



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 10:10 AM UTC

PDB ID : 6TXC / pdb_00006txc
Title : Crystal structure of tetrameric human wt-SAMHD1 (residues 109-626) with GTP, dATP, dCMPNPP and Mg
Authors : Morris, E.R.; Kunzelmann, S.; Caswell, S.J.; Arnold, L.H.; Purkiss, A.; Kelly, G.; Taylor, I.A.
Deposited on : 2020-01-14
Resolution : 2.84 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

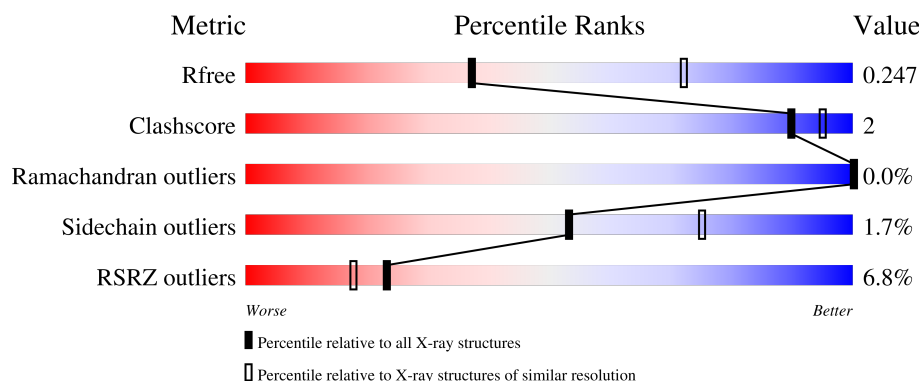
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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

Mol	Chain	Length	Quality of chain
1	A	520	2% 86% 6% • 8%
1	B	520	3% 87% • • 8%
1	C	520	2% 86% 6% • 8%
1	D	520	• 86% 6% • 8%

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Mol	Chain	Length	Quality of chain
1	E	520	
1	F	520	
1	G	520	
1	H	520	
1	I	520	
1	J	520	
1	K	520	
1	L	520	
1	M	520	
1	N	520	
1	O	520	
1	P	520	

2 Entry composition

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

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

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

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

There are 32 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is FE (III) ION (CCD ID: 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 1	Fe 1	0	0
2	D	1	Total 1	Fe 1	0	0
2	E	1	Total 1	Fe 1	0	0
2	F	1	Total 1	Fe 1	0	0
2	G	1	Total 1	Fe 1	0	0
2	H	1	Total 1	Fe 1	0	0
2	I	1	Total 1	Fe 1	0	0
2	J	1	Total 1	Fe 1	0	0
2	K	1	Total 1	Fe 1	0	0
2	L	1	Total 1	Fe 1	0	0
2	M	1	Total 1	Fe 1	0	0
2	N	1	Total 1	Fe 1	0	0
2	O	1	Total 1	Fe 1	0	0
2	P	1	Total 1	Fe 1	0	0

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

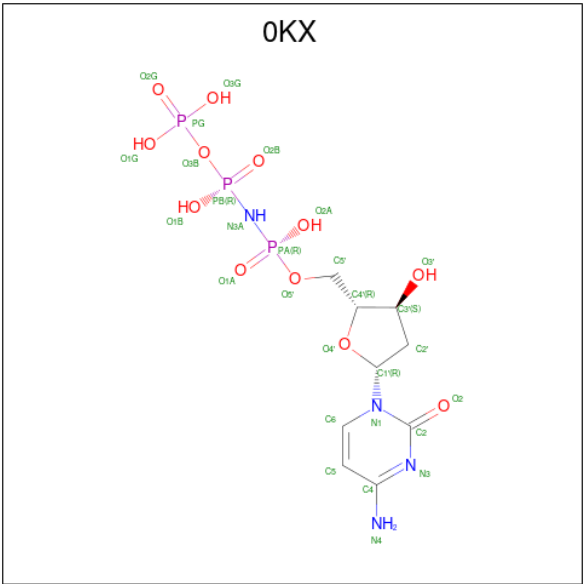
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	Mg 3	0	0
3	B	3	Total 3	Mg 3	0	0
3	C	3	Total 3	Mg 3	0	0
3	D	3	Total 3	Mg 3	0	0
3	E	2	Total 2	Mg 2	0	0

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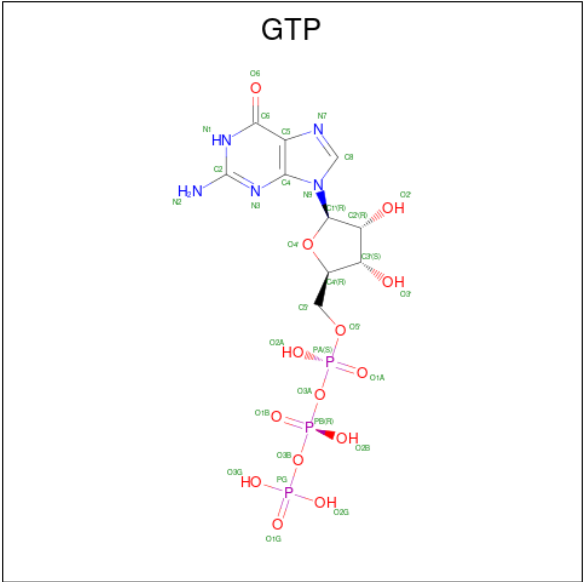
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	2	Total	Mg	0	0
			2	2		
3	G	3	Total	Mg	0	0
			3	3		
3	H	2	Total	Mg	0	0
			2	2		
3	I	3	Total	Mg	0	0
			3	3		
3	J	2	Total	Mg	0	0
			2	2		
3	K	3	Total	Mg	0	0
			3	3		
3	L	3	Total	Mg	0	0
			3	3		
3	M	3	Total	Mg	0	0
			3	3		
3	N	2	Total	Mg	0	0
			2	2		
3	O	2	Total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

- Molecule 4 is 2'-deoxy-5'-O-[(R)-hydroxy{[(R)-hydroxy(phosphonooxy)phosphoryl]amino}phosphoryl]cytidine (CCD ID: 0KX) (formula: C₉H₁₇N₄O₁₂P₃) (labeled as "Ligand of Interest" by depositor).



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

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



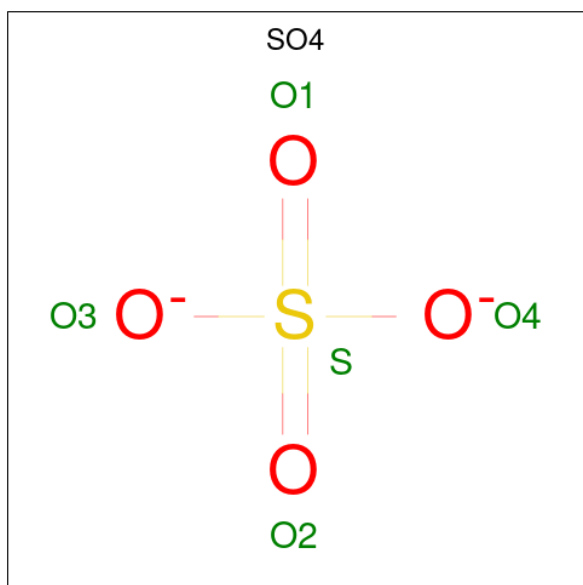
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	E	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	F	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	G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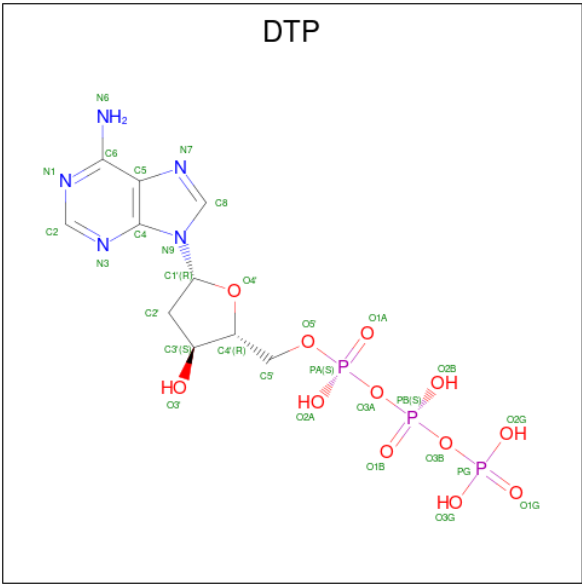
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	O	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	O	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 7 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃) (labeled as "Ligand of Interest" by depositor).



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

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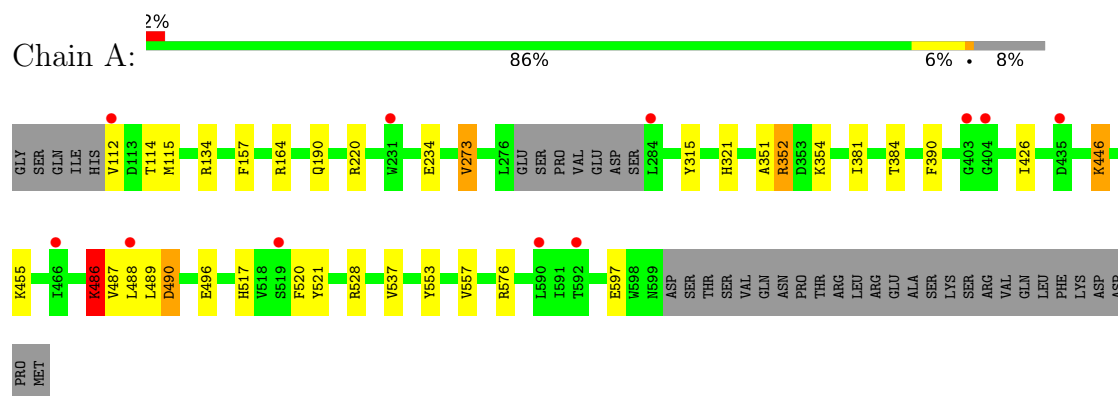
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	M	1	Total 30	C 10	N 5	O 12	P 3	0	0
7	N	1	Total 30	C 10	N 5	O 12	P 3	0	0
7	O	1	Total 30	C 10	N 5	O 12	P 3	0	0
7	P	1	Total 30	C 10	N 5	O 12	P 3	0	0

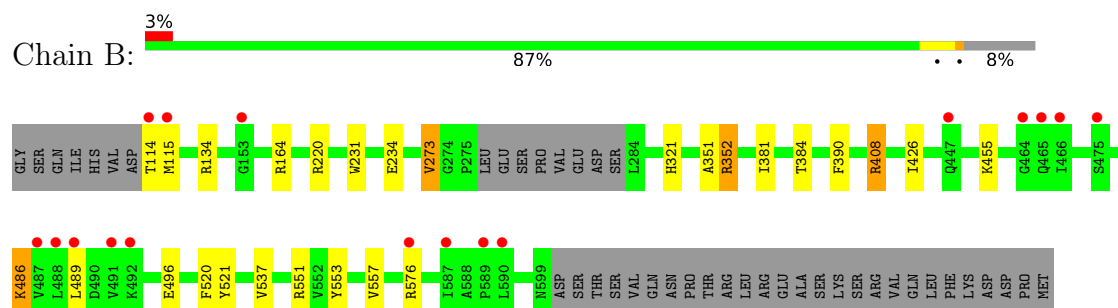
3 Residue-property plots [i](#)

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

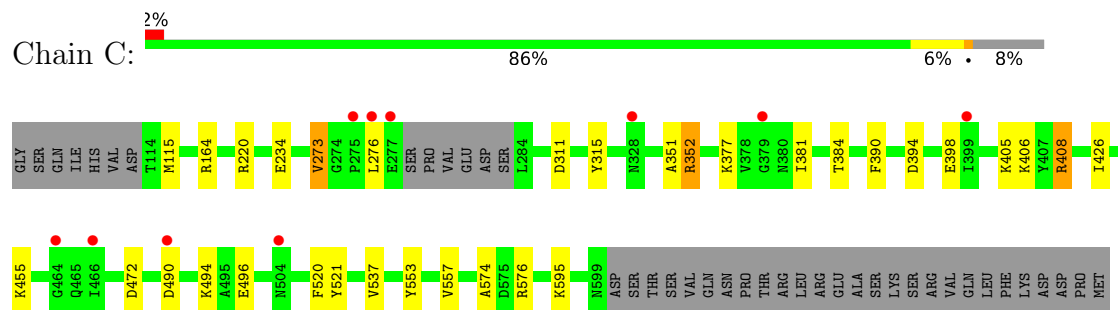
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



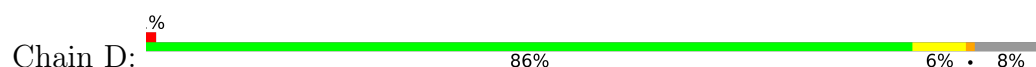
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

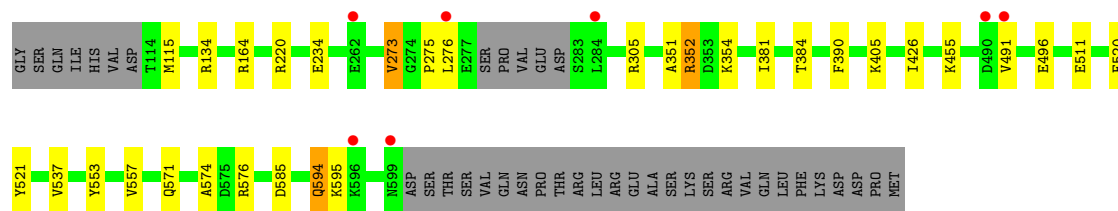


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

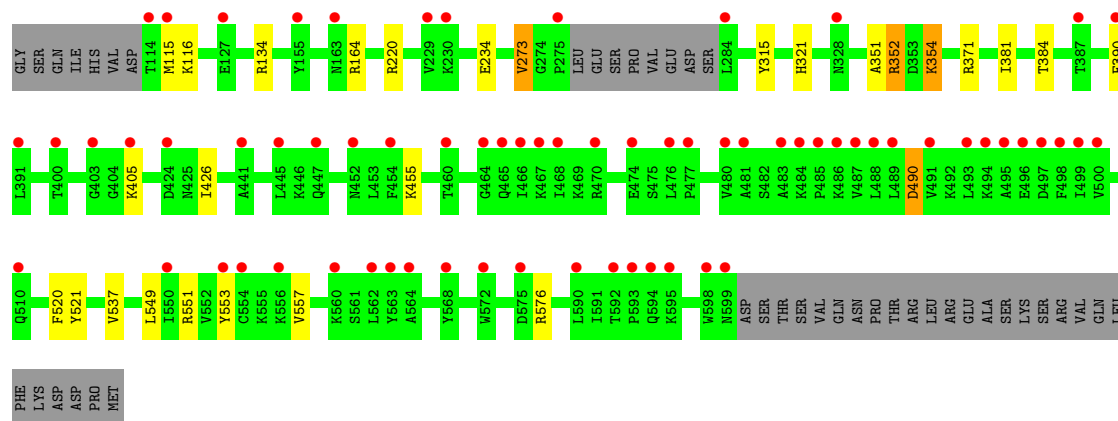
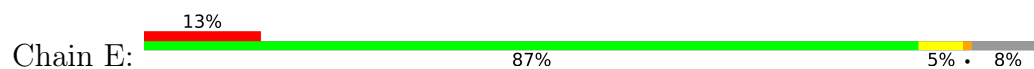


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

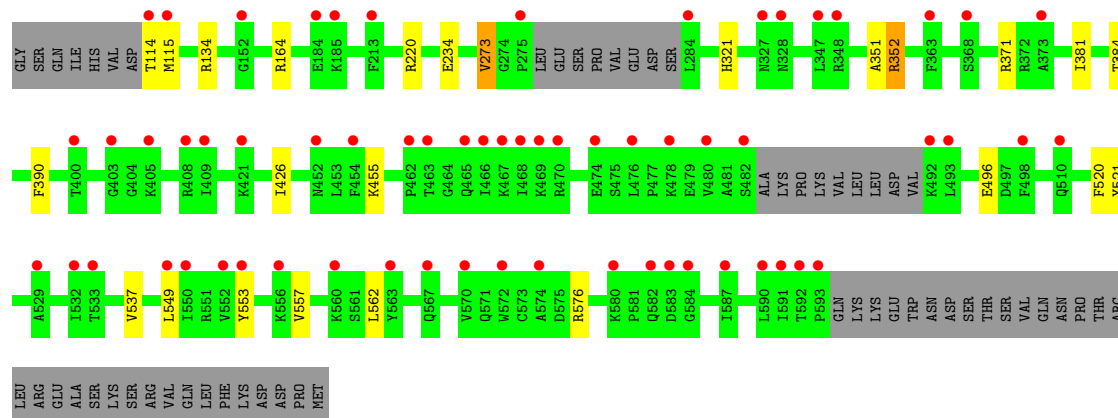
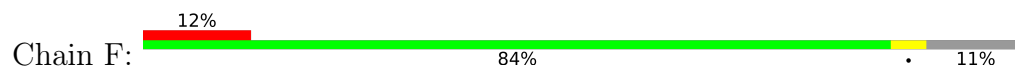




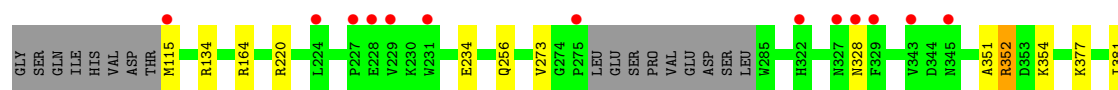
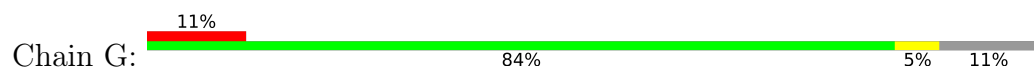
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

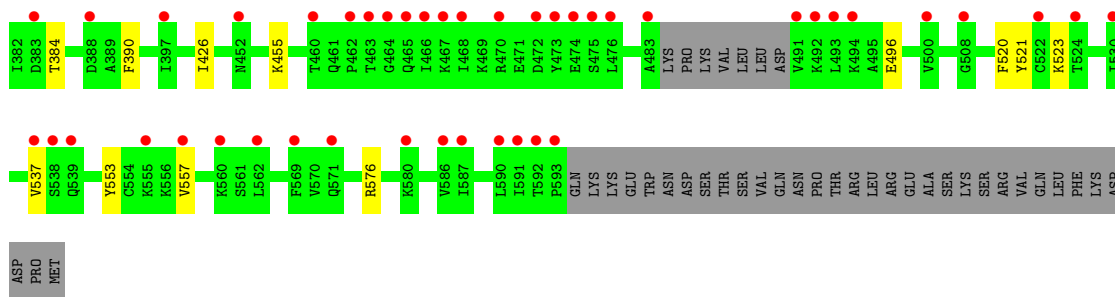


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

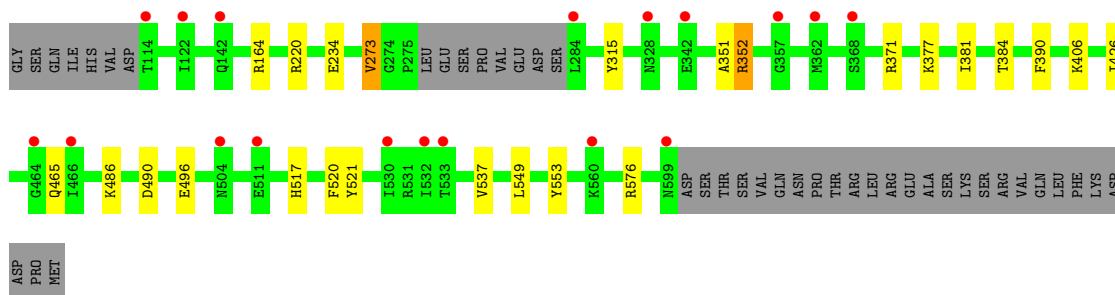
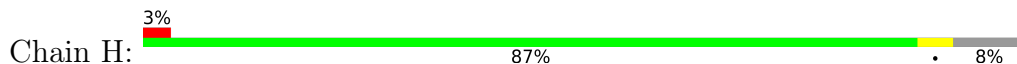


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

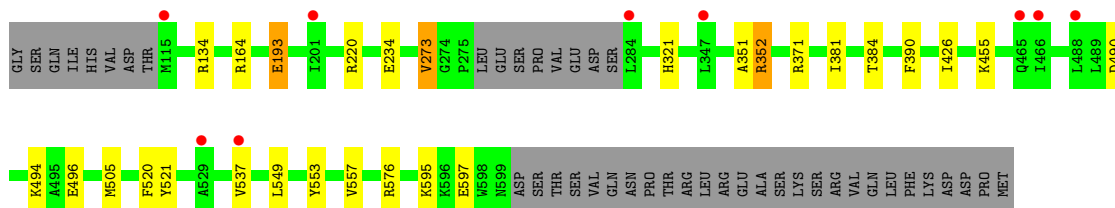
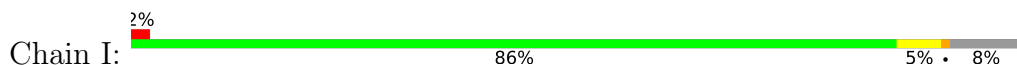




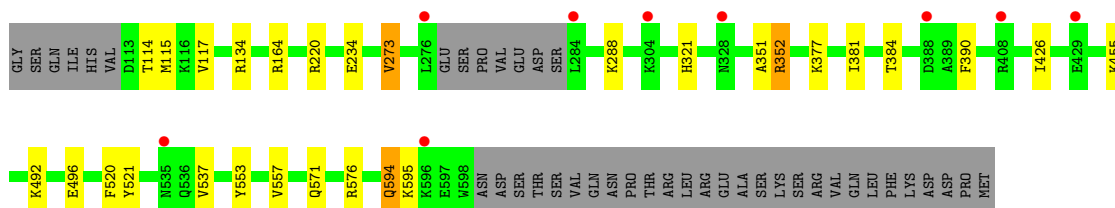
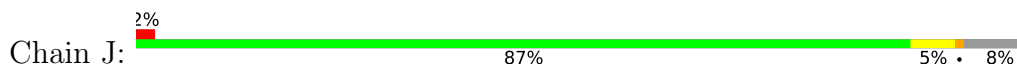
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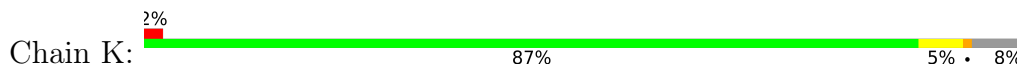
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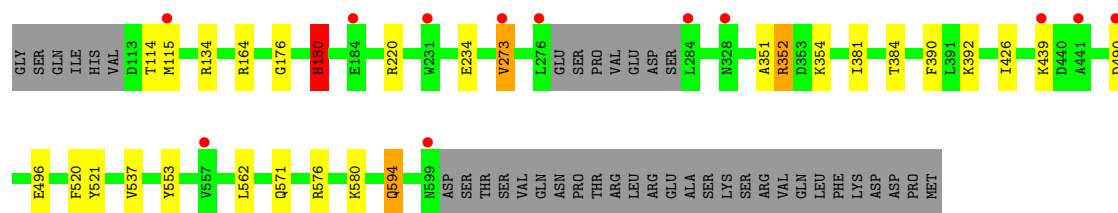


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

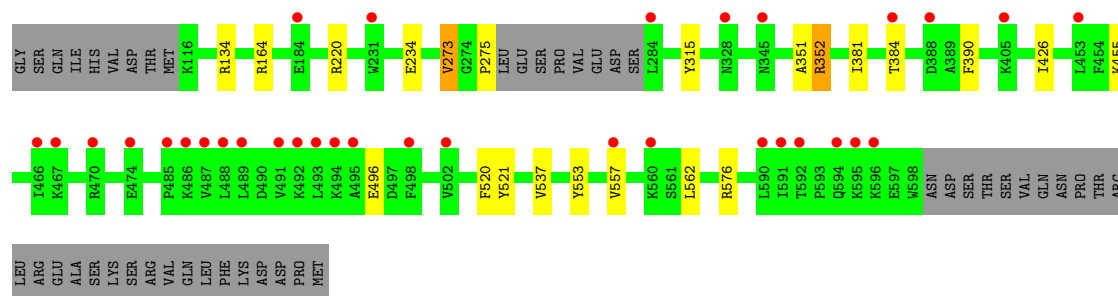
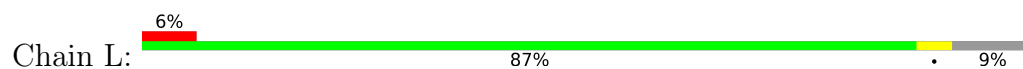


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

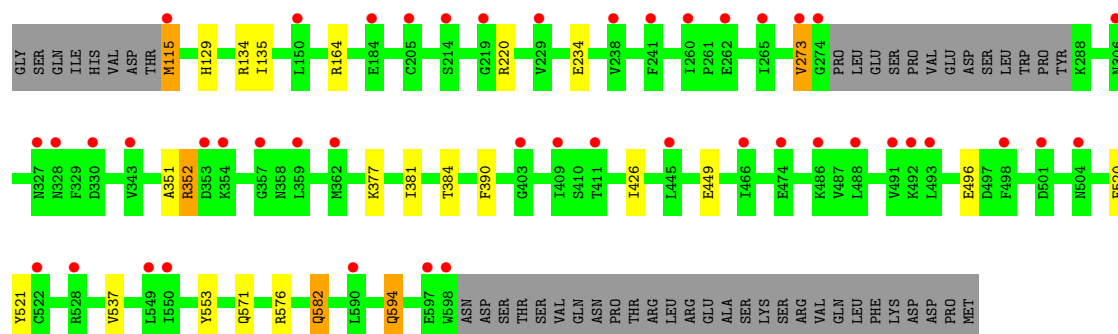
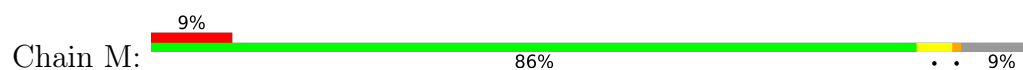




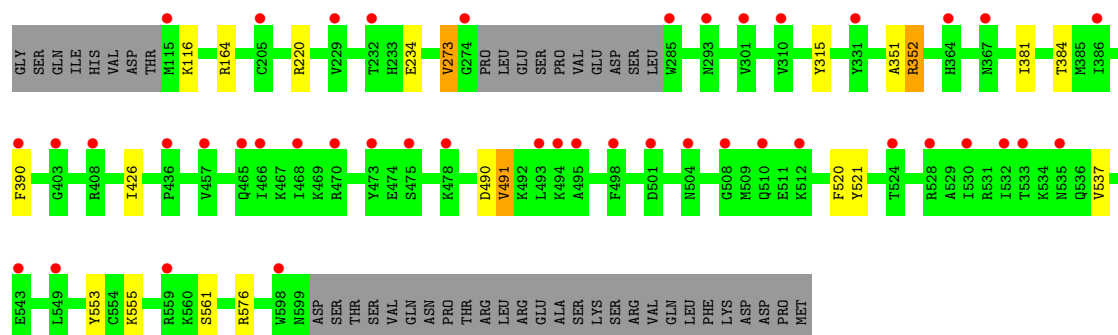
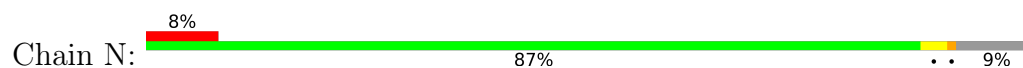
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.11Å 175.24Å 277.27Å 90.00° 94.81° 90.00°	Depositor
Resolution (Å)	276.29 – 2.84 276.29 – 2.84	Depositor EDS
% Data completeness (in resolution range)	72.7 (276.29-2.84) 72.7 (276.29-2.84)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.228 , 0.249 0.227 , 0.247	Depositor DCC
R_{free} test set	8050 reflections (3.55%)	wwPDB-VP
Wilson B-factor (Å ²)	46.2	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	61950	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.94	5/3933 (0.1%)	1.03	11/5335 (0.2%)
1	B	0.92	3/3918 (0.1%)	1.02	8/5310 (0.2%)
1	C	0.90	0/3947	0.99	7/5346 (0.1%)
1	D	0.91	3/3939 (0.1%)	1.00	6/5339 (0.1%)
1	E	0.84	0/3892	0.99	10/5282 (0.2%)
1	F	0.83	0/3784	0.96	6/5129 (0.1%)
1	G	0.82	2/3757 (0.1%)	0.98	6/5099 (0.1%)
1	H	0.85	1/3938 (0.0%)	0.98	5/5333 (0.1%)
1	I	0.84	0/3915	0.97	6/5306 (0.1%)
1	J	0.89	3/3930 (0.1%)	1.00	5/5327 (0.1%)
1	K	0.87	1/3932 (0.0%)	1.00	9/5333 (0.2%)
1	L	0.84	3/3849 (0.1%)	0.98	5/5230 (0.1%)
1	M	0.85	0/3792	0.98	7/5151 (0.1%)
1	N	0.85	3/3849 (0.1%)	0.99	7/5229 (0.1%)
1	O	0.85	0/3769	1.00	11/5116 (0.2%)
1	P	0.84	3/3729 (0.1%)	0.99	7/5064 (0.1%)
All	All	0.87	27/61873 (0.0%)	0.99	116/83929 (0.1%)

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

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

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	489	LEU	C-O	-10.78	1.10	1.24
1	L	275	PRO	C-O	-6.53	1.10	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	486	LYS	C-O	-6.34	1.16	1.24
1	J	164	ARG	CZ-NH2	-6.29	1.25	1.33
1	A	487	VAL	CA-C	6.20	1.60	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	115	MET	CG-SD-CE	11.61	126.44	100.90
1	J	164	ARG	NE-CZ-NH1	10.47	131.97	121.50
1	D	164	ARG	NE-CZ-NH1	10.44	131.94	121.50
1	N	164	ARG	NE-CZ-NH1	10.28	131.78	121.50
1	P	164	ARG	NE-CZ-NH1	10.25	131.75	121.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	486	LYS	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3840	0	3707	17	0
1	B	3825	0	3715	10	0
1	C	3854	0	3758	17	1
1	D	3846	0	3732	16	0
1	E	3799	0	3656	14	0
1	F	3695	0	3560	12	0
1	G	3668	0	3505	14	0
1	H	3845	0	3751	15	0
1	I	3822	0	3705	14	0
1	J	3837	0	3723	15	0
1	K	3839	0	3704	13	0
1	L	3756	0	3583	11	0
1	M	3704	0	3524	12	0
1	N	3757	0	3573	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	3680	0	3508	13	0
1	P	3640	0	3463	14	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	3	0	0	0	0
3	H	2	0	0	0	0
3	I	3	0	0	0	0
3	J	2	0	0	0	0
3	K	3	0	0	0	0
3	L	3	0	0	0	0
3	M	3	0	0	0	0
3	N	2	0	0	0	0
3	O	2	0	0	0	0
3	P	3	0	0	0	0
4	A	28	0	16	1	0
4	B	28	0	16	1	0
4	C	28	0	16	2	0
4	D	28	0	17	1	0
4	E	28	0	17	1	0
4	F	28	0	17	0	0
4	G	28	0	16	0	0
4	H	28	0	16	1	0

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	K	30	0	12	3	0
7	L	30	0	12	0	0
7	M	30	0	12	4	0
7	N	30	0	12	1	0
7	O	30	0	12	2	0
7	P	30	0	12	2	0
All	All	61950	0	58812	220	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 220 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:352:ARG:NH1	7:N:706:DTP:O3G	2.20	0.71
1:M:352:ARG:NH1	7:M:708:DTP:O3G	2.21	0.70
7:E:706:DTP:O2G	5:G:707:GTP:O1B	2.13	0.67
1:I:595:LYS:HZ2	1:I:597:GLU:HG2	1.61	0.65
7:M:708:DTP:O1B	5:O:706:GTP:H5"	1.97	0.64

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

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	477/520 (92%)	463 (97%)	13 (3%)	1 (0%)	43 62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	474/520 (91%)	459 (97%)	14 (3%)	1 (0%)	43	62
1	C	476/520 (92%)	462 (97%)	14 (3%)	0	100	100
1	D	477/520 (92%)	462 (97%)	15 (3%)	0	100	100
1	E	474/520 (91%)	457 (96%)	17 (4%)	0	100	100
1	F	457/520 (88%)	443 (97%)	14 (3%)	0	100	100
1	G	457/520 (88%)	442 (97%)	15 (3%)	0	100	100
1	H	474/520 (91%)	458 (97%)	16 (3%)	0	100	100
1	I	473/520 (91%)	460 (97%)	13 (3%)	0	100	100
1	J	475/520 (91%)	459 (97%)	16 (3%)	0	100	100
1	K	476/520 (92%)	460 (97%)	16 (3%)	0	100	100
1	L	471/520 (91%)	455 (97%)	16 (3%)	0	100	100
1	M	467/520 (90%)	453 (97%)	14 (3%)	0	100	100
1	N	471/520 (91%)	457 (97%)	14 (3%)	0	100	100
1	O	459/520 (88%)	441 (96%)	17 (4%)	1 (0%)	43	62
1	P	455/520 (88%)	441 (97%)	14 (3%)	0	100	100
All	All	7513/8320 (90%)	7272 (97%)	238 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	406/464 (88%)	397 (98%)	9 (2%)	45	69
1	B	404/464 (87%)	397 (98%)	7 (2%)	53	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	409/464 (88%)	401 (98%)	8 (2%)	48	72
1	D	407/464 (88%)	399 (98%)	8 (2%)	48	72
1	E	398/464 (86%)	392 (98%)	6 (2%)	57	77
1	F	390/464 (84%)	384 (98%)	6 (2%)	57	77
1	G	384/464 (83%)	380 (99%)	4 (1%)	68	83
1	H	409/464 (88%)	403 (98%)	6 (2%)	57	77
1	I	404/464 (87%)	397 (98%)	7 (2%)	53	75
1	J	406/464 (88%)	399 (98%)	7 (2%)	53	75
1	K	406/464 (88%)	397 (98%)	9 (2%)	45	69
1	L	391/464 (84%)	386 (99%)	5 (1%)	61	79
1	M	384/464 (83%)	376 (98%)	8 (2%)	47	70
1	N	391/464 (84%)	387 (99%)	4 (1%)	68	83
1	O	385/464 (83%)	379 (98%)	6 (2%)	55	76
1	P	380/464 (82%)	375 (99%)	5 (1%)	61	79
All	All	6354/7424 (86%)	6249 (98%)	105 (2%)	53	75

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	490	ASP
1	K	392	LYS
1	O	582	GLN
1	I	496	GLU
1	J	496	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 138 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	370	HIS
1	N	539	GLN
1	P	235	GLN
1	F	271	GLN
1	F	235	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	OKX	C	706	3	28,29,29	1.13	3 (10%)	39,45,45	1.48	3 (7%)
4	OKX	L	706	3,2	28,29,29	1.52	3 (10%)	39,45,45	1.79	9 (23%)
5	GTP	A	706	3	33,34,34	1.49	6 (18%)	50,54,54	2.06	16 (32%)
5	GTP	F	705	3	33,34,34	1.34	3 (9%)	50,54,54	1.79	11 (22%)
4	OKX	K	706	3,2	28,29,29	1.22	3 (10%)	39,45,45	1.81	7 (17%)
4	OKX	H	705	3,2	28,29,29	1.02	3 (10%)	39,45,45	1.35	5 (12%)
4	OKX	E	704	3,2	28,29,29	1.42	4 (14%)	39,45,45	1.28	3 (7%)
4	OKX	I	705	3,2	28,29,29	1.08	3 (10%)	39,45,45	1.76	6 (15%)
7	DTP	B	708	3	31,32,32	1.70	6 (19%)	46,50,50	1.97	15 (32%)
4	OKX	B	705	3,2	28,29,29	1.51	5 (17%)	39,45,45	2.05	10 (25%)
5	GTP	M	706	3	33,34,34	1.27	5 (15%)	50,54,54	2.03	12 (24%)
6	SO4	A	707	-	4,4,4	0.55	0	6,6,6	0.99	1 (16%)
7	DTP	L	701	3	31,32,32	1.63	7 (22%)	46,50,50	2.75	16 (34%)
7	DTP	A	708	3	31,32,32	1.74	8 (25%)	46,50,50	1.97	15 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	C	708	-	4,4,4	0.77	0	6,6,6	0.41	0
4	OKX	A	705	3,2	28,29,29	1.08	3 (10%)	39,45,45	1.46	5 (12%)
5	GTP	N	705	3	33,34,34	1.56	7 (21%)	50,54,54	1.98	16 (32%)
7	DTP	H	701	3	31,32,32	1.88	10 (32%)	46,50,50	1.86	11 (23%)
4	OKX	F	704	3,2	28,29,29	1.10	3 (10%)	39,45,45	1.73	4 (10%)
7	DTP	D	701	3	31,32,32	1.80	7 (22%)	46,50,50	1.97	12 (26%)
6	SO4	H	707	-	4,4,4	0.53	0	6,6,6	0.49	0
6	SO4	D	708	-	4,4,4	0.60	0	6,6,6	0.27	0
7	DTP	E	706	3	31,32,32	1.99	7 (22%)	46,50,50	2.03	13 (28%)
4	OKX	O	705	3,2	28,29,29	1.17	4 (14%)	39,45,45	1.36	4 (10%)
6	SO4	I	707	-	4,4,4	0.51	0	6,6,6	0.74	0
5	GTP	O	707	3	33,34,34	1.27	4 (12%)	50,54,54	1.78	12 (24%)
7	DTP	F	706	3	31,32,32	1.57	5 (16%)	46,50,50	2.27	17 (36%)
5	GTP	H	706	3	33,34,34	1.55	5 (15%)	50,54,54	1.88	10 (20%)
7	DTP	O	701	3	31,32,32	1.64	6 (19%)	46,50,50	2.32	16 (34%)
7	DTP	I	708	3	31,32,32	1.36	4 (12%)	46,50,50	1.94	14 (30%)
5	GTP	B	706	3	33,34,34	1.39	5 (15%)	50,54,54	1.94	13 (26%)
5	GTP	C	707	3	33,34,34	1.31	5 (15%)	50,54,54	1.68	9 (18%)
7	DTP	P	701	3	31,32,32	2.14	9 (29%)	46,50,50	1.93	14 (30%)
6	SO4	B	707	-	4,4,4	0.66	0	6,6,6	0.86	0
7	DTP	C	701	3	31,32,32	1.27	3 (9%)	46,50,50	2.46	20 (43%)
6	SO4	J	706	-	4,4,4	0.71	0	6,6,6	0.47	0
5	GTP	D	707	3	33,34,34	1.67	8 (24%)	50,54,54	1.89	12 (24%)
4	OKX	M	705	3,2	28,29,29	1.20	3 (10%)	39,45,45	1.63	6 (15%)
5	GTP	G	707	3	33,34,34	1.37	5 (15%)	50,54,54	1.37	8 (16%)
4	OKX	P	706	3,2	28,29,29	1.46	4 (14%)	39,45,45	1.36	4 (10%)
4	OKX	J	704	3,2	28,29,29	1.26	3 (10%)	39,45,45	1.50	6 (15%)
5	GTP	K	707	3	33,34,34	1.29	6 (18%)	50,54,54	1.93	13 (26%)
5	GTP	L	707	3	33,34,34	1.44	5 (15%)	50,54,54	1.68	12 (24%)
7	DTP	K	701	3	31,32,32	1.60	7 (22%)	46,50,50	2.08	13 (28%)
5	GTP	E	705	3	33,34,34	1.34	5 (15%)	50,54,54	1.87	11 (22%)
5	GTP	O	706	3	33,34,34	1.14	2 (6%)	50,54,54	1.93	10 (20%)
6	SO4	M	707	-	4,4,4	0.56	0	6,6,6	0.21	0
7	DTP	N	706	3	31,32,32	1.84	7 (22%)	46,50,50	1.85	10 (21%)
7	DTP	G	701	3	31,32,32	1.70	7 (22%)	46,50,50	1.98	12 (26%)
7	DTP	M	708	3	31,32,32	2.21	7 (22%)	46,50,50	1.72	9 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	L	708	-	4,4,4	0.70	0	6,6,6	0.71	0
4	OKX	N	704	3,2	28,29,29	1.21	3 (10%)	39,45,45	1.43	4 (10%)
7	DTP	J	707	3	31,32,32	1.62	6 (19%)	46,50,50	2.30	14 (30%)
4	OKX	D	706	3,2	28,29,29	1.47	4 (14%)	39,45,45	1.79	7 (17%)
5	GTP	I	706	3	33,34,34	1.40	7 (21%)	50,54,54	1.83	11 (22%)
4	OKX	G	706	3,2	28,29,29	1.34	3 (10%)	39,45,45	1.85	6 (15%)
5	GTP	J	705	3	33,34,34	1.56	5 (15%)	50,54,54	1.88	14 (28%)

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
4	OKX	C	706	3	-	1/19/34/34	0/2/2/2
4	OKX	L	706	3,2	-	4/19/34/34	0/2/2/2
5	GTP	A	706	3	-	1/22/38/38	0/3/3/3
5	GTP	F	705	3	-	0/22/38/38	0/3/3/3
4	OKX	K	706	3,2	-	1/19/34/34	0/2/2/2
4	OKX	H	705	3,2	-	2/19/34/34	0/2/2/2
4	OKX	E	704	3,2	-	4/19/34/34	0/2/2/2
4	OKX	I	705	3,2	-	2/19/34/34	0/2/2/2
7	DTP	B	708	3	-	2/22/34/34	0/3/3/3
4	OKX	B	705	3,2	-	6/19/34/34	0/2/2/2
5	GTP	M	706	3	-	2/22/38/38	0/3/3/3
7	DTP	L	701	3	-	3/22/34/34	0/3/3/3
7	DTP	A	708	3	-	5/22/34/34	0/3/3/3
4	OKX	A	705	3,2	-	1/19/34/34	0/2/2/2
5	GTP	N	705	3	-	4/22/38/38	0/3/3/3
7	DTP	H	701	3	-	6/22/34/34	0/3/3/3
4	OKX	F	704	3,2	-	4/19/34/34	0/2/2/2
7	DTP	D	701	3	-	4/22/34/34	0/3/3/3
7	DTP	E	706	3	-	2/22/34/34	0/3/3/3
4	OKX	O	705	3,2	-	1/19/34/34	0/2/2/2
5	GTP	O	707	3	-	2/22/38/38	0/3/3/3
7	DTP	F	706	3	-	1/22/34/34	0/3/3/3
5	GTP	H	706	3	-	1/22/38/38	0/3/3/3
7	DTP	O	701	3	-	5/22/34/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	DTP	I	708	3	-	5/22/34/34	0/3/3/3
5	GTP	B	706	3	-	4/22/38/38	0/3/3/3
5	GTP	C	707	3	-	4/22/38/38	0/3/3/3
7	DTP	P	701	3	-	1/22/34/34	0/3/3/3
7	DTP	C	701	3	-	3/22/34/34	0/3/3/3
5	GTP	D	707	3	-	2/22/38/38	0/3/3/3
4	OKX	M	705	3,2	-	1/19/34/34	0/2/2/2
5	GTP	G	707	3	-	3/22/38/38	0/3/3/3
4	OKX	P	706	3,2	-	6/19/34/34	0/2/2/2
4	OKX	J	704	3,2	-	2/19/34/34	0/2/2/2
5	GTP	K	707	3	-	2/22/38/38	0/3/3/3
5	GTP	L	707	3	-	3/22/38/38	0/3/3/3
7	DTP	K	701	3	-	0/22/34/34	0/3/3/3
5	GTP	E	705	3	-	3/22/38/38	0/3/3/3
5	GTP	O	706	3	-	3/22/38/38	0/3/3/3
7	DTP	N	706	3	-	3/22/34/34	0/3/3/3
7	DTP	G	701	3	-	3/22/34/34	0/3/3/3
7	DTP	M	708	3	-	2/22/34/34	0/3/3/3
4	OKX	N	704	3,2	-	2/19/34/34	0/2/2/2
7	DTP	J	707	3	-	4/22/34/34	0/3/3/3
4	OKX	D	706	3,2	-	4/19/34/34	0/2/2/2
5	GTP	I	706	3	-	4/22/38/38	0/3/3/3
4	OKX	G	706	3,2	-	7/19/34/34	0/2/2/2
5	GTP	J	705	3	-	1/22/38/38	0/3/3/3

The worst 5 of 243 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	P	701	DTP	PB-O3B	6.56	1.66	1.59
7	M	708	DTP	PB-O3A	5.54	1.65	1.59
4	B	705	OKX	PB-O2B	5.46	1.54	1.46
5	J	705	GTP	C6-N1	-5.26	1.29	1.38
4	L	706	OKX	PB-O2B	5.18	1.54	1.46

The worst 5 of 501 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	701	DTP	C5-C4-N3	-7.41	116.52	126.72
7	L	701	DTP	C4-C5-N7	-7.21	102.34	110.58
4	I	705	0KX	O2B-PB-N3A	-7.11	101.30	111.77
7	K	701	DTP	C5-C4-N3	-6.87	117.25	126.72
7	E	706	DTP	C5-C4-N3	-6.73	117.45	126.72

There are no chirality outliers.

5 of 136 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	705	0KX	PG-O3B-PB-O1B
4	B	705	0KX	PB-O3B-PG-O1G
4	B	705	0KX	PG-O3B-PB-O1B
4	B	705	0KX	PA-N3A-PB-O2B
4	B	705	0KX	PB-N3A-PA-O1A

There are no ring outliers.

32 monomers are involved in 46 short contacts:

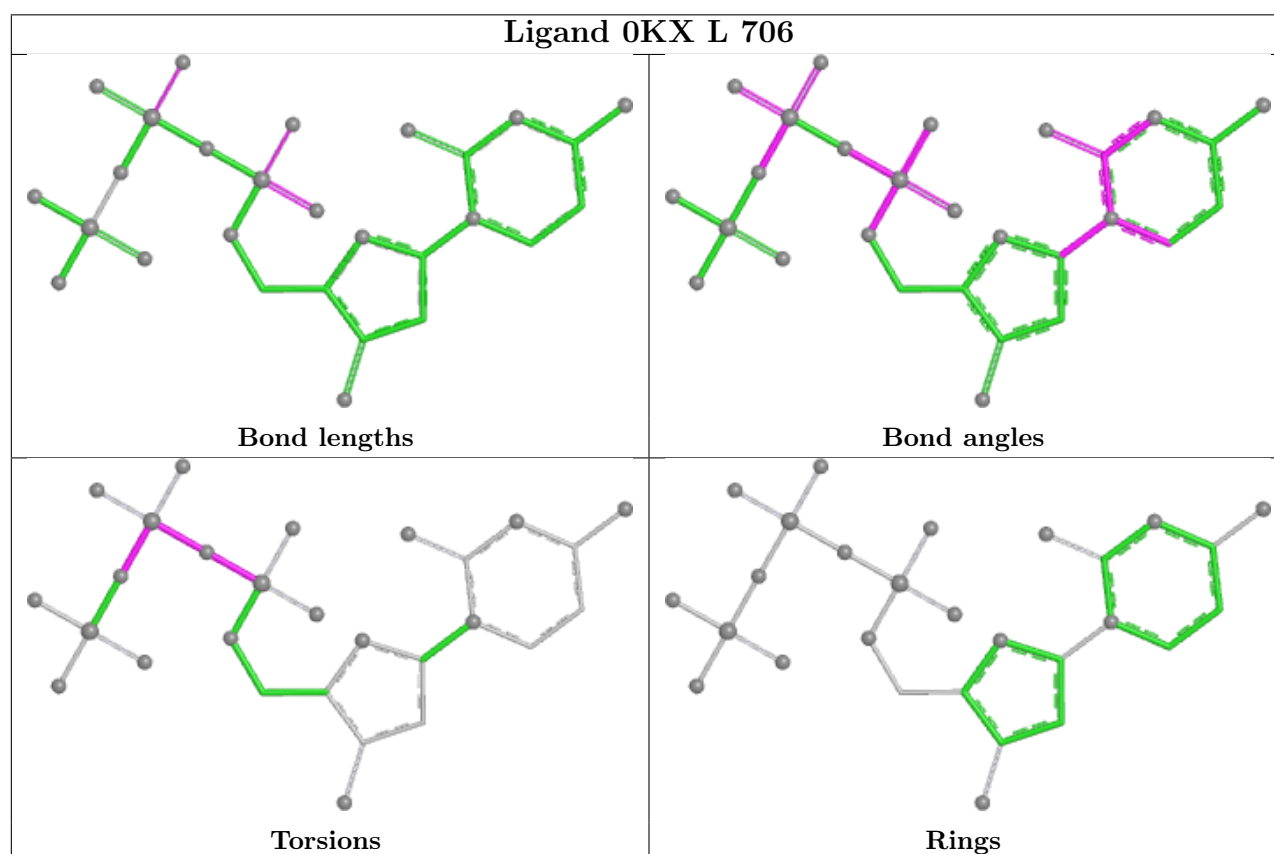
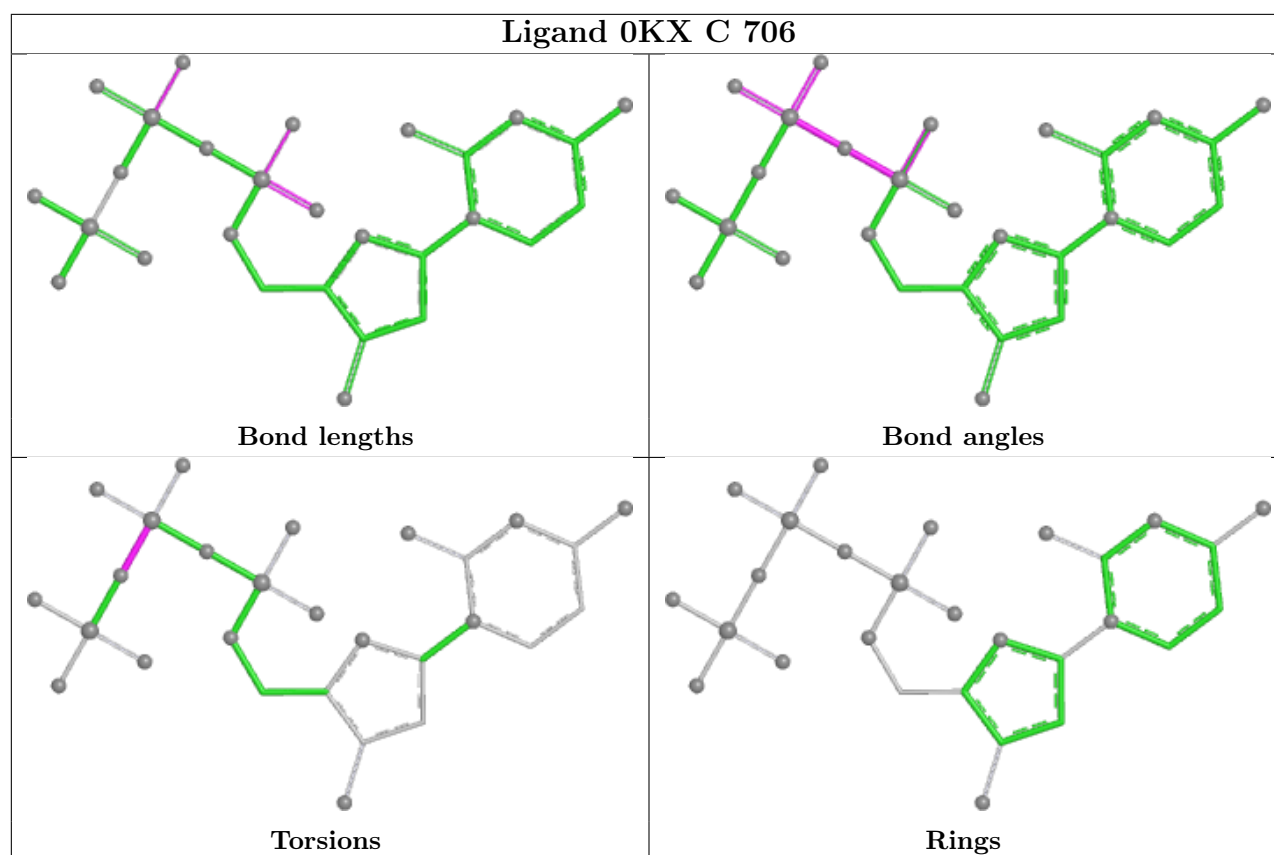
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	706	0KX	2	0
4	L	706	0KX	2	0
5	F	705	GTP	1	0
4	H	705	0KX	1	0
4	E	704	0KX	1	0
7	B	708	DTP	2	0
4	B	705	0KX	1	0
6	A	707	SO4	1	0
7	A	708	DTP	1	0
4	A	705	0KX	1	0
5	N	705	GTP	1	0
7	H	701	DTP	2	0
7	D	701	DTP	2	0
6	H	707	SO4	1	0
6	D	708	SO4	1	0
7	E	706	DTP	3	0
5	O	707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

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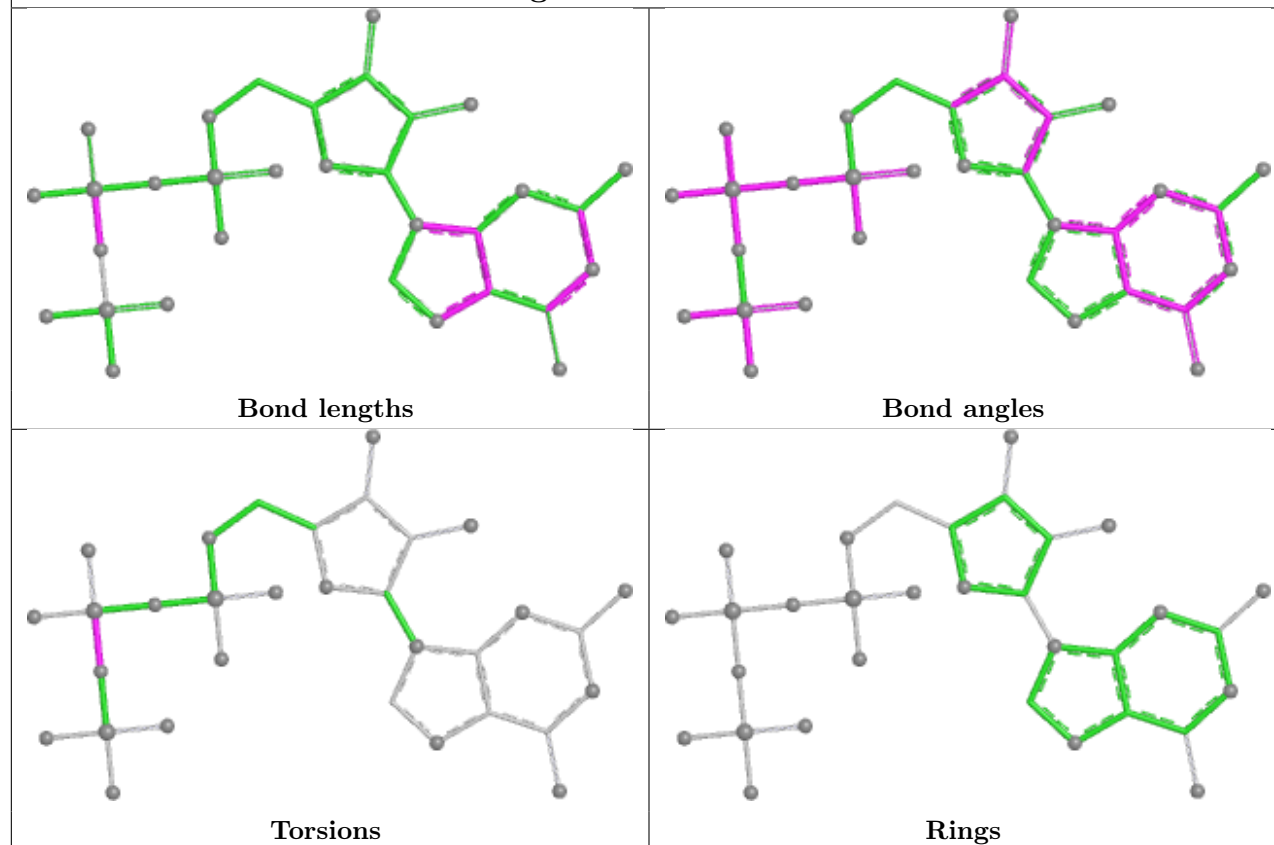
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	K	701	DTP	3	0
5	E	705	GTP	1	0
5	O	706	GTP	1	0
7	N	706	DTP	1	0
7	G	701	DTP	3	0
7	M	708	DTP	4	0
4	N	704	OKX	2	0
7	J	707	DTP	1	0
4	D	706	OKX	1	0
5	J	705	GTP	1	0

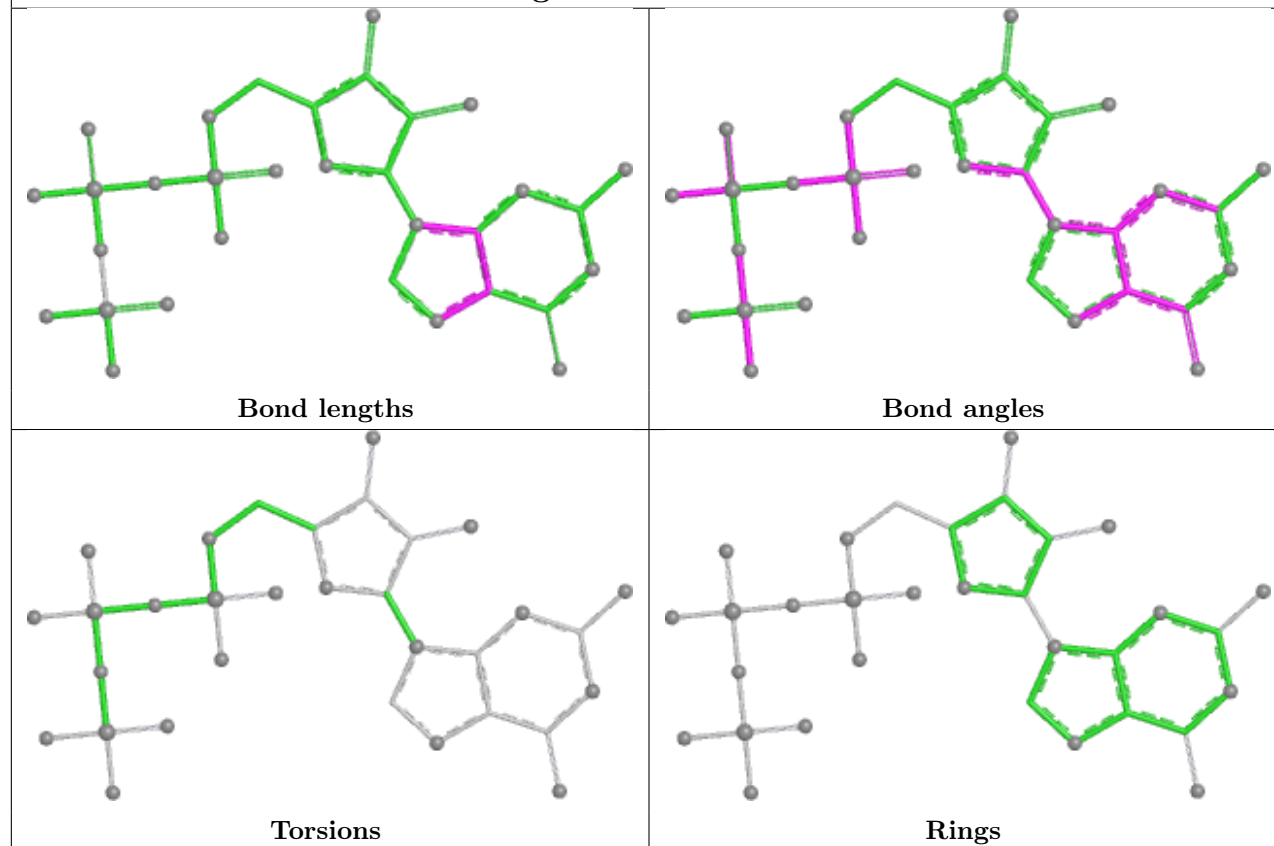
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



