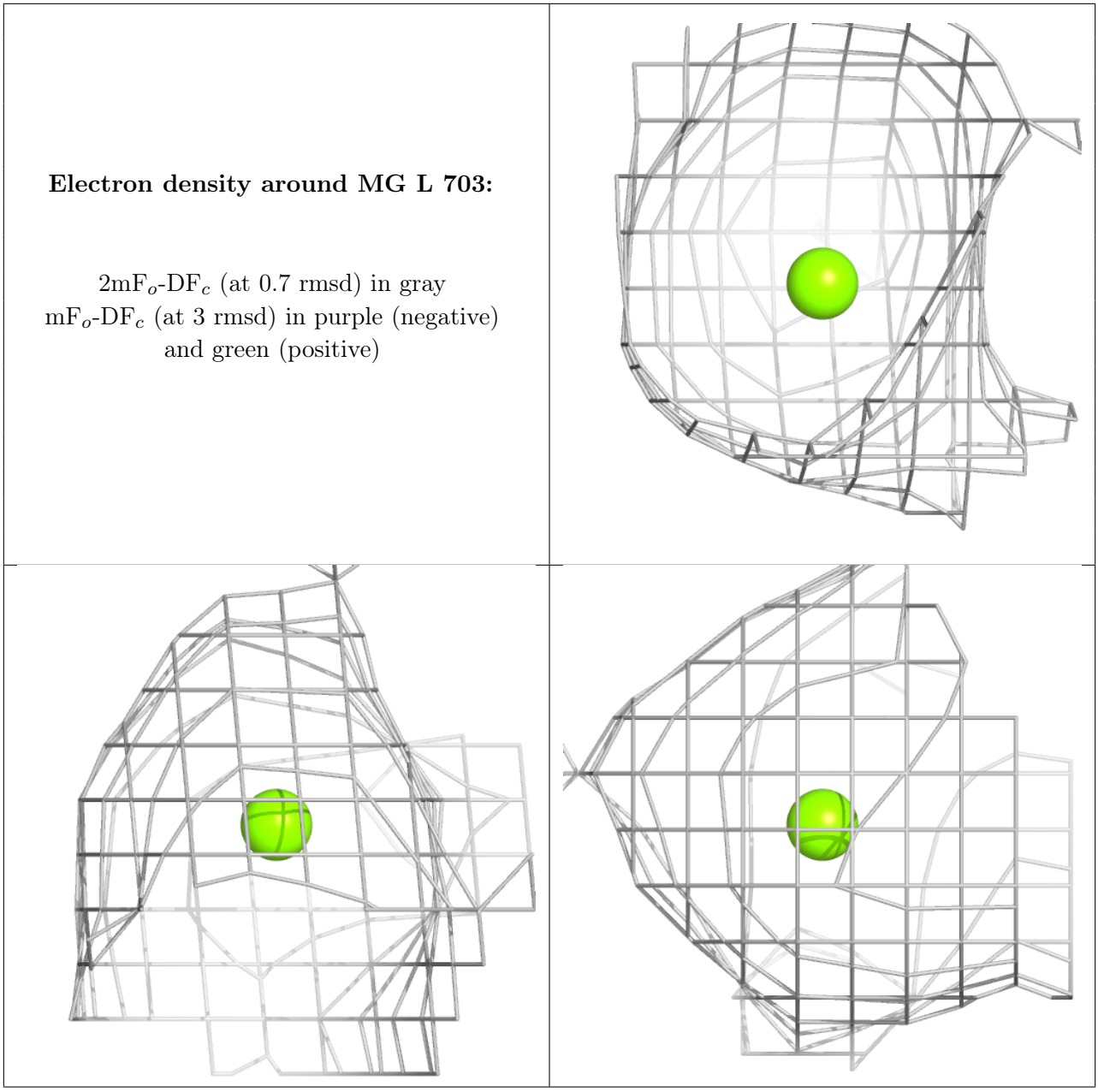
Electron density around MG K 704:

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



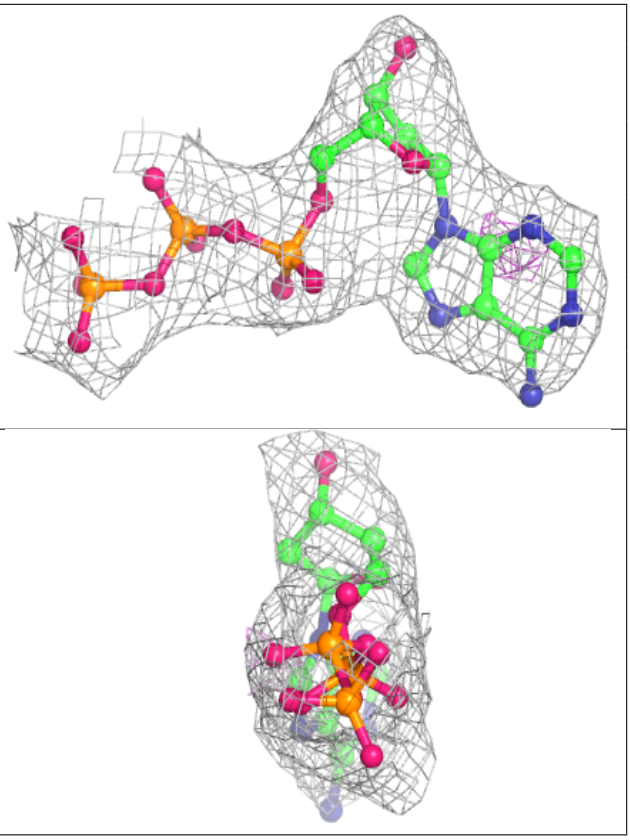
Electron density around MG L 703:

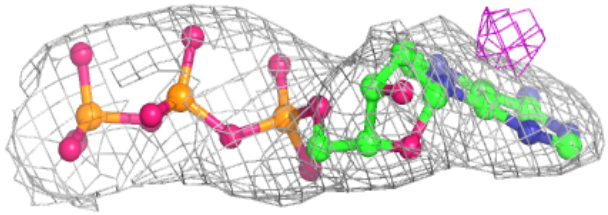
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around DTP N 701:

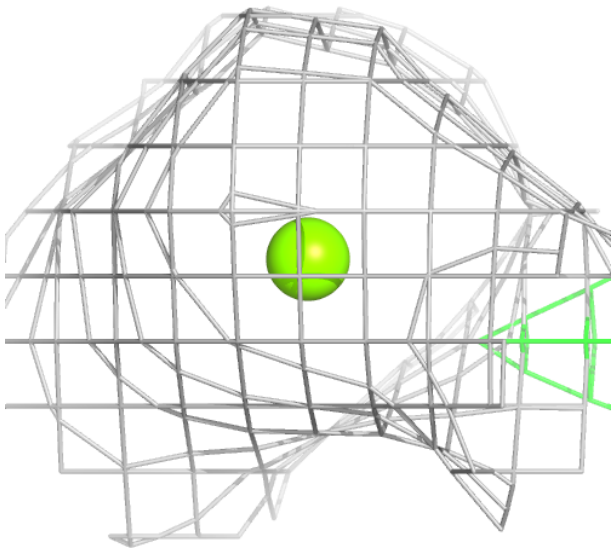
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

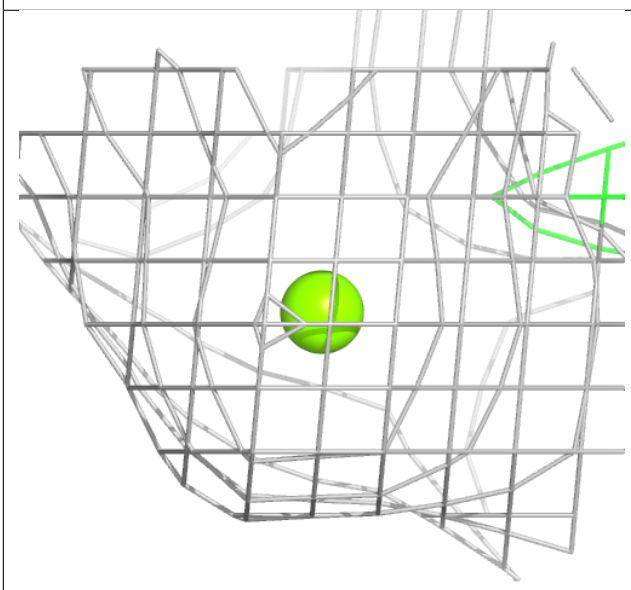


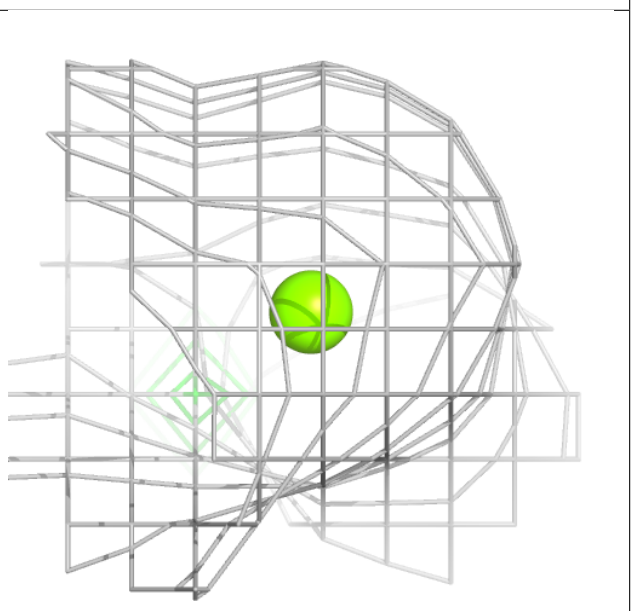


Electron density around MG B 702:

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

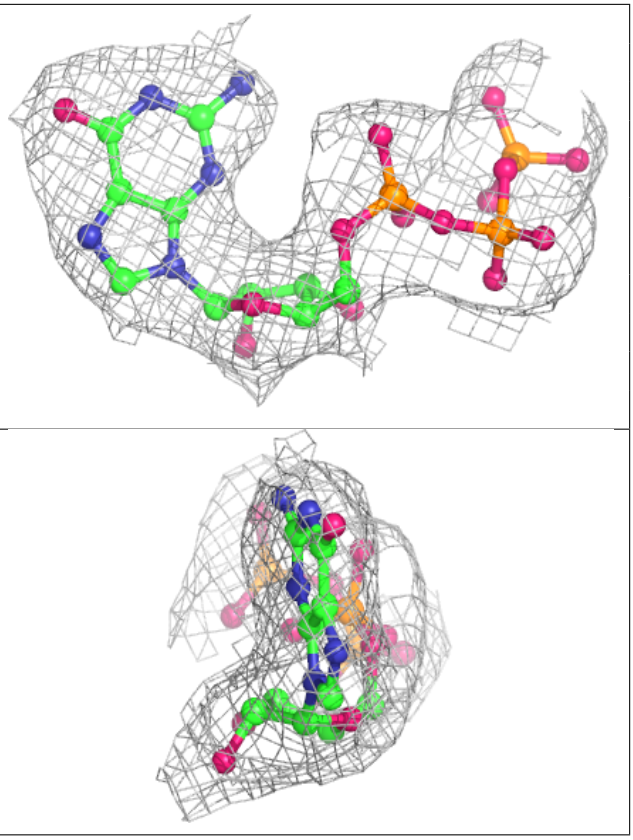


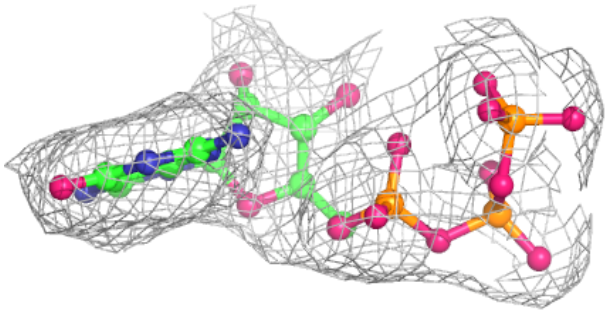




Electron density around GTP G 706:

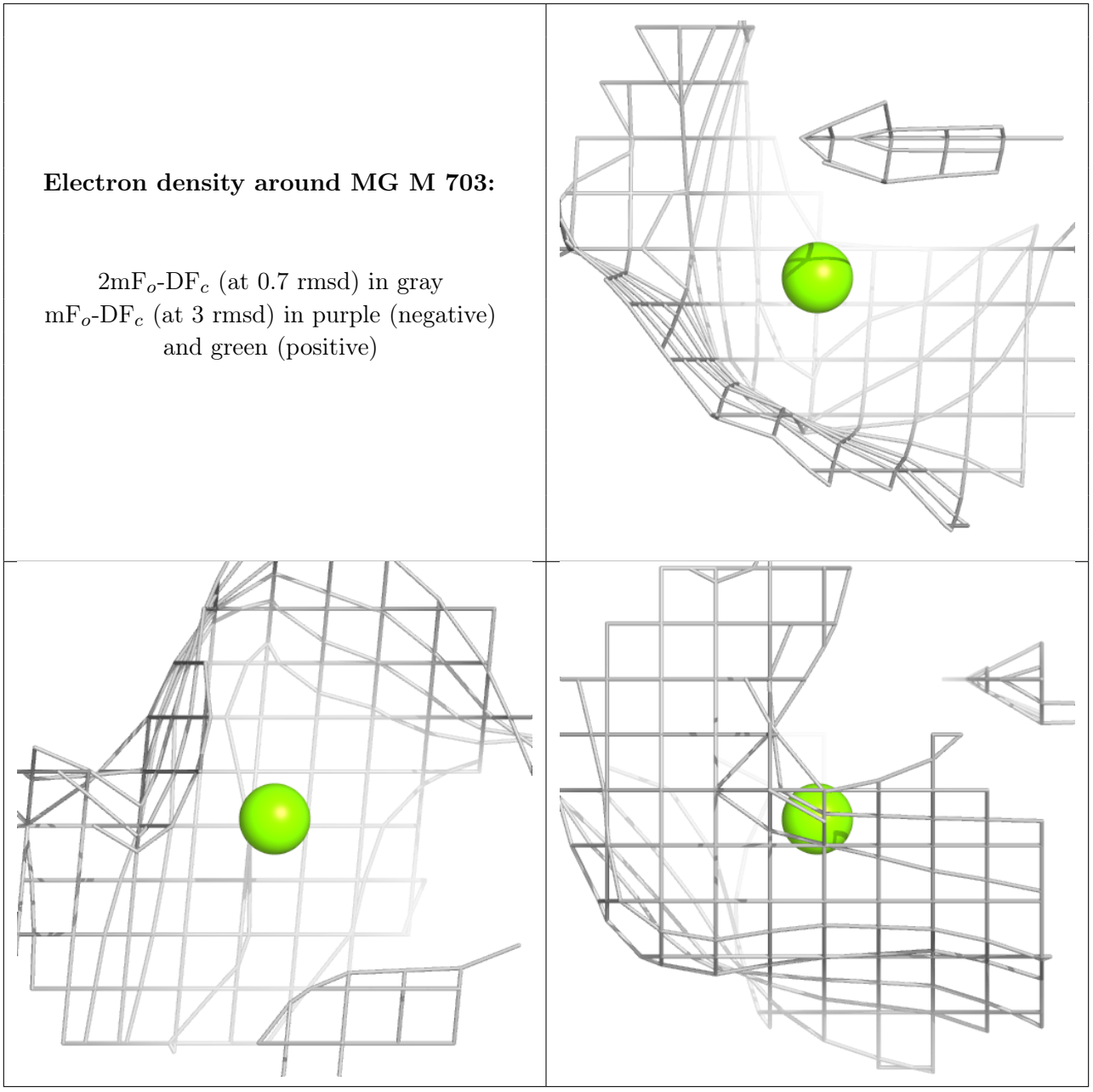
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





