



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 14, 2024 – 12:50 am GMT

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

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

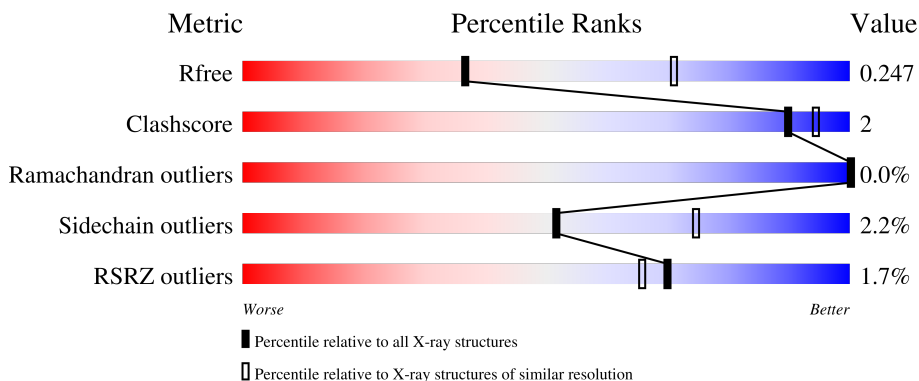
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


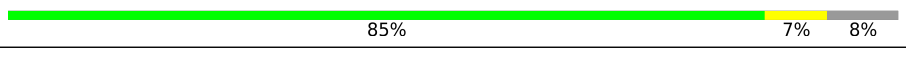
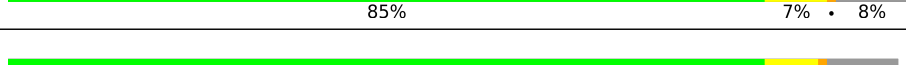

The reported resolution of this entry is 2.84 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	 85% 7% • 8%
1	B	520	 85% 7% • 8%
1	C	520	 85% 7% • 8%
1	D	520	 85% 6% • 8%

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

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

There are 32 discrepancies between the modelled and reference sequences:

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

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

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

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

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

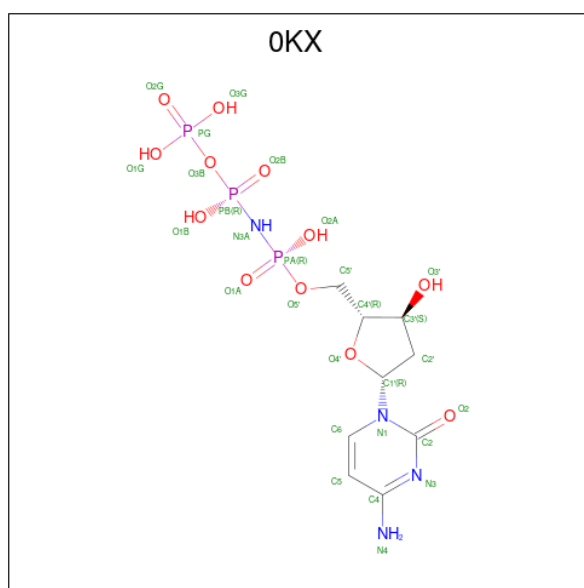
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Mg 3 3	0	0
3	B	3	Total Mg 3 3	0	0
3	C	3	Total Mg 3 3	0	0
3	D	3	Total Mg 3 3	0	0
3	E	2	Total Mg 2 2	0	0

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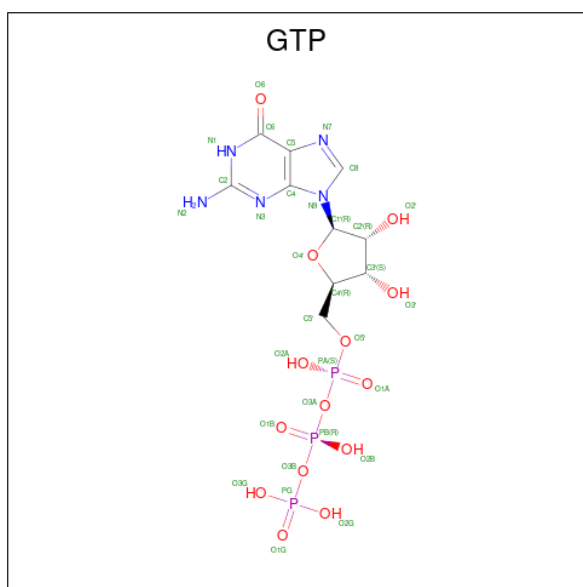
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	2	Total Mg 2 2	0	0
3	G	3	Total Mg 3 3	0	0
3	H	2	Total Mg 2 2	0	0
3	I	3	Total Mg 3 3	0	0
3	J	2	Total Mg 2 2	0	0
3	K	3	Total Mg 3 3	0	0
3	L	3	Total Mg 3 3	0	0
3	M	3	Total Mg 3 3	0	0
3	N	2	Total Mg 2 2	0	0
3	O	2	Total Mg 2 2	0	0
3	P	3	Total Mg 3 3	0	0

- Molecule 4 is 2'-deoxy-5'-O-[(R)-hydroxy{(R)-hydroxy(phosphonoxy)phosphoryl}amino}phosphoryl]cytidine (three-letter code: 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 (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



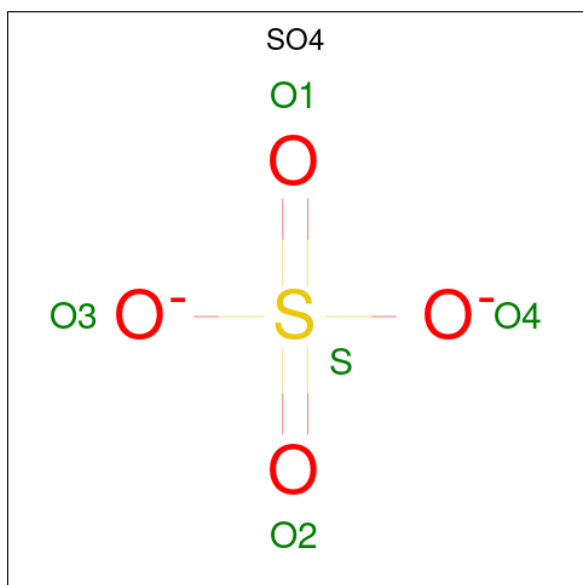
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	Total 32	C 10	N 5	O 14	P 3	0	0
5	B	1	Total 32	C 10	N 5	O 14	P 3	0	0
5	C	1	Total 32	C 10	N 5	O 14	P 3	0	0
5	D	1	Total 32	C 10	N 5	O 14	P 3	0	0
5	E	1	Total 32	C 10	N 5	O 14	P 3	0	0
5	F	1	Total 32	C 10	N 5	O 14	P 3	0	0
5	G	1	Total 32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

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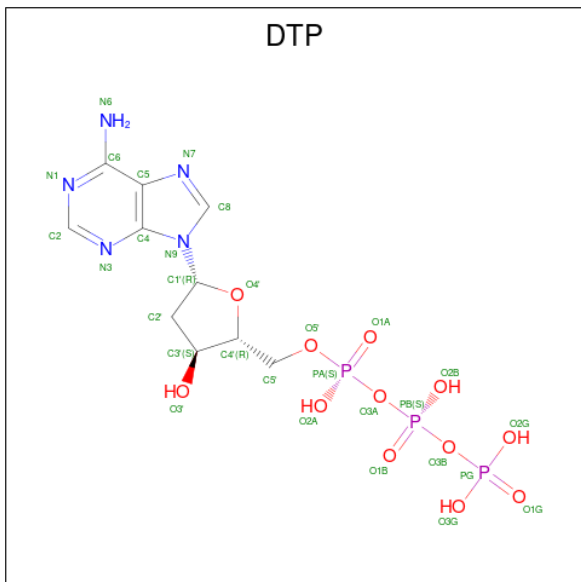
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
5	O	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	O	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 7 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



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

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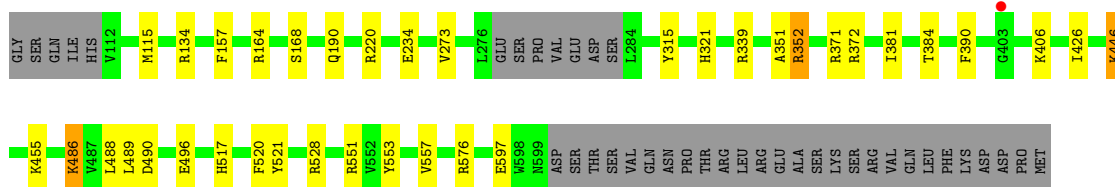
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	M	1	Total 30	10	5	12	3	0	0
7	N	1	Total 30	10	5	12	3	0	0
7	O	1	Total 30	10	5	12	3	0	0
7	P	1	Total 30	10	5	12	3	0	0

3 Residue-property plots


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

- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain A: 




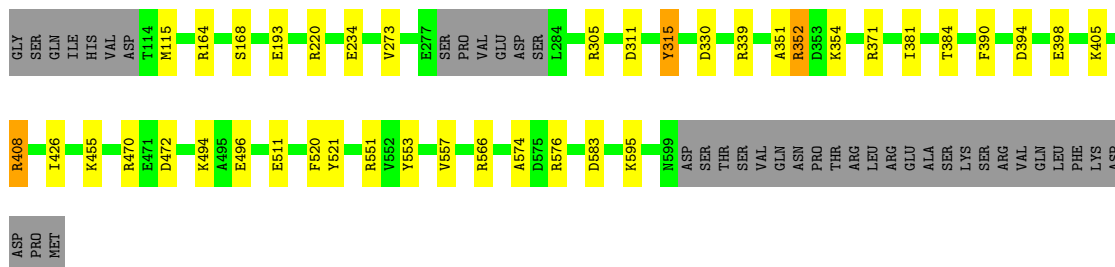
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain B: 




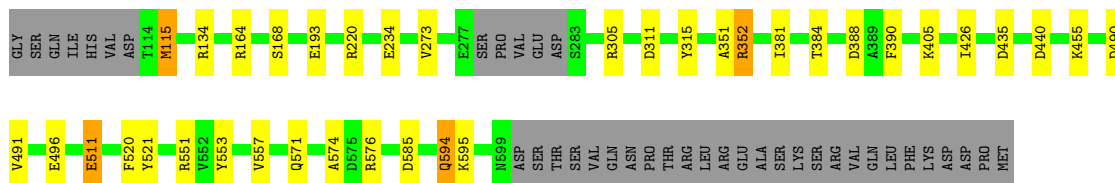
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain C: 

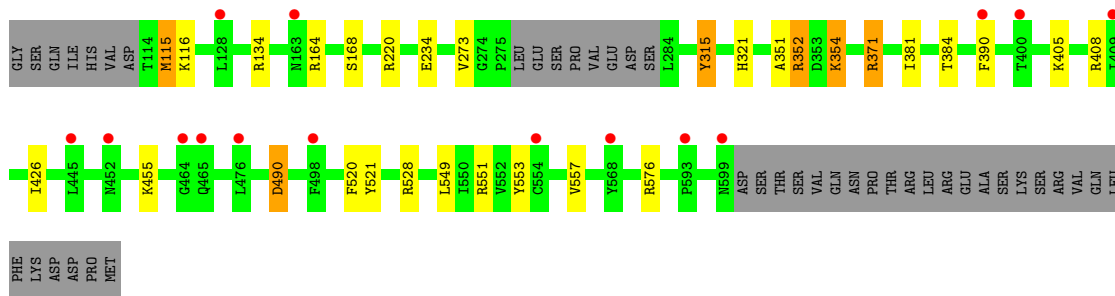
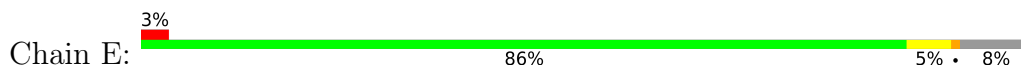


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

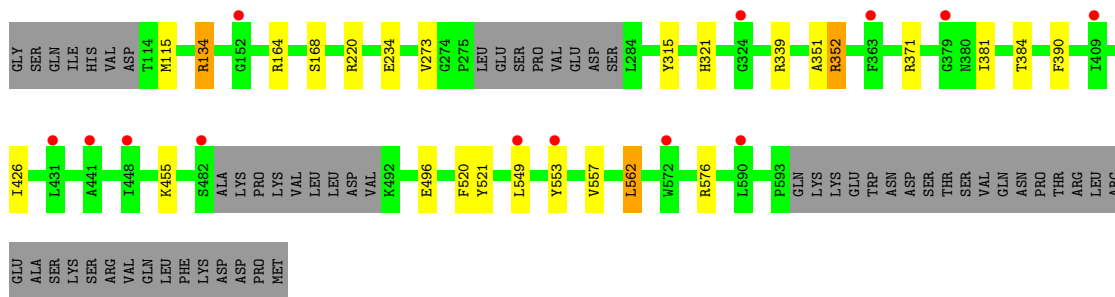
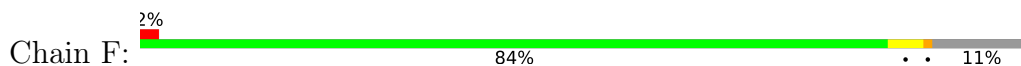
Chain D: 



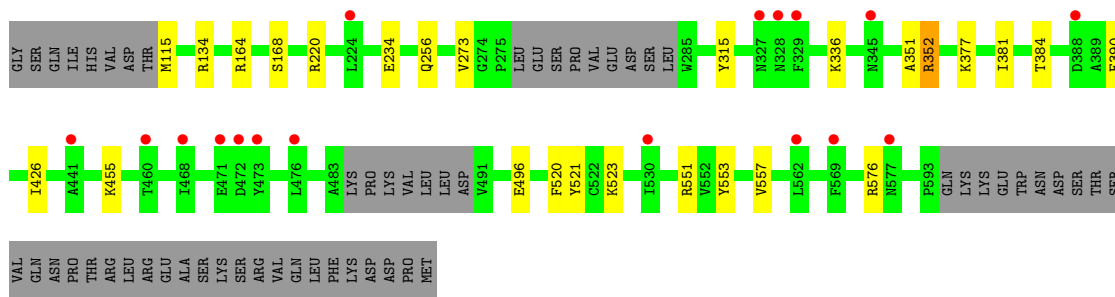
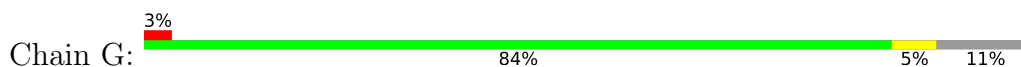
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



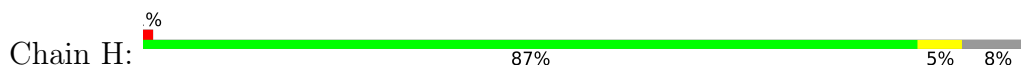
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

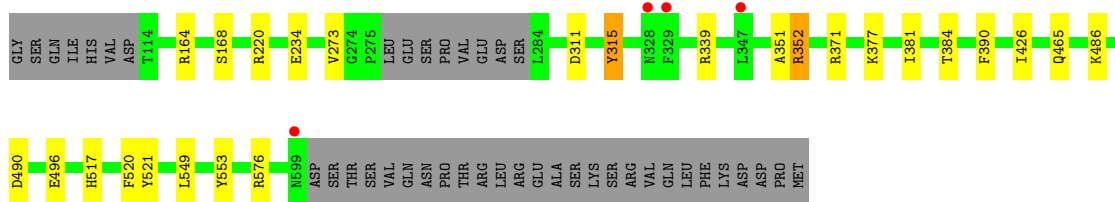


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



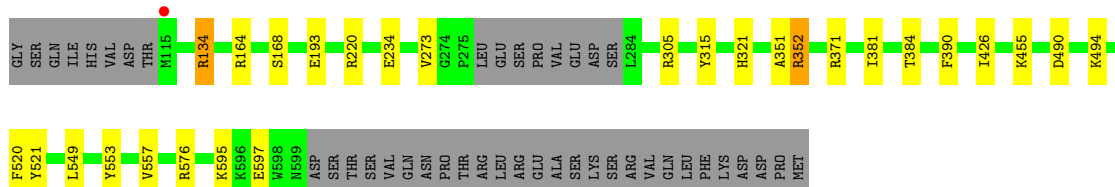
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





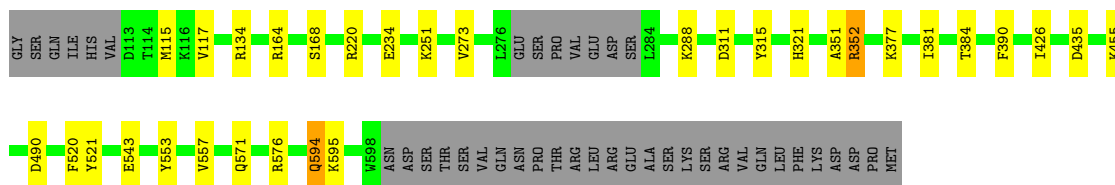
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain I: 86% 5% 8%



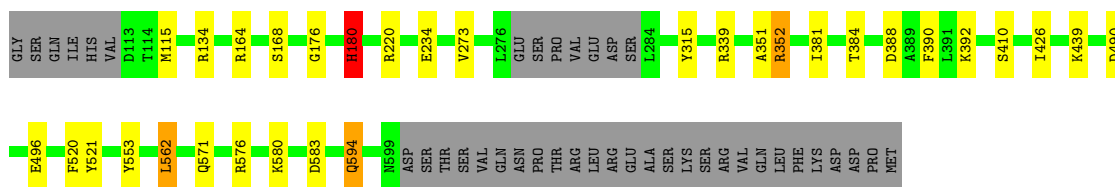
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain J: 86% 6% 8%



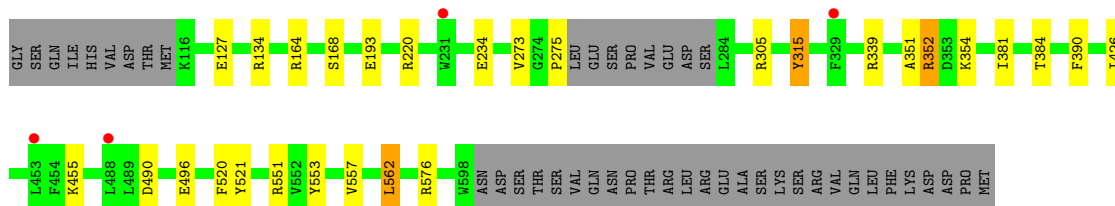
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain K: 86% 5% 8%

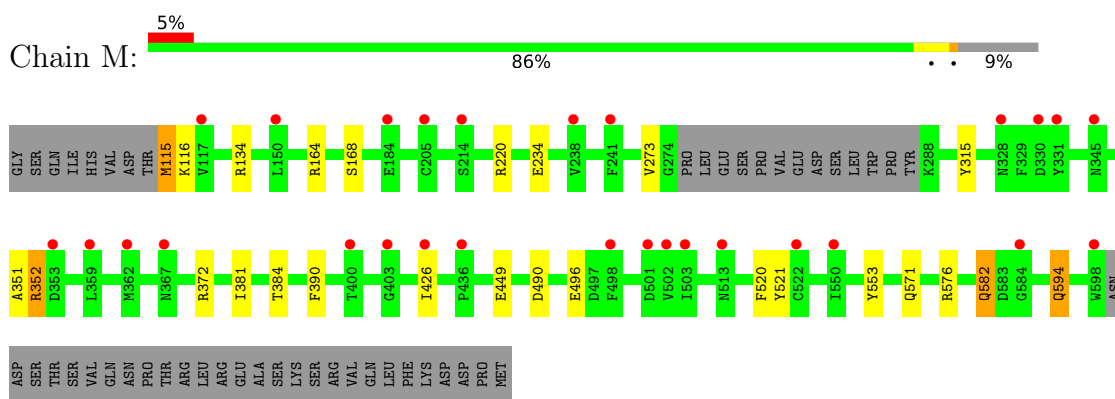


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

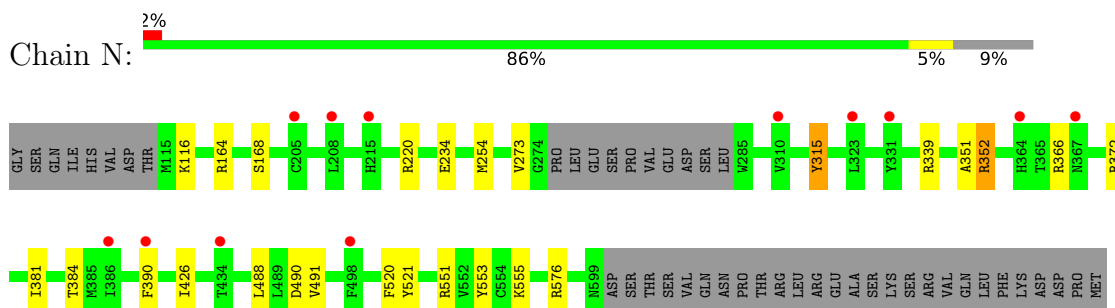
Chain L: 86% 5% 9%



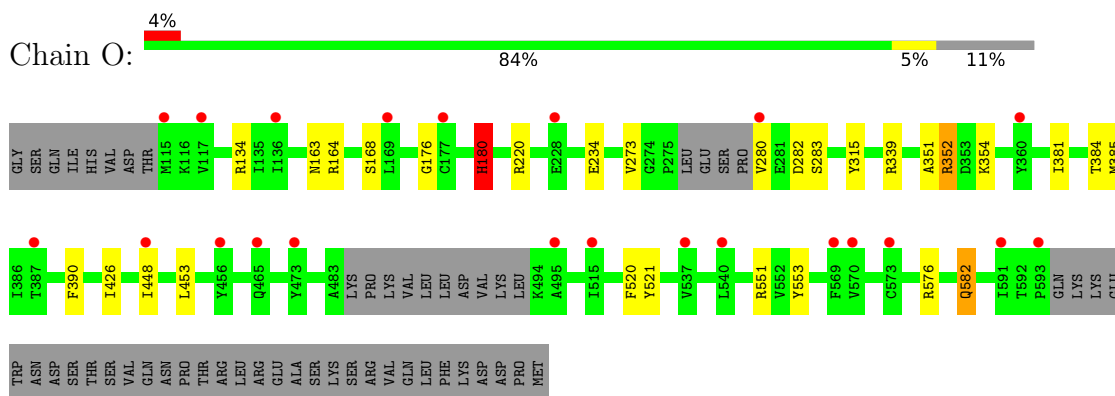
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



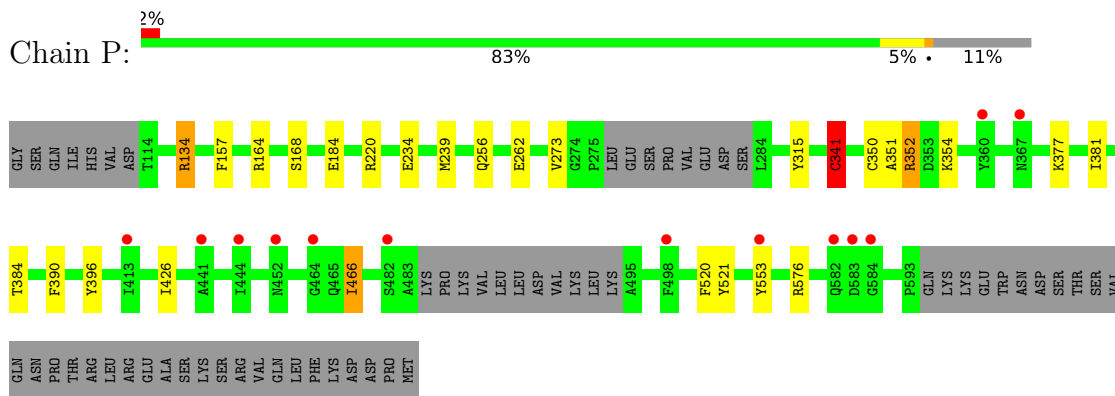
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



4 Data and refinement statistics

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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

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

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

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

All (31) bond length outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	489	LEU	C-O	-6.56	1.10	1.23
1	K	410	SER	CB-OG	-6.51	1.33	1.42
1	L	275	PRO	C-O	-6.38	1.10	1.23
1	D	511	GLU	CB-CG	6.30	1.64	1.52
1	B	263	GLU	CD-OE2	6.29	1.32	1.25
1	P	256	GLN	CG-CD	6.17	1.65	1.51
1	J	164	ARG	CZ-NH2	-5.99	1.25	1.33
1	D	164	ARG	CZ-NH2	-5.83	1.25	1.33
1	L	164	ARG	CZ-NH2	-5.82	1.25	1.33
1	N	164	ARG	CZ-NH1	5.81	1.40	1.33
1	P	262	GLU	CD-OE2	5.79	1.32	1.25
1	P	164	ARG	CZ-NH2	-5.69	1.25	1.33
1	B	114	THR	N-CA	5.63	1.57	1.46
1	P	164	ARG	CZ-NH1	5.58	1.40	1.33
1	N	164	ARG	CZ-NH2	-5.56	1.25	1.33
1	H	164	ARG	CZ-NH2	-5.54	1.25	1.33
1	L	164	ARG	CZ-NH1	5.52	1.40	1.33
1	G	115	MET	N-CA	5.51	1.57	1.46
1	L	127	GLU	CD-OE2	5.50	1.31	1.25
1	D	164	ARG	CZ-NH1	5.45	1.40	1.33
1	C	193	GLU	CD-OE2	5.43	1.31	1.25
1	L	127	GLU	CD-OE1	5.42	1.31	1.25
1	D	193	GLU	CG-CD	5.37	1.60	1.51
1	G	115	MET	CG-SD	5.27	1.94	1.81
1	J	164	ARG	CZ-NH1	5.22	1.39	1.33
1	H	164	ARG	CZ-NH1	5.13	1.39	1.33
1	P	184	GLU	CD-OE1	5.06	1.31	1.25
1	A	446	LYS	CD-CE	5.05	1.63	1.51
1	D	511	GLU	CG-CD	5.03	1.59	1.51