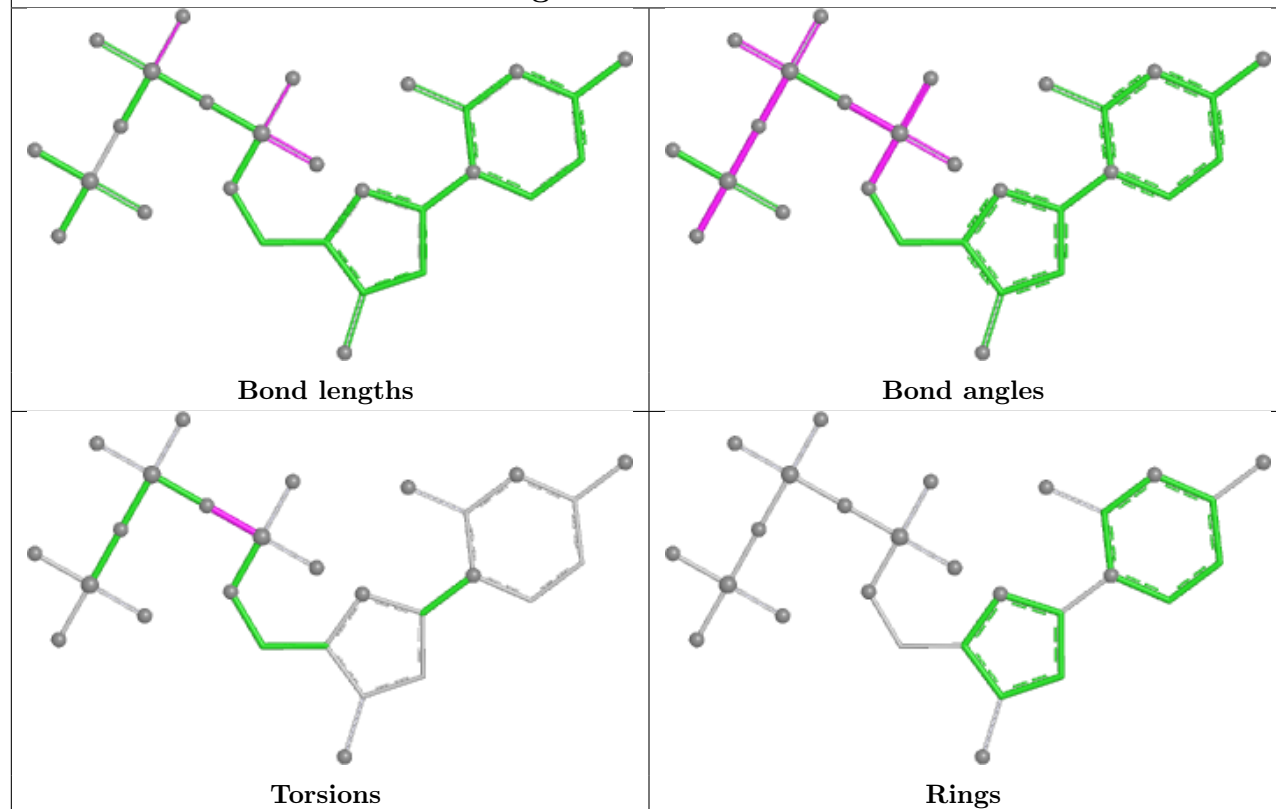
Ligand GTP A 706



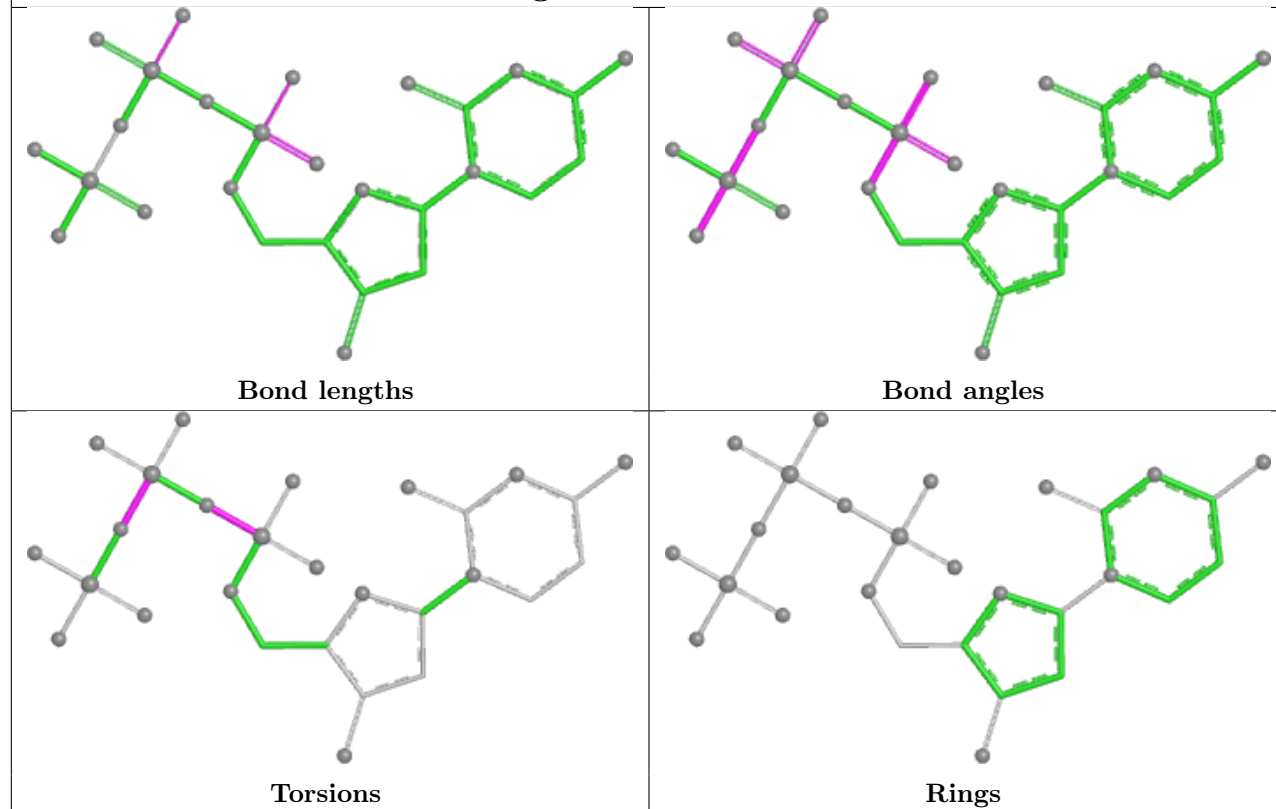
Ligand GTP F 705



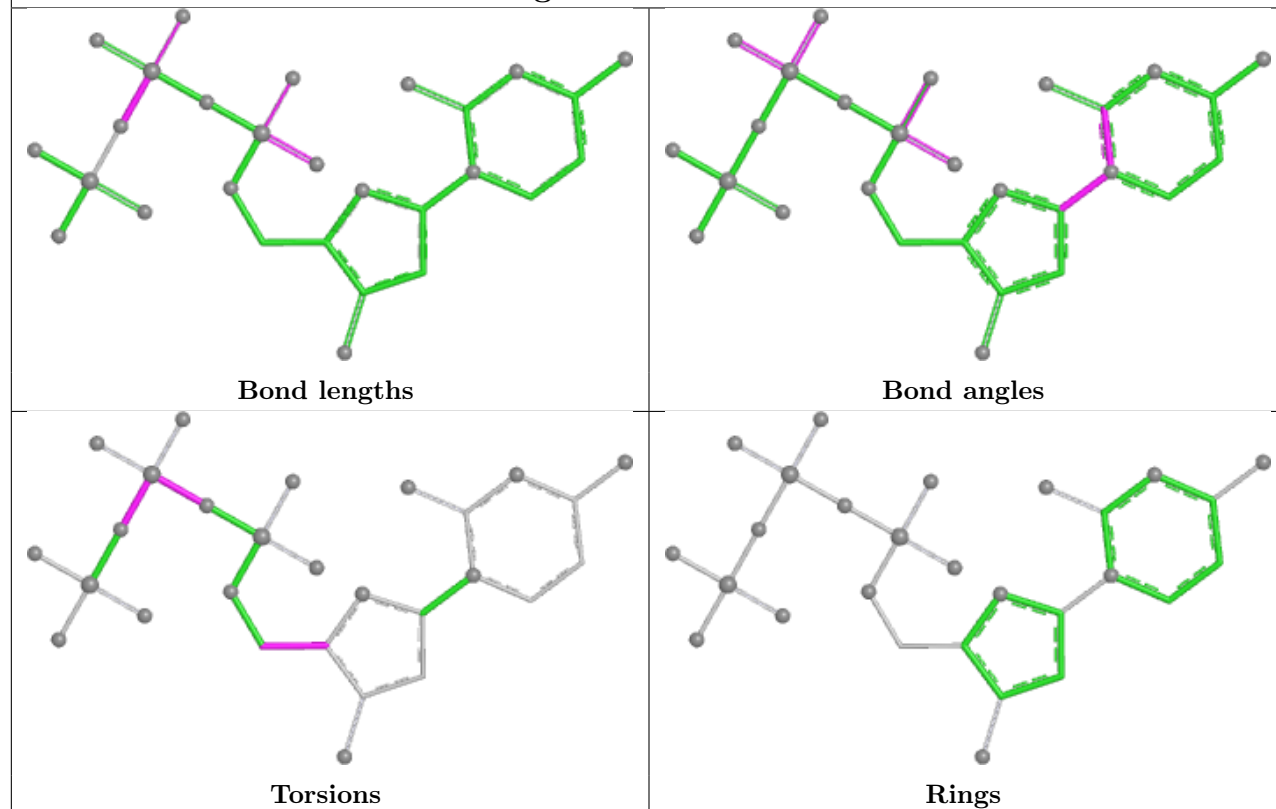
Ligand 0KX K 706



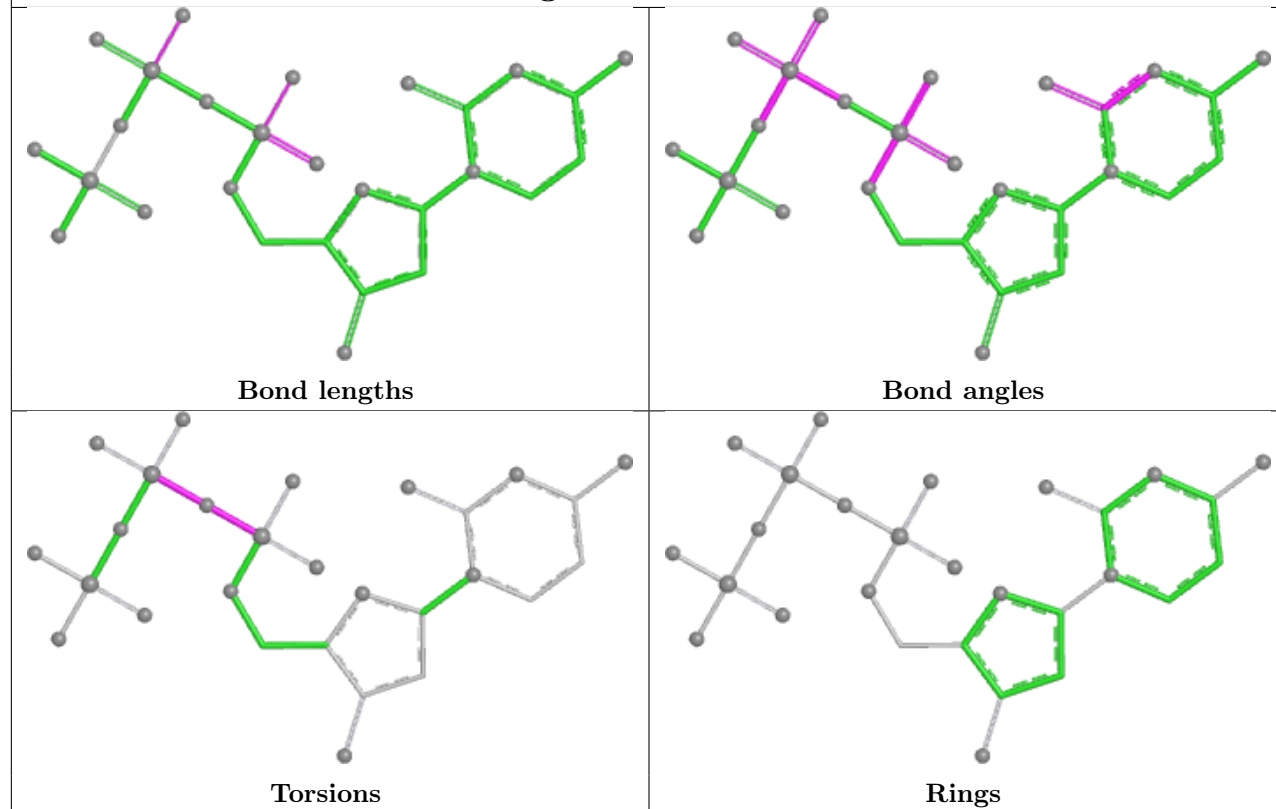
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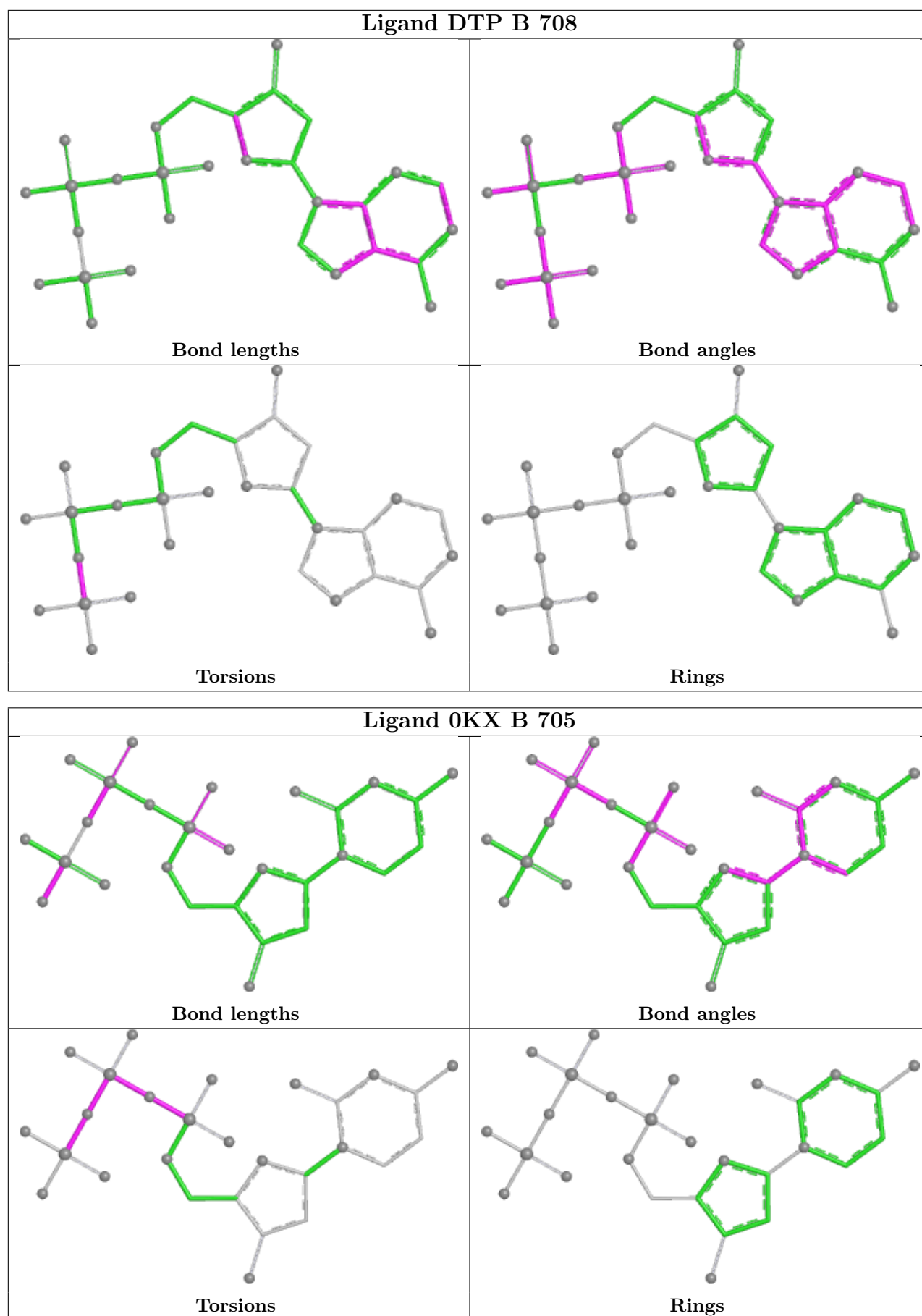


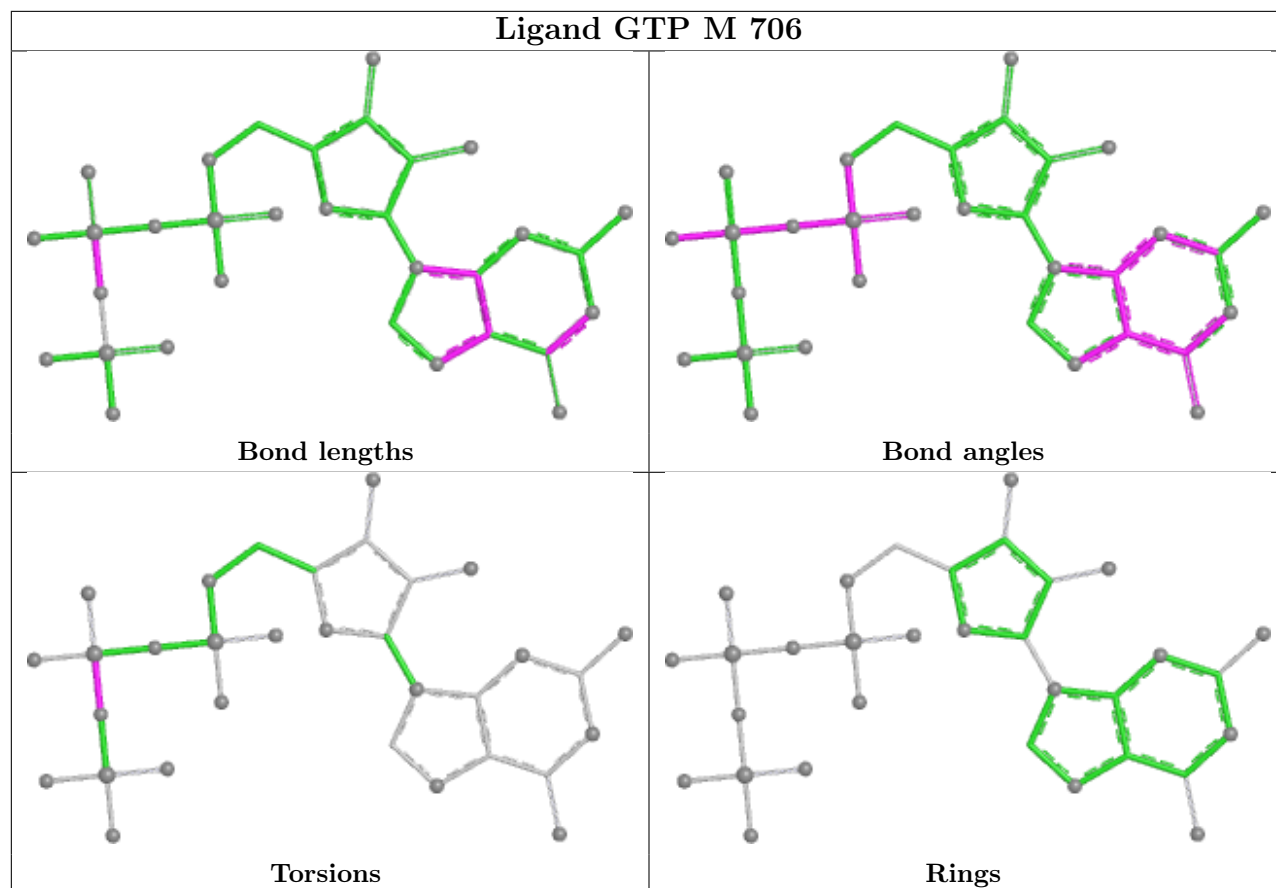
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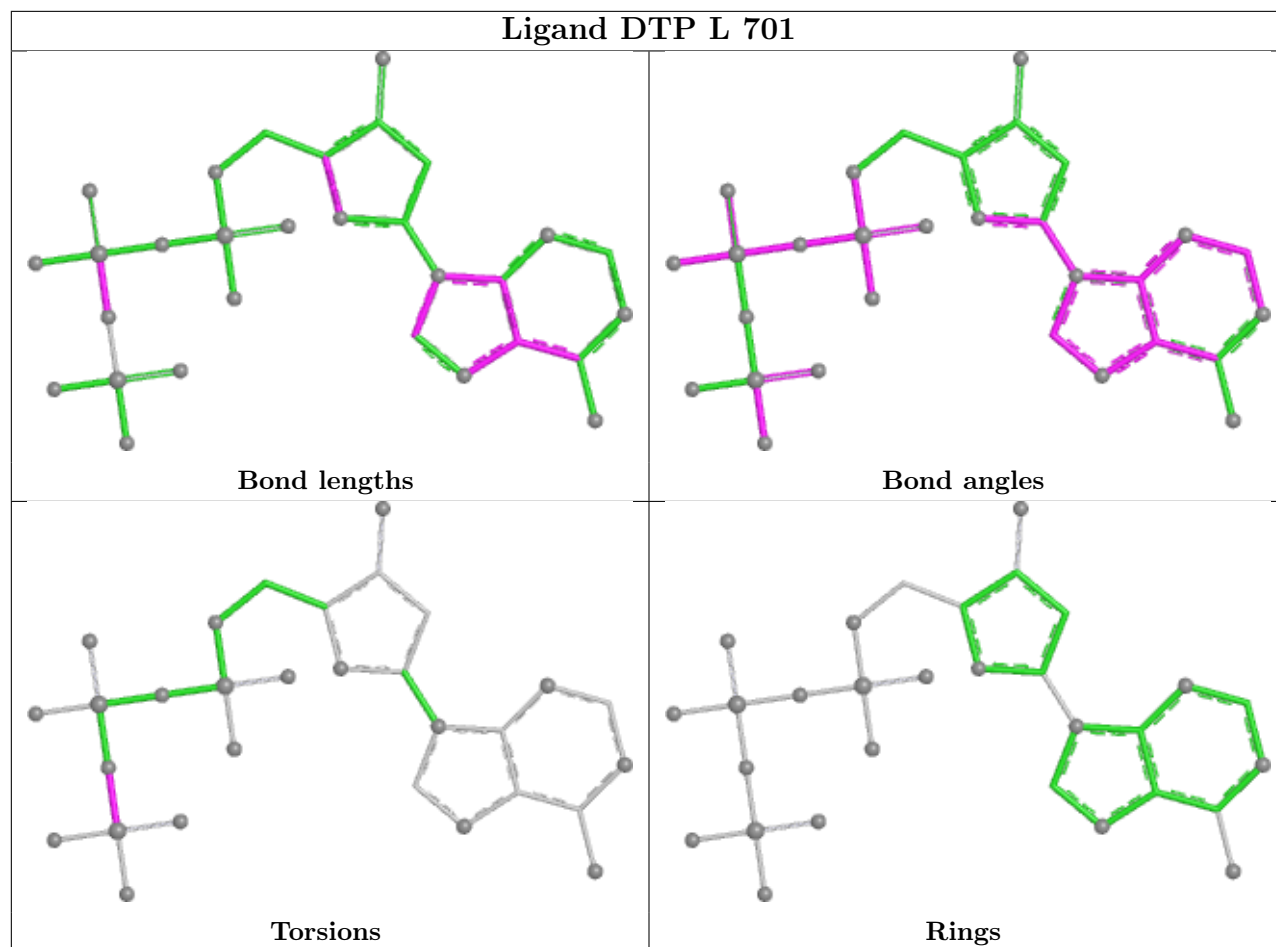
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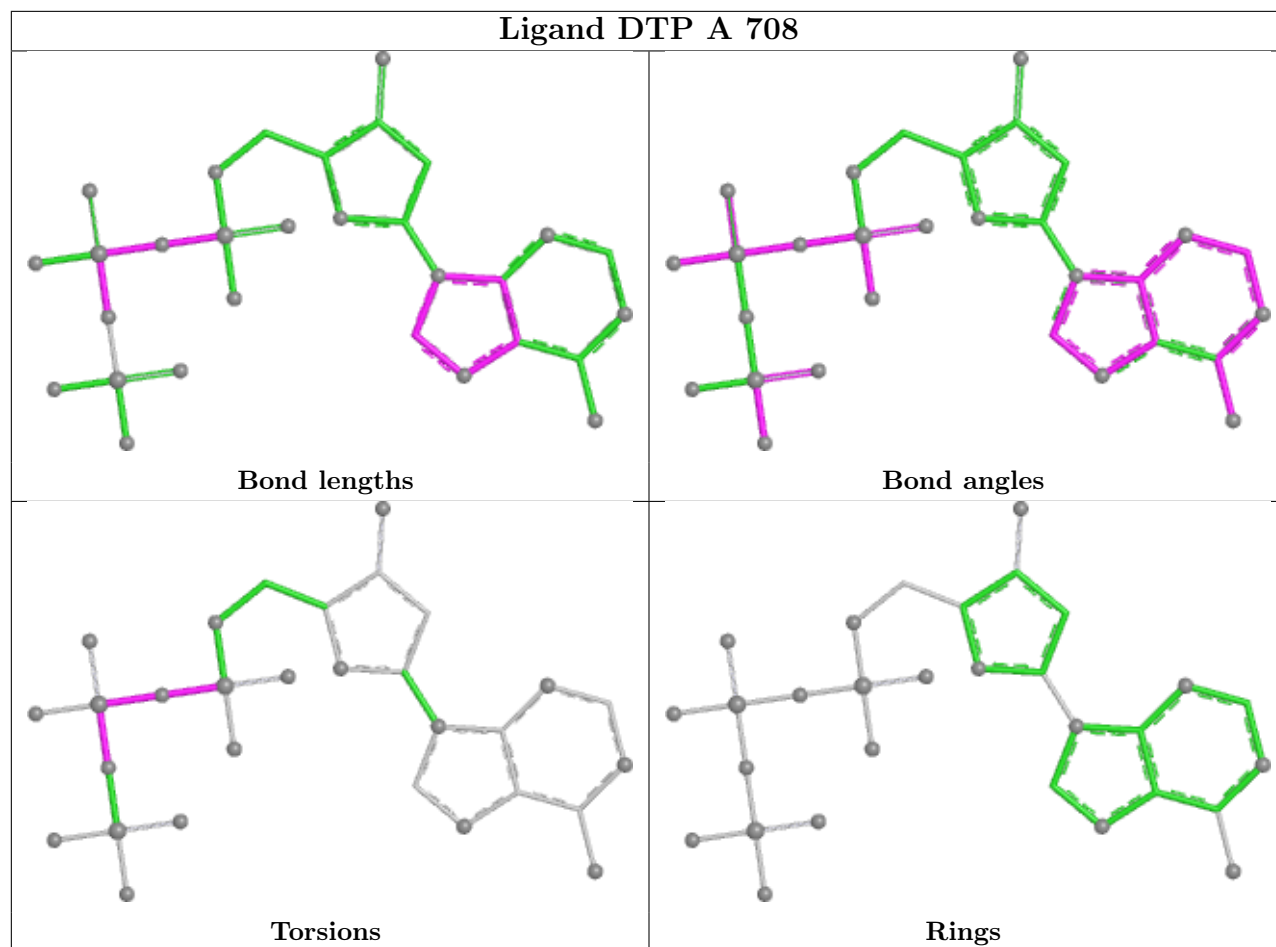




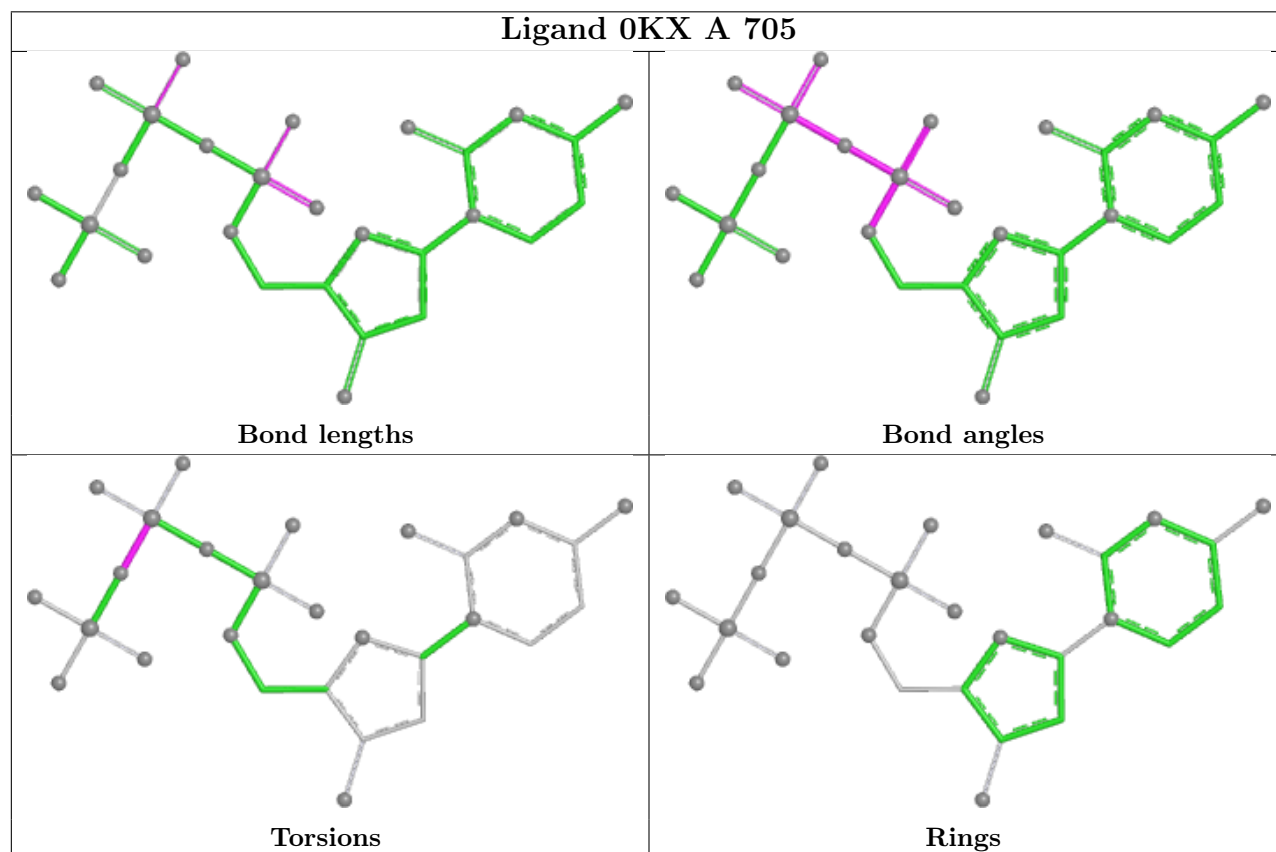
Ligand DTP L 701

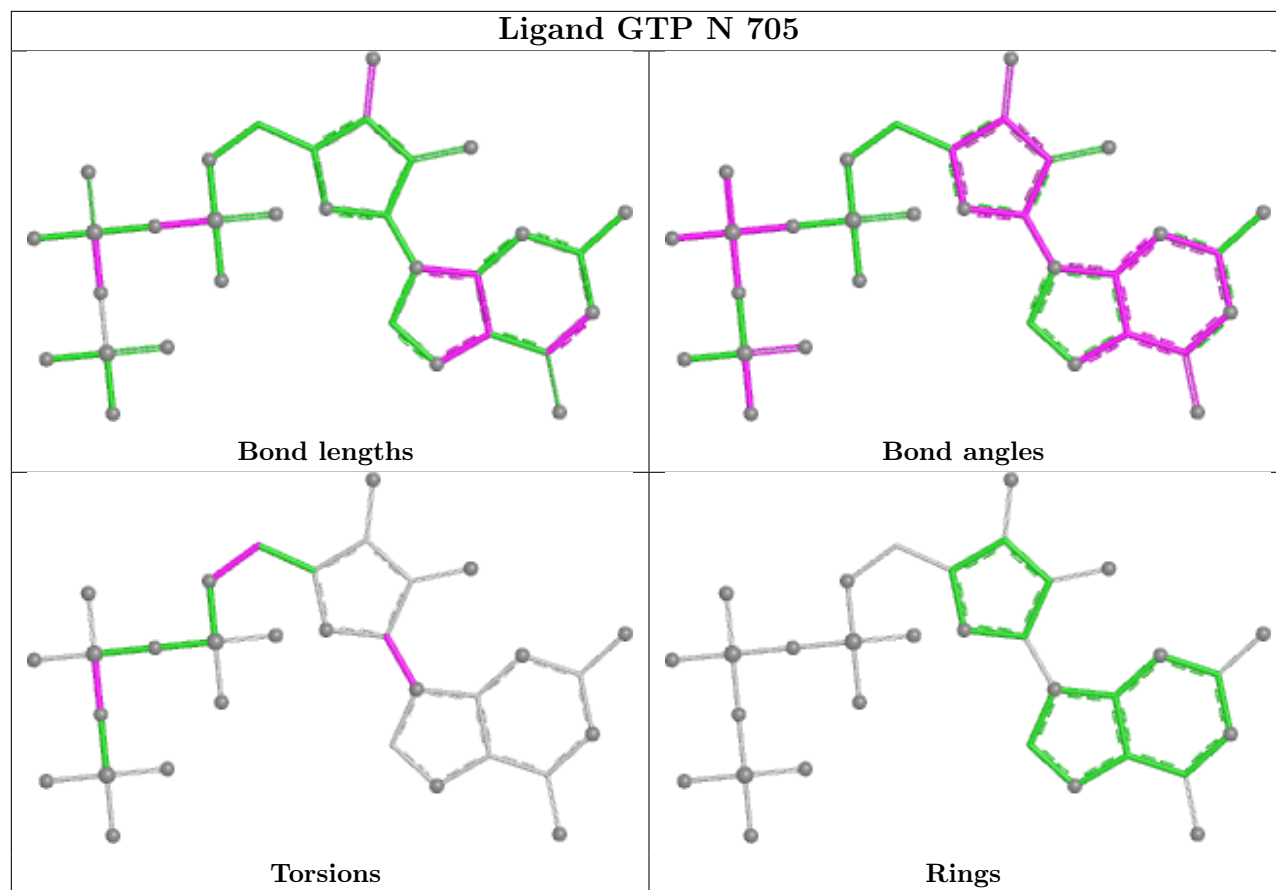


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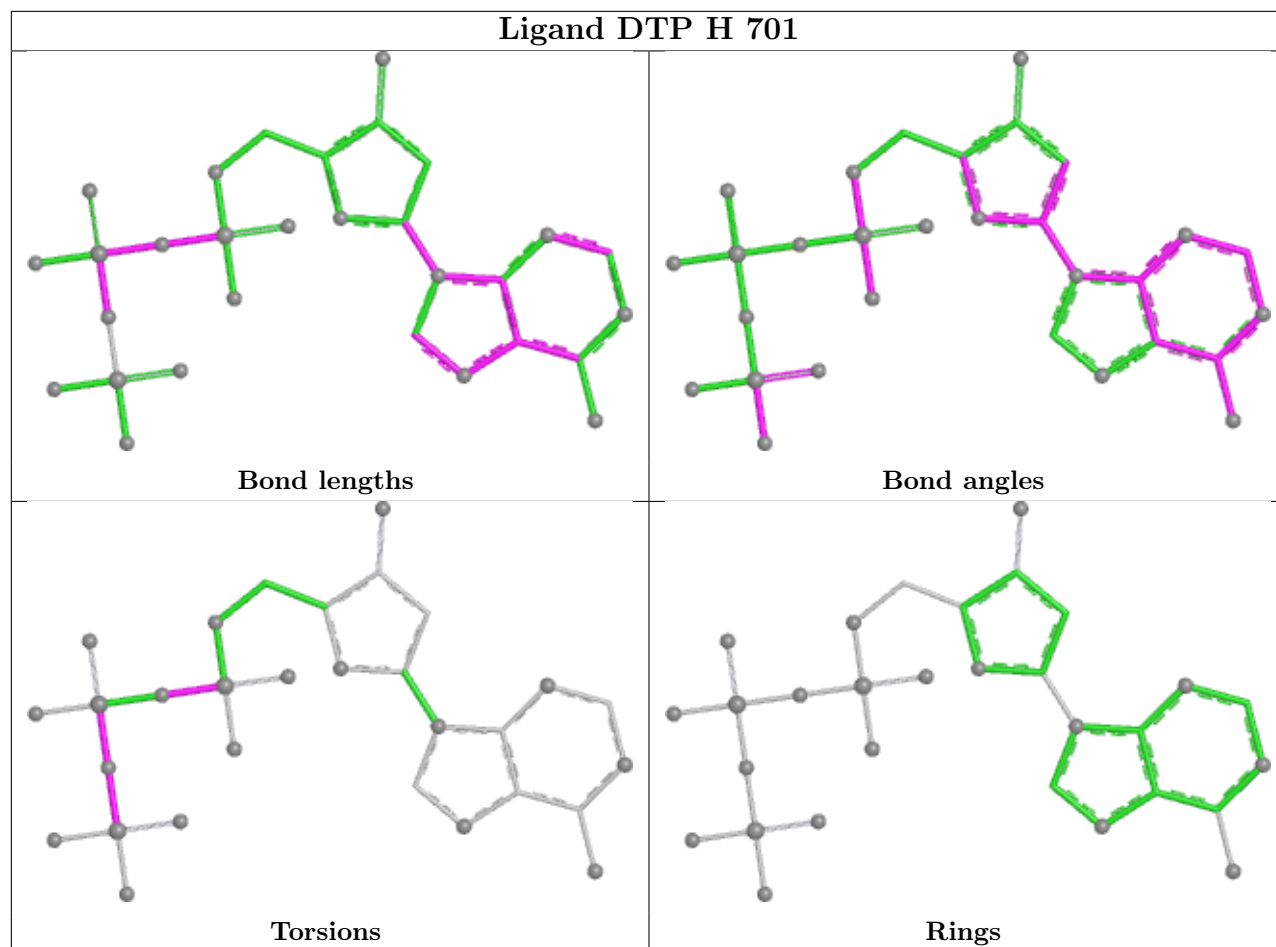


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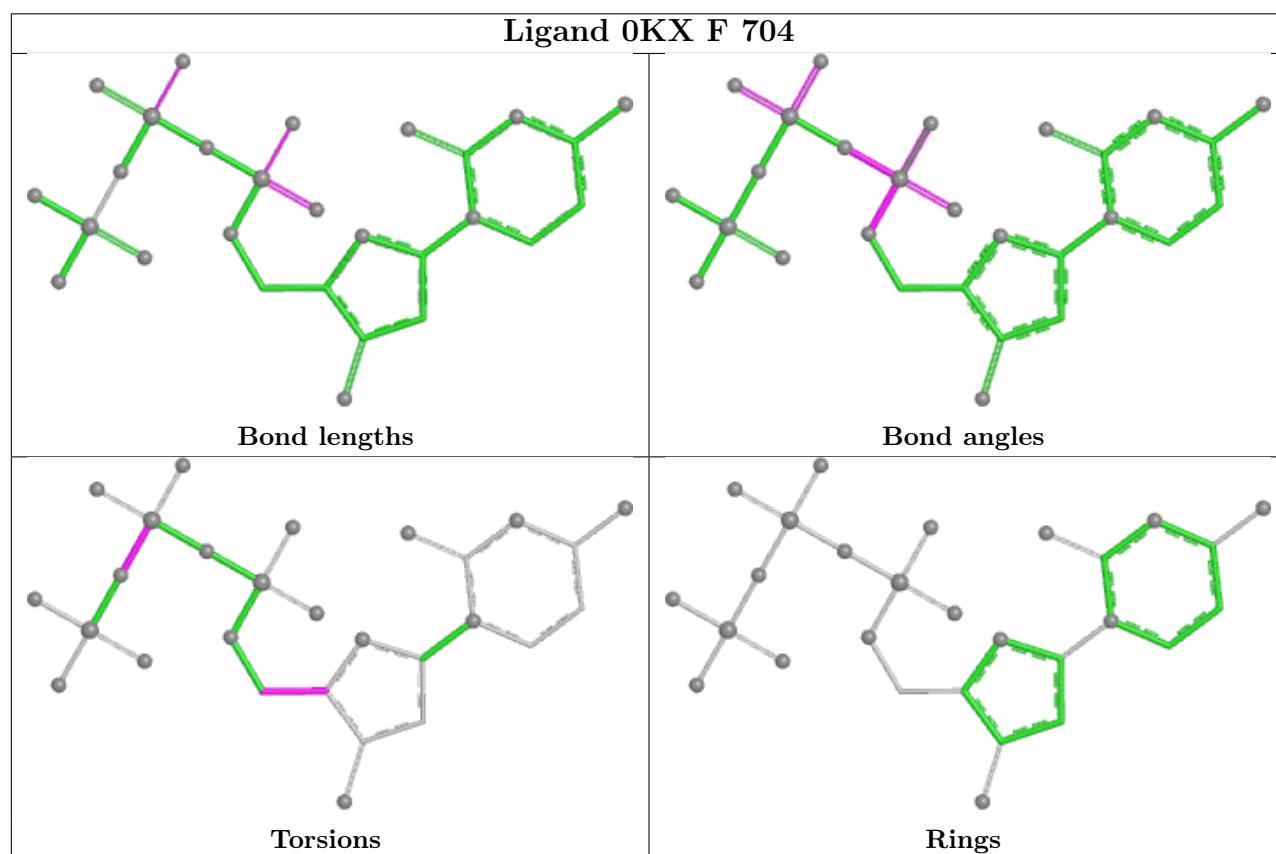


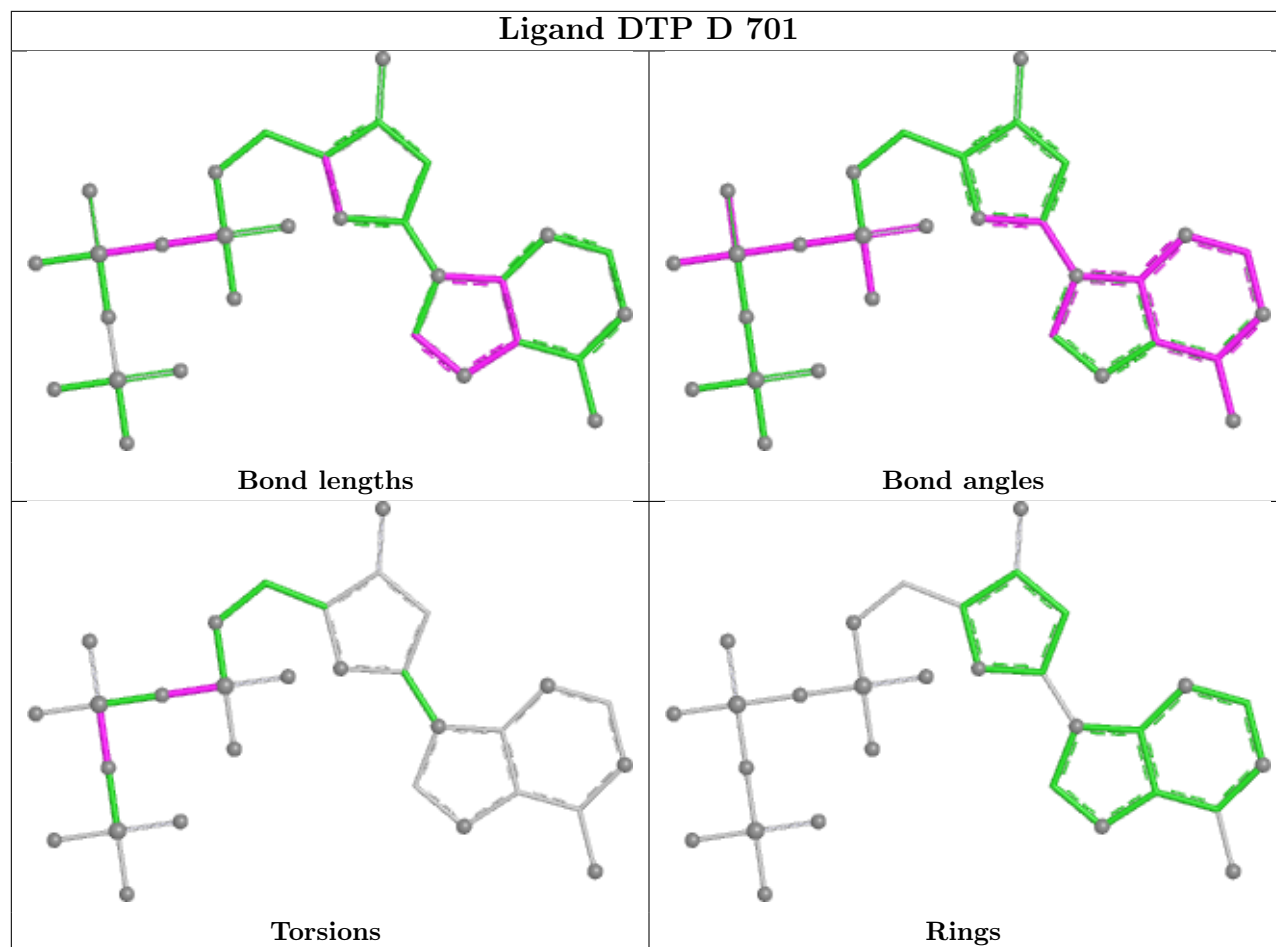


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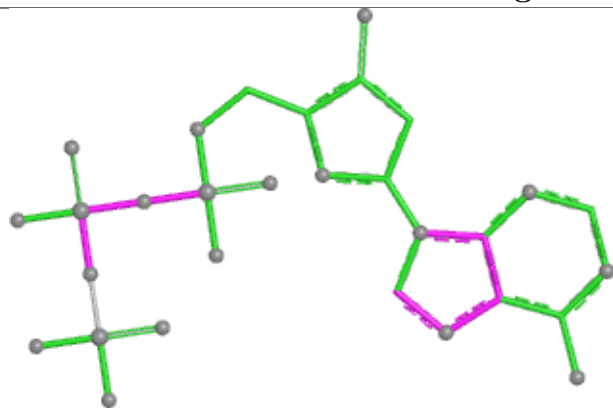


Ligand 0KX F 704

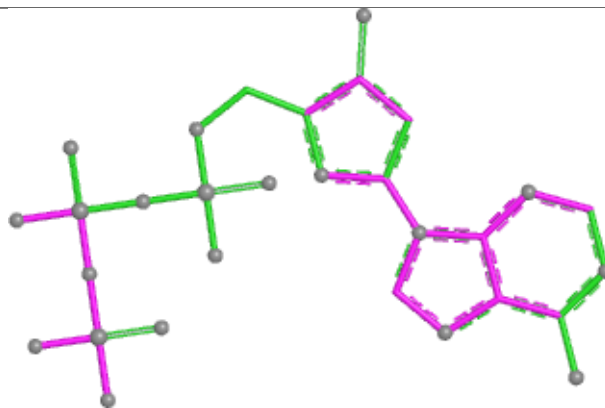




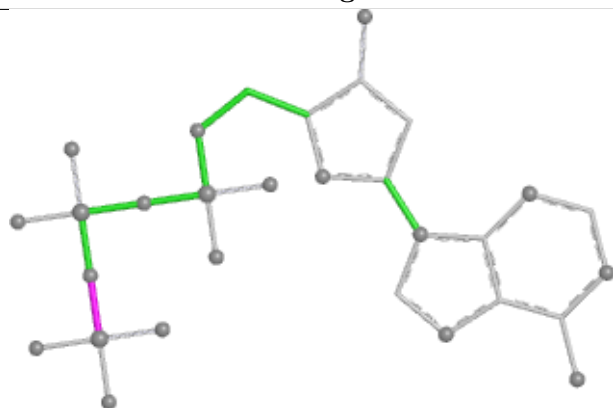
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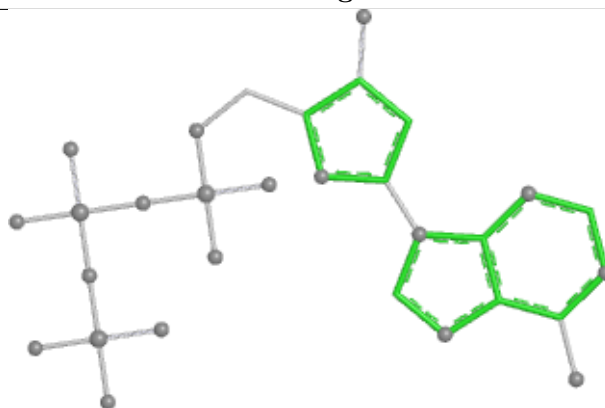
Bond lengths



Bond angles

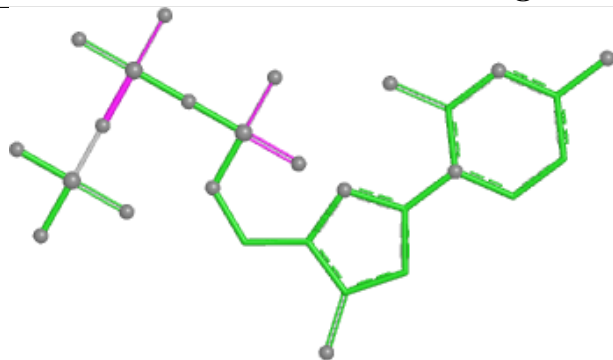


Torsions

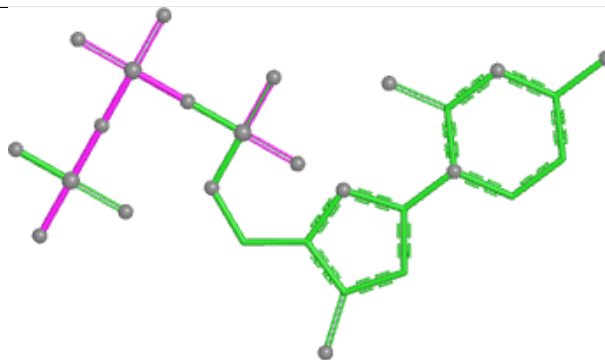


Rings

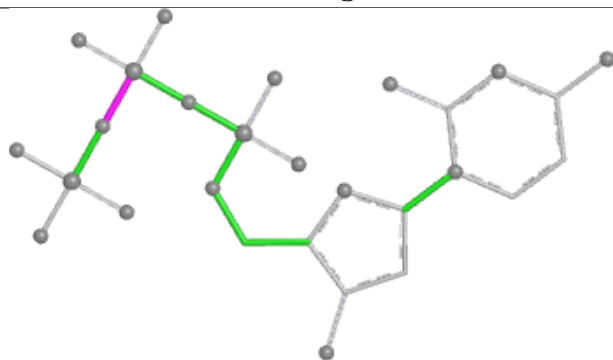
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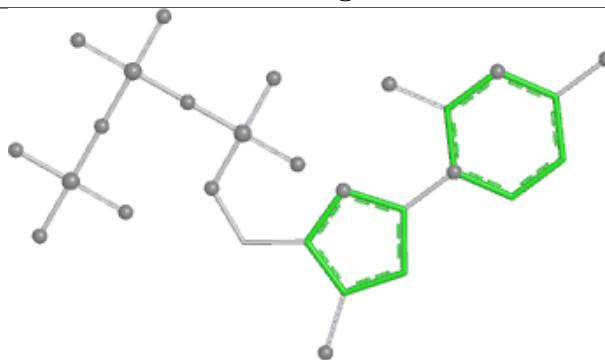
Bond lengths



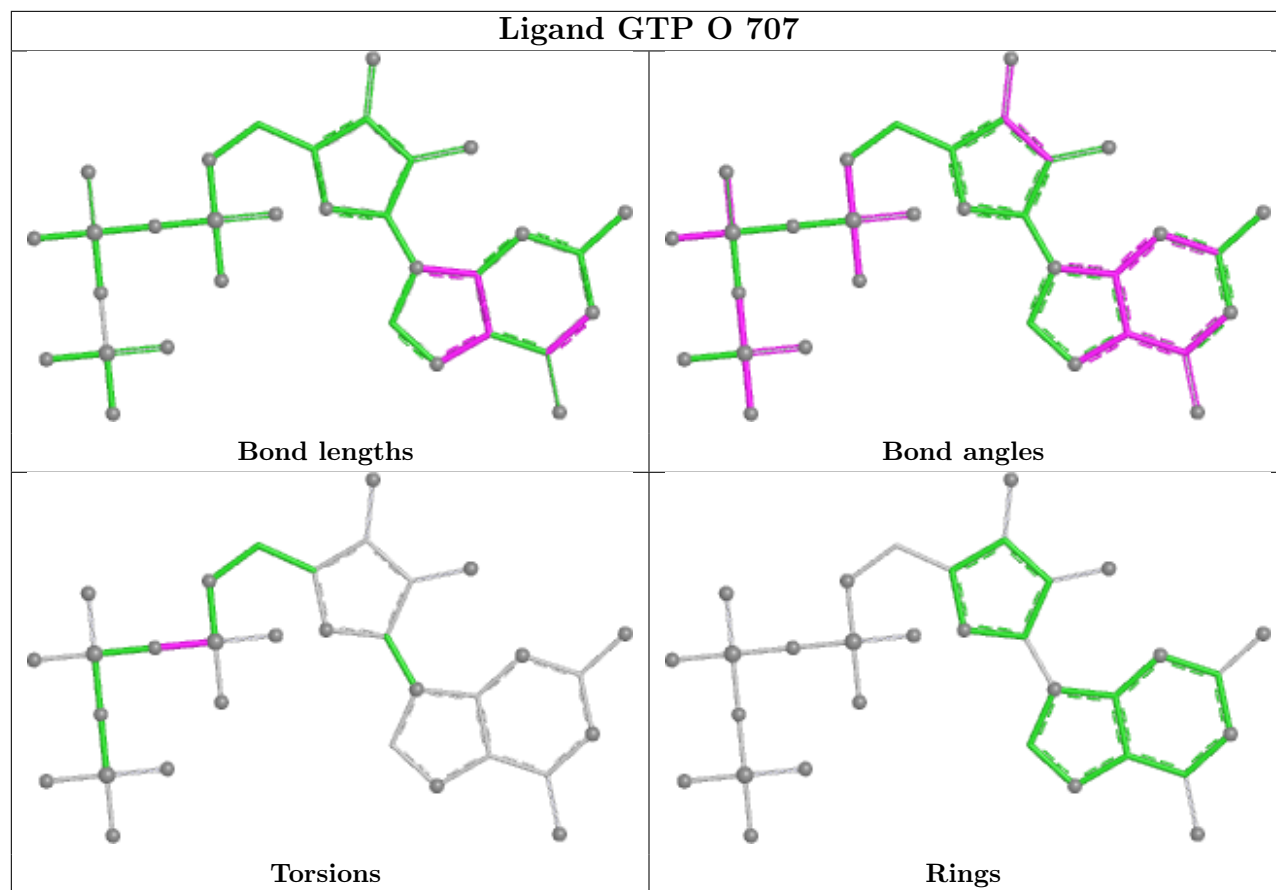
Bond angles



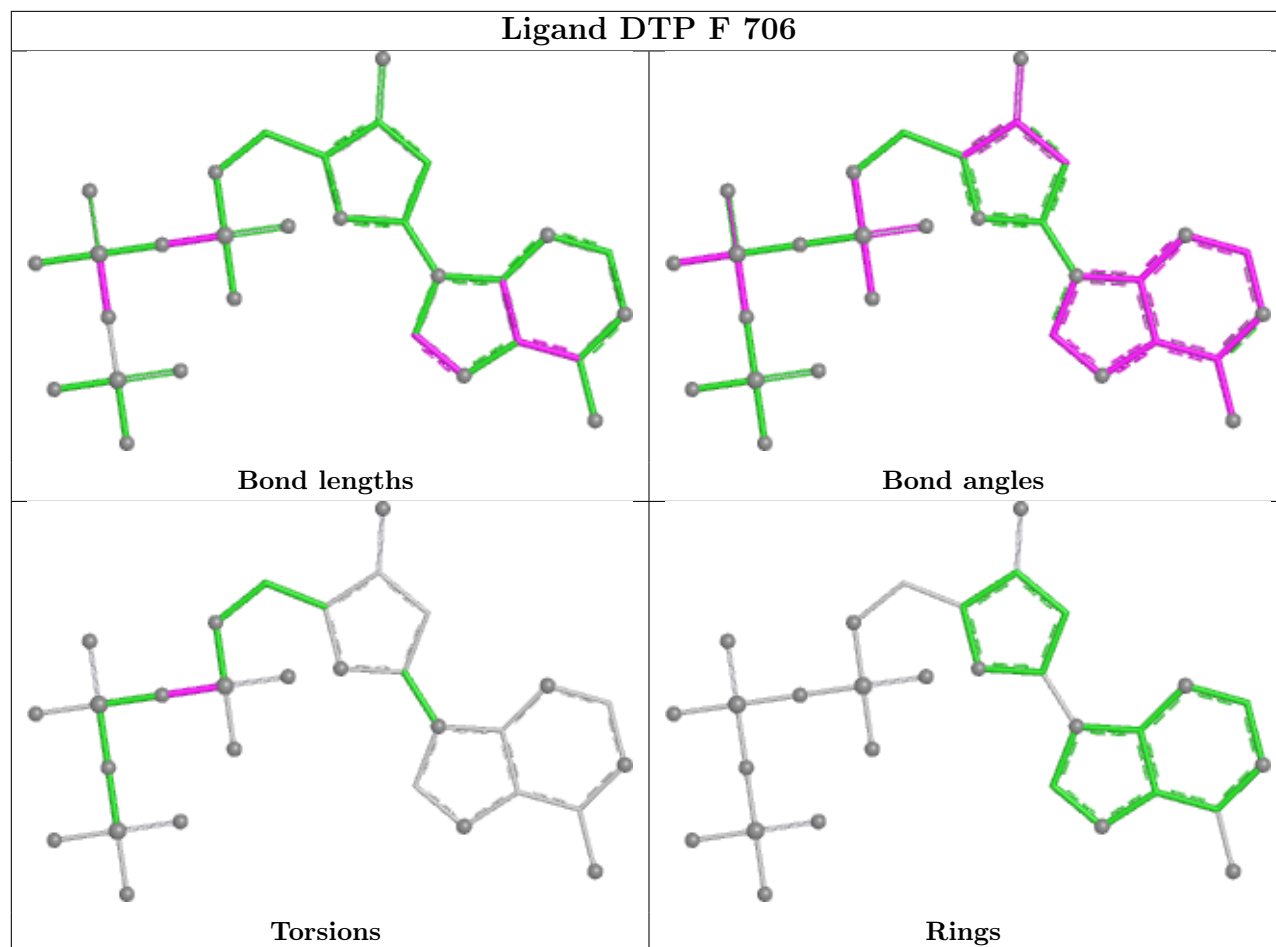
Torsions

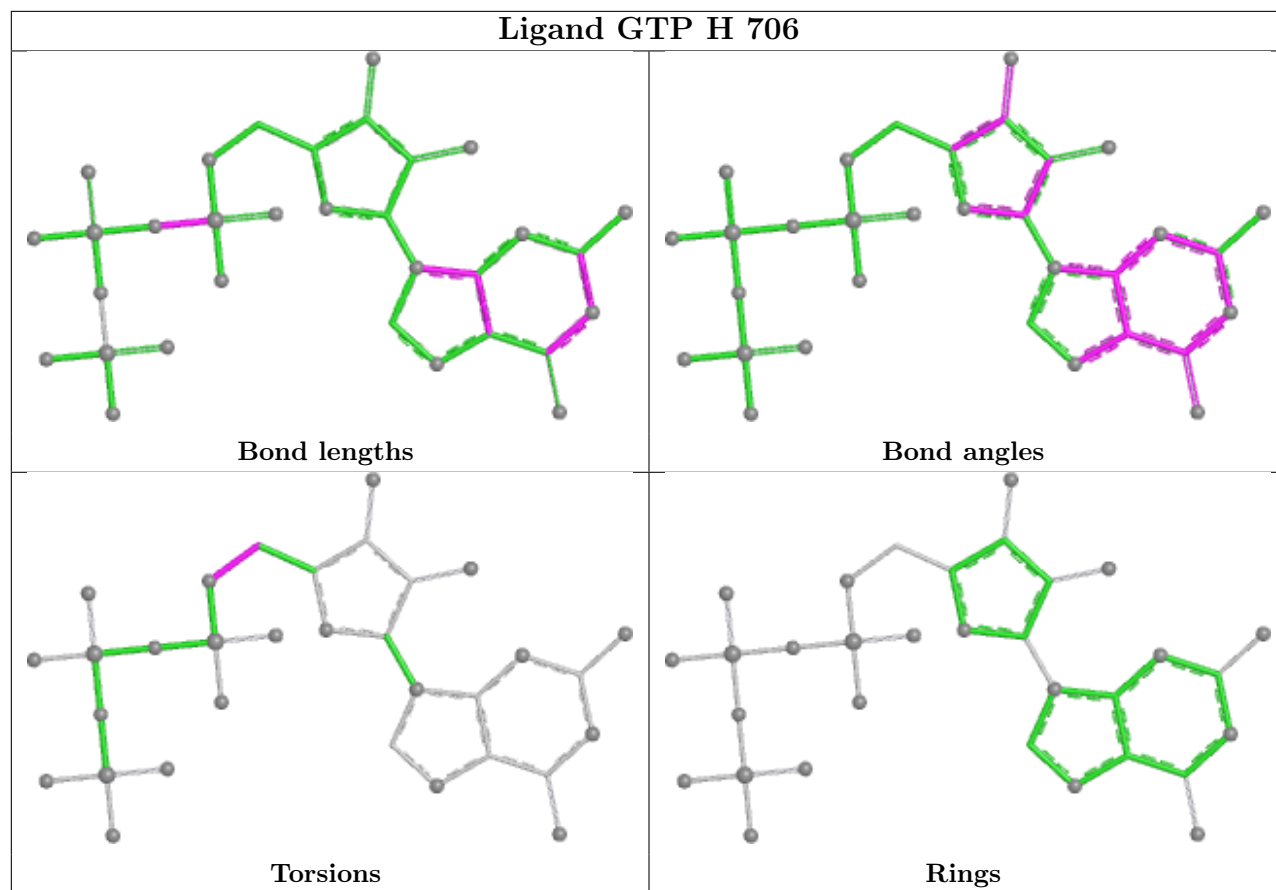


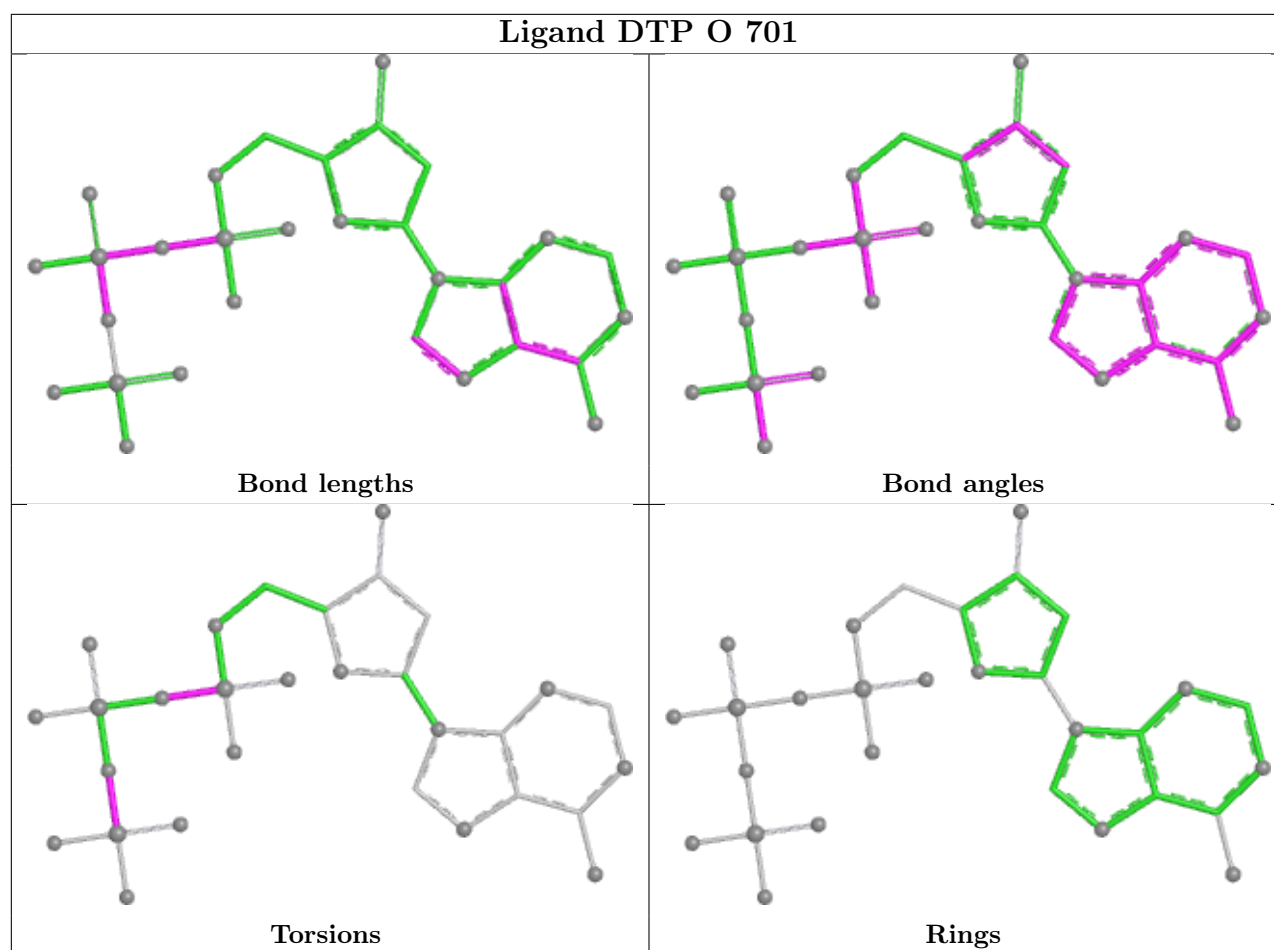
Rings



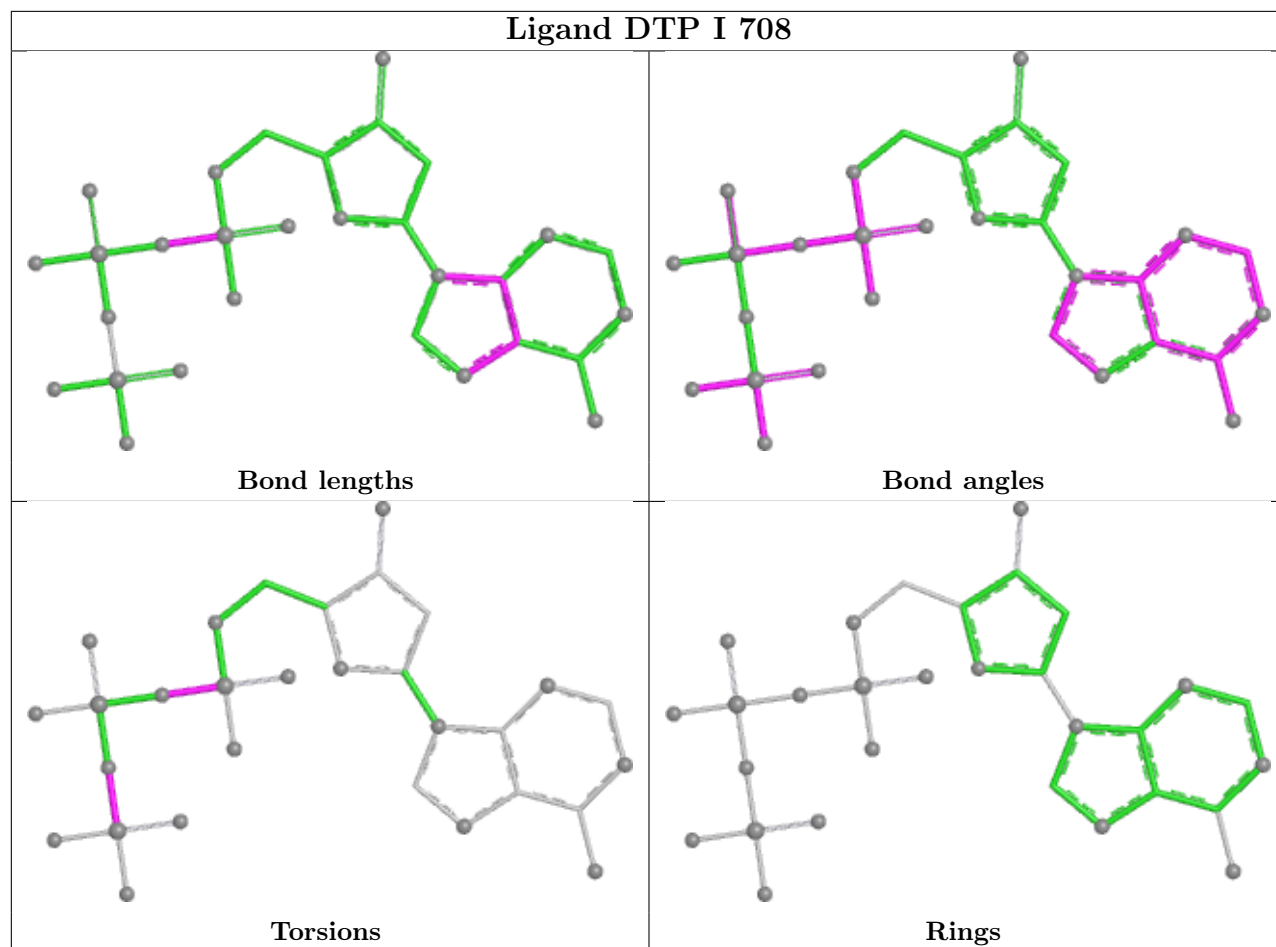
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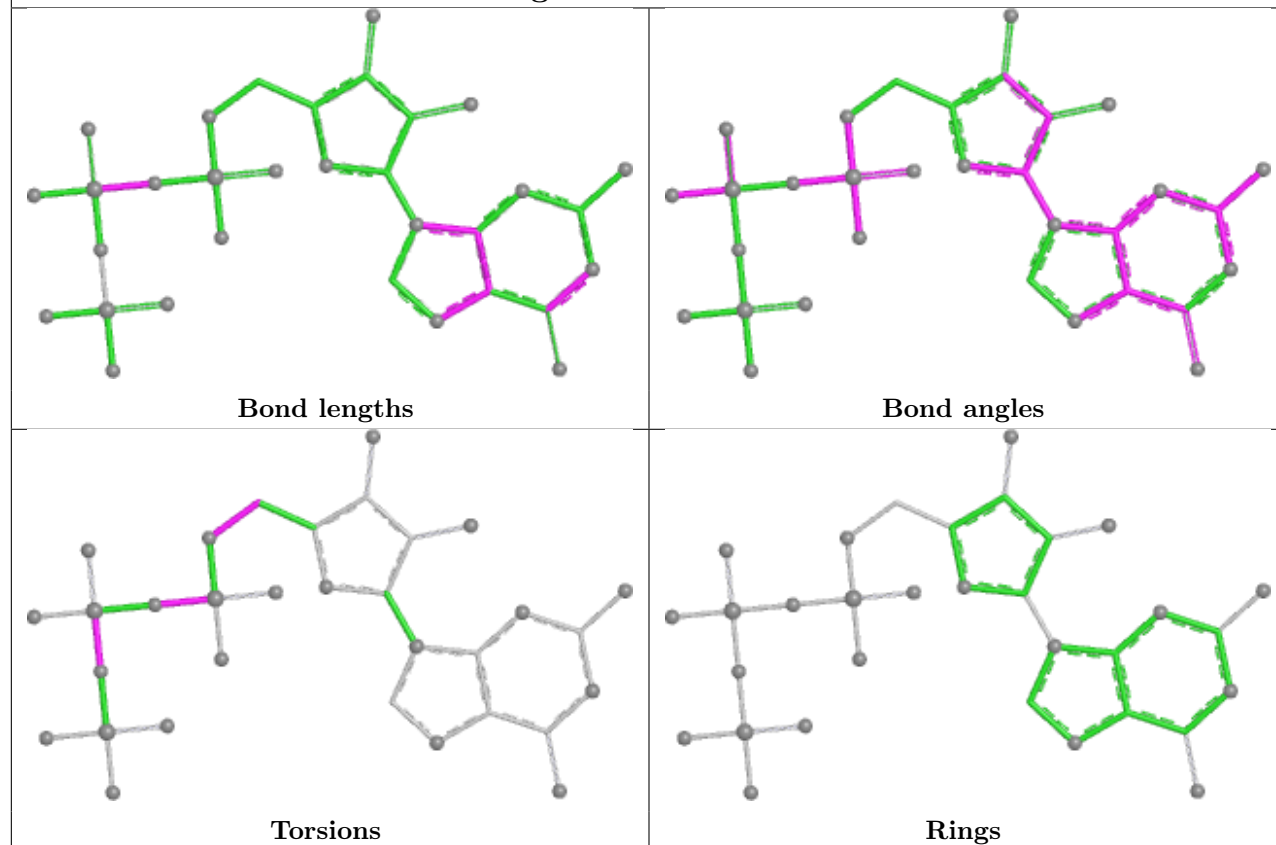