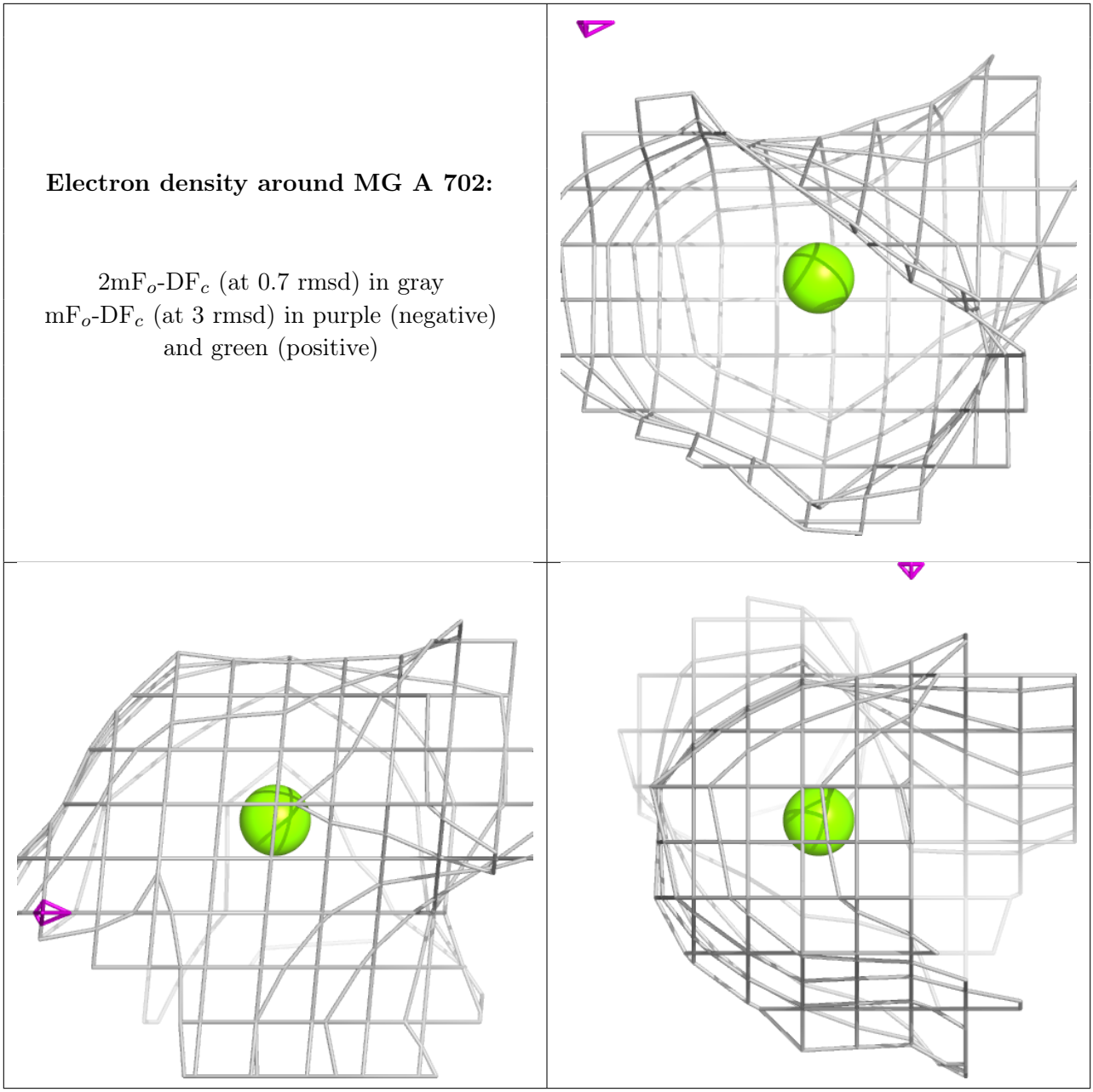
Electron density around MG M 703:

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



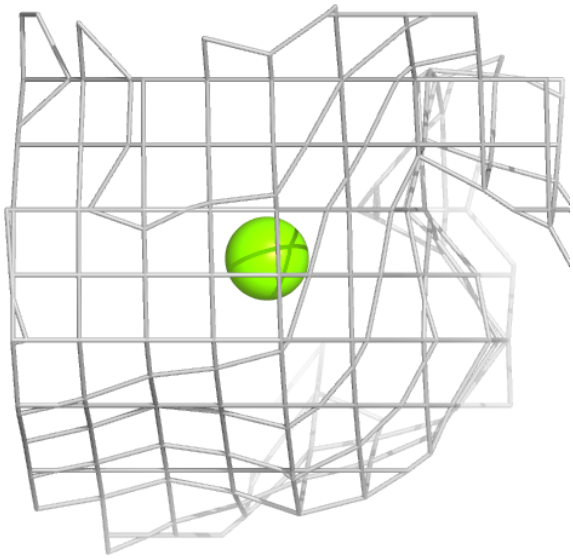
Electron density around MG A 702:

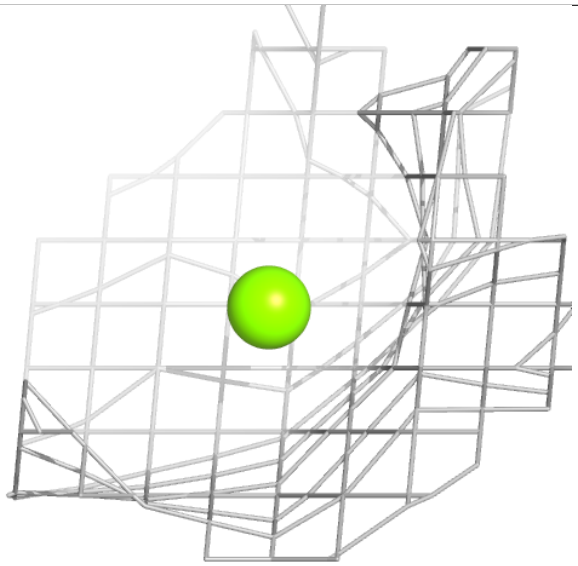
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

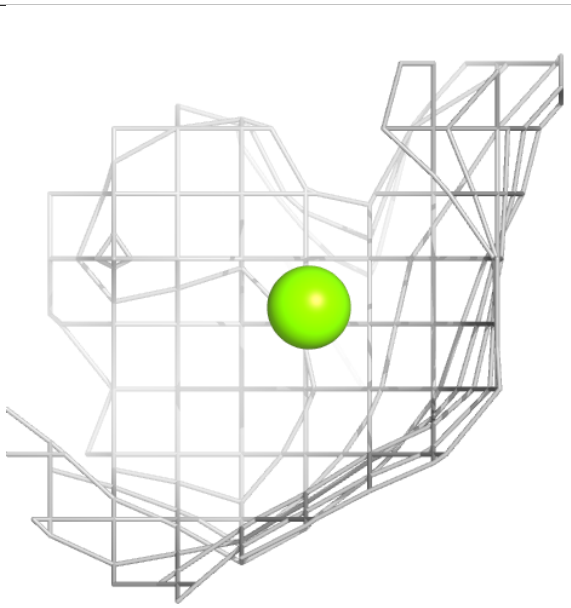


Electron density around MG N 704:

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

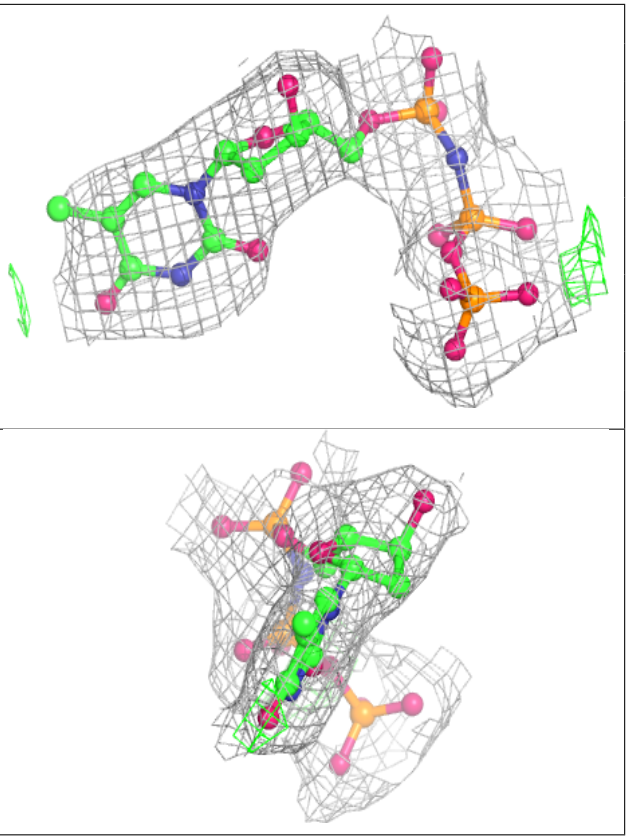


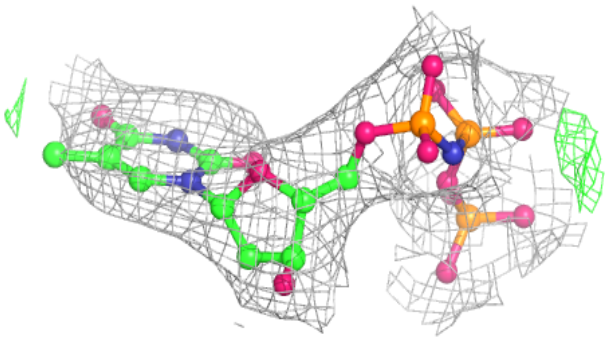




Electron density around 1FZ J 704:

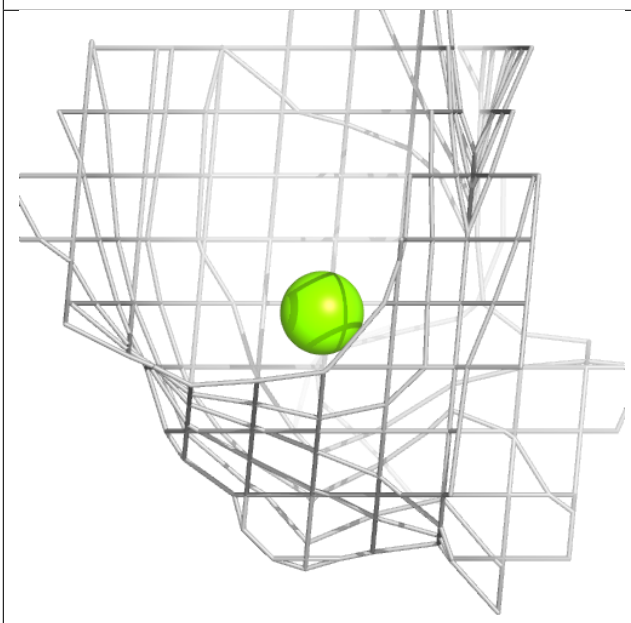
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





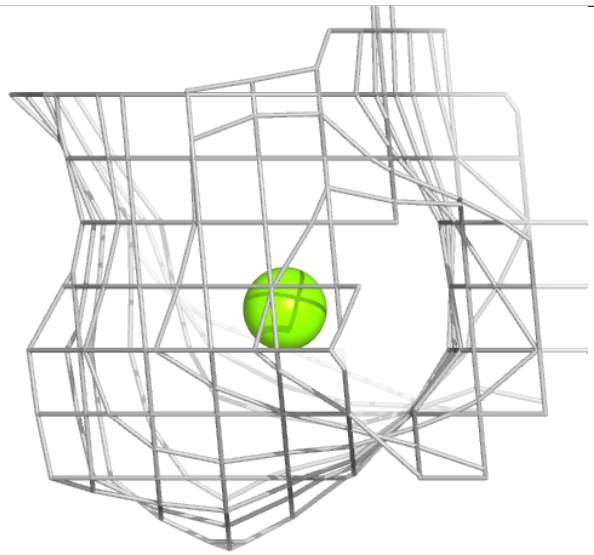
Electron density around MG A 703:

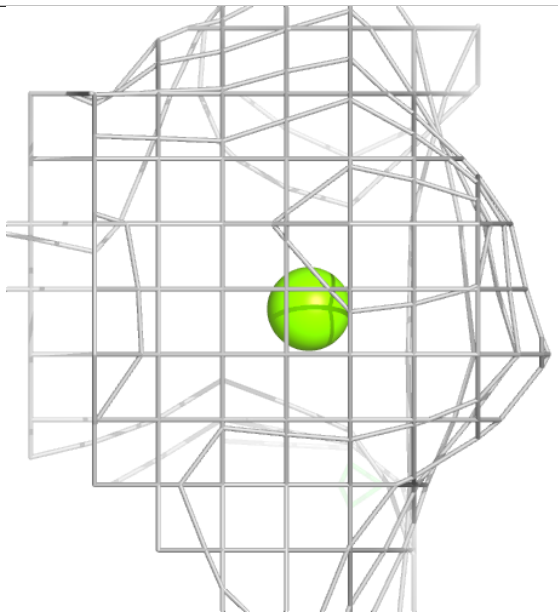
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around MG G 703:

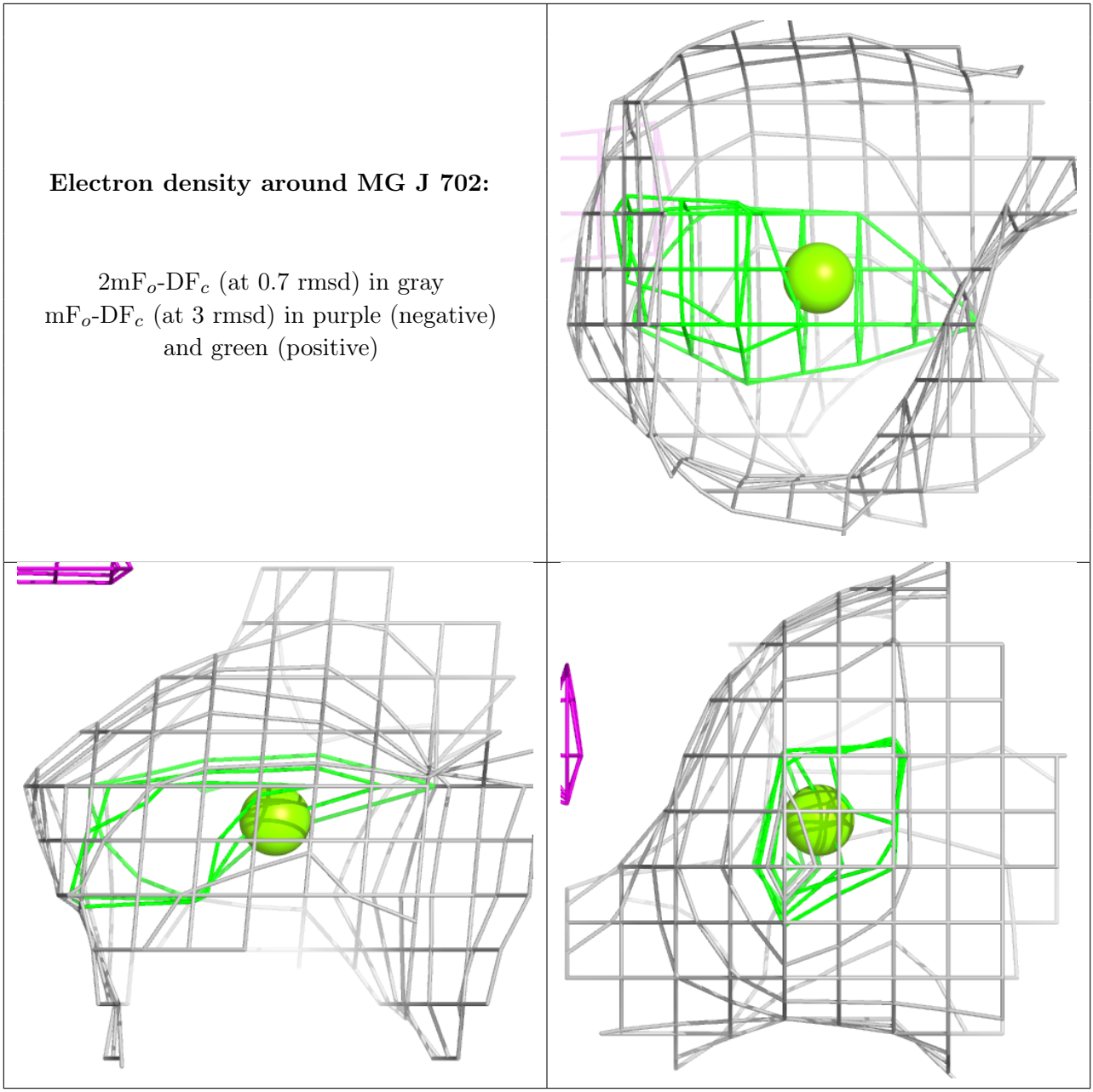
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