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	164	ARG	NE-CZ-NH1	23.34	131.97	120.30
1	D	164	ARG	NE-CZ-NH1	23.28	131.94	120.30
1	N	164	ARG	NE-CZ-NH1	22.96	131.78	120.30
1	P	164	ARG	NE-CZ-NH1	22.90	131.75	120.30
1	L	164	ARG	NE-CZ-NH1	22.63	131.61	120.30
1	H	164	ARG	NE-CZ-NH1	22.61	131.61	120.30
1	N	164	ARG	NE-CZ-NH2	-19.87	110.36	120.30
1	J	164	ARG	NE-CZ-NH2	-19.80	110.40	120.30
1	D	164	ARG	NE-CZ-NH2	-19.57	110.51	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	164	ARG	NE-CZ-NH2	-19.54	110.53	120.30
1	P	164	ARG	NE-CZ-NH2	-19.28	110.66	120.30
1	H	164	ARG	NE-CZ-NH2	-18.97	110.81	120.30
1	G	115	MET	CG-SD-CE	16.40	126.44	100.20
1	O	164	ARG	NE-CZ-NH2	14.89	127.74	120.30
1	F	164	ARG	NE-CZ-NH2	14.75	127.68	120.30
1	E	164	ARG	NE-CZ-NH2	14.71	127.65	120.30
1	C	164	ARG	NE-CZ-NH2	14.60	127.60	120.30
1	I	164	ARG	NE-CZ-NH2	14.59	127.60	120.30
1	K	164	ARG	NE-CZ-NH2	14.57	127.58	120.30
1	B	164	ARG	NE-CZ-NH2	14.53	127.57	120.30
1	A	164	ARG	NE-CZ-NH2	14.34	127.47	120.30
1	E	164	ARG	NE-CZ-NH1	-14.21	113.19	120.30
1	G	164	ARG	NE-CZ-NH2	14.20	127.40	120.30
1	M	164	ARG	NE-CZ-NH2	14.20	127.40	120.30
1	B	164	ARG	NE-CZ-NH1	-13.84	113.38	120.30
1	C	164	ARG	NE-CZ-NH1	-13.82	113.39	120.30
1	A	164	ARG	NE-CZ-NH1	-13.77	113.42	120.30
1	O	164	ARG	NE-CZ-NH1	-13.75	113.43	120.30
1	K	164	ARG	NE-CZ-NH1	-13.66	113.47	120.30
1	G	164	ARG	NE-CZ-NH1	-13.52	113.54	120.30
1	F	164	ARG	NE-CZ-NH1	-13.47	113.57	120.30
1	I	164	ARG	NE-CZ-NH1	-13.45	113.58	120.30
1	M	164	ARG	NE-CZ-NH1	-13.36	113.62	120.30
1	O	551	ARG	NE-CZ-NH1	-12.37	114.11	120.30
1	E	551	ARG	NE-CZ-NH1	-12.18	114.21	120.30
1	B	551	ARG	NE-CZ-NH1	-11.88	114.36	120.30
1	E	551	ARG	NE-CZ-NH2	9.70	125.15	120.30
1	O	551	ARG	NE-CZ-NH2	9.42	125.01	120.30
1	B	490	ASP	CB-CG-OD1	-8.96	110.23	118.30
1	B	551	ARG	NE-CZ-NH2	8.69	124.64	120.30
1	B	511	GLU	OE1-CD-OE2	-7.67	114.10	123.30
1	K	583	ASP	CB-CG-OD2	-7.24	111.78	118.30
1	P	262	GLU	CA-CB-CG	7.23	129.30	113.40
1	D	115	MET	CG-SD-CE	7.17	111.68	100.20
1	M	490	ASP	CB-CG-OD1	7.03	124.63	118.30
1	K	115	MET	CA-CB-CG	6.89	125.02	113.30
1	B	528	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	J	490	ASP	CB-CG-OD1	6.65	124.28	118.30
1	N	254	MET	CG-SD-CE	6.49	110.58	100.20
1	A	372	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	D	490	ASP	CB-CG-OD2	-6.42	112.52	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	134	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	K	580	LYS	CG-CD-CE	6.36	130.99	111.90
1	N	366	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	C	511	GLU	OE1-CD-OE2	6.21	130.75	123.30
1	B	531	ARG	NE-CZ-NH1	-6.19	117.20	120.30
1	D	115	MET	CA-CB-CG	6.19	123.83	113.30
1	K	562	LEU	CB-CG-CD2	6.17	121.48	111.00
1	N	488	LEU	CA-CB-CG	6.12	129.38	115.30
1	I	134	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	I	305	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	J	251	LYS	CD-CE-NZ	6.02	125.54	111.70
1	J	435	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	C	470	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	H	311	ASP	CB-CG-OD2	-5.92	112.98	118.30
1	K	388	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	E	115	MET	CG-SD-CE	5.84	109.55	100.20
1	C	330	ASP	CB-CG-OD2	5.74	123.47	118.30
1	N	551	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	M	449	GLU	CG-CD-OE1	-5.72	106.86	118.30
1	L	490	ASP	CB-CG-OD1	5.71	123.44	118.30
1	D	440	ASP	CB-CG-OD2	-5.71	113.17	118.30
1	D	490	ASP	CB-CG-OD1	5.70	123.43	118.30
1	D	388	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	B	251	LYS	CD-CE-NZ	5.67	124.74	111.70
1	D	435	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	O	582	GLN	CA-CB-CG	5.62	125.77	113.40
1	G	336	LYS	CD-CE-NZ	5.62	124.63	111.70
1	C	305	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	M	372	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	M	582	GLN	CA-CB-CG	5.57	125.64	113.40
1	O	163	ASN	CB-CG-OD1	-5.55	110.51	121.60
1	J	311	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	I	193	GLU	CA-CB-CG	5.53	125.57	113.40
1	A	551	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	F	562	LEU	CB-CG-CD2	5.52	120.39	111.00
1	M	115	MET	CG-SD-CE	5.47	108.96	100.20
1	L	562	LEU	CB-CG-CD2	5.45	120.26	111.00
1	C	566	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	C	371	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	446	LYS	CG-CD-CE	5.40	128.09	111.90
1	N	372	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	F	134	ARG	NE-CZ-NH1	5.29	122.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	551	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	G	551	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	P	466	ILE	CB-CG1-CD1	5.26	128.62	113.90
1	P	239	MET	CG-SD-CE	5.24	108.58	100.20
1	E	408	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	L	305	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	C	583	ASP	CB-CG-OD2	-5.23	113.60	118.30
1	N	555	LYS	CG-CD-CE	5.22	127.57	111.90
1	O	180	HIS	CA-CB-CG	5.22	122.47	113.60
1	E	354	LYS	CD-CE-NZ	-5.21	99.72	111.70
1	B	566	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	K	180	HIS	CA-CB-CG	5.17	122.39	113.60
1	E	528	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	D	311	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	O	282	ASP	CB-CG-OD1	5.12	122.91	118.30
1	L	551	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	M	115	MET	CA-CB-CG	5.09	121.96	113.30
1	E	371	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	K	580	LYS	CD-CE-NZ	5.08	123.40	111.70
1	J	543	GLU	OE1-CD-OE2	-5.08	117.20	123.30
1	E	490	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	D	551	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	371	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	486	LYS	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3840	0	3707	15	0
1	B	3825	0	3715	11	0
1	C	3854	0	3758	17	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3846	0	3732	15	0
1	E	3799	0	3656	14	0
1	F	3695	0	3560	12	0
1	G	3668	0	3505	13	0
1	H	3845	0	3751	15	0
1	I	3822	0	3705	13	0
1	J	3837	0	3723	15	0
1	K	3839	0	3704	12	0
1	L	3756	0	3583	12	0
1	M	3704	0	3524	10	0
1	N	3757	0	3573	12	0
1	O	3680	0	3508	12	0
1	P	3640	0	3463	14	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	3	0	0	0	0
3	H	2	0	0	0	0
3	I	3	0	0	0	0
3	J	2	0	0	0	0
3	K	3	0	0	0	0
3	L	3	0	0	0	0
3	M	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	2	0	0	0	0
3	O	2	0	0	0	0
3	P	3	0	0	0	0
4	A	28	0	16	0	0
4	B	28	0	16	1	0
4	C	28	0	16	2	0
4	D	28	0	17	1	0
4	E	28	0	17	1	0
4	F	28	0	17	0	0
4	G	28	0	16	0	0
4	H	28	0	16	1	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	M	5	0	0	0	0
7	A	30	0	12	0	0
7	B	30	0	12	2	0
7	C	30	0	12	1	0
7	D	30	0	12	1	0
7	E	30	0	12	3	0
7	F	30	0	12	2	0
7	G	30	0	12	2	0
7	H	30	0	12	2	0
7	I	30	0	12	0	0
7	J	30	0	12	1	0
7	K	30	0	12	2	0
7	L	30	0	12	1	0
7	M	30	0	12	4	0
7	N	30	0	12	1	0
7	O	30	0	12	1	0
7	P	30	0	12	2	0
All	All	61950	0	58812	213	1

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

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:352:ARG:NH1	7:N:706:DTP:O3G	2.20	0.71
1:M:352:ARG:NH1	7:M:708:DTP:O3G	2.21	0.70
7:E:706:DTP:O2G	5:G:707:GTP:O1B	2.13	0.67
1:I:595:LYS:HZ2	1:I:597:GLU:HG2	1.62	0.65
7:M:708:DTP:O1B	5:O:706:GTP:H5''	1.97	0.64
1:H:352:ARG:NH1	7:H:701:DTP:O1G	2.33	0.62
7:F:706:DTP:O2B	1:G:377:LYS:NZ	2.32	0.59
1:D:455:LYS:HE3	1:D:557:VAL:HG13	1.85	0.58
1:F:455:LYS:HE3	1:F:557:VAL:HG13	1.85	0.58
1:L:352:ARG:HG3	1:L:521:TYR:CE1	2.39	0.57
1:O:352:ARG:HG3	1:O:521:TYR:CE1	2.39	0.57
1:N:352:ARG:HG3	1:N:521:TYR:CE1	2.40	0.57
1:E:352:ARG:HG3	1:E:521:TYR:CE1	2.40	0.57
1:D:352:ARG:HG3	1:D:521:TYR:CE1	2.40	0.56
1:I:352:ARG:HG3	1:I:521:TYR:CE1	2.40	0.56
1:J:352:ARG:HG3	1:J:521:TYR:CE1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:491:VAL:HG13	1:G:256:GLN:O	2.04	0.56
1:G:352:ARG:NH1	7:G:701:DTP:O3G	2.38	0.55
1:H:234:GLU:HB3	1:H:273:VAL:HG12	1.88	0.55
4:B:705:0KX:O2G	4:B:705:0KX:O2B	2.24	0.55
1:J:234:GLU:HB3	1:J:273:VAL:HG12	1.89	0.55
1:K:571:GLN:HE22	1:K:594:GLN:HE22	1.54	0.55
1:B:455:LYS:HE3	1:B:557:VAL:HG13	1.89	0.55
1:L:234:GLU:HB3	1:L:273:VAL:HG12	1.89	0.55
1:P:234:GLU:HB3	1:P:273:VAL:HG12	1.88	0.55
1:F:234:GLU:HB3	1:F:273:VAL:HG12	1.88	0.54
1:K:234:GLU:HB3	1:K:273:VAL:HG12	1.89	0.54
1:E:455:LYS:HE3	1:E:557:VAL:HG13	1.89	0.54
1:H:517:HIS:ND1	6:H:707:SO4:O1	2.36	0.54
1:H:315:TYR:CG	4:H:705:0KX:H9	2.43	0.54
1:A:190:GLN:HE21	1:H:486:LYS:HD2	1.72	0.54
1:O:385:MET:SD	1:O:448:ILE:HD11	2.47	0.54
1:H:352:ARG:HG3	1:H:521:TYR:CE1	2.43	0.54
1:C:394:ASP:O	1:C:408:ARG:HG3	2.08	0.53
1:O:234:GLU:HB3	1:O:273:VAL:HG12	1.89	0.53
1:B:234:GLU:HB3	1:B:273:VAL:HG12	1.90	0.53
1:E:234:GLU:HB3	1:E:273:VAL:HG12	1.89	0.53
1:N:234:GLU:HB3	1:N:273:VAL:HG12	1.91	0.53
1:P:341:CYS:SG	1:P:350:CYS:CB	2.96	0.53
1:M:234:GLU:HB3	1:M:273:VAL:HG12	1.91	0.53
1:G:234:GLU:HB3	1:G:273:VAL:HG12	1.89	0.53
1:C:394:ASP:O	1:C:408:ARG:CG	2.56	0.53
1:K:352:ARG:NH1	7:K:701:DTP:O3G	2.40	0.53
1:E:354:LYS:NZ	7:E:706:DTP:O3B	2.42	0.53
1:I:234:GLU:HB3	1:I:273:VAL:HG12	1.90	0.52
7:M:708:DTP:H1'	1:P:157:PHE:CE2	2.45	0.52
1:J:377:LYS:NZ	7:K:701:DTP:O2B	2.36	0.52
1:M:571:GLN:HE22	1:M:594:GLN:NE2	2.07	0.52
1:A:234:GLU:HB3	1:A:273:VAL:HG12	1.90	0.52
1:F:352:ARG:NH1	7:F:706:DTP:O3G	2.37	0.52
1:C:234:GLU:HB3	1:C:273:VAL:HG12	1.92	0.52
1:D:234:GLU:HB3	1:D:273:VAL:HG12	1.90	0.52
1:E:116:LYS:NZ	5:E:705:GTP:O1G	2.41	0.51
7:B:708:DTP:O1B	5:D:707:GTP:O2A	2.29	0.50
1:D:305:ARG:NH1	6:D:708:SO4:O2	2.45	0.50
1:K:571:GLN:HE22	1:K:594:GLN:NE2	2.10	0.50
1:A:352:ARG:HG3	1:A:521:TYR:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:TYR:OH	4:C:706:0KX:O2G	2.21	0.49
1:K:352:ARG:HG3	1:K:521:TYR:CE2	2.48	0.49
1:G:352:ARG:HG3	1:G:521:TYR:CE2	2.48	0.49
4:D:706:0KX:O2G	4:D:706:0KX:O2B	2.30	0.49
1:P:352:ARG:HG3	1:P:521:TYR:CE2	2.47	0.49
1:K:176:GLY:O	1:K:180:HIS:HB2	2.12	0.49
1:I:321:HIS:CE1	1:J:321:HIS:CE1	3.00	0.48
1:H:351:ALA:O	1:H:520:PHE:HA	2.14	0.48
1:O:176:GLY:O	1:O:180:HIS:HB2	2.13	0.48
1:C:351:ALA:O	1:C:520:PHE:HA	2.14	0.48
1:L:315:TYR:CG	4:L:706:0KX:H9	2.47	0.48
1:N:315:TYR:CD1	4:N:704:0KX:H9	2.48	0.48
1:B:351:ALA:O	1:B:520:PHE:HA	2.14	0.48
1:B:352:ARG:HG3	1:B:521:TYR:CE2	2.48	0.48
1:C:352:ARG:HG3	1:C:521:TYR:CE2	2.48	0.48
1:F:352:ARG:HG3	1:F:521:TYR:CE2	2.48	0.48
1:J:351:ALA:O	1:J:520:PHE:HA	2.14	0.48
1:M:352:ARG:HG3	1:M:521:TYR:CE2	2.49	0.48
1:K:351:ALA:O	1:K:520:PHE:HA	2.14	0.48
1:M:351:ALA:O	1:M:520:PHE:HA	2.14	0.48
1:O:351:ALA:O	1:O:520:PHE:HA	2.14	0.48
1:E:351:ALA:O	1:E:520:PHE:HA	2.14	0.48
1:I:595:LYS:NZ	1:I:597:GLU:HG2	2.29	0.48
1:N:351:ALA:O	1:N:520:PHE:HA	2.14	0.48
1:P:352:ARG:HG3	1:P:521:TYR:CZ	2.49	0.48
1:G:351:ALA:O	1:G:520:PHE:HA	2.14	0.47
1:A:157:PHE:CE2	7:D:701:DTP:H1'	2.50	0.47
1:A:351:ALA:O	1:A:520:PHE:HA	2.14	0.47
1:F:351:ALA:O	1:F:520:PHE:HA	2.14	0.47
1:I:351:ALA:O	1:I:520:PHE:HA	2.14	0.47
1:J:352:ARG:NH1	7:J:707:DTP:O3G	2.46	0.47
1:L:351:ALA:O	1:L:520:PHE:HA	2.14	0.47
1:N:352:ARG:HG3	1:N:521:TYR:CZ	2.49	0.47
1:P:351:ALA:O	1:P:520:PHE:HA	2.14	0.47
5:F:705:GTP:H5''	7:H:701:DTP:O1B	2.14	0.47
1:C:352:ARG:HG3	1:C:521:TYR:CZ	2.50	0.47
1:D:351:ALA:O	1:D:520:PHE:HA	2.14	0.47
1:F:352:ARG:HG3	1:F:521:TYR:CZ	2.49	0.47
1:E:315:TYR:OH	4:E:704:0KX:O1G	2.32	0.47
1:B:354:LYS:NZ	7:B:708:DTP:O1A	2.31	0.47
1:C:398:GLU:HG2	1:C:408:ARG:NH2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:352:ARG:HG3	1:E:521:TYR:CZ	2.50	0.47
1:B:352:ARG:HG3	1:B:521:TYR:CZ	2.50	0.47
1:O:352:ARG:HG3	1:O:521:TYR:CZ	2.50	0.47
1:M:381:ILE:HD13	1:M:553:TYR:CG	2.50	0.46
1:D:352:ARG:HG3	1:D:521:TYR:CZ	2.50	0.46
1:J:381:ILE:HD13	1:J:553:TYR:CG	2.50	0.46
1:J:455:LYS:HE3	1:J:557:VAL:HG13	1.98	0.46
1:L:381:ILE:HD13	1:L:553:TYR:CG	2.50	0.46
1:A:352:ARG:HG3	1:A:521:TYR:CZ	2.50	0.46
1:G:455:LYS:HE3	1:G:557:VAL:HG13	1.97	0.46
1:L:352:ARG:HG3	1:L:521:TYR:CZ	2.50	0.46
1:G:381:ILE:HD13	1:G:553:TYR:CG	2.50	0.46
1:J:352:ARG:HG3	1:J:521:TYR:CZ	2.51	0.46
1:D:381:ILE:HD13	1:D:553:TYR:CG	2.51	0.46
1:K:352:ARG:HG3	1:K:521:TYR:CZ	2.50	0.46
1:O:381:ILE:HD13	1:O:553:TYR:CG	2.51	0.46
1:I:381:ILE:HD13	1:I:553:TYR:CG	2.51	0.46
1:I:352:ARG:HG3	1:I:521:TYR:CZ	2.50	0.46
1:D:571:GLN:NE2	1:D:594:GLN:HE22	2.14	0.45
1:F:381:ILE:HD13	1:F:553:TYR:CD2	2.51	0.45
1:L:381:ILE:HD13	1:L:553:TYR:CD2	2.52	0.45
1:O:381:ILE:HD13	1:O:553:TYR:CD2	2.51	0.45
1:E:381:ILE:HD13	1:E:553:TYR:CG	2.52	0.45
1:G:352:ARG:HG3	1:G:521:TYR:CZ	2.51	0.45
1:H:381:ILE:HD13	1:H:553:TYR:CG	2.52	0.45
1:L:455:LYS:HE3	1:L:557:VAL:HG13	1.98	0.45
1:M:381:ILE:HD13	1:M:553:TYR:CD2	2.52	0.45
1:A:381:ILE:HD13	1:A:553:TYR:CG	2.52	0.45
1:C:455:LYS:HE3	1:C:557:VAL:HG13	1.97	0.45
1:D:381:ILE:HD13	1:D:553:TYR:CD2	2.52	0.45
1:N:381:ILE:HD13	1:N:553:TYR:CG	2.51	0.45
5:O:707:GTP:O1B	5:O:707:GTP:O2A	2.35	0.45
1:B:381:ILE:HD13	1:B:553:TYR:CG	2.52	0.45
7:E:706:DTP:O2B	1:H:377:LYS:NZ	2.47	0.45
1:H:381:ILE:HD13	1:H:553:TYR:CD2	2.52	0.45
1:P:381:ILE:HD13	1:P:553:TYR:CG	2.52	0.45
1:C:381:ILE:HD13	1:C:553:TYR:CG	2.52	0.45
1:F:381:ILE:HD13	1:F:553:TYR:CG	2.51	0.45
1:C:381:ILE:HD13	1:C:553:TYR:CD2	2.52	0.44
1:I:455:LYS:HE3	1:I:557:VAL:HG13	1.99	0.44
1:K:381:ILE:HD13	1:K:553:TYR:CG	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:ILE:HD13	1:B:553:TYR:CD2	2.53	0.44
1:G:381:ILE:HD13	1:G:553:TYR:CD2	2.52	0.44
1:G:390:PHE:CZ	1:G:426:ILE:CG2	3.01	0.44
1:L:354:LYS:NZ	7:L:701:DTP:O1A	2.46	0.44
1:A:455:LYS:HE3	1:A:557:VAL:HG13	1.99	0.44
1:B:220:ARG:NH1	1:B:384:THR:HG22	2.32	0.44
1:I:381:ILE:HD13	1:I:553:TYR:CD2	2.52	0.44
1:J:390:PHE:CZ	1:J:426:ILE:CG2	3.01	0.44
1:K:381:ILE:HD13	1:K:553:TYR:CD2	2.53	0.44
1:P:381:ILE:HD13	1:P:553:TYR:CD2	2.52	0.44
1:J:381:ILE:HD13	1:J:553:TYR:CD2	2.52	0.44
1:A:517:HIS:ND1	6:A:707:SO4:O2	2.44	0.44
1:B:390:PHE:CZ	1:B:426:ILE:CG2	3.01	0.44
1:N:390:PHE:CZ	1:N:426:ILE:CG2	3.01	0.44
1:J:571:GLN:NE2	1:J:594:GLN:HE22	2.16	0.44
1:L:390:PHE:CZ	1:L:426:ILE:CG2	3.01	0.44
1:P:354:LYS:NZ	7:P:701:DTP:O1A	2.38	0.44
1:E:381:ILE:HD13	1:E:553:TYR:CD2	2.53	0.43
1:M:352:ARG:HG3	1:M:521:TYR:CZ	2.52	0.43
1:D:220:ARG:NH1	1:D:384:THR:HG22	2.33	0.43
1:F:390:PHE:CZ	1:F:426:ILE:CG2	3.01	0.43
1:H:220:ARG:NH1	1:H:384:THR:HG22	2.34	0.43
1:M:390:PHE:CZ	1:M:426:ILE:CG2	3.01	0.43
1:O:390:PHE:CZ	1:O:426:ILE:CG2	3.02	0.43
1:A:381:ILE:HD13	1:A:553:TYR:CD2	2.53	0.43
1:A:390:PHE:CZ	1:A:426:ILE:CG2	3.01	0.43
1:E:390:PHE:CZ	1:E:426:ILE:CG2	3.01	0.43
1:G:220:ARG:NH1	1:G:384:THR:HG22	2.33	0.43
1:K:390:PHE:CZ	1:K:426:ILE:CG2	3.01	0.43
1:C:394:ASP:O	1:C:408:ARG:HG2	2.19	0.43
1:N:381:ILE:HD13	1:N:553:TYR:CD2	2.53	0.43
1:C:390:PHE:CZ	1:C:426:ILE:CG2	3.01	0.43
1:F:220:ARG:NH1	1:F:384:THR:HG22	2.33	0.43
1:I:390:PHE:CZ	1:I:426:ILE:CG2	3.02	0.43
1:P:390:PHE:CZ	1:P:426:ILE:CG2	3.01	0.43
1:A:321:HIS:CE1	1:B:321:HIS:CE1	3.07	0.43
1:D:390:PHE:CZ	1:D:426:ILE:CG2	3.01	0.43
1:H:486:LYS:HE3	1:H:486:LYS:HB2	1.86	0.43
7:M:708:DTP:O2B	1:P:377:LYS:NZ	2.49	0.43
1:H:390:PHE:CZ	1:H:426:ILE:CG2	3.01	0.43
1:K:220:ARG:NH1	1:K:384:THR:HG22	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:220:ARG:NH1	1:M:384:THR:HG22	2.34	0.42
1:H:352:ARG:HG3	1:H:521:TYR:CZ	2.54	0.42
1:L:315:TYR:CD1	4:L:706:0KX:H9	2.54	0.42
1:I:220:ARG:NH1	1:I:384:THR:HG22	2.34	0.42
1:J:220:ARG:NH1	1:J:384:THR:HG22	2.34	0.42
1:P:220:ARG:NH1	1:P:384:THR:HG22	2.34	0.42
1:L:220:ARG:NH1	1:L:384:THR:HG22	2.34	0.42
1:O:220:ARG:NH1	1:O:384:THR:HG22	2.35	0.42
1:A:220:ARG:NH1	1:A:384:THR:HG22	2.35	0.42
1:E:220:ARG:NH1	1:E:384:THR:HG22	2.35	0.42
1:J:117:VAL:O	5:J:705:GTP:O2'	2.31	0.42
1:D:594:GLN:HG2	1:D:595:LYS:N	2.34	0.42
1:O:354:LYS:NZ	7:O:701:DTP:O1A	2.43	0.42
1:J:594:GLN:HG2	1:J:595:LYS:N	2.35	0.41
1:N:116:LYS:NZ	5:N:705:GTP:O2G	2.53	0.41
1:C:574:ALA:HB1	1:C:595:LYS:HD3	2.02	0.41
1:O:448:ILE:HD13	1:O:453:LEU:CD2	2.51	0.41
1:C:311:ASP:OD2	4:C:706:0KX:N3A	2.52	0.41
1:A:528:ARG:HH12	1:D:585:ASP:HB3	1.86	0.41
1:C:354:LYS:NZ	7:C:701:DTP:O1A	2.49	0.41
1:D:574:ALA:HB1	1:D:595:LYS:HD3	2.02	0.41
1:G:523:LYS:NZ	7:G:701:DTP:O2G	2.49	0.41
1:H:371:ARG:HH22	1:H:549:LEU:HD21	1.86	0.41
1:N:220:ARG:NH1	1:N:384:THR:HG22	2.35	0.41
1:P:341:CYS:SG	1:P:350:CYS:HB2	2.61	0.41
1:C:220:ARG:NH1	1:C:384:THR:HG22	2.36	0.41
1:E:371:ARG:HH22	1:E:549:LEU:HD21	1.85	0.41
1:F:371:ARG:HH22	1:F:549:LEU:HD21	1.86	0.41
1:P:352:ARG:HH12	7:P:701:DTP:PG	2.44	0.41
1:N:315:TYR:CG	4:N:704:0KX:H9	2.57	0.40
1:A:597:GLU:OE1	1:A:597:GLU:N	2.55	0.40
1:E:321:HIS:CE1	1:F:321:HIS:CE1	3.09	0.40
1:I:371:ARG:HH22	1:I:549:LEU:HD21	1.87	0.40

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

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	477/520 (92%)	463 (97%)	13 (3%)	1 (0%)	47	69
1	B	474/520 (91%)	459 (97%)	14 (3%)	1 (0%)	47	69
1	C	476/520 (92%)	462 (97%)	14 (3%)	0	100	100
1	D	477/520 (92%)	462 (97%)	15 (3%)	0	100	100
1	E	474/520 (91%)	457 (96%)	17 (4%)	0	100	100
1	F	457/520 (88%)	443 (97%)	14 (3%)	0	100	100
1	G	457/520 (88%)	442 (97%)	15 (3%)	0	100	100
1	H	474/520 (91%)	458 (97%)	16 (3%)	0	100	100
1	I	473/520 (91%)	460 (97%)	13 (3%)	0	100	100
1	J	475/520 (91%)	459 (97%)	16 (3%)	0	100	100
1	K	476/520 (92%)	460 (97%)	16 (3%)	0	100	100
1	L	471/520 (91%)	455 (97%)	16 (3%)	0	100	100
1	M	467/520 (90%)	453 (97%)	14 (3%)	0	100	100
1	N	471/520 (91%)	457 (97%)	14 (3%)	0	100	100
1	O	459/520 (88%)	441 (96%)	17 (4%)	1 (0%)	47	69
1	P	455/520 (88%)	441 (97%)	14 (3%)	0	100	100
All	All	7513/8320 (90%)	7272 (97%)	238 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	406/464 (88%)	394 (97%)	12 (3%)	41	65
1	B	404/464 (87%)	395 (98%)	9 (2%)	52	75
1	C	409/464 (88%)	399 (98%)	10 (2%)	49	72
1	D	407/464 (88%)	397 (98%)	10 (2%)	47	71
1	E	398/464 (86%)	390 (98%)	8 (2%)	55	76
1	F	390/464 (84%)	381 (98%)	9 (2%)	50	73
1	G	384/464 (83%)	378 (98%)	6 (2%)	62	81
1	H	409/464 (88%)	401 (98%)	8 (2%)	55	76
1	I	404/464 (87%)	397 (98%)	7 (2%)	60	80
1	J	406/464 (88%)	398 (98%)	8 (2%)	55	76
1	K	406/464 (88%)	393 (97%)	13 (3%)	39	63
1	L	391/464 (84%)	383 (98%)	8 (2%)	55	76
1	M	384/464 (83%)	374 (97%)	10 (3%)	46	70
1	N	391/464 (84%)	384 (98%)	7 (2%)	59	78
1	O	385/464 (83%)	376 (98%)	9 (2%)	50	73
1	P	380/464 (82%)	373 (98%)	7 (2%)	59	78
All	All	6354/7424 (86%)	6213 (98%)	141 (2%)	52	75