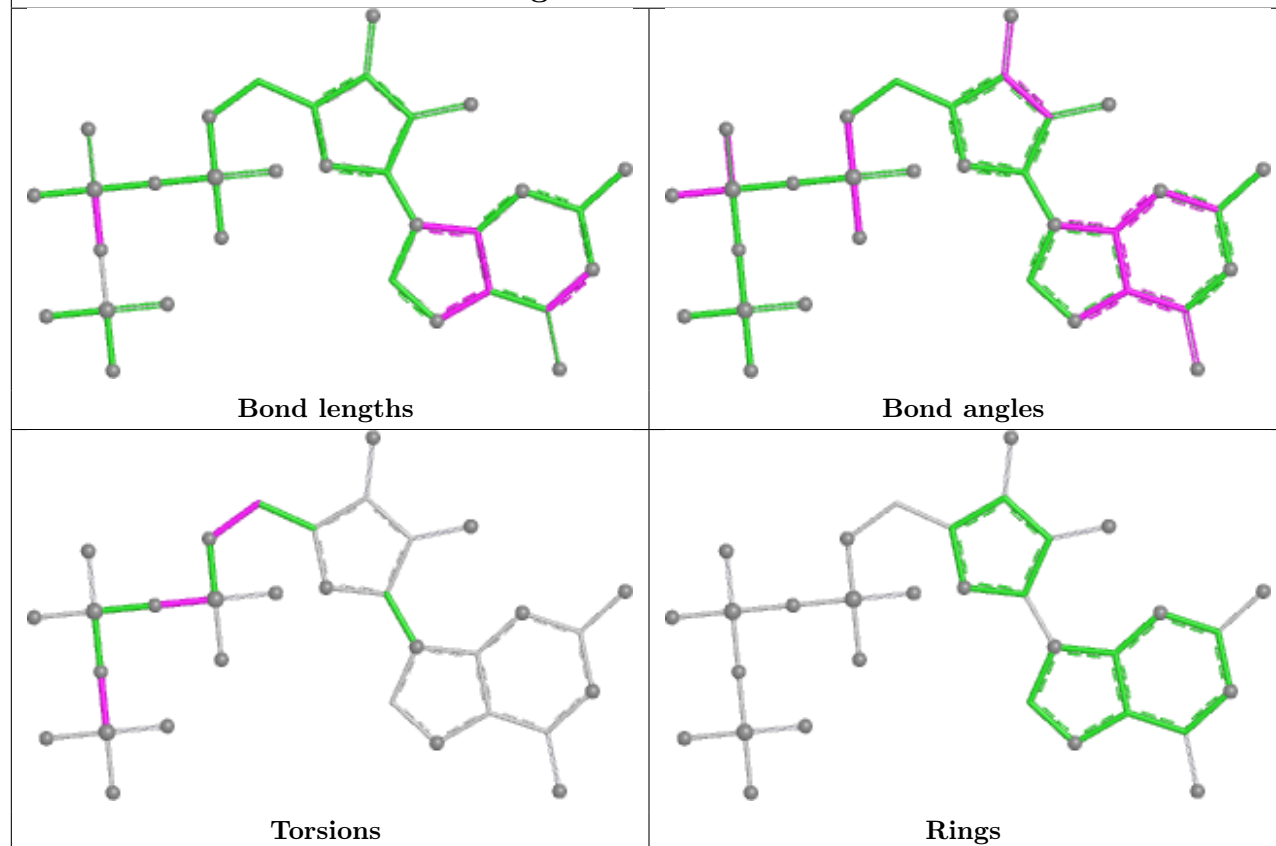
Ligand DTP I 708

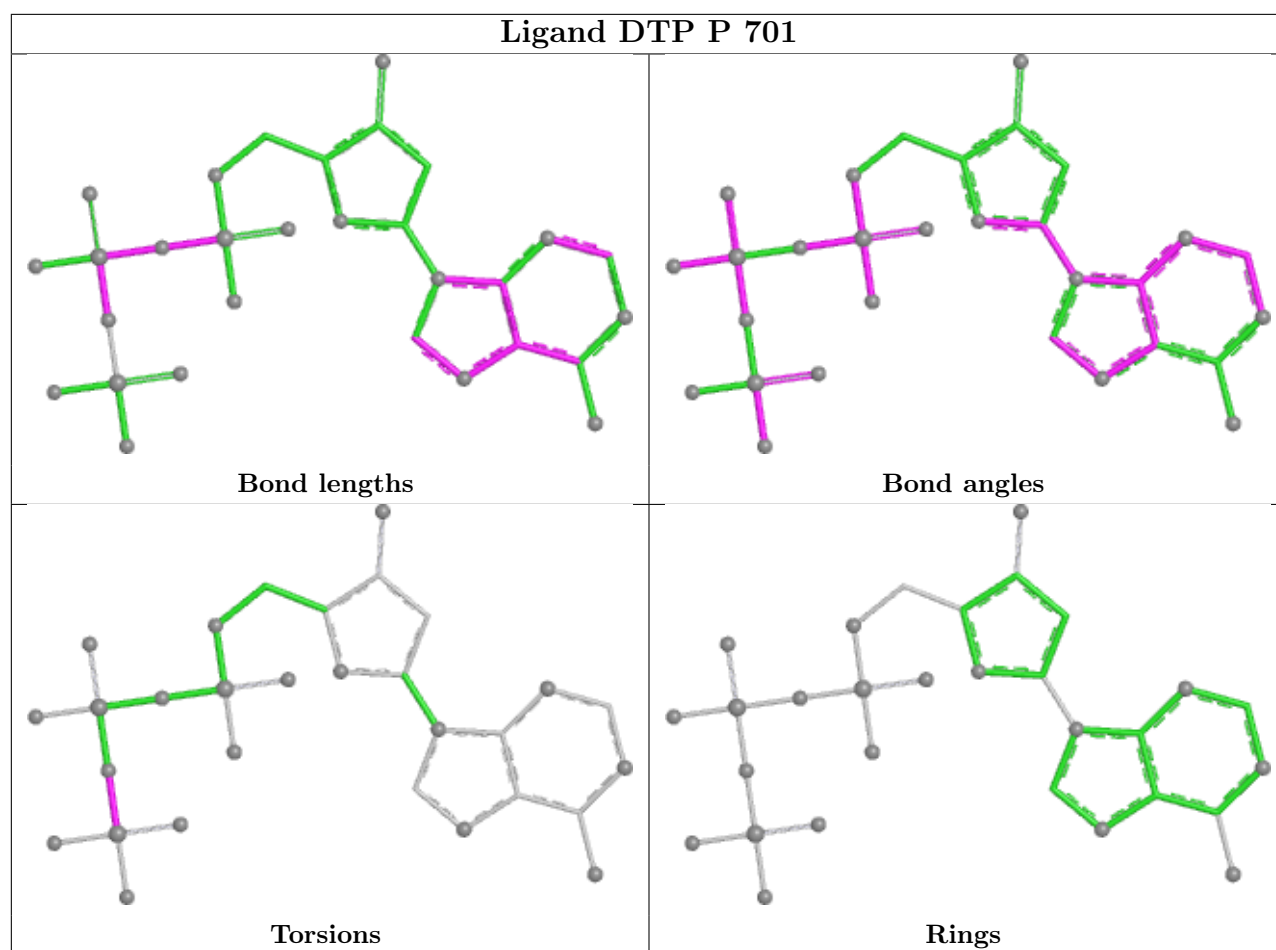


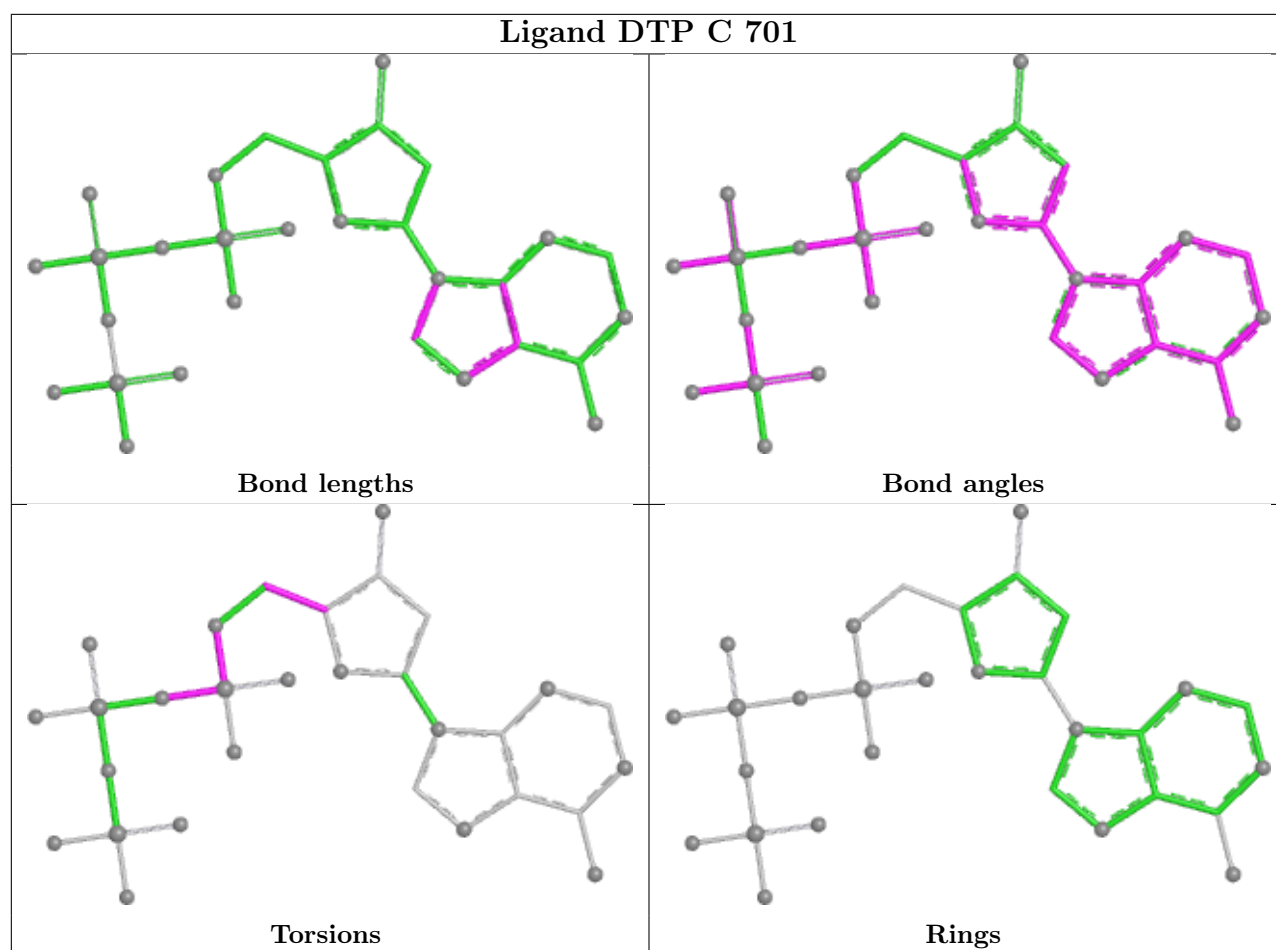
Ligand GTP B 706

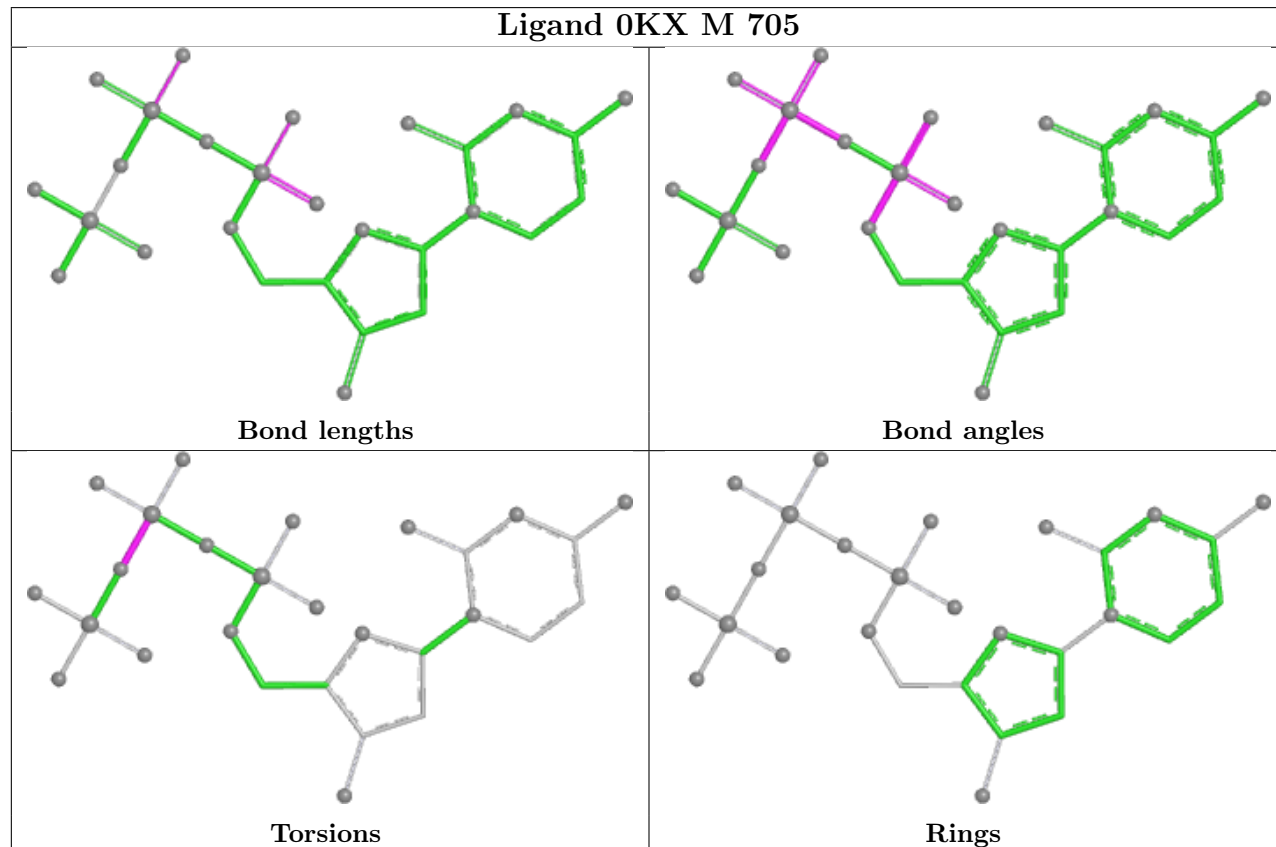
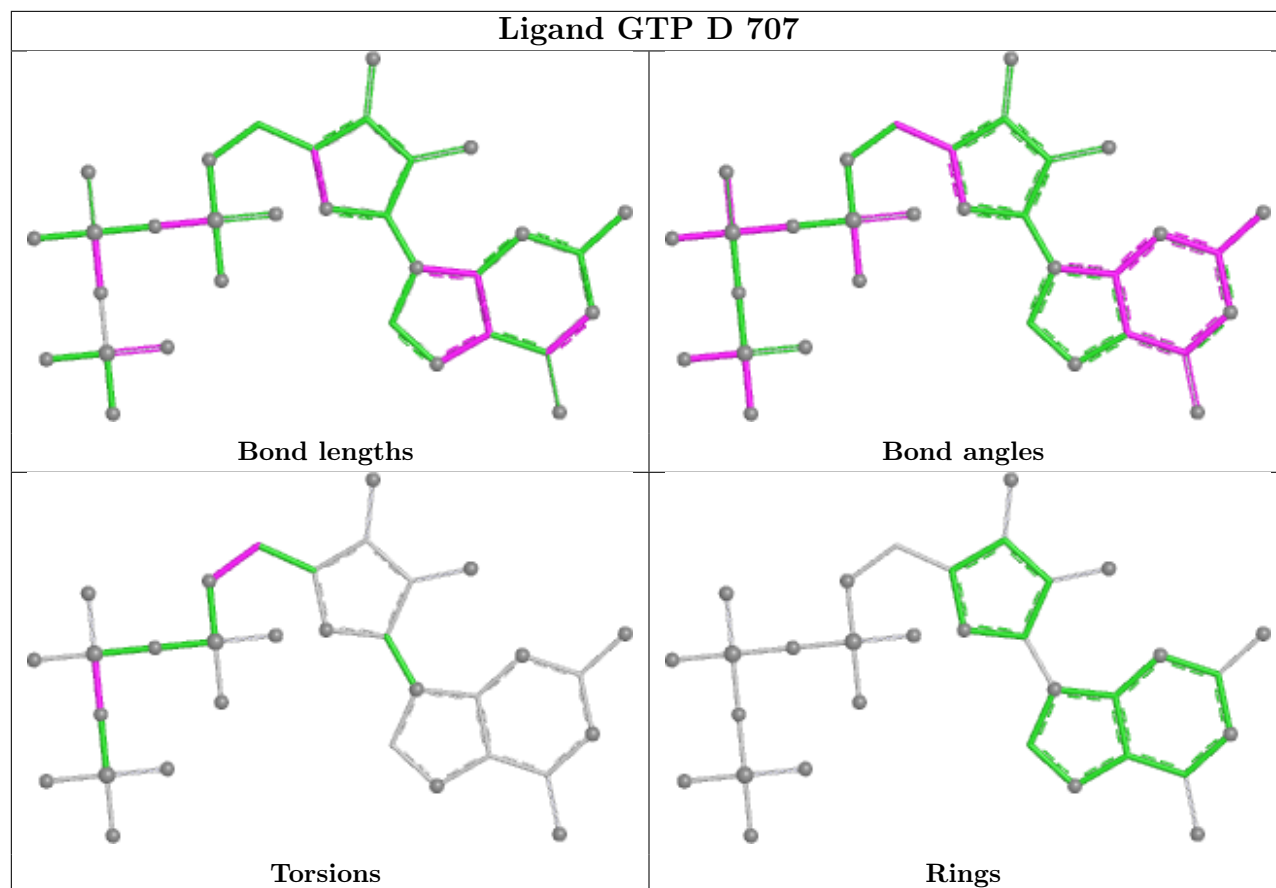


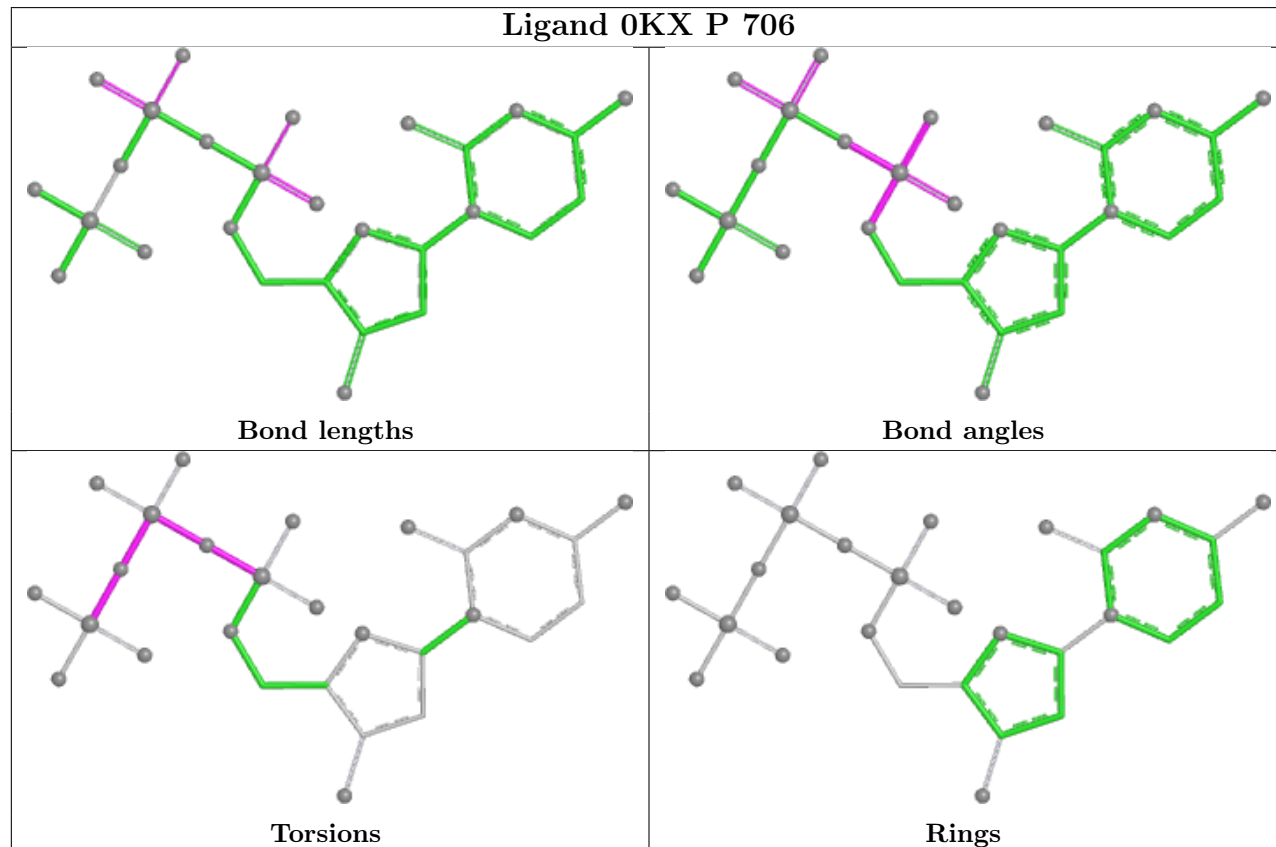
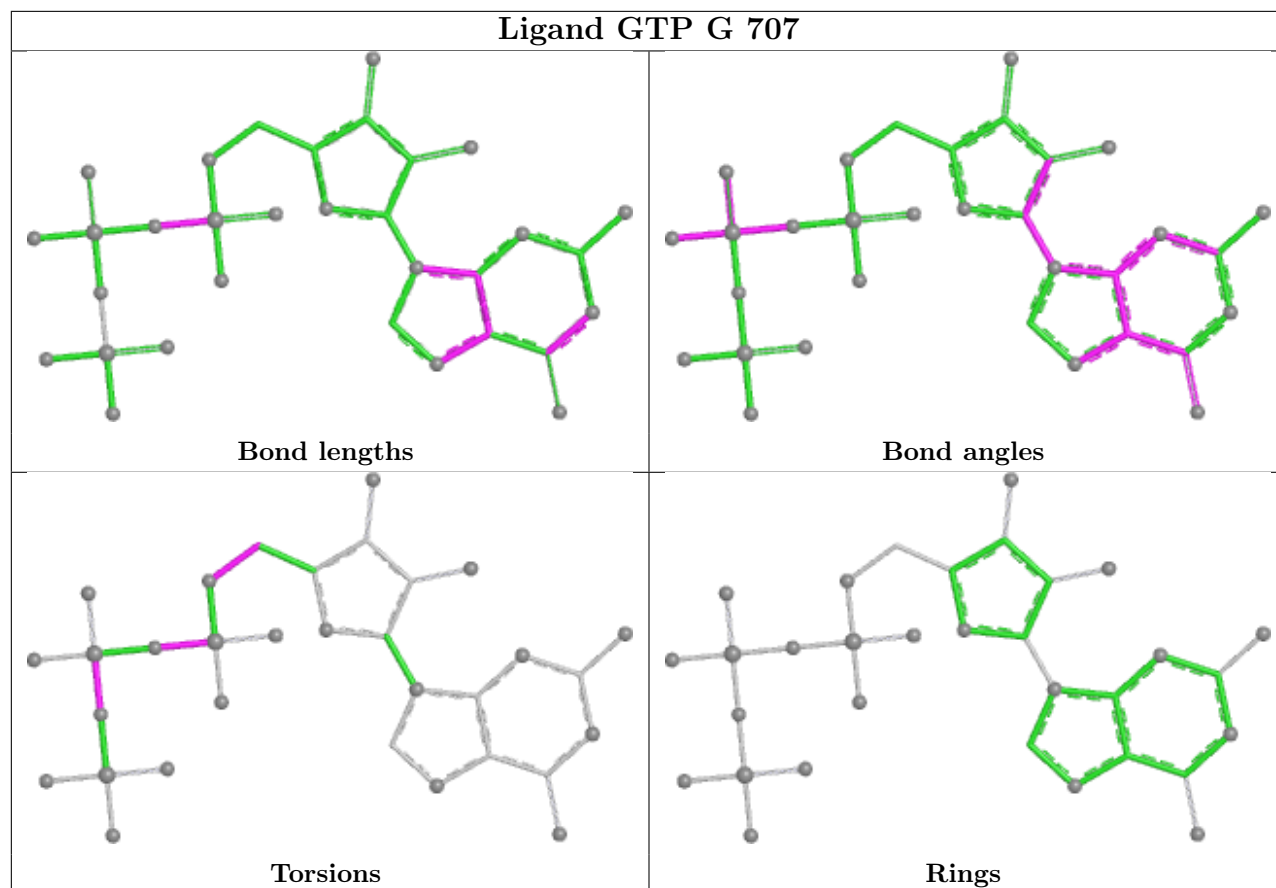
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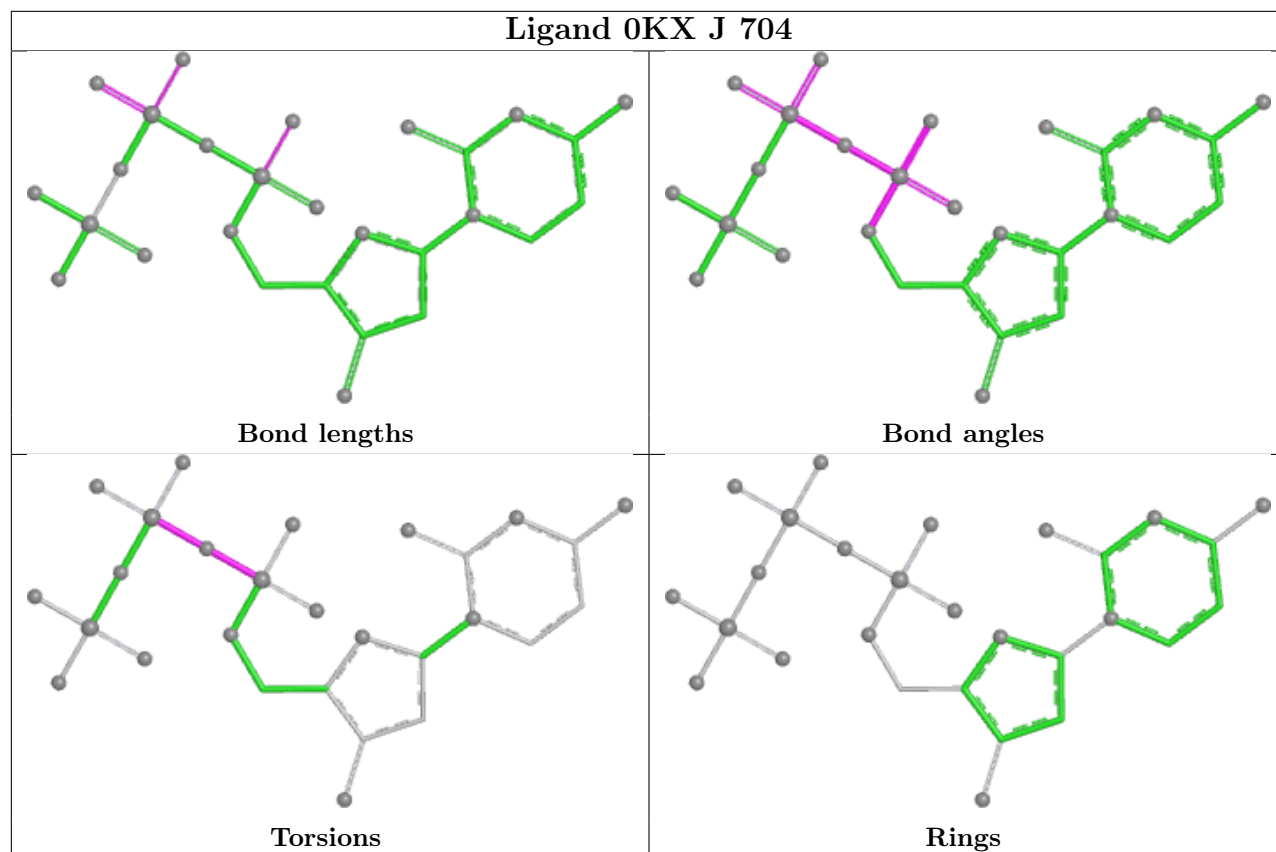




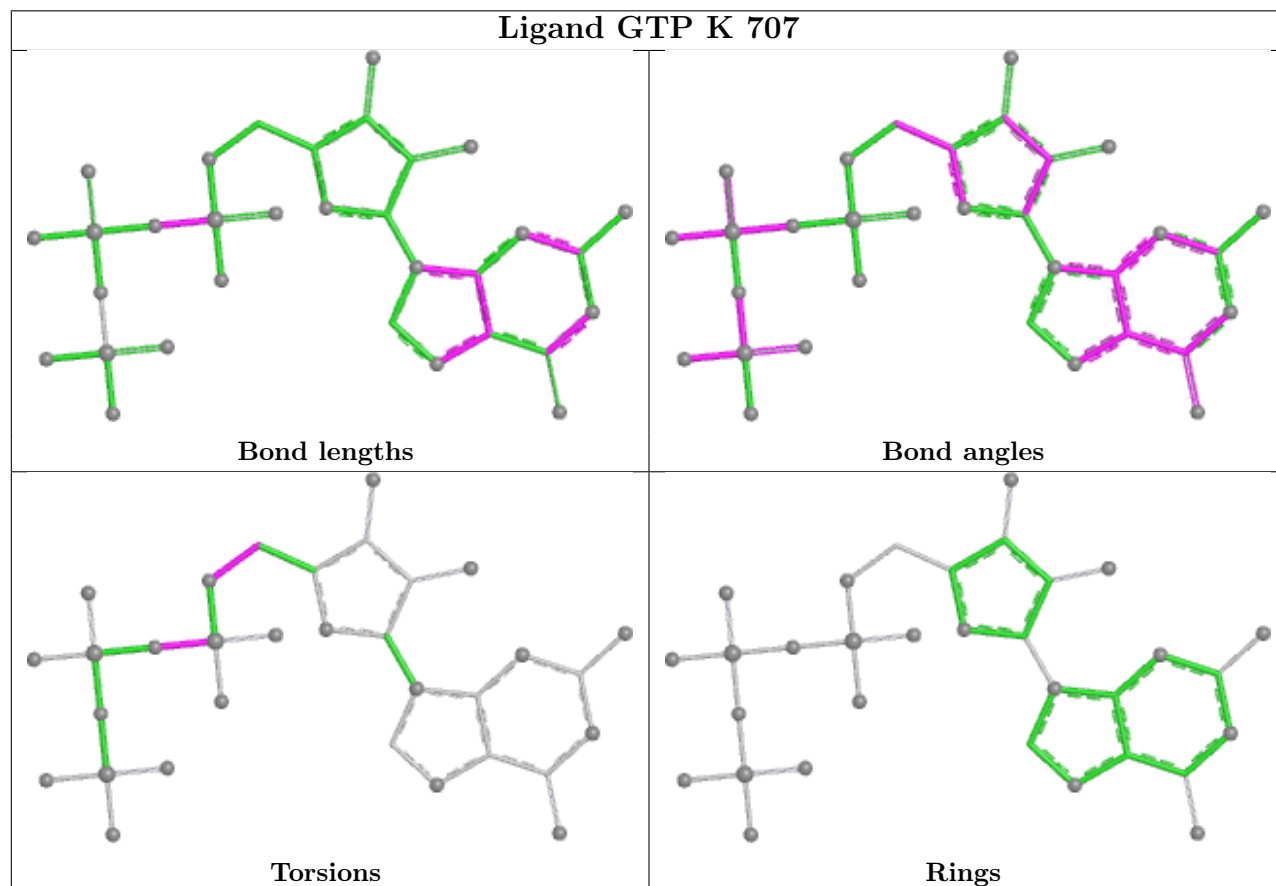


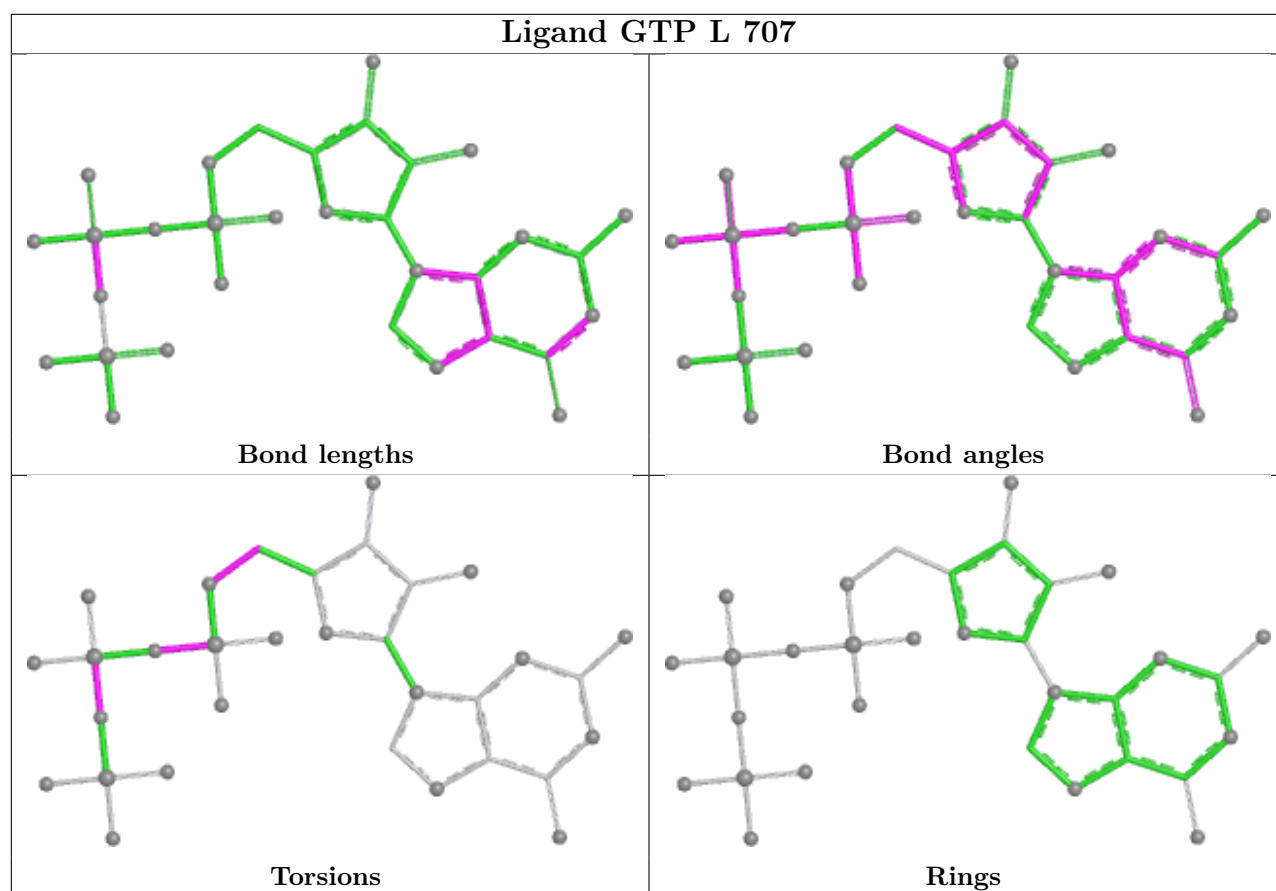


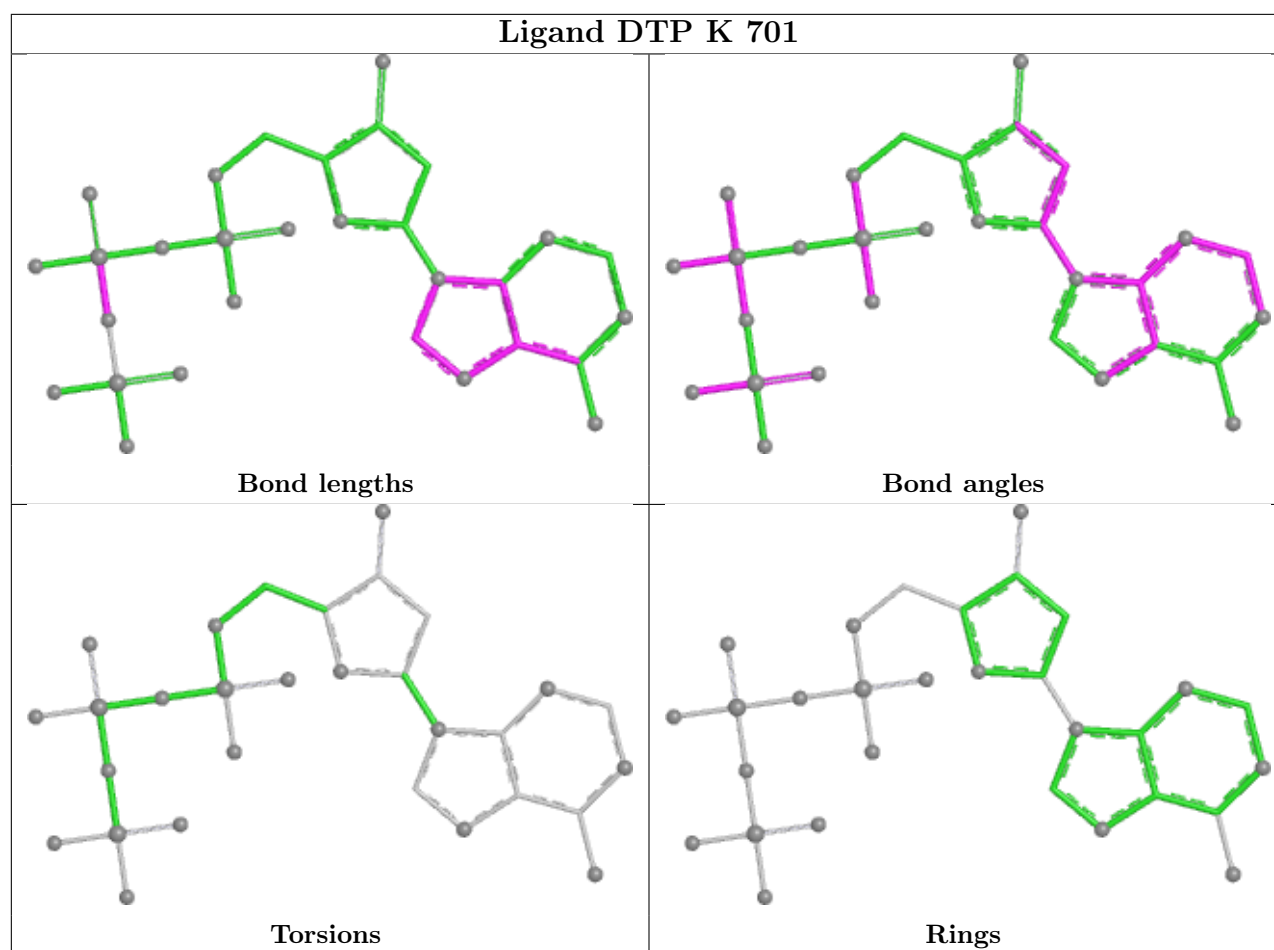
Ligand 0KX J 704



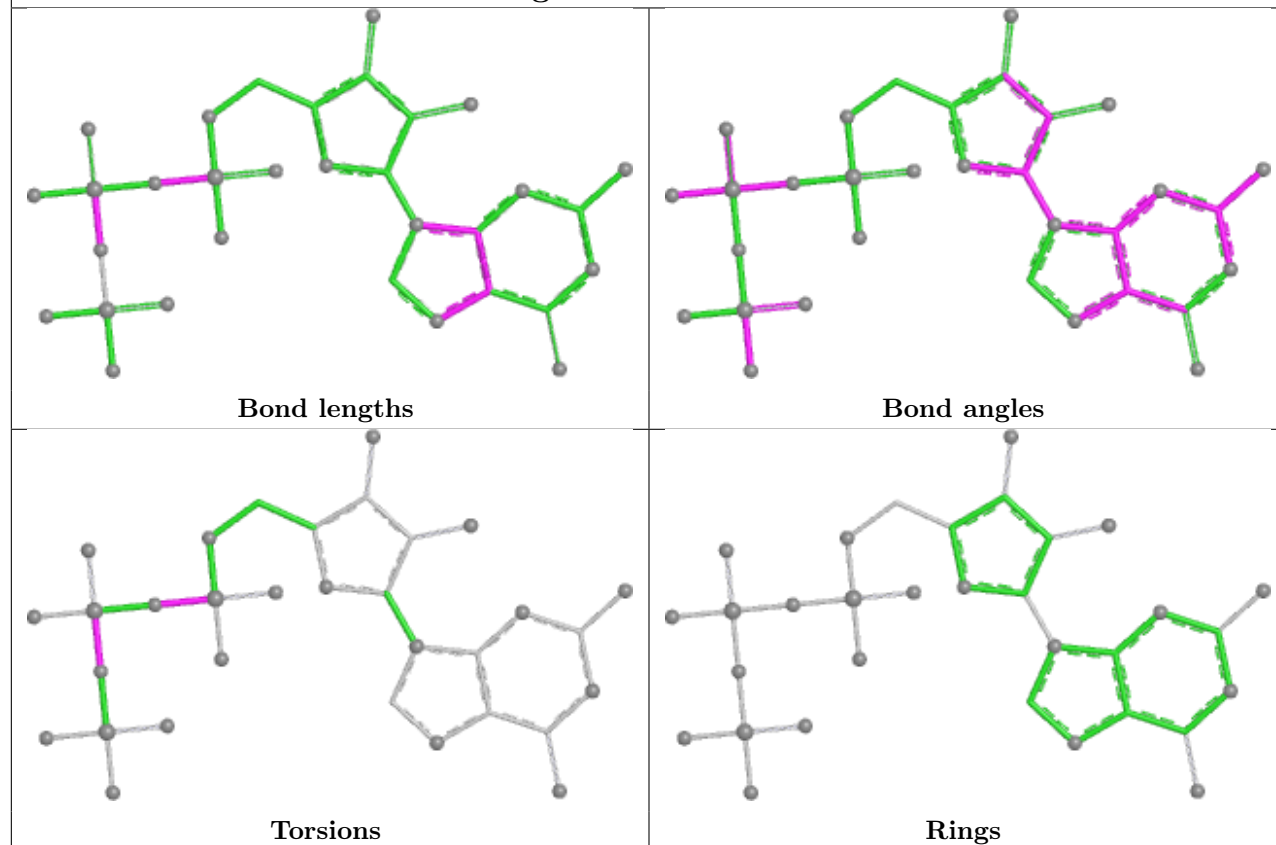
Ligand GTP K 707



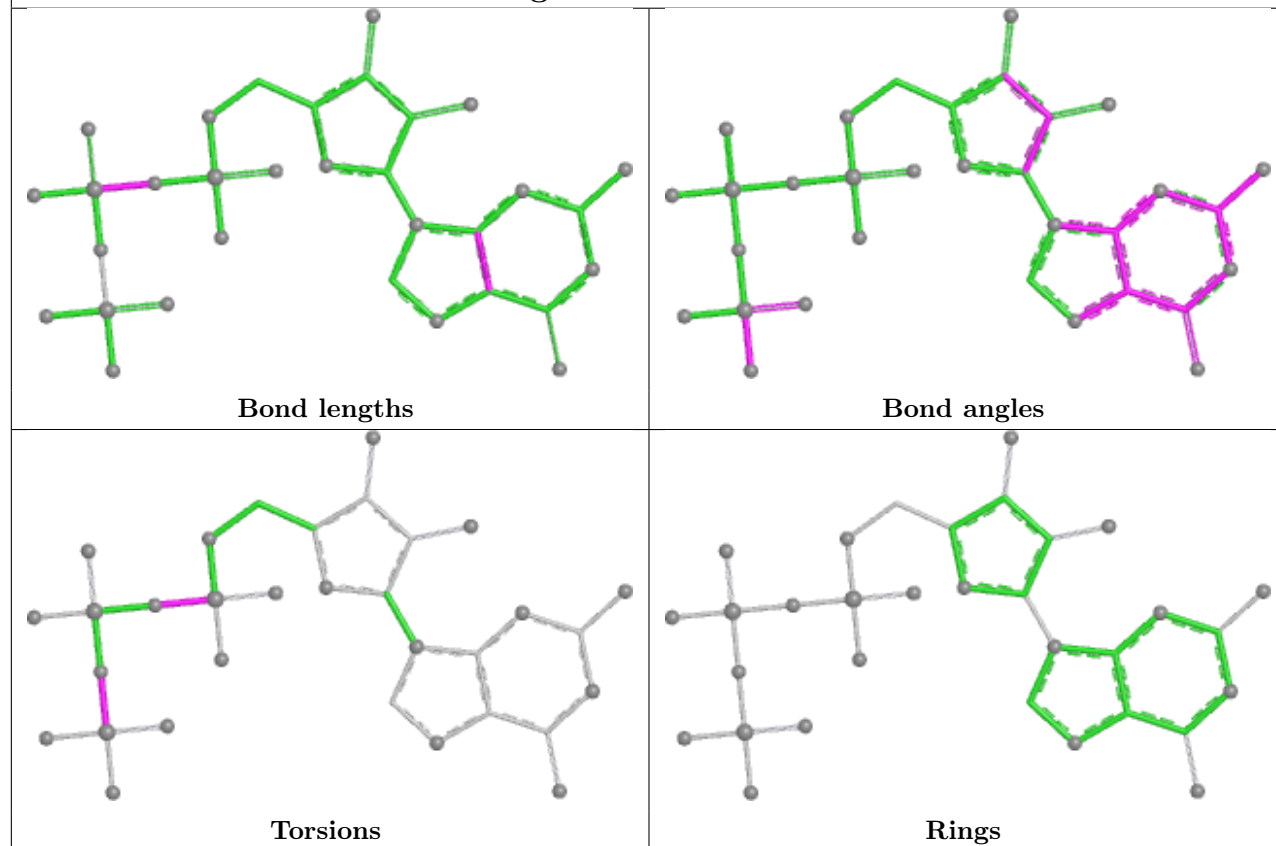


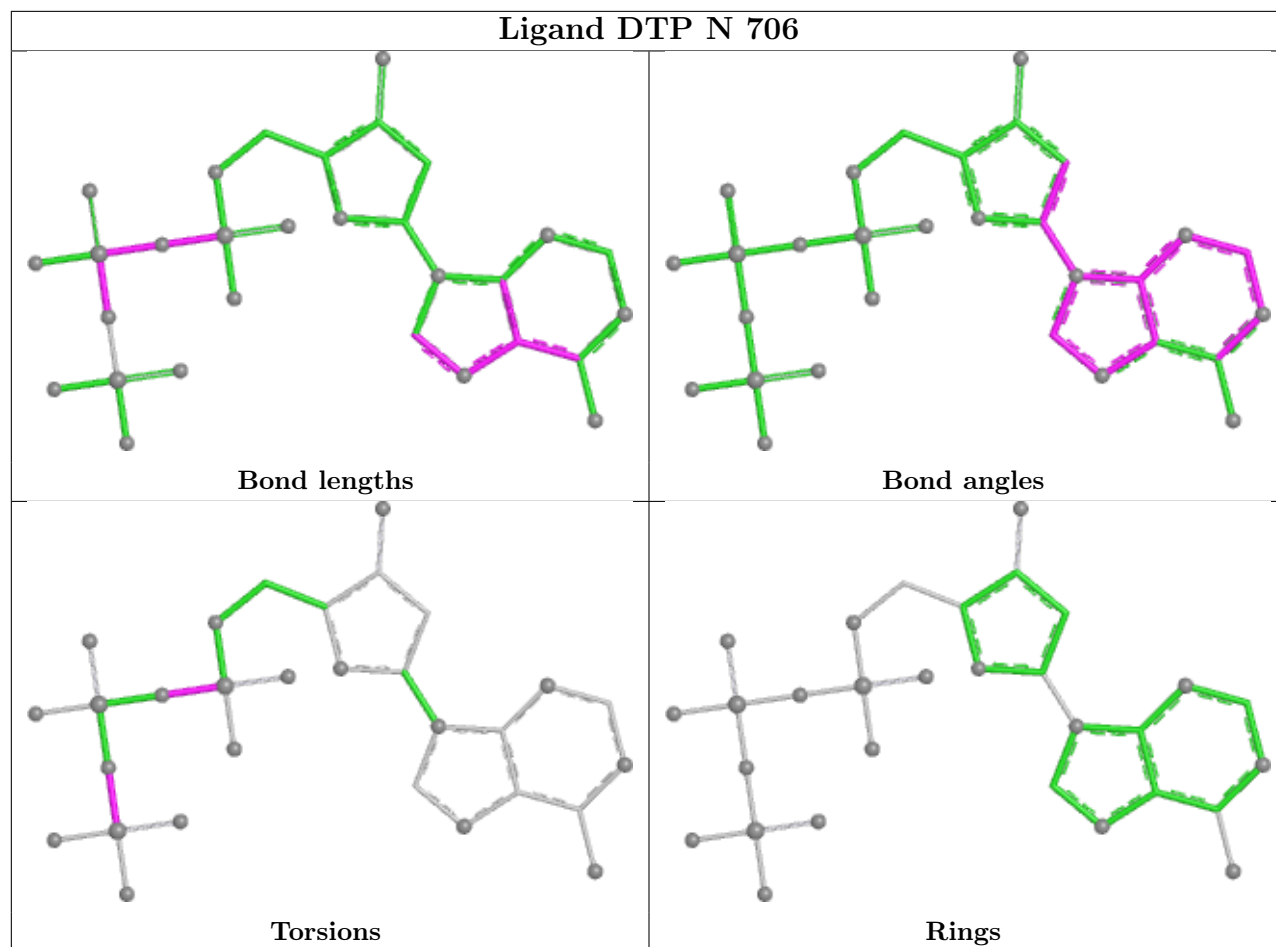


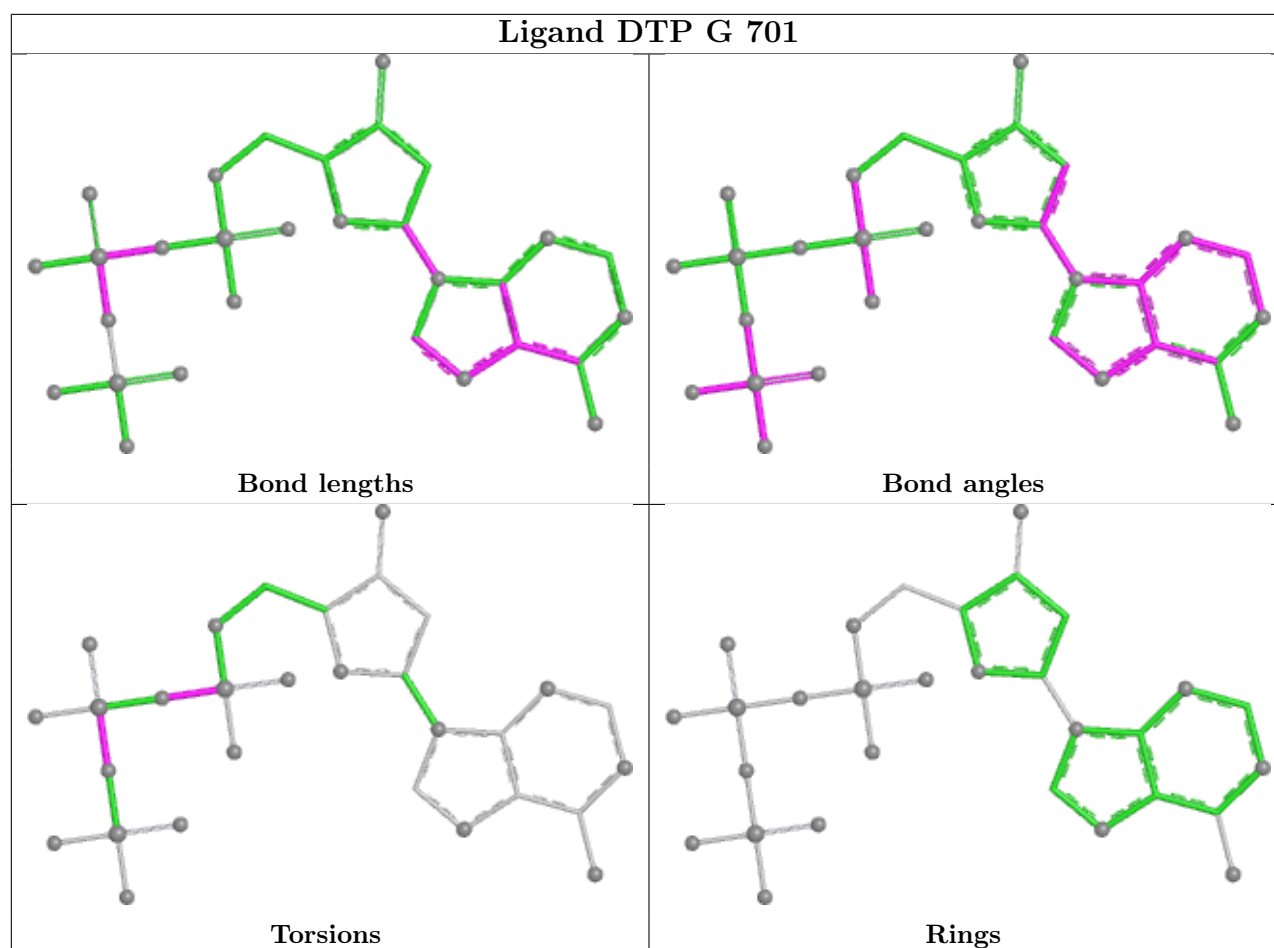
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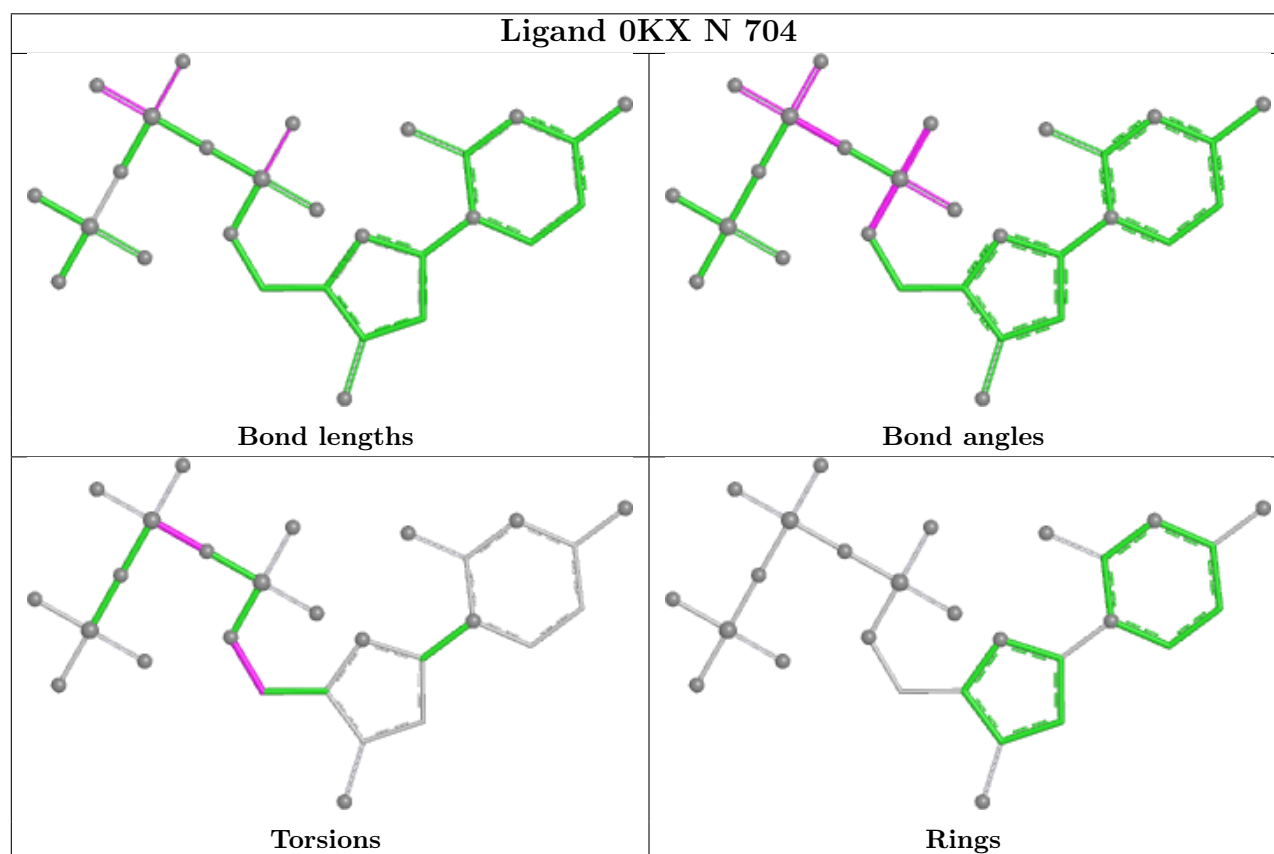
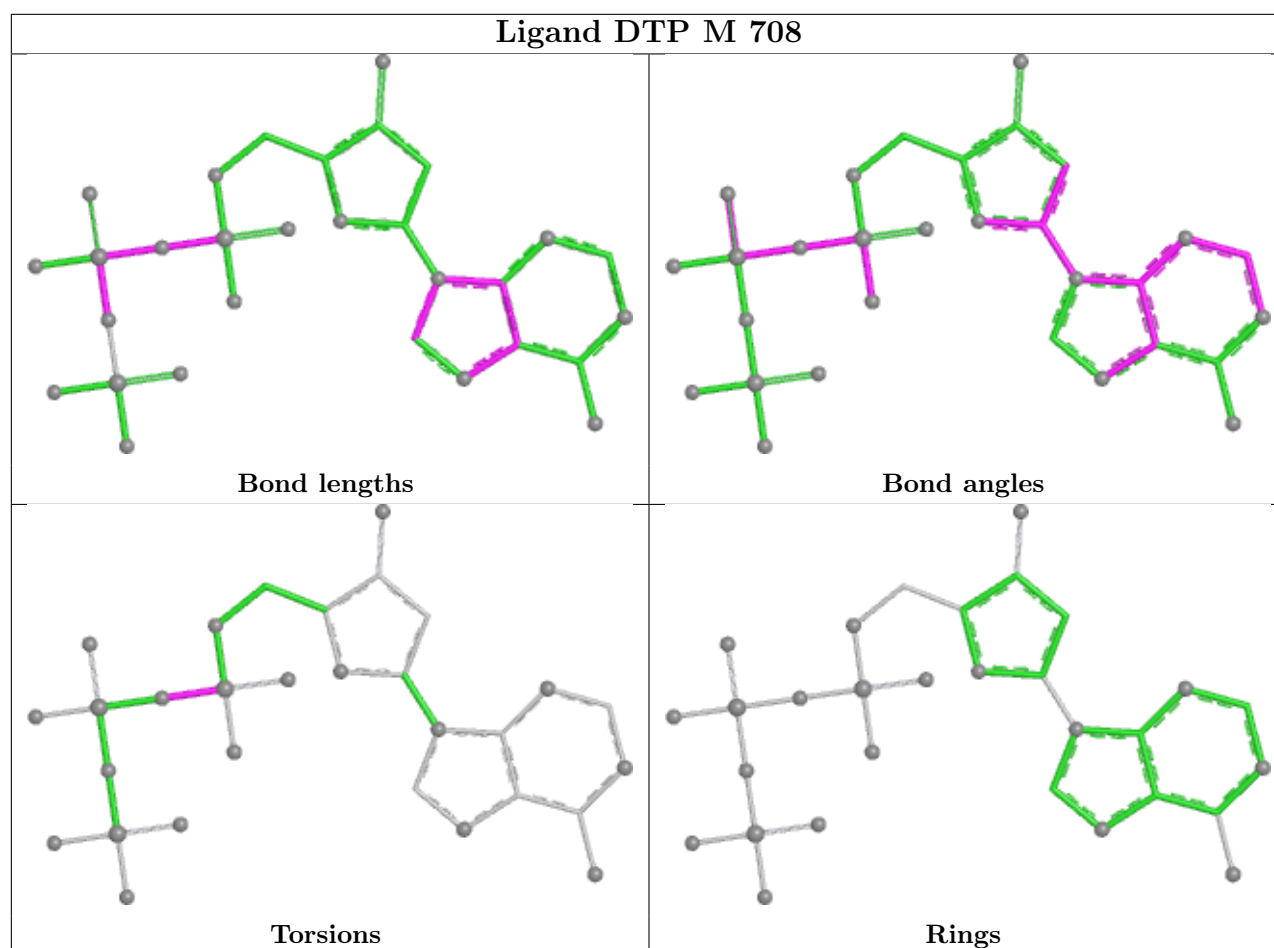