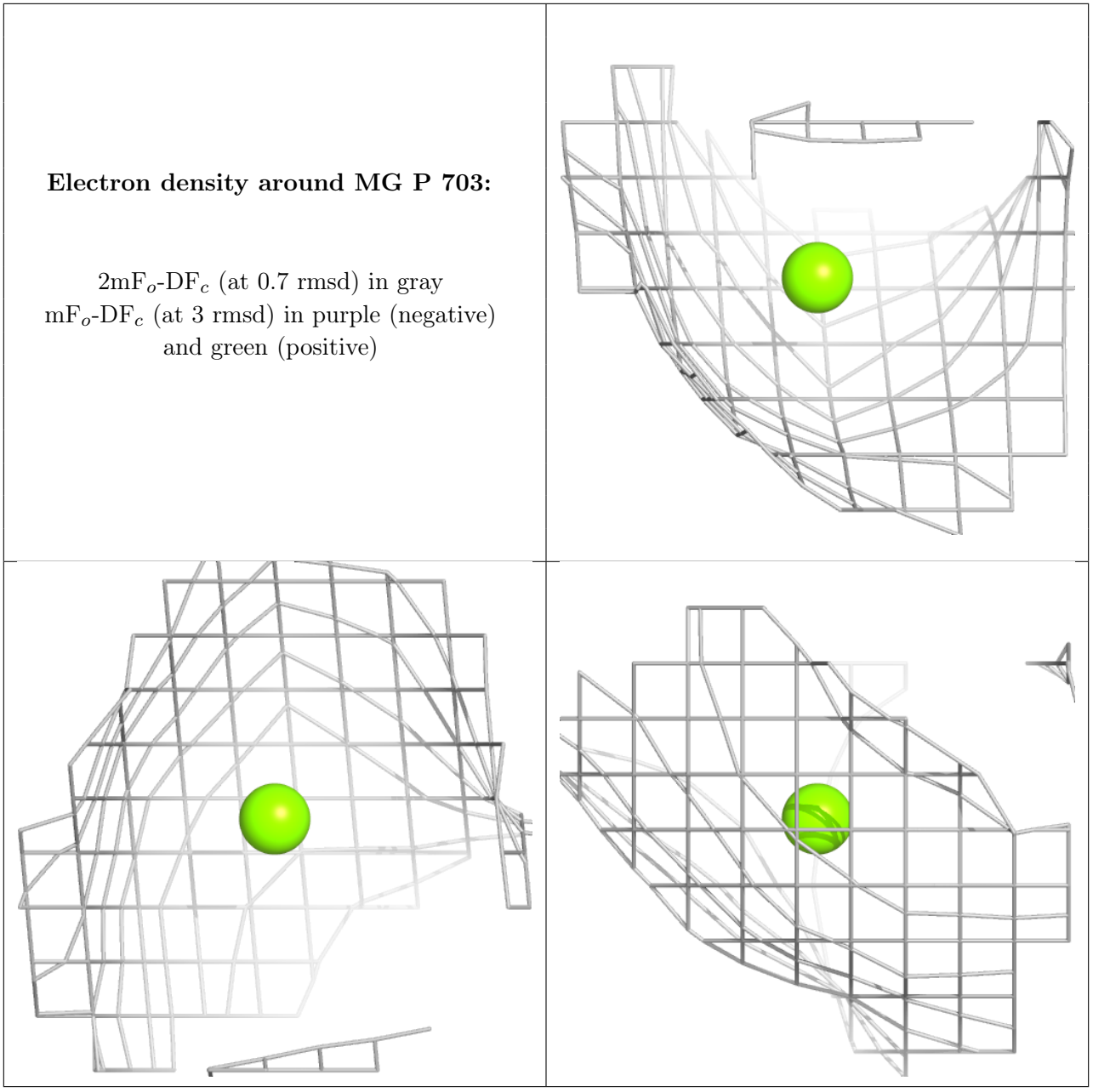
Electron density around MG J 702:

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



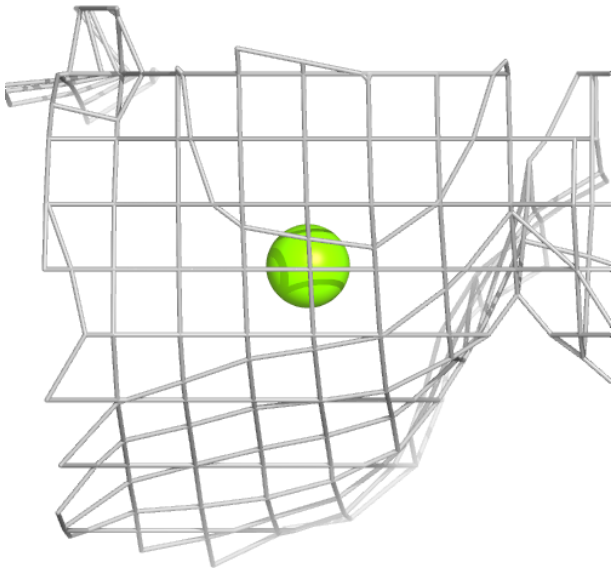
Electron density around MG P 703:

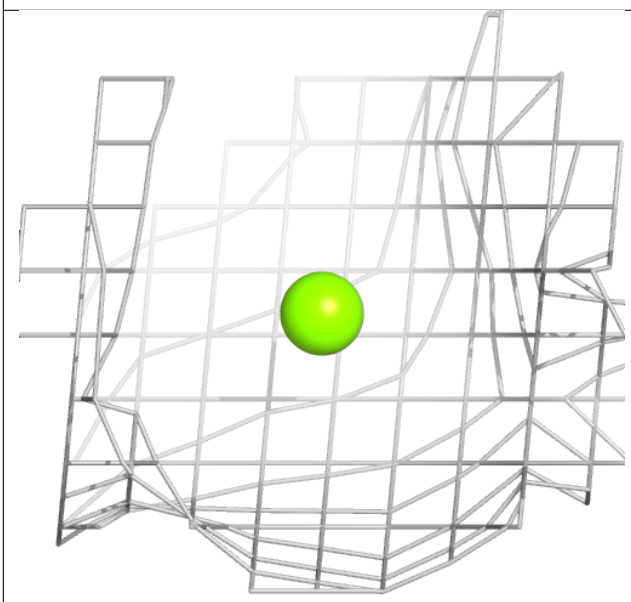
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

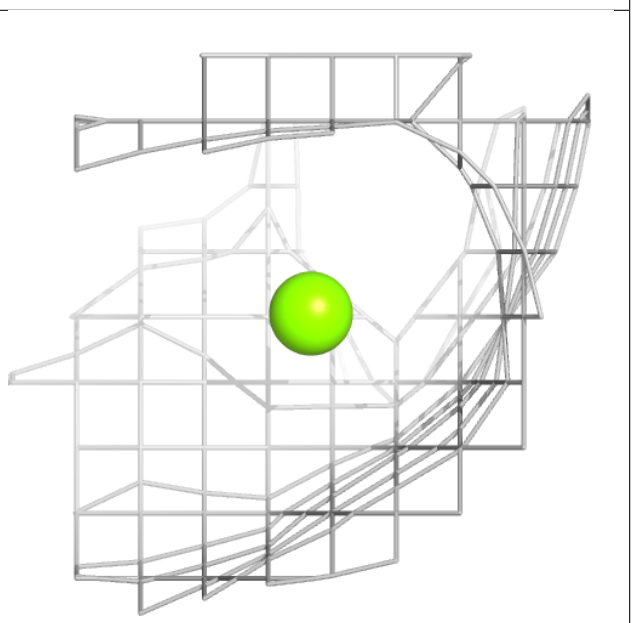


Electron density around MG J 703:

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

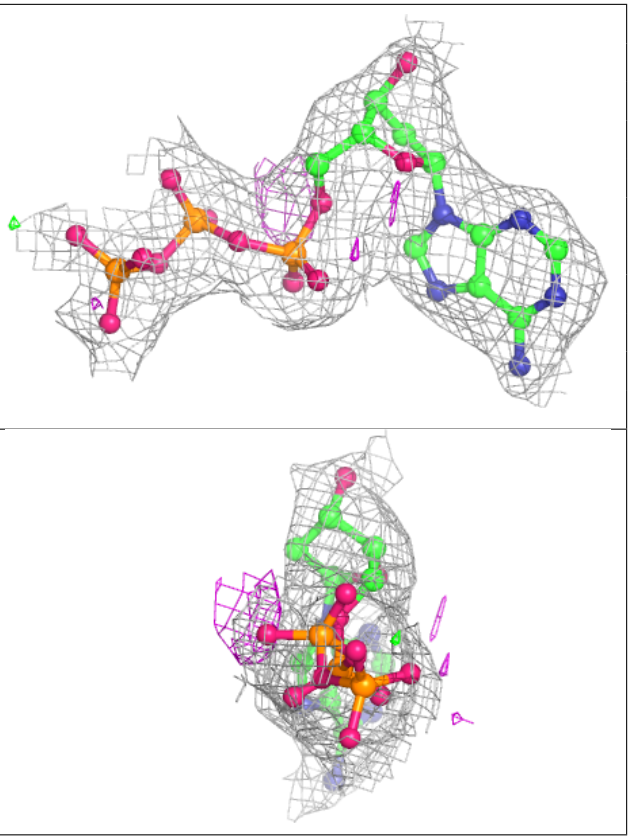


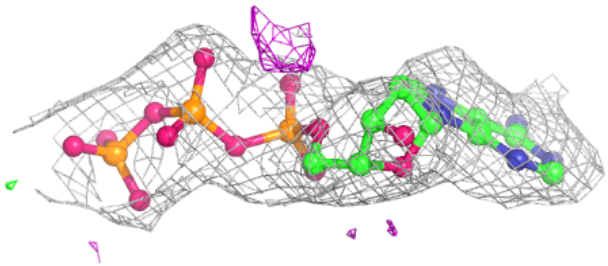




Electron density around DTP A 706:

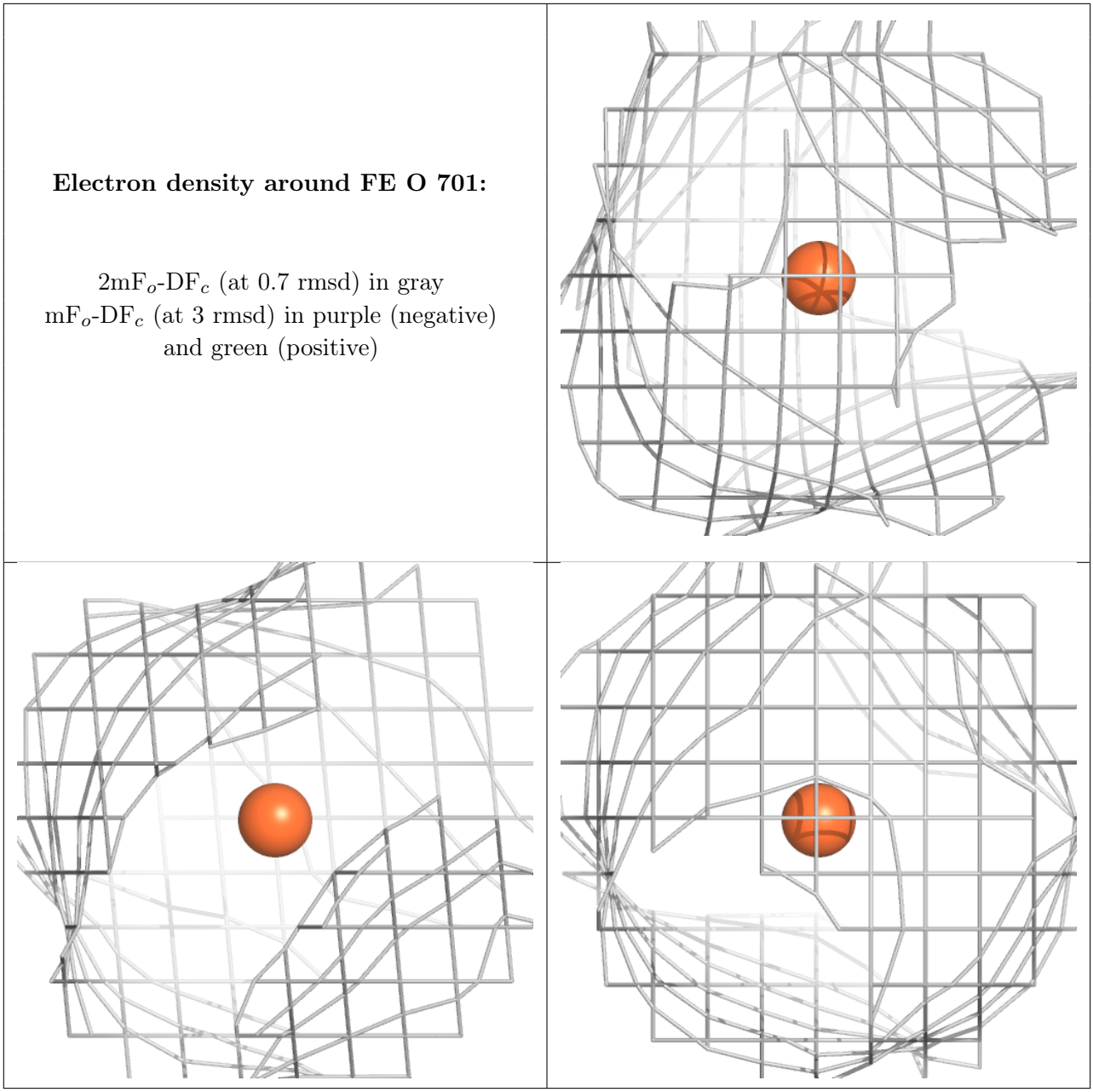
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