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	MET
1	A	134	ARG
1	A	168	SER
1	A	315	TYR
1	A	339	ARG
1	A	352	ARG
1	A	406	LYS
1	A	446	LYS

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Mol	Chain	Res	Type
1	A	488	LEU
1	A	490	ASP
1	A	496	GLU
1	A	576	ARG
1	B	115	MET
1	B	134	ARG
1	B	168	SER
1	B	231	TRP
1	B	315	TYR
1	B	352	ARG
1	B	408	ARG
1	B	496	GLU
1	B	576	ARG
1	C	115	MET
1	C	168	SER
1	C	315	TYR
1	C	339	ARG
1	C	352	ARG
1	C	405	LYS
1	C	408	ARG
1	C	494	LYS
1	C	496	GLU
1	C	576	ARG
1	D	115	MET
1	D	134	ARG
1	D	168	SER
1	D	315	TYR
1	D	352	ARG
1	D	405	LYS
1	D	496	GLU
1	D	511	GLU
1	D	576	ARG
1	D	594	GLN
1	E	115	MET
1	E	134	ARG
1	E	168	SER
1	E	315	TYR
1	E	352	ARG
1	E	405	LYS
1	E	490	ASP
1	E	576	ARG
1	F	115	MET

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Mol	Chain	Res	Type
1	F	134	ARG
1	F	168	SER
1	F	315	TYR
1	F	339	ARG
1	F	352	ARG
1	F	496	GLU
1	F	562	LEU
1	F	576	ARG
1	G	134	ARG
1	G	168	SER
1	G	315	TYR
1	G	352	ARG
1	G	496	GLU
1	G	576	ARG
1	H	168	SER
1	H	315	TYR
1	H	339	ARG
1	H	352	ARG
1	H	465	GLN
1	H	490	ASP
1	H	496	GLU
1	H	576	ARG
1	I	134	ARG
1	I	168	SER
1	I	315	TYR
1	I	352	ARG
1	I	490	ASP
1	I	494	LYS
1	I	576	ARG
1	J	115	MET
1	J	134	ARG
1	J	168	SER
1	J	288	LYS
1	J	315	TYR
1	J	352	ARG
1	J	576	ARG
1	J	594	GLN
1	K	134	ARG
1	K	168	SER
1	K	180	HIS
1	K	315	TYR
1	K	339	ARG

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Mol	Chain	Res	Type
1	K	352	ARG
1	K	392	LYS
1	K	439	LYS
1	K	490	ASP
1	K	496	GLU
1	K	562	LEU
1	K	576	ARG
1	K	594	GLN
1	L	134	ARG
1	L	168	SER
1	L	315	TYR
1	L	339	ARG
1	L	352	ARG
1	L	496	GLU
1	L	562	LEU
1	L	576	ARG
1	M	115	MET
1	M	116	LYS
1	M	134	ARG
1	M	168	SER
1	M	315	TYR
1	M	352	ARG
1	M	496	GLU
1	M	576	ARG
1	M	582	GLN
1	M	594	GLN
1	N	168	SER
1	N	315	TYR
1	N	339	ARG
1	N	352	ARG
1	N	490	ASP
1	N	491	VAL
1	N	576	ARG
1	O	134	ARG
1	O	168	SER
1	O	180	HIS
1	O	280	VAL
1	O	315	TYR
1	O	339	ARG
1	O	352	ARG
1	O	576	ARG
1	O	582	GLN

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Mol	Chain	Res	Type
1	P	134	ARG
1	P	168	SER
1	P	315	TYR
1	P	341	CYS
1	P	352	ARG
1	P	466	ILE
1	P	576	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	GLN
1	A	210	HIS
1	A	271	GLN
1	A	370	HIS
1	A	375	GLN
1	A	380	ASN
1	B	210	HIS
1	B	271	GLN
1	B	321	HIS
1	B	375	GLN
1	B	380	ASN
1	C	210	HIS
1	C	271	GLN
1	C	375	GLN
1	C	380	ASN
1	D	210	HIS
1	D	271	GLN
1	D	370	HIS
1	D	375	GLN
1	D	380	ASN
1	D	571	GLN
1	D	594	GLN
1	E	210	HIS
1	E	271	GLN
1	E	370	HIS
1	E	375	GLN
1	E	380	ASN
1	F	210	HIS
1	F	271	GLN
1	F	375	GLN
1	F	380	ASN

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Mol	Chain	Res	Type
1	G	210	HIS
1	G	271	GLN
1	G	370	HIS
1	G	375	GLN
1	G	380	ASN
1	H	210	HIS
1	H	271	GLN
1	H	375	GLN
1	H	380	ASN
1	H	465	GLN
1	I	271	GLN
1	I	375	GLN
1	I	380	ASN
1	J	271	GLN
1	J	370	HIS
1	J	375	GLN
1	J	380	ASN
1	J	571	GLN
1	J	594	GLN
1	K	271	GLN
1	K	375	GLN
1	K	380	ASN
1	K	571	GLN
1	L	271	GLN
1	L	375	GLN
1	L	380	ASN
1	M	210	HIS
1	M	271	GLN
1	M	370	HIS
1	M	375	GLN
1	M	380	ASN
1	M	571	GLN
1	N	271	GLN
1	N	370	HIS
1	N	375	GLN
1	N	380	ASN
1	O	210	HIS
1	O	271	GLN
1	O	370	HIS
1	O	375	GLN
1	O	380	ASN
1	P	210	HIS

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Mol	Chain	Res	Type
1	P	271	GLN
1	P	375	GLN
1	P	380	ASN
1	P	425	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	G	706	3,2	28,29,29	1.29	3 (10%)	40,45,45	1.78	7 (17%)
7	DTP	F	706	3	26,32,32	1.09	2 (7%)	30,50,50	1.53	7 (23%)
5	GTP	O	707	3	26,34,34	0.88	1 (3%)	32,54,54	1.80	11 (34%)
6	SO4	A	707	-	4,4,4	0.47	0	6,6,6	0.98	1 (16%)
6	SO4	H	707	-	4,4,4	0.45	0	6,6,6	0.51	0
4	OKX	O	705	3,2	28,29,29	1.14	3 (10%)	40,45,45	1.34	4 (10%)
4	OKX	J	704	3,2	28,29,29	1.22	3 (10%)	40,45,45	1.45	6 (15%)
7	DTP	B	708	3	26,32,32	1.35	4 (15%)	30,50,50	1.77	9 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	DTP	C	701	3	26,32,32	0.86	1 (3%)	30,50,50	2.02	12 (40%)
5	GTP	I	706	3	26,34,34	1.09	2 (7%)	32,54,54	1.67	8 (25%)
4	OKX	A	705	3,2	28,29,29	1.05	3 (10%)	40,45,45	1.48	5 (12%)
4	OKX	B	705	3,2	28,29,29	1.46	4 (14%)	40,45,45	1.98	11 (27%)
5	GTP	E	705	3	26,34,34	0.79	0	32,54,54	1.47	5 (15%)
6	SO4	M	707	-	4,4,4	0.47	0	6,6,6	0.18	0
4	OKX	C	706	3	28,29,29	1.10	3 (10%)	40,45,45	1.46	3 (7%)
5	GTP	H	706	3	26,34,34	1.52	3 (11%)	32,54,54	1.70	7 (21%)
7	DTP	A	708	3	26,32,32	0.82	1 (3%)	30,50,50	1.48	5 (16%)
5	GTP	A	706	3	26,34,34	1.19	3 (11%)	32,54,54	1.74	10 (31%)
7	DTP	O	701	3	26,32,32	0.96	1 (3%)	30,50,50	1.63	8 (26%)
5	GTP	B	706	3	26,34,34	1.15	1 (3%)	32,54,54	1.78	9 (28%)
6	SO4	D	708	-	4,4,4	0.53	0	6,6,6	0.27	0
7	DTP	E	706	3	26,32,32	1.12	3 (11%)	30,50,50	1.23	3 (10%)
5	GTP	M	706	3	26,34,34	1.09	1 (3%)	32,54,54	1.61	6 (18%)
7	DTP	K	701	3	26,32,32	0.89	1 (3%)	30,50,50	1.62	8 (26%)
7	DTP	L	701	3	26,32,32	1.12	3 (11%)	30,50,50	2.01	7 (23%)
7	DTP	D	701	3	26,32,32	1.14	4 (15%)	30,50,50	1.47	4 (13%)
5	GTP	C	707	3	26,34,34	1.08	1 (3%)	32,54,54	1.44	5 (15%)
7	DTP	M	708	3	26,32,32	1.12	3 (11%)	30,50,50	1.27	4 (13%)
4	OKX	D	706	3,2	28,29,29	1.42	4 (14%)	40,45,45	1.83	8 (20%)
7	DTP	G	701	3	26,32,32	0.94	0	30,50,50	1.56	7 (23%)
4	OKX	L	706	3,2	28,29,29	1.47	3 (10%)	40,45,45	1.74	9 (22%)
4	OKX	I	705	3,2	28,29,29	1.05	3 (10%)	40,45,45	1.75	5 (12%)
5	GTP	J	705	3	26,34,34	1.52	2 (7%)	32,54,54	1.77	7 (21%)
7	DTP	J	707	3	26,32,32	1.11	1 (3%)	30,50,50	1.99	8 (26%)
4	OKX	E	704	3,2	28,29,29	1.37	4 (14%)	40,45,45	1.27	3 (7%)
5	GTP	O	706	3	26,34,34	0.82	0	32,54,54	1.74	9 (28%)
6	SO4	J	706	-	4,4,4	0.64	0	6,6,6	0.45	0
7	DTP	I	708	3	26,32,32	0.84	0	30,50,50	1.66	9 (30%)
4	OKX	P	706	3,2	28,29,29	1.41	4 (14%)	40,45,45	1.33	4 (10%)
6	SO4	C	708	-	4,4,4	0.70	0	6,6,6	0.37	0
6	SO4	L	708	-	4,4,4	0.62	0	6,6,6	0.70	0
4	OKX	F	704	3,2	28,29,29	1.07	3 (10%)	40,45,45	1.83	5 (12%)
5	GTP	K	707	3	26,34,34	0.99	2 (7%)	32,54,54	1.87	8 (25%)
7	DTP	P	701	3	26,32,32	1.14	3 (11%)	30,50,50	1.35	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OKX	N	704	3,2	28,29,29	1.17	3 (10%)	40,45,45	1.37	4 (10%)
6	SO4	I	707	-	4,4,4	0.43	0	6,6,6	0.81	0
7	DTP	N	706	3	26,32,32	1.06	2 (7%)	30,50,50	1.47	5 (16%)
4	OKX	M	705	3,2	28,29,29	1.16	3 (10%)	40,45,45	1.57	6 (15%)
5	GTP	D	707	3	26,34,34	1.33	4 (15%)	32,54,54	1.72	10 (31%)
5	GTP	N	705	3	26,34,34	1.22	2 (7%)	32,54,54	1.83	9 (28%)
5	GTP	L	707	3	26,34,34	1.16	3 (11%)	32,54,54	1.80	8 (25%)
4	OKX	K	706	3,2	28,29,29	1.18	3 (10%)	40,45,45	1.71	7 (17%)
5	GTP	F	705	3	26,34,34	0.98	0	32,54,54	1.92	9 (28%)
4	OKX	H	705	3,2	28,29,29	0.99	3 (10%)	40,45,45	1.28	5 (12%)
7	DTP	H	701	3	26,32,32	1.25	2 (7%)	30,50,50	1.68	8 (26%)
5	GTP	G	707	3	26,34,34	1.10	2 (7%)	32,54,54	1.25	3 (9%)
6	SO4	B	707	-	4,4,4	0.59	0	6,6,6	0.87	0

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

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

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

All (110) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	705	GTP	C6-N1	-5.95	1.29	1.37
5	H	706	GTP	C6-N1	-5.40	1.29	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	705	0KX	PB-O2B	5.22	1.54	1.46
4	L	706	0KX	PB-O2B	4.96	1.54	1.46
4	D	706	0KX	PB-O2B	4.66	1.53	1.46
4	P	706	0KX	PB-O2B	4.65	1.53	1.46
4	G	706	0KX	PB-O2B	4.36	1.53	1.46
4	E	704	0KX	PB-O2B	4.23	1.52	1.46
5	A	706	GTP	C6-N1	-3.92	1.32	1.37
4	J	704	0KX	PB-O2B	3.85	1.52	1.46
5	D	707	GTP	C6-N1	-3.74	1.32	1.37
4	K	706	0KX	PB-O2B	3.73	1.52	1.46
4	N	704	0KX	PB-O2B	3.72	1.52	1.46
5	M	706	GTP	C6-N1	-3.64	1.32	1.37
5	N	705	GTP	C6-N1	-3.57	1.32	1.37
7	H	701	DTP	C2-N3	3.48	1.37	1.32
4	D	706	0KX	PA-O1A	3.45	1.51	1.46
4	M	705	0KX	PB-O2B	3.38	1.51	1.46
7	P	701	DTP	C2-N3	3.37	1.37	1.32
7	L	701	DTP	C2-N3	3.18	1.37	1.32
7	F	706	DTP	C2-N3	3.15	1.37	1.32
4	O	705	0KX	PB-O2B	3.12	1.51	1.46
4	H	705	0KX	PB-O2B	3.08	1.51	1.46
4	K	706	0KX	PA-O1A	3.03	1.51	1.46
4	F	704	0KX	PA-O1A	3.02	1.50	1.46
4	E	704	0KX	PA-O1A	3.01	1.50	1.46
5	C	707	GTP	C6-N1	-3.00	1.33	1.37
4	L	706	0KX	PA-O1A	2.97	1.50	1.46
4	O	705	0KX	PA-O1A	2.96	1.50	1.46
4	P	706	0KX	PA-O1A	2.93	1.50	1.46
4	A	705	0KX	PB-O2B	2.93	1.50	1.46
4	M	705	0KX	PA-O1A	2.89	1.50	1.46
4	G	706	0KX	PA-O1A	2.86	1.50	1.46
4	C	706	0KX	PA-O2A	-2.83	1.49	1.56
4	J	704	0KX	PA-O1A	2.82	1.50	1.46
5	K	707	GTP	C6-N1	-2.80	1.33	1.37
4	I	705	0KX	PB-O2B	2.79	1.50	1.46
4	A	705	0KX	PA-O1A	2.78	1.50	1.46
4	C	706	0KX	PB-O2B	2.78	1.50	1.46
7	B	708	DTP	C2-N3	2.73	1.36	1.32
4	F	704	0KX	PB-O2B	2.71	1.50	1.46
5	G	707	GTP	C6-N1	-2.62	1.34	1.37
5	I	706	GTP	C6-N1	-2.61	1.34	1.37
7	M	708	DTP	C5-N7	-2.59	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	705	OKX	PA-O2A	-2.58	1.49	1.56
7	H	701	DTP	C5-C4	2.56	1.47	1.40
7	D	701	DTP	C5-C4	2.56	1.47	1.40
4	A	705	OKX	PA-O2A	-2.55	1.49	1.56
4	E	704	OKX	PA-O2A	-2.54	1.49	1.56
4	P	706	OKX	PA-O2A	-2.53	1.49	1.56
4	H	705	OKX	PA-O1A	2.53	1.50	1.46
4	N	704	OKX	PA-O1A	2.52	1.50	1.46
7	B	708	DTP	C5-C4	2.51	1.47	1.40
4	C	706	OKX	PA-O1A	2.51	1.50	1.46
5	D	707	GTP	C4-N3	-2.49	1.31	1.37
4	L	706	OKX	PA-O2A	-2.48	1.50	1.56
7	M	708	DTP	C2-N3	2.48	1.36	1.32
5	H	706	GTP	C4-N3	-2.48	1.31	1.37
7	K	701	DTP	C5-N7	-2.47	1.30	1.39
7	D	701	DTP	C2-N3	2.46	1.36	1.32
5	L	707	GTP	C6-N1	-2.42	1.34	1.37
4	I	705	OKX	PA-O2A	-2.40	1.50	1.56
7	B	708	DTP	O4'-C4'	-2.40	1.39	1.45
7	N	706	DTP	C5-C4	2.39	1.47	1.40
4	M	705	OKX	PA-O2A	-2.38	1.50	1.56
4	D	706	OKX	PA-O2A	-2.37	1.50	1.56
7	B	708	DTP	C2-N1	2.37	1.38	1.33
5	D	707	GTP	O4'-C4'	-2.35	1.39	1.45
4	B	705	OKX	PB-O3B	2.34	1.62	1.59
5	L	707	GTP	O4'-C1'	-2.34	1.37	1.41
7	E	706	DTP	C4-N3	-2.32	1.32	1.35
7	E	706	DTP	C5-N7	-2.30	1.31	1.39
7	E	706	DTP	C2-N3	2.30	1.35	1.32
7	A	708	DTP	C5-N7	-2.29	1.31	1.39
4	I	705	OKX	PA-O1A	2.29	1.49	1.46
5	O	707	GTP	C6-N1	-2.29	1.34	1.37
5	N	705	GTP	O3'-C3'	2.28	1.48	1.43
5	B	706	GTP	C6-N1	-2.28	1.34	1.37
4	E	704	OKX	PB-O3B	2.26	1.61	1.59
4	G	706	OKX	PB-O1B	-2.26	1.50	1.56
4	D	706	OKX	PB-O1B	-2.26	1.50	1.56
7	J	707	DTP	C5-C4	2.26	1.46	1.40
4	F	704	OKX	PA-O2A	-2.26	1.50	1.56
5	L	707	GTP	C5-C4	2.25	1.48	1.43
5	H	706	GTP	C2-N1	-2.25	1.32	1.37
4	B	705	OKX	PA-O1A	2.24	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	P	701	DTP	C5-C4	2.24	1.46	1.40
5	D	707	GTP	PG-O3G	-2.23	1.46	1.54
7	L	701	DTP	C6-C5	2.23	1.51	1.43
5	G	707	GTP	C4-N3	-2.20	1.32	1.37
5	J	705	GTP	C4-N3	-2.20	1.32	1.37
4	P	706	OKX	PB-O1B	-2.20	1.50	1.56
4	N	704	OKX	PB-O1B	-2.18	1.50	1.56
5	I	706	GTP	O3'-C3'	2.18	1.48	1.43
7	M	708	DTP	C5-C4	2.16	1.46	1.40
4	K	706	OKX	PA-O2A	-2.16	1.50	1.56
4	H	705	OKX	PA-O2A	-2.13	1.51	1.56
7	D	701	DTP	O4'-C4'	-2.13	1.40	1.45
7	O	701	DTP	C5-C4	2.13	1.46	1.40
7	N	706	DTP	C2-N3	2.09	1.35	1.32
5	K	707	GTP	C2-N3	2.08	1.38	1.33
5	A	706	GTP	C5-C4	2.07	1.48	1.43
5	A	706	GTP	C2-N1	-2.05	1.32	1.37
7	P	701	DTP	C5-N7	-2.05	1.32	1.39
4	J	704	OKX	PB-O1B	-2.04	1.51	1.56
7	D	701	DTP	C5-N7	-2.03	1.32	1.39
7	L	701	DTP	O4'-C4'	-2.02	1.40	1.45
7	F	706	DTP	C5-C4	2.01	1.46	1.40
4	O	705	OKX	PB-O3B	2.01	1.61	1.59
7	C	701	DTP	C5-N7	-2.01	1.32	1.39