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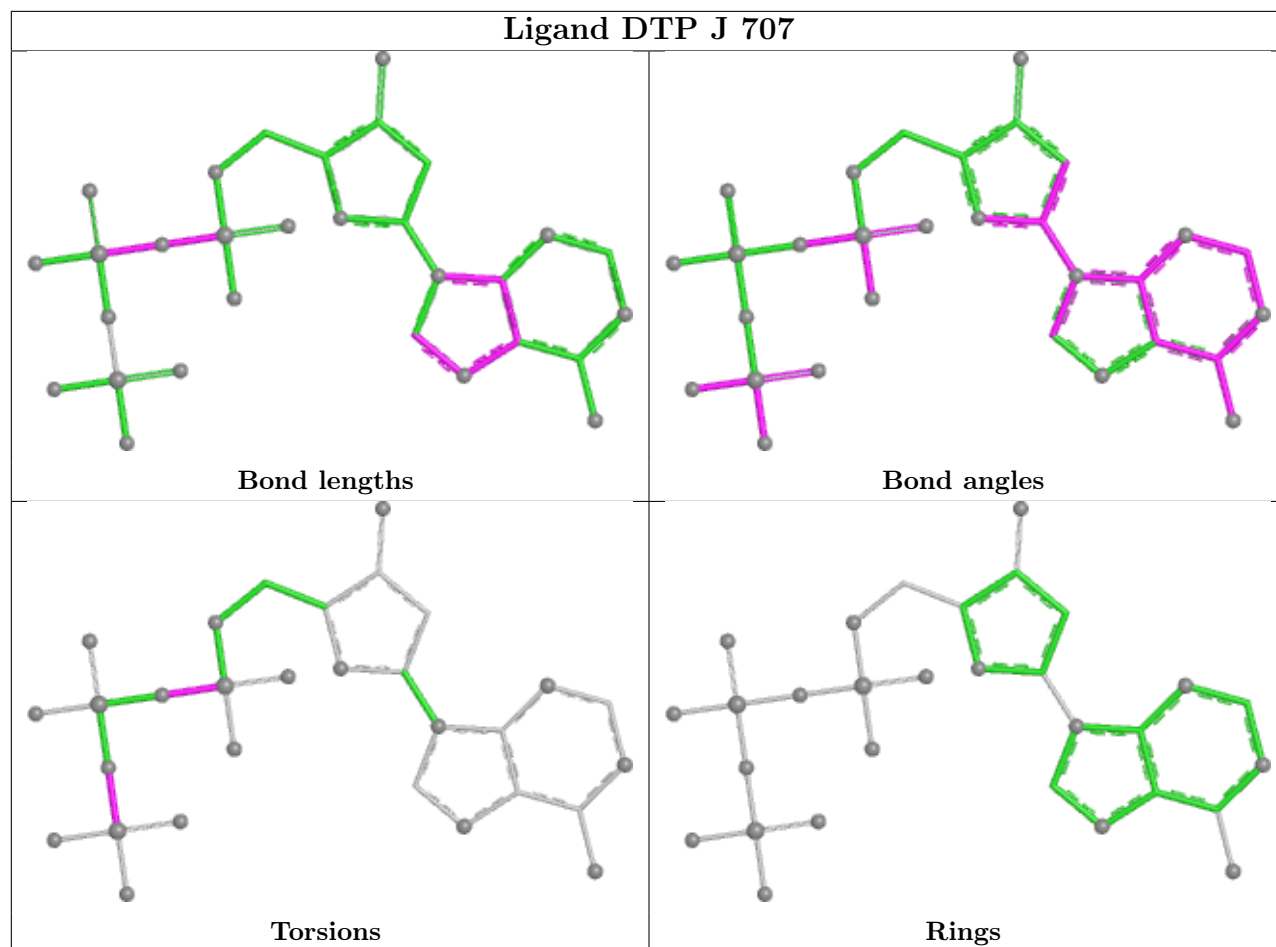




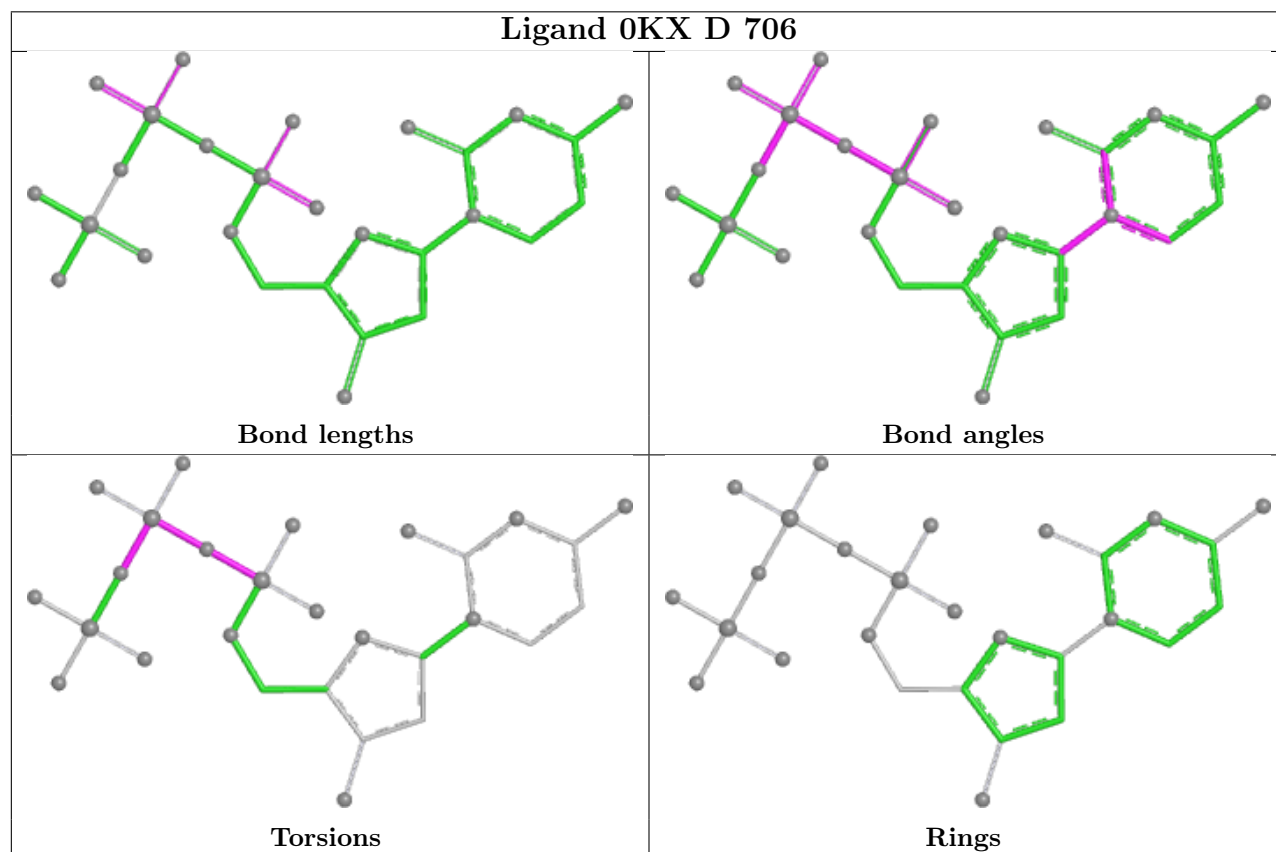




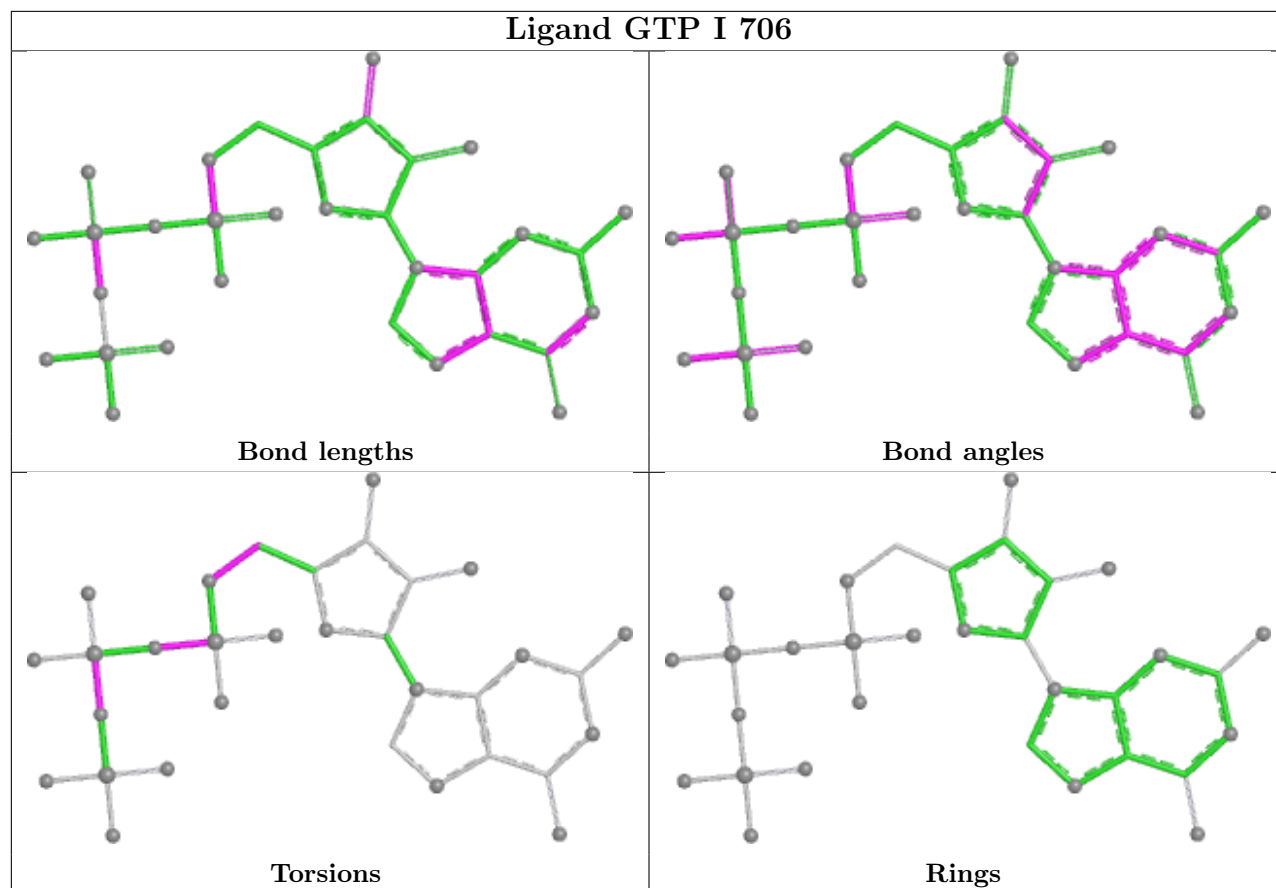
Ligand DTP J 707



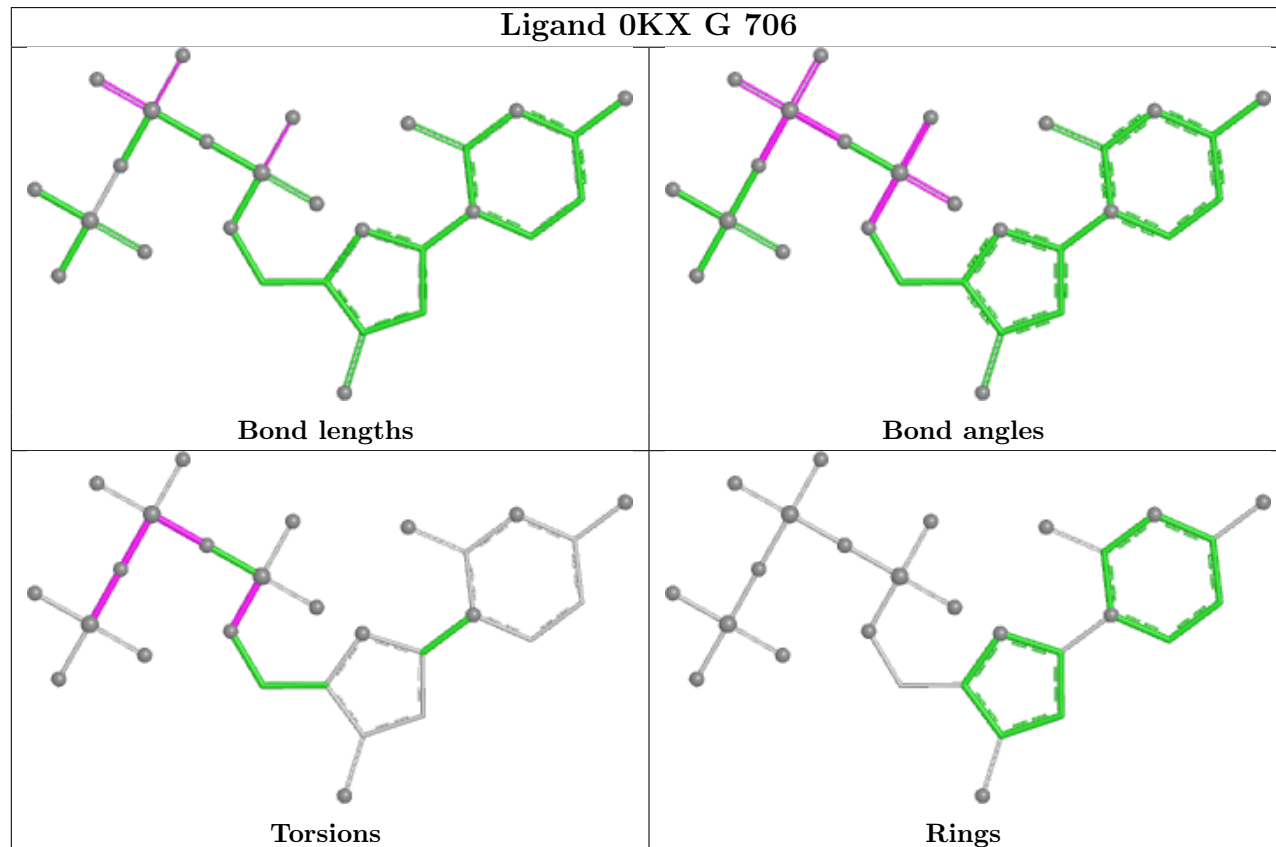
Ligand 0KX D 706

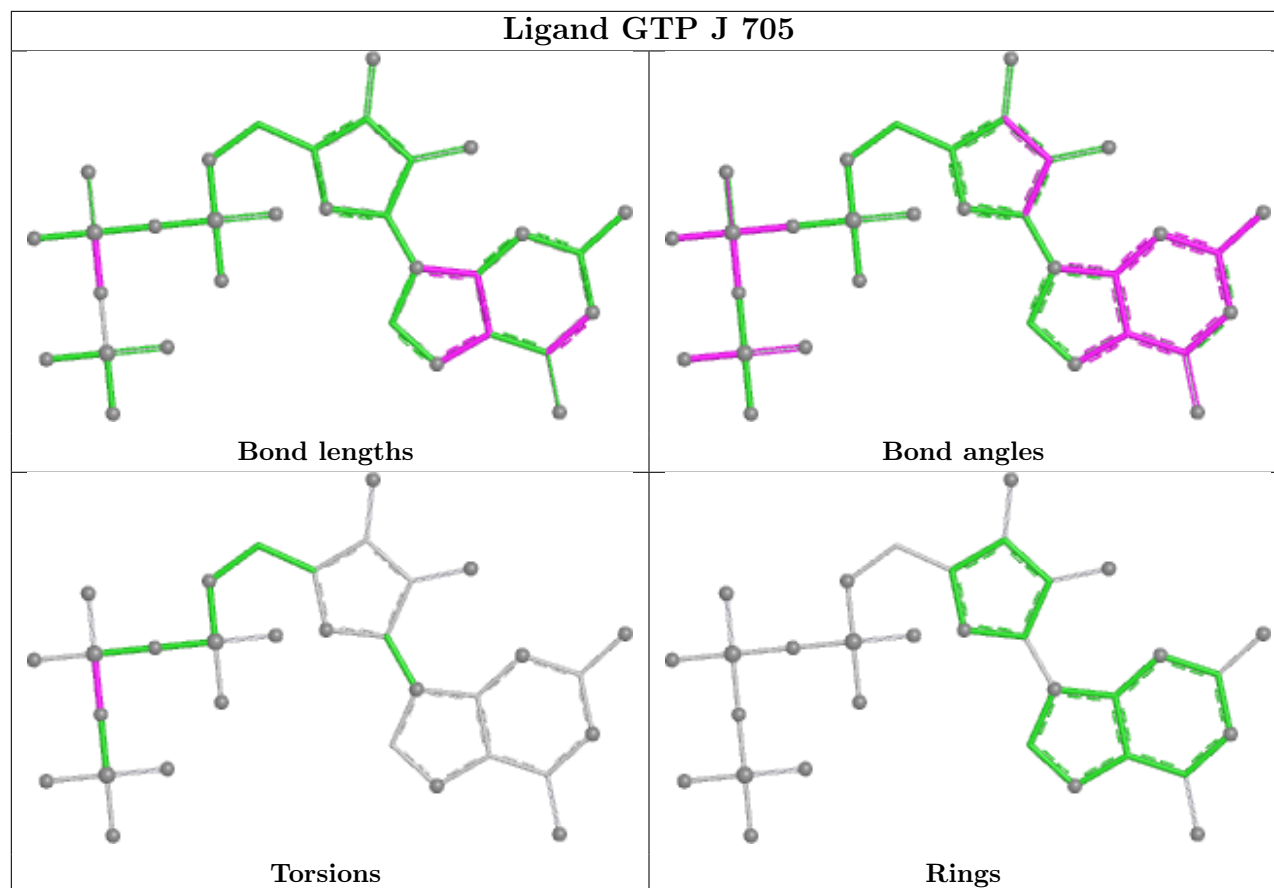


Ligand GTP I 706



Ligand 0KX G 706





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	481/520 (92%)	0.47	11 (2%) 61 52	21, 41, 68, 81	0
1	B	478/520 (91%)	0.48	17 (3%) 46 37	18, 37, 79, 110	0
1	C	480/520 (92%)	0.39	10 (2%) 63 55	17, 36, 58, 90	0
1	D	481/520 (92%)	0.39	7 (1%) 72 65	18, 37, 58, 83	0
1	E	478/520 (91%)	1.04	69 (14%) 6 4	36, 66, 114, 142	0
1	F	463/520 (89%)	1.06	63 (13%) 7 4	39, 64, 105, 120	0
1	G	463/520 (89%)	1.02	57 (12%) 8 6	35, 61, 107, 120	0
1	H	478/520 (91%)	0.66	18 (3%) 44 35	28, 50, 74, 86	0
1	I	477/520 (91%)	0.53	9 (1%) 66 59	25, 50, 74, 93	0
1	J	479/520 (92%)	0.50	9 (1%) 66 59	21, 41, 72, 87	0
1	K	480/520 (92%)	0.52	12 (2%) 58 49	25, 45, 68, 81	0
1	L	475/520 (91%)	0.74	33 (6%) 23 17	25, 49, 91, 120	0
1	M	471/520 (90%)	1.16	45 (9%) 13 11	49, 75, 98, 107	0
1	N	475/520 (91%)	1.11	44 (9%) 14 11	44, 68, 89, 105	0
1	O	465/520 (89%)	1.03	61 (13%) 7 5	36, 64, 104, 124	0
1	P	461/520 (88%)	0.90	48 (10%) 11 9	36, 57, 104, 120	0
All	All	7585/8320 (91%)	0.75	513 (6%) 23 18	17, 52, 95, 142	0

The worst 5 of 513 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	274	GLY	5.0
1	F	466	ILE	4.7
1	P	483	ALA	4.3
1	G	491	VAL	4.3
1	I	115	MET	4.2

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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	J	706	5/5	0.77	0.14	70,72,73,74	0
6	SO4	H	707	5/5	0.80	0.12	94,94,94,95	0
6	SO4	I	707	5/5	0.81	0.12	92,93,97,97	0
6	SO4	B	707	5/5	0.82	0.12	67,68,70,71	0
6	SO4	L	708	5/5	0.82	0.12	72,75,77,80	0
3	MG	I	702	1/1	0.83	0.15	55,55,55,55	0
3	MG	N	702	1/1	0.85	0.18	40,40,40,40	0
3	MG	P	703	1/1	0.86	0.10	39,39,39,39	0
6	SO4	A	707	5/5	0.87	0.12	83,84,84,85	0
6	SO4	D	708	5/5	0.87	0.10	69,71,72,73	0
6	SO4	M	707	5/5	0.87	0.09	88,89,90,92	0
3	MG	M	703	1/1	0.88	0.20	46,46,46,46	0
3	MG	F	702	1/1	0.89	0.27	35,35,35,35	0
3	MG	D	703	1/1	0.90	0.08	32,32,32,32	0
3	MG	P	704	1/1	0.91	0.20	28,28,28,28	0
3	MG	A	703	1/1	0.91	0.20	16,16,16,16	0
3	MG	E	702	1/1	0.91	0.24	32,32,32,32	0
6	SO4	C	708	5/5	0.91	0.08	57,57,59,60	0
3	MG	M	702	1/1	0.91	0.09	59,59,59,59	0
3	MG	J	702	1/1	0.92	0.08	17,17,17,17	0
3	MG	I	703	1/1	0.92	0.18	20,20,20,20	0
4	OKX	M	705	28/28	0.92	0.10	52,56,59,61	0
3	MG	K	704	1/1	0.93	0.13	19,19,19,19	0
3	MG	H	703	1/1	0.93	0.17	25,25,25,25	0
3	MG	G	704	1/1	0.94	0.17	33,33,33,33	0
3	MG	N	703	1/1	0.94	0.07	40,40,40,40	0
3	MG	L	704	1/1	0.94	0.15	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	B	703	1/1	0.94	0.12	13,13,13,13	0
3	MG	H	704	1/1	0.94	0.06	37,37,37,37	0
4	OKX	O	705	28/28	0.94	0.09	48,51,56,59	0
5	GTP	F	705	32/32	0.94	0.09	44,48,53,55	0
5	GTP	H	706	32/32	0.94	0.08	36,39,43,45	0
5	GTP	N	705	32/32	0.94	0.08	50,52,54,54	0
7	DTP	F	706	30/30	0.94	0.08	36,39,45,47	0
4	OKX	F	704	28/28	0.95	0.08	42,47,50,52	0
4	OKX	G	706	28/28	0.95	0.08	40,45,47,49	0
3	MG	K	705	1/1	0.95	0.06	30,30,30,30	0
4	OKX	N	704	28/28	0.95	0.08	51,54,55,55	0
3	MG	F	703	1/1	0.95	0.07	44,44,44,44	0
3	MG	K	703	1/1	0.95	0.10	68,68,68,68	0
3	MG	C	704	1/1	0.95	0.16	13,13,13,13	0
5	GTP	M	706	32/32	0.95	0.07	48,51,56,56	0
3	MG	P	705	1/1	0.95	0.04	43,43,43,43	0
7	DTP	E	706	30/30	0.95	0.07	28,29,34,34	0
5	GTP	O	706	32/32	0.95	0.07	45,50,58,61	0
7	DTP	G	701	30/30	0.95	0.07	41,44,52,54	0
7	DTP	P	701	30/30	0.95	0.07	44,45,49,51	0
5	GTP	O	707	32/32	0.96	0.06	37,41,47,48	0
4	OKX	L	706	28/28	0.96	0.07	31,35,39,41	0
3	MG	G	703	1/1	0.96	0.07	52,52,52,52	0
3	MG	D	704	1/1	0.96	0.14	13,13,13,13	0
3	MG	B	704	1/1	0.96	0.09	20,20,20,20	0
4	OKX	P	706	28/28	0.96	0.07	40,43,50,53	0
5	GTP	E	705	32/32	0.96	0.06	45,49,55,57	0
4	OKX	C	706	28/28	0.96	0.07	19,21,26,27	0
3	MG	B	702	1/1	0.96	0.10	61,61,61,61	0
5	GTP	I	706	32/32	0.96	0.06	26,29,37,38	0
5	GTP	K	707	32/32	0.96	0.06	36,40,44,46	0
3	MG	A	704	1/1	0.96	0.06	20,20,20,20	0
4	OKX	H	705	28/28	0.96	0.07	38,40,42,44	0
7	DTP	H	701	30/30	0.96	0.07	39,43,49,52	0
7	DTP	J	707	30/30	0.96	0.07	19,21,23,23	0
7	DTP	L	701	30/30	0.96	0.07	26,28,31,32	0
7	DTP	M	708	30/30	0.96	0.07	41,45,58,59	0
7	DTP	N	706	30/30	0.96	0.07	38,43,48,50	0
7	DTP	O	701	30/30	0.96	0.07	44,46,49,49	0
4	OKX	I	705	28/28	0.96	0.07	28,31,33,34	0
3	MG	J	703	1/1	0.97	0.07	18,18,18,18	0
4	OKX	A	705	28/28	0.97	0.06	23,29,32,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	D	705	1/1	0.97	0.05	23,23,23,23	0
5	GTP	A	706	32/32	0.97	0.06	21,23,27,29	0
5	GTP	B	706	32/32	0.97	0.06	20,22,26,27	0
4	OKX	D	706	28/28	0.97	0.07	21,23,27,30	0
4	OKX	E	704	28/28	0.97	0.06	42,45,48,50	0
5	GTP	G	707	32/32	0.97	0.06	30,31,32,33	0
7	DTP	A	708	30/30	0.97	0.06	21,25,26,28	0
7	DTP	B	708	30/30	0.97	0.06	15,16,19,19	0
7	DTP	D	701	30/30	0.97	0.07	20,25,28,30	0
3	MG	A	702	1/1	0.97	0.07	48,48,48,48	0
3	MG	E	703	1/1	0.97	0.04	52,52,52,52	0
5	GTP	J	705	32/32	0.97	0.06	21,23,25,26	0
3	MG	O	703	1/1	0.97	0.14	31,31,31,31	0
7	DTP	I	708	30/30	0.97	0.06	30,33,38,39	0
5	GTP	L	707	32/32	0.97	0.06	21,24,26,27	0
7	DTP	K	701	30/30	0.97	0.06	25,28,30,30	0
3	MG	O	704	1/1	0.97	0.04	43,43,43,43	0
4	OKX	J	704	28/28	0.97	0.06	23,26,28,29	0
4	OKX	K	706	28/28	0.97	0.06	31,34,38,40	0
3	MG	L	703	1/1	0.97	0.07	37,37,37,37	0
3	MG	C	705	1/1	0.97	0.03	24,24,24,24	0
3	MG	G	705	1/1	0.98	0.05	25,25,25,25	0
3	MG	C	703	1/1	0.98	0.06	32,32,32,32	0
7	DTP	C	701	30/30	0.98	0.05	16,18,23,24	0
3	MG	M	704	1/1	0.98	0.04	49,49,49,49	0
4	OKX	B	705	28/28	0.98	0.05	19,22,24,25	0
2	FE	I	701	1/1	0.98	0.03	25,25,25,25	0
5	GTP	C	707	32/32	0.98	0.05	21,23,26,27	0
5	GTP	D	707	32/32	0.98	0.05	16,17,19,20	0
2	FE	J	701	1/1	0.99	0.02	18,18,18,18	0
3	MG	I	704	1/1	0.99	0.05	23,23,23,23	0
2	FE	N	701	1/1	0.99	0.03	38,38,38,38	0
2	FE	E	701	1/1	0.99	0.02	42,42,42,42	0
3	MG	L	705	1/1	0.99	0.04	22,22,22,22	0
2	FE	B	701	1/1	0.99	0.02	16,16,16,16	0
2	FE	F	701	1/1	1.00	0.01	33,33,33,33	0
2	FE	G	702	1/1	1.00	0.01	30,30,30,30	0
2	FE	H	702	1/1	1.00	0.03	26,26,26,26	0
2	FE	C	702	1/1	1.00	0.02	17,17,17,17	0
2	FE	D	702	1/1	1.00	0.03	14,14,14,14	0
2	FE	K	702	1/1	1.00	0.02	28,28,28,28	0
2	FE	L	702	1/1	1.00	0.02	25,25,25,25	0

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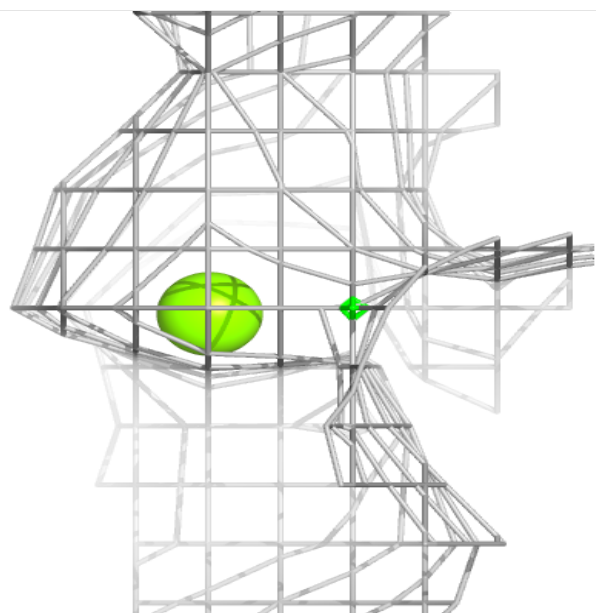
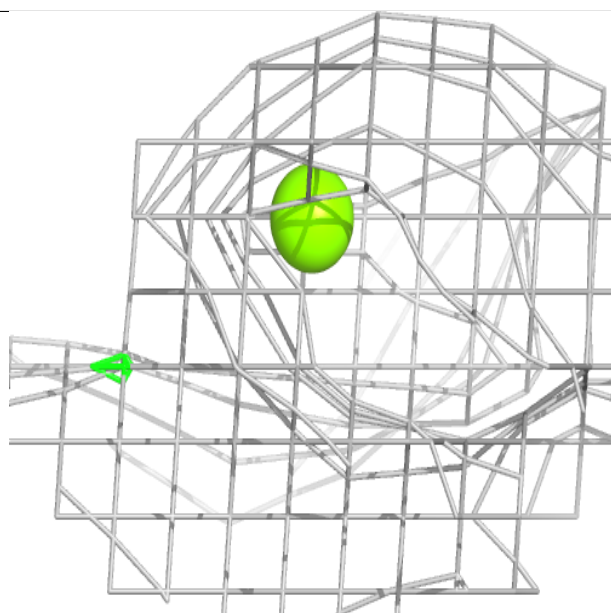
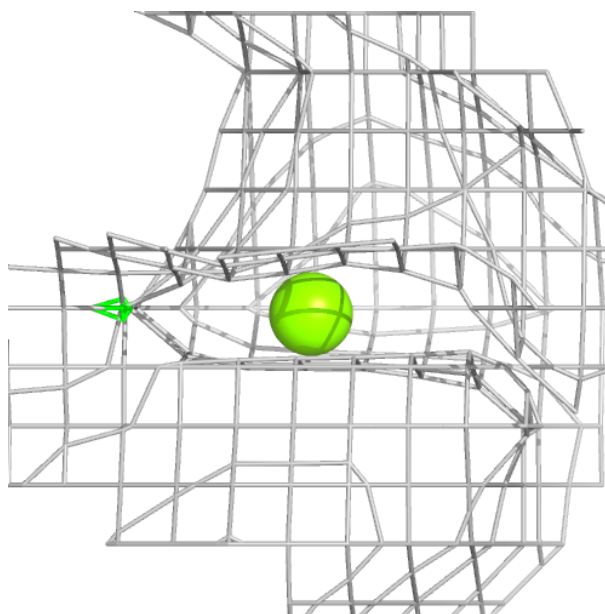
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FE	M	701	1/1	1.00	0.02	44,44,44,44	0
2	FE	A	701	1/1	1.00	0.02	22,22,22,22	0
2	FE	O	702	1/1	1.00	0.02	39,39,39,39	0
2	FE	P	702	1/1	1.00	0.01	30,30,30,30	0

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.

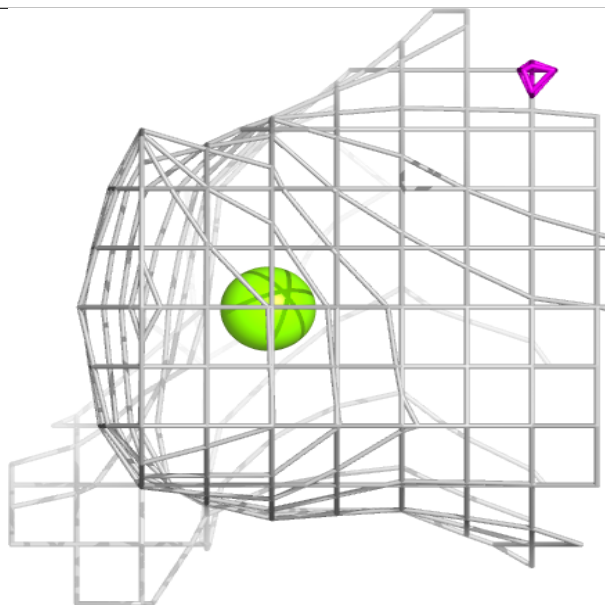
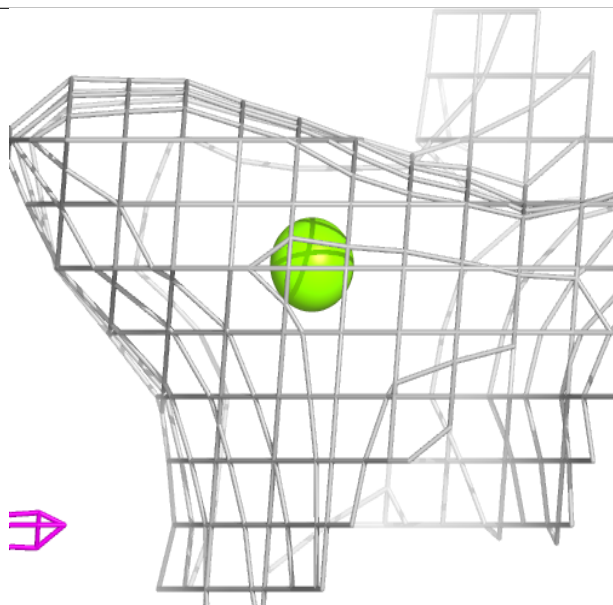
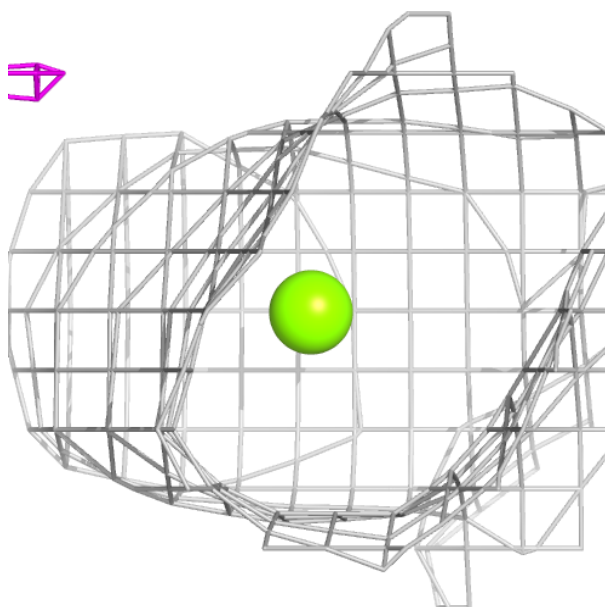
Electron density around MG I 702:

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



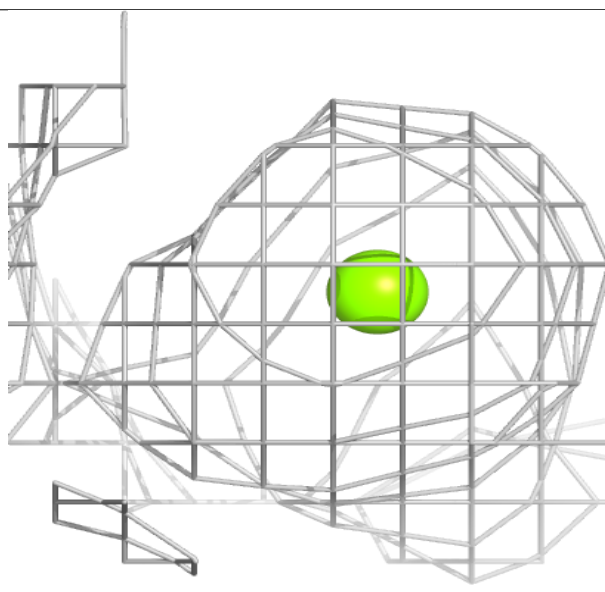
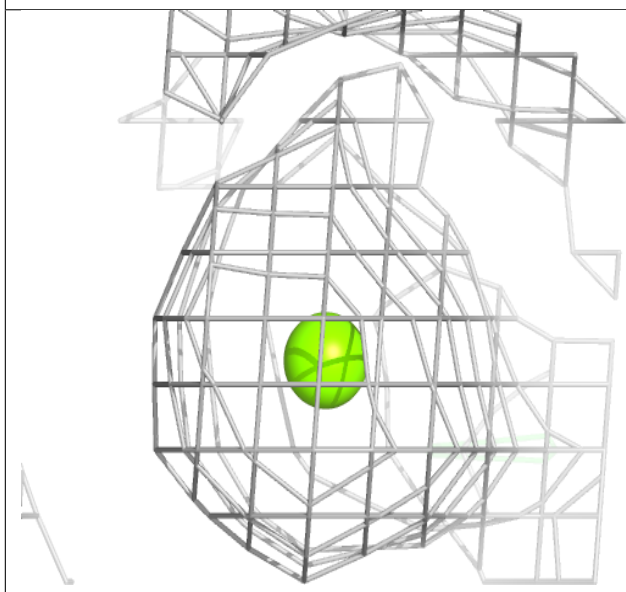
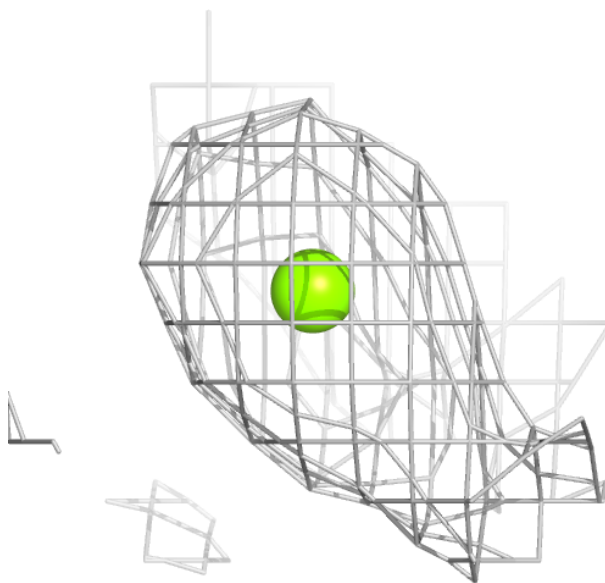
Electron density around MG N 702:

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and green (positive)



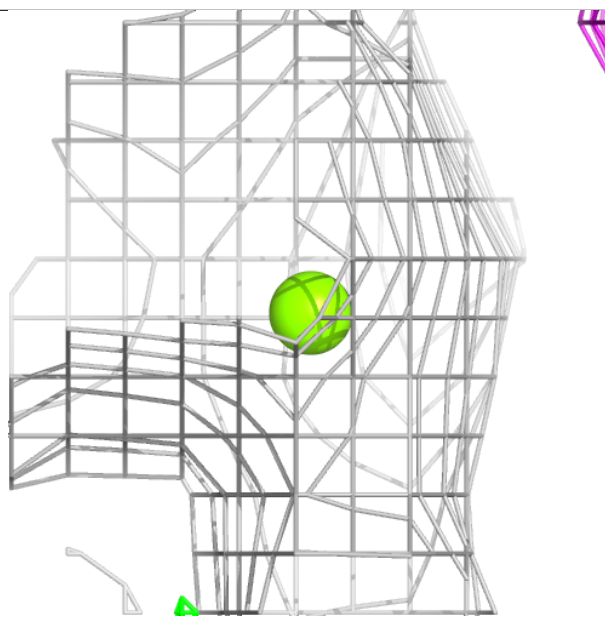
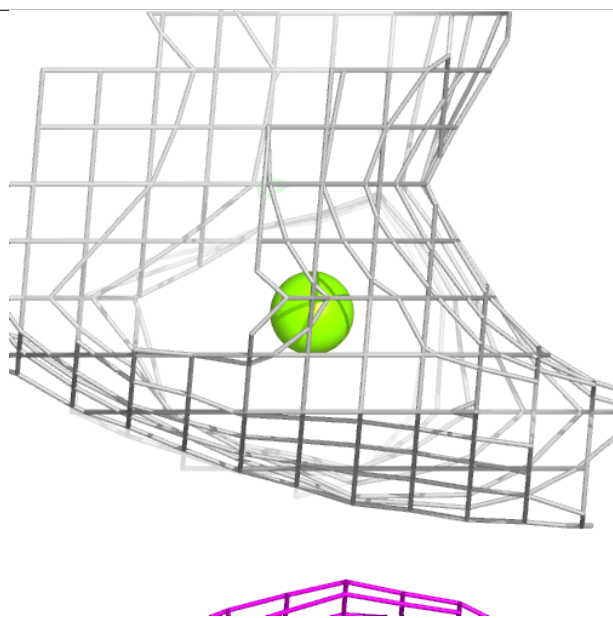
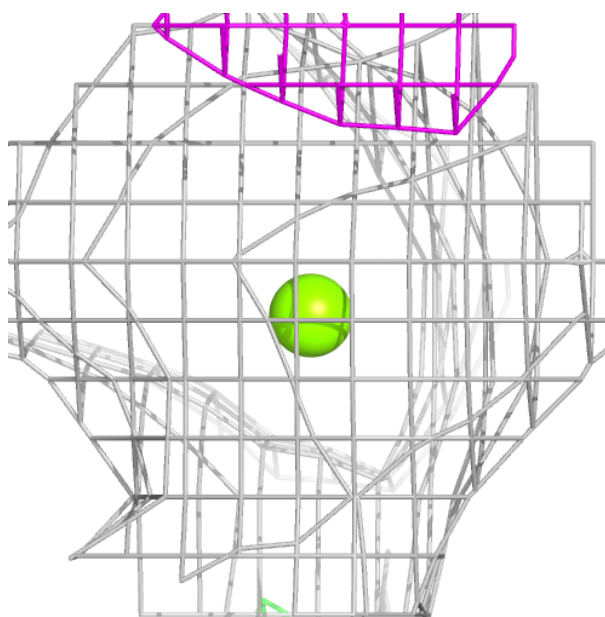
Electron density around MG P 703:

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and green (positive)



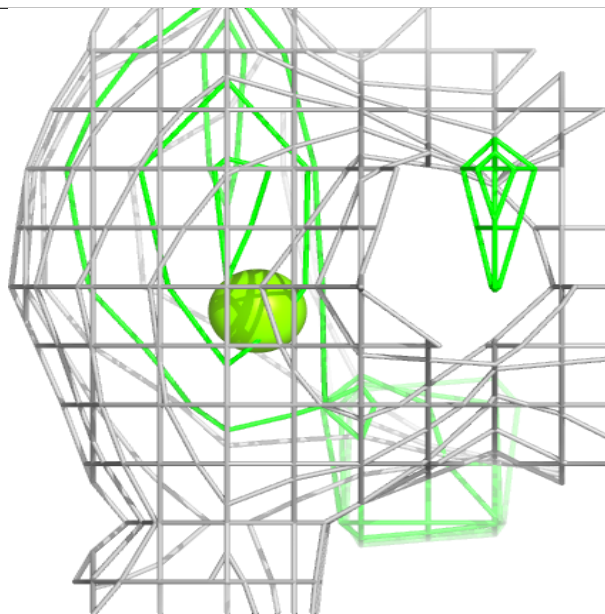
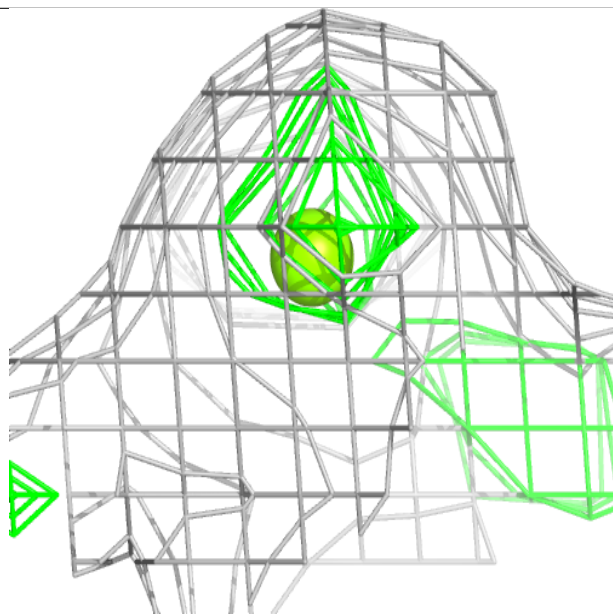
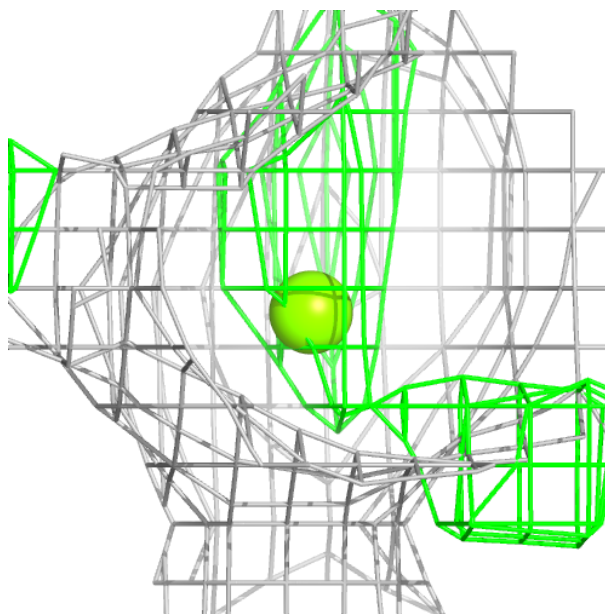
Electron density around MG M 703:

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and green (positive)



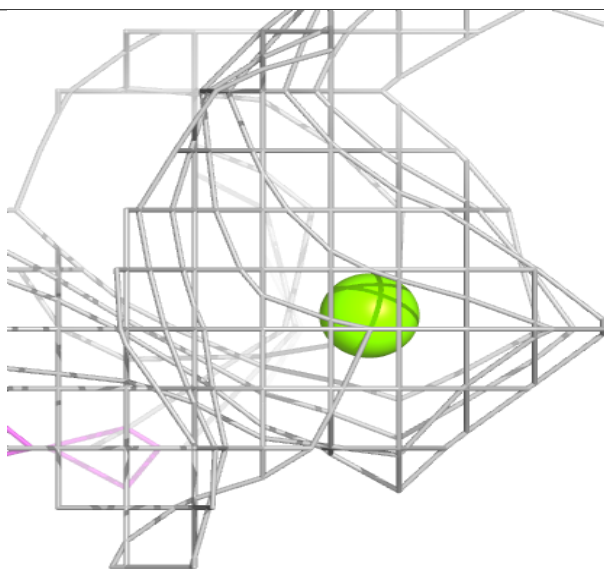
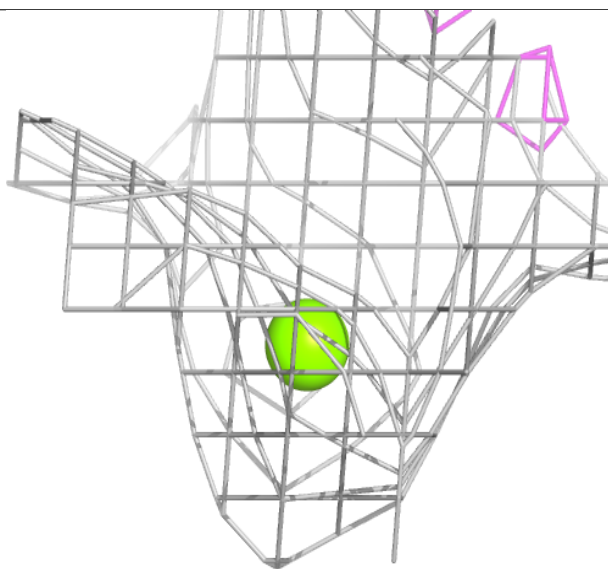
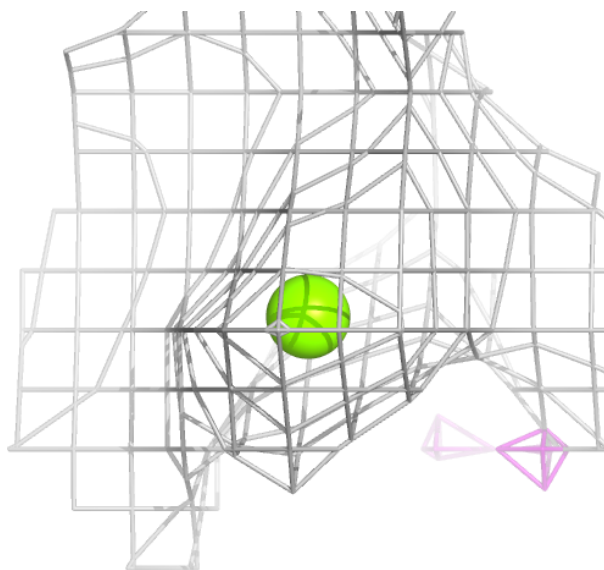
Electron density around MG F 702:

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and green (positive)



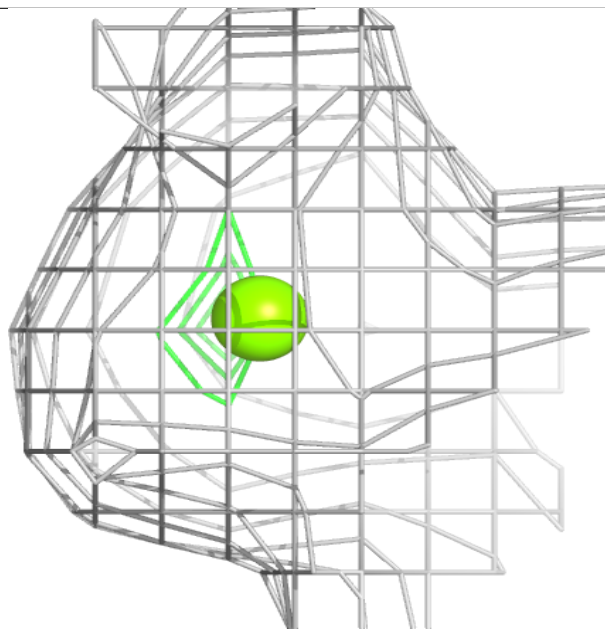
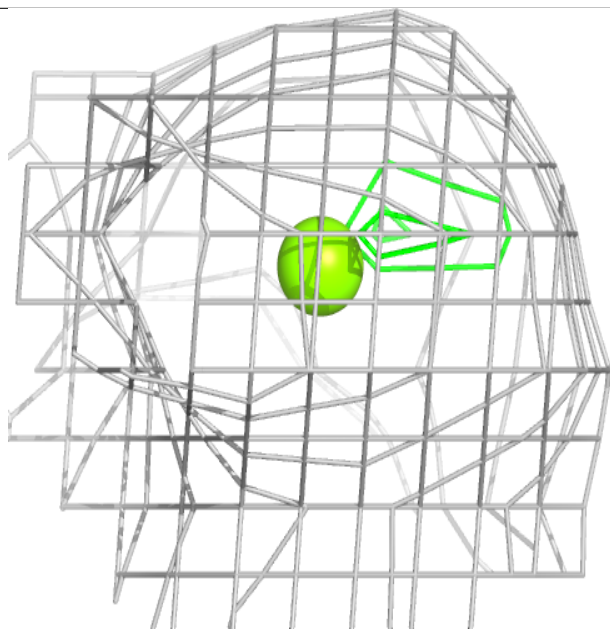
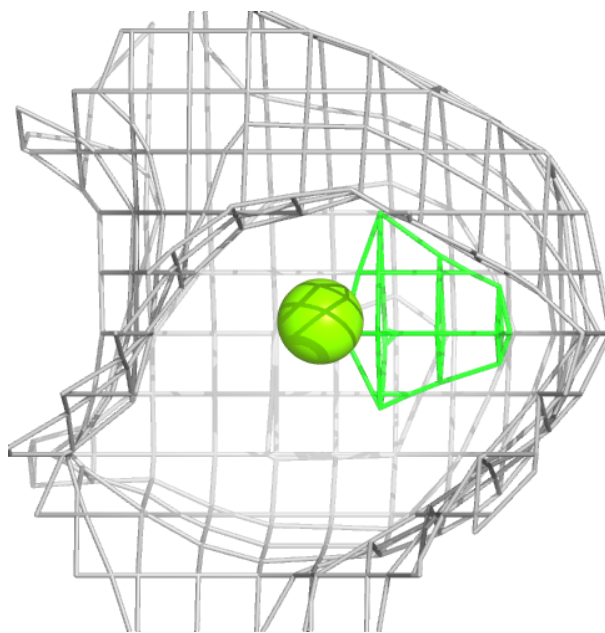
Electron density around MG D 703:

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



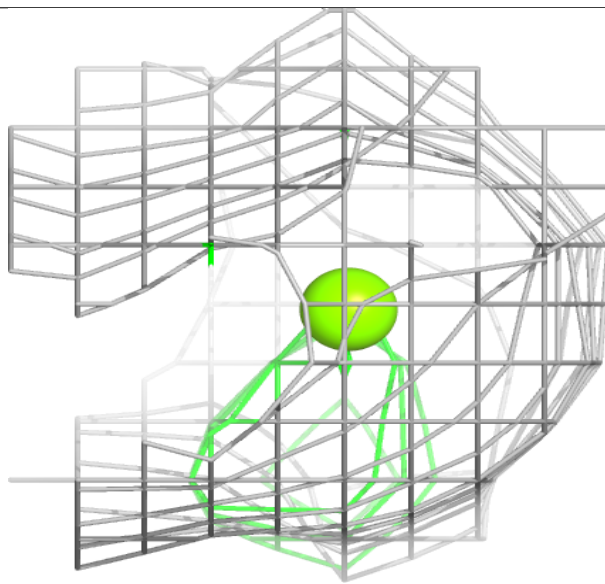
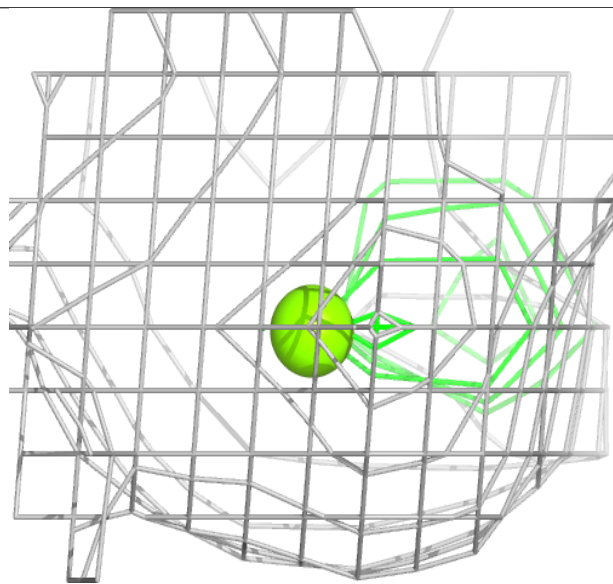
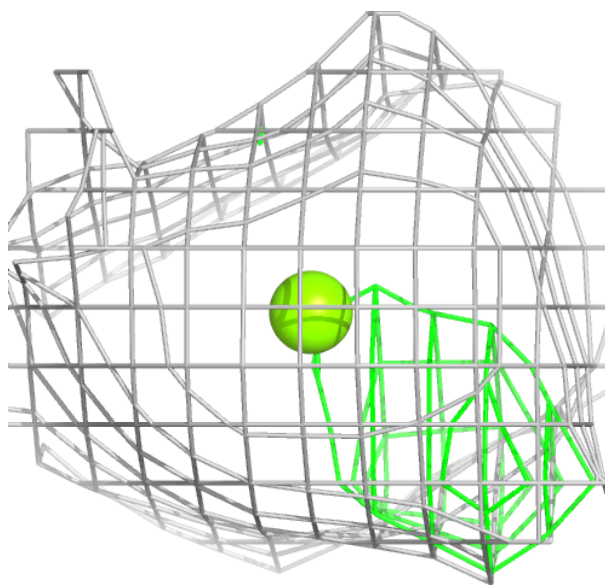
Electron density around MG P 704:

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



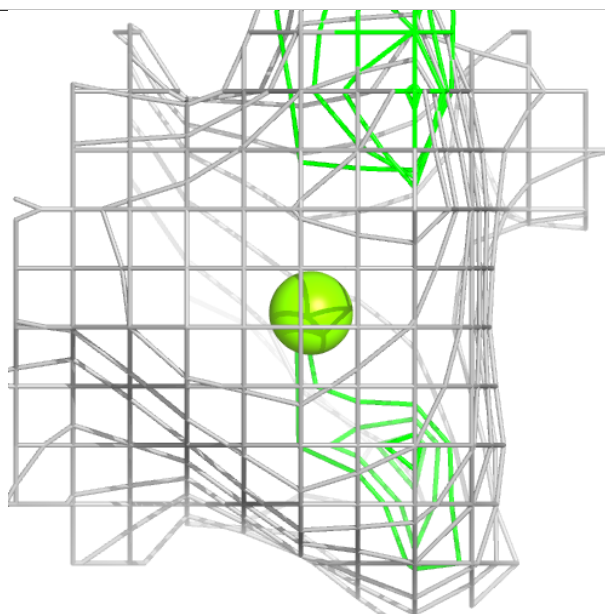
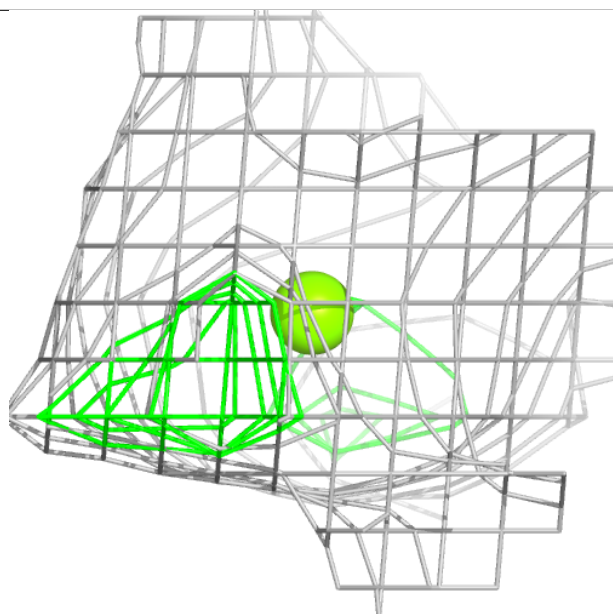
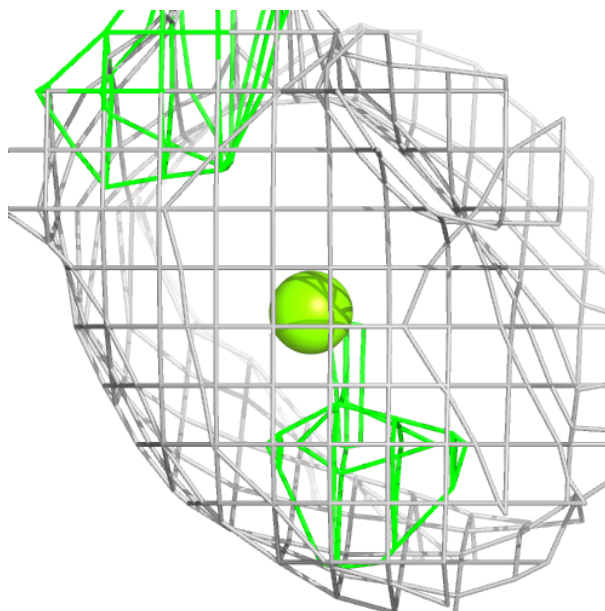
Electron density around MG A 703:

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



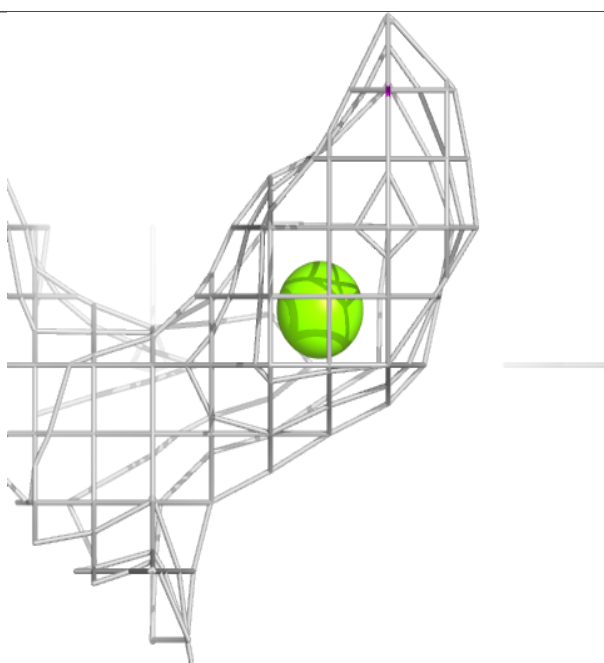
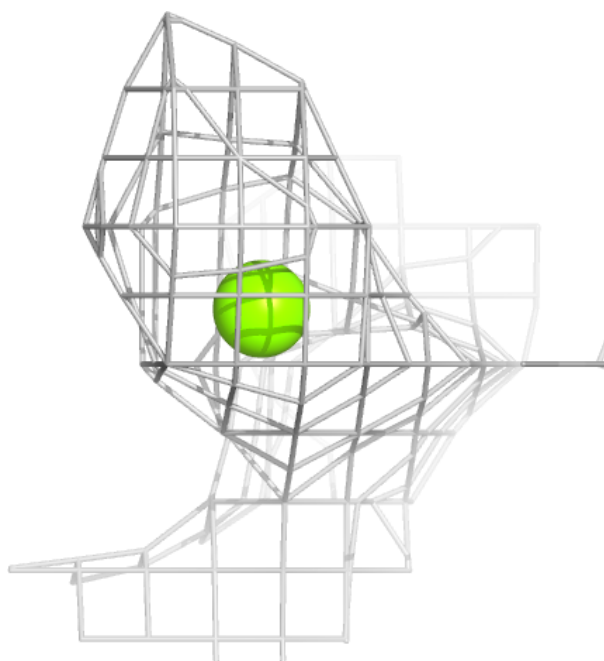
Electron density around MG E 702:

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



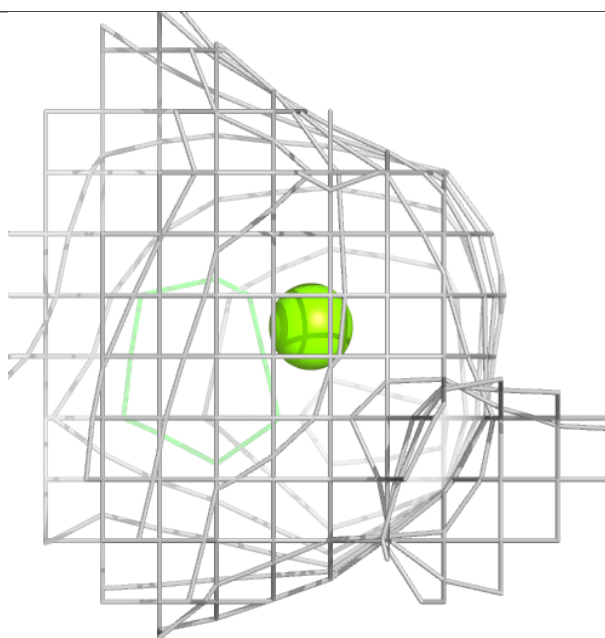
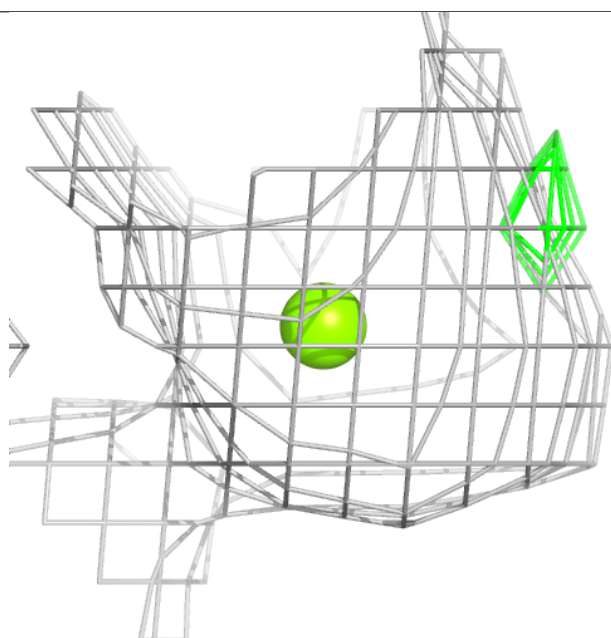
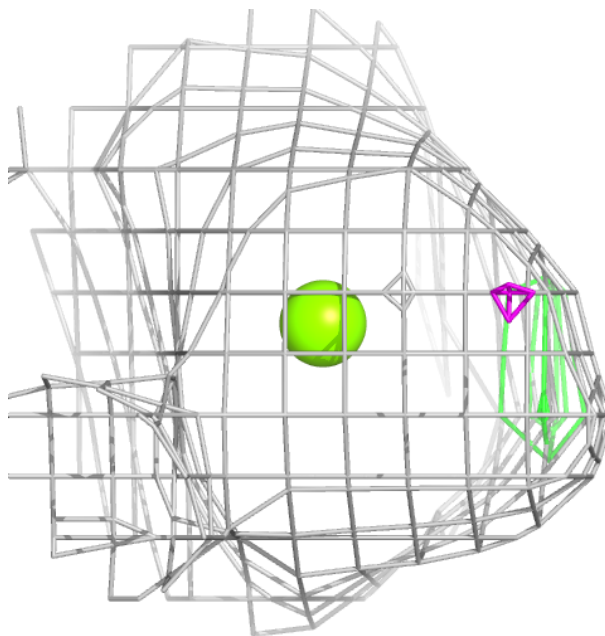
Electron density around MG M 702:

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



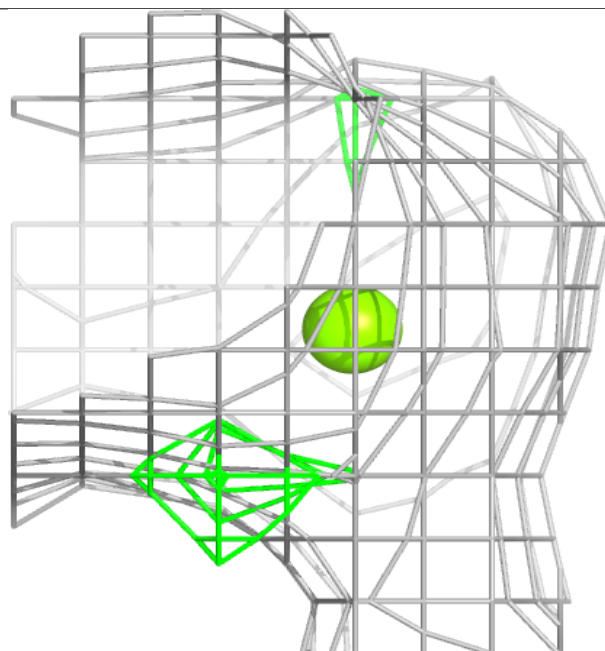
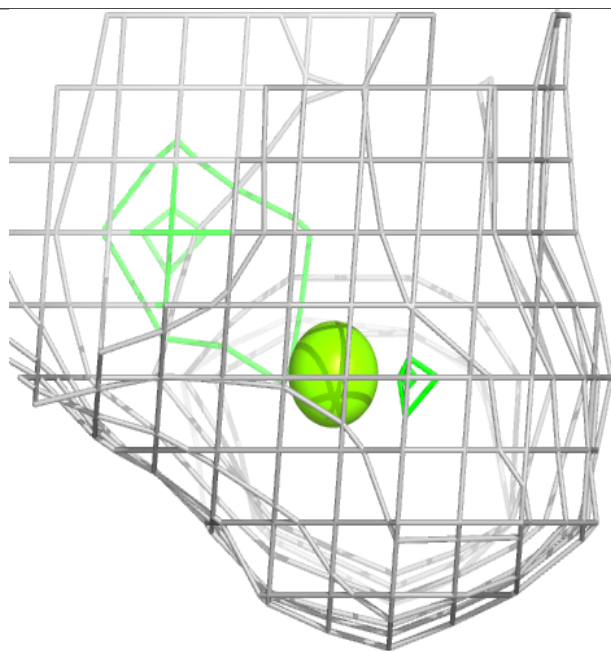
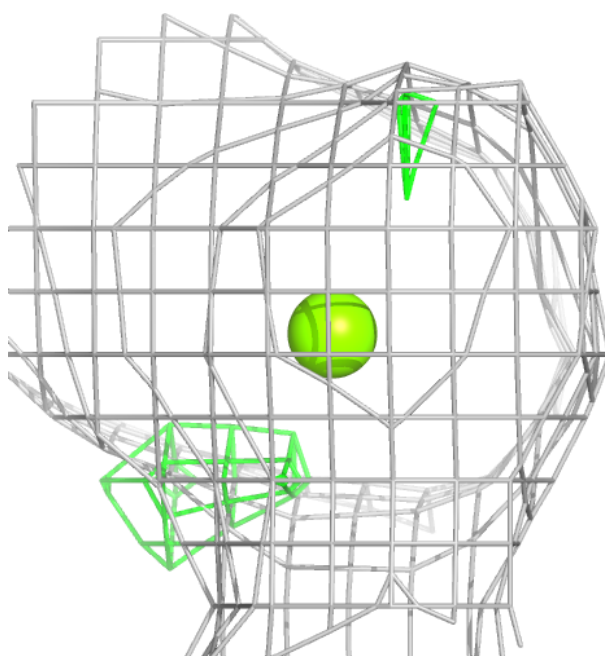
Electron density around MG J 702:

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



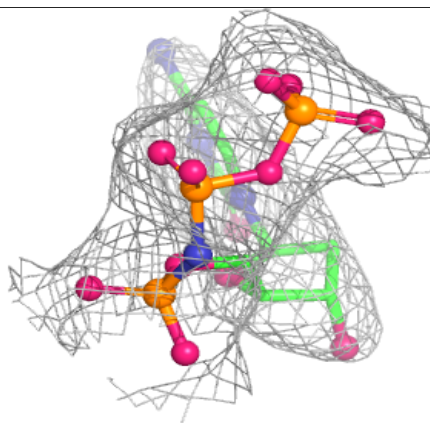
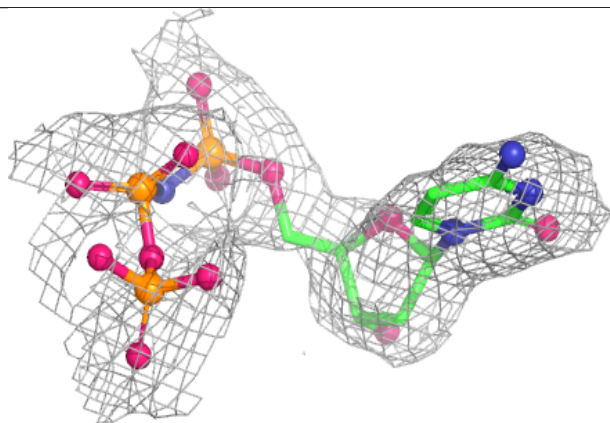
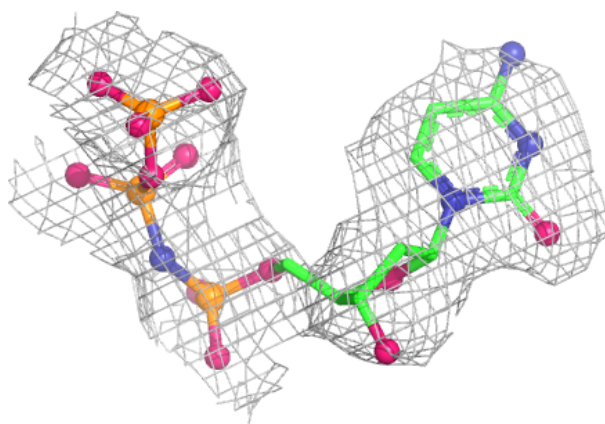
Electron density around MG I 703:

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



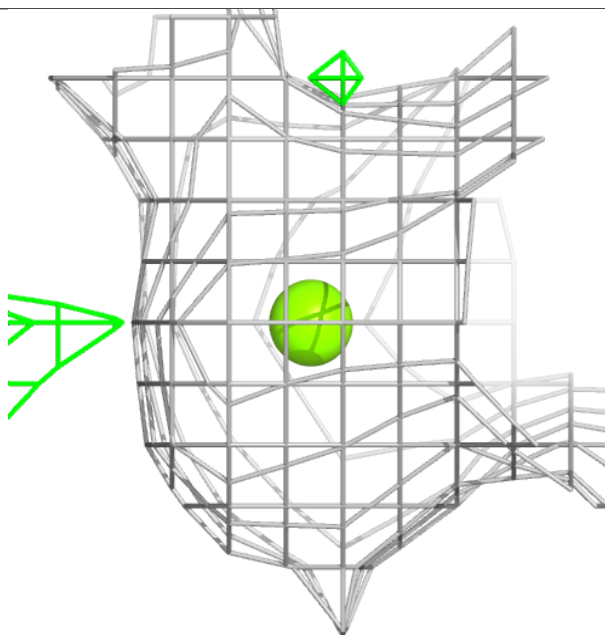
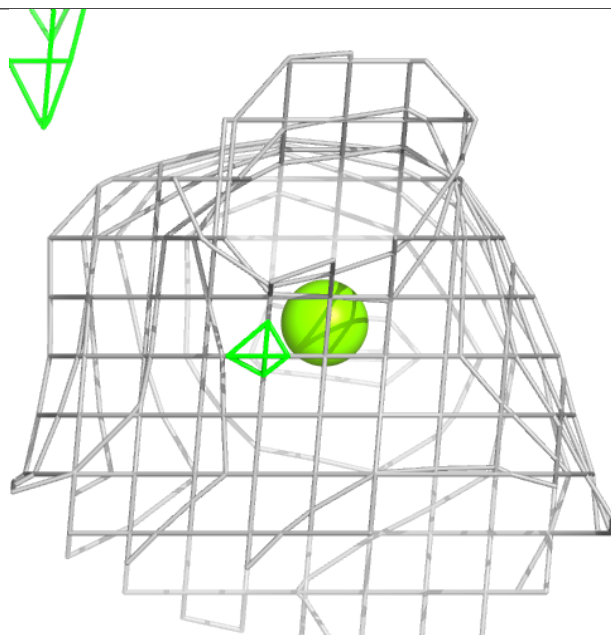
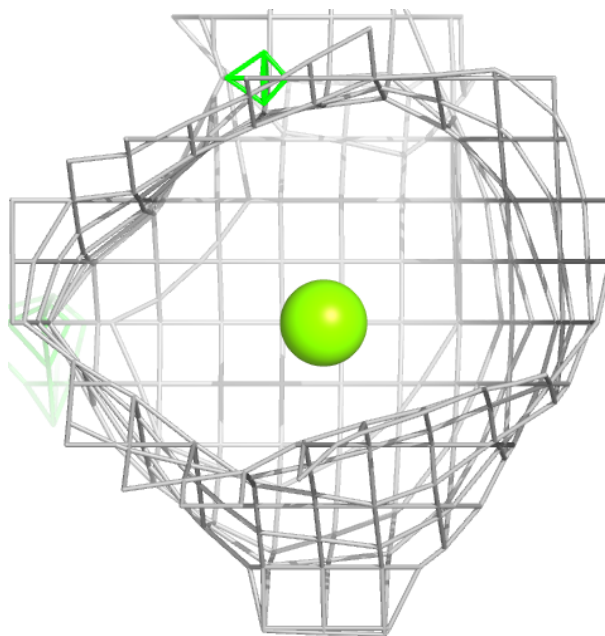
Electron density around 0KX M 705:

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



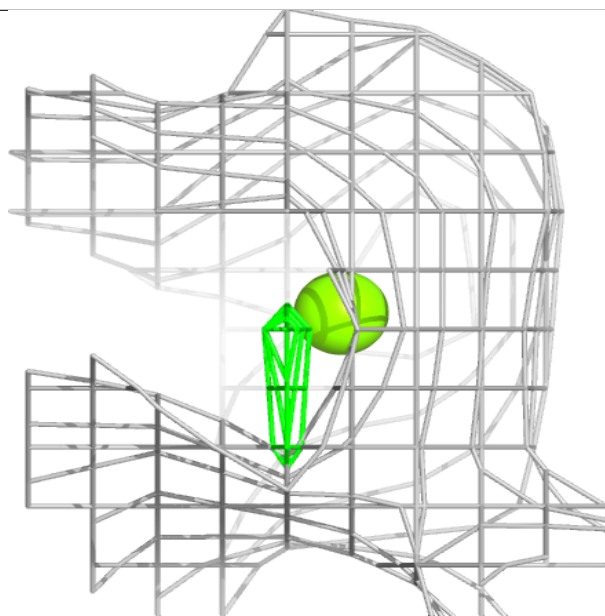
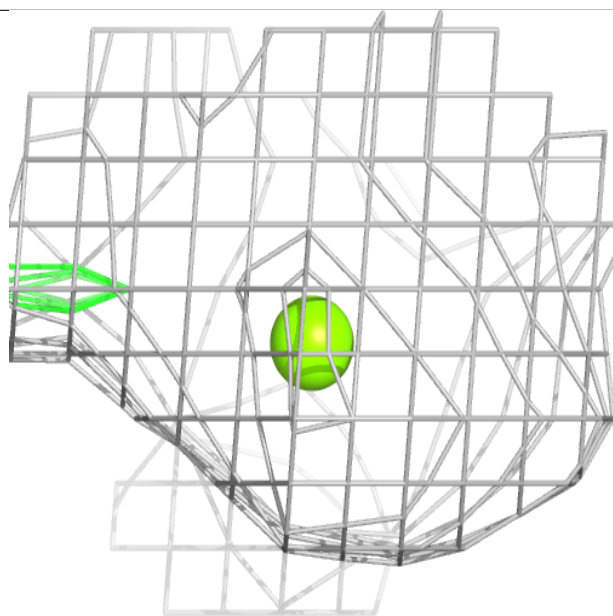
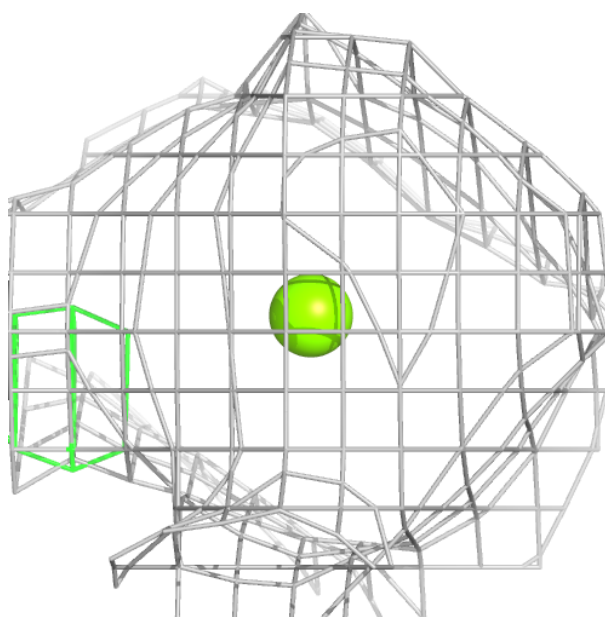
Electron density around MG K 704:

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



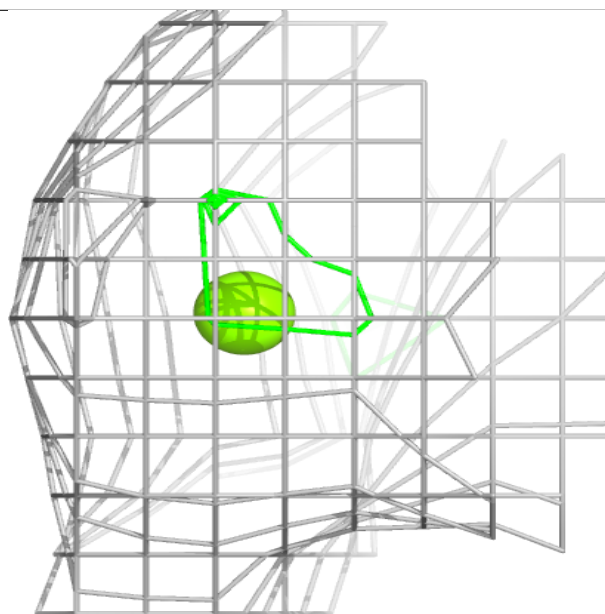
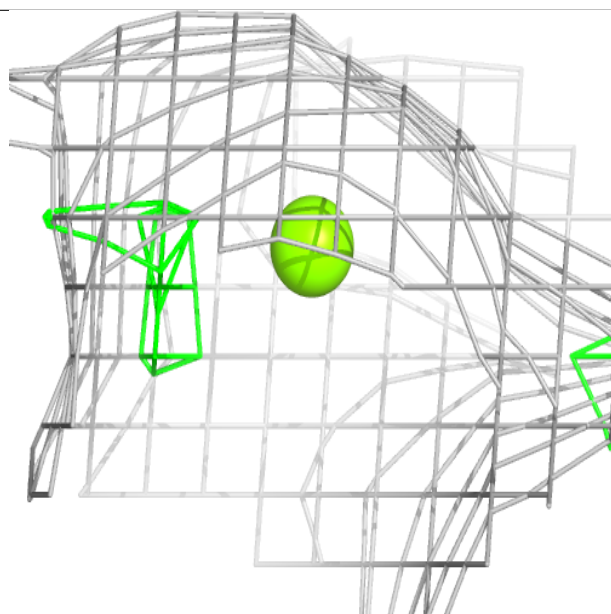
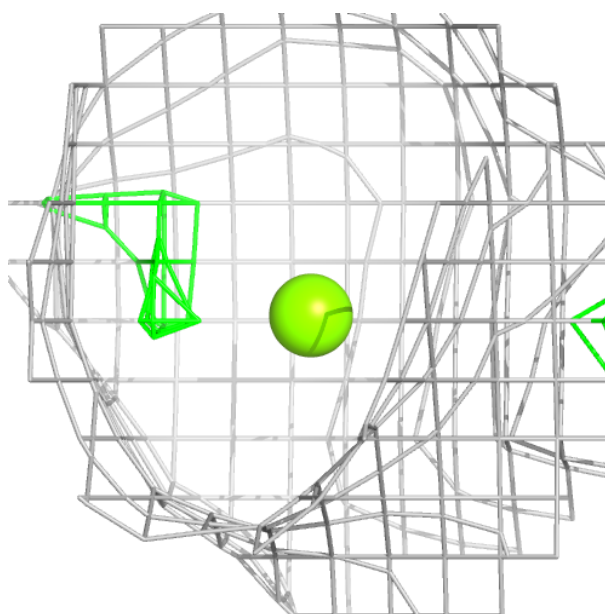
Electron density around MG H 703:

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



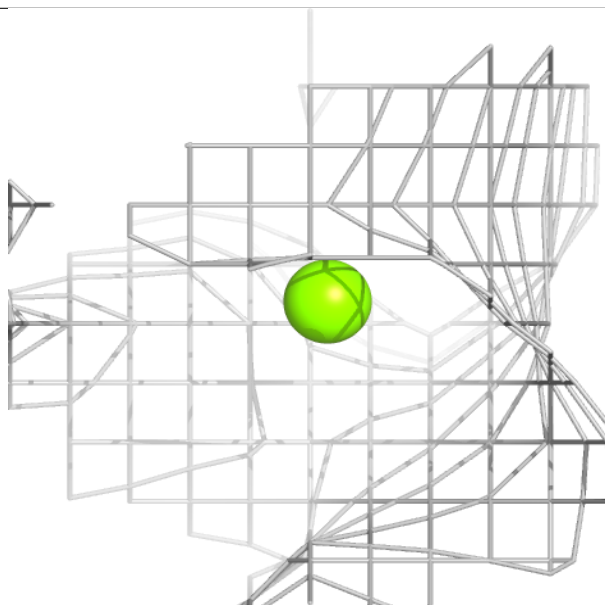
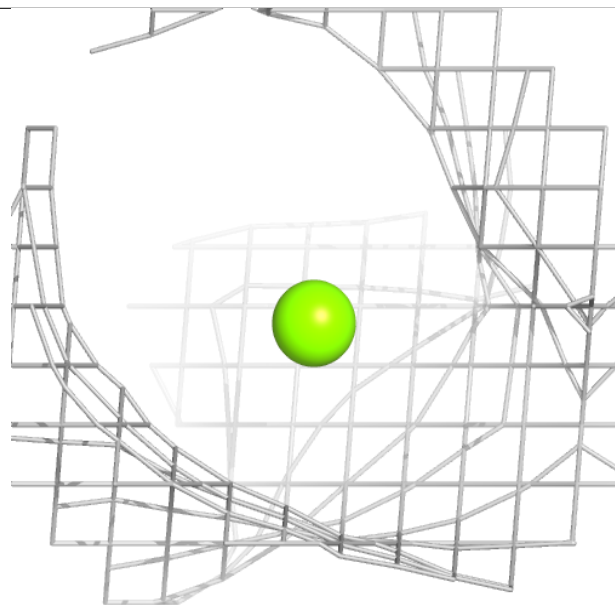
Electron density around MG G 704:

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



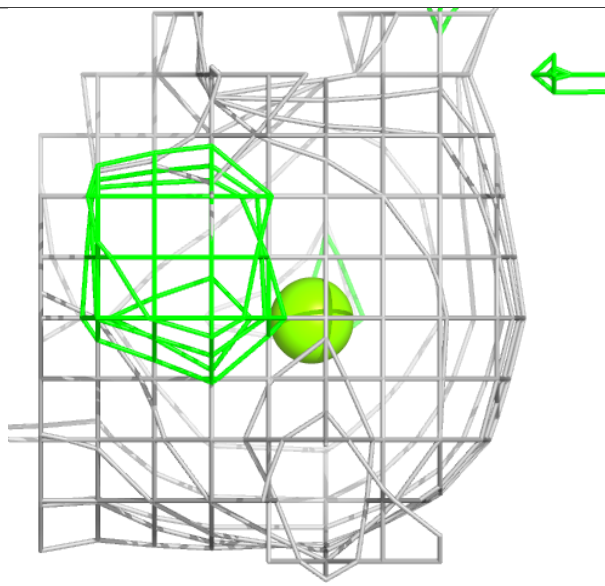
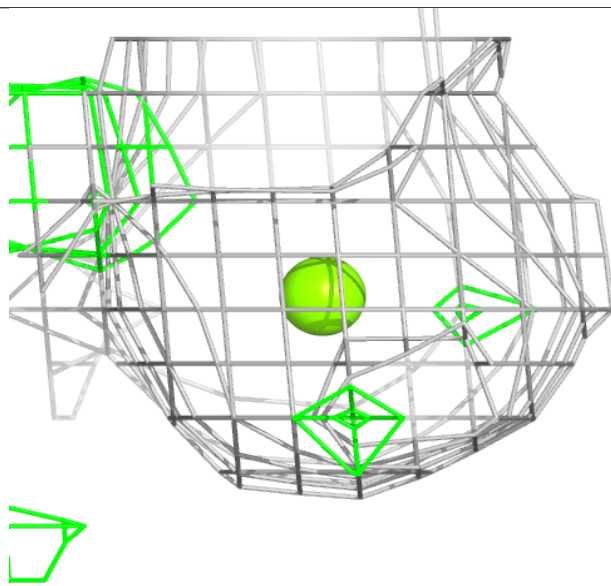
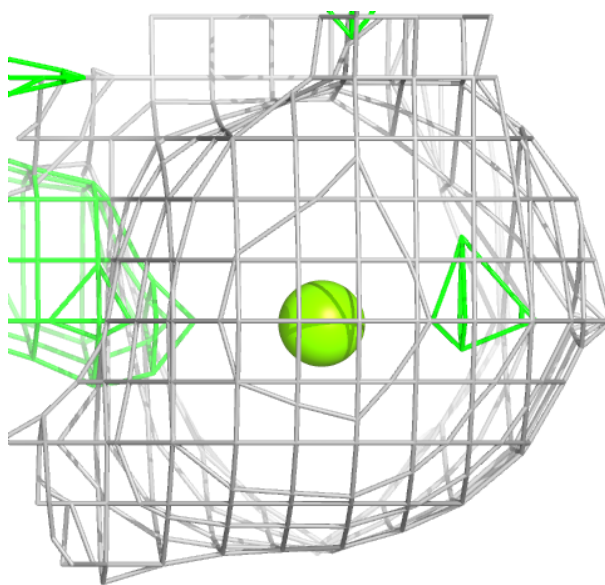
Electron density around MG N 703:

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



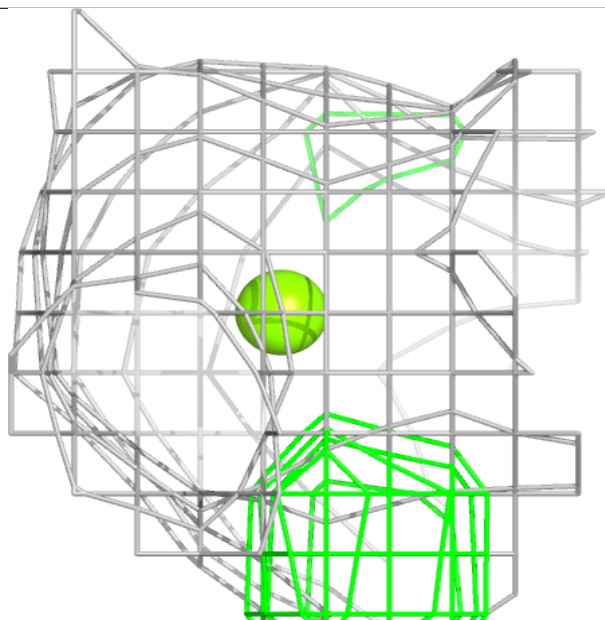
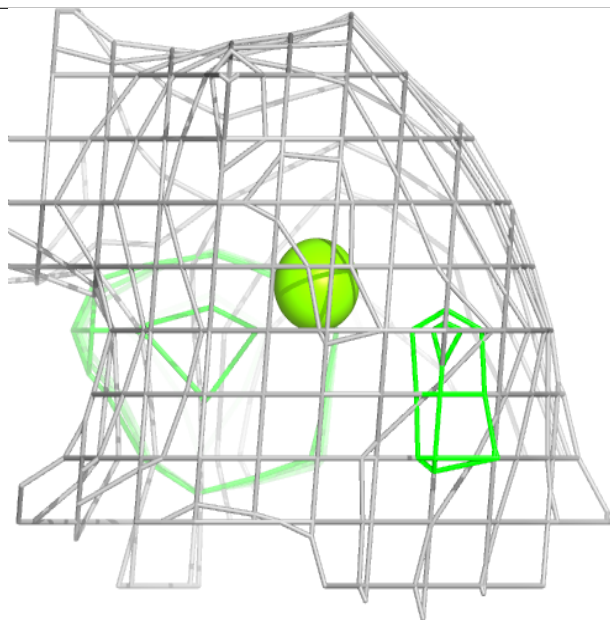
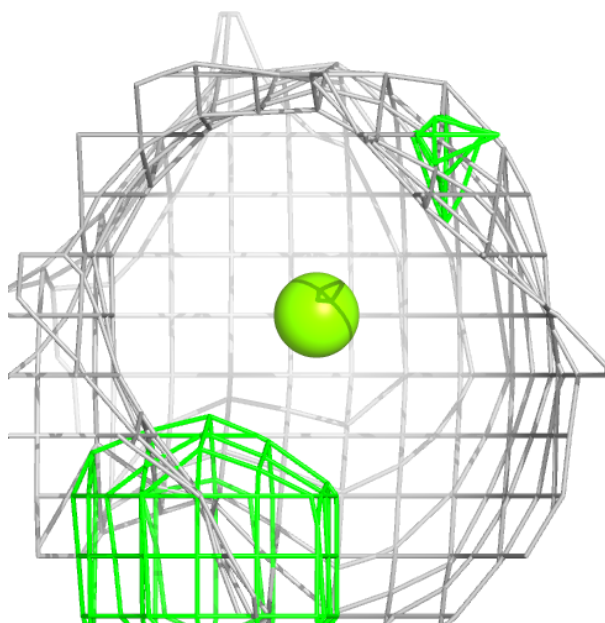
Electron density around MG L 704:

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



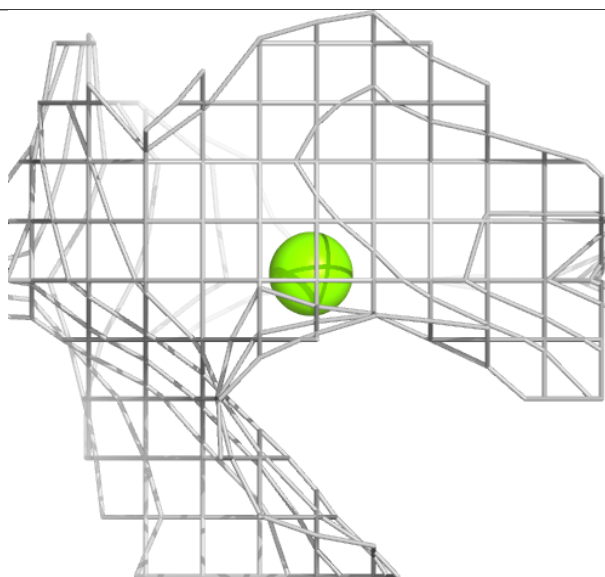
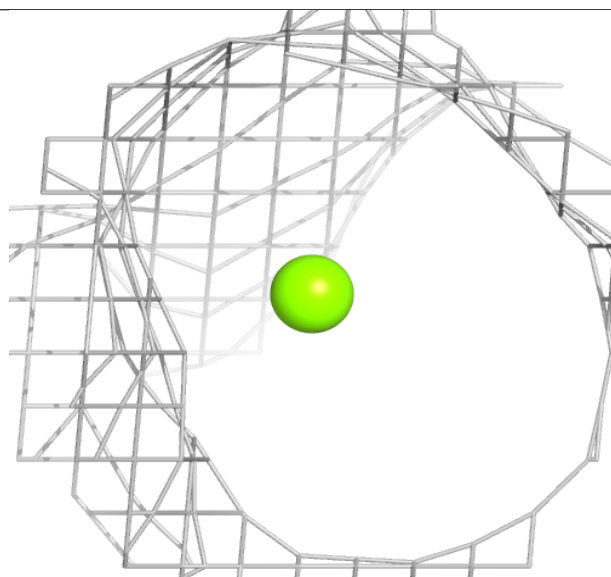
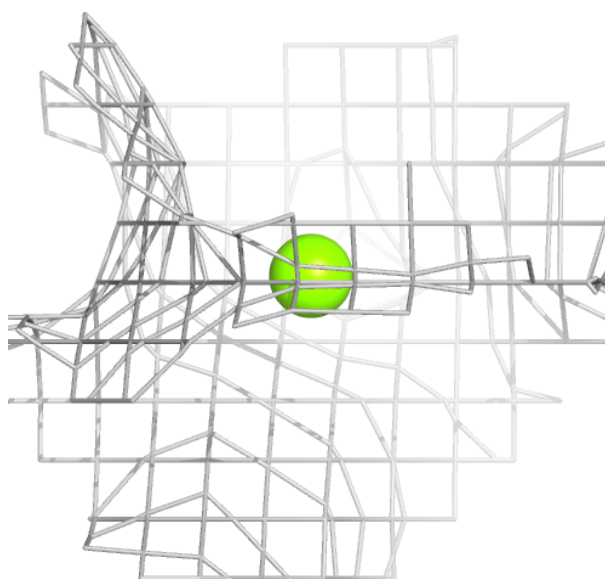
Electron density around MG B 703:

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



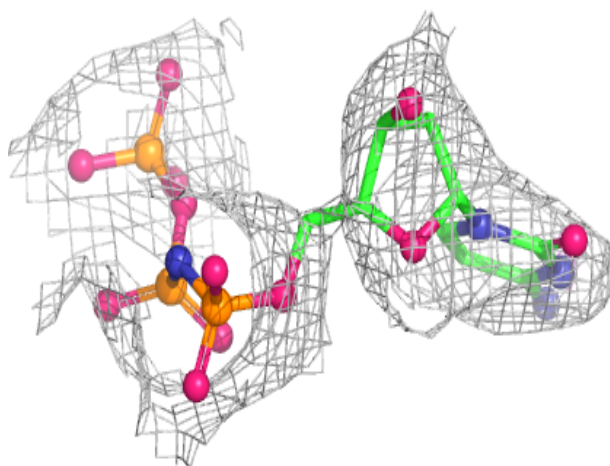
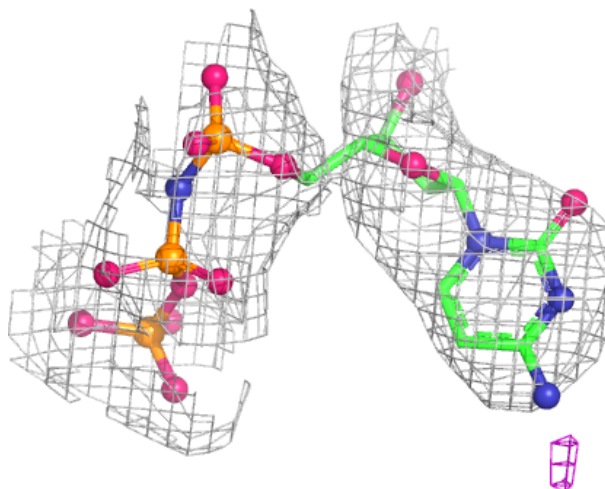
Electron density around MG H 704:

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



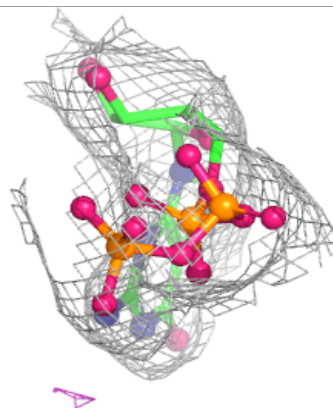
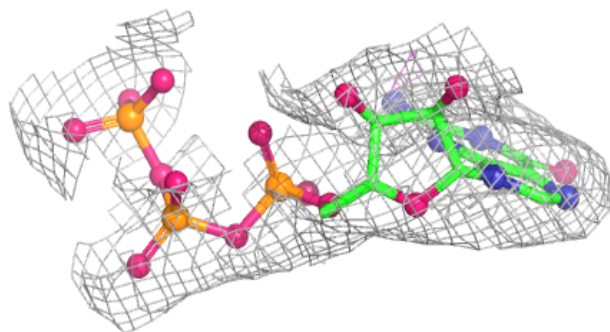
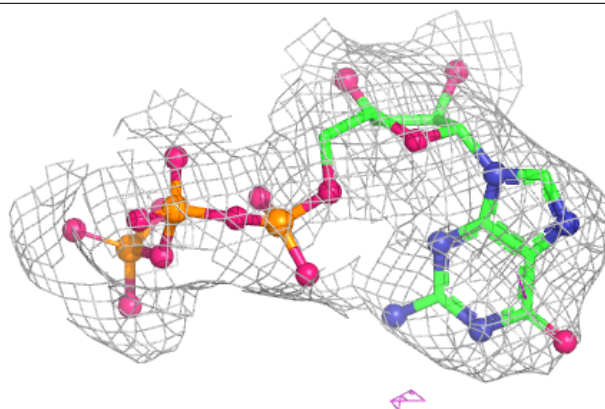
Electron density around 0KX O 705:

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

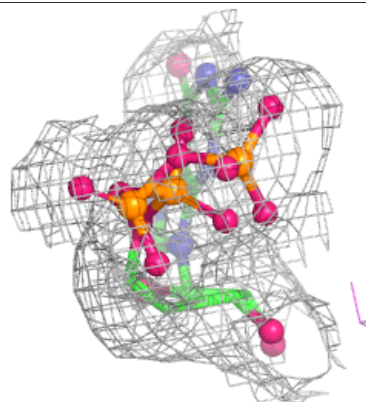
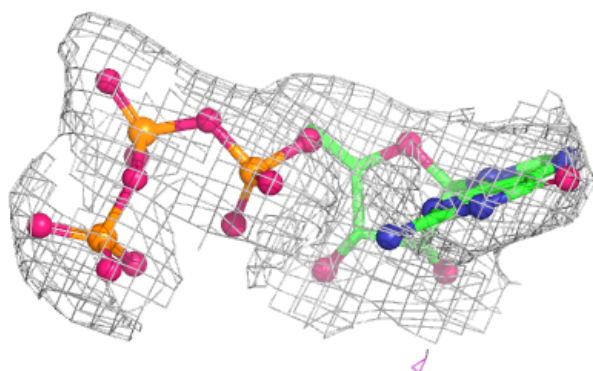
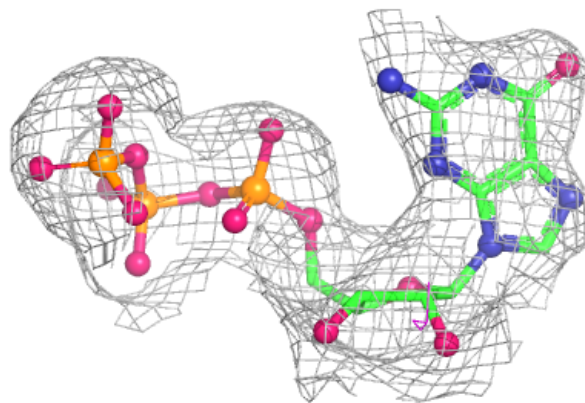


Electron density around GTP F 705:

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

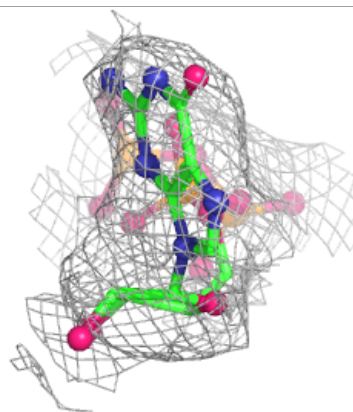
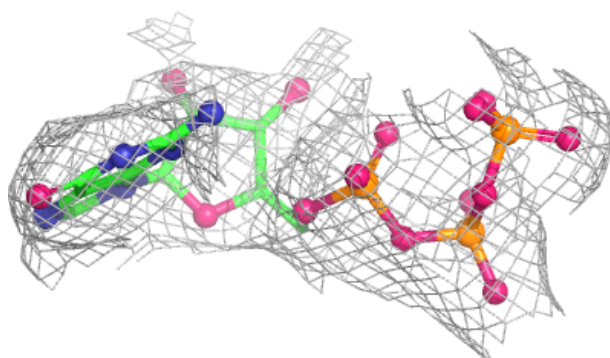
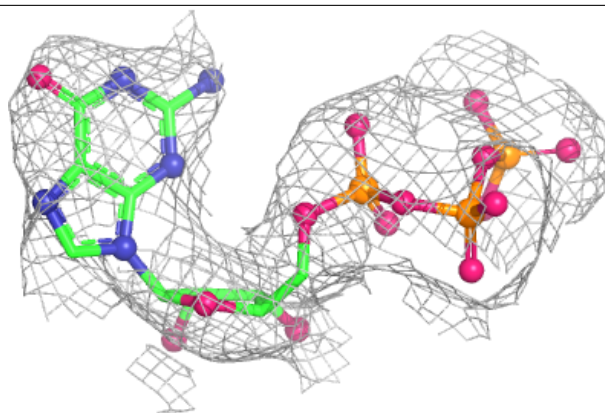
**Electron density around GTP H 706:**

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

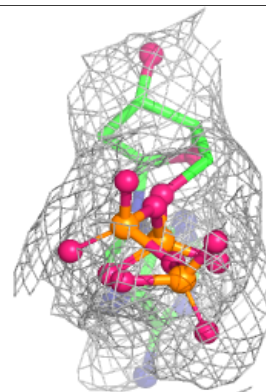
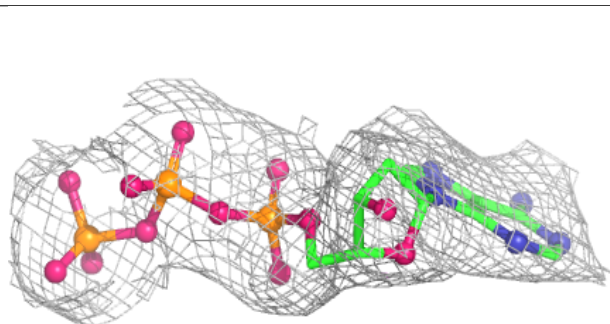
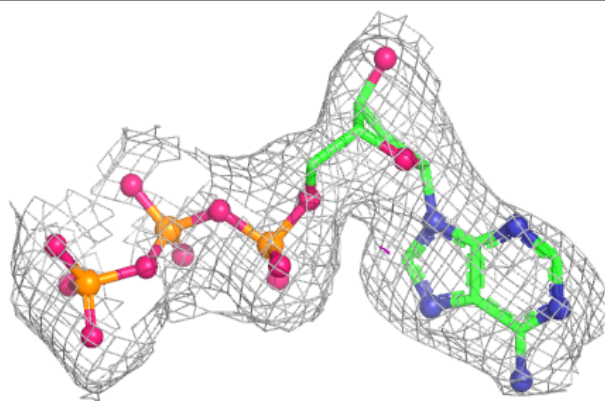


Electron density around GTP N 705:

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

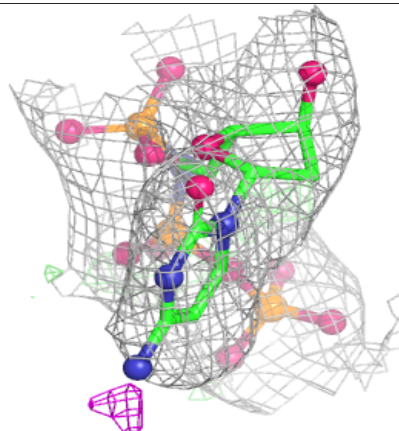
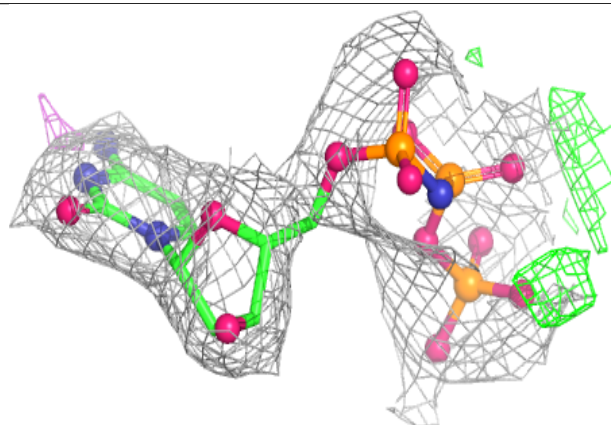
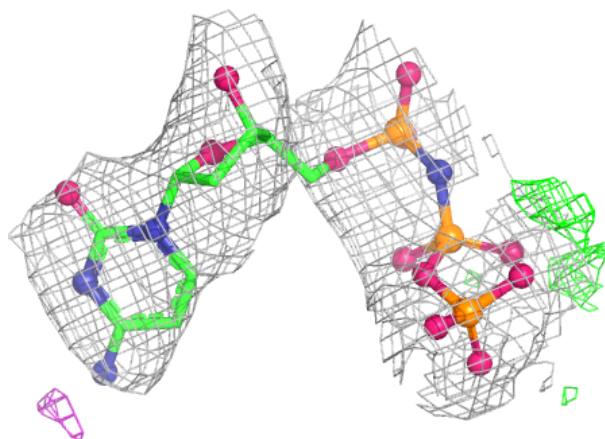
**Electron density around DTP F 706:**

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



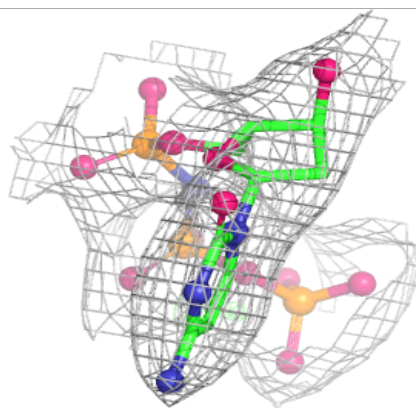
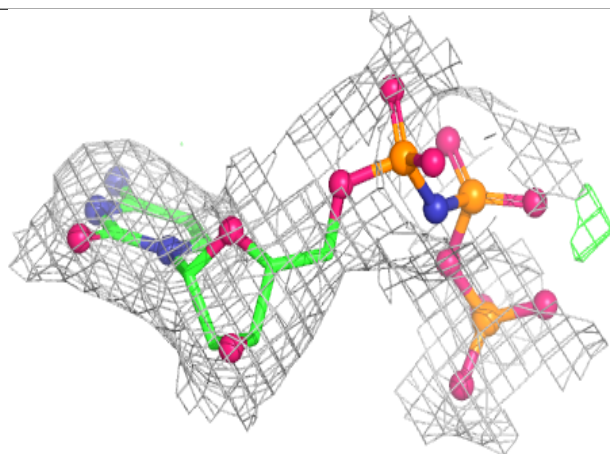
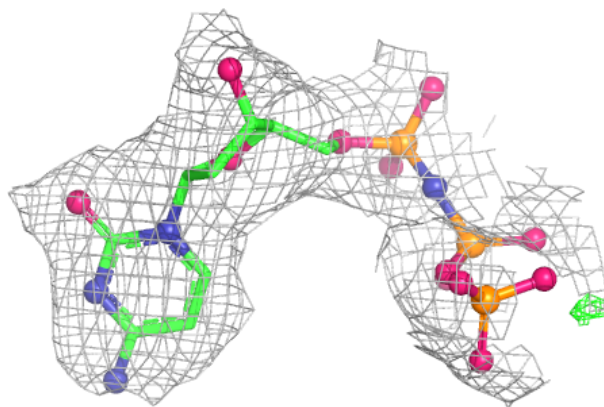
Electron density around 0KX F 704:

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



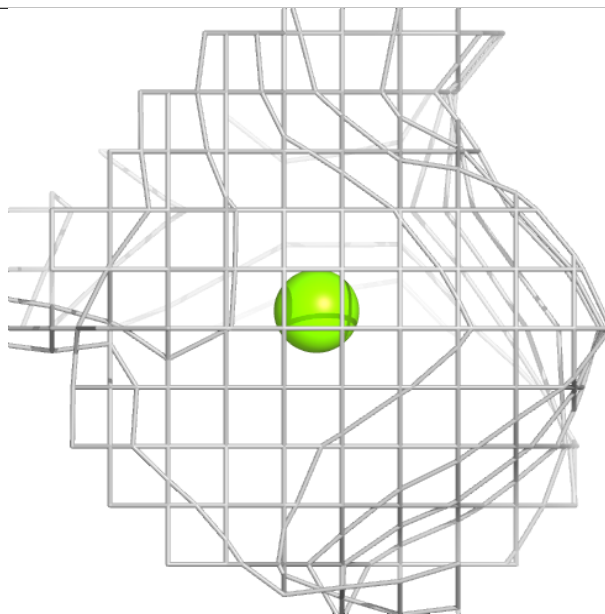
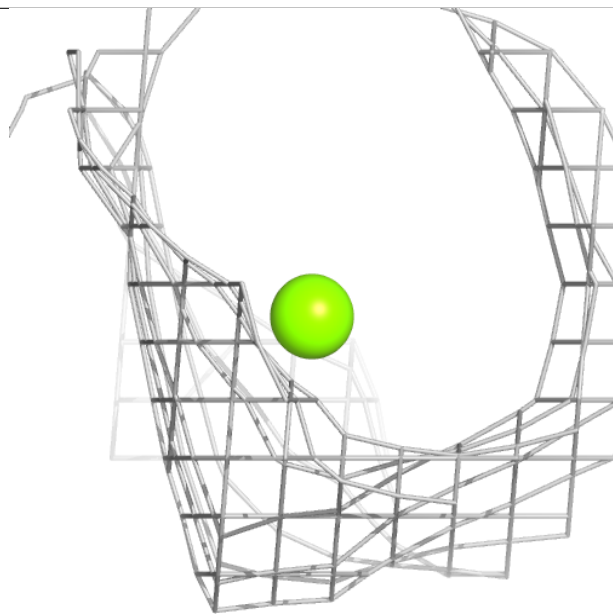
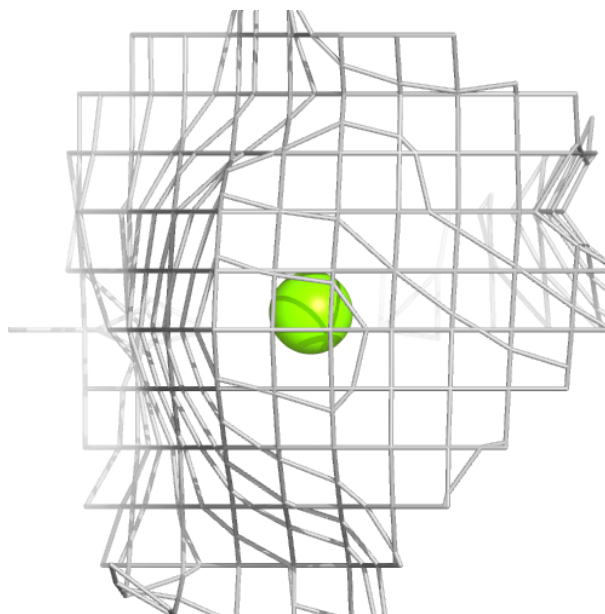
Electron density around 0KX G 706:

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



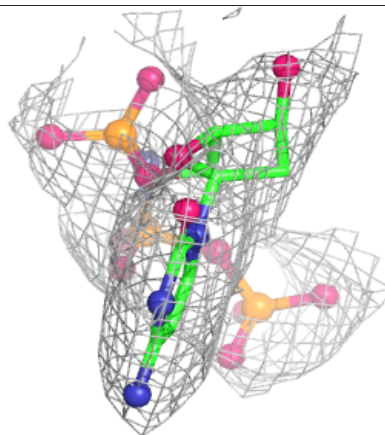
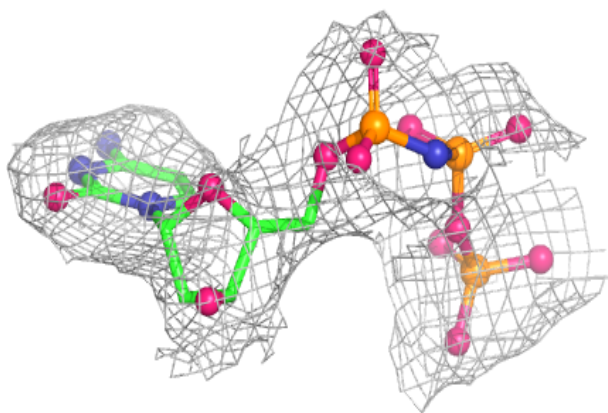
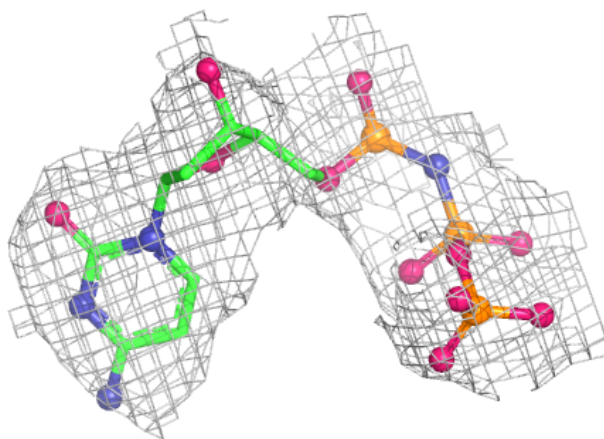
Electron density around MG K 705:

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



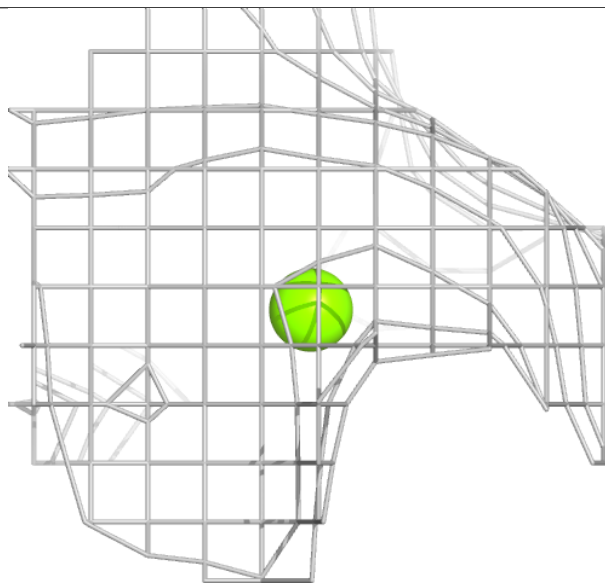
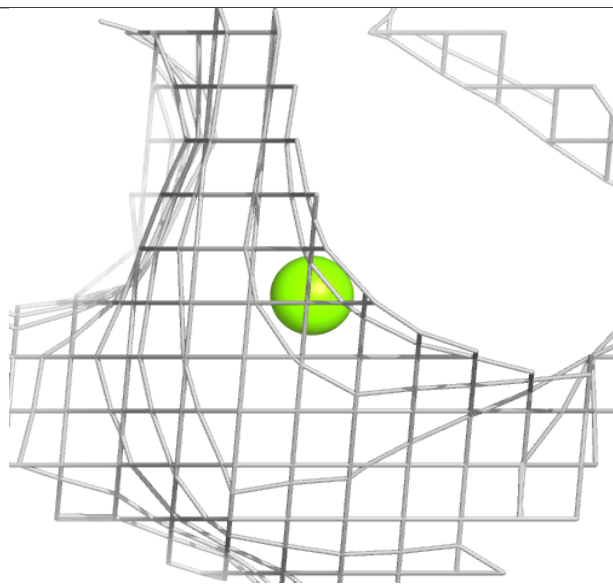
Electron density around 0KX N 704:

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



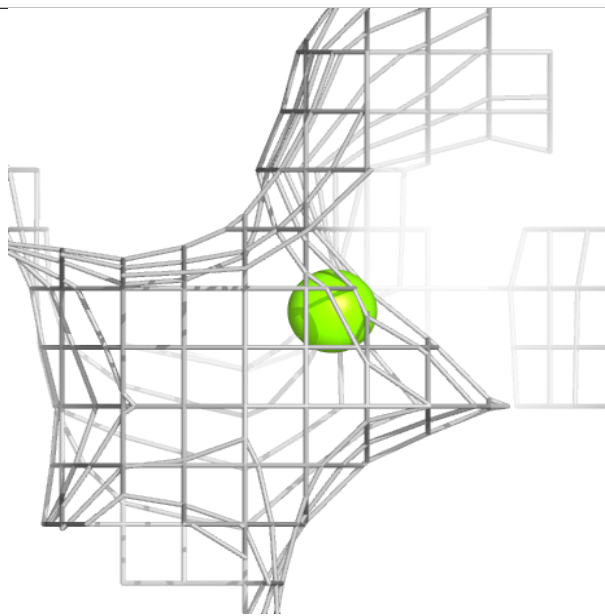
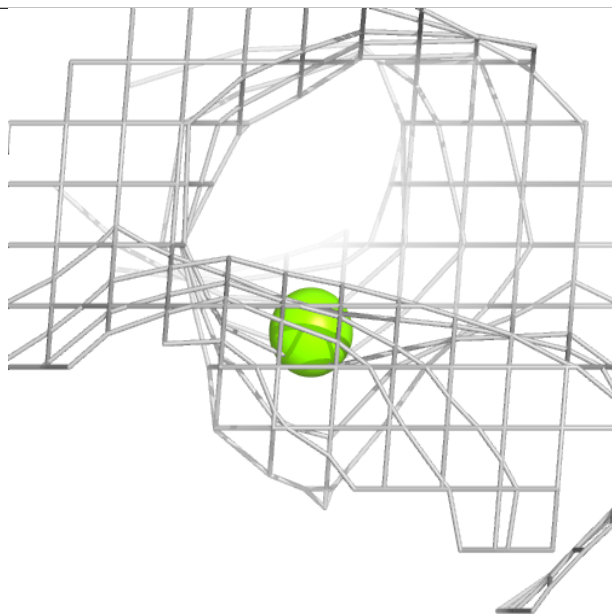
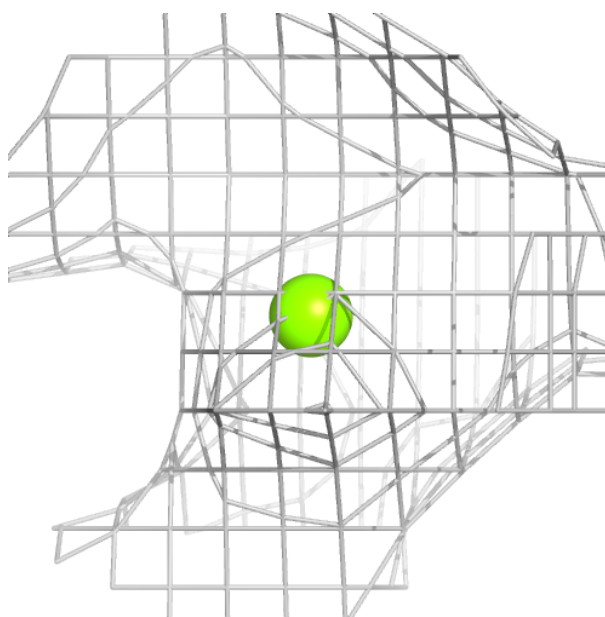
Electron density around MG F 703:

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



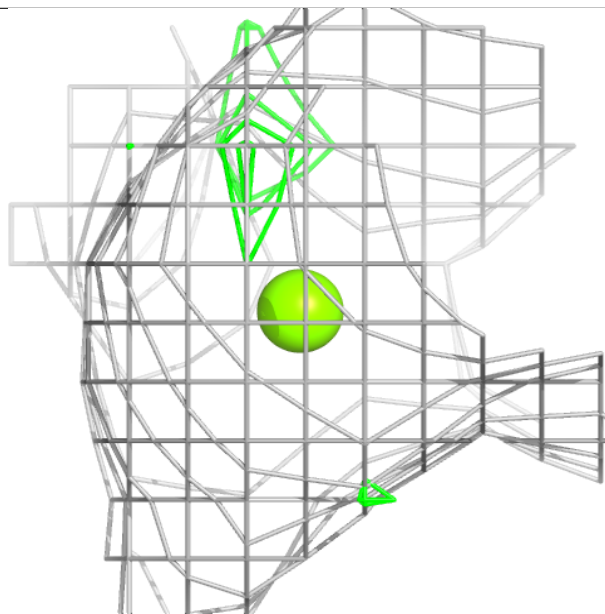
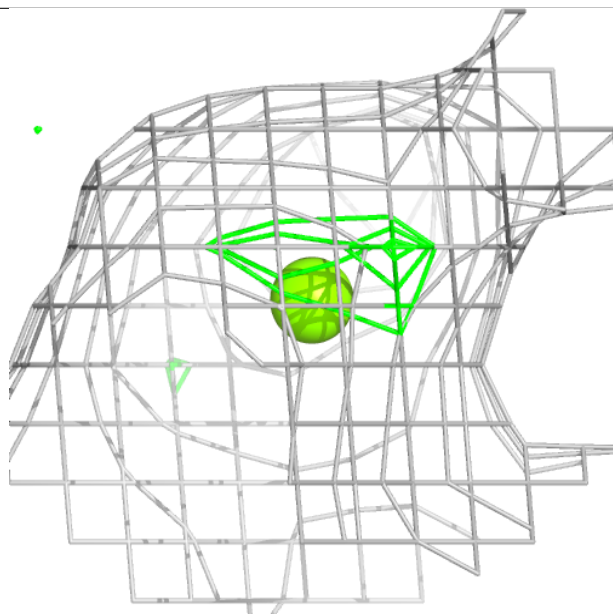
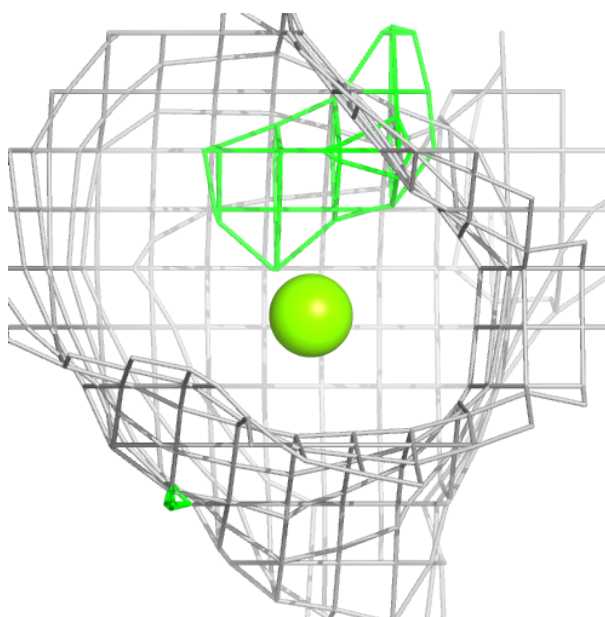
Electron density around MG K 703:

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



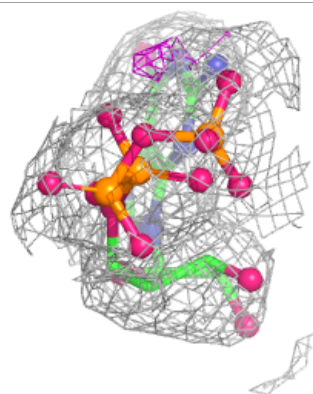
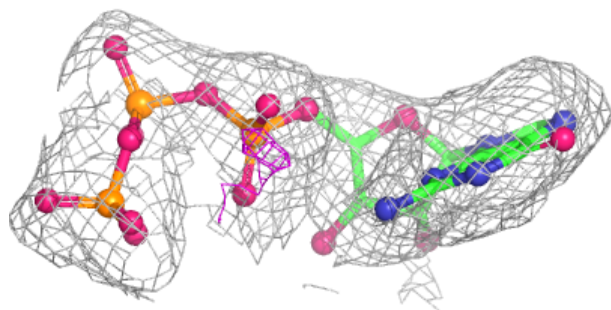
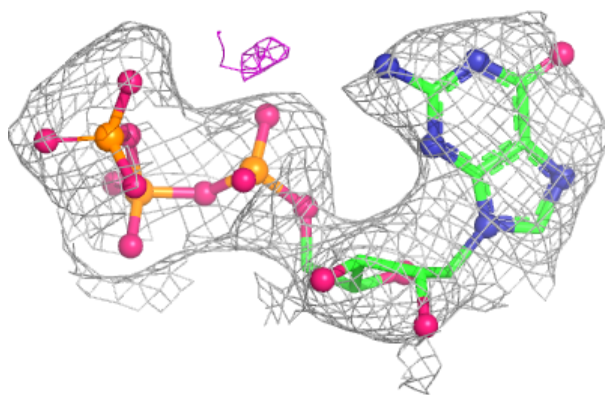
Electron density around MG C 704:

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



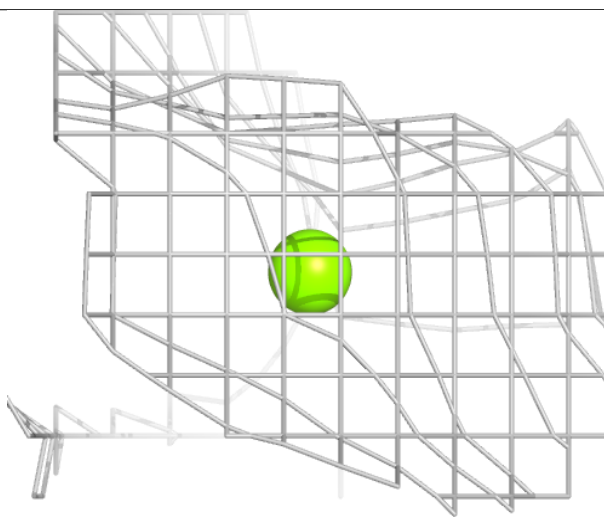
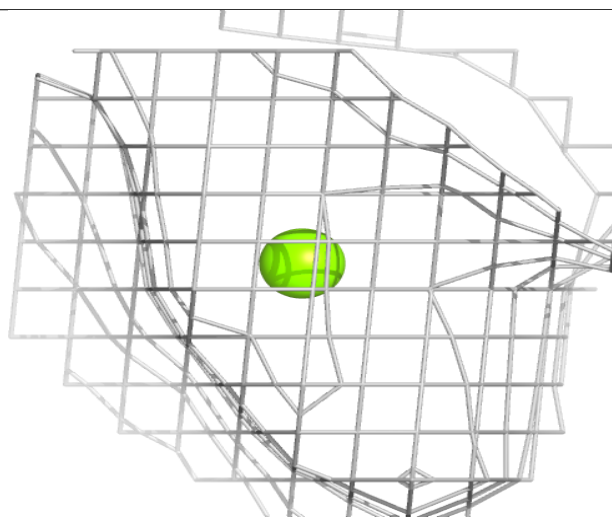
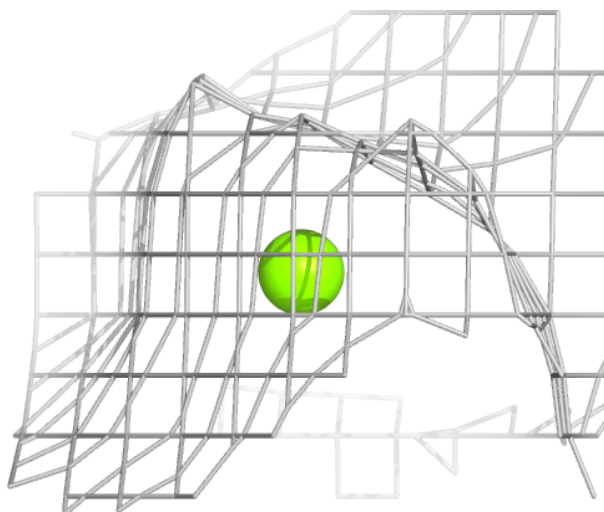
Electron density around GTP M 706:

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



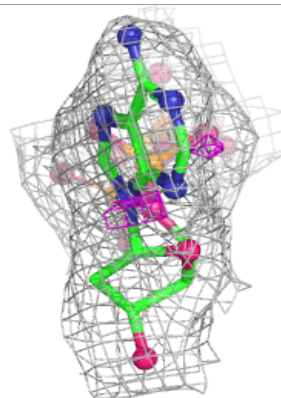
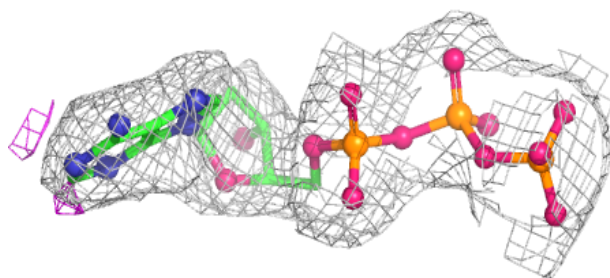
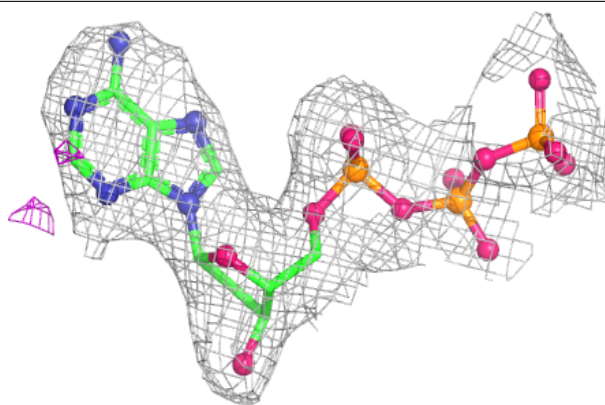
Electron density around MG P 705:

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

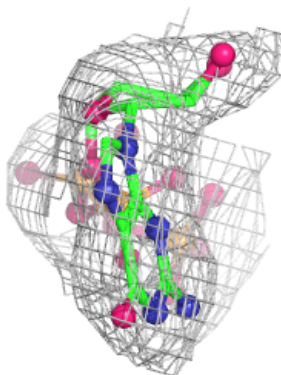
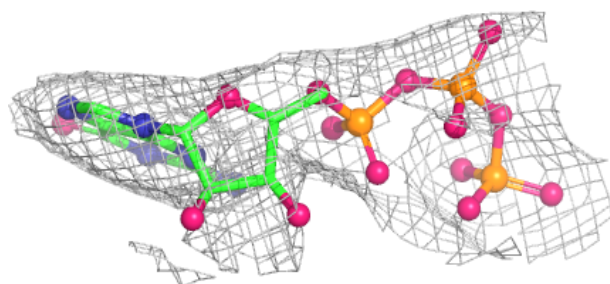
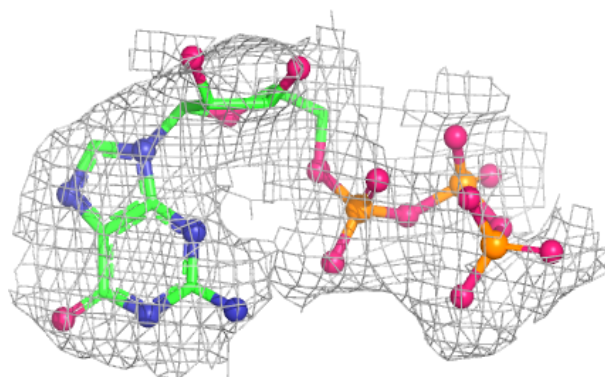


Electron density around DTP E 706:

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

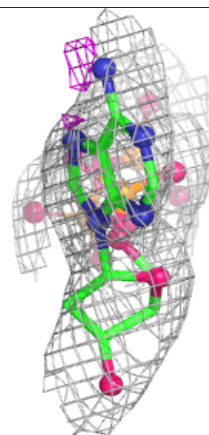
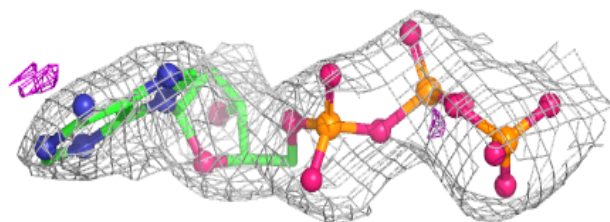
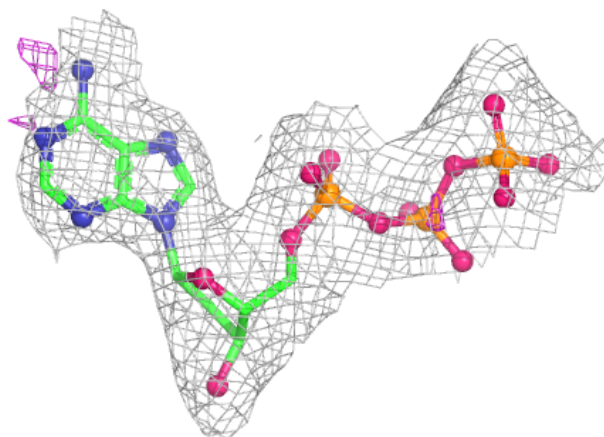
**Electron density around GTP O 706:**

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



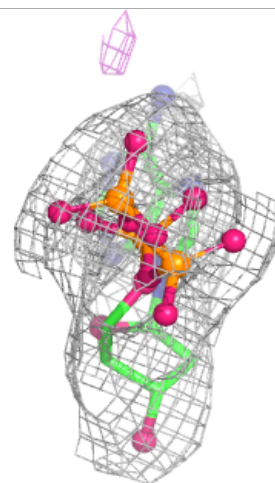
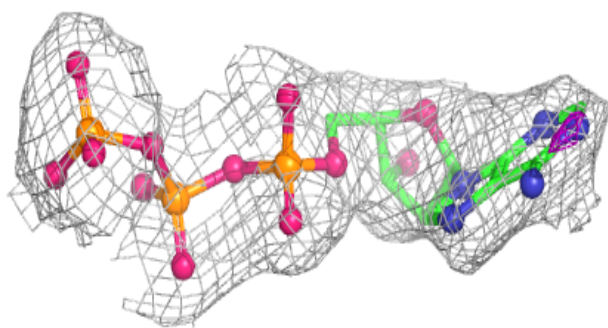
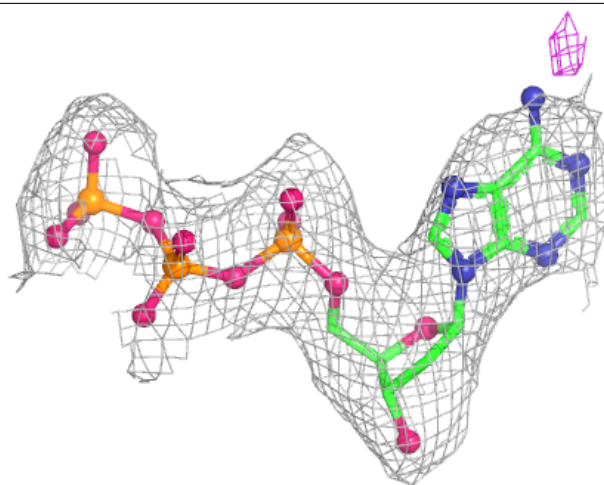
Electron density around DTP G 701:

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



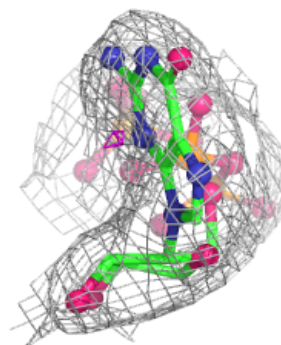
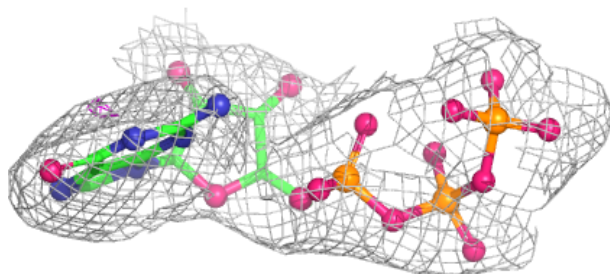
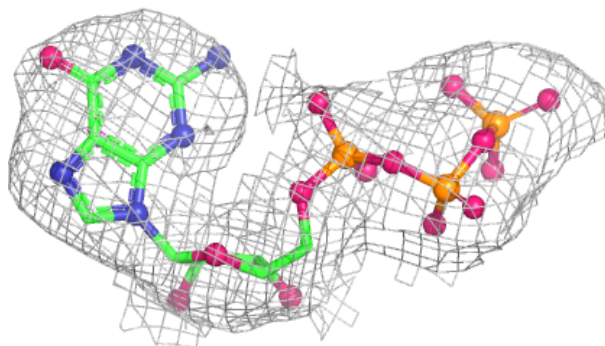
Electron density around DTP P 701:

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

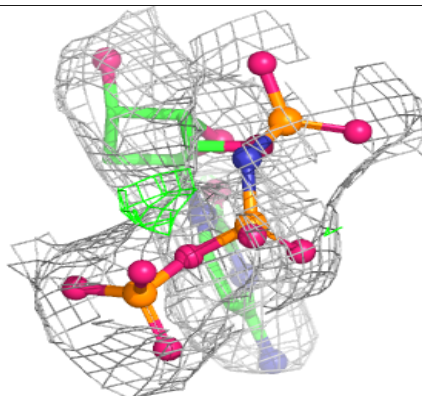
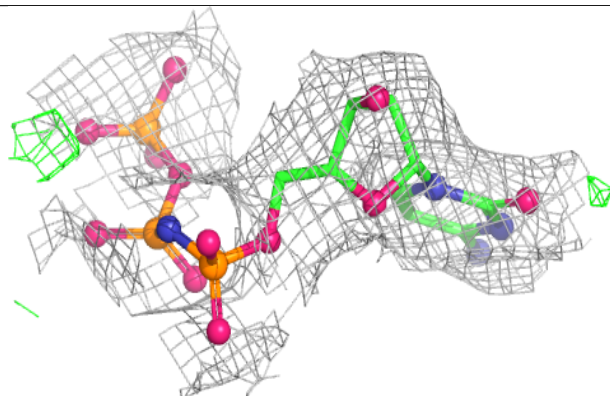
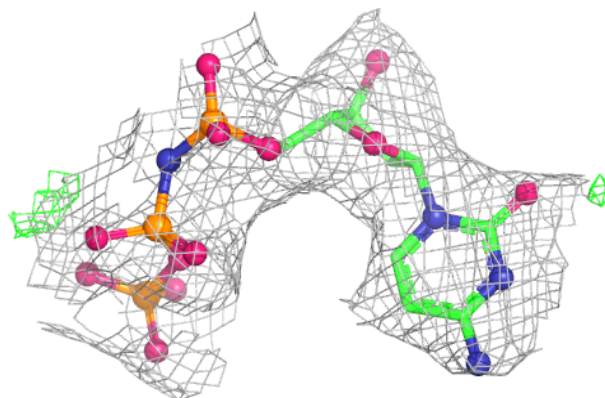


Electron density around GTP O 707:

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

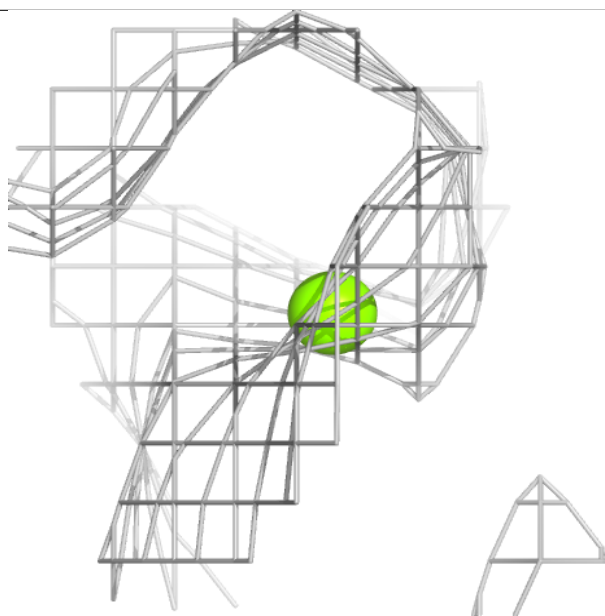
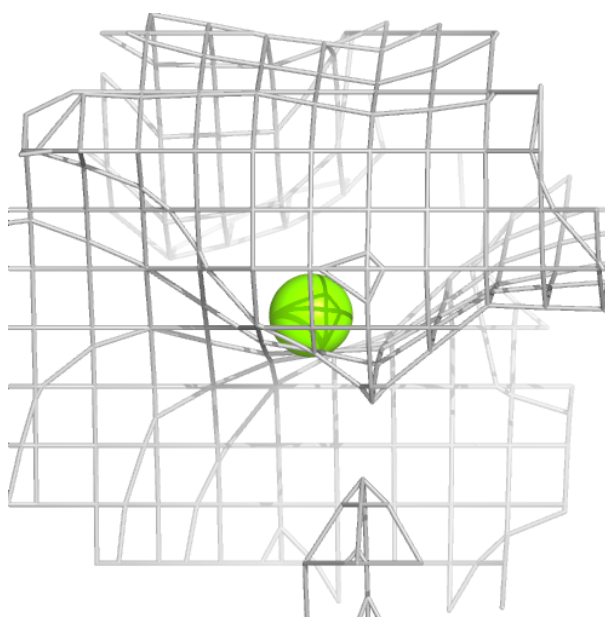
**Electron density around 0KX L 706:**

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



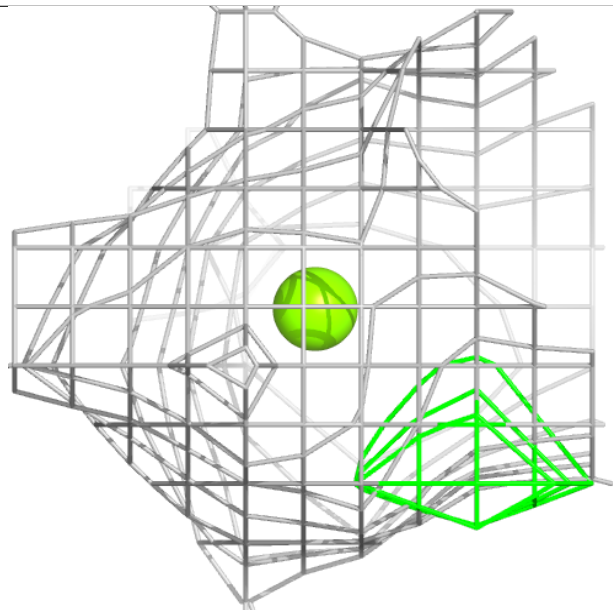
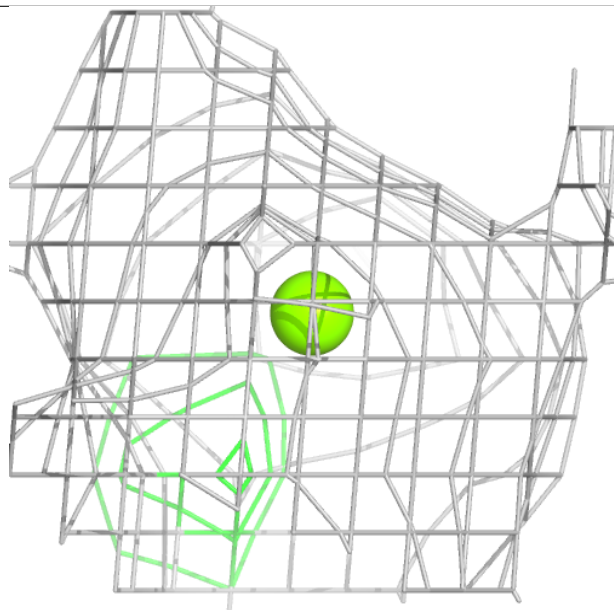
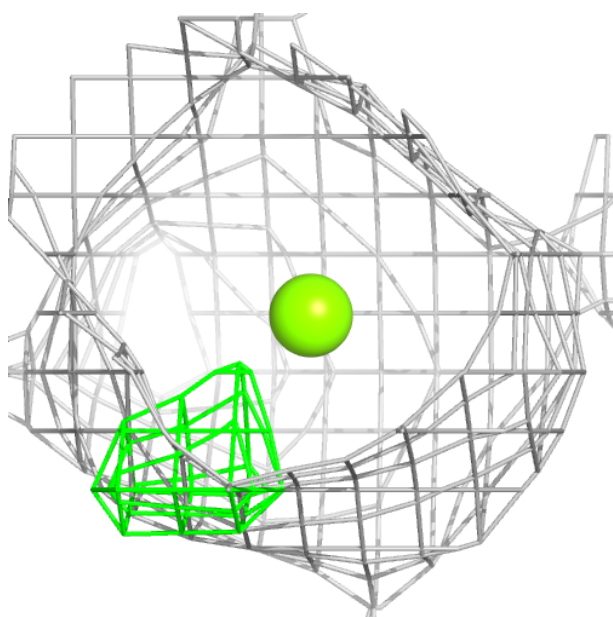
Electron density around MG G 703:

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



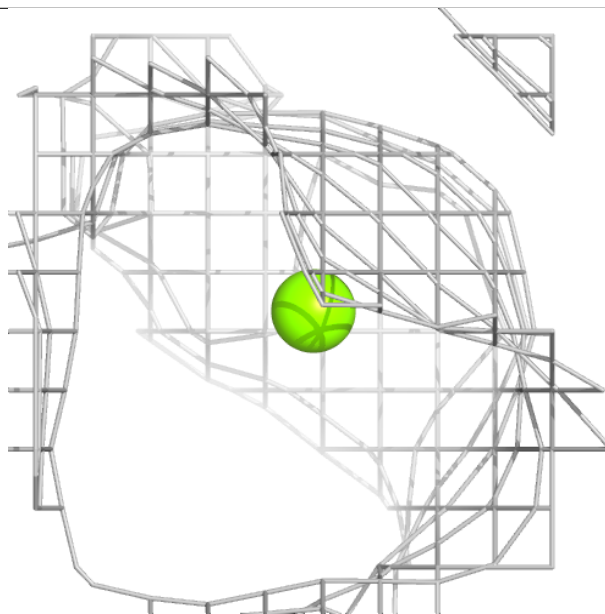
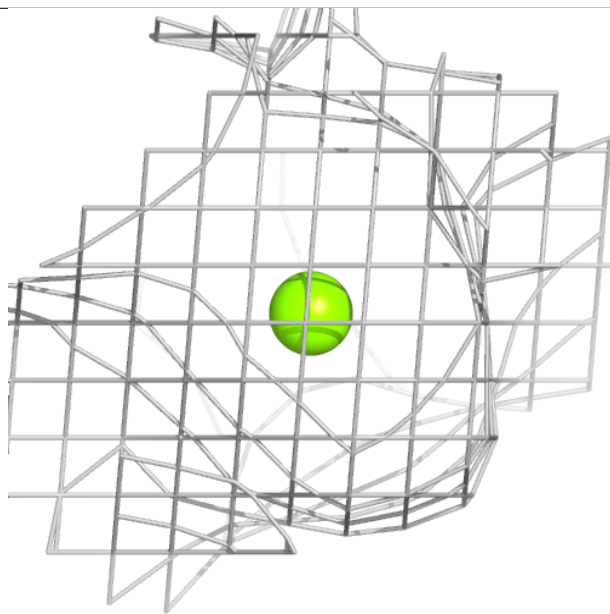
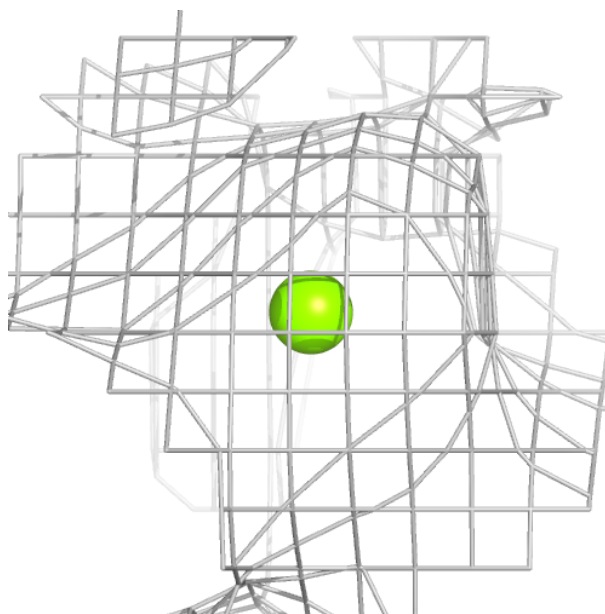
Electron density around MG D 704:

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



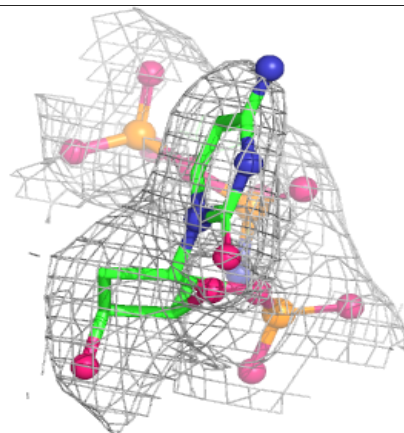
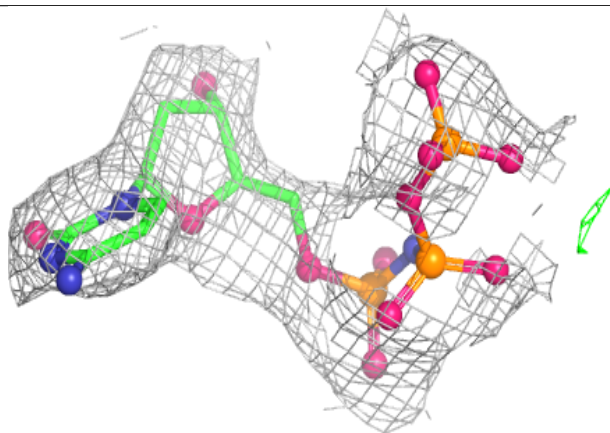
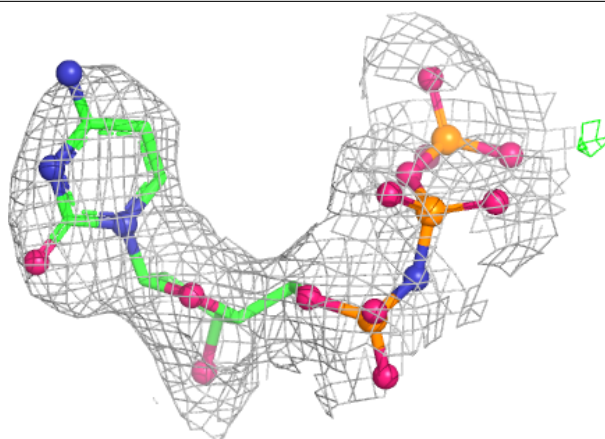
Electron density around MG B 704:

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

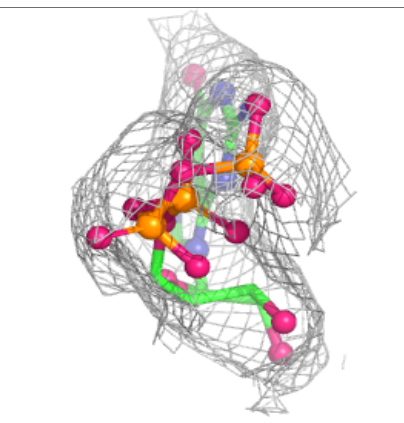
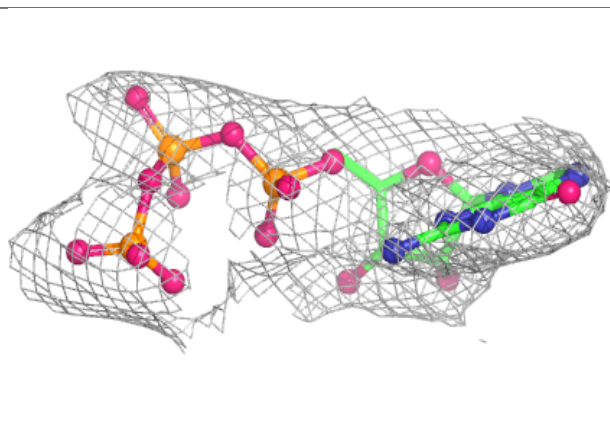
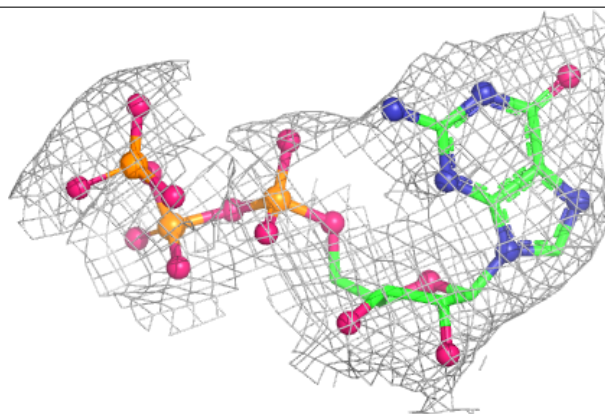


Electron density around 0KX P 706:

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

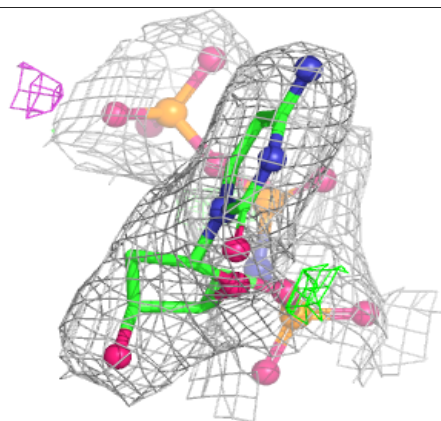
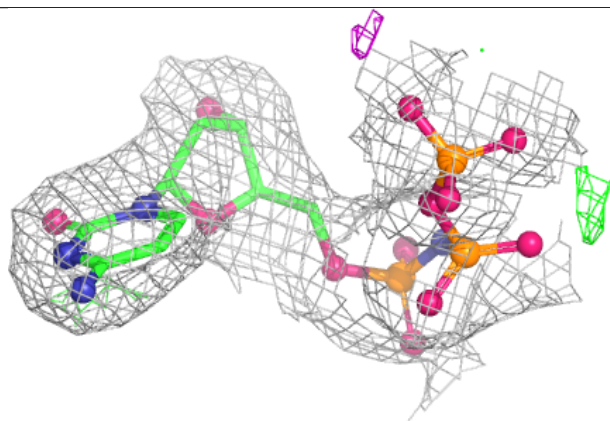
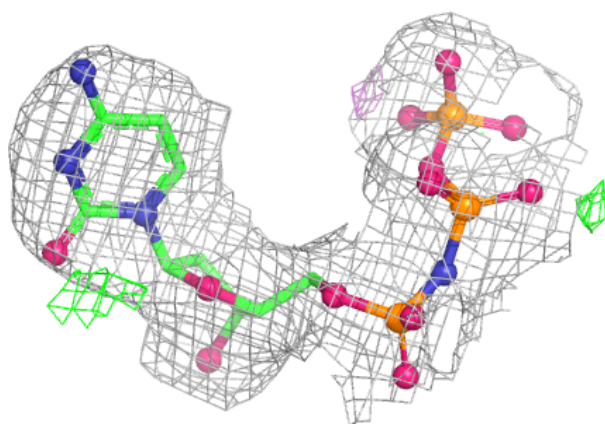
**Electron density around GTP E 705:**

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



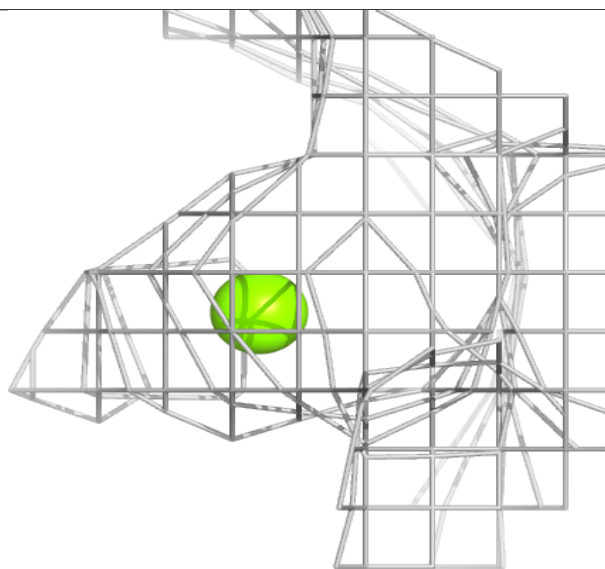
Electron density around 0KX C 706:

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



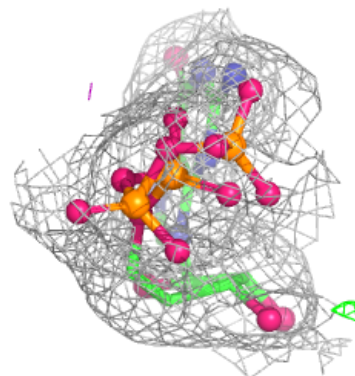
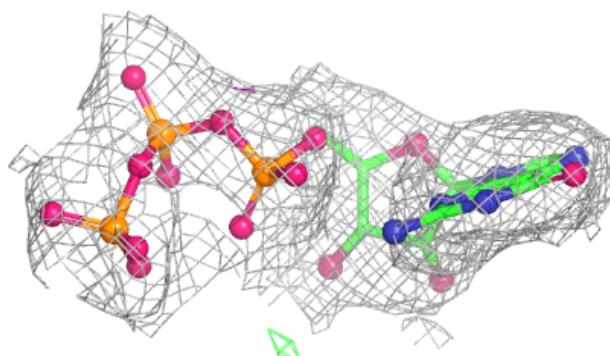
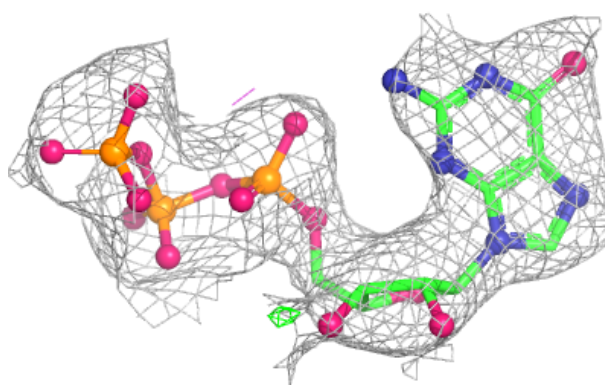
Electron density around MG B 702:

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

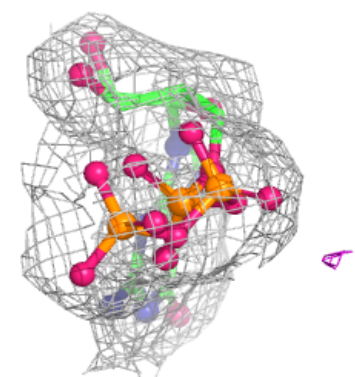
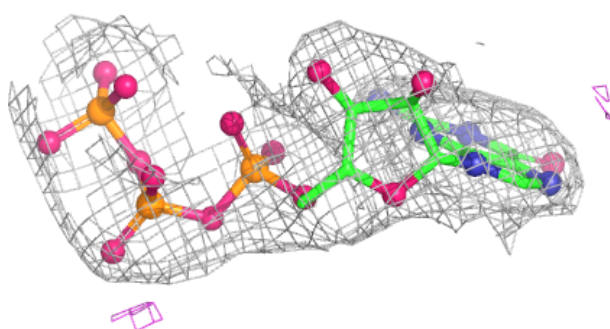
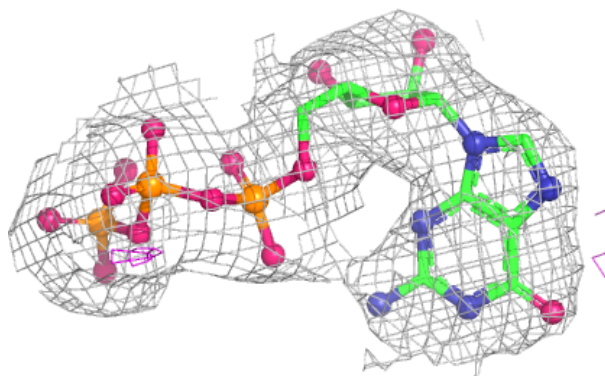


Electron density around GTP I 706:

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

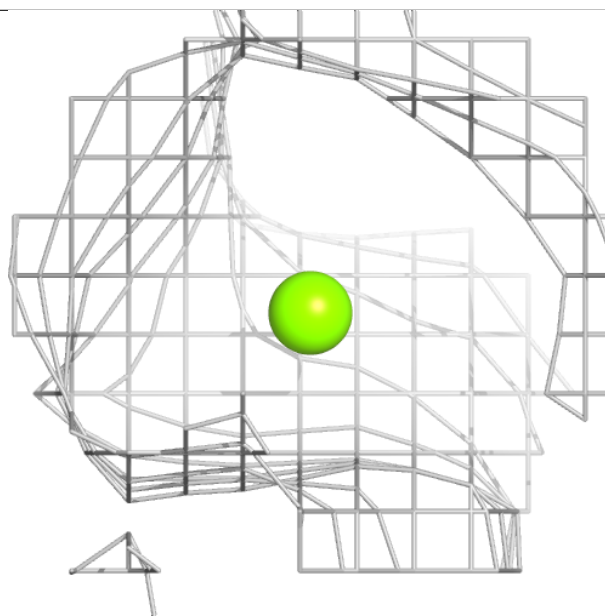
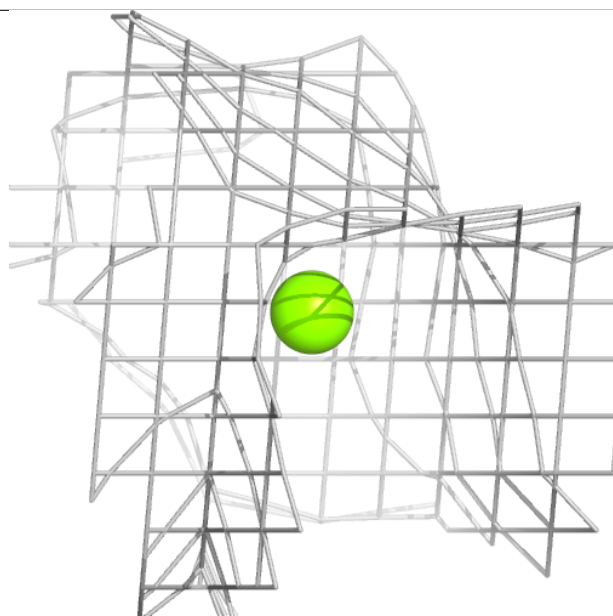
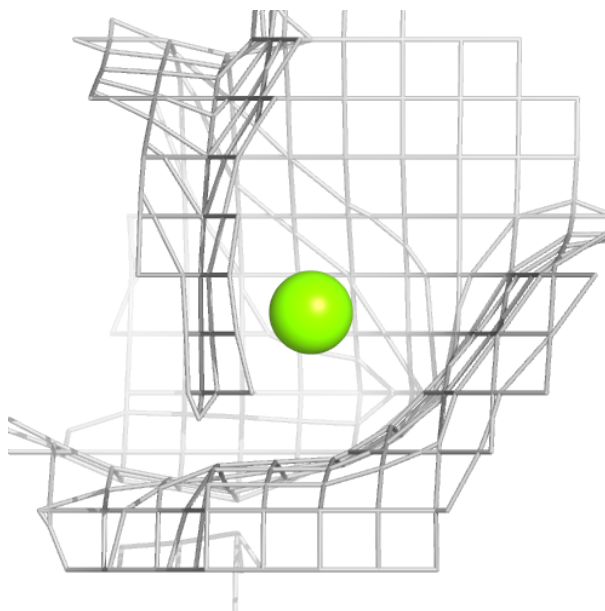
**Electron density around GTP K 707:**

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



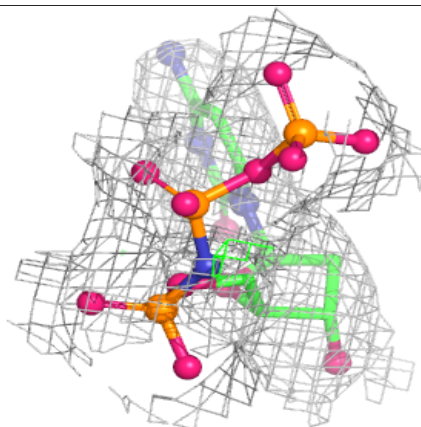
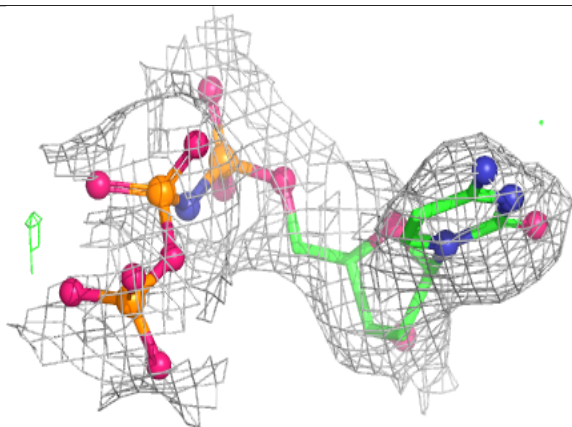
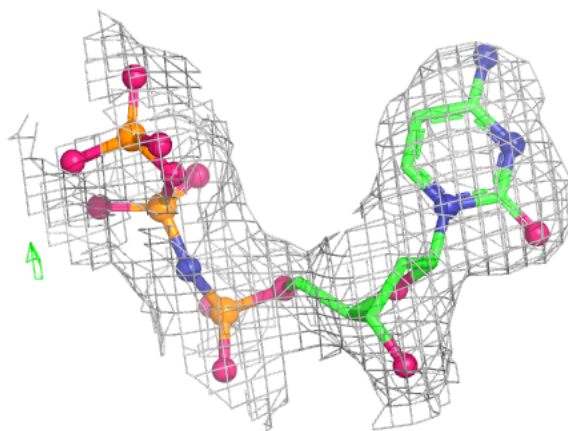
Electron density around MG A 704:

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

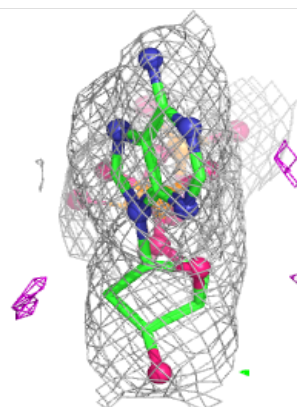
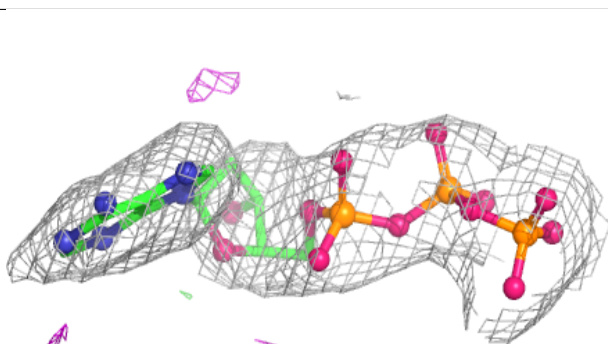
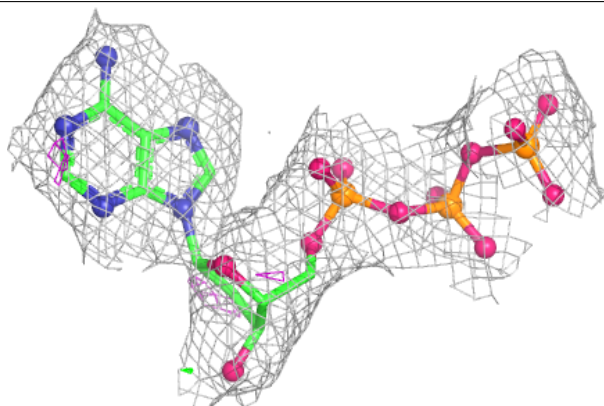


Electron density around 0KX H 705:

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

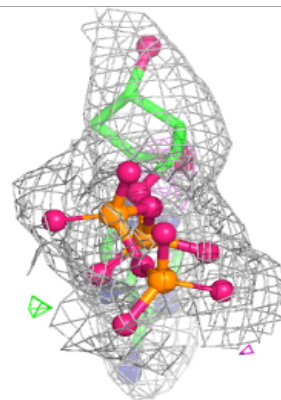
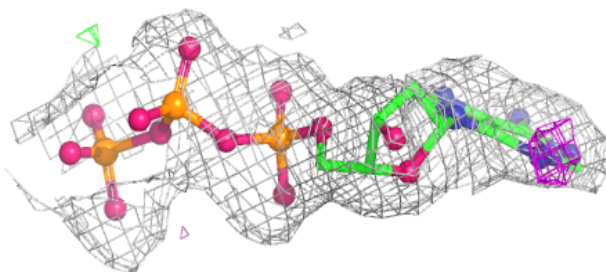
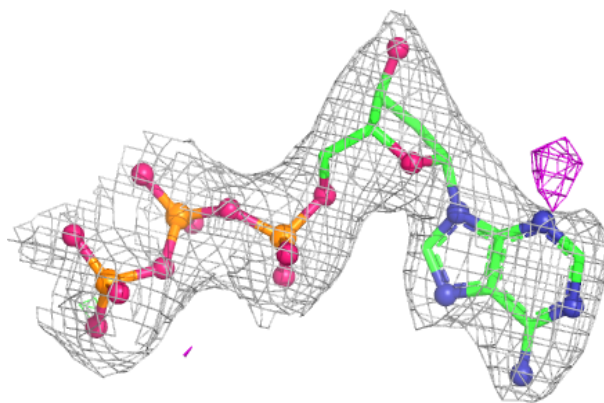
**Electron density around DTP H 701:**

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

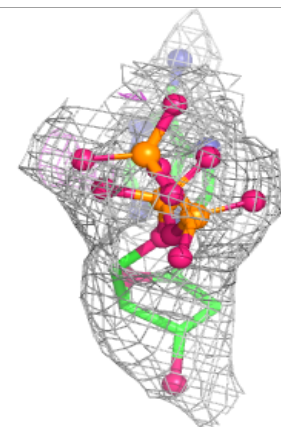
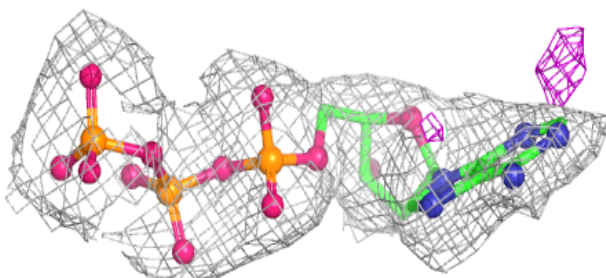
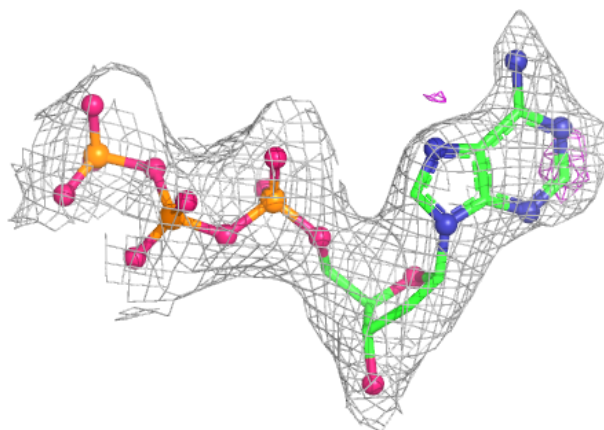


Electron density around DTP J 707:

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

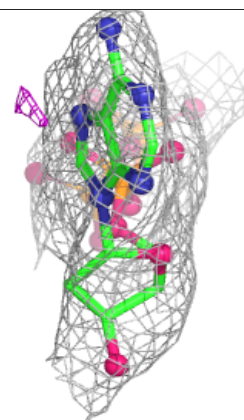
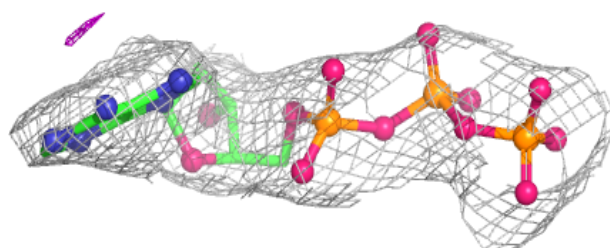
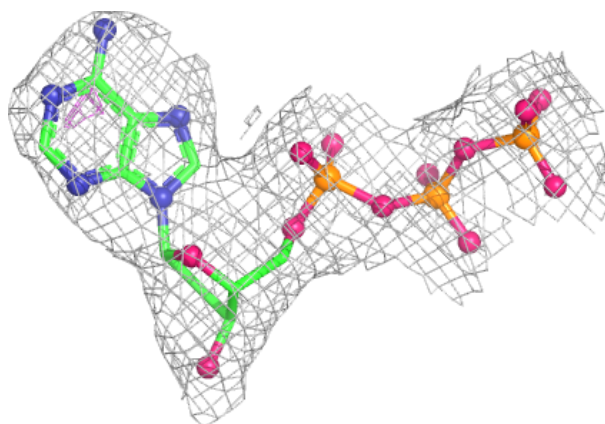
**Electron density around DTP L 701:**

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

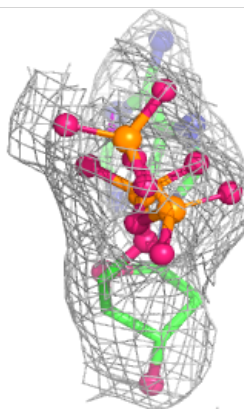
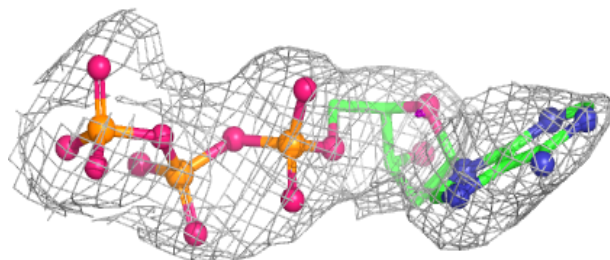
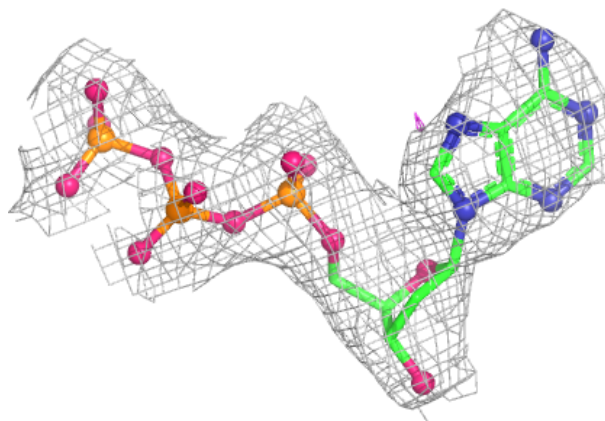


Electron density around DTP M 708:

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

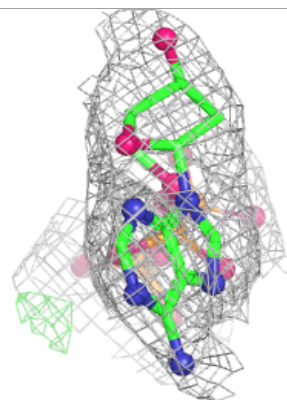
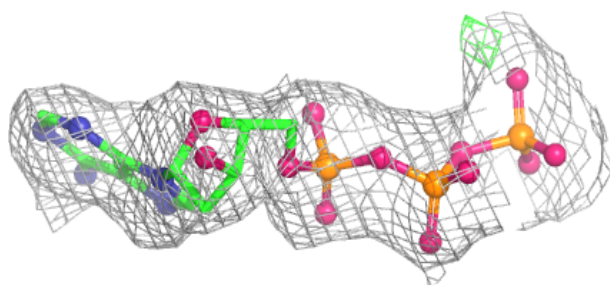
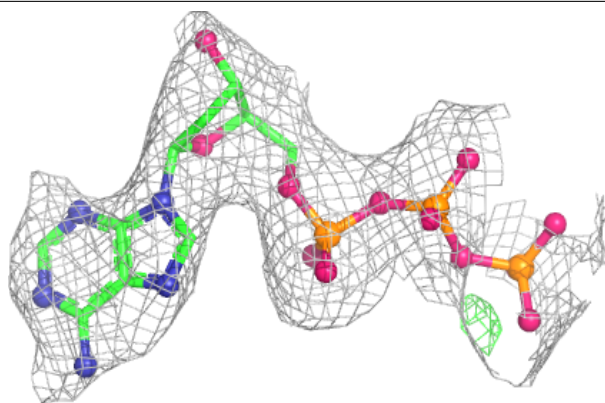
**Electron density around DTP N 706:**

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

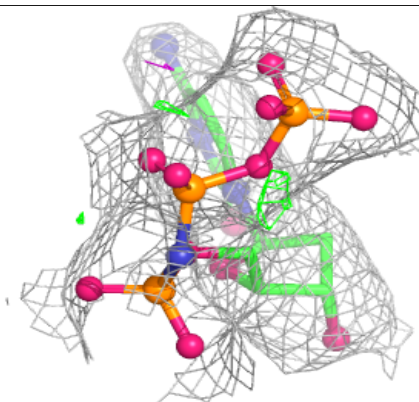
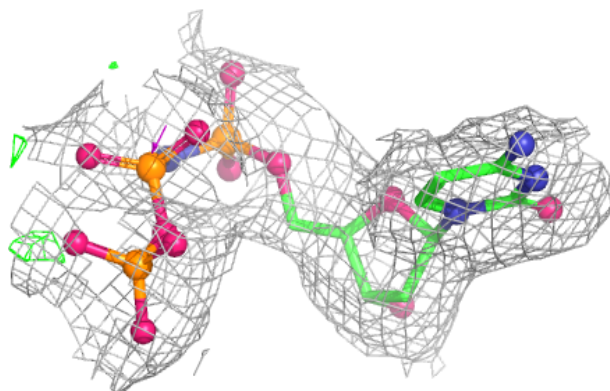
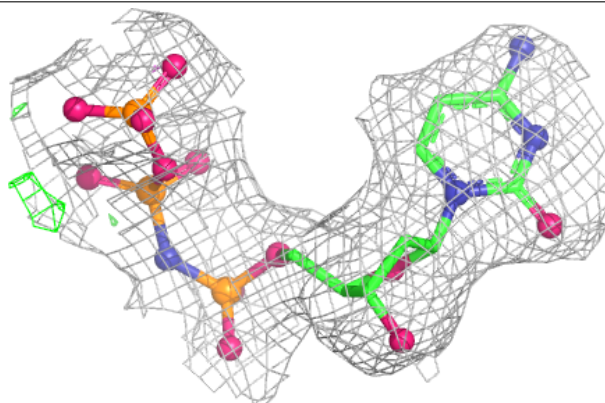


Electron density around DTP O 701:

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

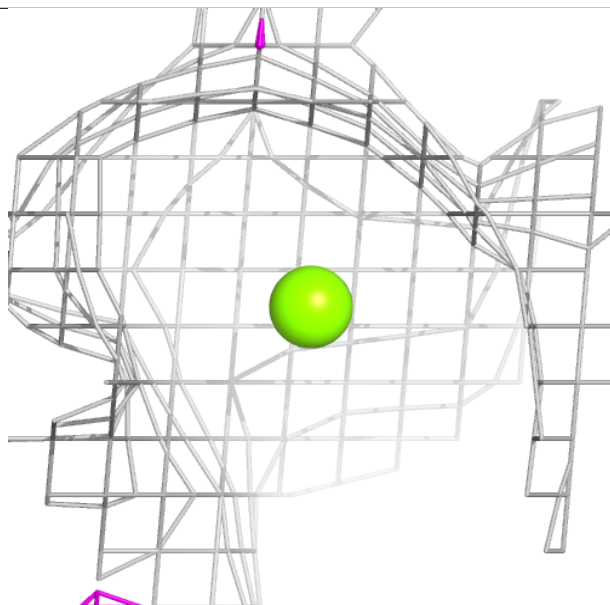
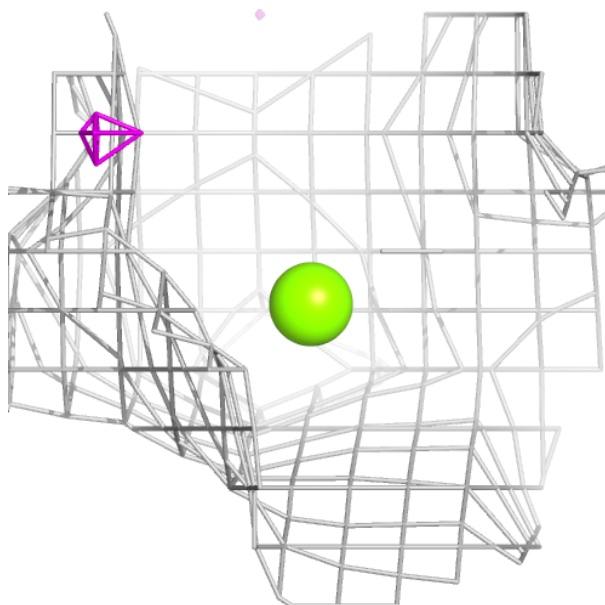
**Electron density around OKX I 705:**

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



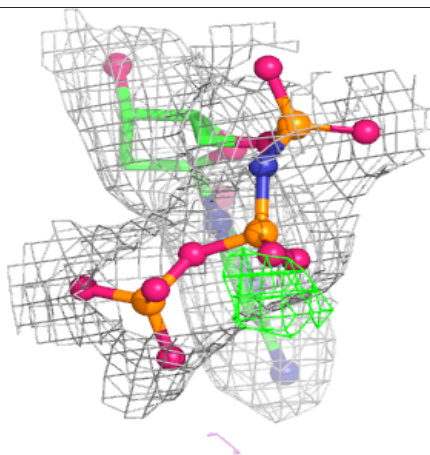
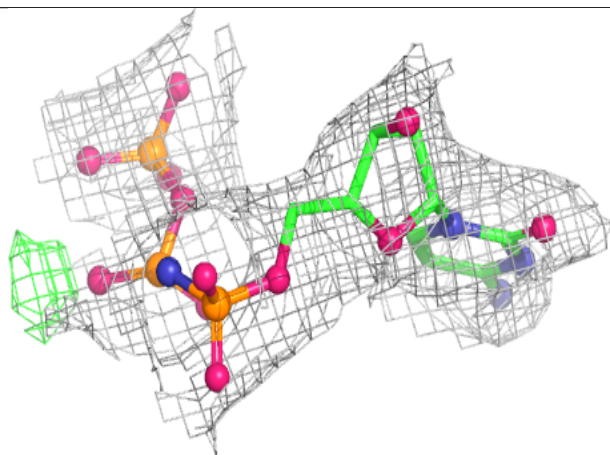
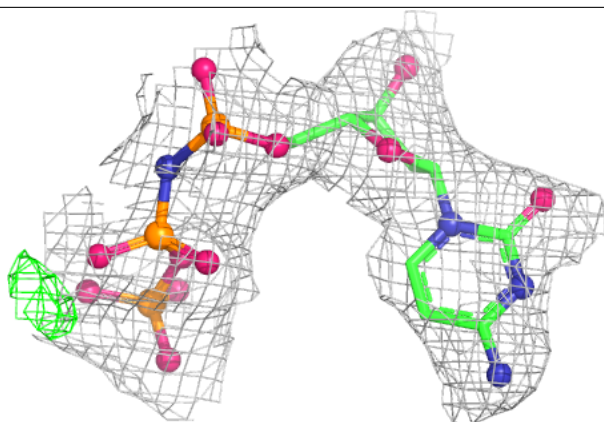
Electron density around MG J 703:

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



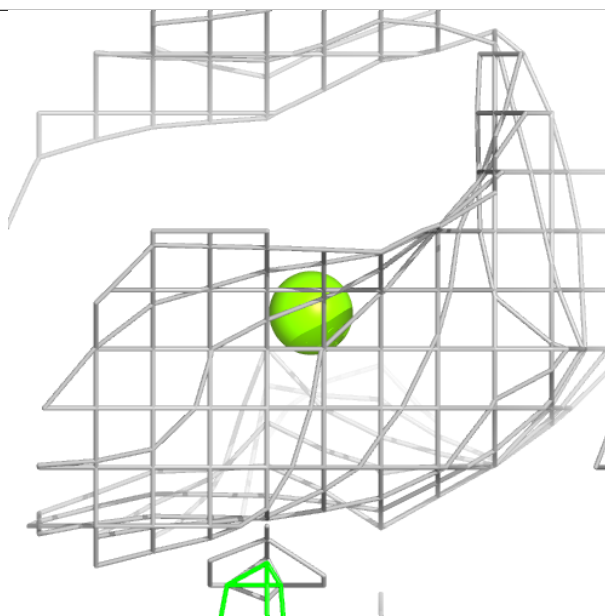
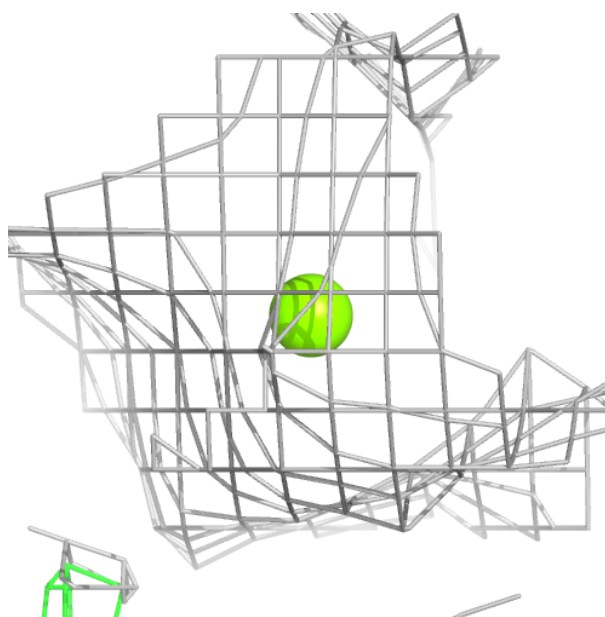
Electron density around 0KX A 705:

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



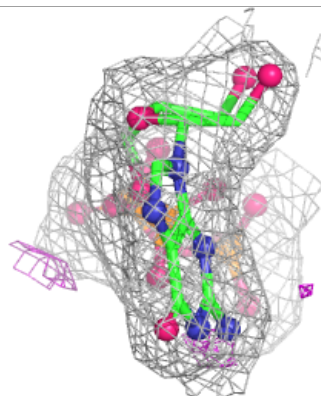
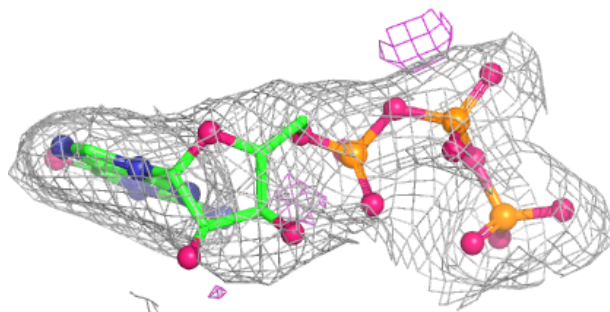
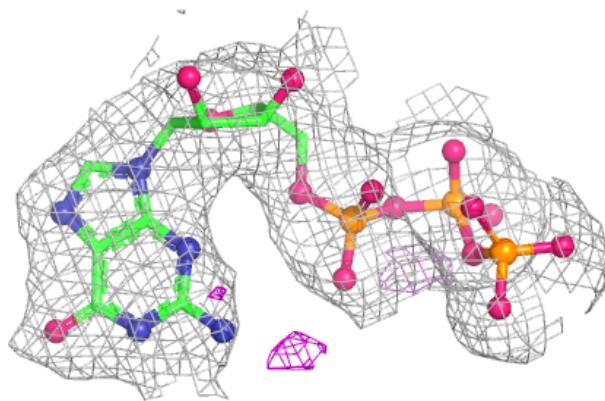
Electron density around MG D 705:

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

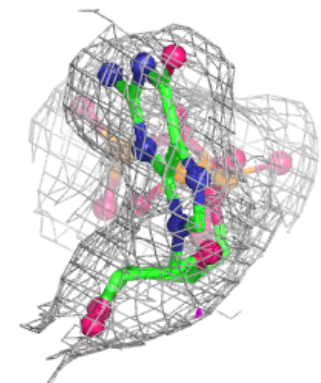
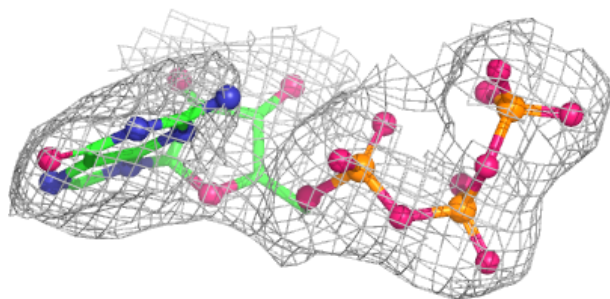
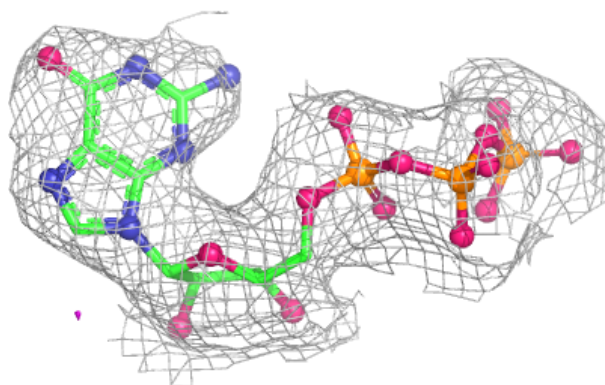


Electron density around GTP A 706:

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

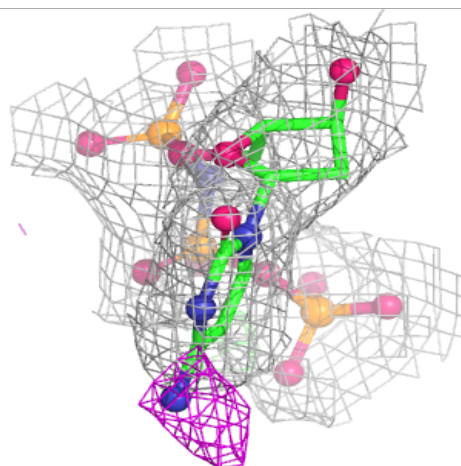
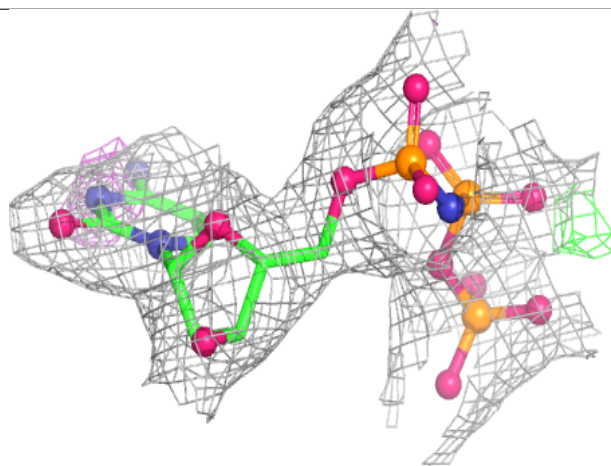
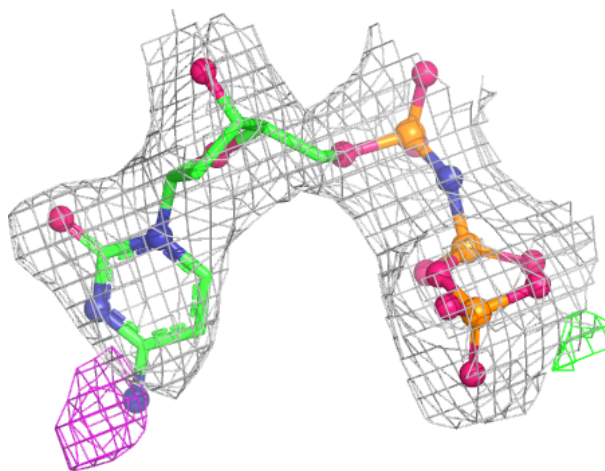
**Electron density around GTP B 706:**

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



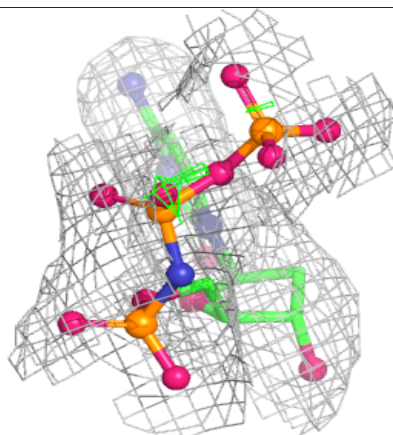
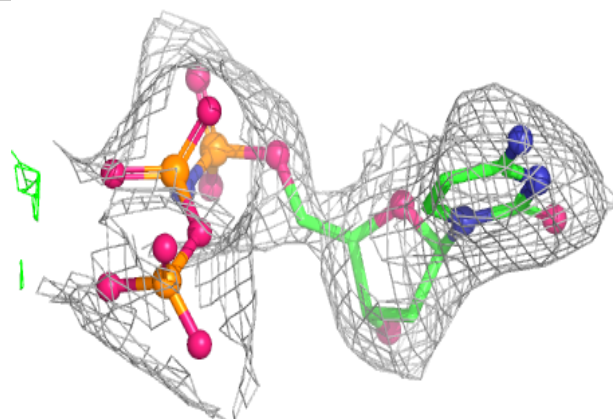
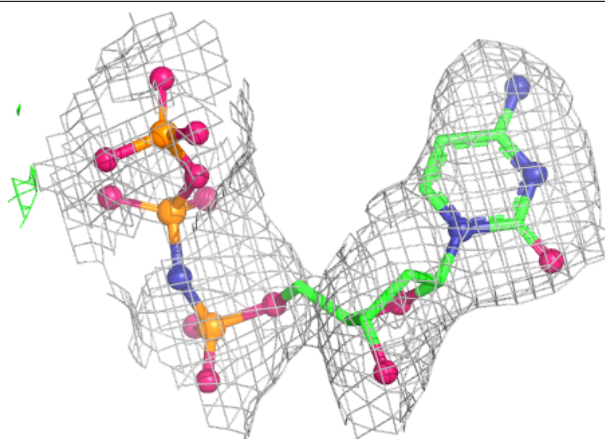
Electron density around 0KX D 706:

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

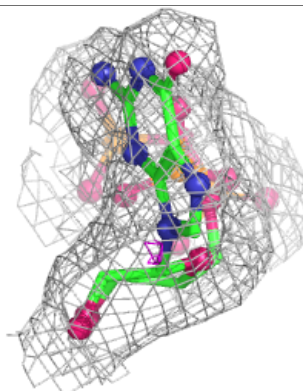
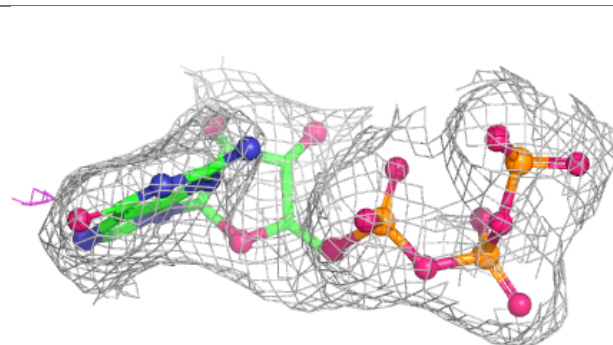
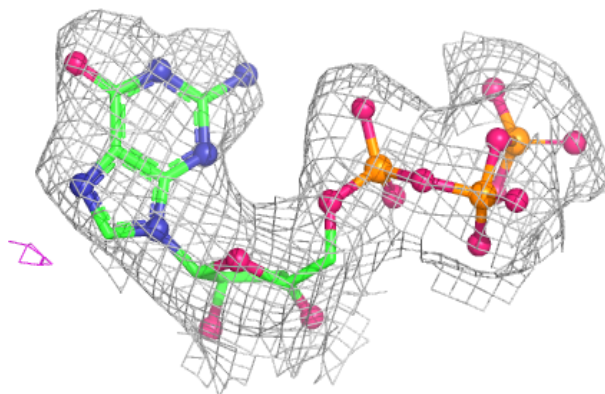


Electron density around 0KX E 704:

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

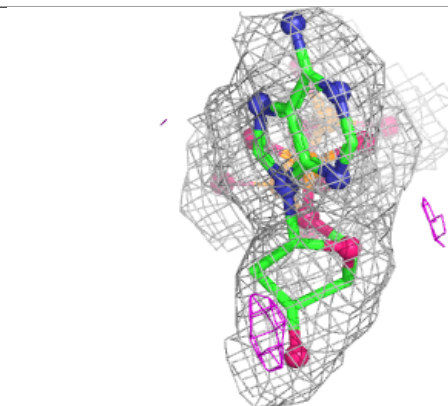
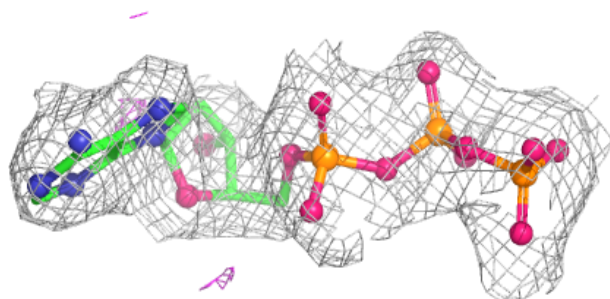
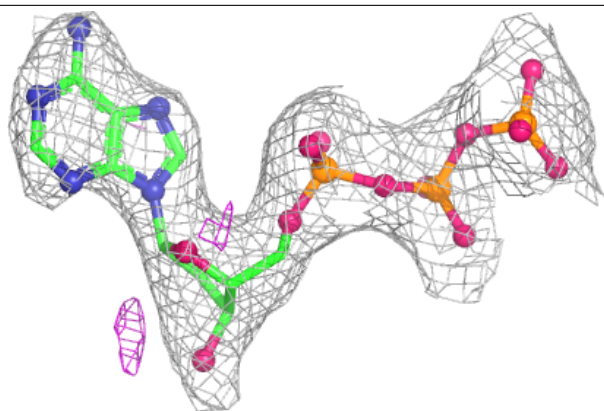
**Electron density around GTP G 707:**

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

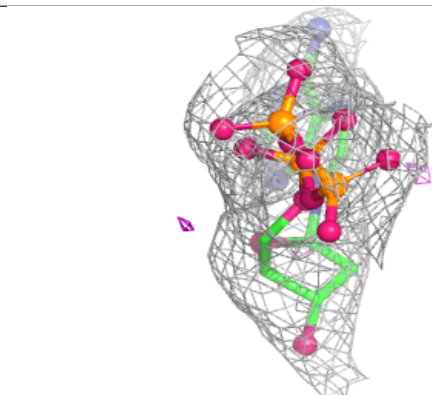
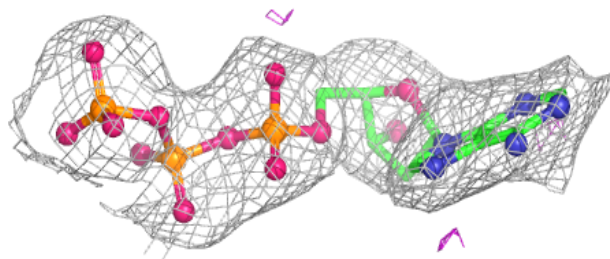
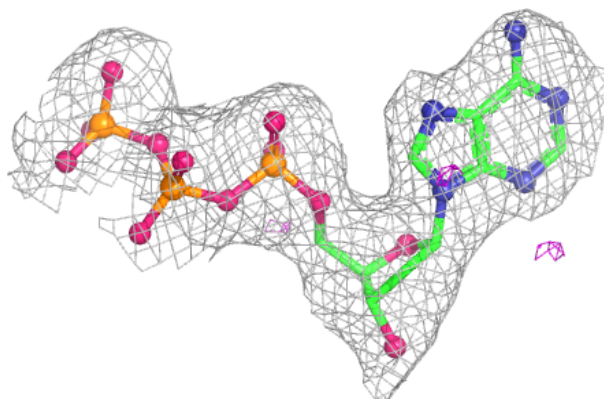


Electron density around DTP A 708:

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

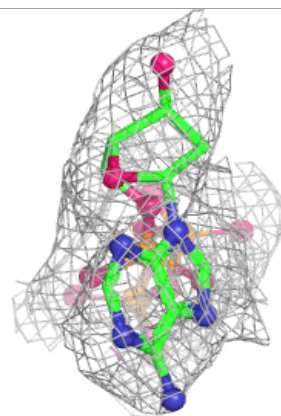
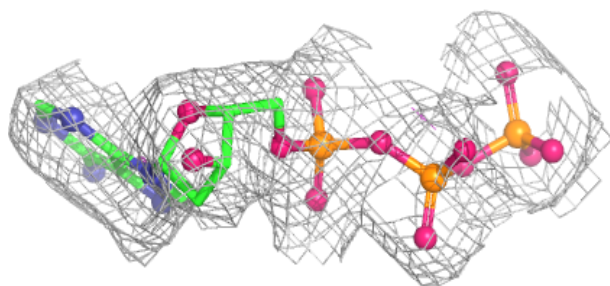
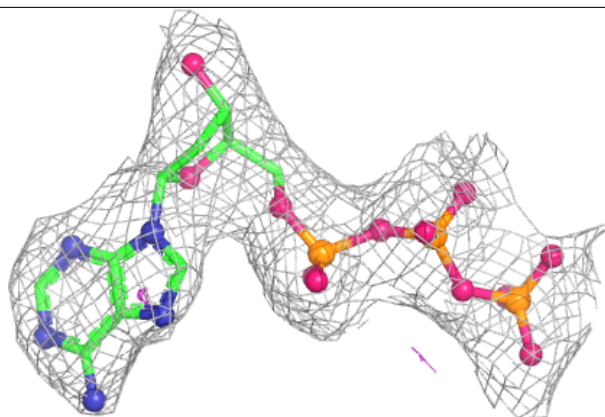
**Electron density around DTP B 708:**

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



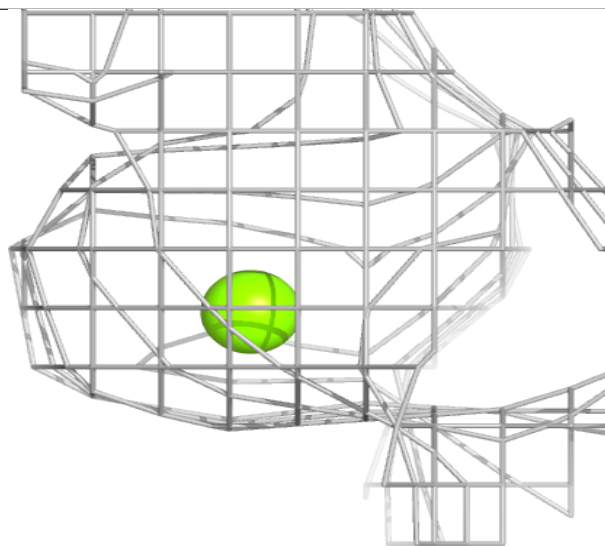
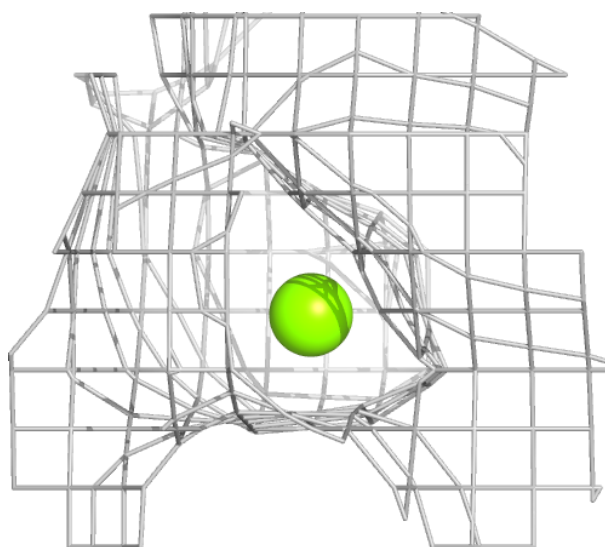
Electron density around DTP D 701:

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



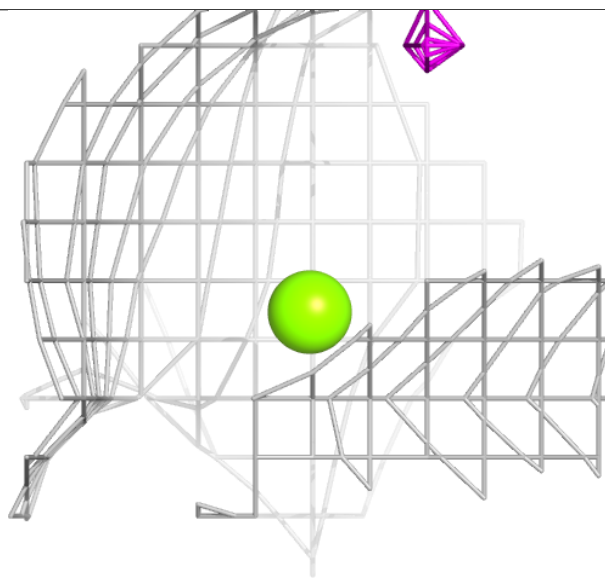
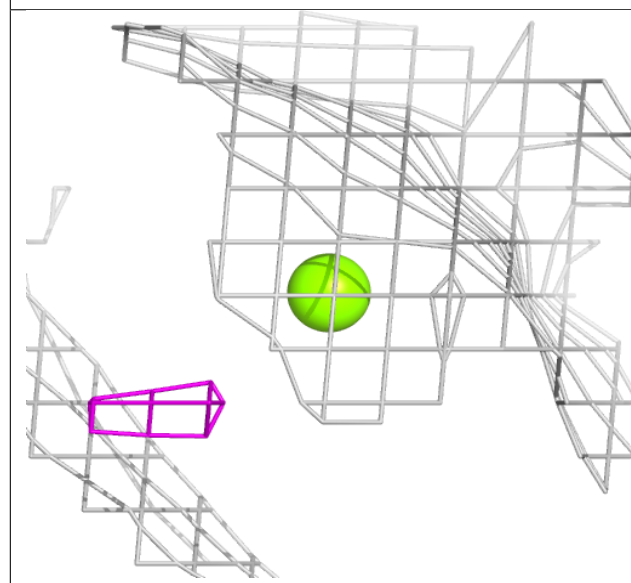
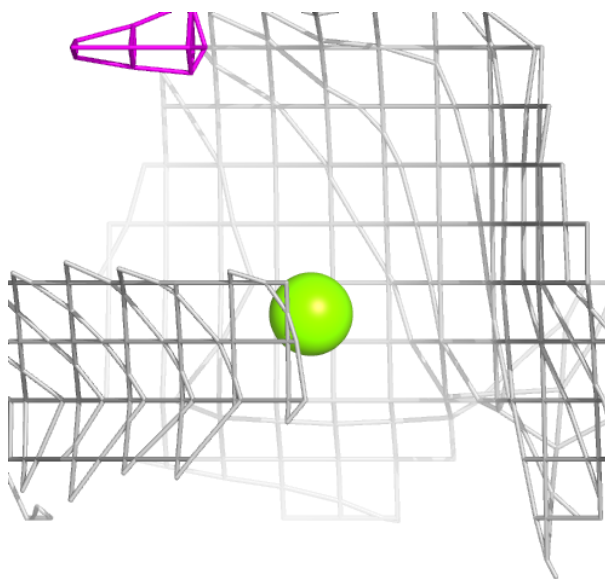
Electron density around MG A 702:

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



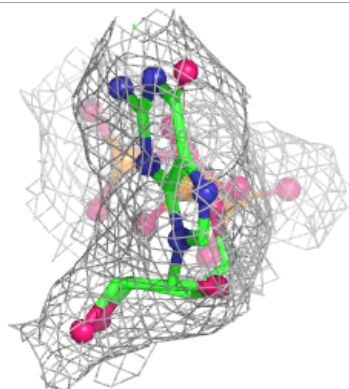
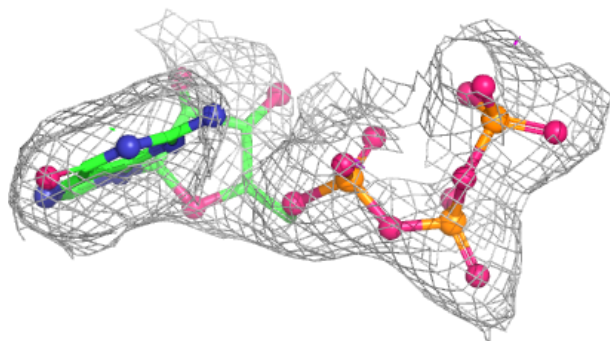
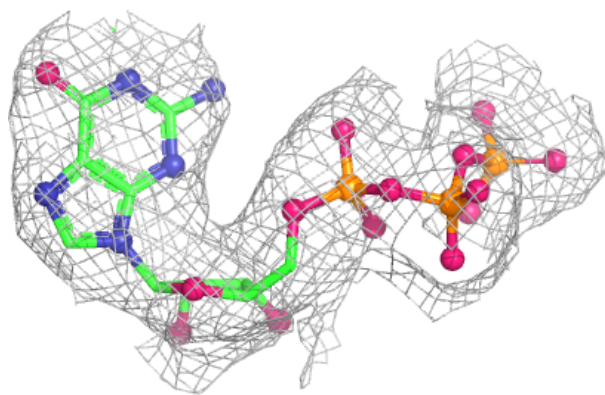
Electron density around MG E 703:

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



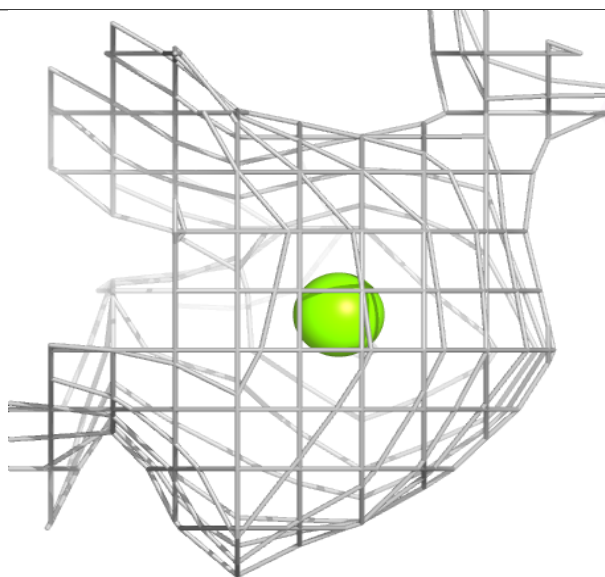
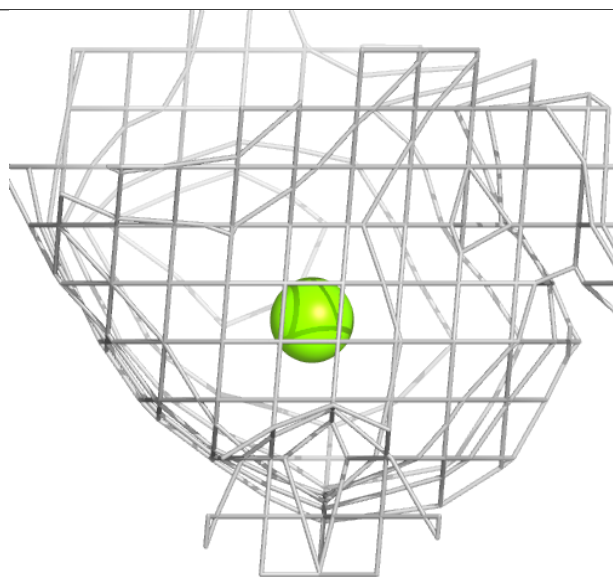
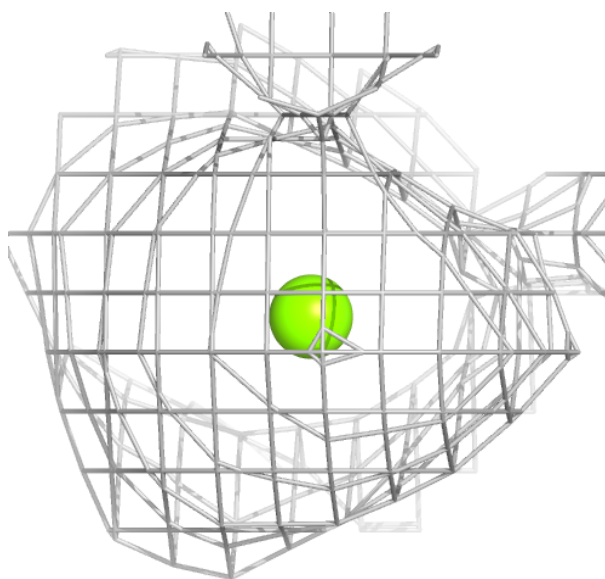
Electron density around GTP J 705:

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



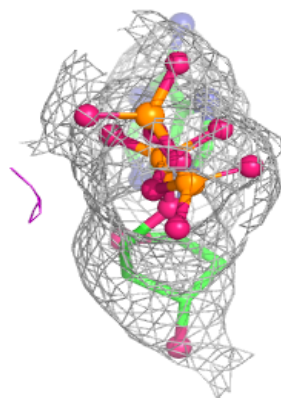
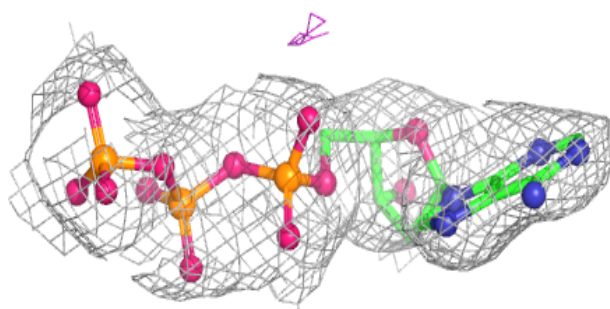
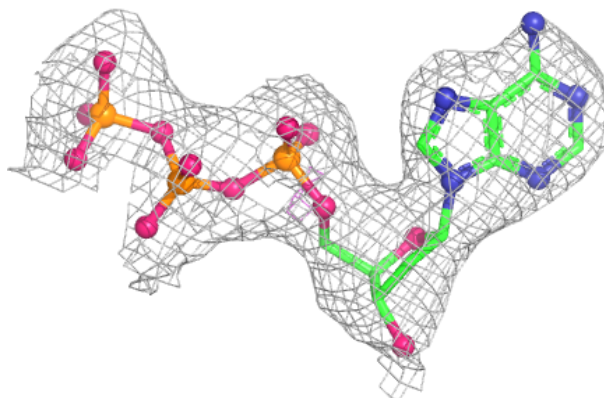
Electron density around MG O 703:

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

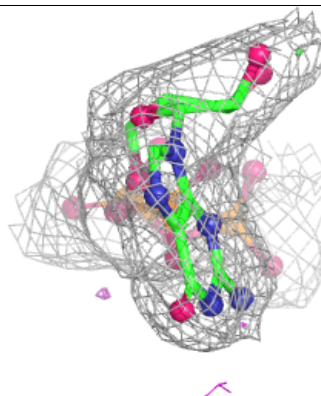
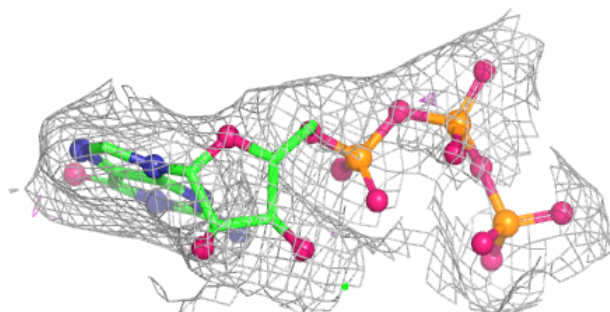
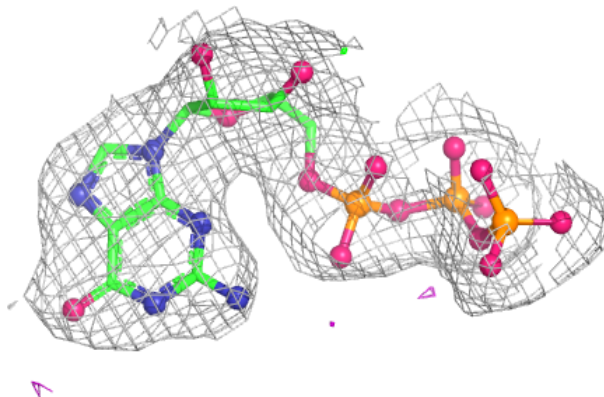


Electron density around DTP I 708:

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

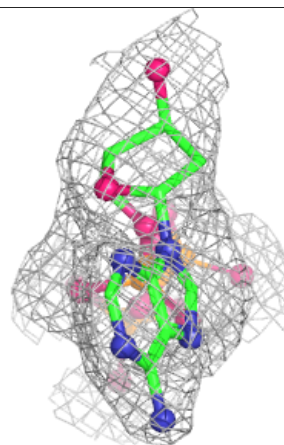
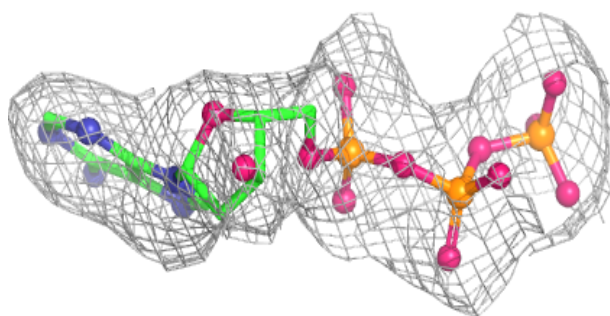
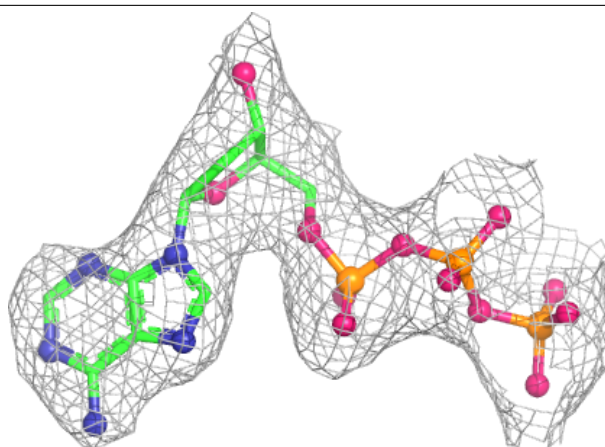
**Electron density around GTP L 707:**

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



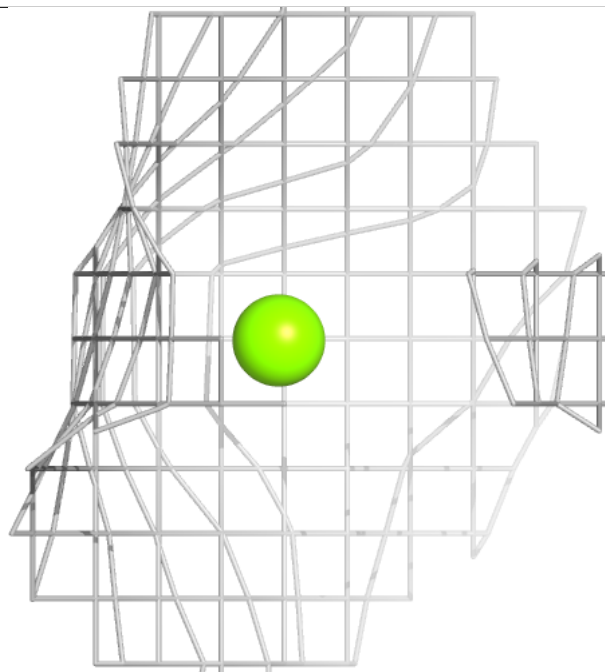
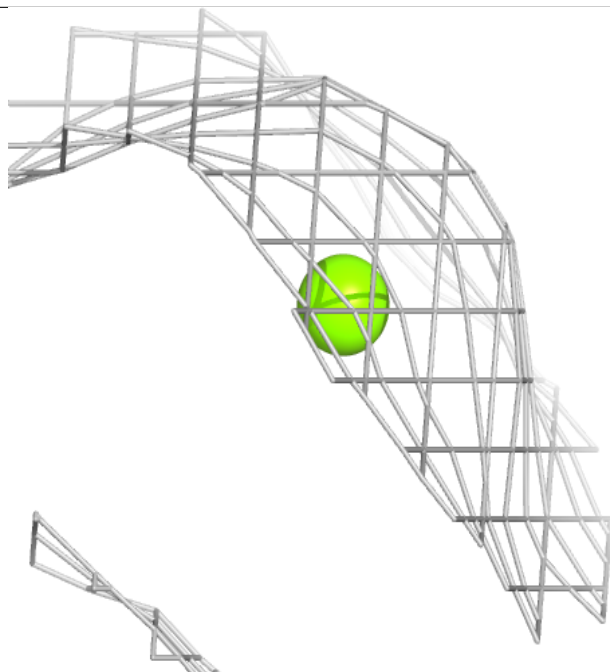
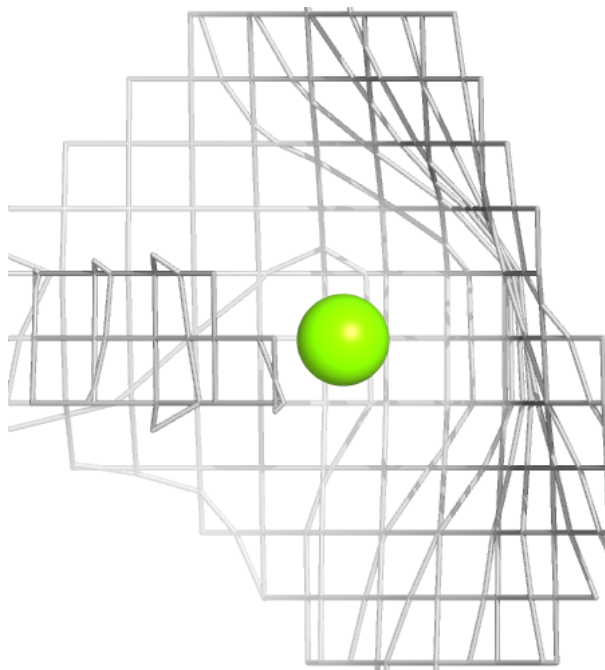
Electron density around DTP K 701:

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



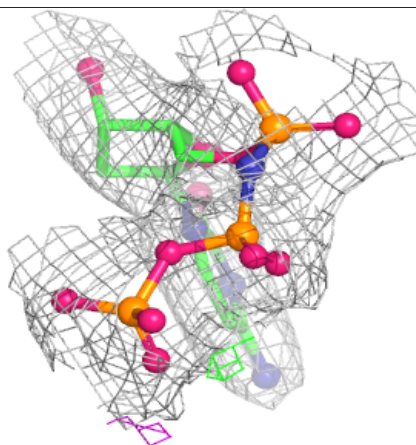
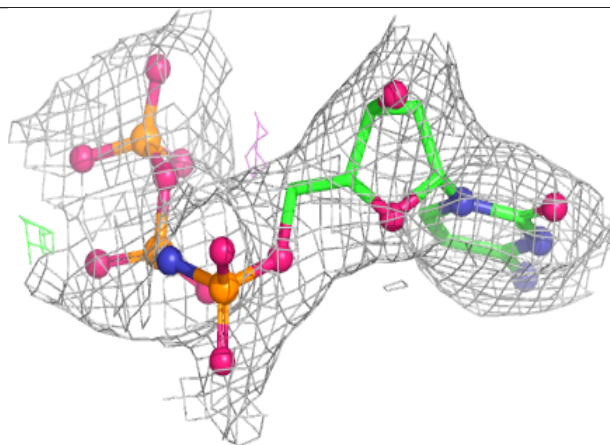
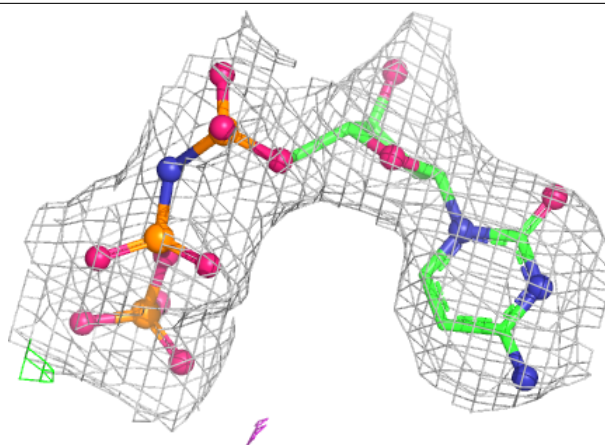
Electron density around MG O 704:

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



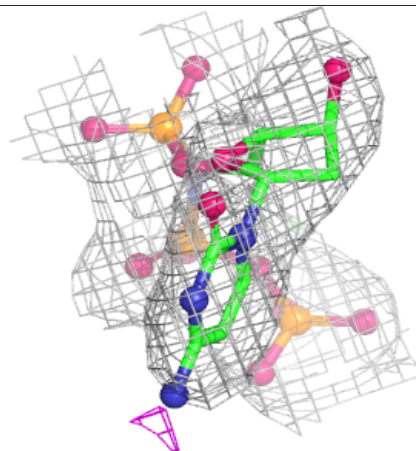
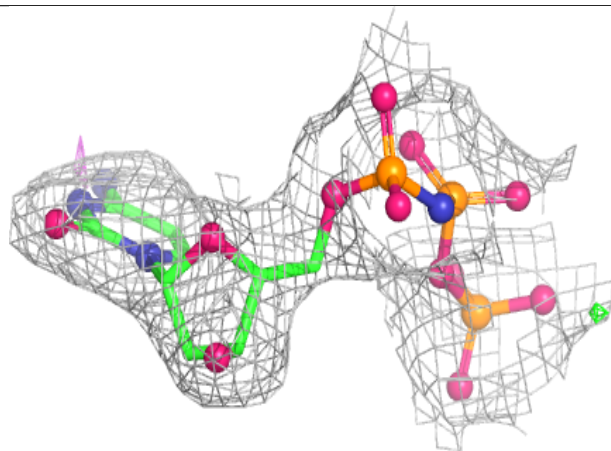
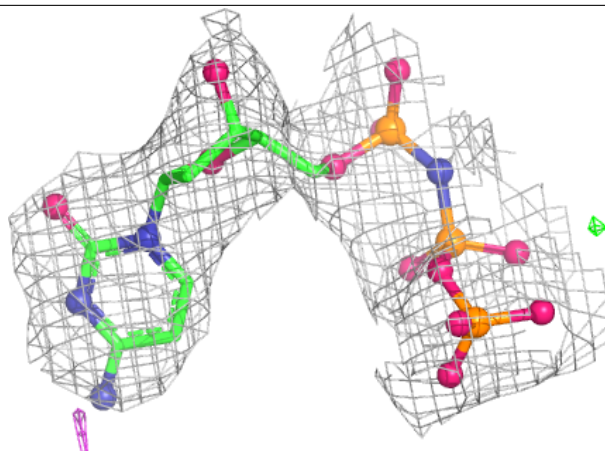
Electron density around 0KX J 704:

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



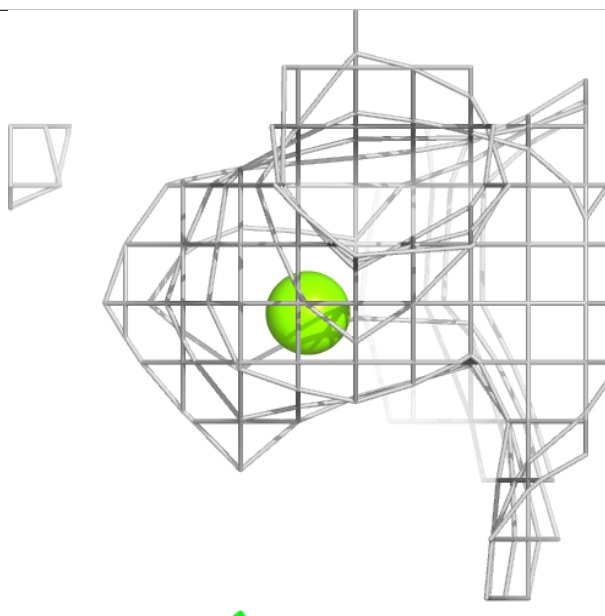
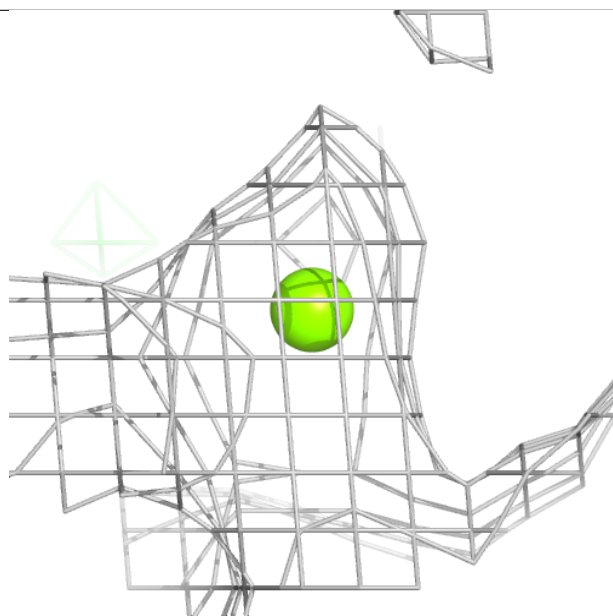
Electron density around 0KX K 706:

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



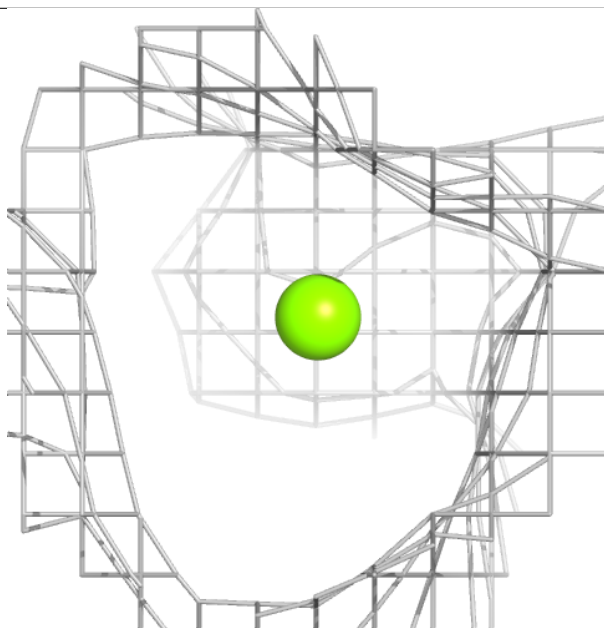
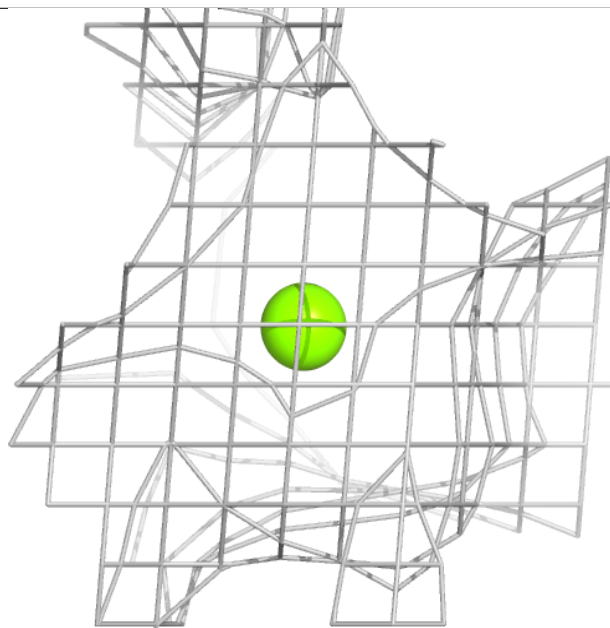
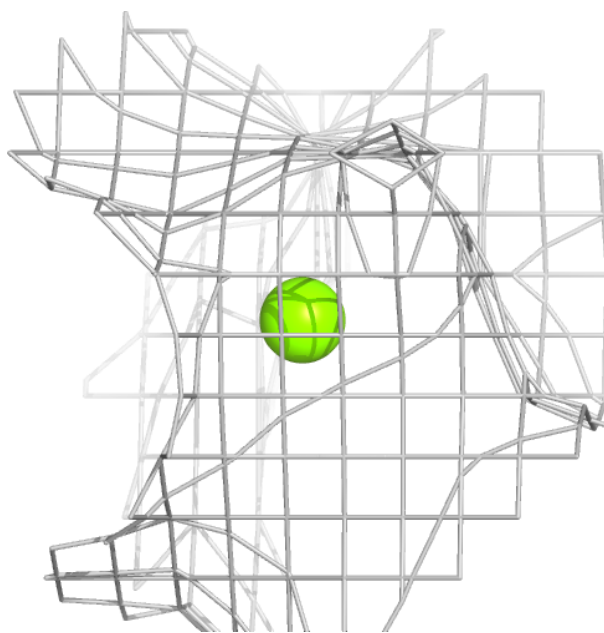
Electron density around MG L 703:

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



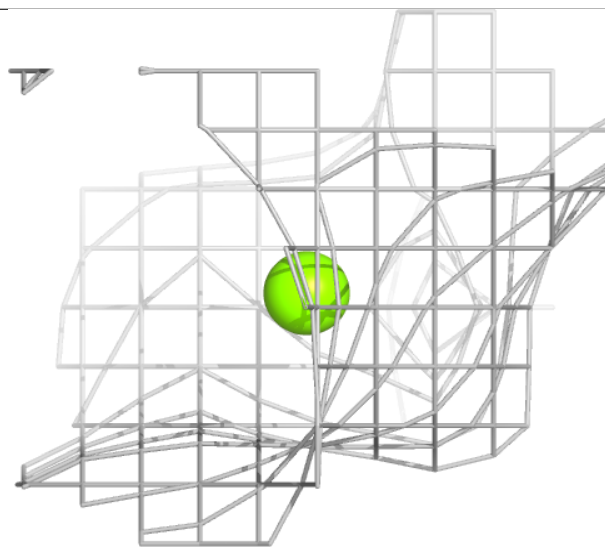
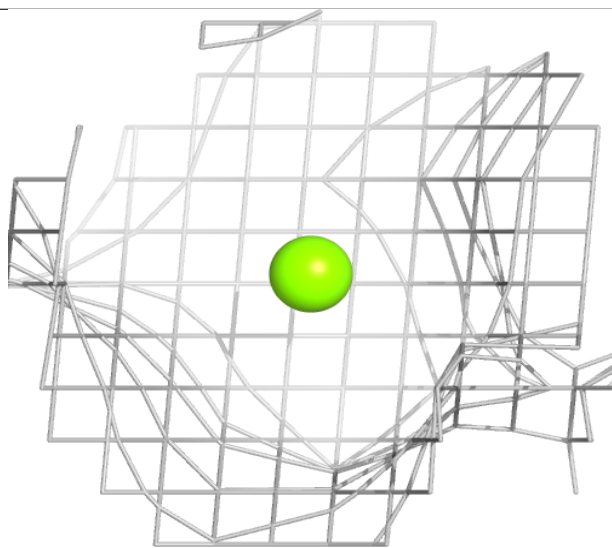
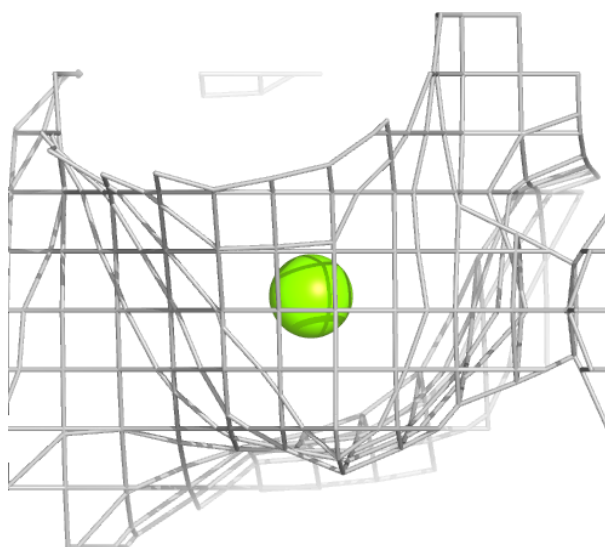
Electron density around MG C 705:

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



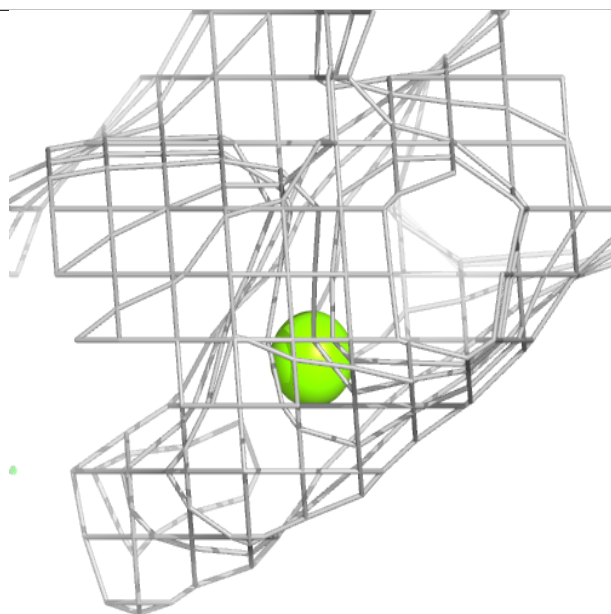
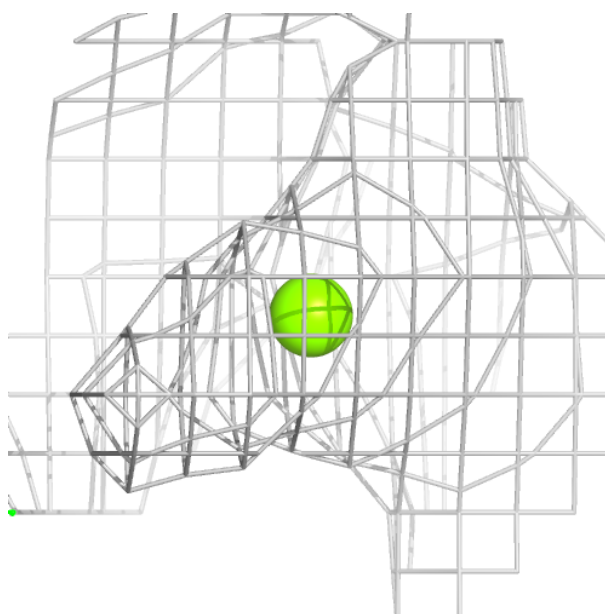
Electron density around MG G 705:

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



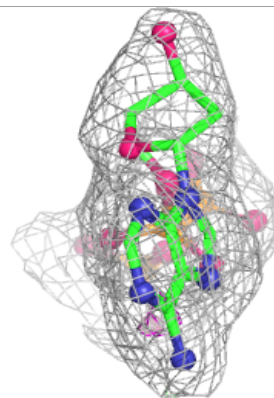
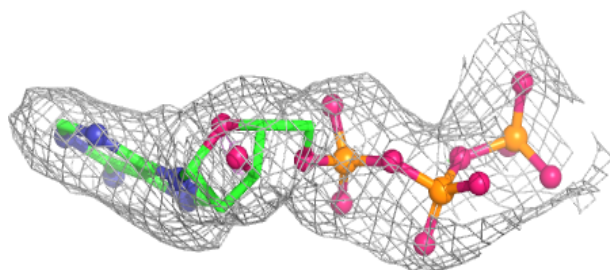
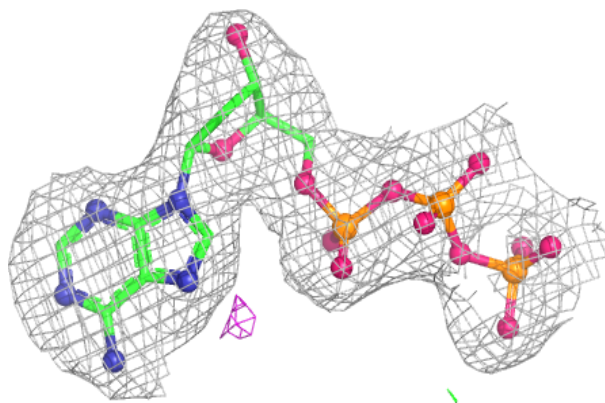
Electron density around MG C 703:

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



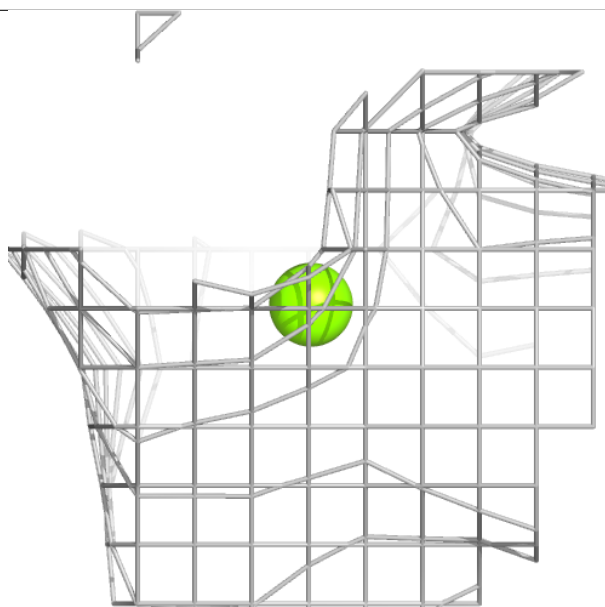
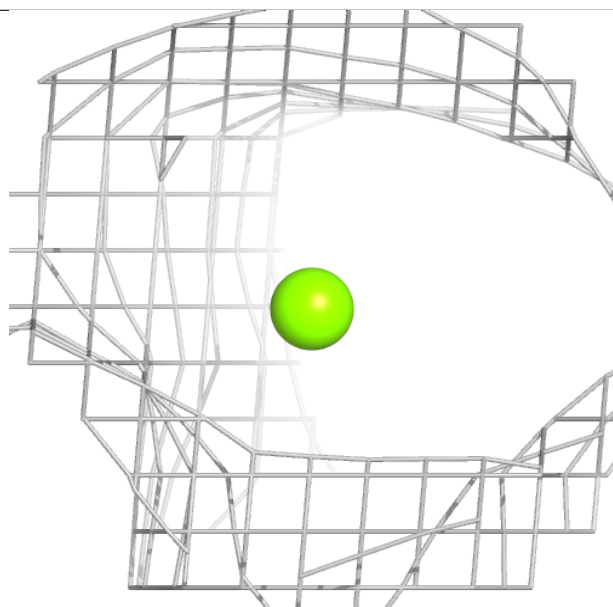
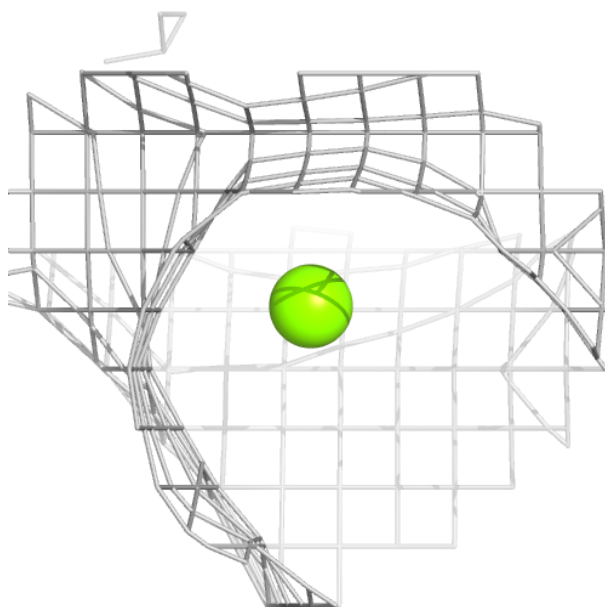
Electron density around DTP C 701:

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



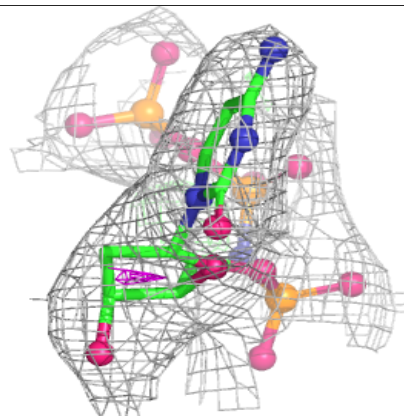
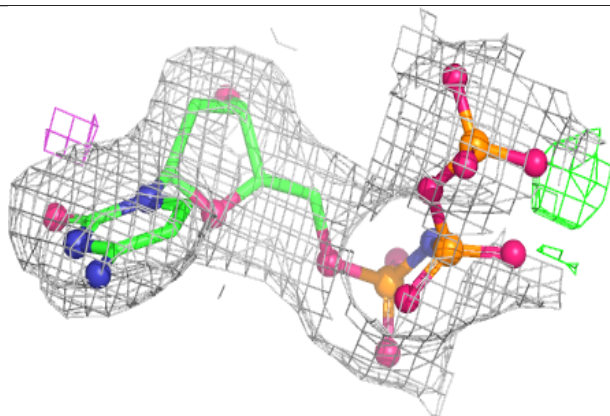
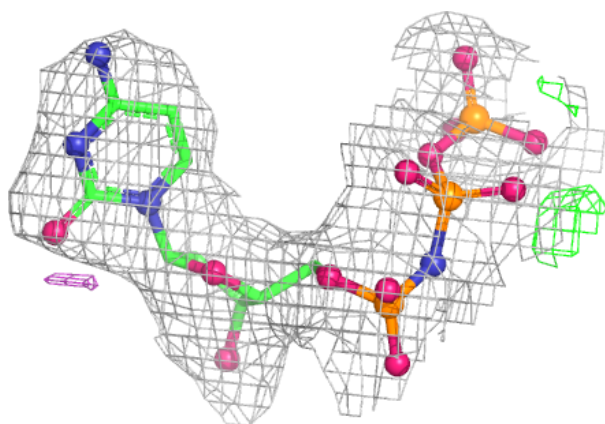
Electron density around MG M 704:

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



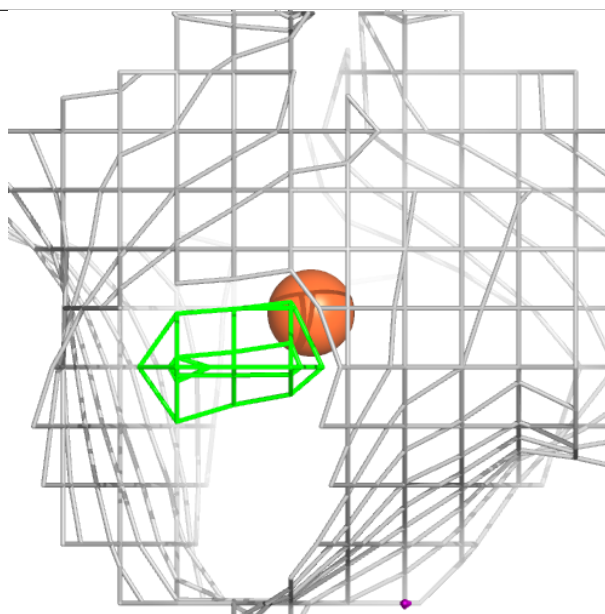
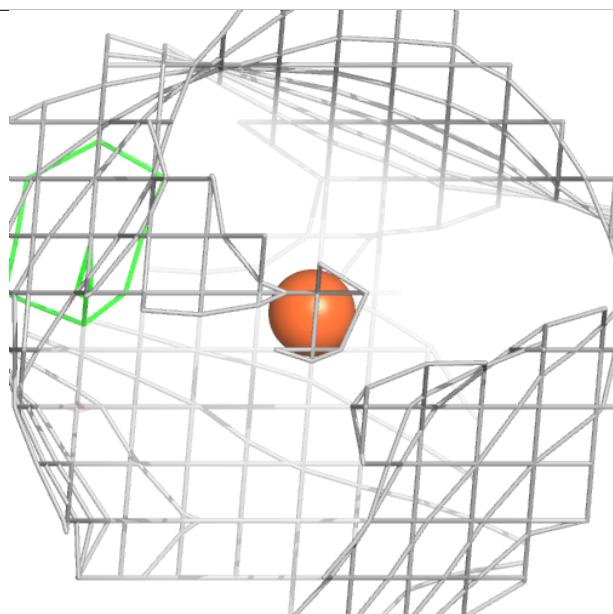
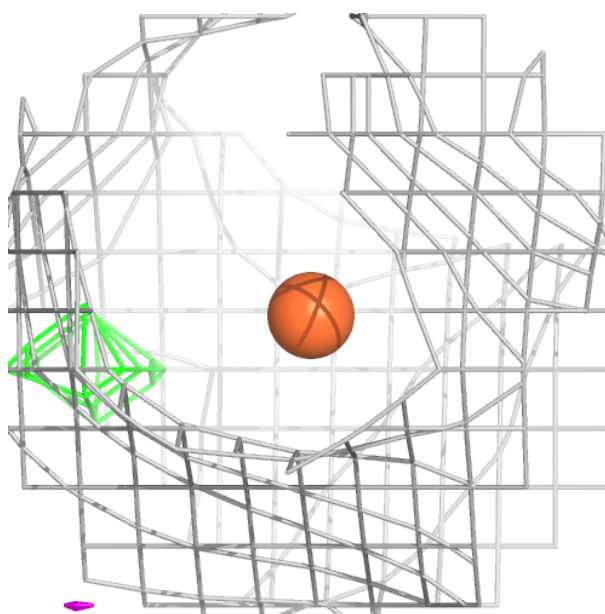
Electron density around 0KX B 705:

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



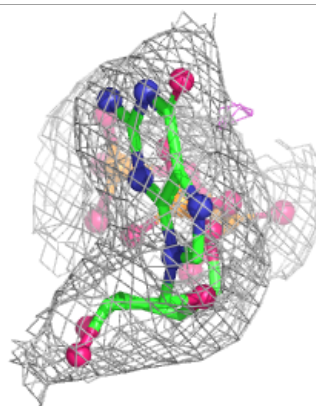
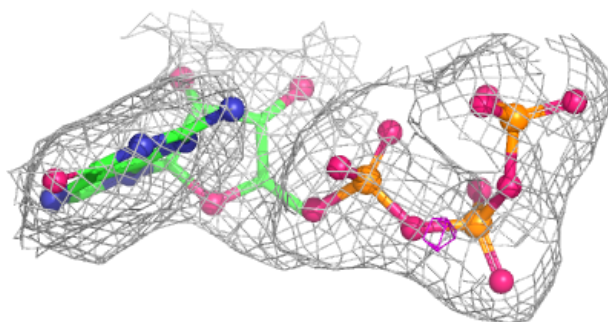
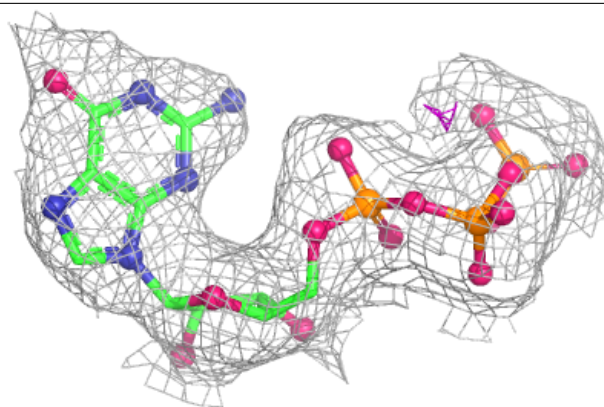
Electron density around FE I 701:

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

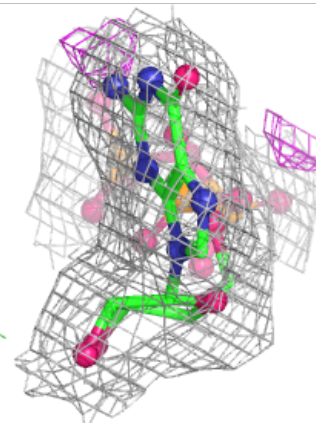
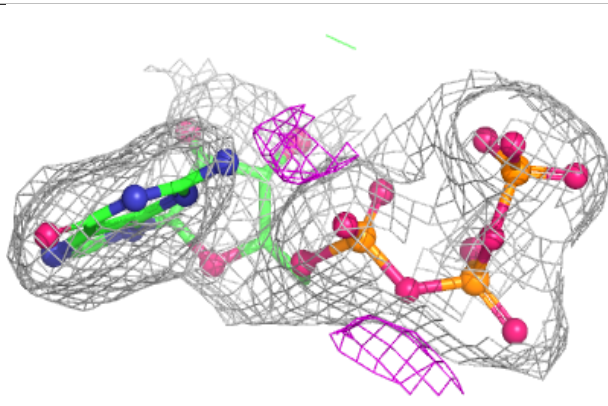
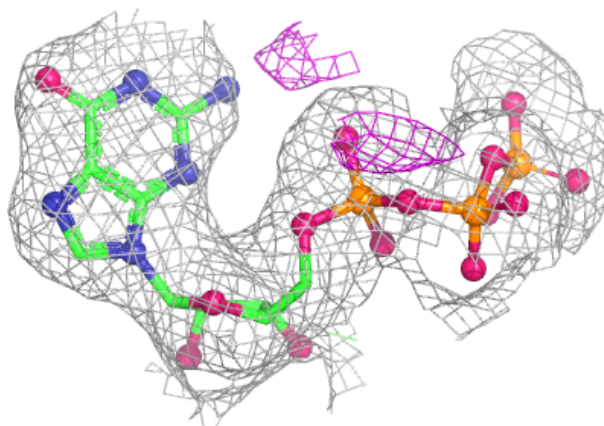


Electron density around GTP C 707:

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

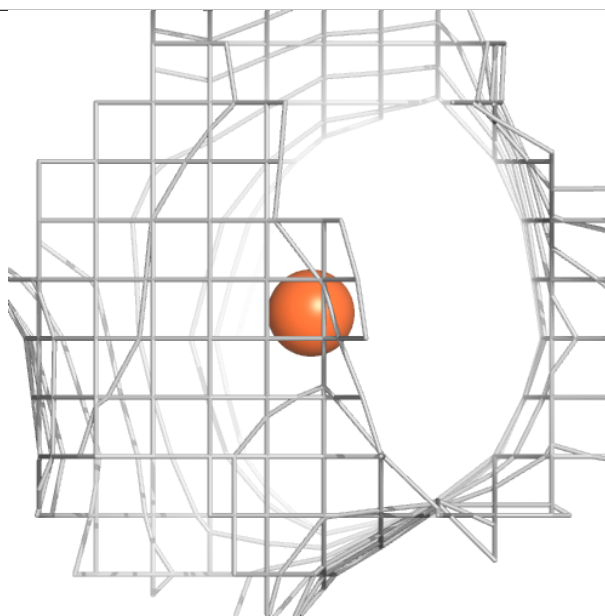
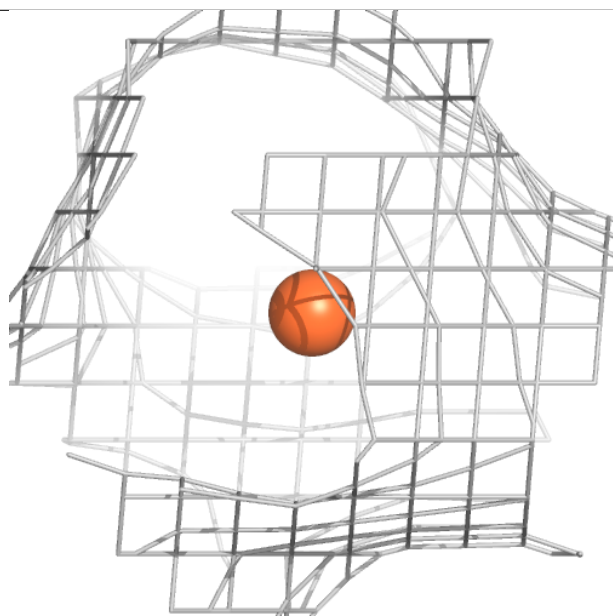
**Electron density around GTP D 707:**

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



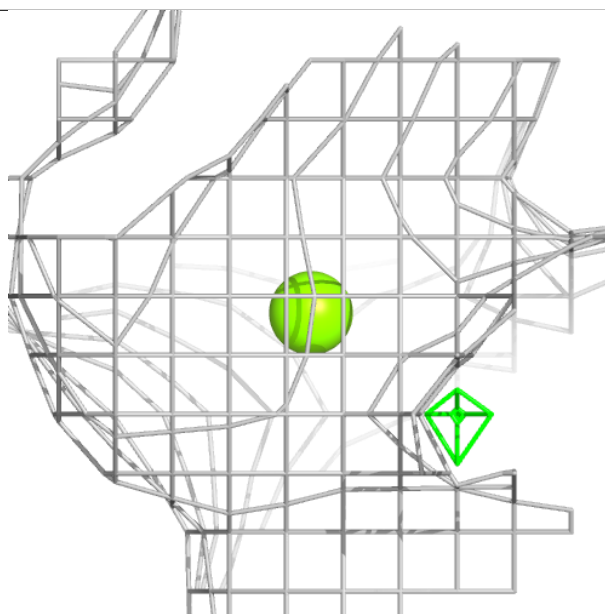
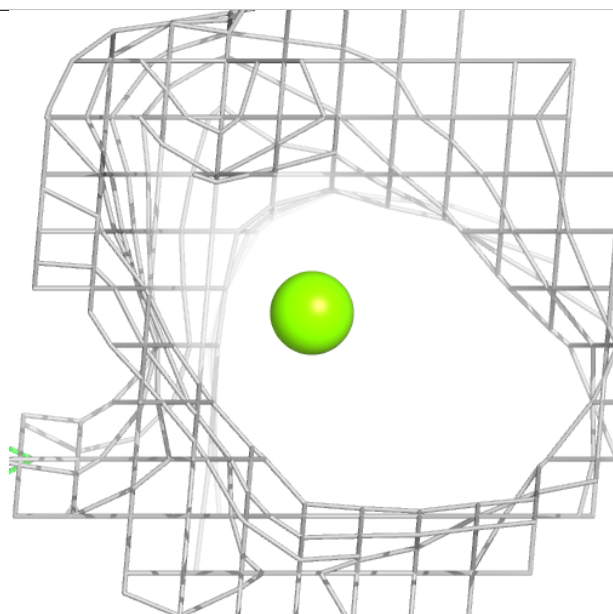
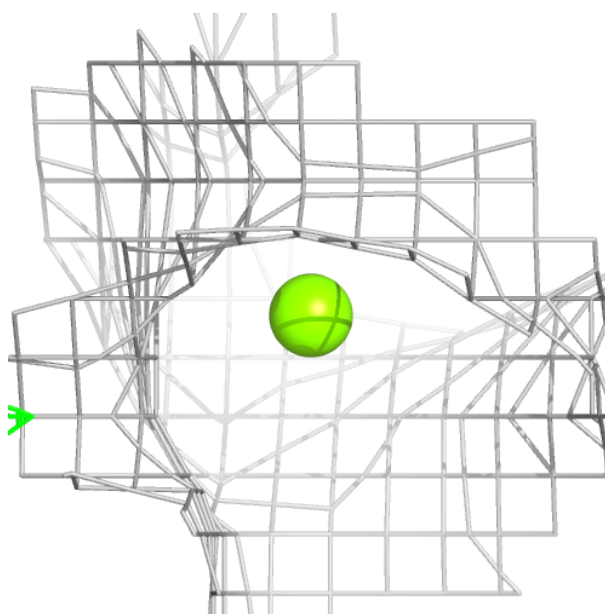
Electron density around FE J 701:

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



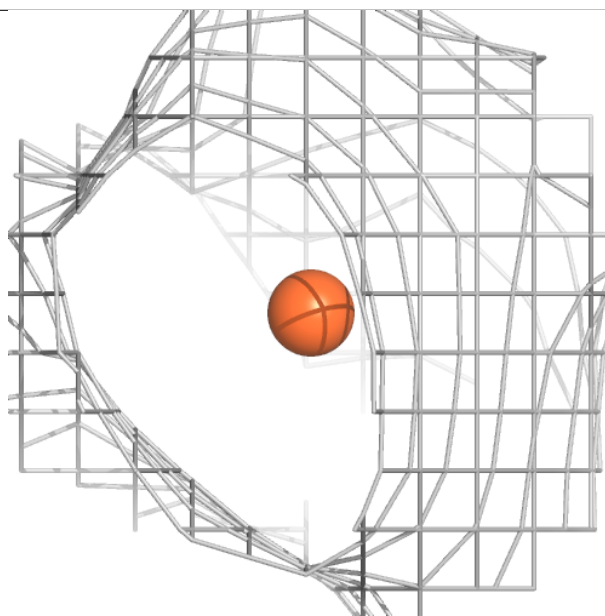
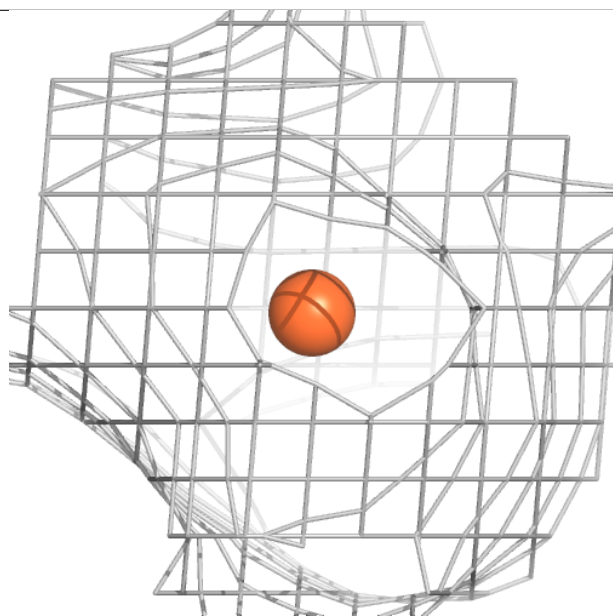
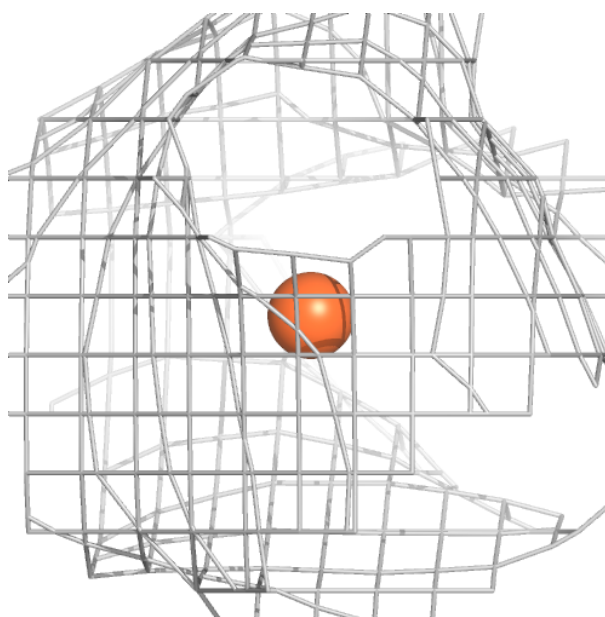
Electron density around MG I 704:

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



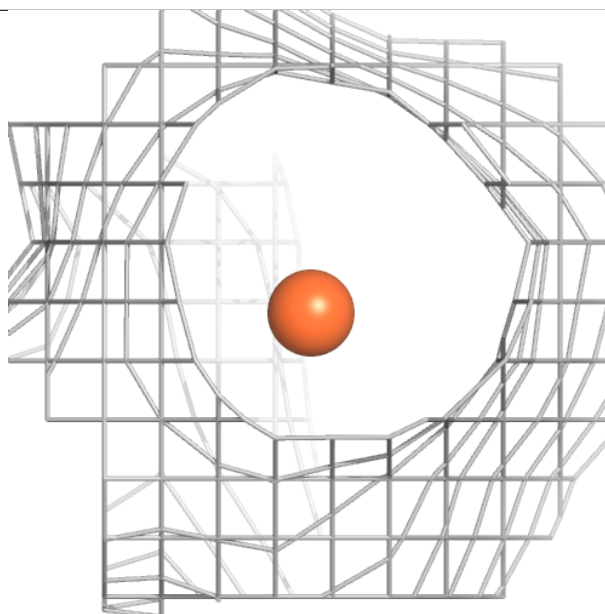
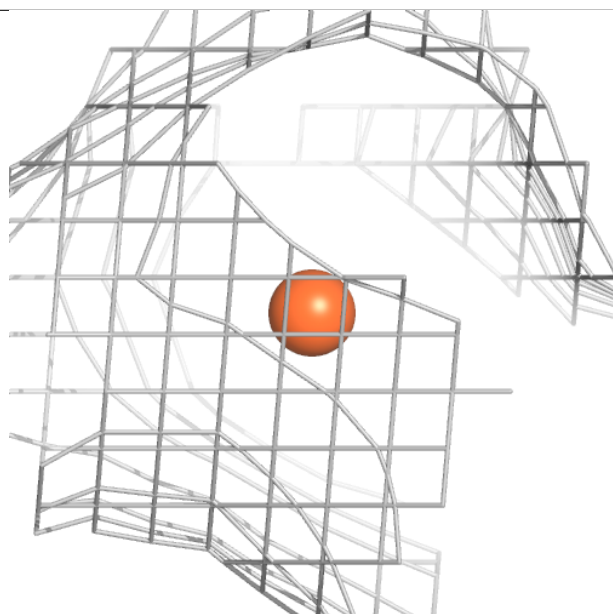
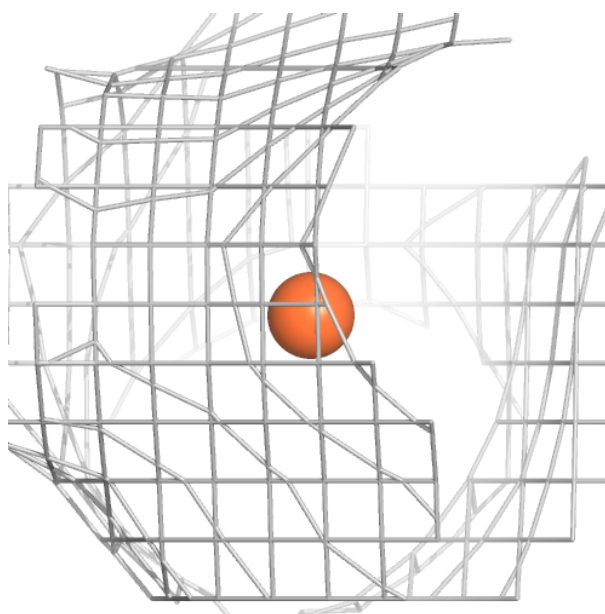
Electron density around FE N 701:

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



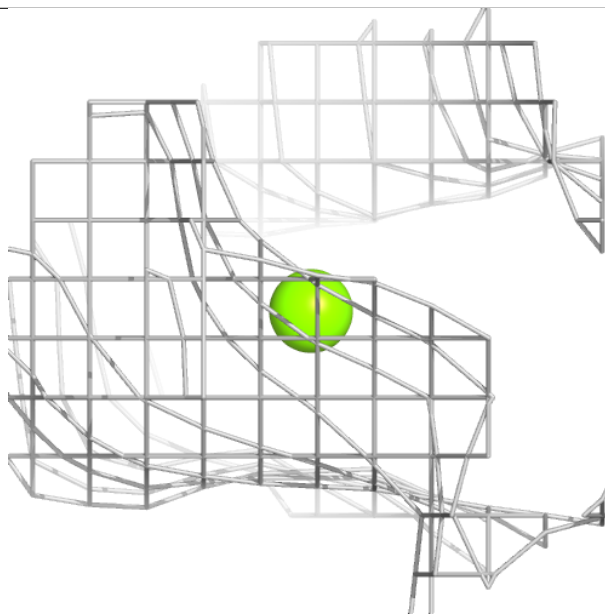
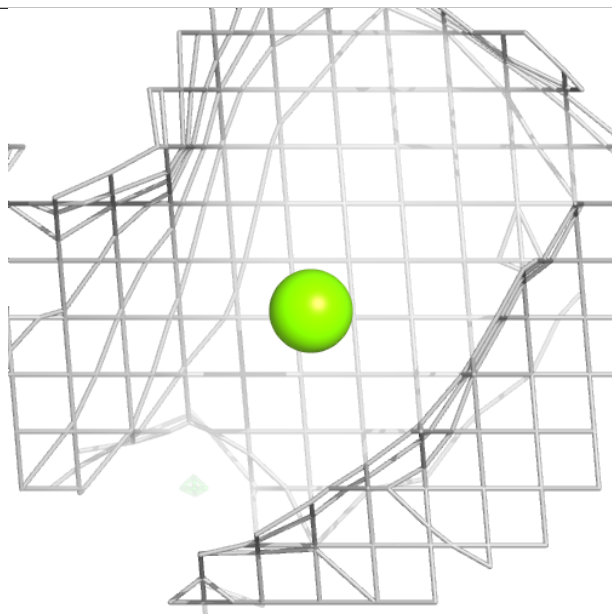
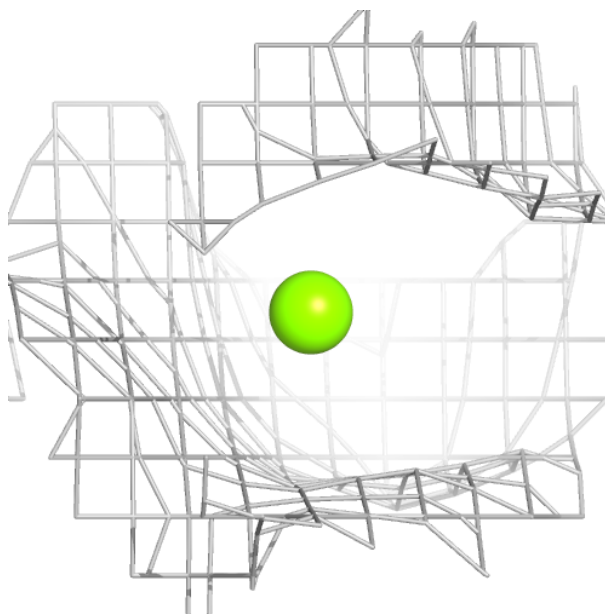
Electron density around FE E 701:

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



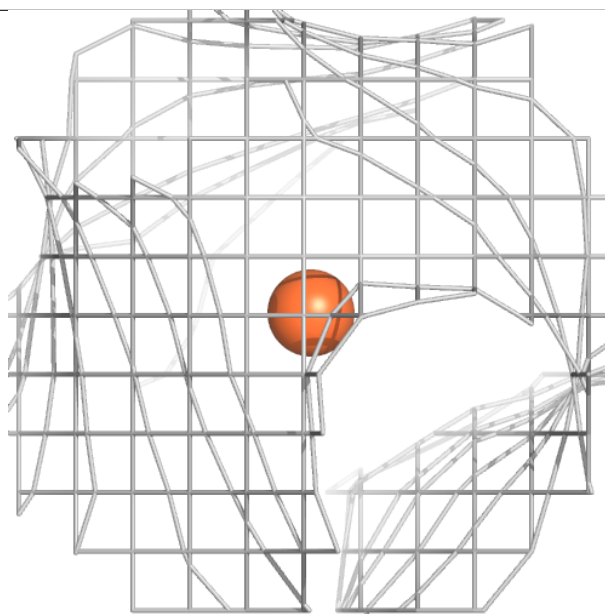
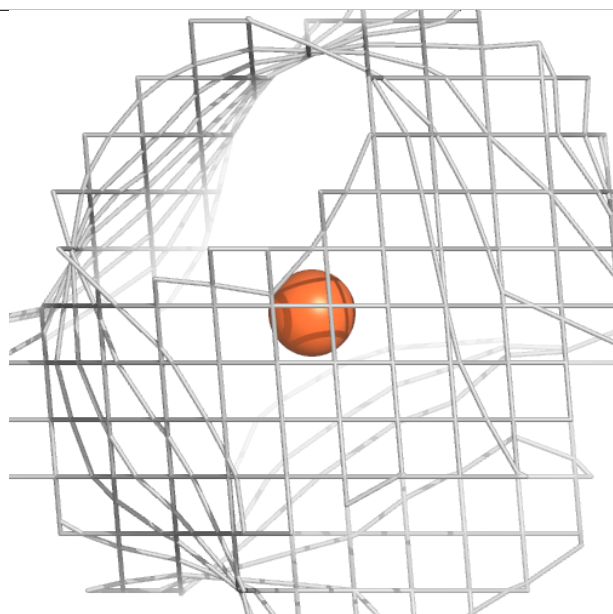
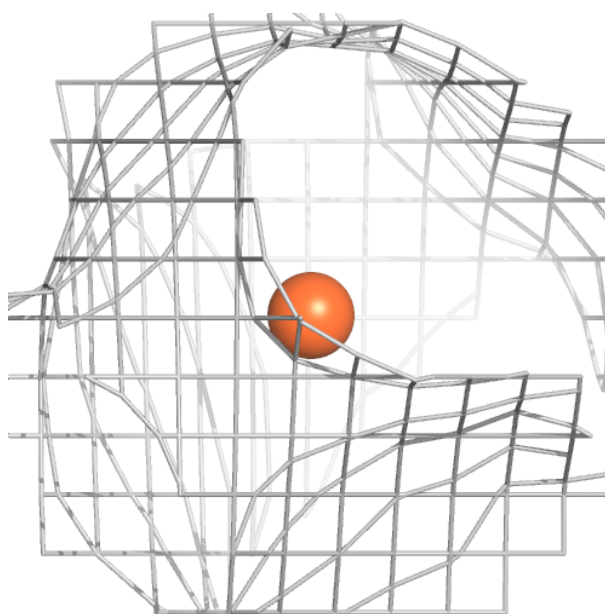
Electron density around MG L 705:

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



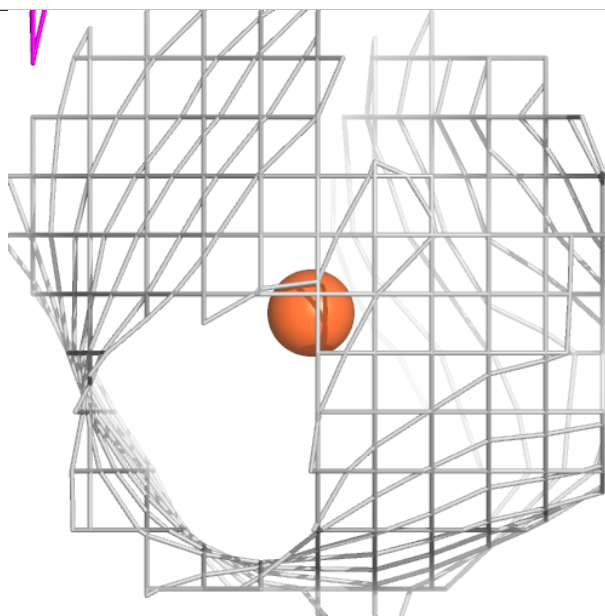
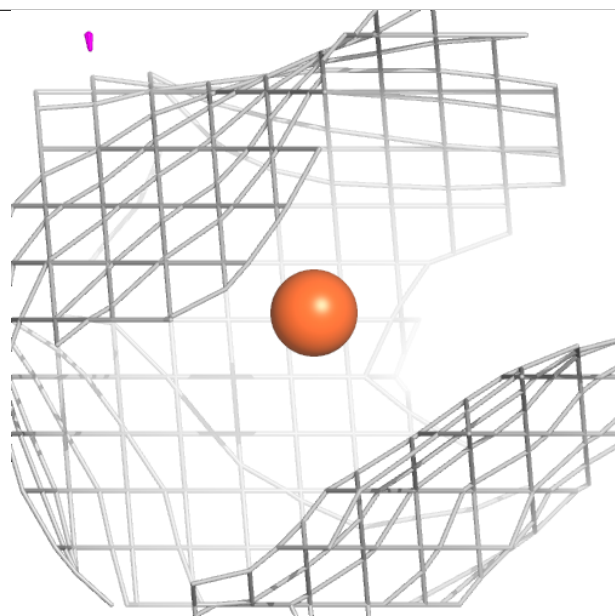
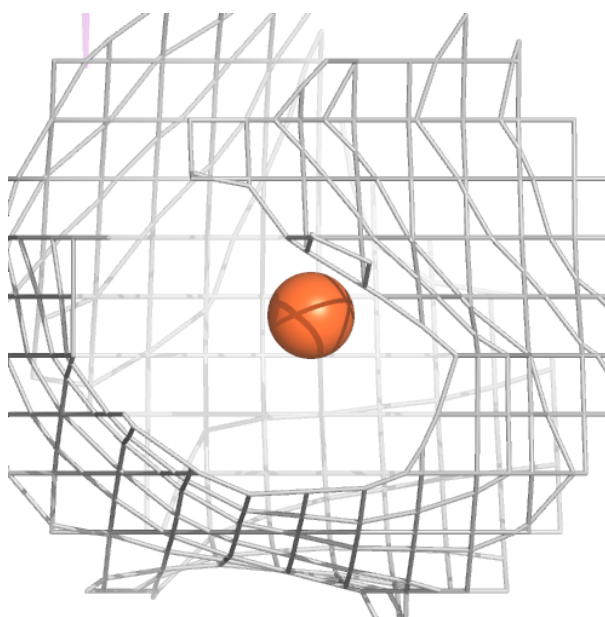
Electron density around FE B 701:

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



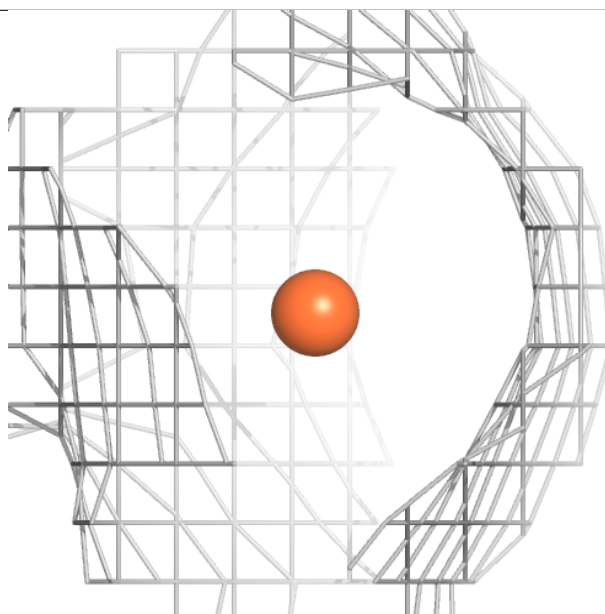
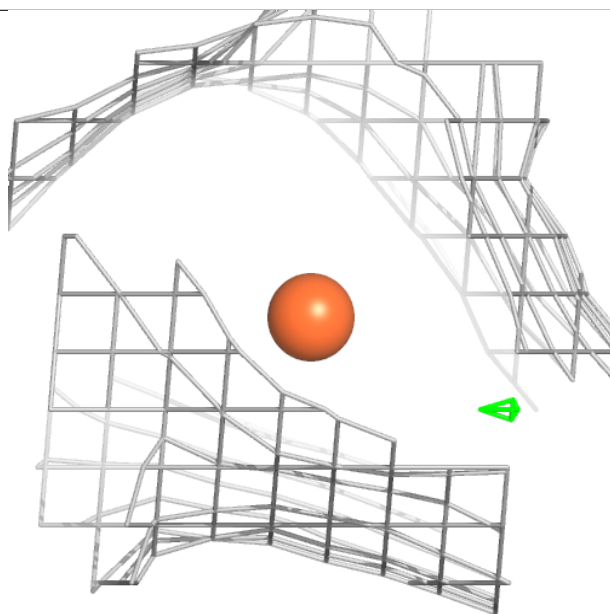
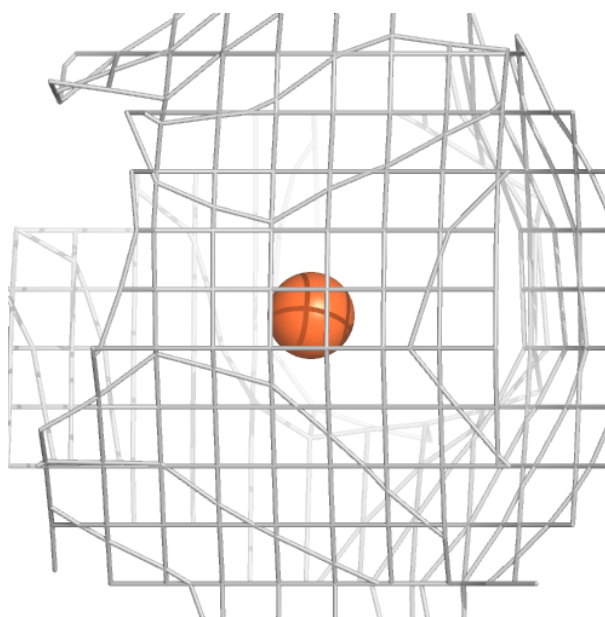
Electron density around FE F 701:

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



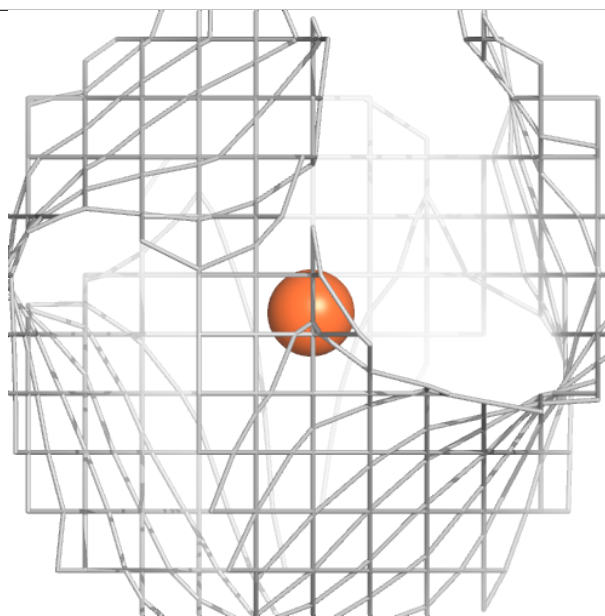
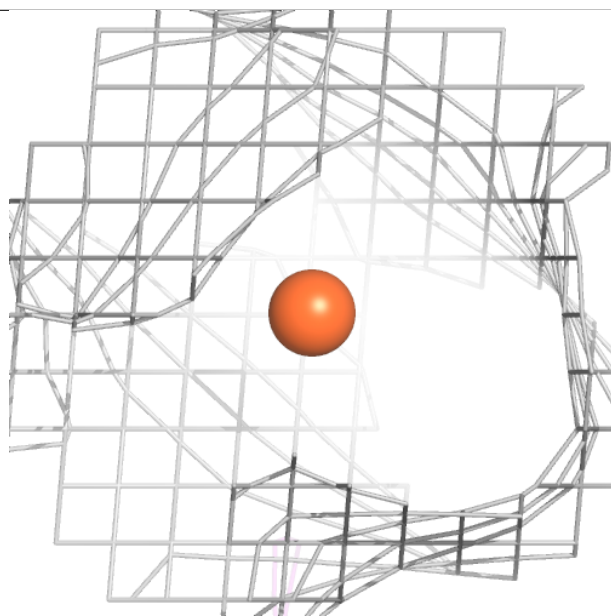
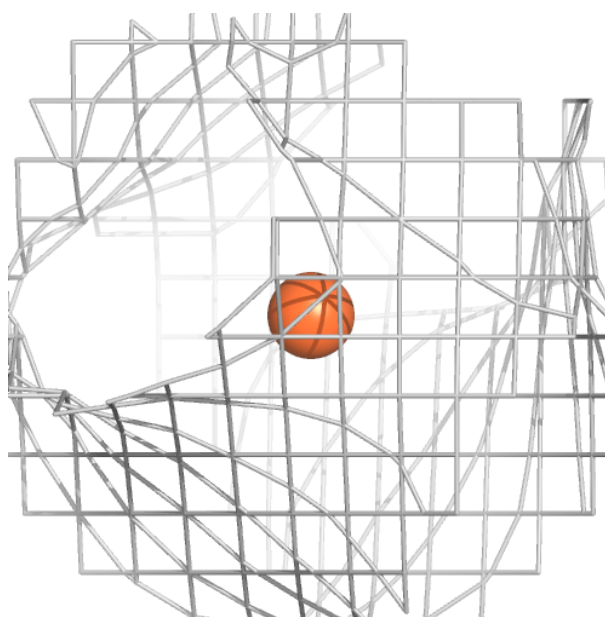
Electron density around FE G 702:

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



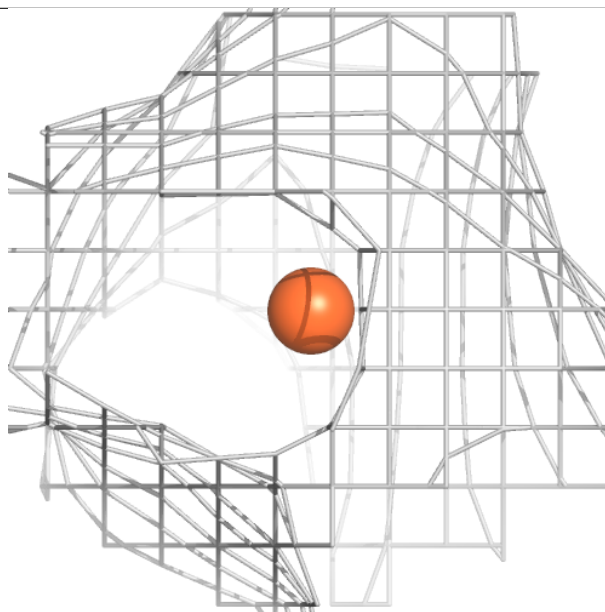
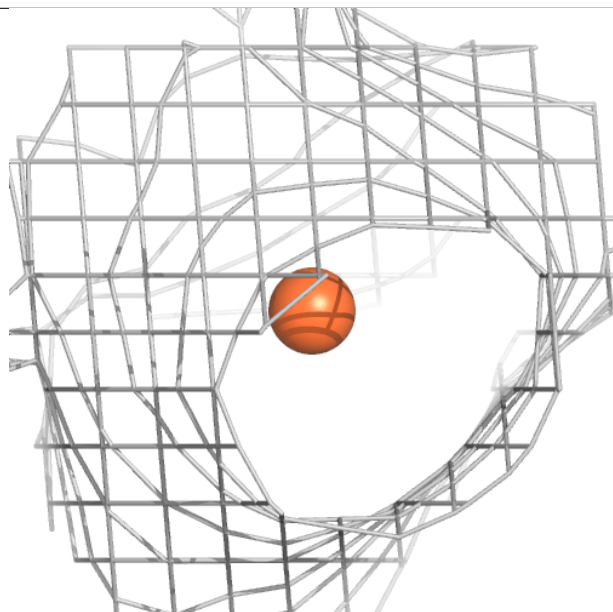
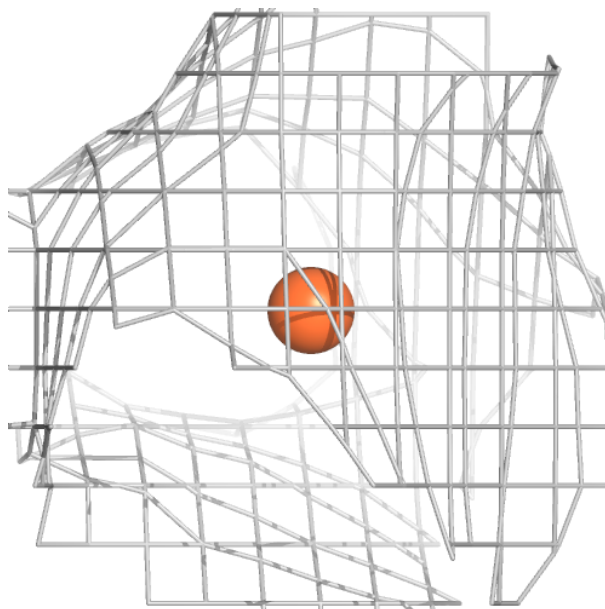
Electron density around FE H 702:

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



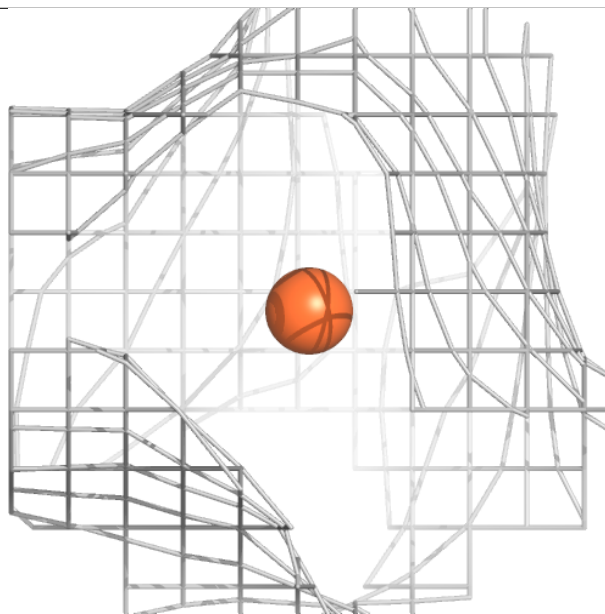
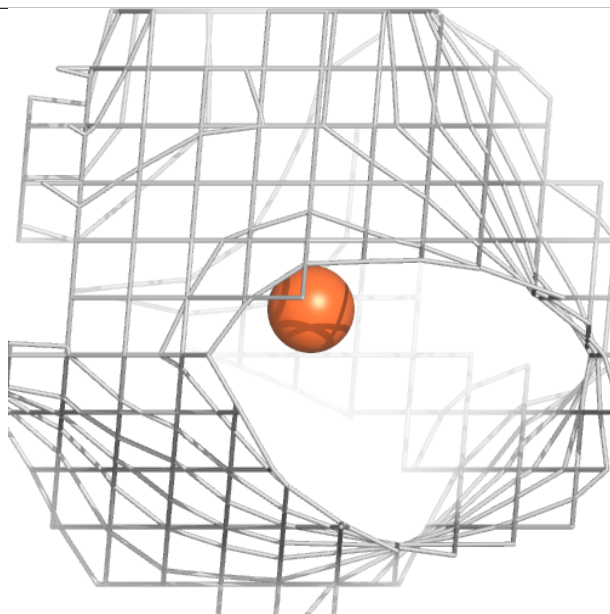
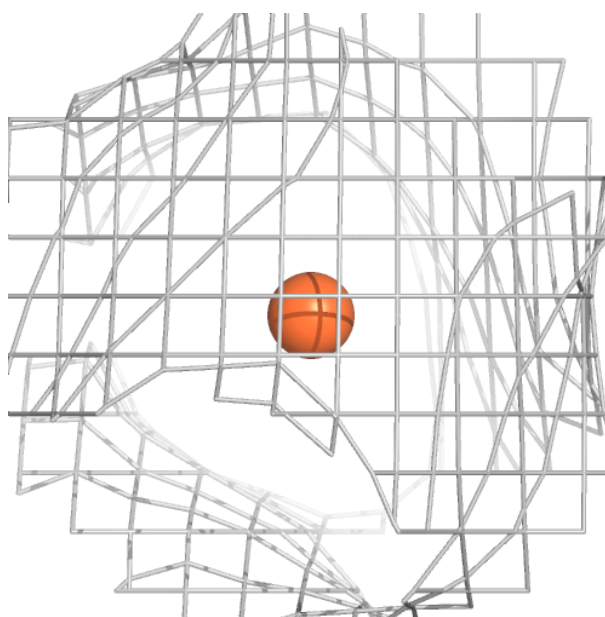
Electron density around FE C 702:

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



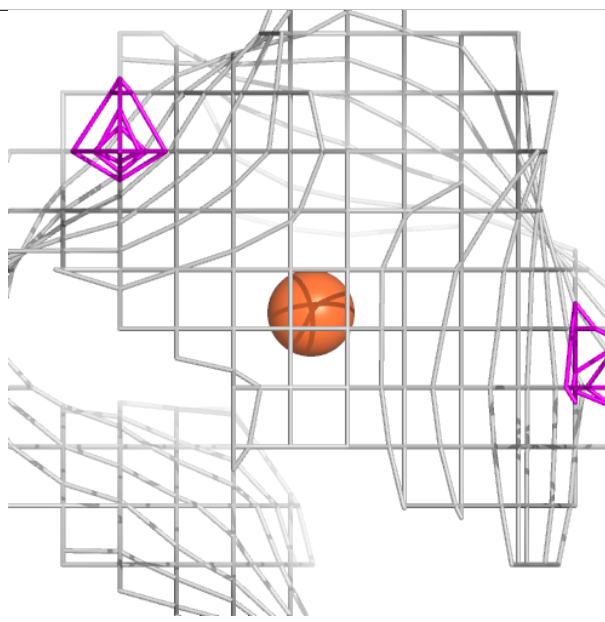
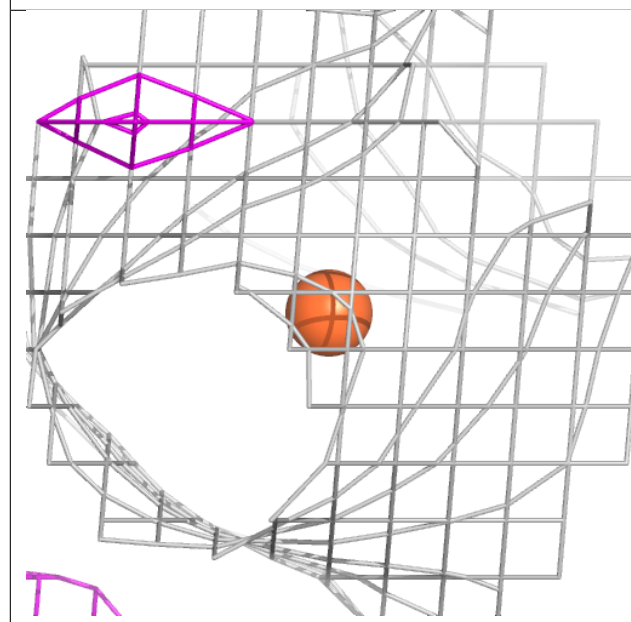
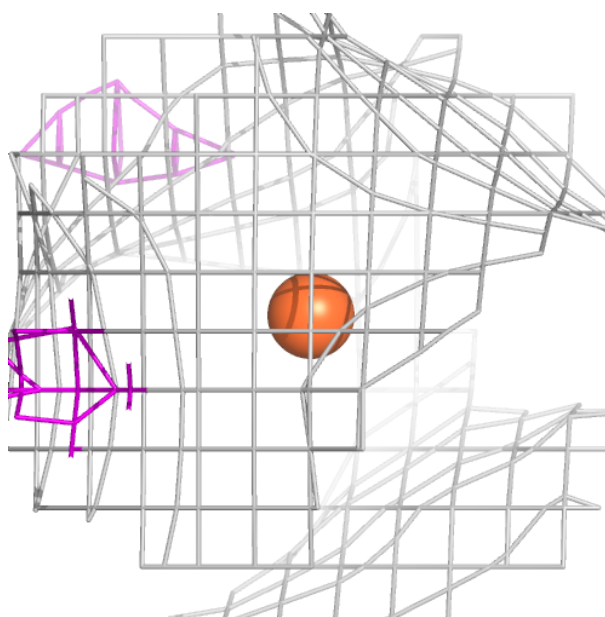
Electron density around FE D 702:

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



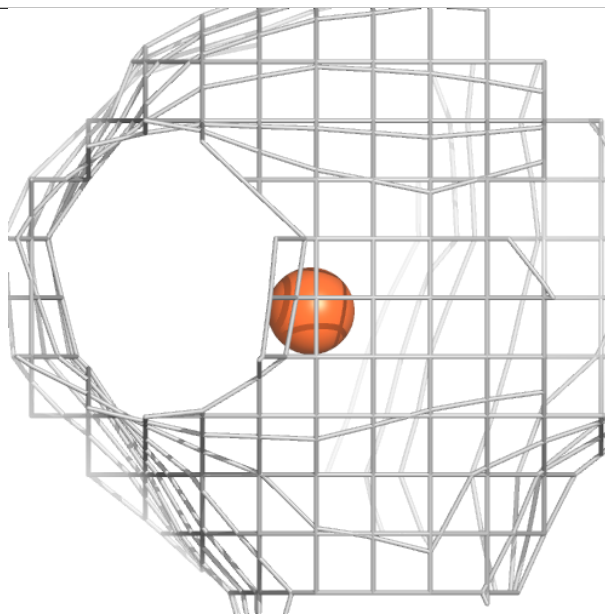
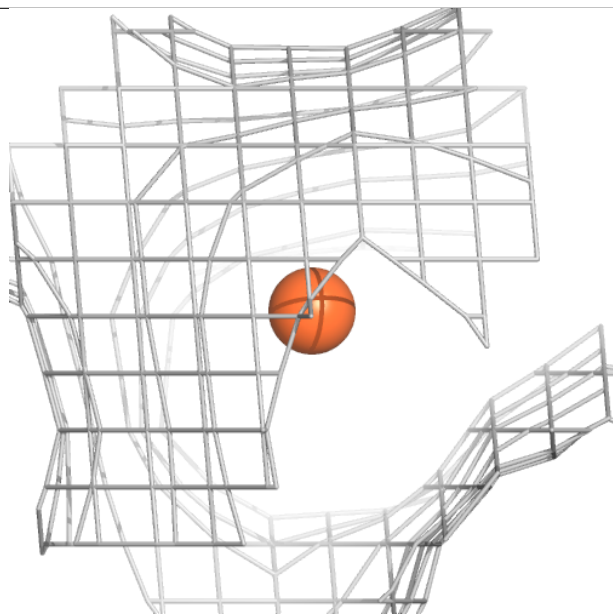
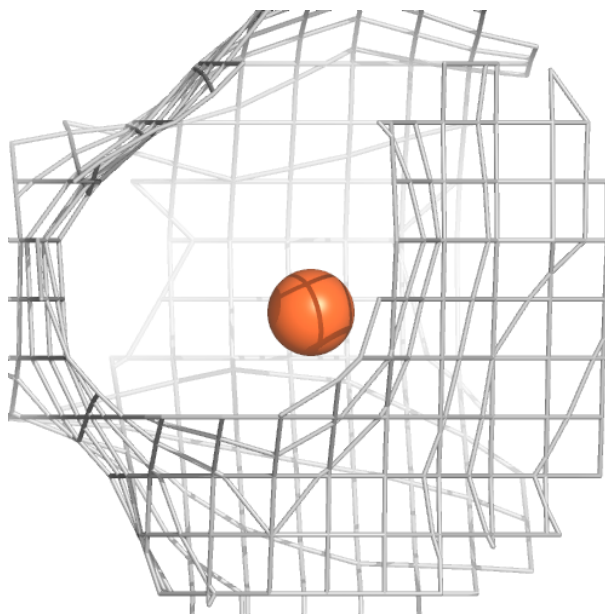
Electron density around FE K 702:

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



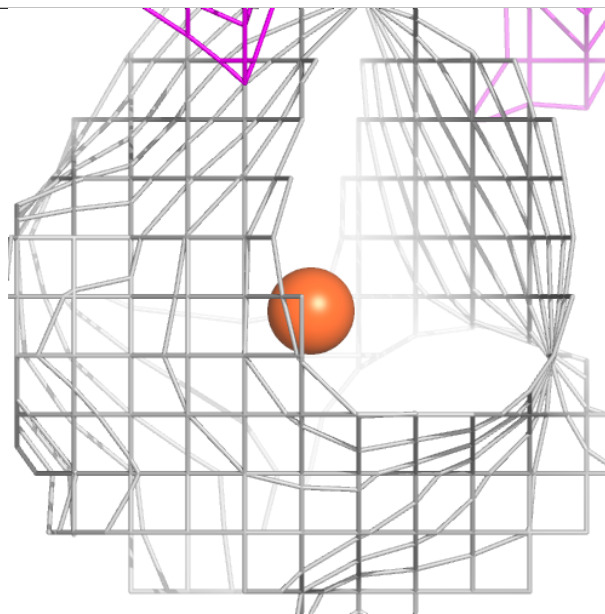
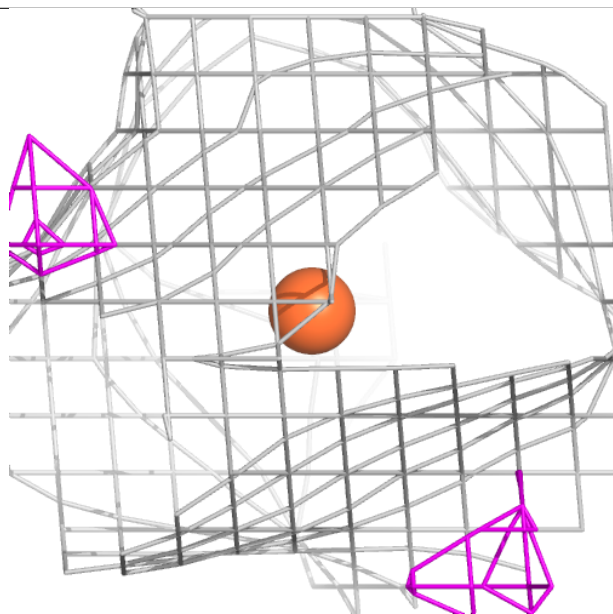
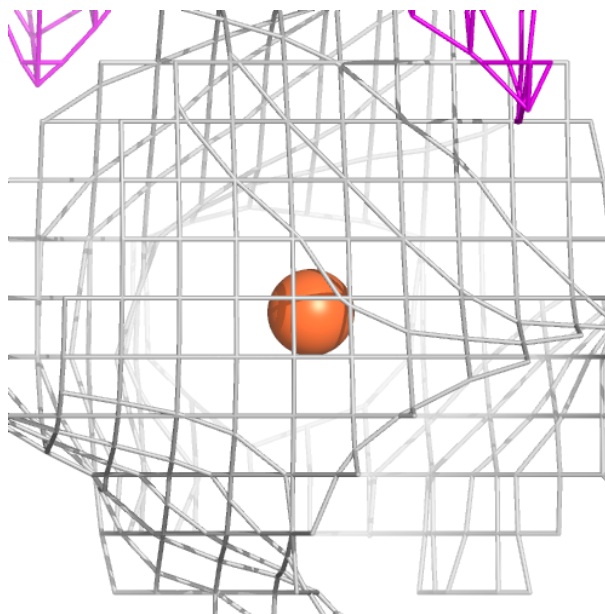
Electron density around FE L 702:

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



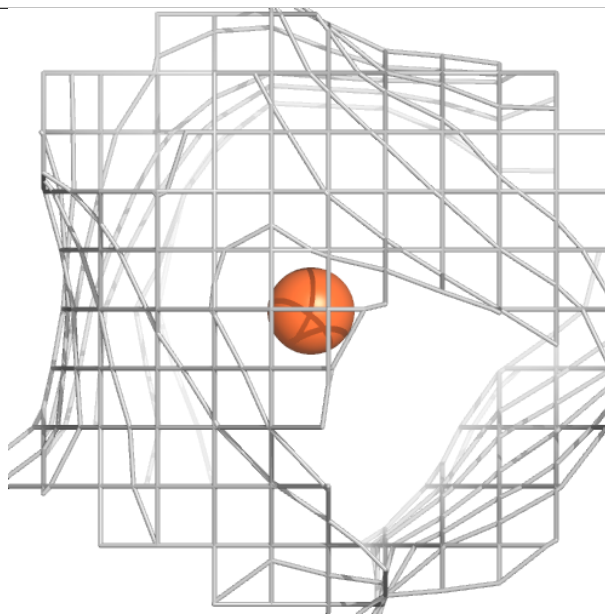
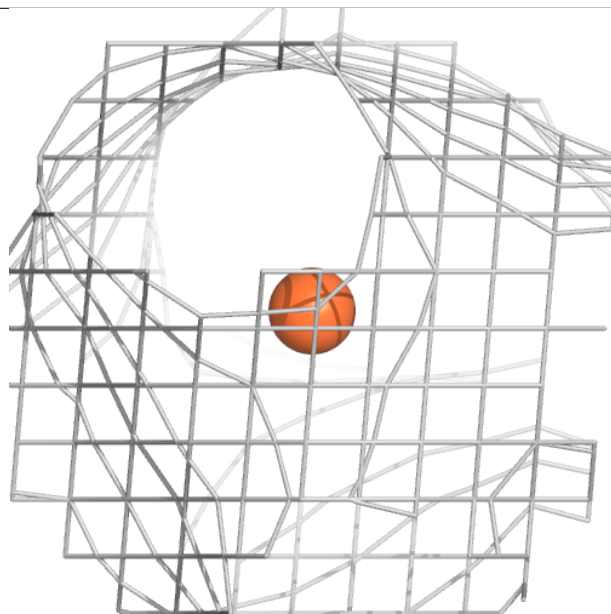
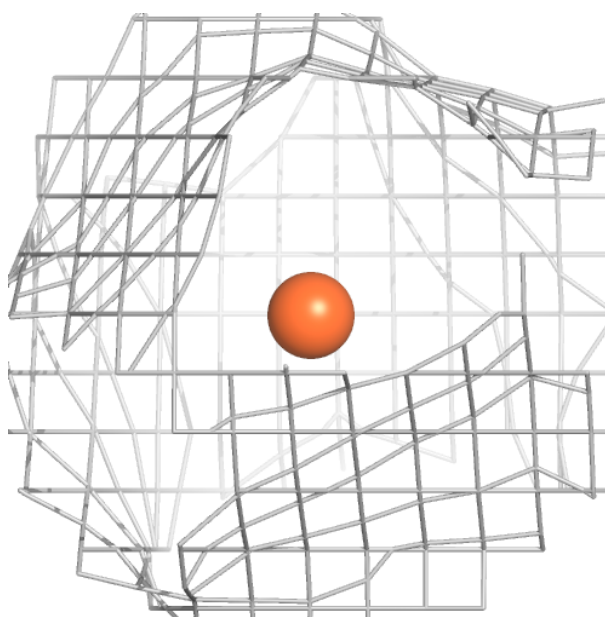
Electron density around FE M 701:

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



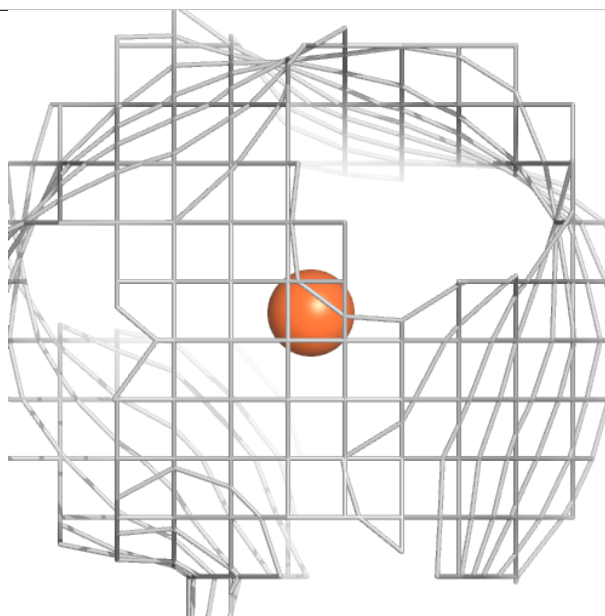
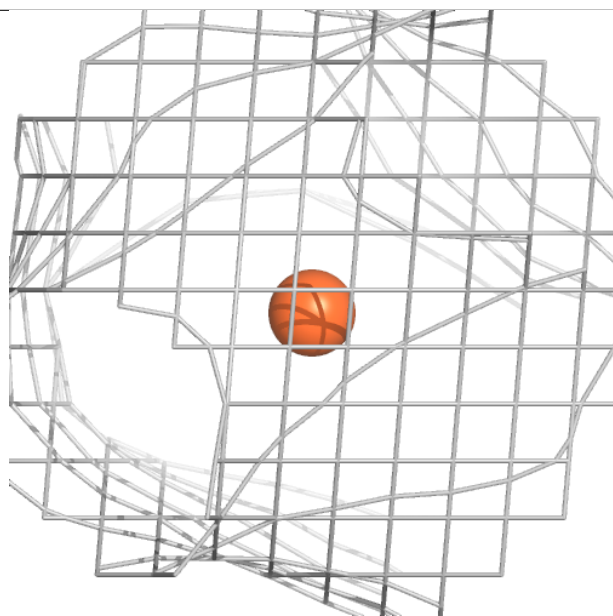
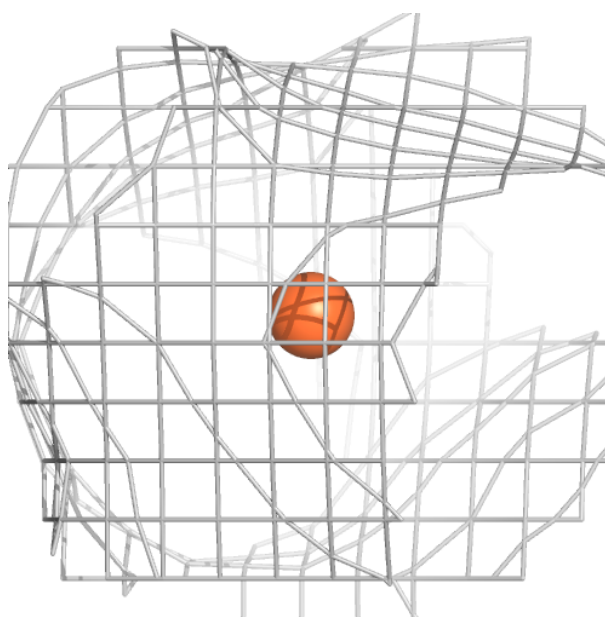
Electron density around FE A 701:

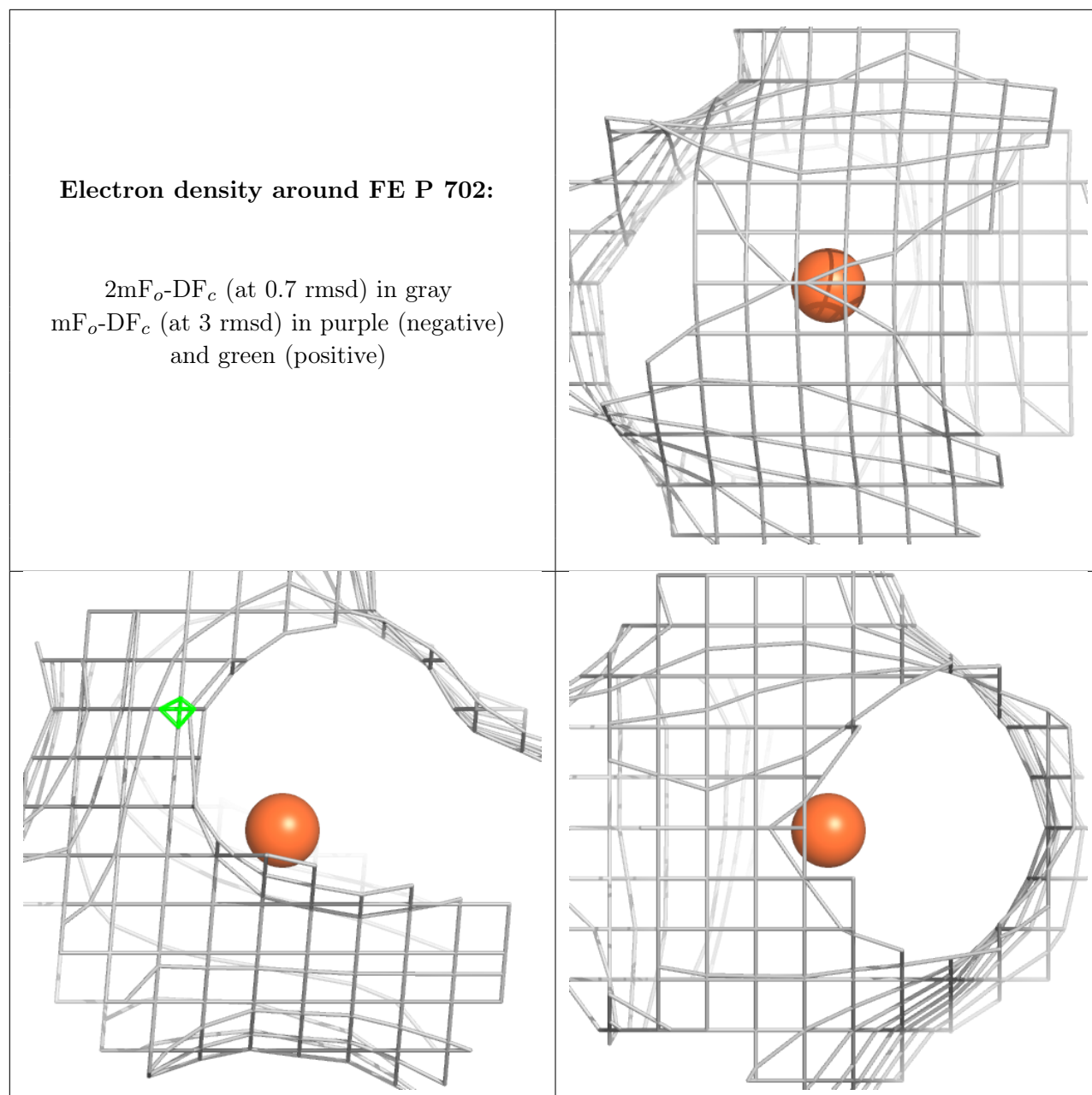
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.