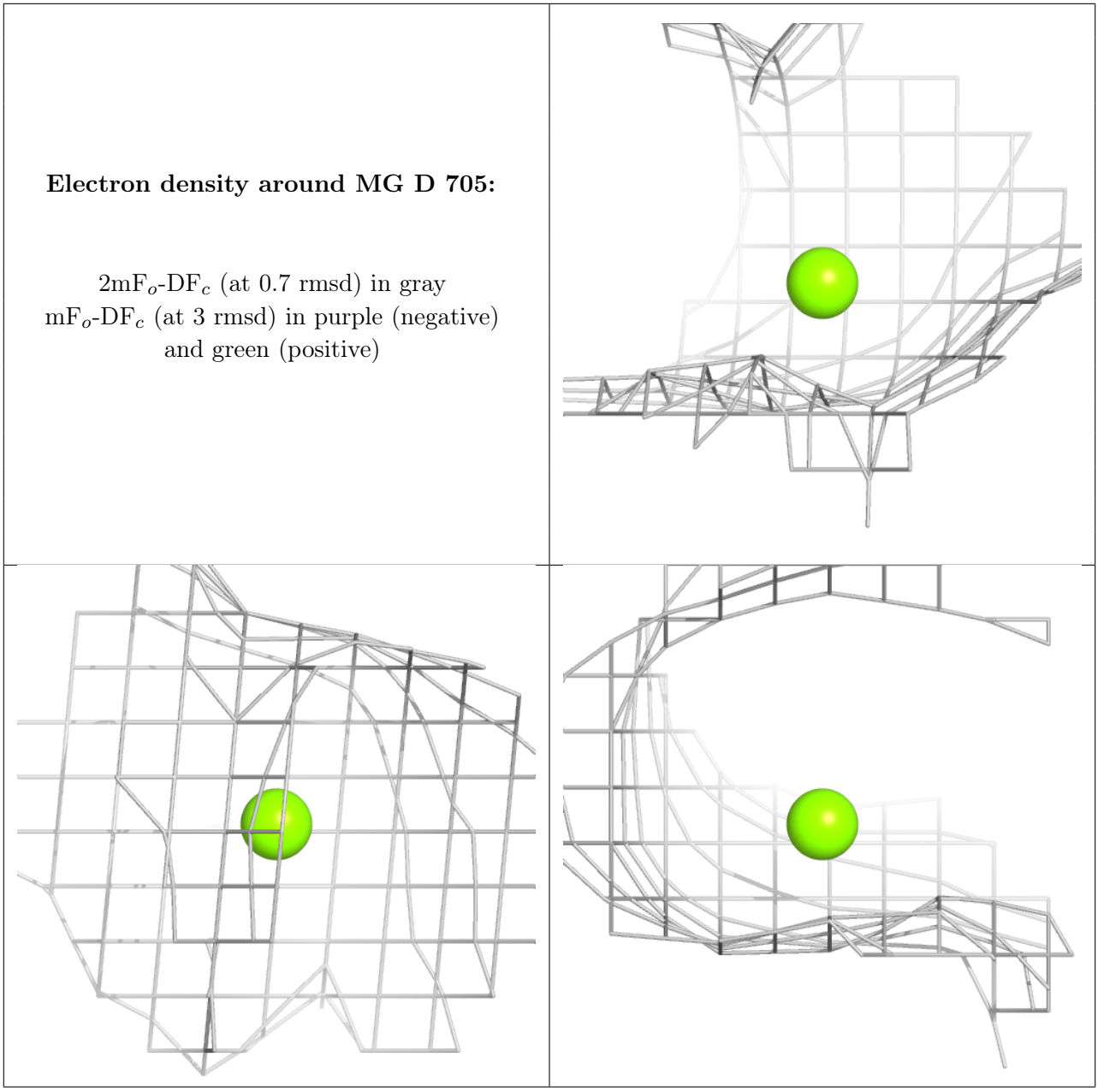
Electron density around FE O 701:

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



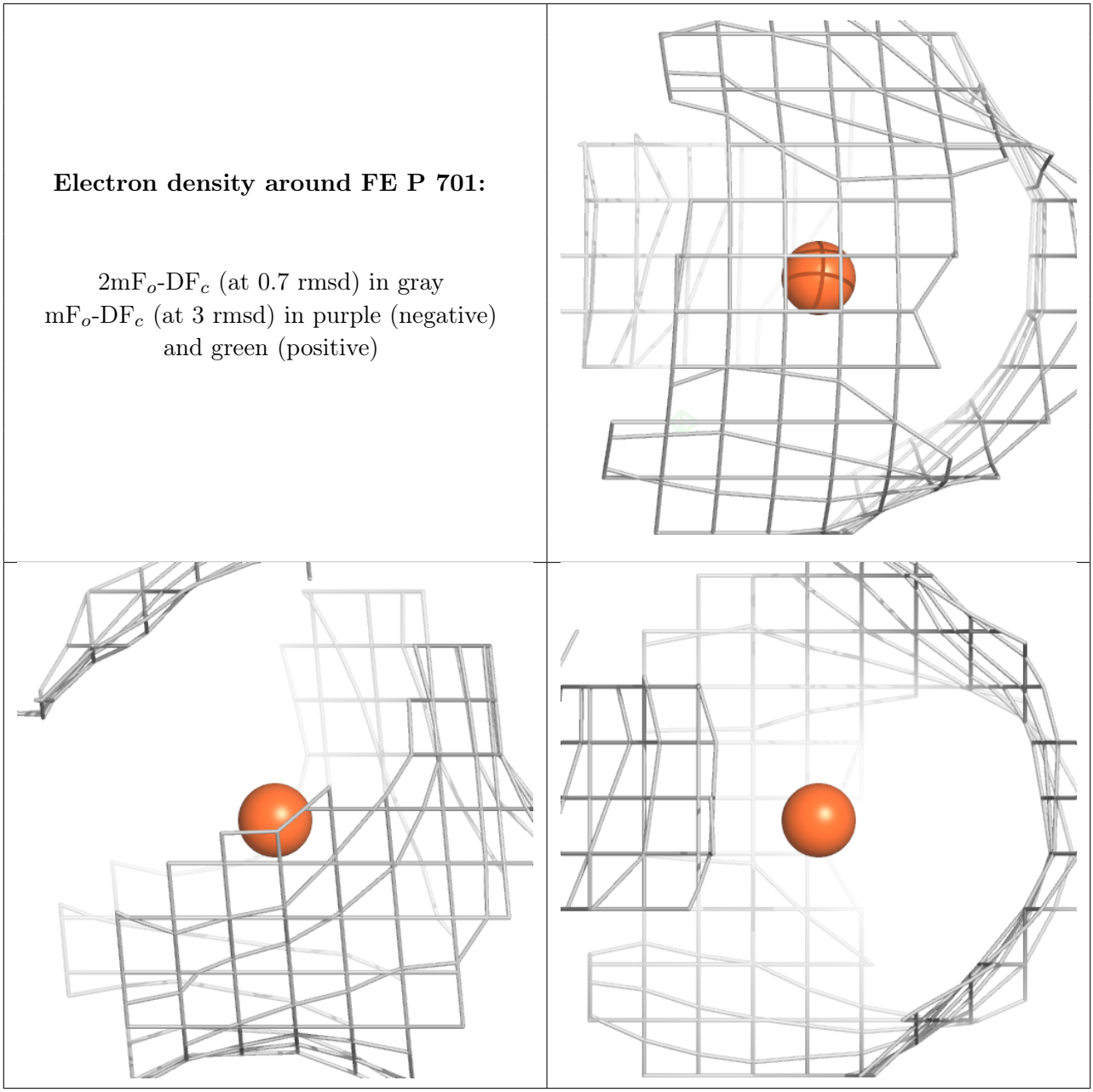
Electron density around MG D 705:

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



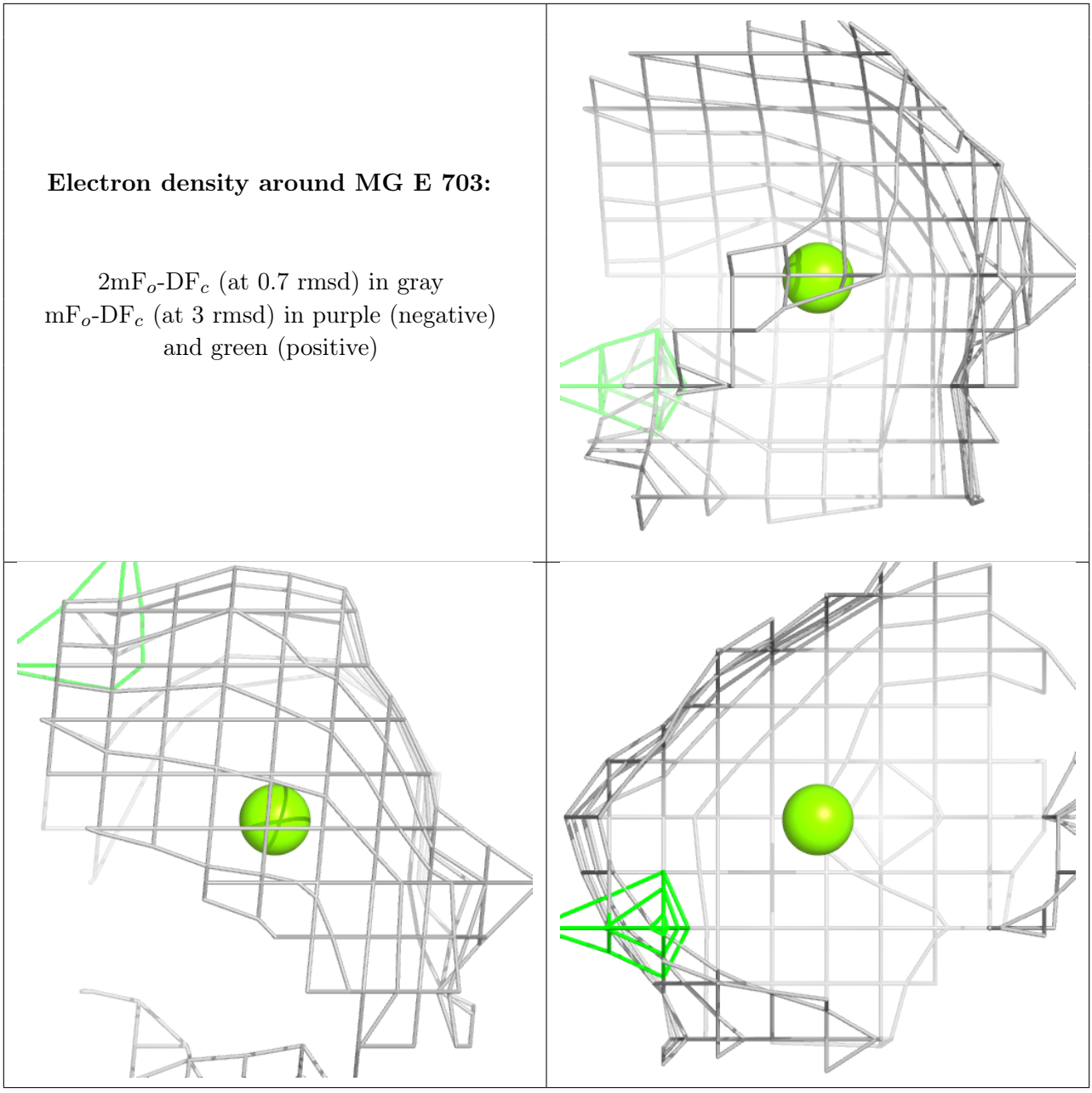
Electron density around FE P 701:

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



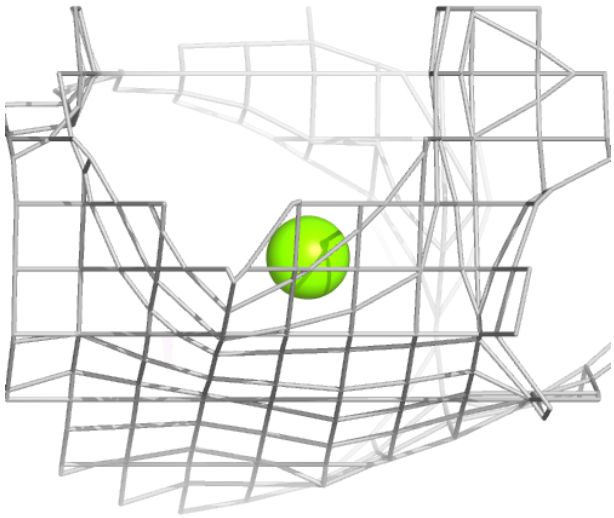
Electron density around MG E 703:

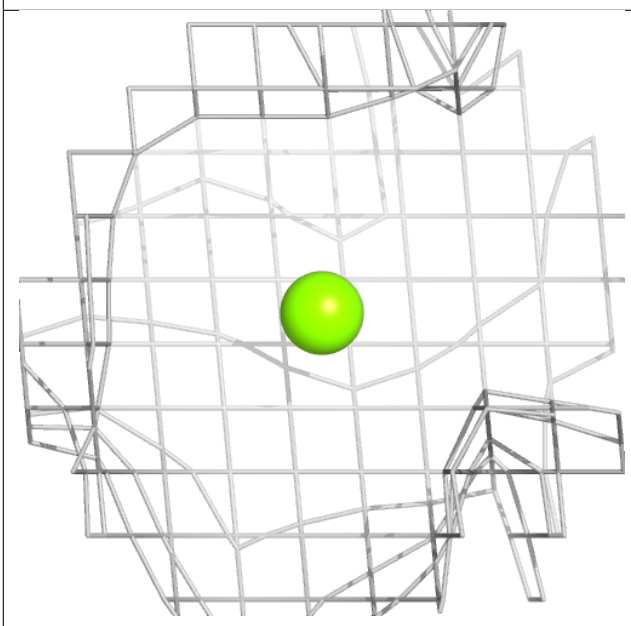
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

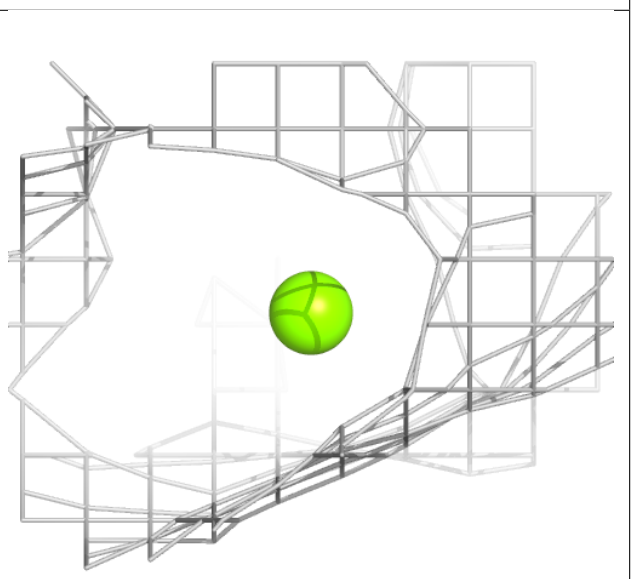


Electron density around MG L 704:

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

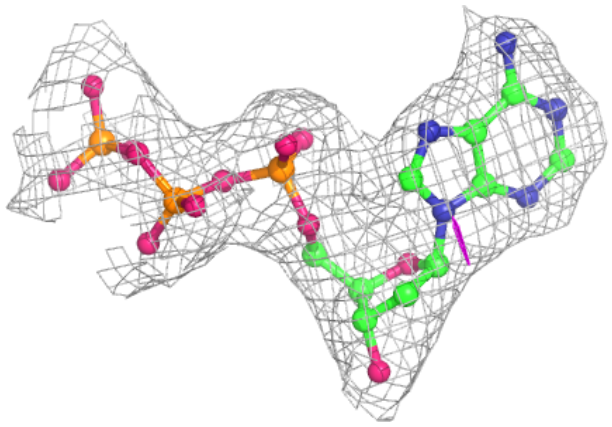


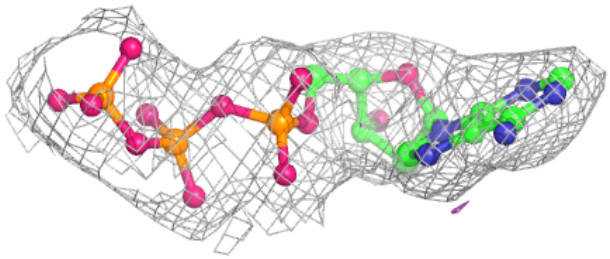


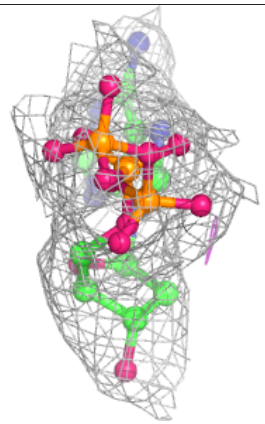


Electron density around DTP C 701:

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

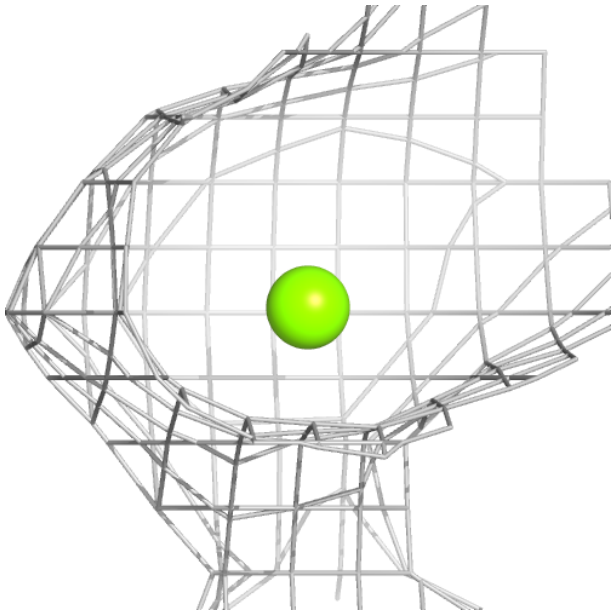


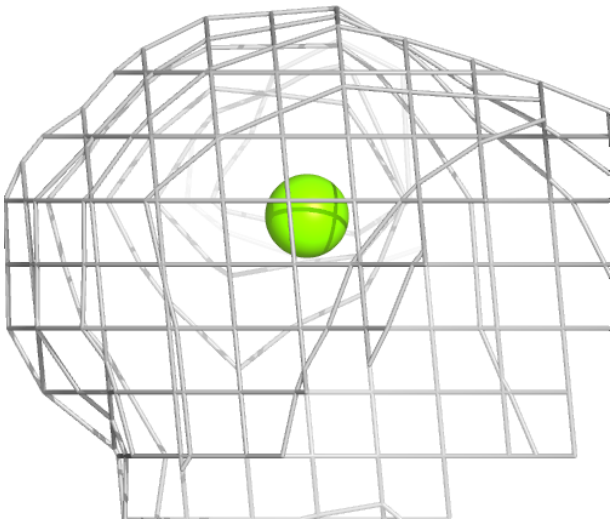


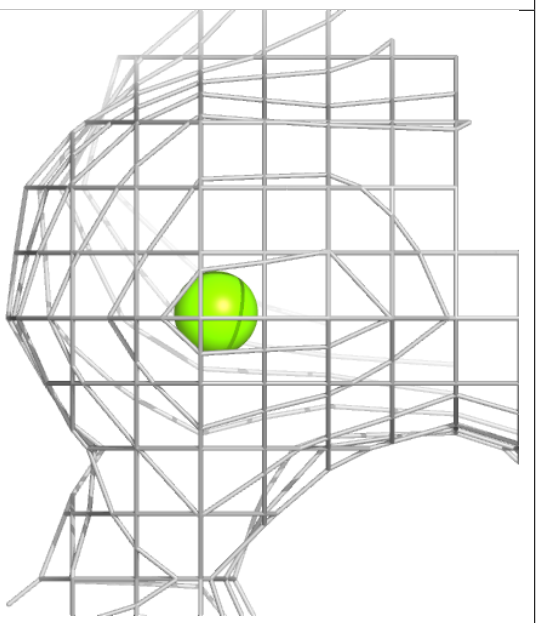


Electron density around MG F 702:

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

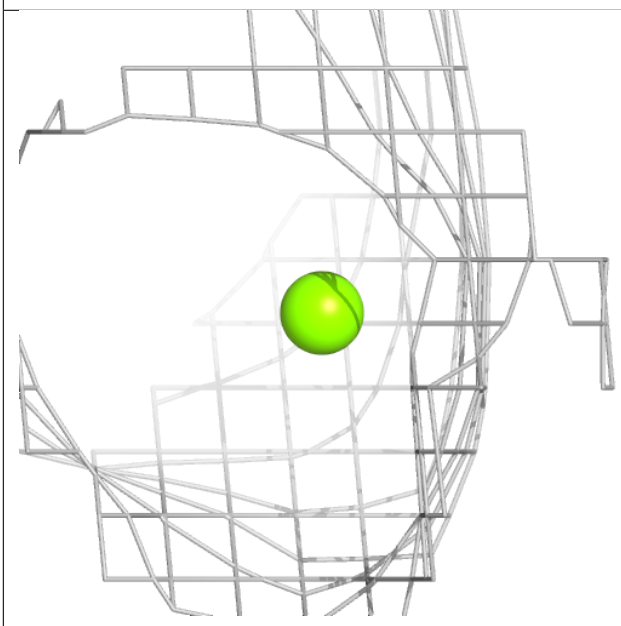


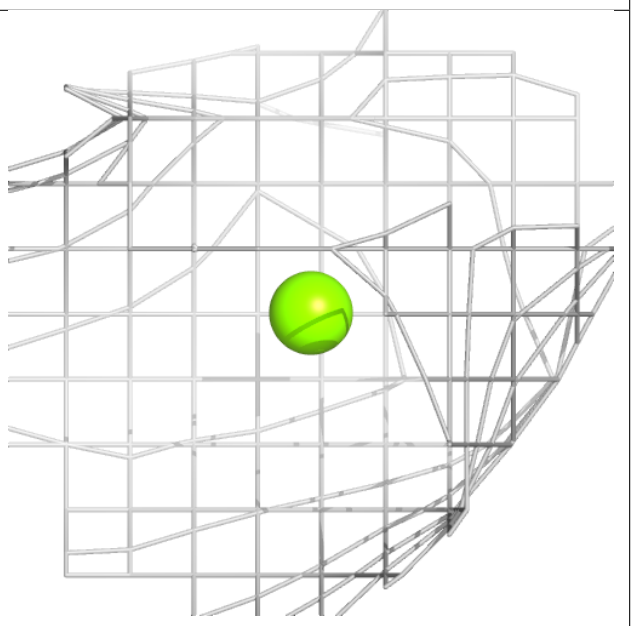




Electron density around MG F 703:

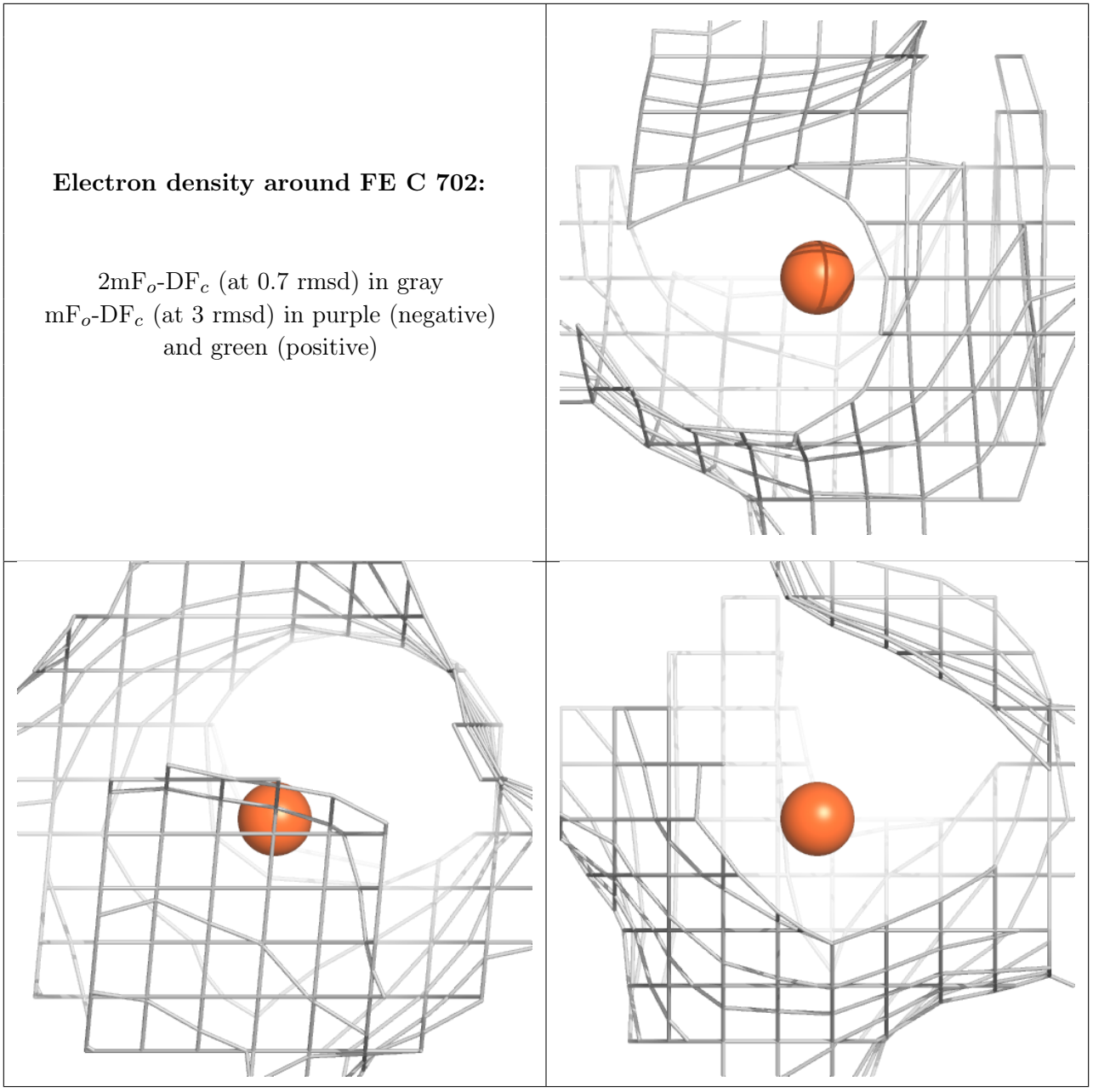
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





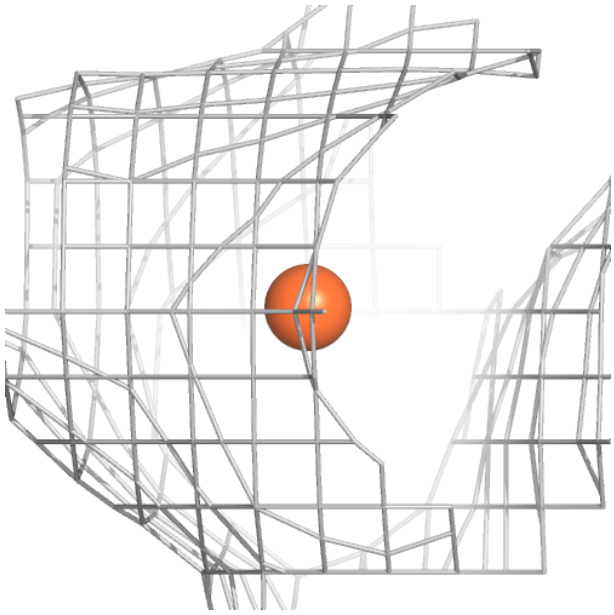
Electron density around FE C 702:

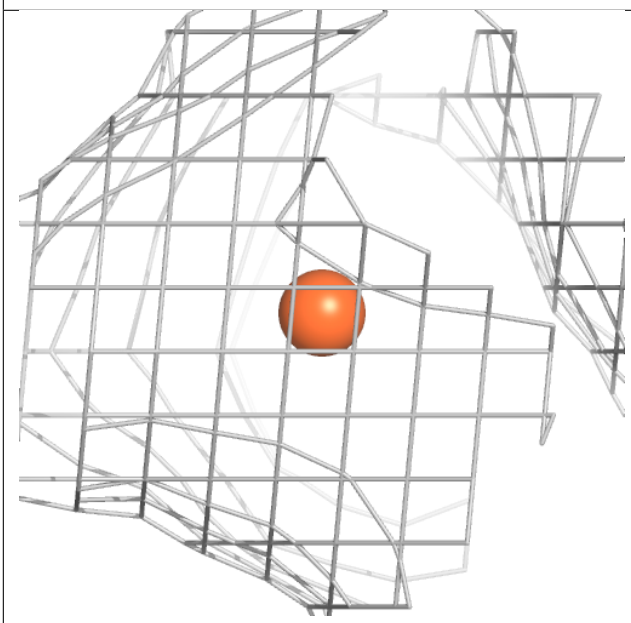
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

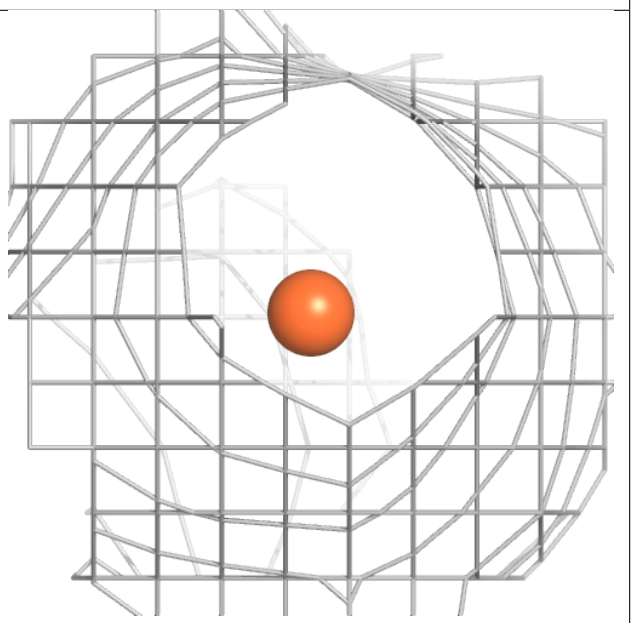


Electron density around FE E 701:

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

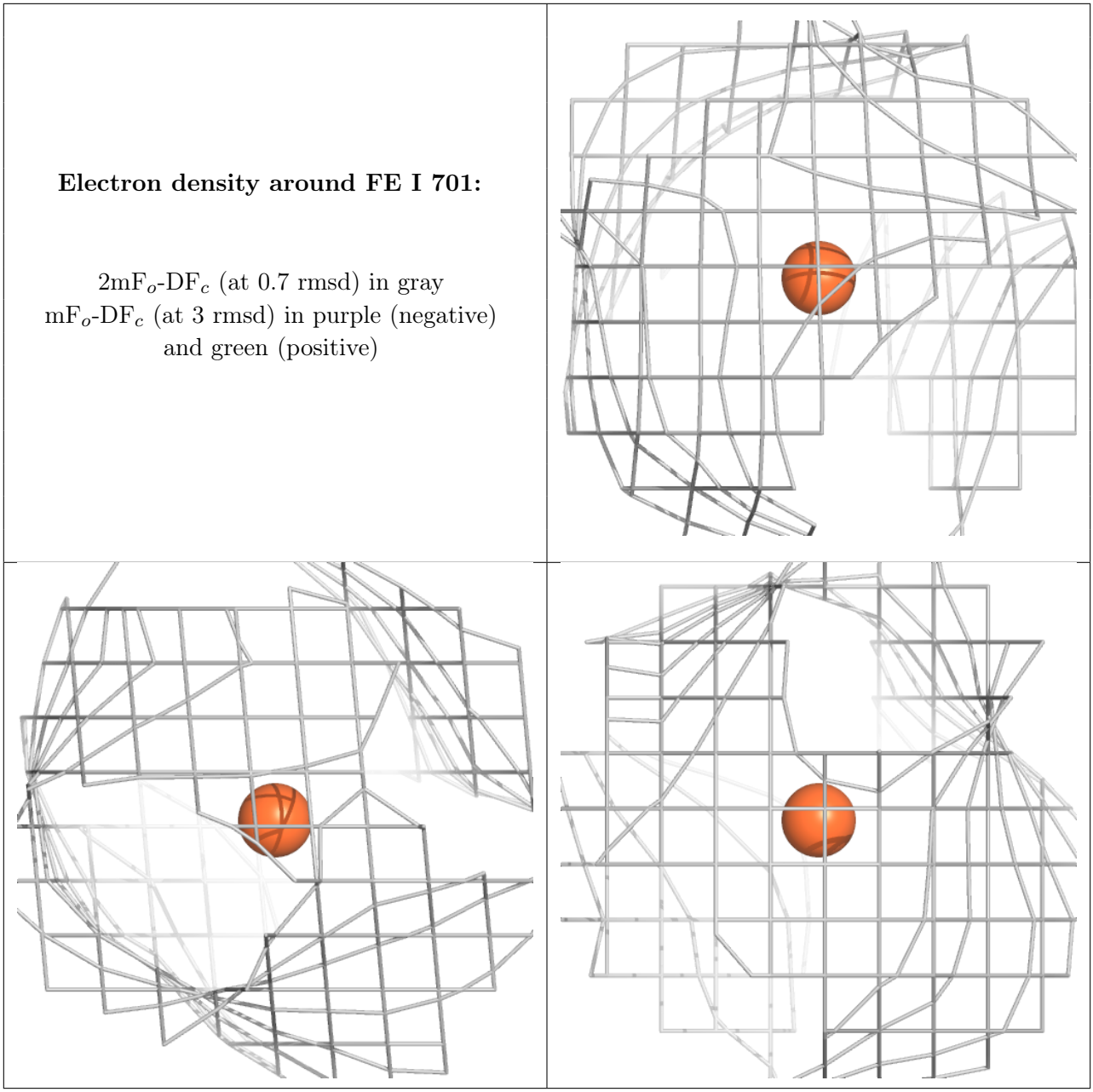






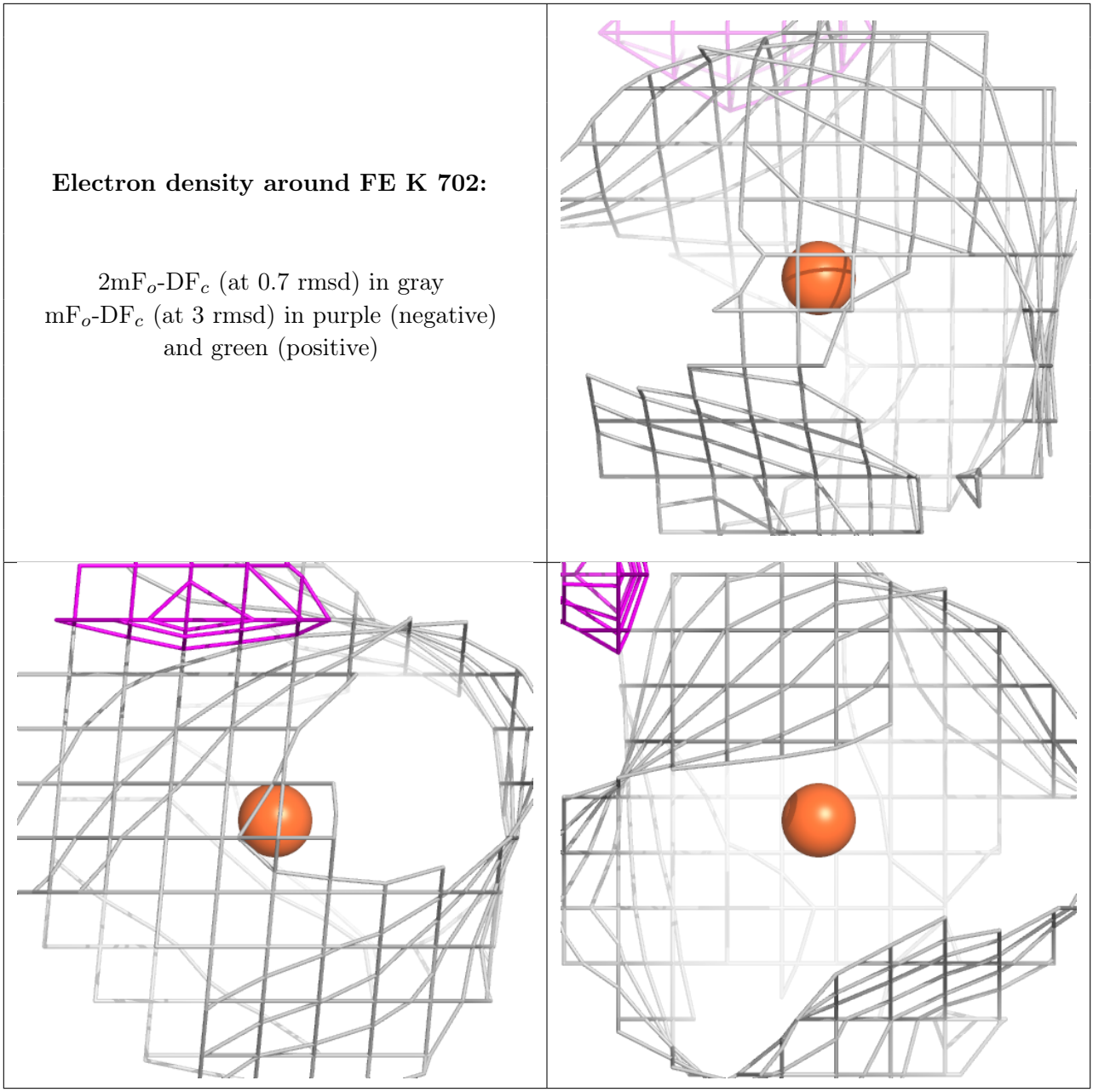
Electron density around FE I 701:

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



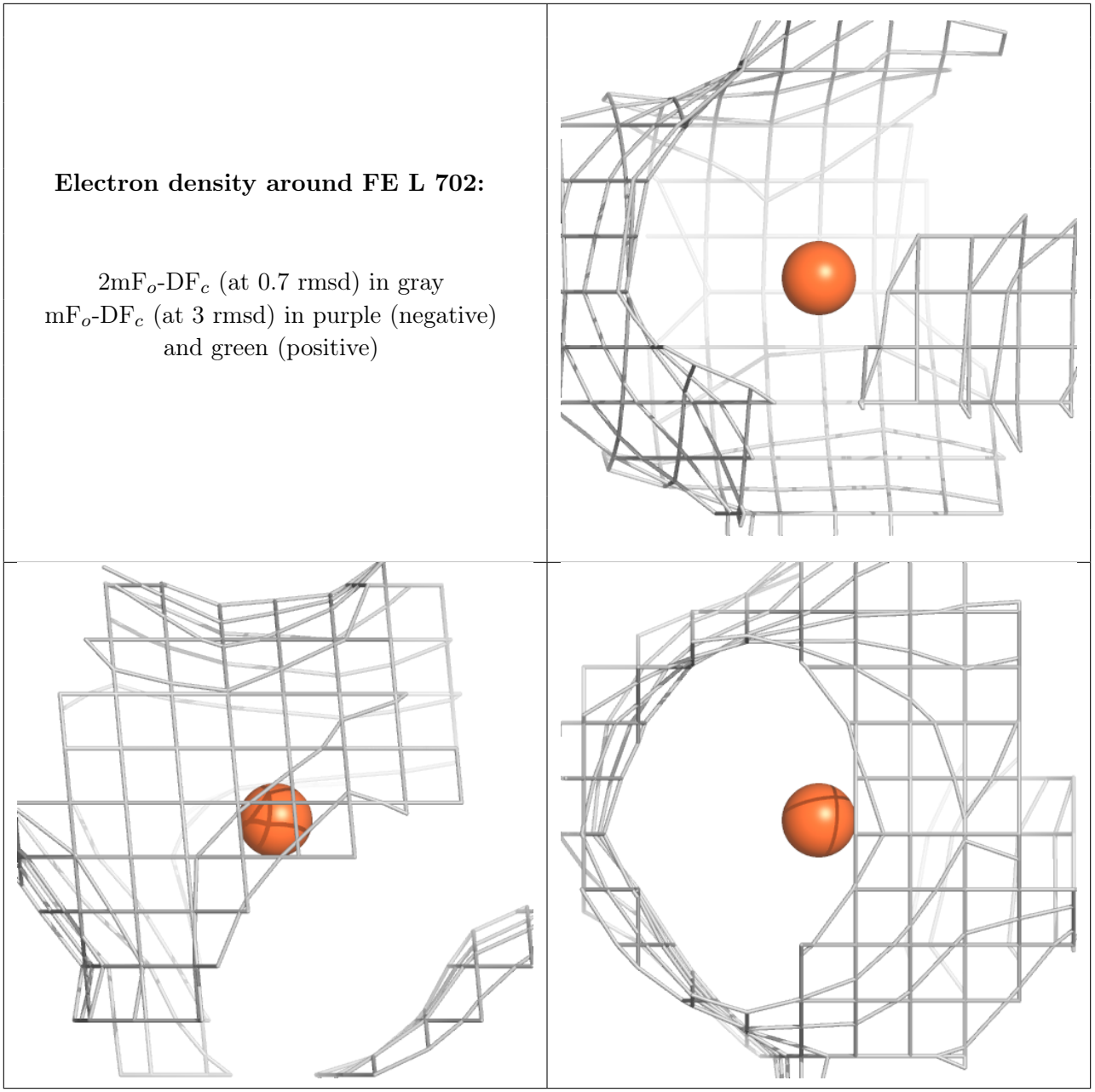
Electron density around FE K 702:

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



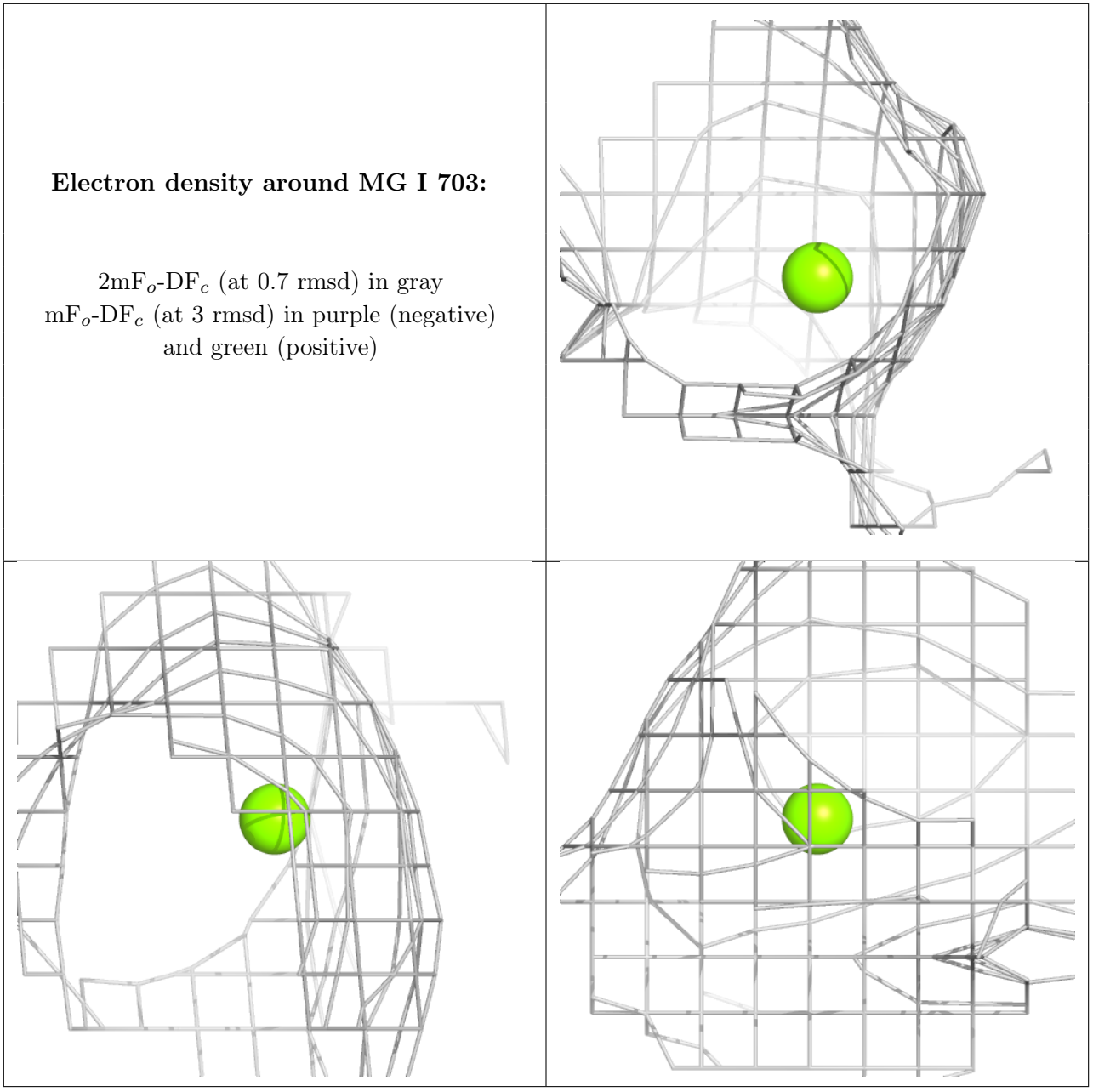
Electron density around FE L 702:

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



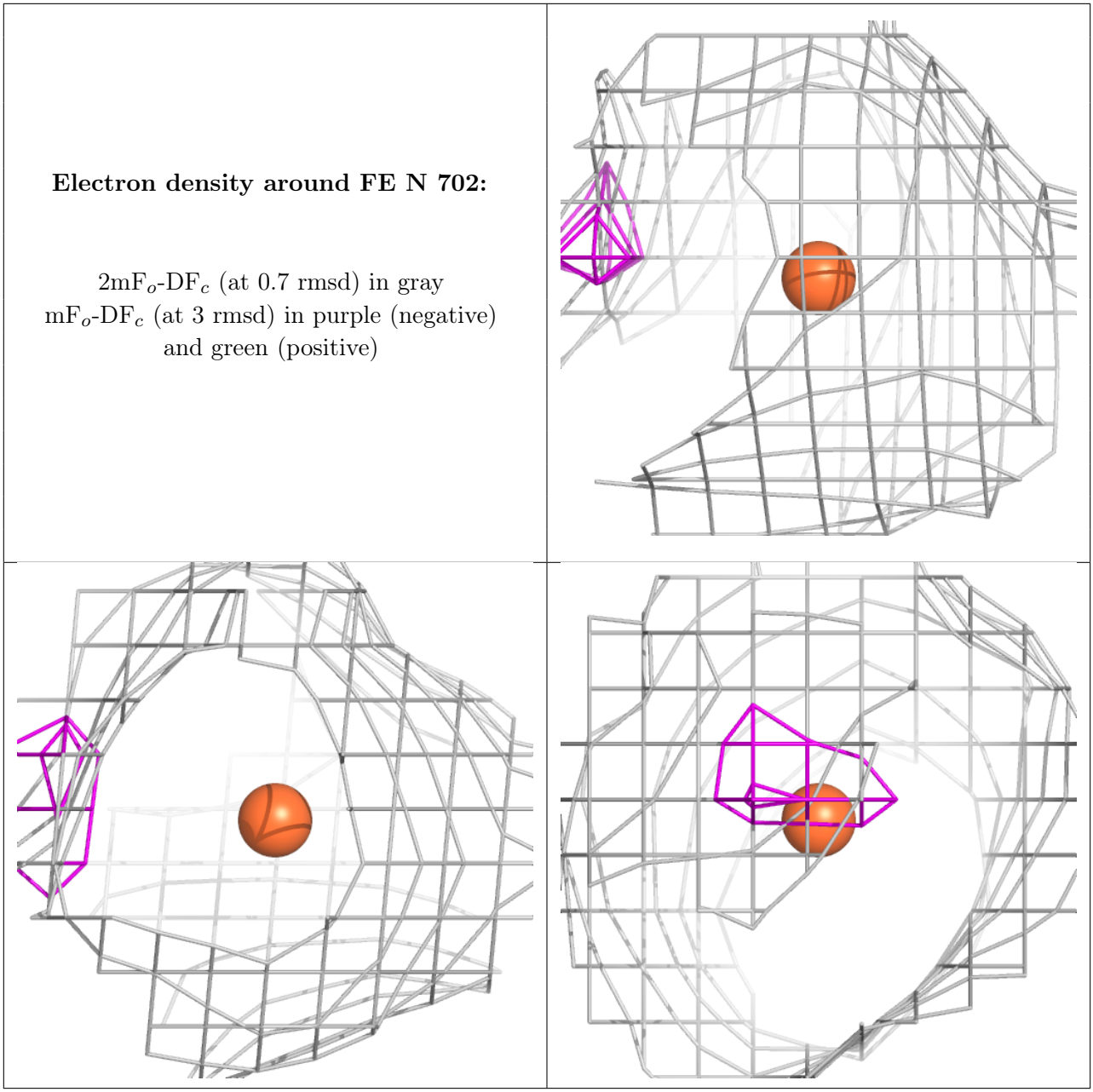
Electron density around MG I 703:

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



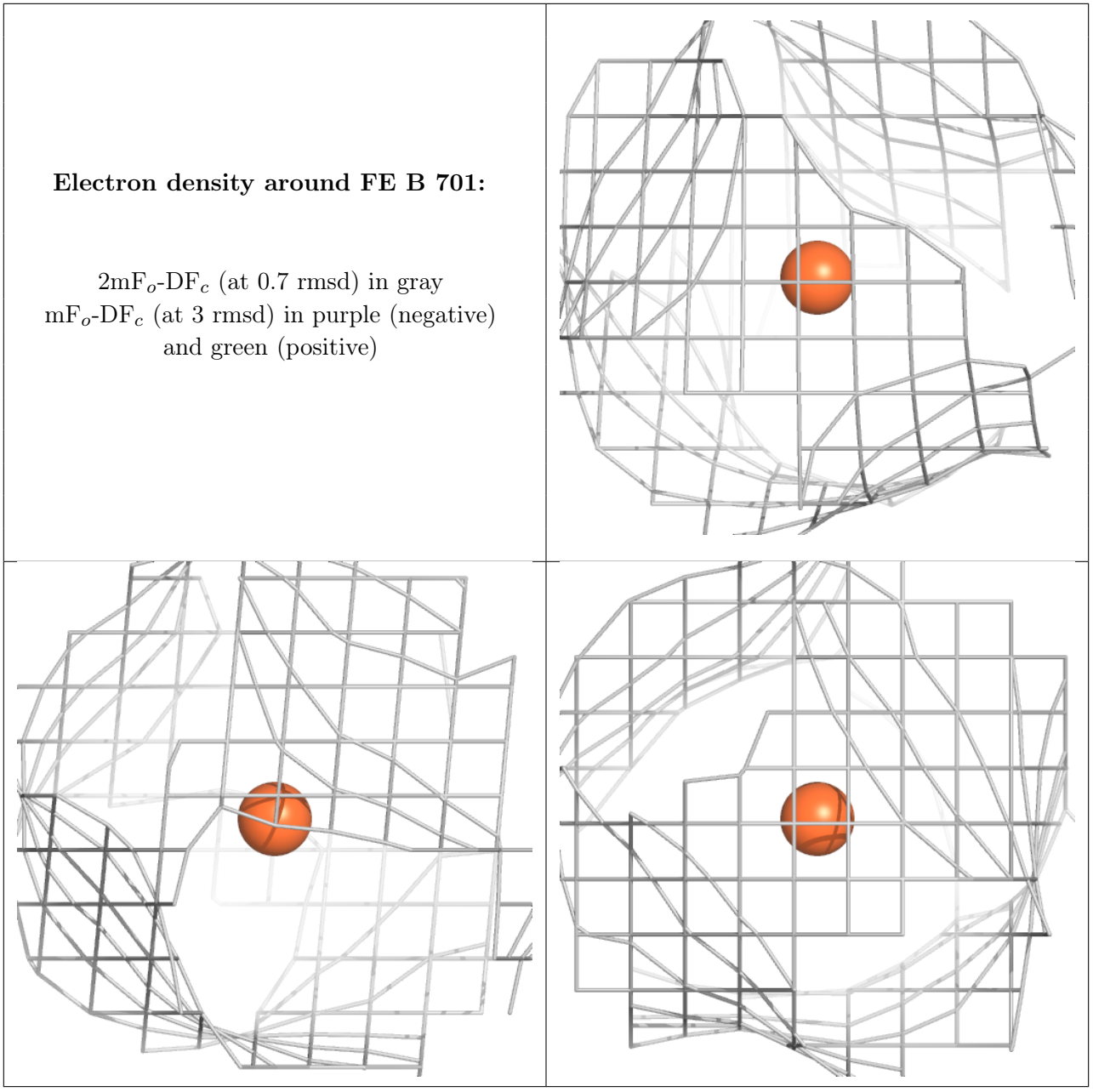
Electron density around FE N 702:

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



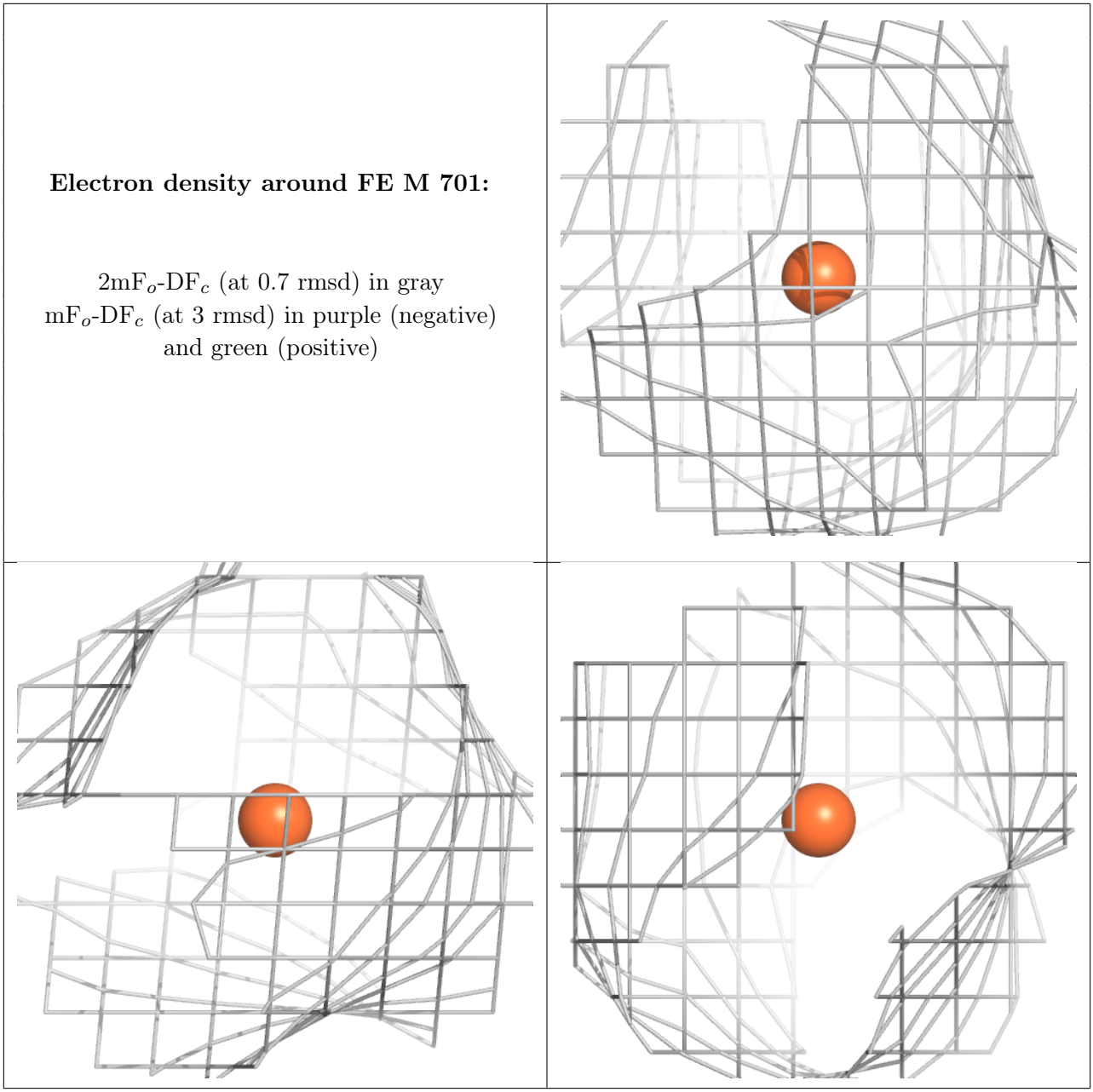
Electron density around FE B 701:

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



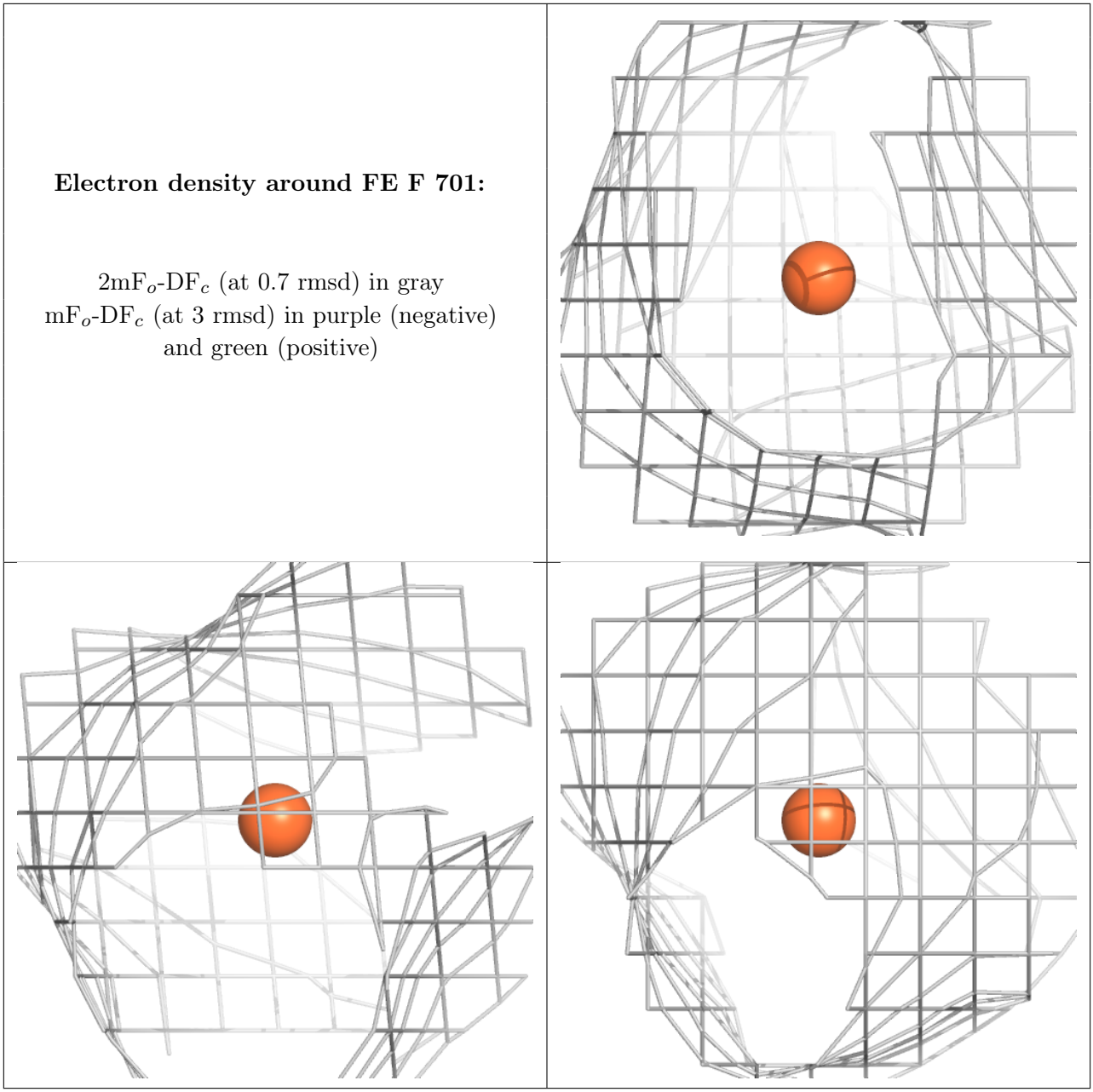
Electron density around FE M 701:

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



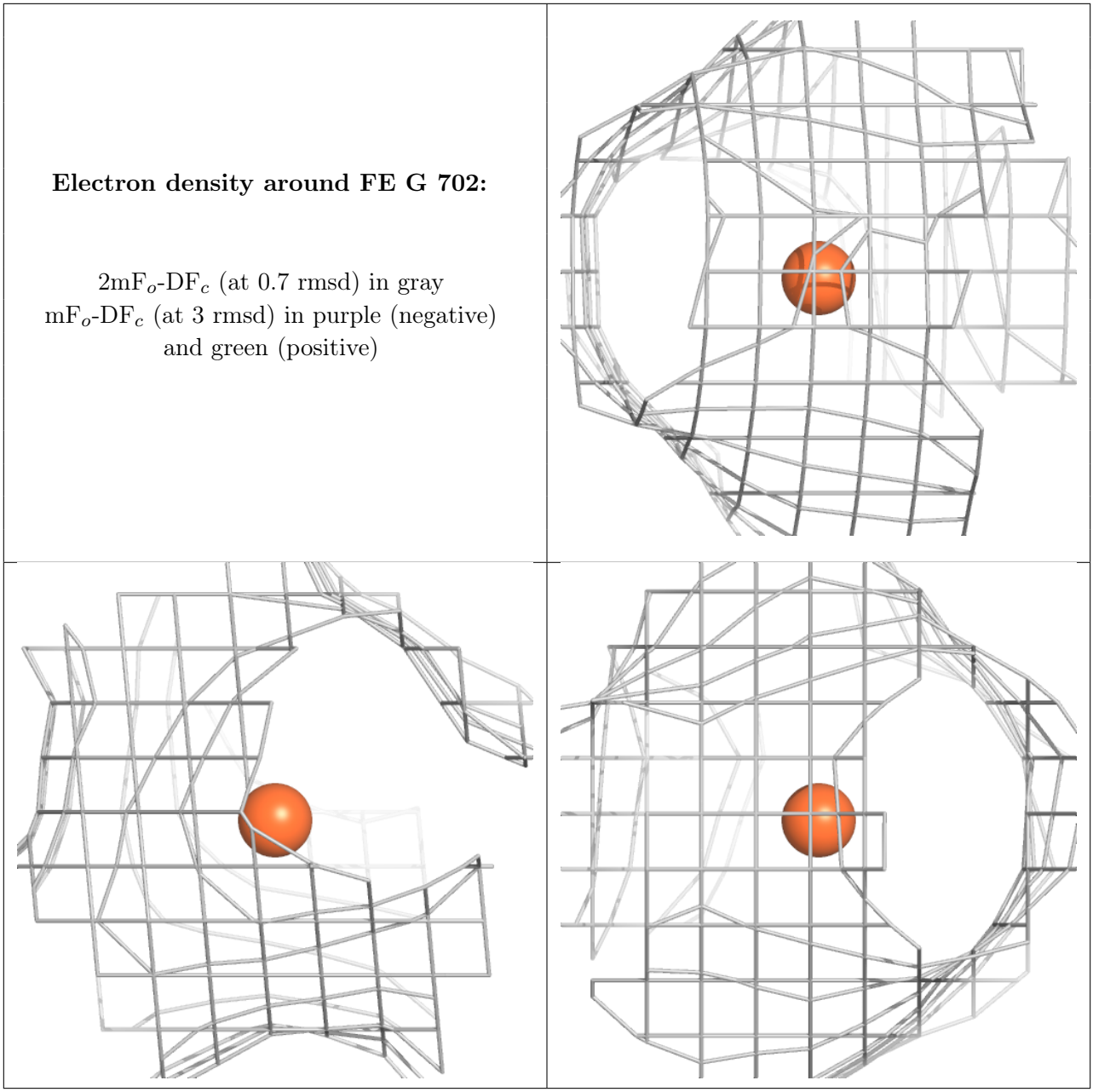
Electron density around FE F 701:

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



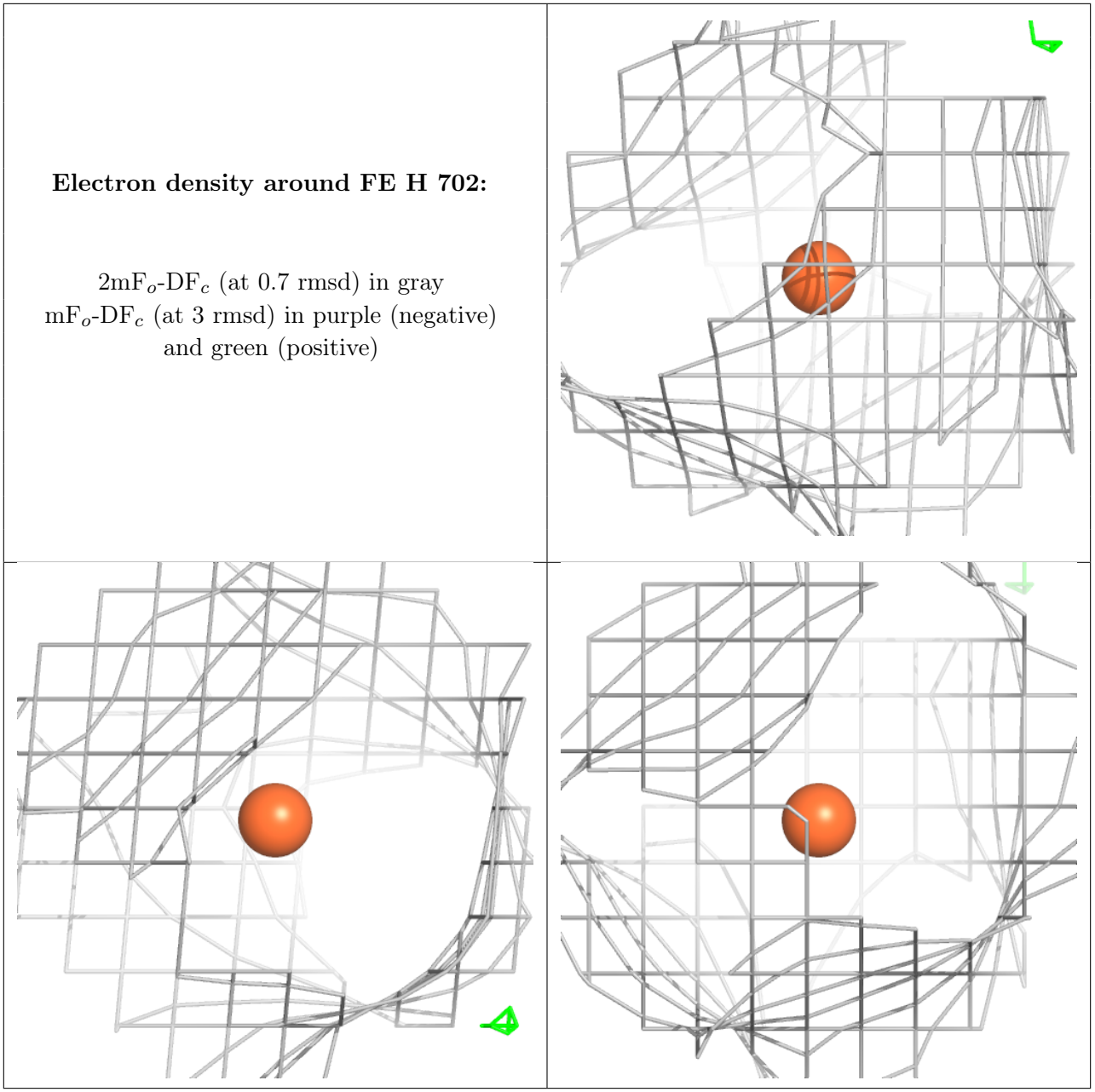
Electron density around FE G 702:

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



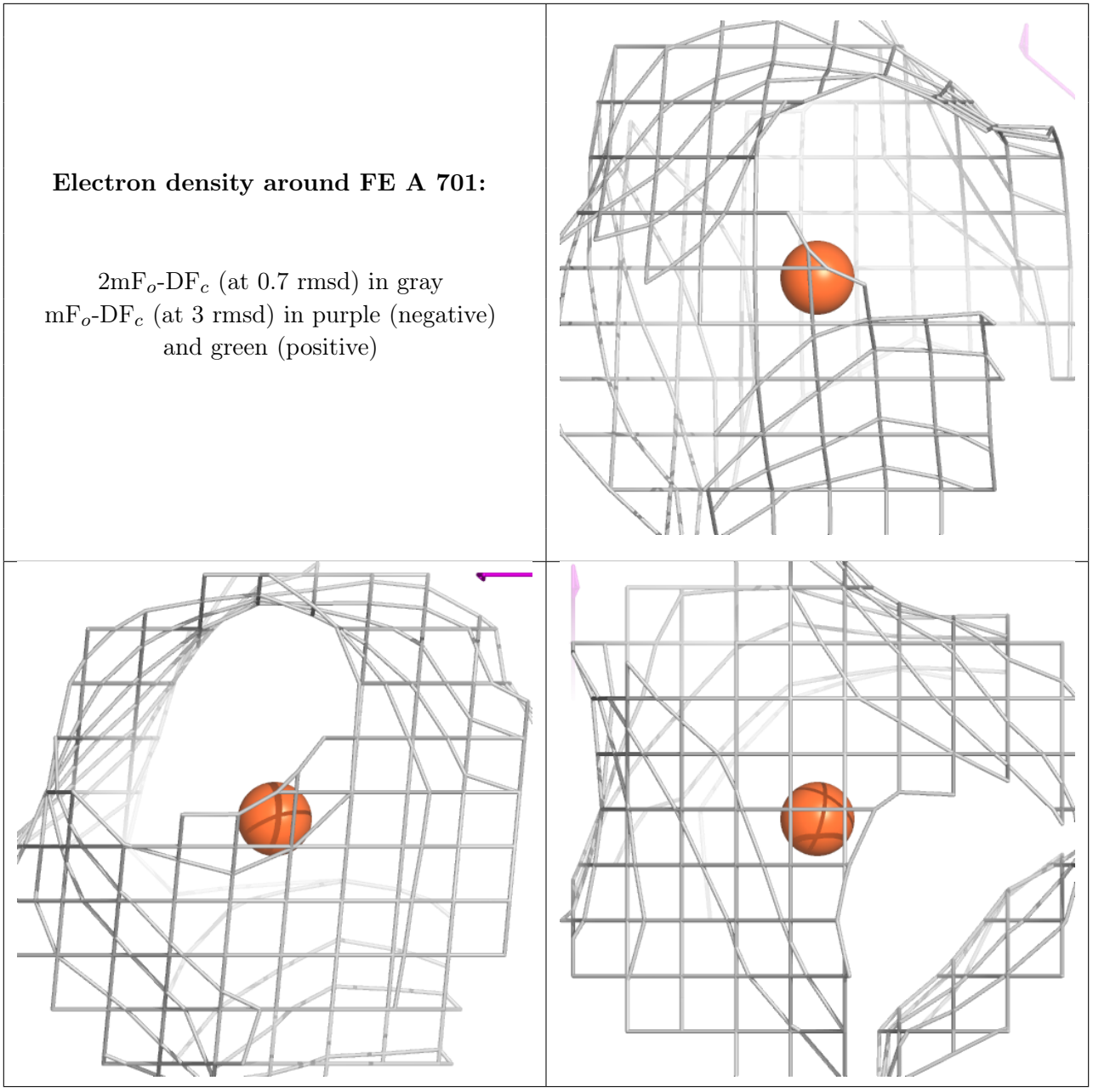
Electron density around FE H 702:

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



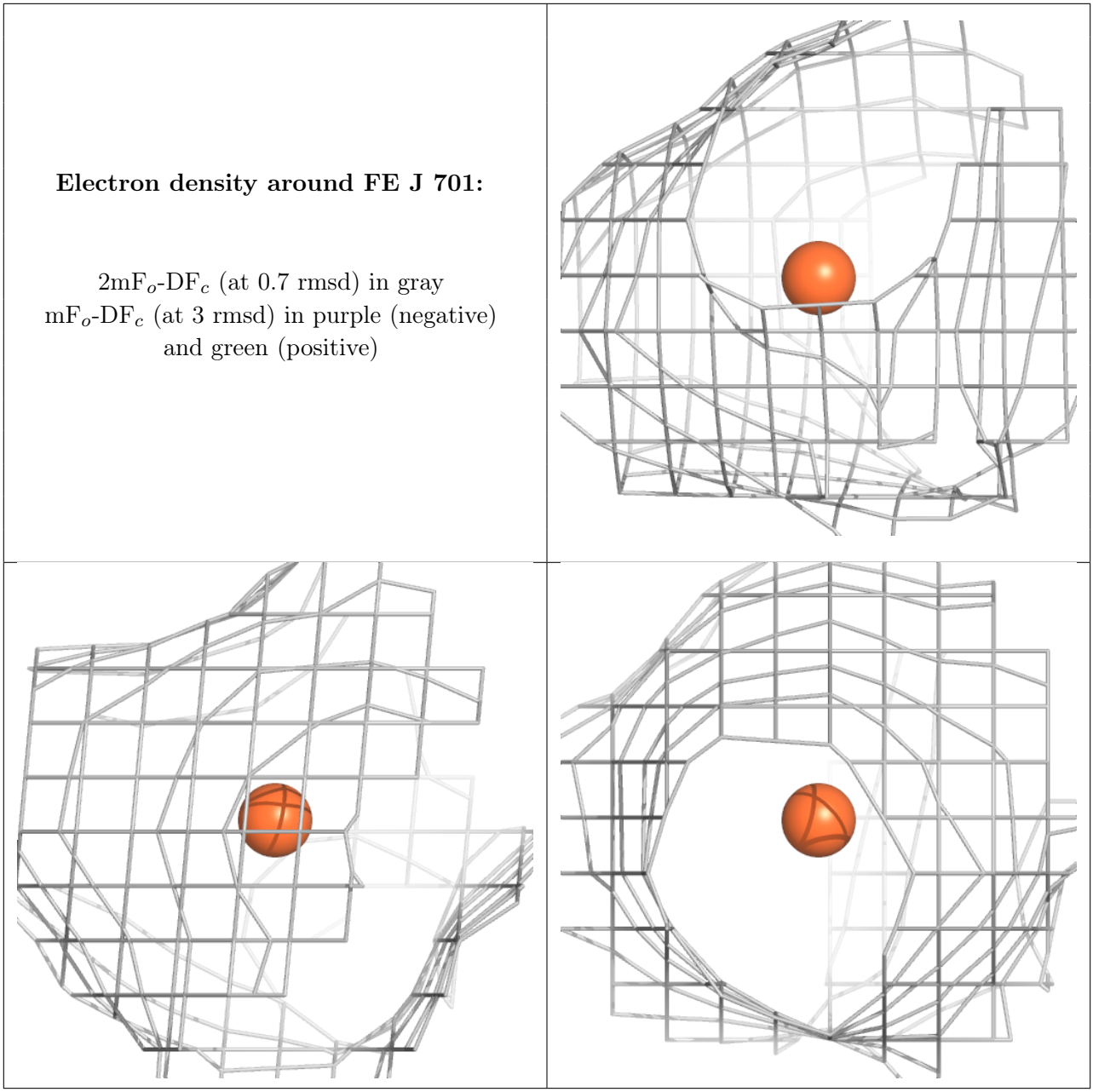
Electron density around FE A 701:

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



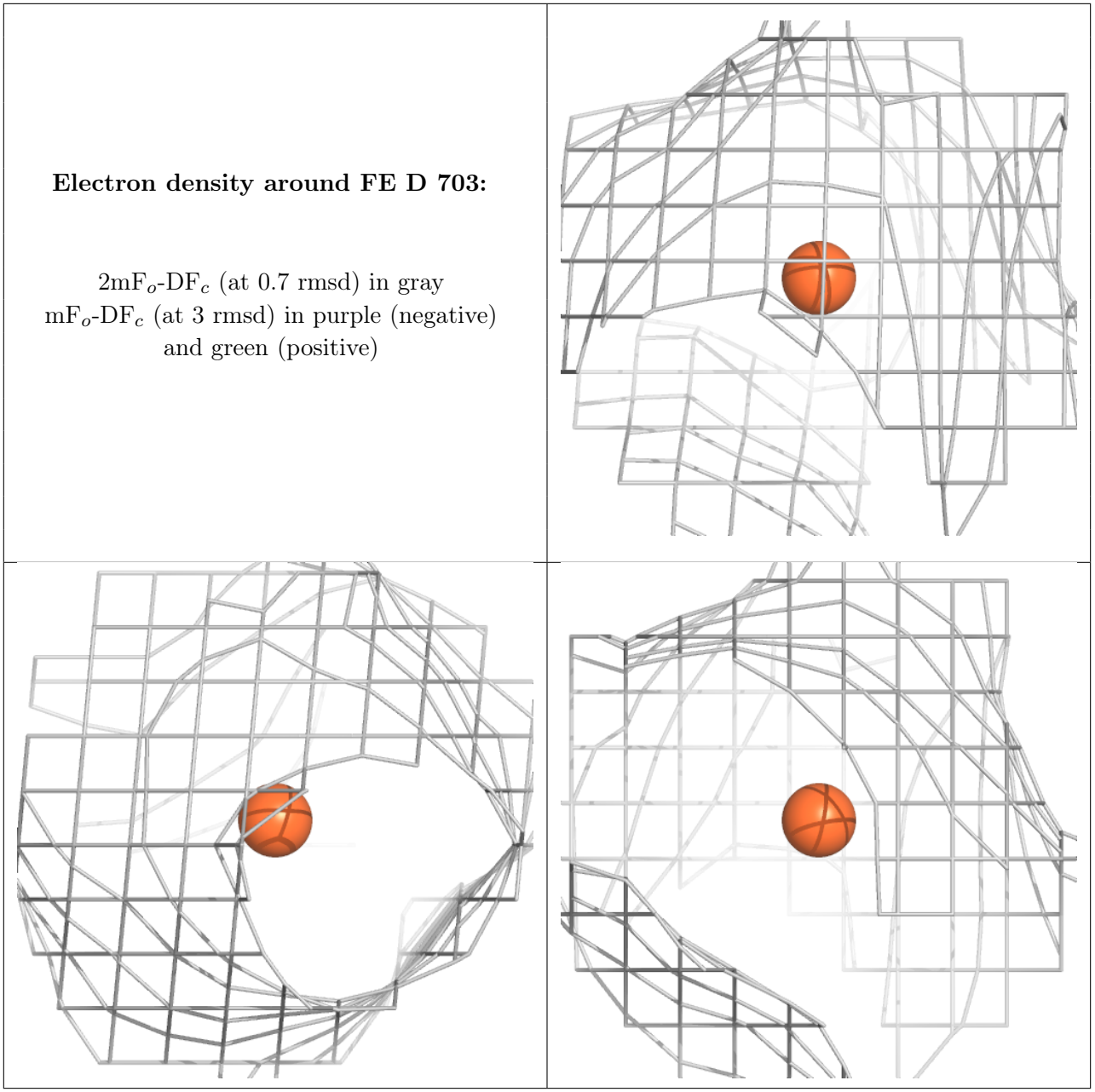
Electron density around FE J 701:

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



Electron density around FE 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)



6.5 Other polymers

There are no such residues in this entry.