All (325) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	705	OKX	O2B-PB-N3A	-7.11	101.30	111.77
7	L	701	DTP	C4-C5-N7	-6.77	102.34	109.40
4	B	705	OKX	O1B-PB-O2B	6.53	123.61	109.92
4	C	706	OKX	O1B-PB-O2B	6.23	122.98	109.92
4	L	706	OKX	O1B-PB-O2B	5.64	121.75	109.92
4	F	704	OKX	O1A-PA-N3A	-5.64	103.47	111.77
4	M	705	OKX	O1B-PB-O2B	5.49	121.43	109.92
4	I	705	OKX	O1B-PB-O2B	5.46	121.37	109.92
4	D	706	OKX	O1A-PA-N3A	-5.32	103.94	111.77
4	F	704	OKX	O1B-PB-O2B	5.31	121.05	109.92
4	A	705	OKX	O1B-PB-O2B	5.21	120.85	109.92
4	D	706	OKX	O1B-PB-O2B	5.11	120.63	109.92
4	P	706	OKX	O1B-PB-O2B	5.05	120.51	109.92
4	E	704	OKX	O1B-PB-O2B	5.04	120.49	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	706	0KX	O3B-PB-N3A	-5.04	92.62	106.59
4	K	706	0KX	O1B-PB-O2B	5.04	120.48	109.92
7	J	707	DTP	N3-C2-N1	-4.94	120.95	128.68
4	N	704	0KX	O1B-PB-O2B	4.93	120.27	109.92
4	J	704	0KX	O1B-PB-O2B	4.89	120.16	109.92
5	F	705	GTP	PA-O3A-PB	-4.83	116.26	132.83
5	L	707	GTP	C3'-C2'-C1'	4.72	108.09	100.98
7	C	701	DTP	O5'-PA-O1A	-4.72	90.64	109.07
5	N	705	GTP	C3'-C2'-C1'	4.70	108.05	100.98
5	F	705	GTP	O5'-PA-O1A	-4.67	90.81	109.07
5	B	706	GTP	PA-O3A-PB	-4.67	116.81	132.83
7	I	708	DTP	N3-C2-N1	-4.65	121.40	128.68
4	K	706	0KX	O1A-PA-N3A	4.65	118.62	111.77
4	H	705	0KX	O1B-PB-O2B	4.60	119.58	109.92
7	O	701	DTP	N3-C2-N1	-4.39	121.82	128.68
5	K	707	GTP	PA-O3A-PB	-4.38	117.81	132.83
4	G	706	0KX	O5'-PA-O1A	-4.33	97.59	114.24
7	H	701	DTP	C2'-C1'-N9	4.33	124.25	114.27
7	B	708	DTP	O2G-PG-O1G	4.28	127.43	110.68
7	N	706	DTP	N3-C2-N1	-4.26	122.02	128.68
4	G	706	0KX	O1B-PB-O2B	4.26	118.84	109.92
7	C	701	DTP	N3-C2-N1	-4.20	122.11	128.68
7	J	707	DTP	C2'-C1'-N9	4.20	123.97	114.27
4	G	706	0KX	O2B-PB-N3A	4.18	117.92	111.77
4	L	706	0KX	O2A-PA-O1A	4.15	118.62	109.92
4	O	705	0KX	O3B-PB-N3A	-4.12	95.16	106.59
4	B	705	0KX	O2A-PA-O1A	4.11	118.54	109.92
5	N	705	GTP	C5-C6-N1	4.10	121.19	113.95
5	H	706	GTP	O6-C6-N1	-4.07	115.84	120.65
4	B	705	0KX	O5'-PA-O1A	-4.06	98.61	114.24
5	O	707	GTP	PA-O3A-PB	-4.06	118.89	132.83
4	F	704	0KX	PB-O3B-PG	-4.05	118.35	132.62
4	A	705	0KX	O1A-PA-N3A	-4.00	105.87	111.77
4	K	706	0KX	O5'-PA-O1A	-3.99	98.91	114.24
7	J	707	DTP	N6-C6-N1	3.93	126.73	118.57
4	C	706	0KX	O2B-PB-N3A	-3.93	105.99	111.77
4	B	705	0KX	O3B-PB-N3A	3.90	117.40	106.59
7	L	701	DTP	O3G-PG-O2G	3.86	122.41	107.64
5	L	707	GTP	PA-O3A-PB	-3.85	119.61	132.83
5	O	706	GTP	C3'-C2'-C1'	3.85	106.77	100.98
5	J	705	GTP	C2-N1-C6	-3.84	118.03	125.10
4	E	704	0KX	O2A-PA-O1A	3.80	117.90	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	707	GTP	PB-O3B-PG	-3.80	119.80	132.83
5	K	707	GTP	C3'-C2'-C1'	3.73	106.60	100.98
7	C	701	DTP	C2'-C1'-N9	3.73	122.86	114.27
4	O	705	0KX	O2A-PA-O1A	3.72	117.73	109.92
7	K	701	DTP	N3-C2-N1	-3.69	122.91	128.68
5	I	706	GTP	C3'-C2'-C1'	3.68	106.52	100.98
5	M	706	GTP	C5-C6-N1	3.68	120.44	113.95
4	O	705	0KX	O1B-PB-O2B	3.68	117.63	109.92
4	P	706	0KX	O2A-PA-O1A	3.67	117.61	109.92
4	D	706	0KX	O2A-PA-O1A	3.66	117.60	109.92
5	J	705	GTP	C5-C6-N1	3.65	120.41	113.95
4	N	704	0KX	O5'-PA-O1A	-3.64	100.26	114.24
5	A	706	GTP	PA-O3A-PB	-3.62	120.40	132.83
5	D	707	GTP	C2-N1-C6	-3.61	118.46	125.10
4	G	706	0KX	O2A-PA-O1A	3.61	117.48	109.92
7	A	708	DTP	N3-C2-N1	-3.59	123.07	128.68
4	A	705	0KX	O2A-PA-O1A	3.59	117.44	109.92
5	O	707	GTP	O6-C6-C5	-3.52	117.49	124.37
4	K	706	0KX	O2A-PA-O5'	3.49	116.21	106.75
4	M	705	0KX	O5'-PA-O1A	-3.49	100.81	114.24
4	K	706	0KX	O2A-PA-O1A	3.48	117.22	109.92
7	G	701	DTP	N3-C2-N1	-3.48	123.24	128.68
5	I	706	GTP	PA-O3A-PB	-3.46	120.94	132.83
4	L	706	0KX	O5'-PA-O1A	-3.44	101.00	114.24
5	G	707	GTP	PB-O3B-PG	-3.44	121.02	132.83
5	K	707	GTP	C5-C6-N1	3.42	119.99	113.95
5	E	705	GTP	C3'-C2'-C1'	3.41	106.12	100.98
4	N	704	0KX	O2A-PA-O1A	3.36	116.97	109.92
7	H	701	DTP	N3-C2-N1	-3.35	123.44	128.68
4	M	705	0KX	O2A-PA-O1A	3.34	116.93	109.92
7	B	708	DTP	N3-C2-N1	-3.33	123.47	128.68
7	D	701	DTP	N6-C6-N1	3.32	125.46	118.57
4	D	706	0KX	O2B-PB-N3A	3.28	116.61	111.77
5	M	706	GTP	PB-O3B-PG	-3.28	121.56	132.83
4	J	704	0KX	O2A-PA-O1A	3.28	116.80	109.92
5	C	707	GTP	O5'-PA-O1A	-3.28	96.26	109.07
5	N	705	GTP	PA-O3A-PB	-3.27	121.60	132.83
4	F	704	0KX	O2A-PA-O5'	-3.27	97.88	106.75
4	F	704	0KX	O2A-PA-O1A	3.27	116.77	109.92
5	E	705	GTP	PA-O3A-PB	-3.26	121.63	132.83
5	A	706	GTP	C3'-C2'-C1'	3.26	105.89	100.98
7	L	701	DTP	N3-C2-N1	-3.25	123.60	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	706	GTP	PA-O3A-PB	-3.23	121.74	132.83
7	A	708	DTP	O3G-PG-O2G	3.22	119.96	107.64
7	F	706	DTP	N3-C2-N1	-3.21	123.67	128.68
5	B	706	GTP	PB-O3B-PG	-3.18	121.90	132.83
7	O	701	DTP	O5'-PA-O1A	-3.17	96.66	109.07
5	O	706	GTP	O4'-C1'-C2'	-3.14	102.34	106.93
5	B	706	GTP	C3'-C2'-C1'	3.12	105.68	100.98
4	H	705	OKX	O2A-PA-O1A	3.10	116.42	109.92
5	M	706	GTP	O6-C6-C5	-3.10	118.32	124.37
5	H	706	GTP	C5-C6-N1	3.10	119.42	113.95
7	C	701	DTP	C5-C6-N6	-3.09	115.65	120.35
7	D	701	DTP	C5-C6-N6	-3.09	115.65	120.35
5	O	707	GTP	O5'-PA-O1A	-3.09	96.99	109.07
5	J	705	GTP	C3'-C2'-C1'	3.07	105.60	100.98
7	C	701	DTP	N6-C6-N1	3.05	124.91	118.57
7	G	701	DTP	O3G-PG-O3B	-3.02	94.51	104.64
4	J	704	OKX	O5'-PA-O1A	-3.02	102.64	114.24
5	A	706	GTP	O3G-PG-O2G	3.01	119.13	107.64
5	D	707	GTP	O2A-PA-O1A	3.00	127.08	112.24
4	I	705	OKX	O2A-PA-O1A	3.00	116.21	109.92
7	D	701	DTP	O2A-PA-O1A	2.98	126.97	112.24
7	E	706	DTP	C4-C5-N7	-2.98	106.30	109.40
5	F	705	GTP	O6-C6-C5	-2.98	118.56	124.37
4	M	705	OKX	O3B-PB-N3A	-2.97	98.36	106.59
4	J	704	OKX	O1A-PA-N3A	-2.97	107.40	111.77
5	O	706	GTP	PB-O3B-PG	-2.96	122.66	132.83
4	D	706	OKX	PB-O3B-PG	-2.93	122.29	132.62
4	B	705	OKX	C1'-N1-C2	2.92	122.87	117.74
7	J	707	DTP	C2-N1-C6	2.91	123.73	118.75
7	G	701	DTP	C2'-C1'-N9	2.90	120.95	114.27
5	J	705	GTP	N2-C2-N3	-2.89	114.10	119.74
4	B	705	OKX	O2A-PA-O5'	2.88	114.55	106.75
5	O	707	GTP	C5-C6-N1	2.88	119.04	113.95
5	F	705	GTP	O2A-PA-O1A	2.88	126.47	112.24
4	H	705	OKX	O5'-PA-O1A	-2.87	103.19	114.24
4	J	704	OKX	O2A-PA-O5'	2.85	114.46	106.75
5	D	707	GTP	C5-C6-N1	2.84	118.97	113.95
7	G	701	DTP	O3G-PG-O1G	2.84	121.80	110.68
5	C	707	GTP	O2B-PB-O1B	2.83	126.25	112.24
7	F	706	DTP	O5'-PA-O1A	-2.83	98.02	109.07
5	H	706	GTP	O4'-C1'-C2'	2.82	111.05	106.93
5	I	706	GTP	O2A-PA-O5'	2.81	120.81	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	707	GTP	C3'-C2'-C1'	2.81	105.21	100.98
7	B	708	DTP	C4'-O4'-C1'	2.79	116.20	109.45
7	K	701	DTP	C2'-C1'-N9	2.77	120.66	114.27
5	J	705	GTP	O3G-PG-O1G	2.77	121.51	110.68
5	N	705	GTP	O3'-C3'-C2'	2.76	120.74	111.82
7	G	701	DTP	O5'-PA-O1A	-2.75	98.32	109.07
7	K	701	DTP	C4-C5-N7	-2.74	106.54	109.40
7	A	708	DTP	O2A-PA-O1A	2.74	125.77	112.24
7	P	701	DTP	N3-C2-N1	-2.74	124.40	128.68
4	L	706	OKX	O1A-PA-N3A	2.74	115.80	111.77
7	P	701	DTP	C4-C5-N7	-2.73	106.56	109.40
7	F	706	DTP	C4-C5-N7	-2.72	106.56	109.40
5	M	706	GTP	O2A-PA-O1A	2.72	125.68	112.24
5	J	705	GTP	PA-O3A-PB	-2.70	123.55	132.83
7	M	708	DTP	N3-C2-N1	-2.70	124.45	128.68
7	B	708	DTP	PB-O3B-PG	-2.70	123.56	132.83
4	H	705	OKX	O2A-PA-O5'	2.70	114.07	106.75
7	B	708	DTP	O2G-PG-O3B	-2.69	95.61	104.64
5	I	706	GTP	O6-C6-N1	-2.69	117.47	120.65
5	J	705	GTP	N1-C2-N3	2.68	128.33	123.32
4	L	706	OKX	C1'-N1-C2	2.68	122.44	117.74
7	P	701	DTP	O3G-PG-O2G	2.68	117.86	107.64
5	D	707	GTP	O4'-C4'-C5'	-2.67	100.60	109.37
5	N	705	GTP	O6-C6-C5	-2.66	119.17	124.37
5	C	707	GTP	C3'-C2'-C1'	2.66	104.98	100.98
4	L	706	OKX	O2-C2-N3	-2.66	118.01	122.33
5	O	706	GTP	C5-C6-N1	2.66	118.64	113.95
5	B	706	GTP	O2A-PA-O1A	2.65	125.34	112.24
4	D	706	OKX	O3B-PB-N3A	-2.65	99.25	106.59
7	N	706	DTP	C4-C5-N7	-2.64	106.65	109.40
7	J	707	DTP	O3G-PG-O2G	2.64	117.73	107.64
5	O	706	GTP	PA-O3A-PB	-2.64	123.77	132.83
7	I	708	DTP	N6-C6-N1	2.63	124.04	118.57
5	L	707	GTP	O4'-C4'-C5'	-2.63	100.72	109.37
7	D	701	DTP	N3-C2-N1	-2.63	124.57	128.68
7	H	701	DTP	O3G-PG-O2G	2.63	117.68	107.64
7	N	706	DTP	C2'-C1'-N9	2.62	120.32	114.27
5	D	707	GTP	O6-C6-C5	-2.62	119.26	124.37
5	E	705	GTP	N2-C2-N1	2.60	122.24	116.71
5	D	707	GTP	PA-O3A-PB	-2.58	123.96	132.83
5	O	706	GTP	O3G-PG-O2G	2.58	117.50	107.64
4	L	706	OKX	O2-C2-N1	2.57	124.20	118.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	701	DTP	PA-O3A-PB	-2.57	124.02	132.83
7	P	701	DTP	O5'-PA-O1A	-2.56	99.05	109.07
7	L	701	DTP	PB-O3B-PG	-2.56	124.03	132.83
5	F	705	GTP	O2B-PB-O1B	2.56	124.89	112.24
5	I	706	GTP	O3G-PG-O1G	2.56	120.70	110.68
5	A	706	GTP	O3G-PG-O1G	2.56	120.69	110.68
5	O	707	GTP	C3'-C2'-C1'	2.55	104.82	100.98
5	B	706	GTP	O5'-PA-O1A	-2.54	99.13	109.07
5	K	707	GTP	O3G-PG-O1G	2.54	120.63	110.68
7	H	701	DTP	PB-O3B-PG	-2.54	124.11	132.83
5	O	706	GTP	O6-C6-C5	-2.54	119.42	124.37
7	J	707	DTP	C5-C6-N6	-2.53	116.51	120.35
5	M	706	GTP	C3'-C2'-C1'	2.53	104.78	100.98
5	M	706	GTP	O5'-PA-O1A	-2.53	99.20	109.07
5	G	707	GTP	PA-O3A-PB	-2.52	124.16	132.83
5	I	706	GTP	C5-C6-N1	2.52	118.40	113.95
5	B	706	GTP	O6-C6-C5	-2.51	119.46	124.37
7	I	708	DTP	PB-O3B-PG	-2.51	124.22	132.83
4	G	706	OKX	PB-O3B-PG	-2.51	123.79	132.62
7	J	707	DTP	O2G-PG-O1G	2.50	120.47	110.68
7	L	701	DTP	O2B-PB-O1B	2.49	124.57	112.24
4	B	705	OKX	O2-C2-N3	-2.49	118.28	122.33
7	F	706	DTP	O3'-C3'-C4'	-2.49	100.59	110.10
5	C	707	GTP	C5-C6-N1	2.48	118.34	113.95
5	L	707	GTP	O2B-PB-O1B	2.48	124.52	112.24
5	F	705	GTP	O2G-PG-O3B	-2.48	96.31	104.64
7	H	701	DTP	O4'-C1'-C2'	-2.48	101.57	106.25
5	D	707	GTP	O2G-PG-O1G	2.47	120.36	110.68
5	A	706	GTP	C5-C6-N1	2.46	118.30	113.95
7	I	708	DTP	O2G-PG-O1G	2.46	120.32	110.68
5	H	706	GTP	C2-N1-C6	-2.46	120.57	125.10
4	M	705	OKX	O2B-PB-N3A	-2.46	108.15	111.77
4	D	706	OKX	C1'-N1-C6	-2.45	116.70	121.55
5	O	706	GTP	C8-N7-C5	2.45	107.66	102.99
7	M	708	DTP	C2'-C1'-N9	2.45	119.92	114.27
7	N	706	DTP	PB-O3B-PG	-2.44	124.45	132.83
5	K	707	GTP	O3G-PG-O3B	-2.44	96.45	104.64
4	A	705	OKX	O2B-PB-N3A	-2.43	108.19	111.77
4	J	704	OKX	O2B-PB-N3A	2.43	115.35	111.77
5	A	706	GTP	C2-N1-C6	-2.43	120.63	125.10
7	L	701	DTP	PA-O3A-PB	-2.42	124.52	132.83
4	D	706	OKX	C1'-N1-C2	2.42	121.97	117.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	705	GTP	PB-O3B-PG	-2.41	124.54	132.83
5	A	706	GTP	O2B-PB-O1B	2.41	124.16	112.24
4	N	704	0KX	O2B-PB-N3A	2.41	115.31	111.77
7	C	701	DTP	O3G-PG-O1G	2.40	120.08	110.68
5	F	705	GTP	O6-C6-N1	2.39	123.47	120.65
5	O	707	GTP	O6-C6-N1	2.39	123.47	120.65
5	B	706	GTP	C5-C6-N1	2.38	118.15	113.95
5	O	707	GTP	O3'-C3'-C2'	2.38	119.51	111.82
5	A	706	GTP	O2A-PA-O1A	2.37	123.97	112.24
7	K	701	DTP	C3'-C2'-C1'	2.37	108.47	102.54
7	J	707	DTP	PB-O3B-PG	-2.37	124.69	132.83
4	G	706	0KX	O2A-PA-O5'	2.36	113.15	106.75
7	O	701	DTP	N6-C6-N1	2.36	123.48	118.57
5	E	705	GTP	C8-N7-C5	2.35	107.47	102.99
7	C	701	DTP	O3G-PG-O3B	-2.35	96.76	104.64
7	K	701	DTP	O3G-PG-O1G	2.35	119.87	110.68
5	N	705	GTP	O4'-C4'-C3'	2.35	109.76	105.11
4	B	705	0KX	C1'-N1-C6	-2.34	116.92	121.55
4	I	705	0KX	O2-C2-N3	-2.34	118.52	122.33
7	K	701	DTP	O2B-PB-O1B	2.33	123.77	112.24
4	B	705	0KX	O1B-PB-O3B	-2.33	96.87	104.64
5	C	707	GTP	O3'-C3'-C2'	2.33	119.35	111.82
5	N	705	GTP	O2B-PB-O1B	2.32	123.72	112.24
7	K	701	DTP	O5'-PA-O1A	-2.32	100.01	109.07
5	N	705	GTP	O3G-PG-O2G	2.31	116.48	107.64
4	L	706	0KX	O1B-PB-O3B	-2.31	96.95	104.64
7	I	708	DTP	O5'-PA-O1A	-2.31	100.06	109.07
5	B	706	GTP	O2B-PB-O1B	2.30	123.61	112.24
7	B	708	DTP	O5'-PA-O1A	-2.29	100.12	109.07
7	F	706	DTP	PA-O3A-PB	-2.29	124.97	132.83
4	L	706	0KX	C1'-N1-C6	-2.29	117.03	121.55
4	H	705	0KX	O3B-PG-O2G	-2.28	98.52	111.19
7	C	701	DTP	O2B-PB-O1B	2.28	123.51	112.24
5	G	707	GTP	C3'-C2'-C1'	2.28	104.41	100.98
4	A	705	0KX	PB-O3B-PG	-2.27	124.61	132.62
5	F	705	GTP	C5-C6-N1	2.27	117.96	113.95
5	N	705	GTP	C2-N1-C6	-2.26	120.93	125.10
5	L	707	GTP	O5'-PA-O1A	-2.26	100.25	109.07
4	P	706	0KX	O1A-PA-N3A	2.26	115.09	111.77
5	B	706	GTP	N2-C2-N1	2.25	121.50	116.71
5	H	706	GTP	O3'-C3'-C4'	2.25	117.55	111.05
4	C	706	0KX	O1A-PA-N3A	-2.24	108.47	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	701	DTP	C2'-C3'-C4'	2.24	107.42	102.76
5	D	707	GTP	PB-O3B-PG	-2.23	125.16	132.83
7	B	708	DTP	C4-C5-N7	-2.23	107.07	109.40
7	I	708	DTP	PA-O3A-PB	-2.23	125.19	132.83
5	L	707	GTP	O6-C6-N1	2.22	123.28	120.65
7	E	706	DTP	O2G-PG-O1G	2.22	119.38	110.68
5	A	706	GTP	O2G-PG-O1G	-2.21	102.01	110.68
5	A	706	GTP	O3'-C3'-C4'	-2.21	104.66	111.05
5	O	707	GTP	O2A-PA-O1A	2.20	123.13	112.24
4	P	706	OKX	O5'-PA-O1A	-2.20	105.78	114.24
7	M	708	DTP	C4-C5-N7	-2.20	107.11	109.40
4	K	706	OKX	O1B-PB-O3B	-2.20	97.31	104.64
7	H	701	DTP	C4'-O4'-C1'	2.19	114.75	109.45
7	N	706	DTP	C2-N1-C6	2.19	122.50	118.75
7	C	701	DTP	O2A-PA-O5'	2.19	117.91	107.75
7	O	701	DTP	O3G-PG-O2G	2.19	116.00	107.64
7	H	701	DTP	N6-C6-N1	2.19	123.11	118.57
4	K	706	OKX	O3B-PG-O2G	-2.18	99.07	111.19
5	L	707	GTP	PB-O3B-PG	-2.18	125.34	132.83
7	K	701	DTP	PB-O3B-PG	-2.17	125.37	132.83
6	A	707	SO4	O3-S-O2	-2.17	97.97	109.31
7	A	708	DTP	C2-N1-C6	2.17	122.46	118.75
7	A	708	DTP	N6-C6-N1	2.15	123.03	118.57
7	G	701	DTP	O2G-PG-O3B	2.15	111.83	104.64
5	I	706	GTP	O2B-PB-O1B	2.15	122.85	112.24
7	O	701	DTP	C5-C6-N6	-2.14	117.09	120.35
5	O	707	GTP	O2B-PB-O1B	2.14	122.84	112.24
7	H	701	DTP	O5'-PA-O1A	-2.12	100.78	109.07
7	E	706	DTP	C2'-C3'-C4'	2.12	107.17	102.76
7	G	701	DTP	C4-C5-N7	-2.11	107.19	109.40
4	M	705	OKX	O2A-PA-O5'	2.11	112.45	106.75
5	H	706	GTP	PB-O3B-PG	-2.10	125.61	132.83
7	B	708	DTP	O3G-PG-O1G	-2.10	102.47	110.68
7	B	708	DTP	O2B-PB-O1B	2.10	122.60	112.24
5	D	707	GTP	N2-C2-N3	-2.09	115.66	119.74
7	F	706	DTP	PB-O3B-PG	-2.09	125.65	132.83
5	E	705	GTP	O3G-PG-O2G	2.08	115.59	107.64
7	I	708	DTP	C5-C6-N6	-2.08	117.19	120.35
5	O	707	GTP	O3G-PG-O3B	-2.08	97.67	104.64
4	B	705	OKX	PB-O3B-PG	-2.07	125.32	132.62
7	O	701	DTP	C4-C5-N7	-2.06	107.25	109.40
5	O	706	GTP	N2-C2-N1	2.06	121.10	116.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	708	DTP	O3G-PG-O2G	2.05	115.47	107.64
5	O	707	GTP	O3G-PG-O2G	2.05	115.47	107.64
7	C	701	DTP	C4'-O4'-C1'	2.04	114.39	109.45
5	K	707	GTP	C8-N7-C5	2.04	106.88	102.99
4	E	704	0KX	C1'-N1-C2	2.04	121.32	117.74
7	L	701	DTP	O5'-PA-O1A	-2.04	101.11	109.07
5	K	707	GTP	O6-C6-C5	-2.04	120.40	124.37
7	O	701	DTP	O2A-PA-O5'	2.03	117.19	107.75
7	C	701	DTP	O4'-C1'-C2'	-2.03	102.41	106.25
4	O	705	0KX	O3B-PG-O2G	-2.03	99.93	111.19
5	L	707	GTP	C2'-C3'-C4'	-2.03	98.70	102.64
7	M	708	DTP	N6-C6-N1	2.03	122.78	118.57
7	F	706	DTP	C2'-C3'-C4'	2.02	106.98	102.76
4	B	705	0KX	O4'-C1'-N1	-2.02	104.24	107.86
4	I	705	0KX	O3B-PB-N3A	2.02	112.20	106.59
5	I	706	GTP	PB-O3B-PG	-2.02	125.90	132.83
7	I	708	DTP	C2-N1-C6	2.00	122.18	118.75

There are no chirality outliers.

All (126) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	705	0KX	PG-O3B-PB-O1B
4	A	705	0KX	PG-O3B-PB-O2B
4	B	705	0KX	PB-O3B-PG-O1G
4	B	705	0KX	PG-O3B-PB-O1B
4	B	705	0KX	PG-O3B-PB-O2B
4	B	705	0KX	PA-N3A-PB-O2B
4	B	705	0KX	PB-N3A-PA-O1A
4	C	706	0KX	PG-O3B-PB-O1B
4	C	706	0KX	PG-O3B-PB-O2B
4	D	706	0KX	PG-O3B-PB-O1B
4	D	706	0KX	PG-O3B-PB-O2B
4	D	706	0KX	PA-N3A-PB-O2B
4	E	704	0KX	PG-O3B-PB-O1B
4	E	704	0KX	PG-O3B-PB-O2B
4	E	704	0KX	PA-N3A-PB-O2B
4	F	704	0KX	PG-O3B-PB-O1B
4	F	704	0KX	PG-O3B-PB-O2B
4	G	706	0KX	PB-O3B-PG-O1G
4	G	706	0KX	PG-O3B-PB-O1B
4	G	706	0KX	PG-O3B-PB-O2B

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Mol	Chain	Res	Type	Atoms
4	G	706	0KX	PA-N3A-PB-O2B
4	G	706	0KX	C5'-O5'-PA-O1A
4	G	706	0KX	C5'-O5'-PA-N3A
4	H	705	0KX	PG-O3B-PB-O1B
4	H	705	0KX	PG-O3B-PB-O2B
4	I	705	0KX	PA-N3A-PB-O3B
4	I	705	0KX	PB-N3A-PA-O1A
4	J	704	0KX	PA-N3A-PB-O2B
4	J	704	0KX	PB-N3A-PA-O1A
4	K	706	0KX	PB-N3A-PA-O1A
4	L	706	0KX	PG-O3B-PB-O1B
4	L	706	0KX	PG-O3B-PB-O2B
4	L	706	0KX	PA-N3A-PB-O2B
4	L	706	0KX	PB-N3A-PA-O1A
4	N	704	0KX	PA-N3A-PB-O2B
4	O	705	0KX	PG-O3B-PB-O1B
4	O	705	0KX	PG-O3B-PB-O2B
4	P	706	0KX	PG-O3B-PB-O1B
4	P	706	0KX	PG-O3B-PB-O2B
4	P	706	0KX	PA-N3A-PB-O2B
4	P	706	0KX	PB-N3A-PA-O1A
7	E	706	DTP	PB-O3B-PG-O2G
7	H	701	DTP	PB-O3B-PG-O2G
4	F	704	0KX	C3'-C4'-C5'-O5'
5	O	706	GTP	PB-O3A-PA-O1A
5	O	707	GTP	PB-O3A-PA-O1A
7	L	701	DTP	PB-O3B-PG-O1G
7	O	701	DTP	PB-O3B-PG-O1G
4	P	706	0KX	PB-O3B-PG-O1G
7	N	706	DTP	PB-O3B-PG-O3G
4	F	704	0KX	O4'-C4'-C5'-O5'
7	C	701	DTP	O4'-C4'-C5'-O5'
5	I	706	GTP	PB-O3A-PA-O2A
5	M	706	GTP	PG-O3B-PB-O1B
5	N	705	GTP	PG-O3B-PB-O1B
7	A	708	DTP	PA-O3A-PB-O1B
7	G	701	DTP	PB-O3A-PA-O2A
7	H	701	DTP	PB-O3A-PA-O2A
7	J	707	DTP	PB-O3A-PA-O2A
4	D	706	0KX	PB-N3A-PA-O5'
4	H	705	0KX	PB-N3A-PA-O5'
4	E	704	0KX	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	N	704	0KX	C4'-C5'-O5'-PA
5	I	706	GTP	C4'-C5'-O5'-PA
5	N	705	GTP	C4'-C5'-O5'-PA
4	I	705	0KX	C4'-C5'-O5'-PA
5	B	706	GTP	PB-O3A-PA-O2A
5	N	705	GTP	PG-O3B-PB-O2B
5	O	706	GTP	PB-O3A-PA-O2A
5	O	707	GTP	PB-O3A-PA-O2A
7	D	701	DTP	PB-O3A-PA-O2A
7	I	708	DTP	PB-O3A-PA-O2A
7	M	708	DTP	PB-O3A-PA-O2A
7	O	701	DTP	PB-O3A-PA-O2A
5	C	707	GTP	C4'-C5'-O5'-PA
5	H	706	GTP	C4'-C5'-O5'-PA
4	F	704	0KX	C4'-C5'-O5'-PA
5	L	707	GTP	C4'-C5'-O5'-PA
5	B	706	GTP	PG-O3B-PB-O1B
5	C	707	GTP	PB-O3A-PA-O2A
5	D	707	GTP	C4'-C5'-O5'-PA
5	E	705	GTP	PG-O3B-PB-O1B
7	A	708	DTP	PA-O3A-PB-O2B
7	A	708	DTP	PB-O3A-PA-O1A
7	A	708	DTP	PB-O3A-PA-O2A
7	C	701	DTP	PB-O3A-PA-O2A
7	H	701	DTP	PG-O3B-PB-O1B
5	K	707	GTP	C4'-C5'-O5'-PA
4	K	706	0KX	C4'-C5'-O5'-PA
4	P	706	0KX	PB-O3B-PG-O2G
5	C	707	GTP	PB-O3B-PG-O1G
7	I	708	DTP	PB-O3B-PG-O1G
5	C	707	GTP	PB-O3B-PG-O3G
5	O	706	GTP	PB-O3B-PG-O3G
7	B	708	DTP	PB-O3B-PG-O2G
7	B	708	DTP	PB-O3B-PG-O3G
7	E	706	DTP	PB-O3B-PG-O3G
7	H	701	DTP	PB-O3B-PG-O3G
7	I	708	DTP	PB-O3B-PG-O2G
7	I	708	DTP	PB-O3B-PG-O3G
7	J	707	DTP	PB-O3B-PG-O2G
7	J	707	DTP	PB-O3B-PG-O3G
7	L	701	DTP	PB-O3B-PG-O2G
7	L	701	DTP	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
7	O	701	DTP	PB-O3B-PG-O2G
7	O	701	DTP	PB-O3B-PG-O3G
7	P	701	DTP	PB-O3B-PG-O3G
5	A	706	GTP	PG-O3B-PB-O2B
5	B	706	GTP	PG-O3B-PB-O2B
5	D	707	GTP	PG-O3B-PB-O2B
5	G	707	GTP	PB-O3A-PA-O1A
5	K	707	GTP	PB-O3A-PA-O1A
5	L	707	GTP	PB-O3A-PA-O1A
7	D	701	DTP	PG-O3B-PB-O1B
7	D	701	DTP	PB-O3A-PA-O1A
7	H	701	DTP	PB-O3A-PA-O1A
7	I	708	DTP	PB-O3A-PA-O1A
7	J	707	DTP	PB-O3A-PA-O1A
7	M	708	DTP	PB-O3A-PA-O1A
7	N	706	DTP	PB-O3A-PA-O2A
7	O	701	DTP	PB-O3A-PA-O1A
5	B	706	GTP	C4'-C5'-O5'-PA
5	G	707	GTP	C4'-C5'-O5'-PA
7	C	701	DTP	C5'-O5'-PA-O1A
7	C	701	DTP	C3'-C4'-C5'-O5'
7	H	701	DTP	PB-O3B-PG-O1G

There are no ring outliers.

32 monomers are involved in 42 short contacts:

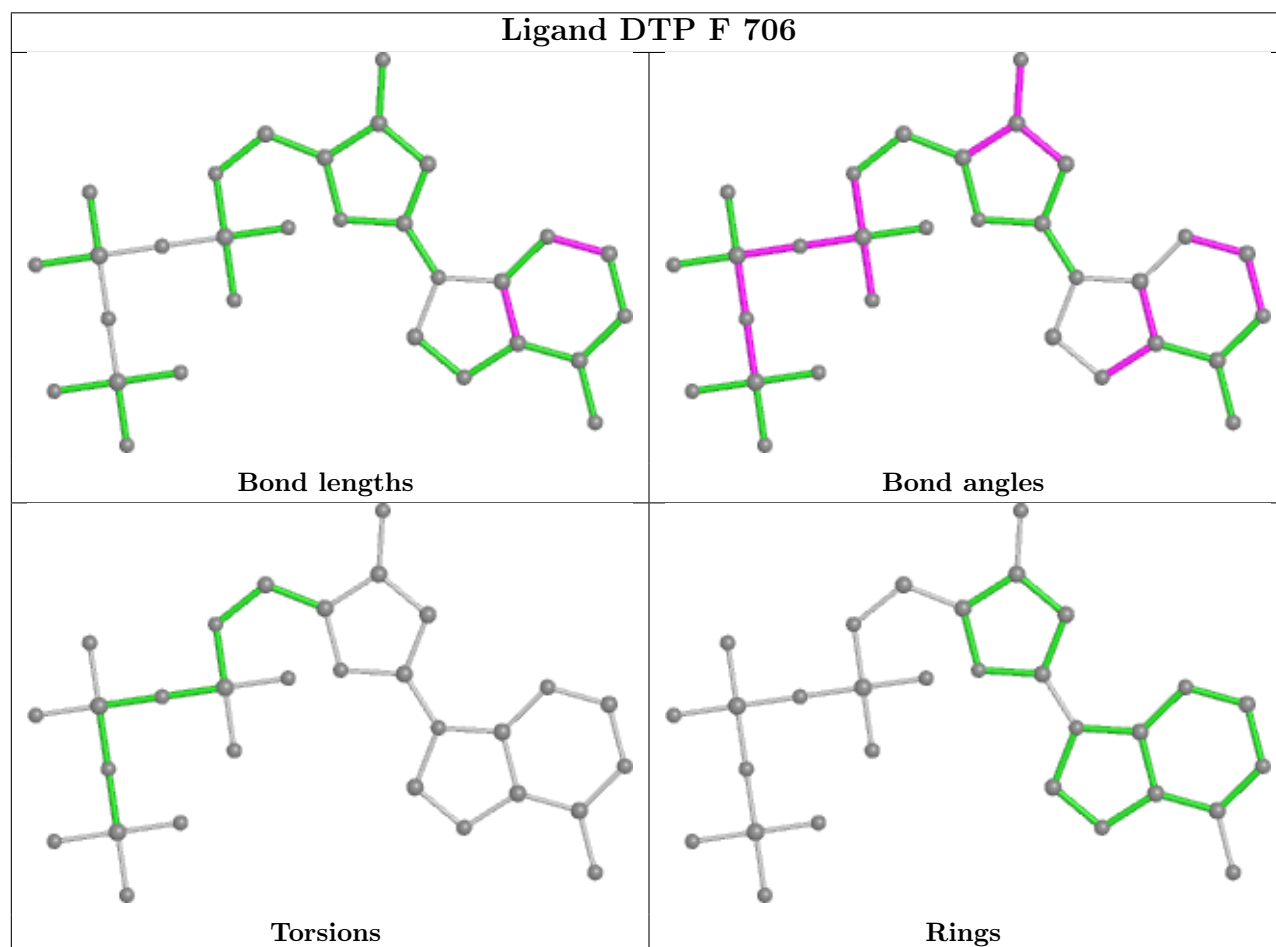
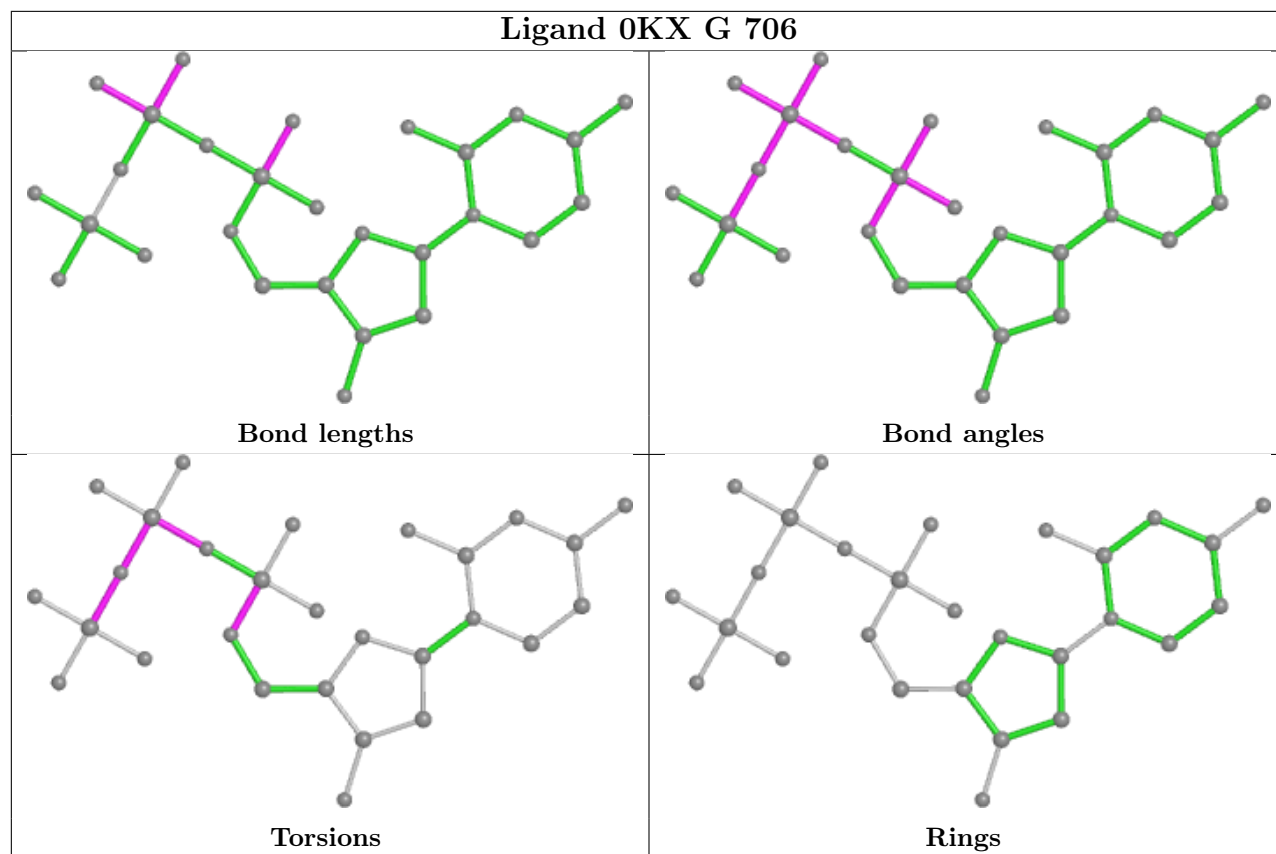
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	706	DTP	2	0
5	O	707	GTP	1	0
6	A	707	SO4	1	0
6	H	707	SO4	1	0
7	B	708	DTP	2	0
7	C	701	DTP	1	0
4	B	705	OKX	1	0
5	E	705	GTP	1	0
4	C	706	OKX	2	0
7	O	701	DTP	1	0
6	D	708	SO4	1	0
7	E	706	DTP	3	0
7	K	701	DTP	2	0
7	L	701	DTP	1	0
7	D	701	DTP	1	0

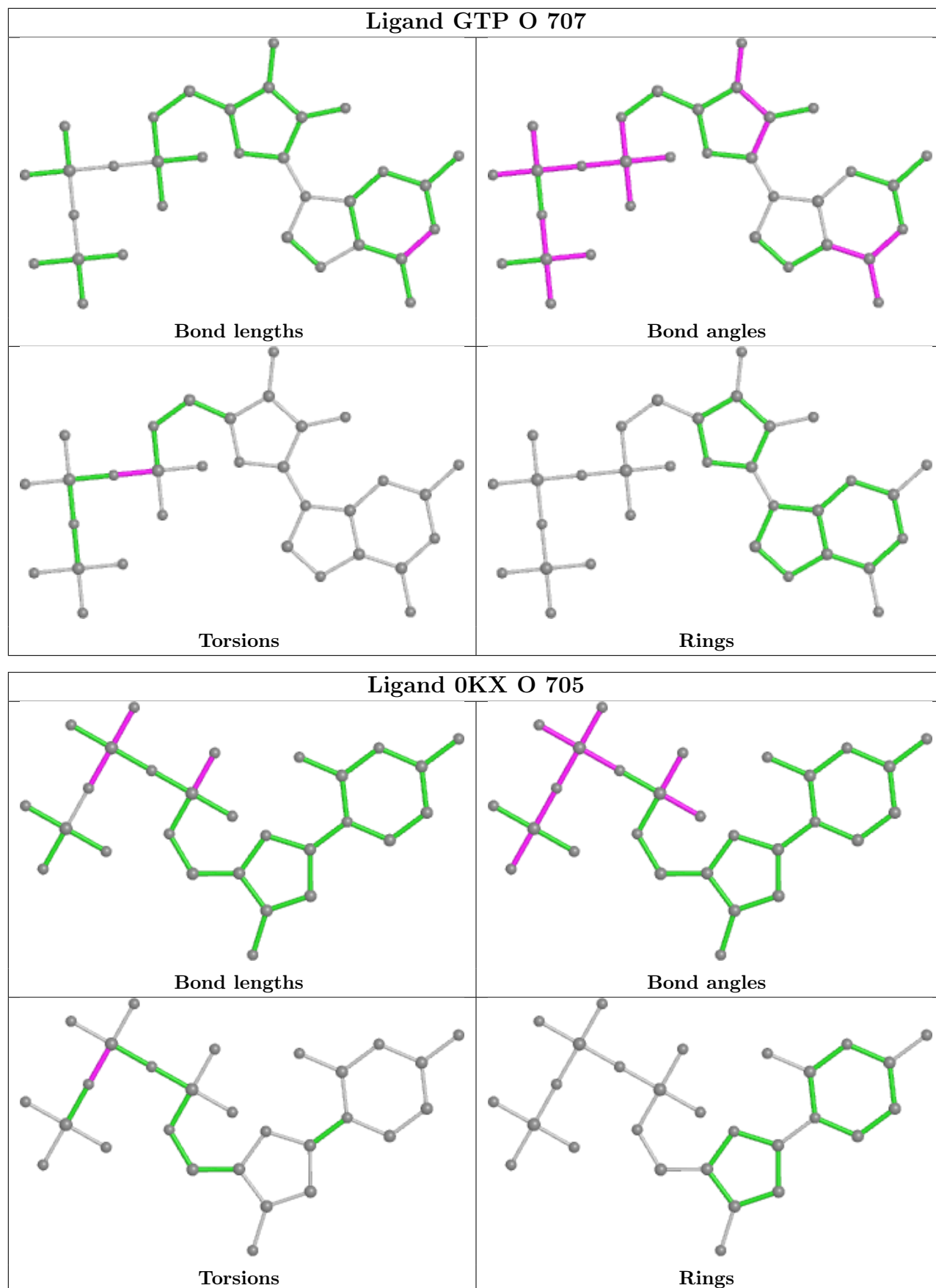
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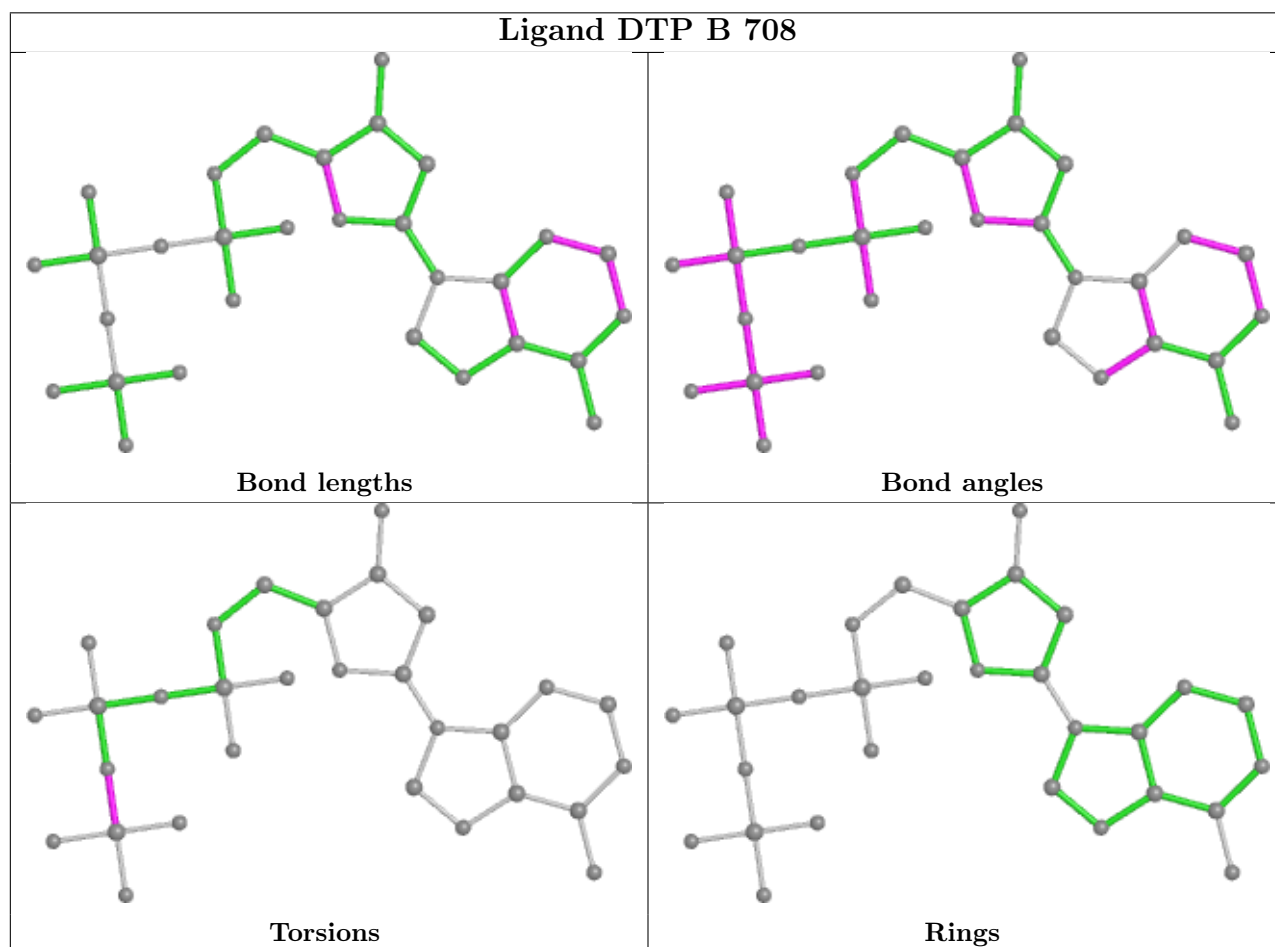
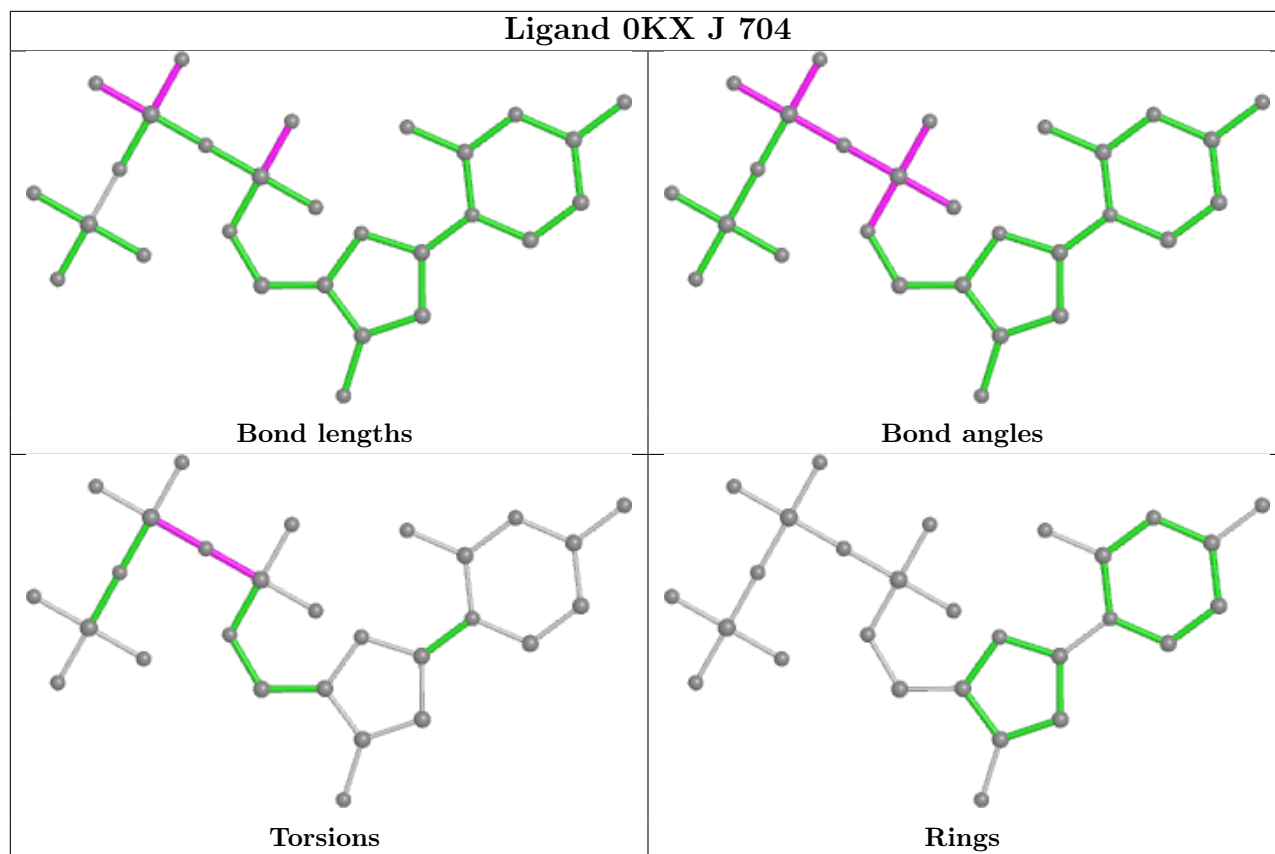
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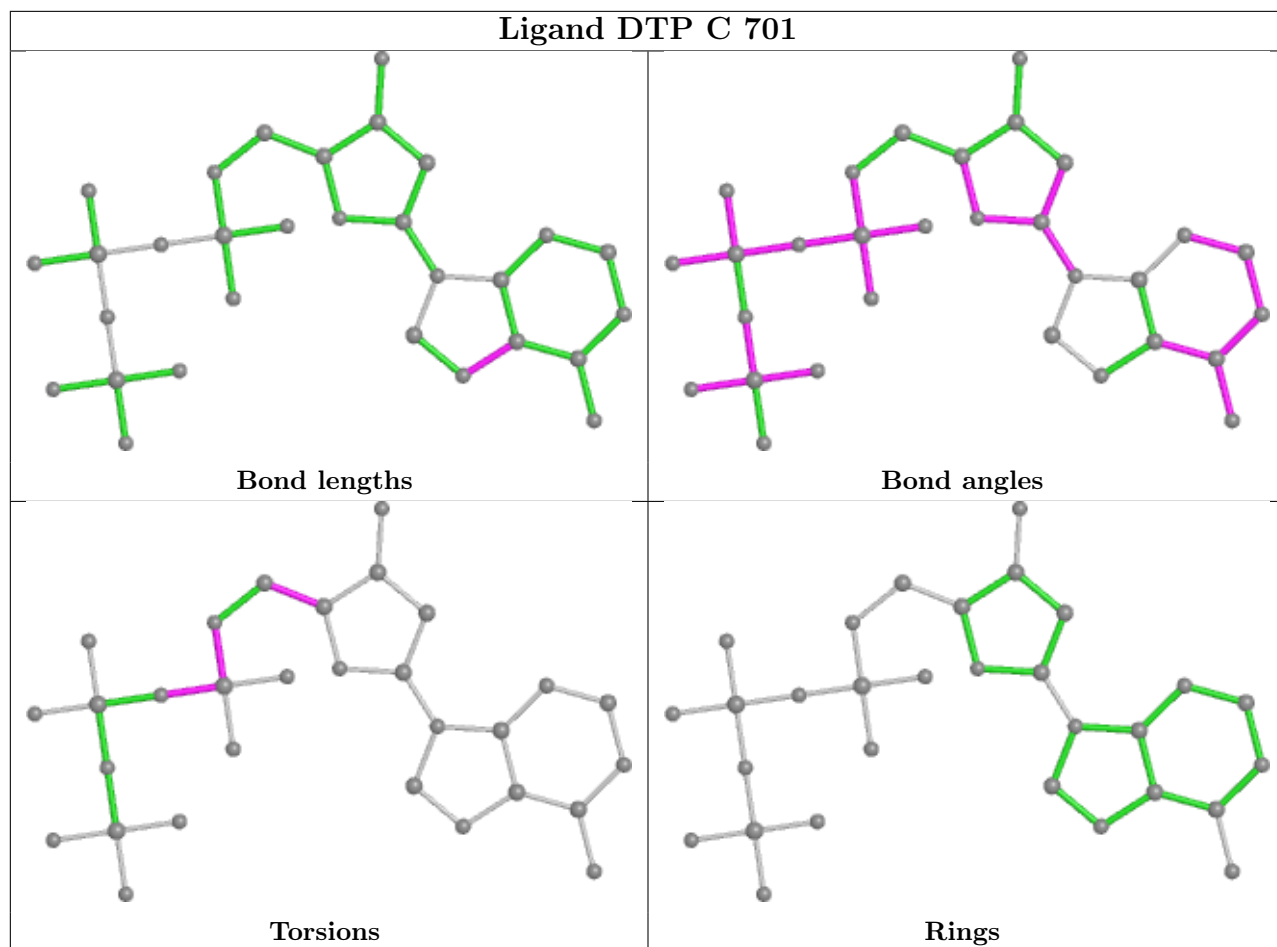
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	M	708	DTP	4	0
4	D	706	OKX	1	0
7	G	701	DTP	2	0
4	L	706	OKX	2	0
5	J	705	GTP	1	0
7	J	707	DTP	1	0
4	E	704	OKX	1	0
5	O	706	GTP	1	0
7	P	701	DTP	2	0
4	N	704	OKX	2	0
7	N	706	DTP	1	0
5	D	707	GTP	1	0
5	N	705	GTP	1	0
5	F	705	GTP	1	0
4	H	705	OKX	1	0
7	H	701	DTP	2	0
5	G	707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

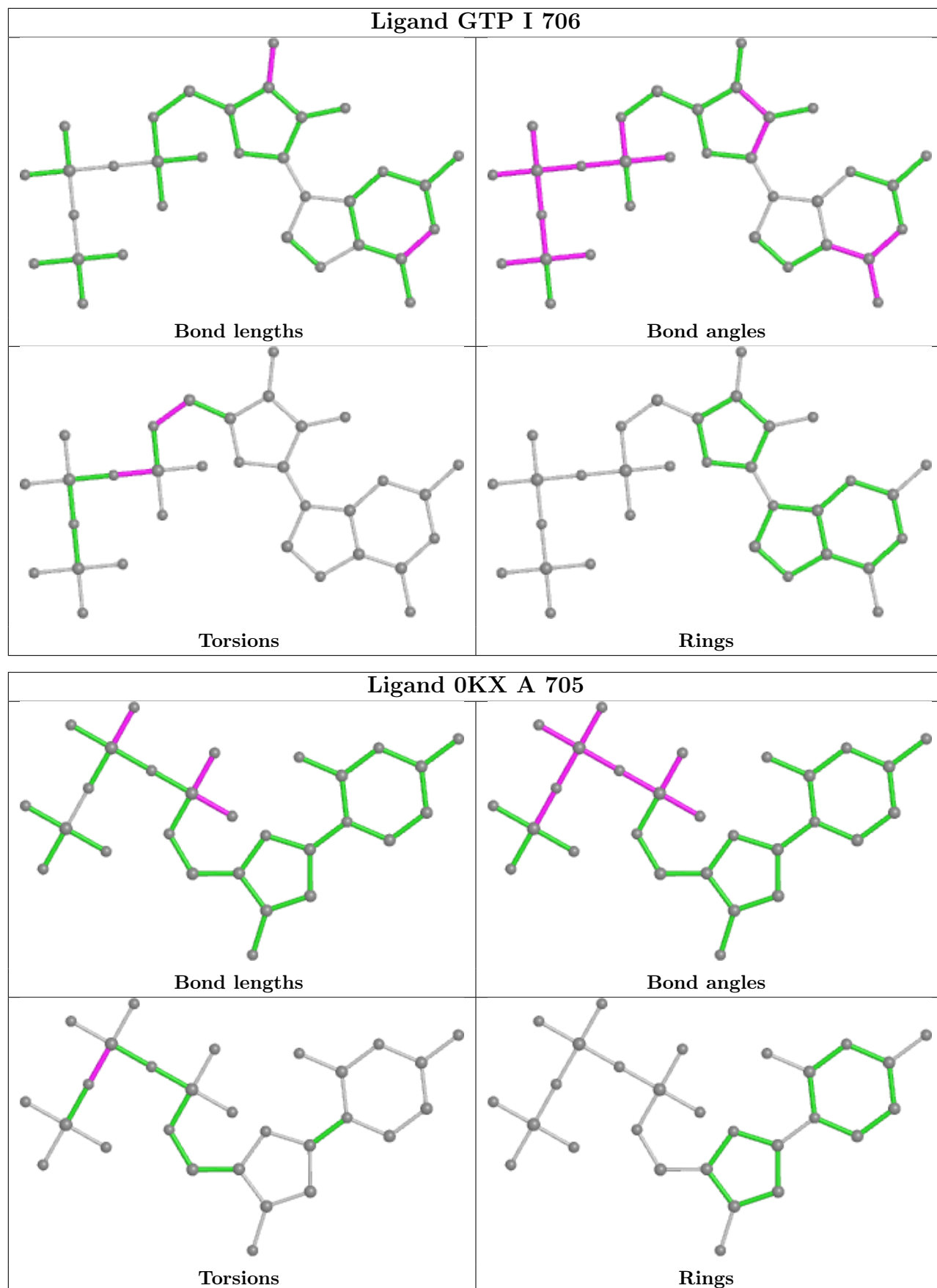
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

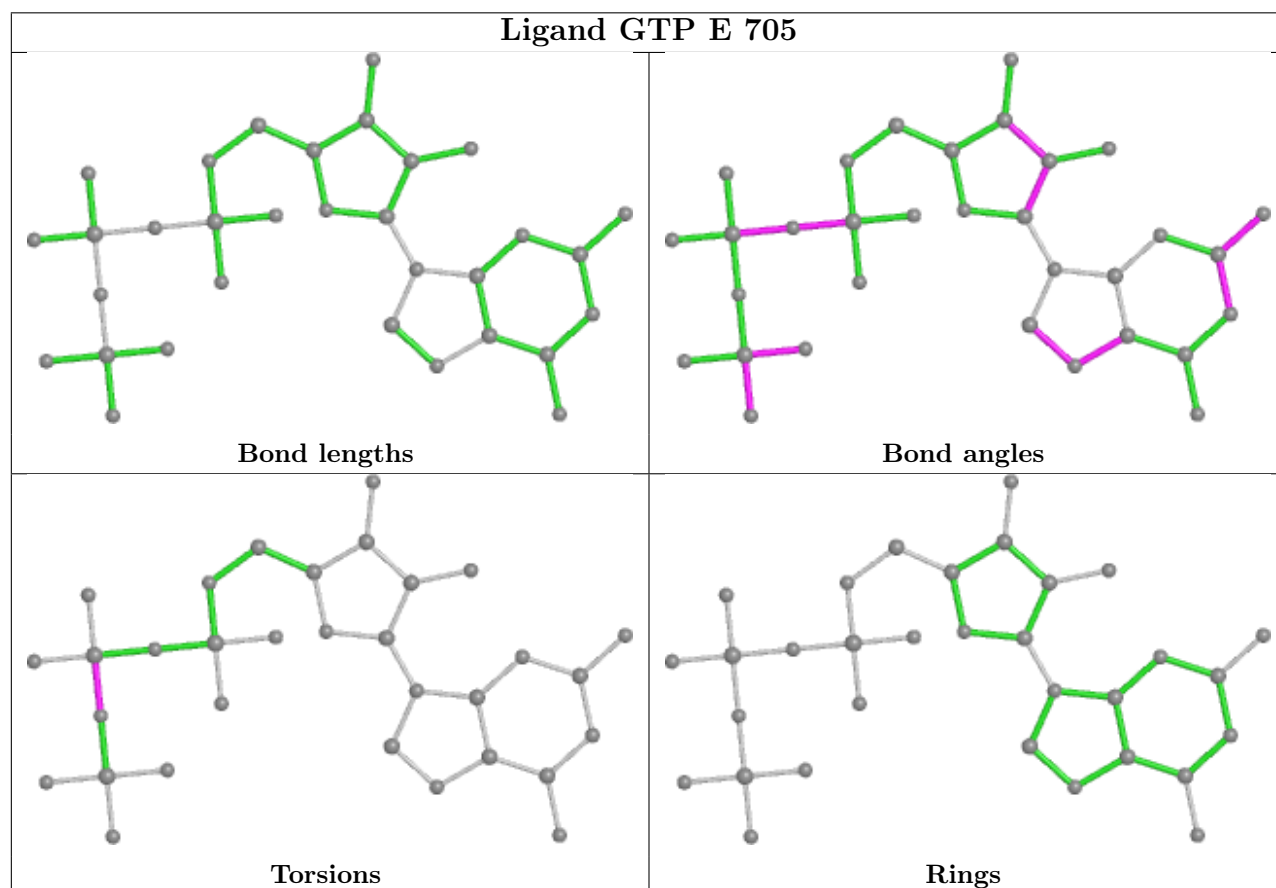
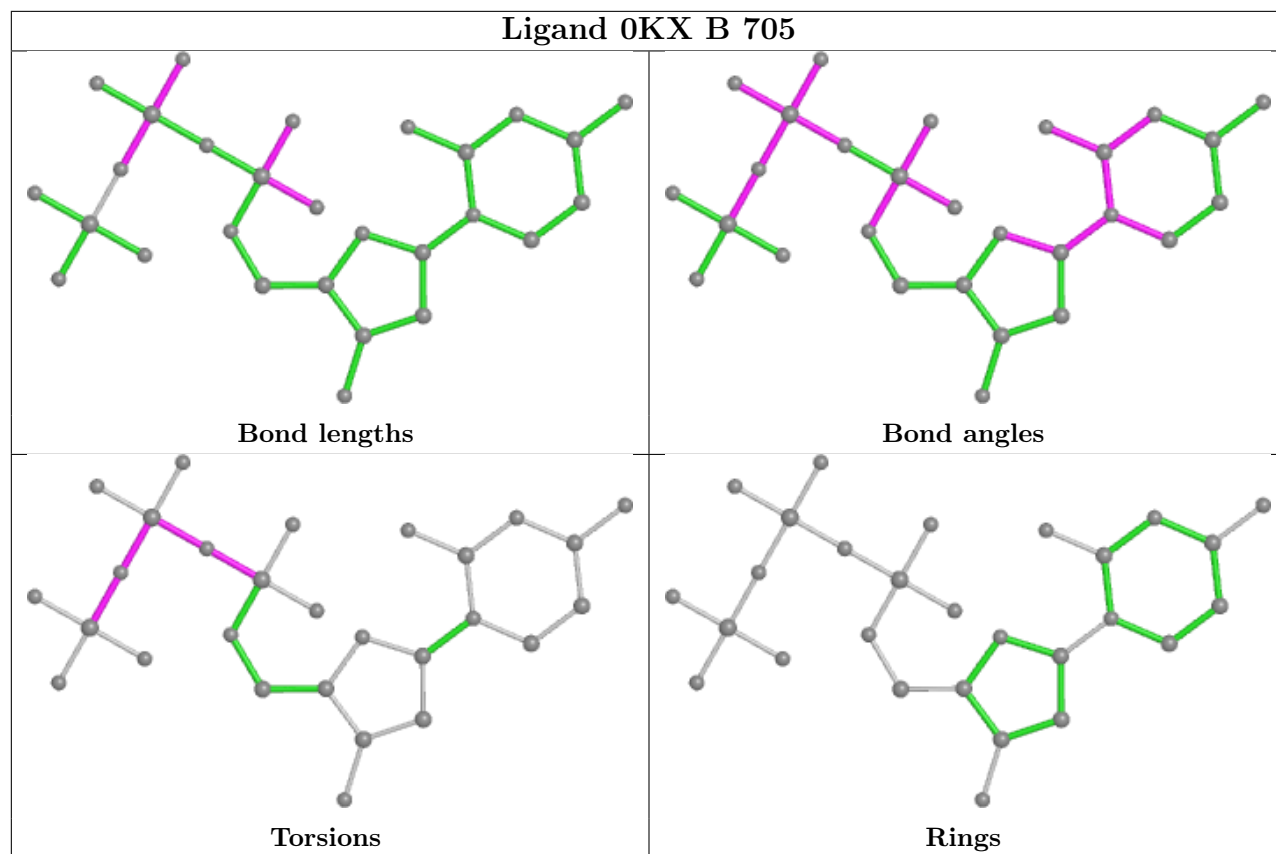


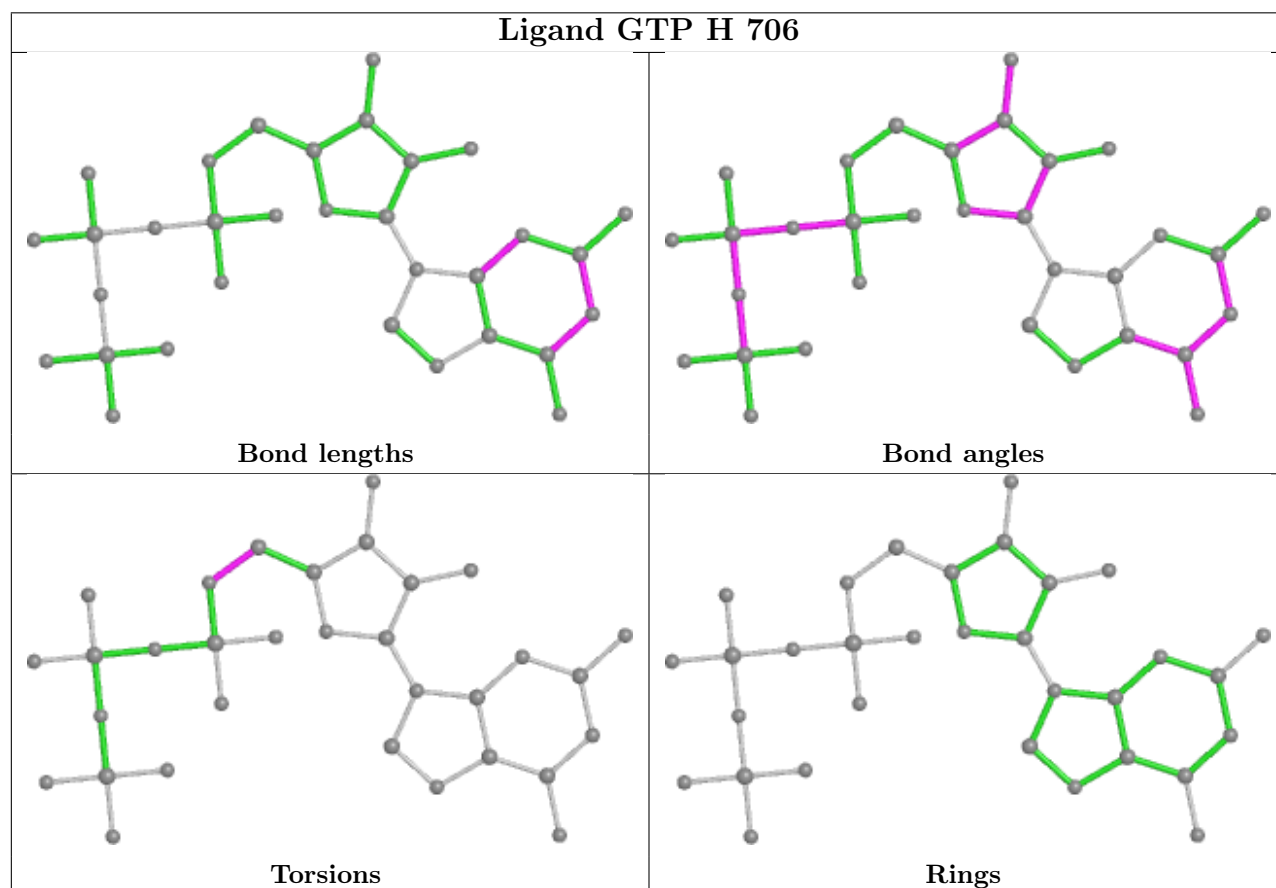
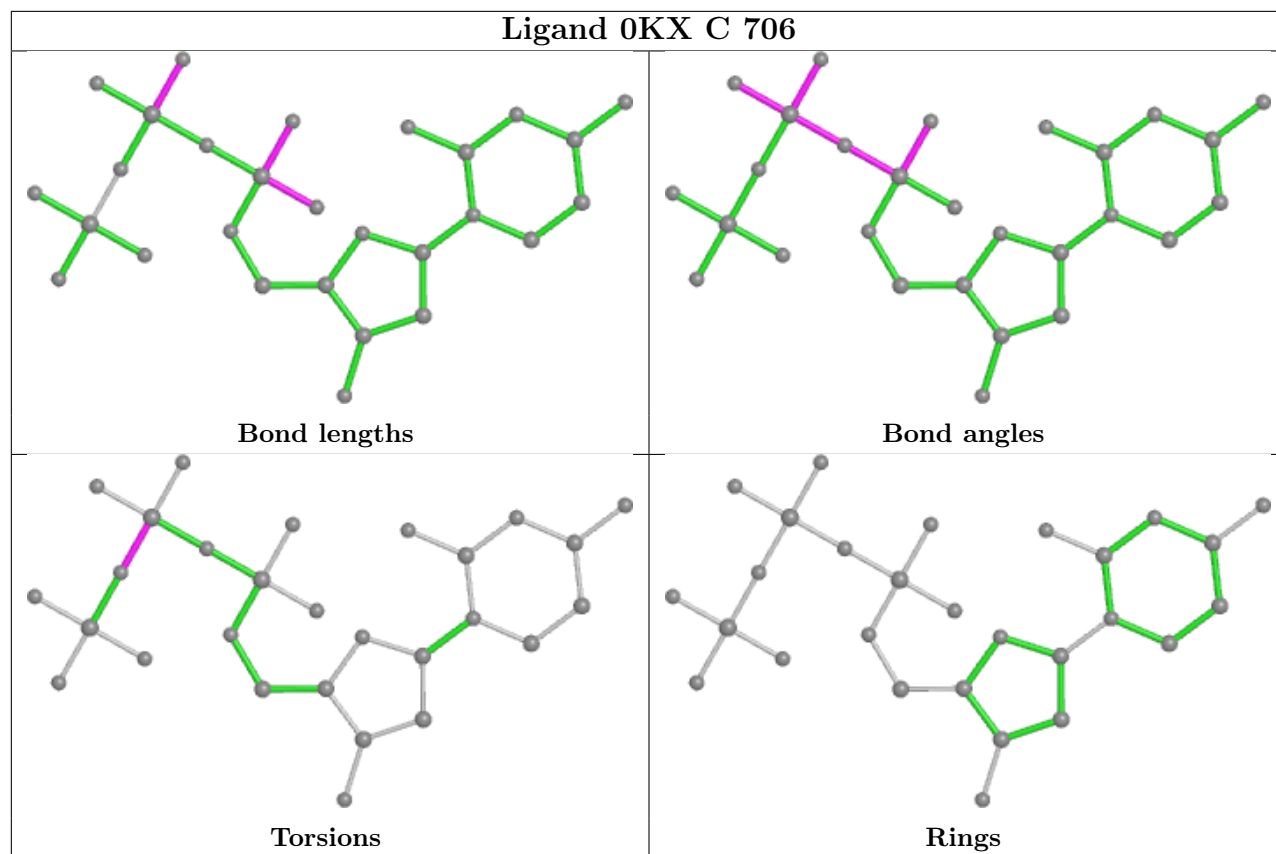


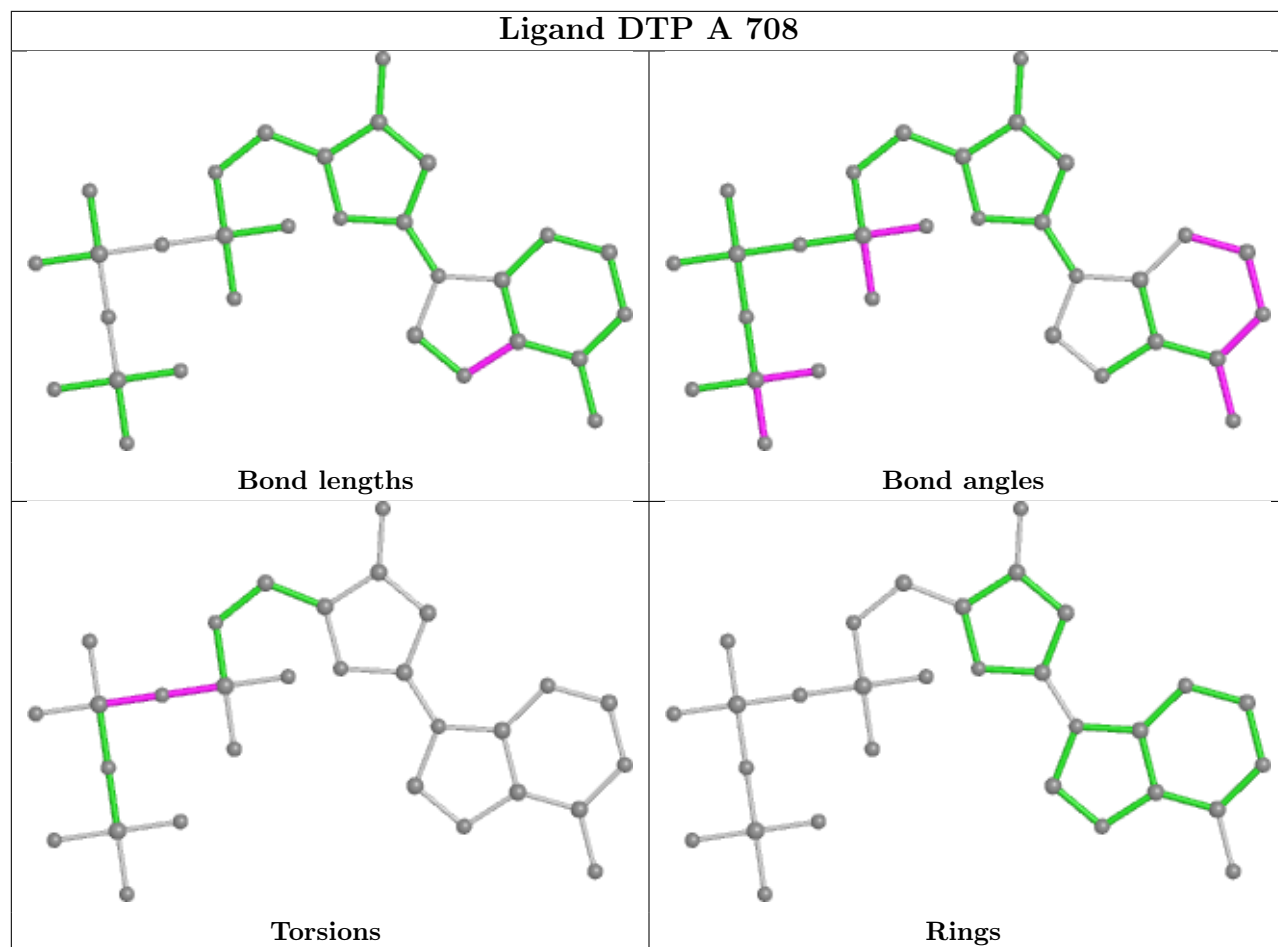


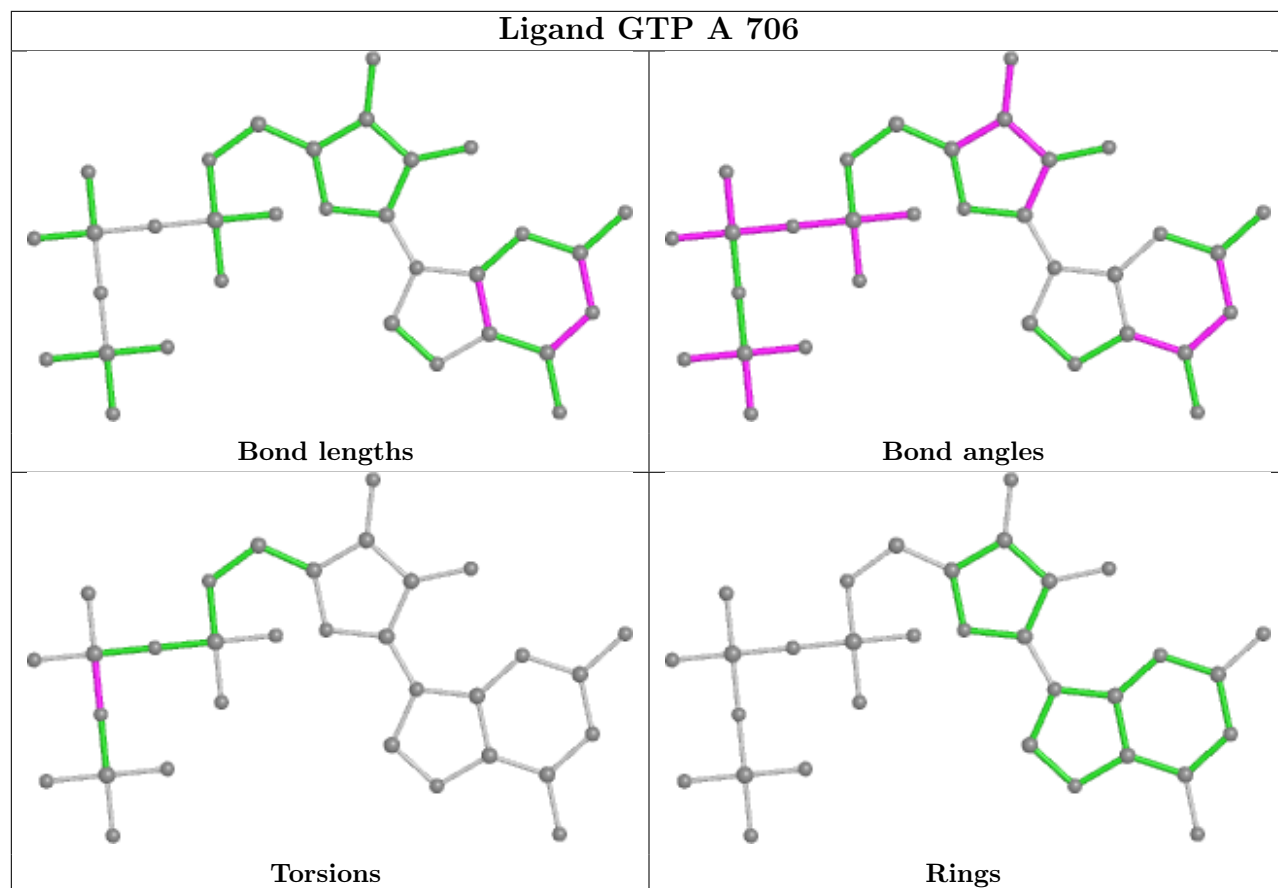


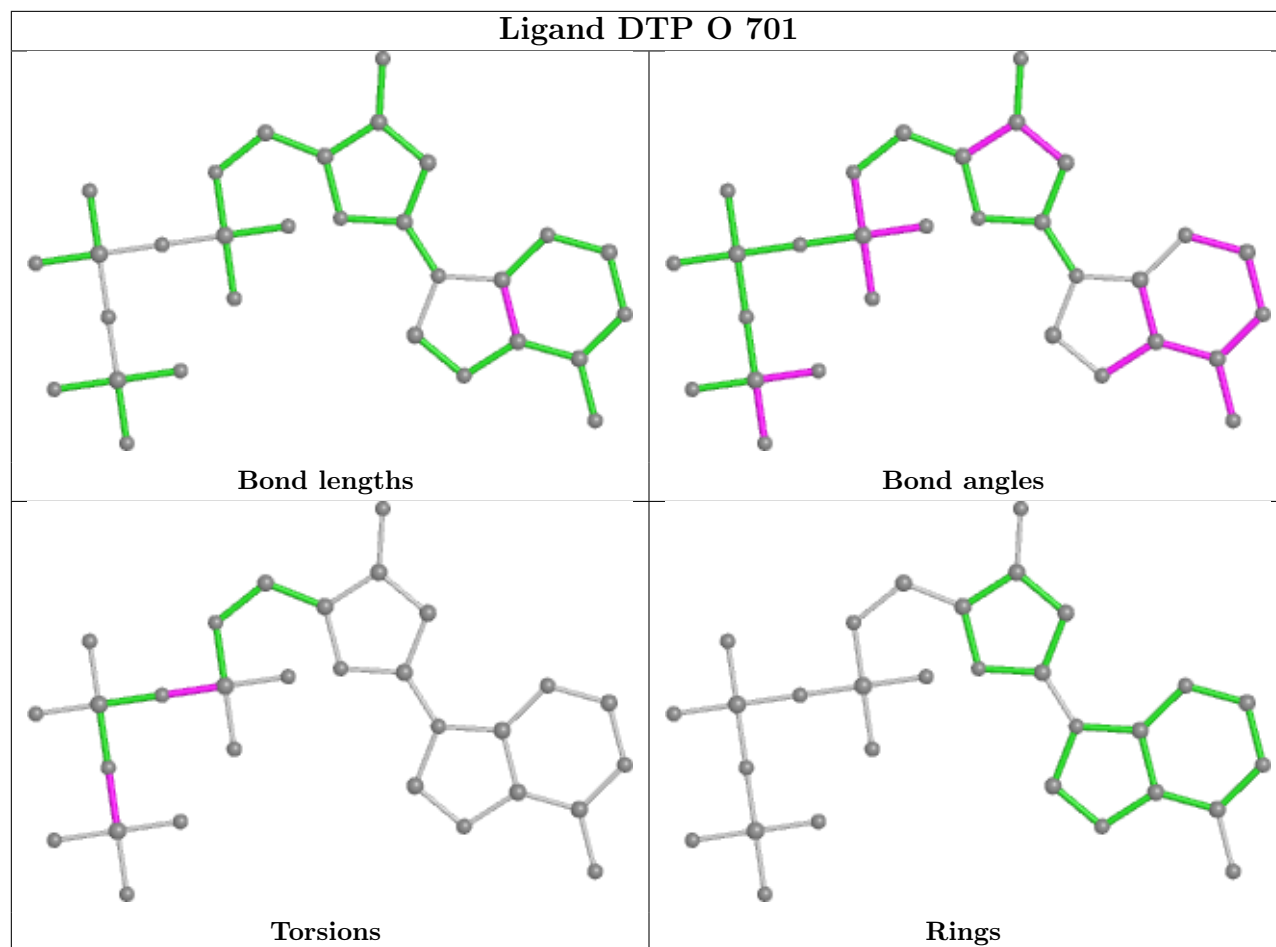


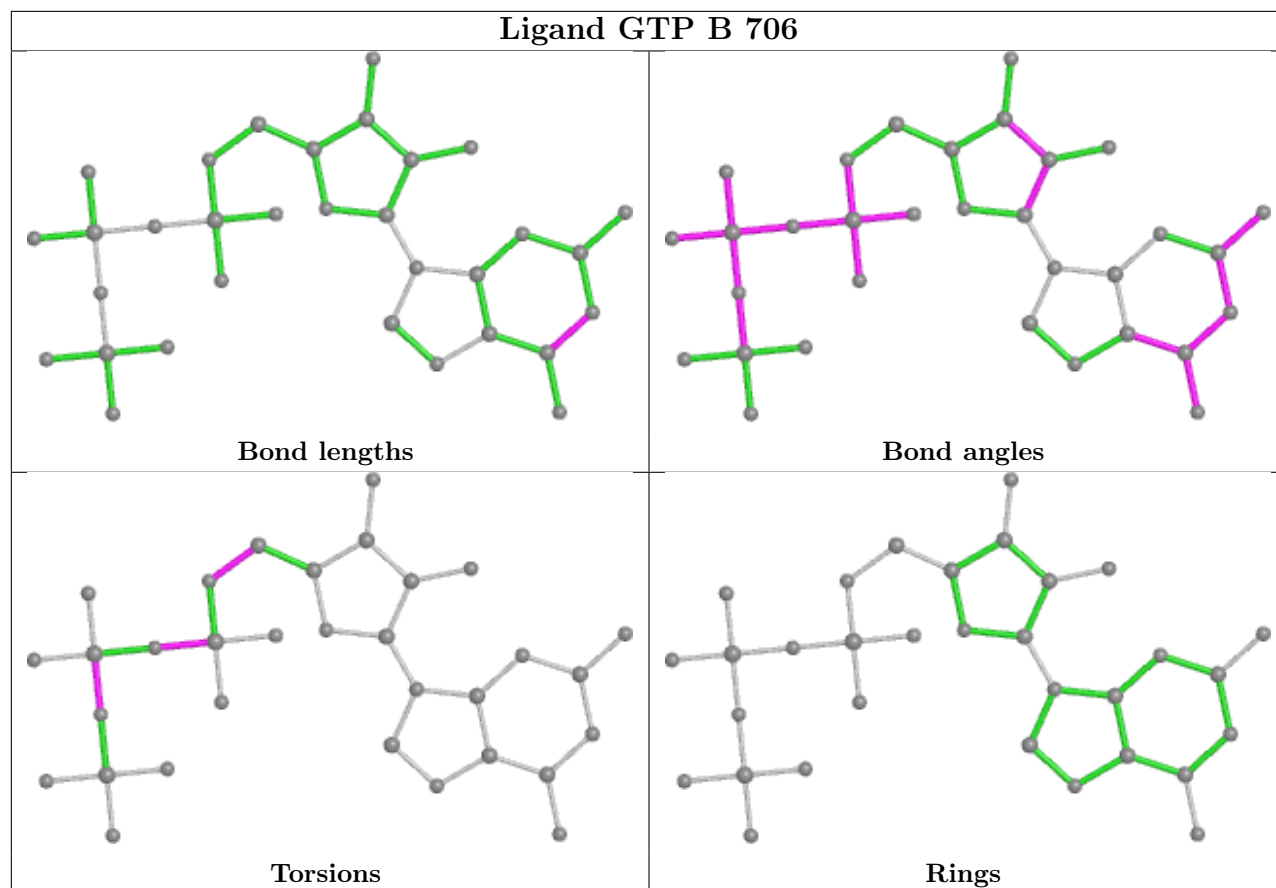


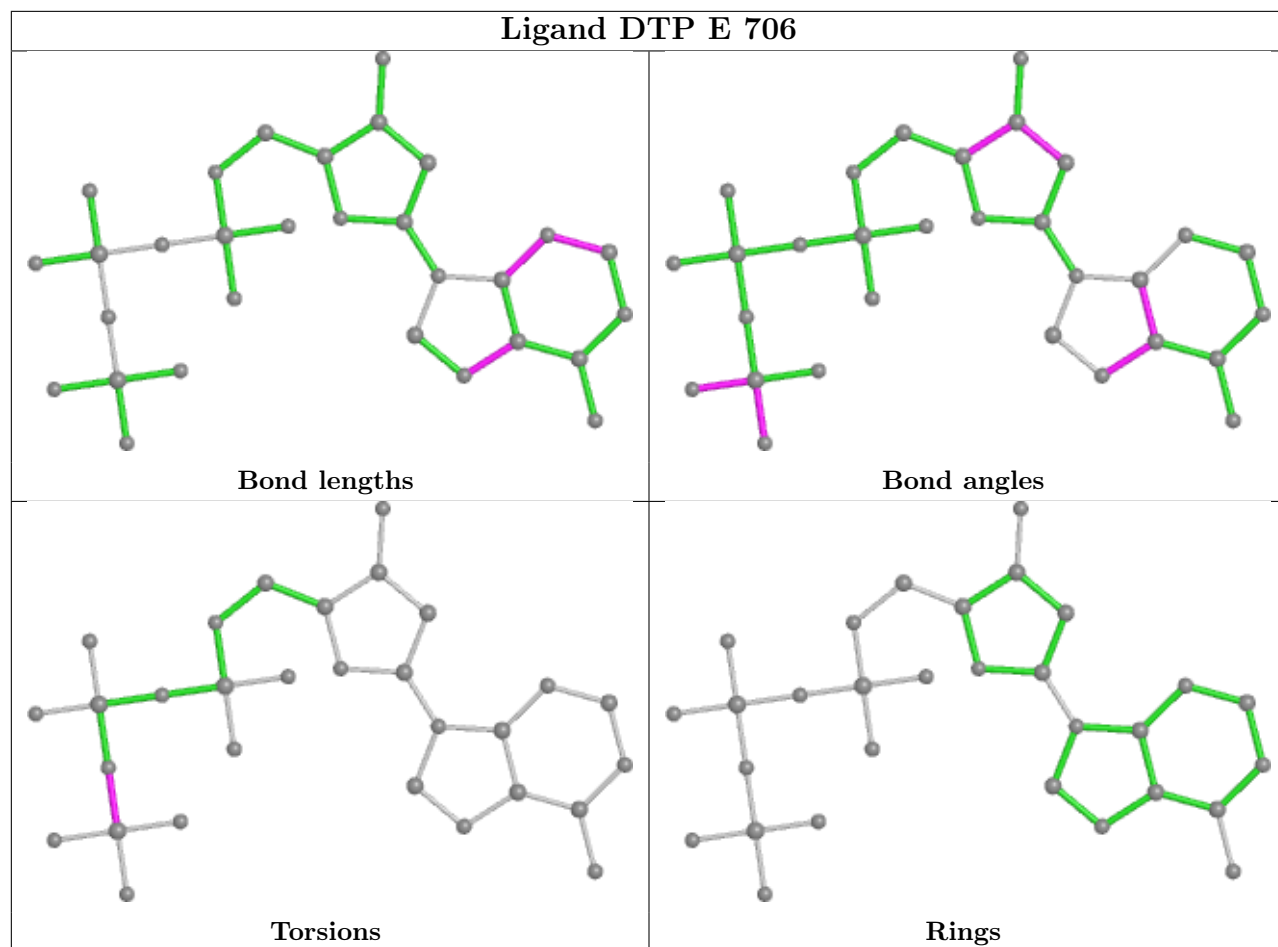


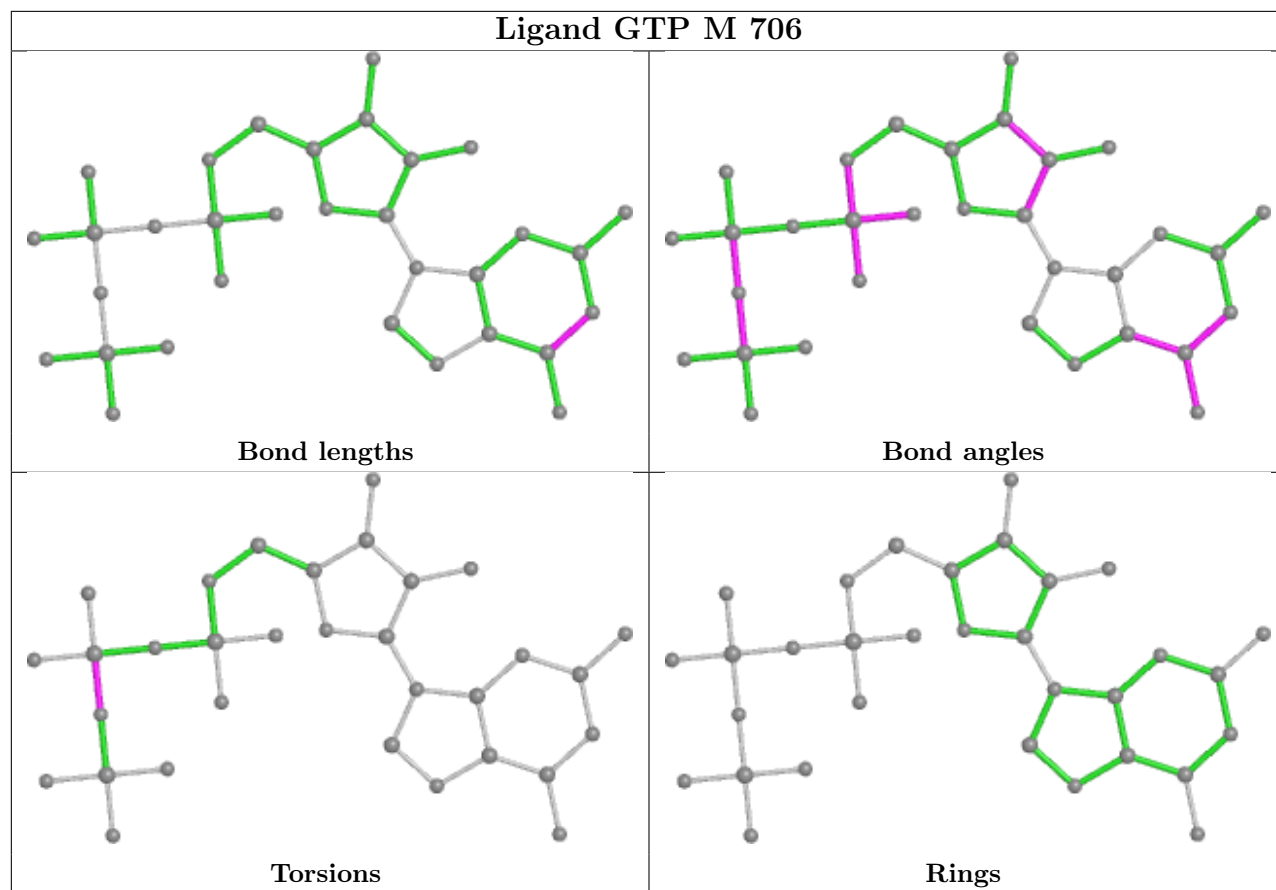


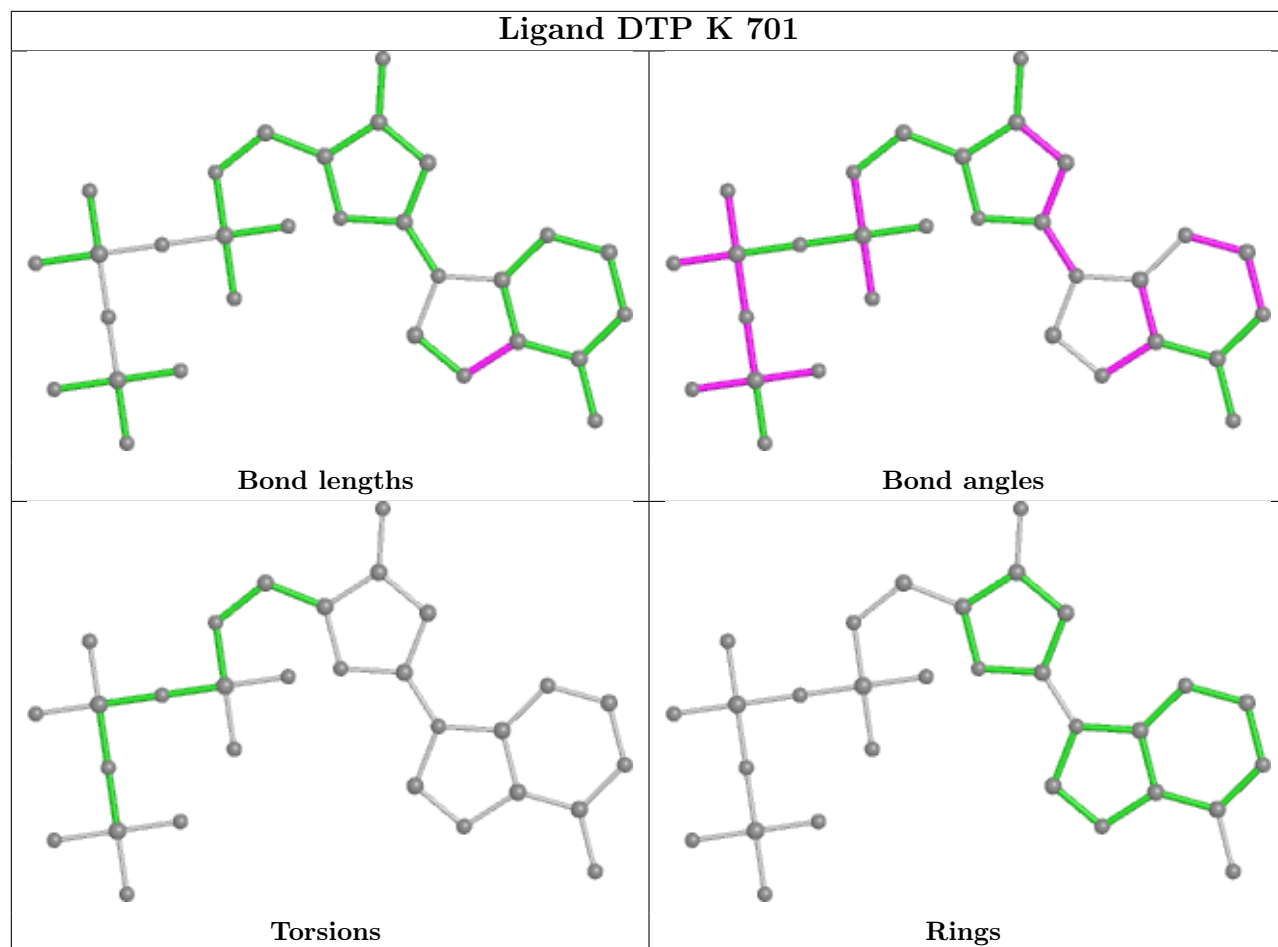


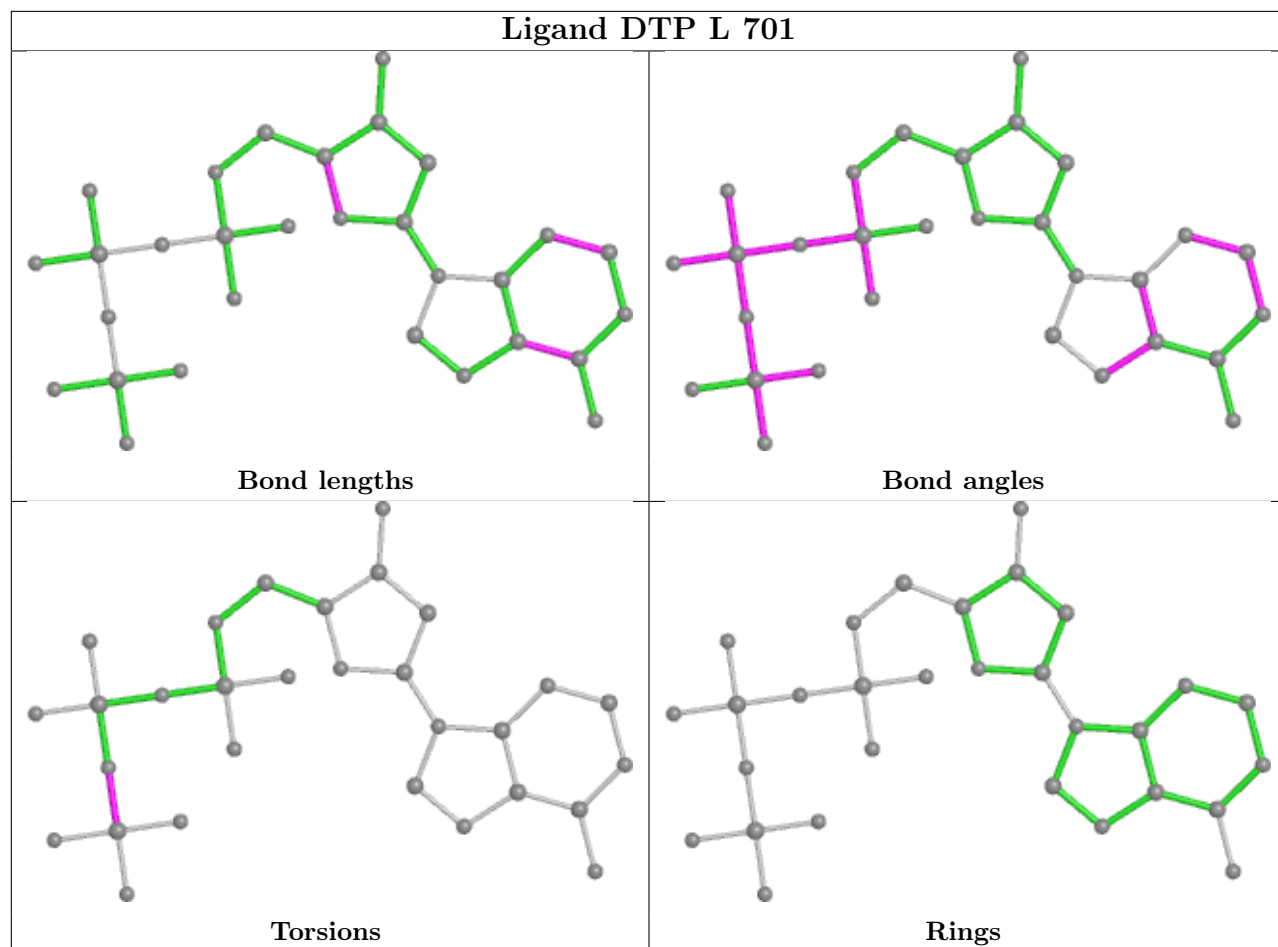


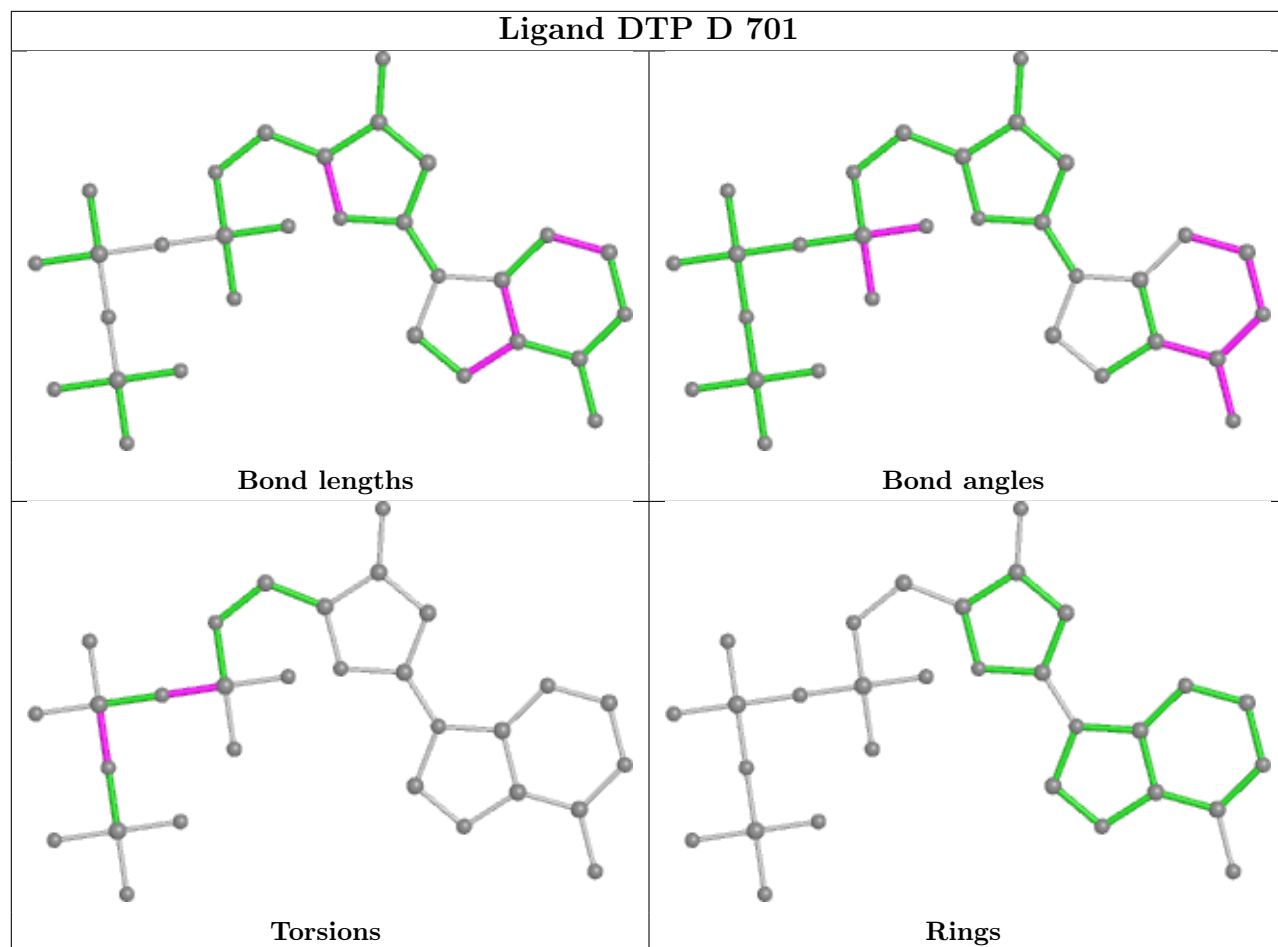


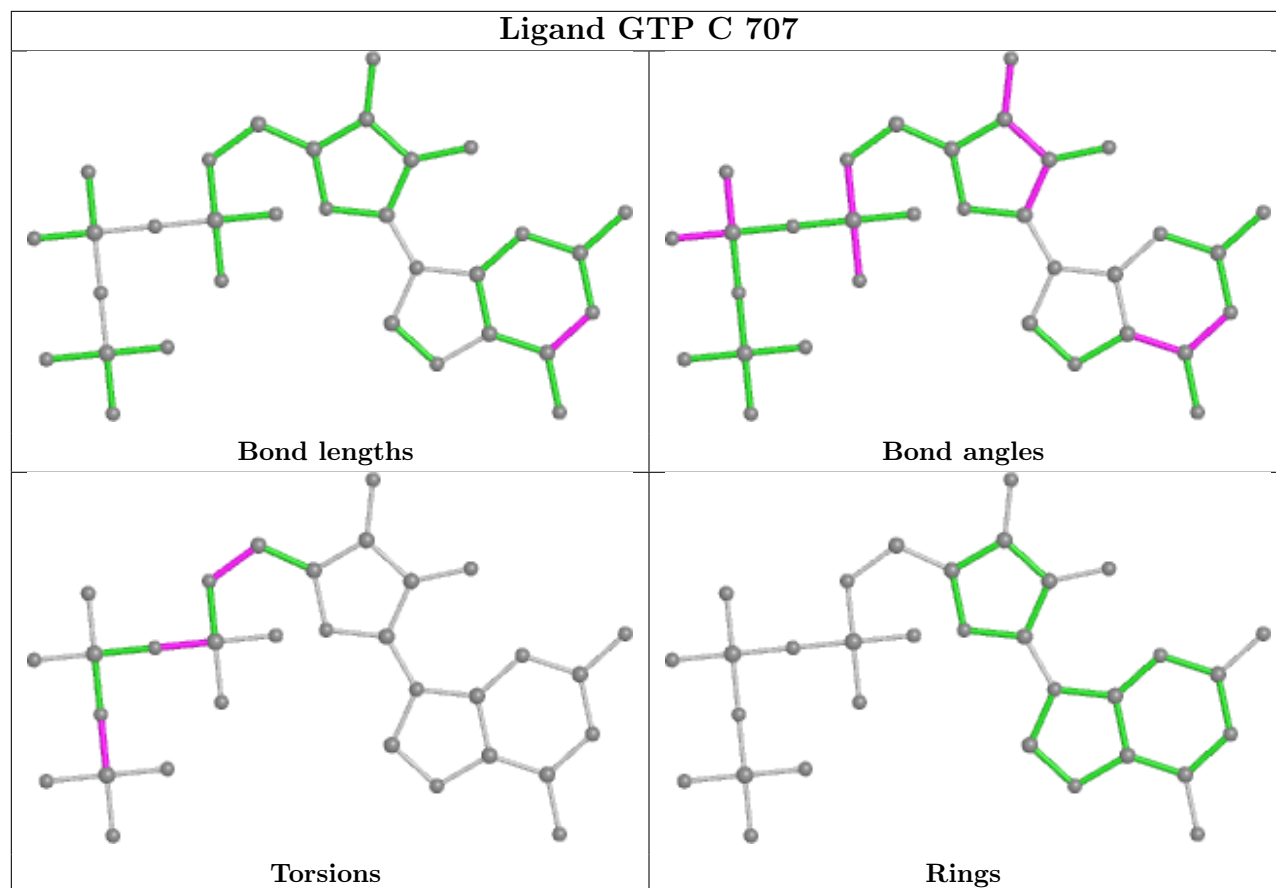


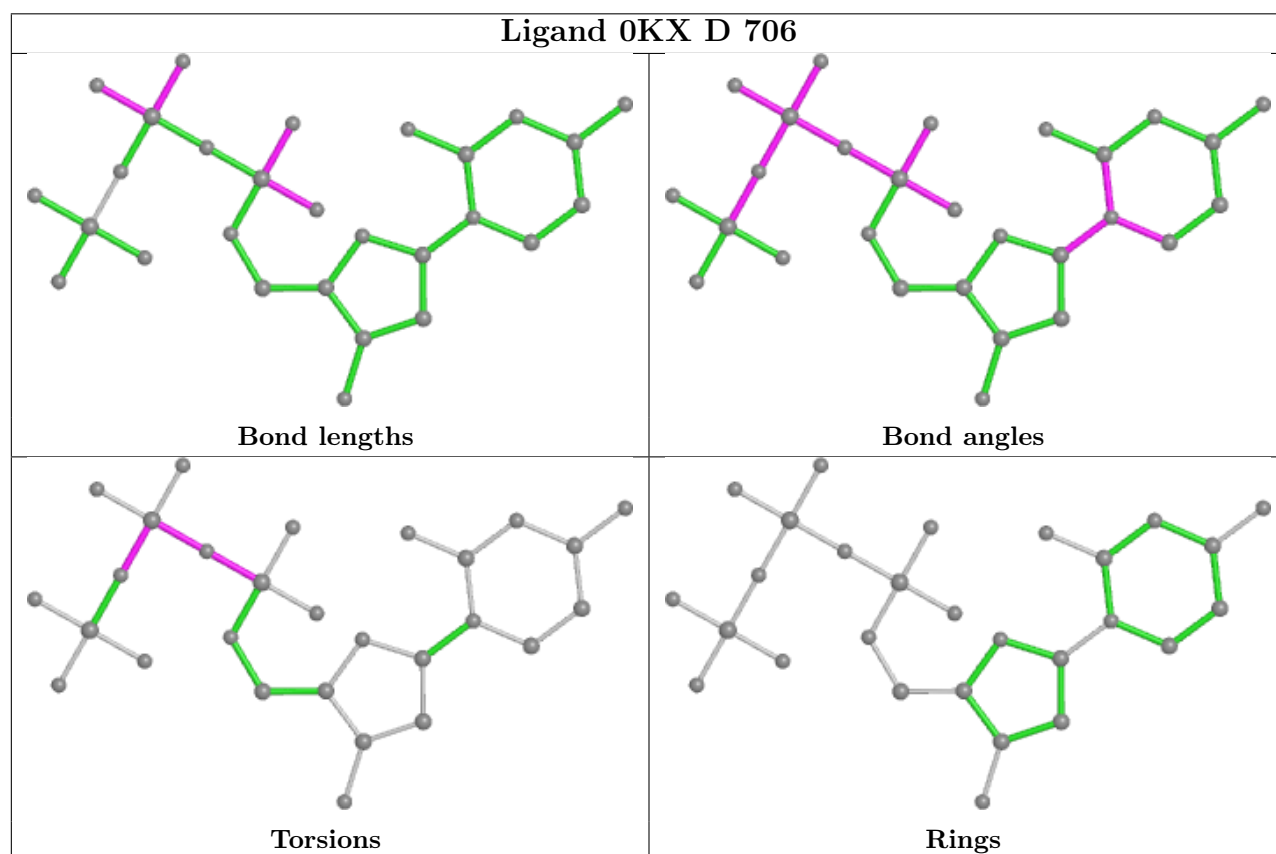
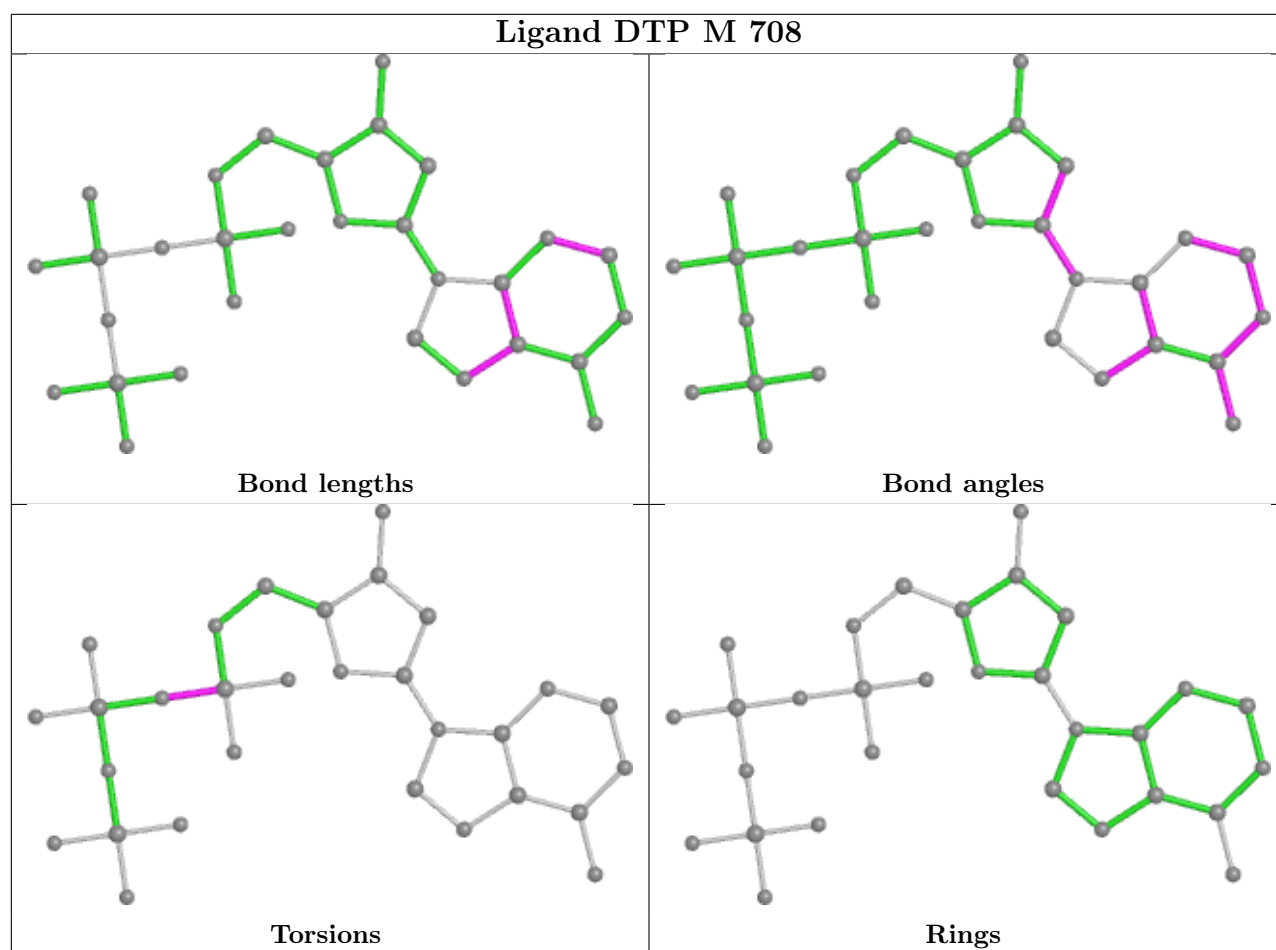


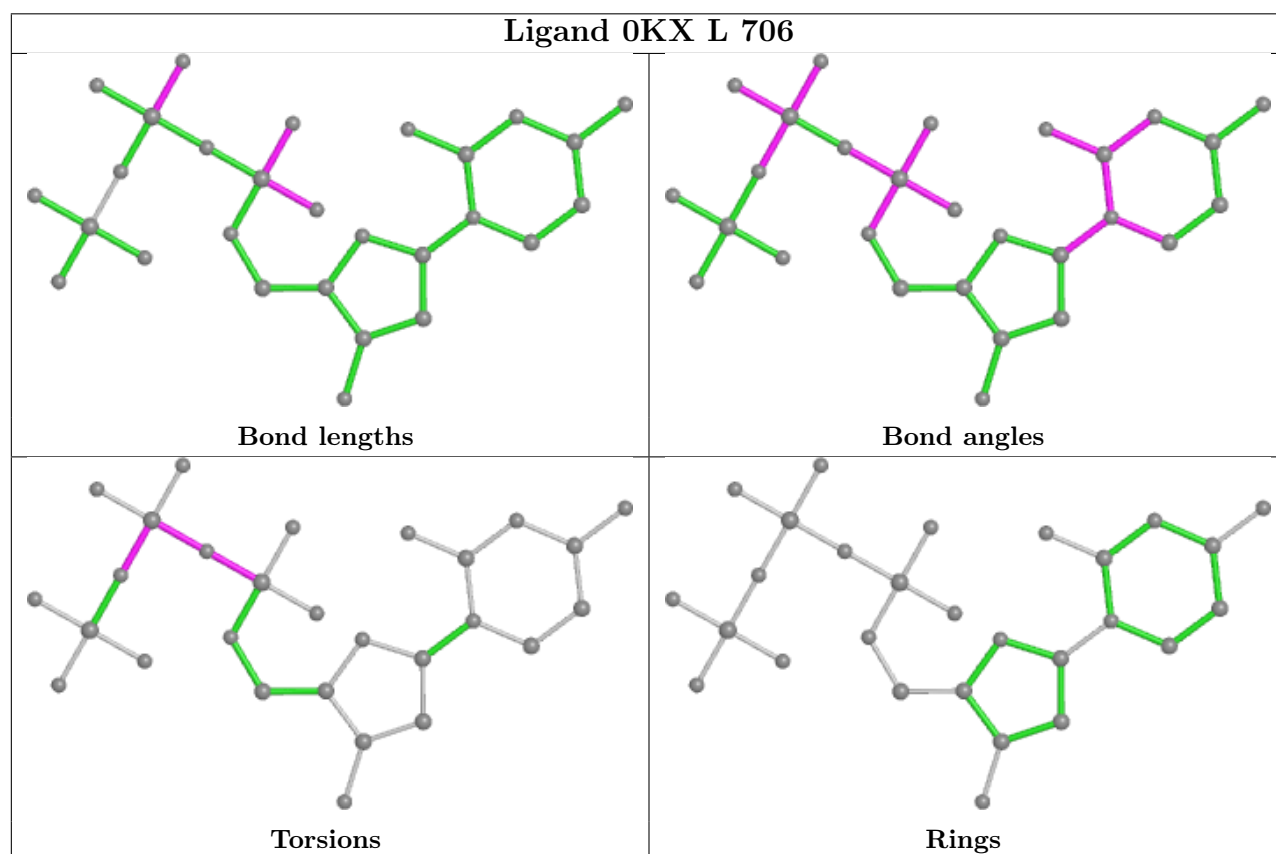
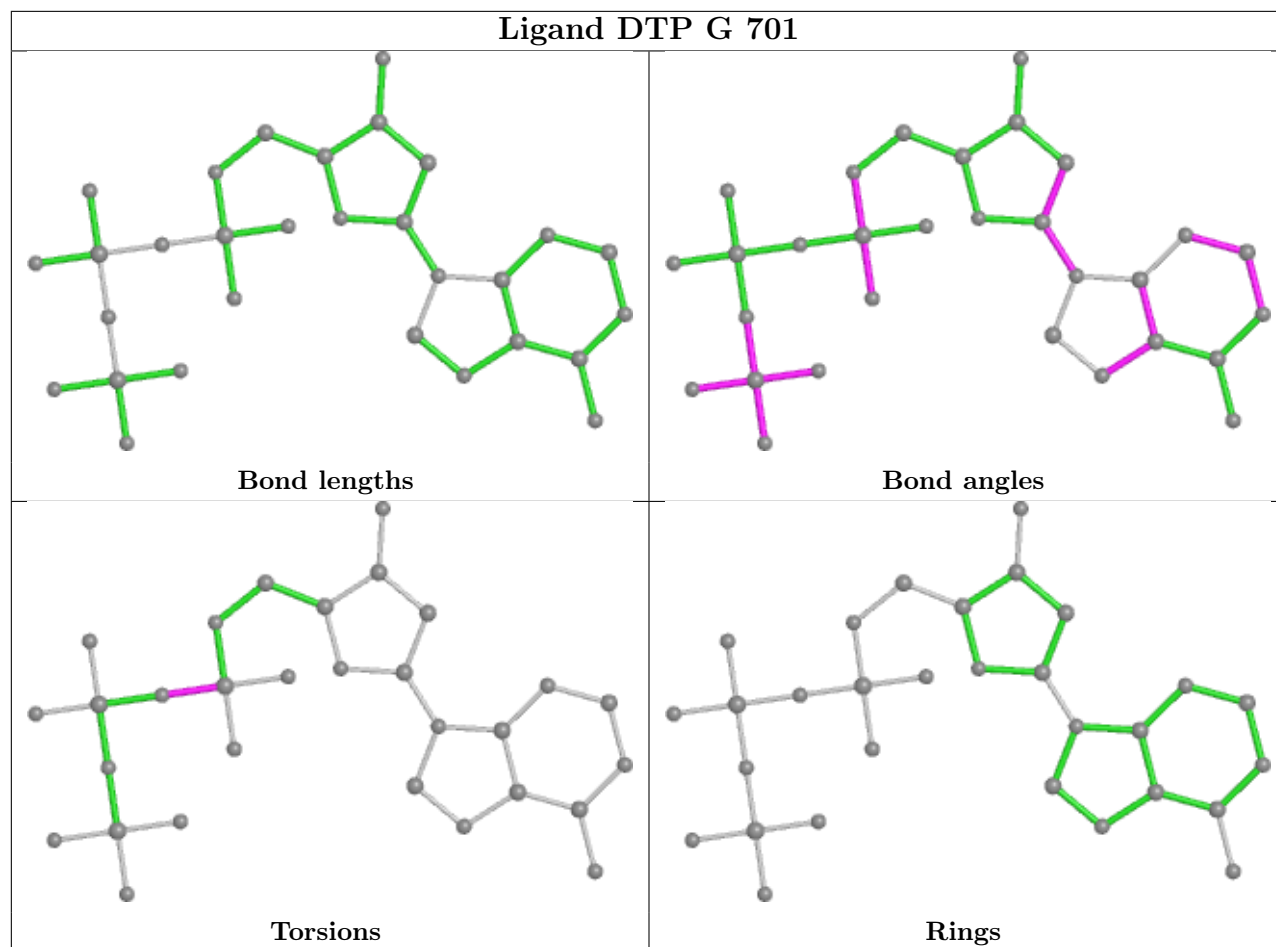


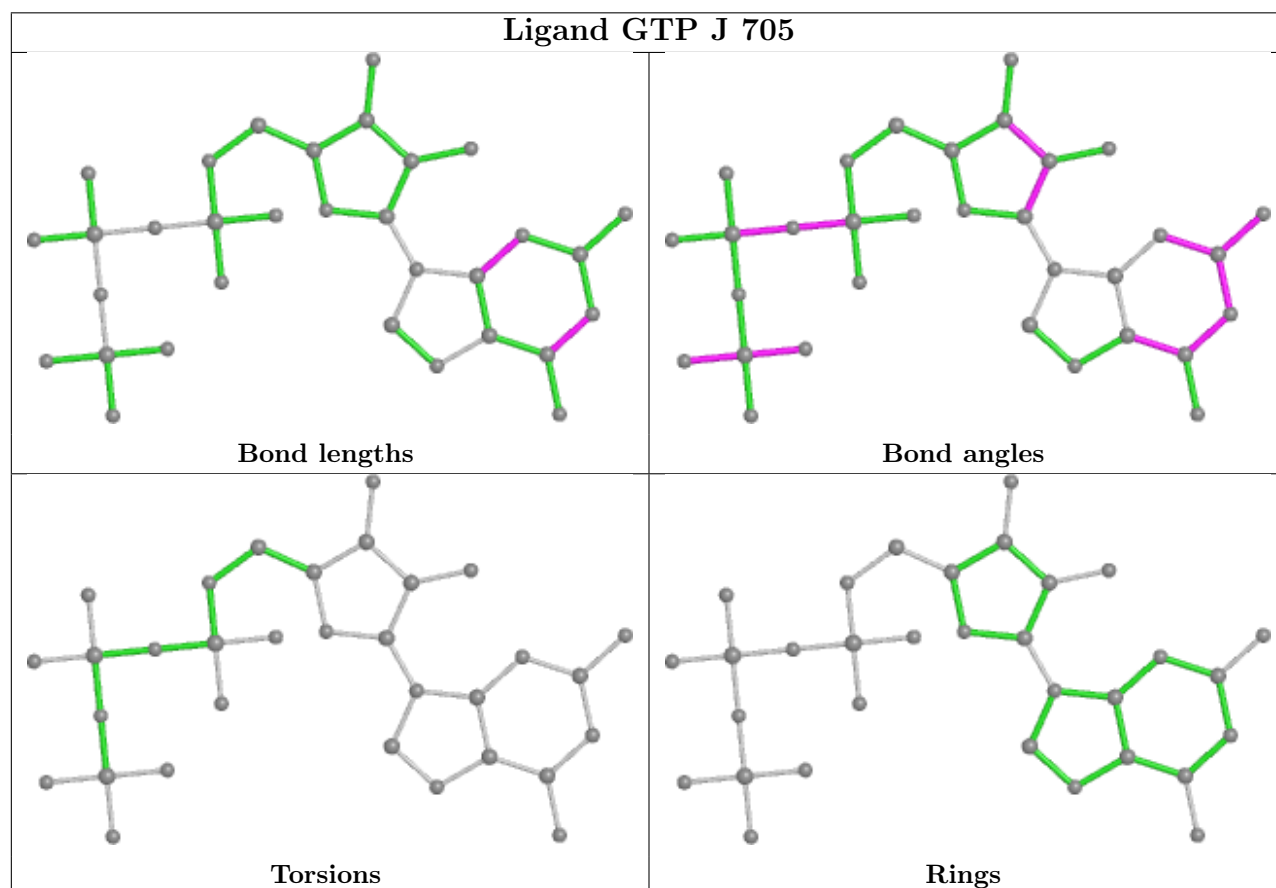
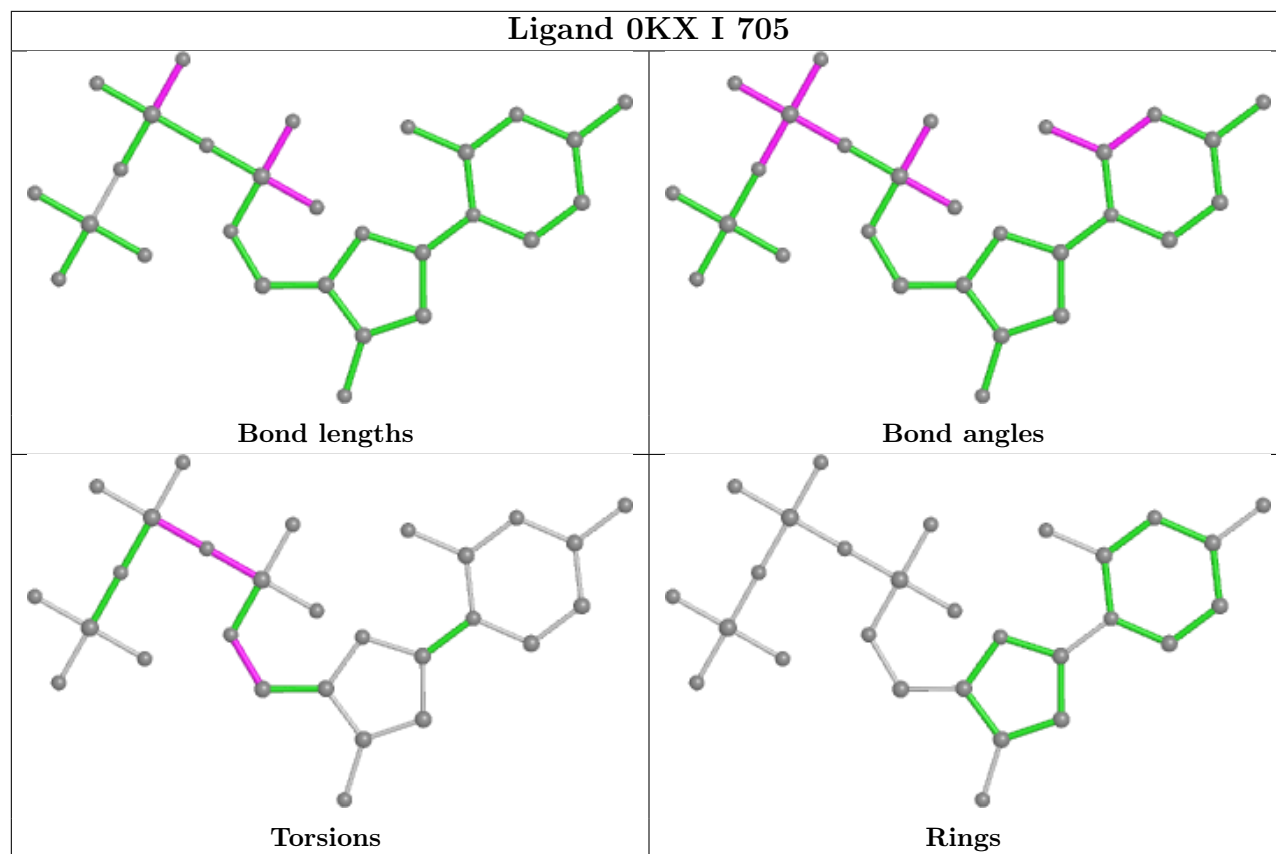


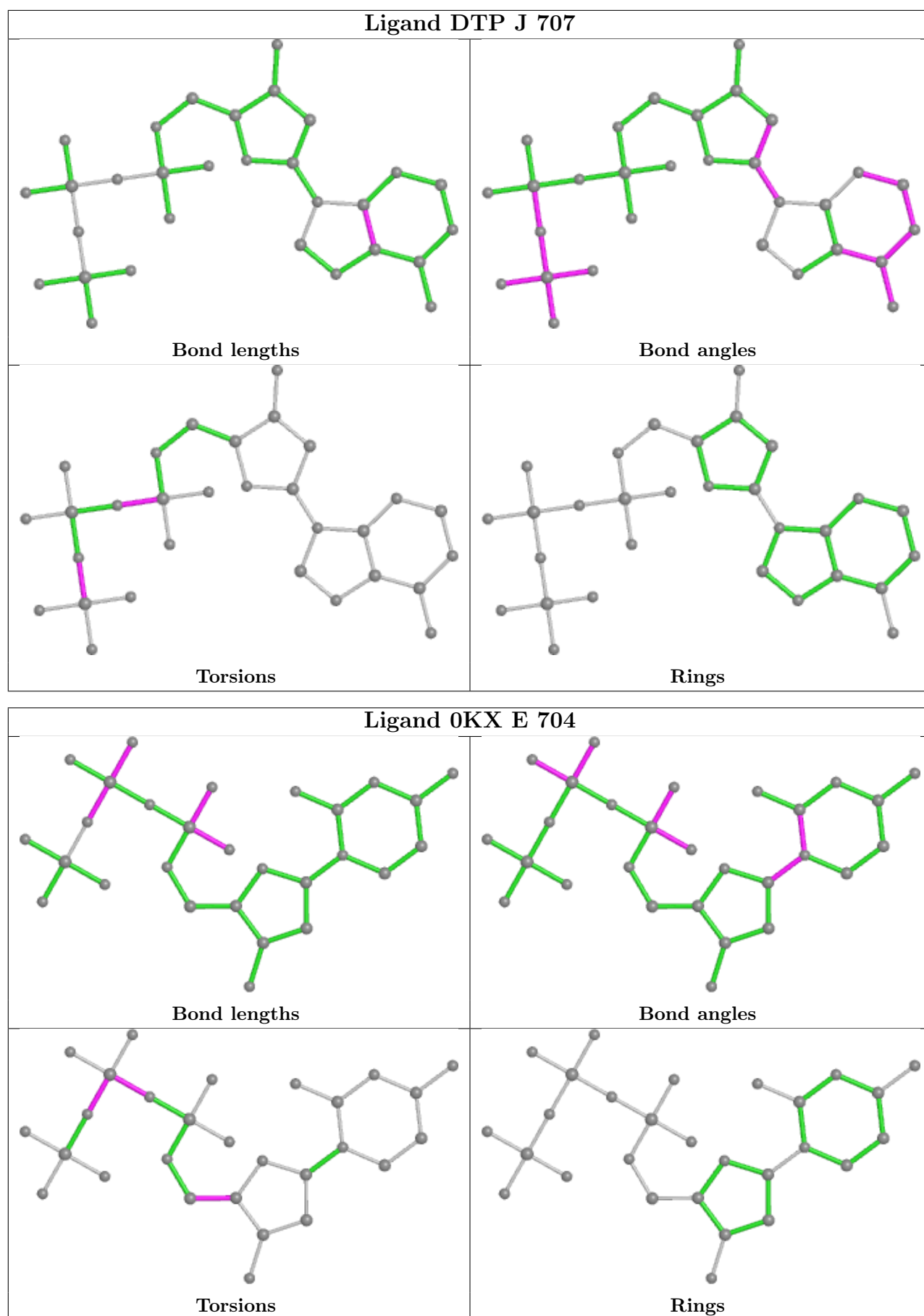


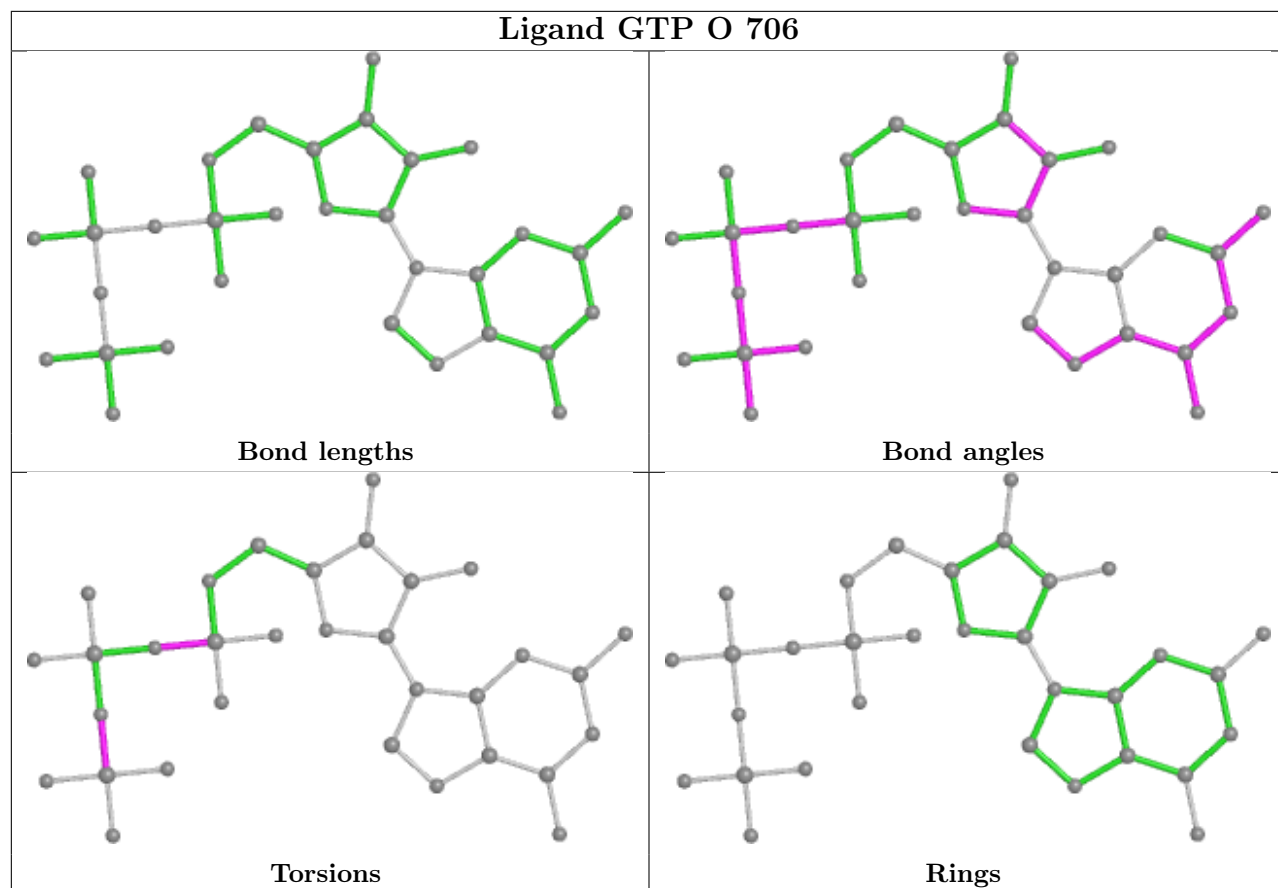


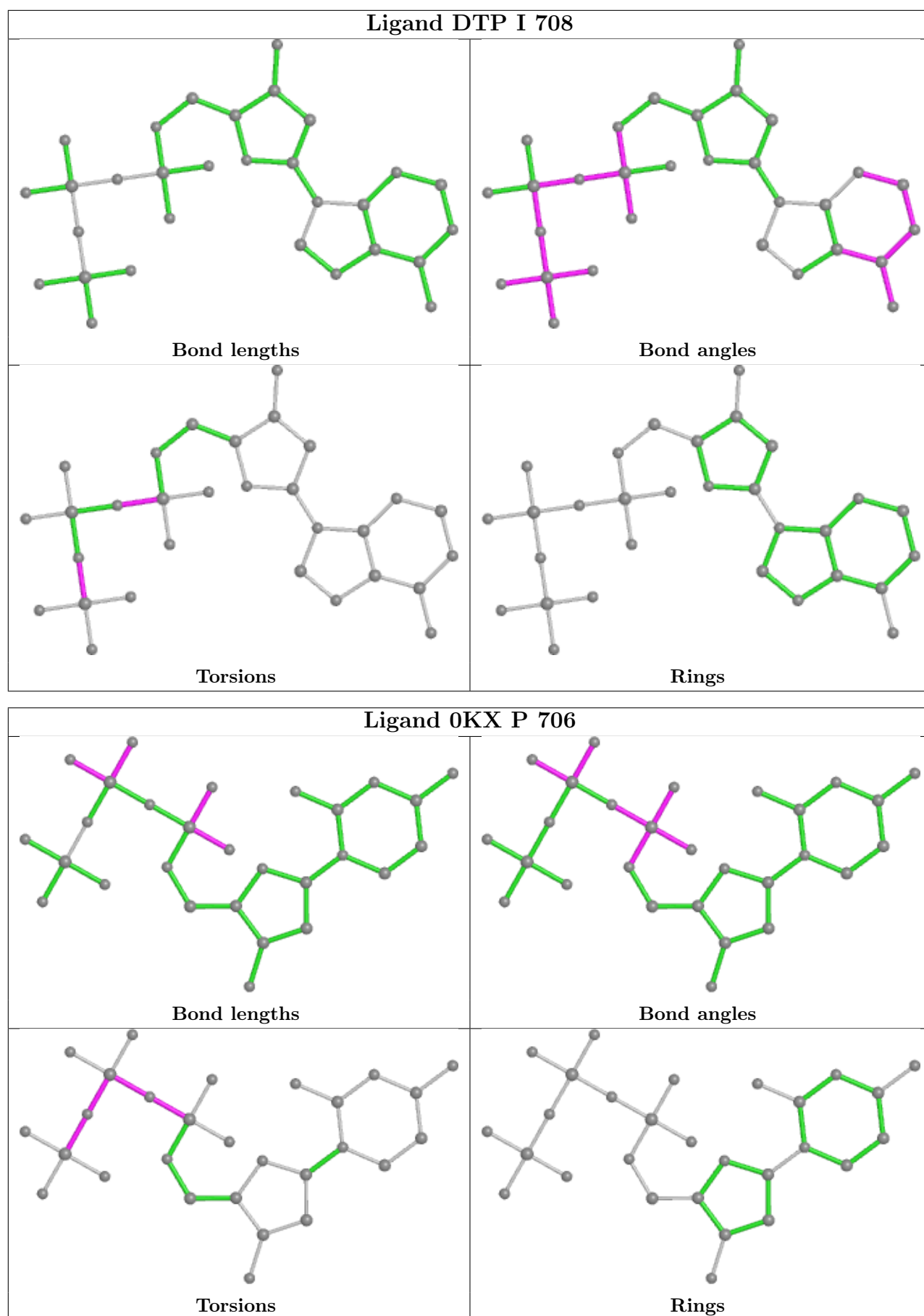


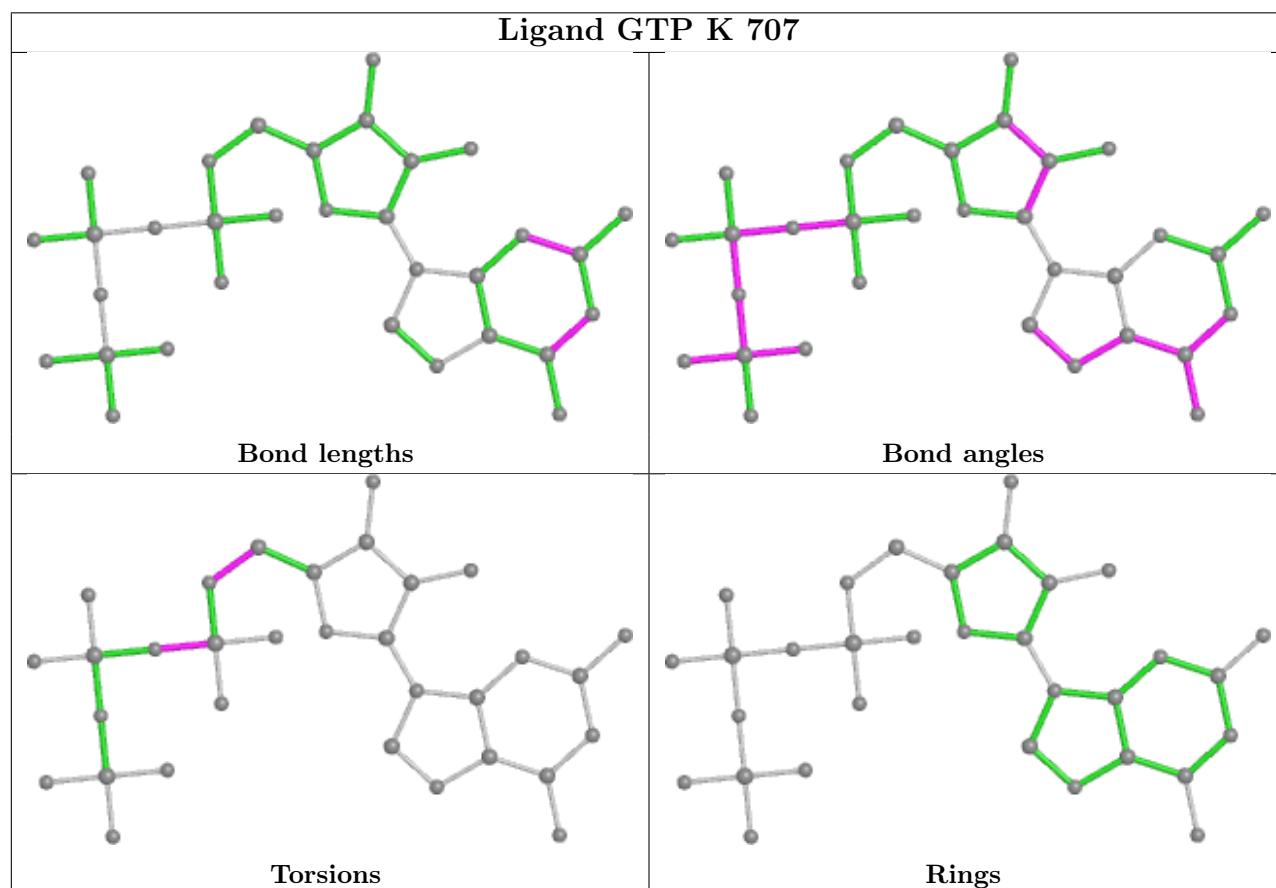
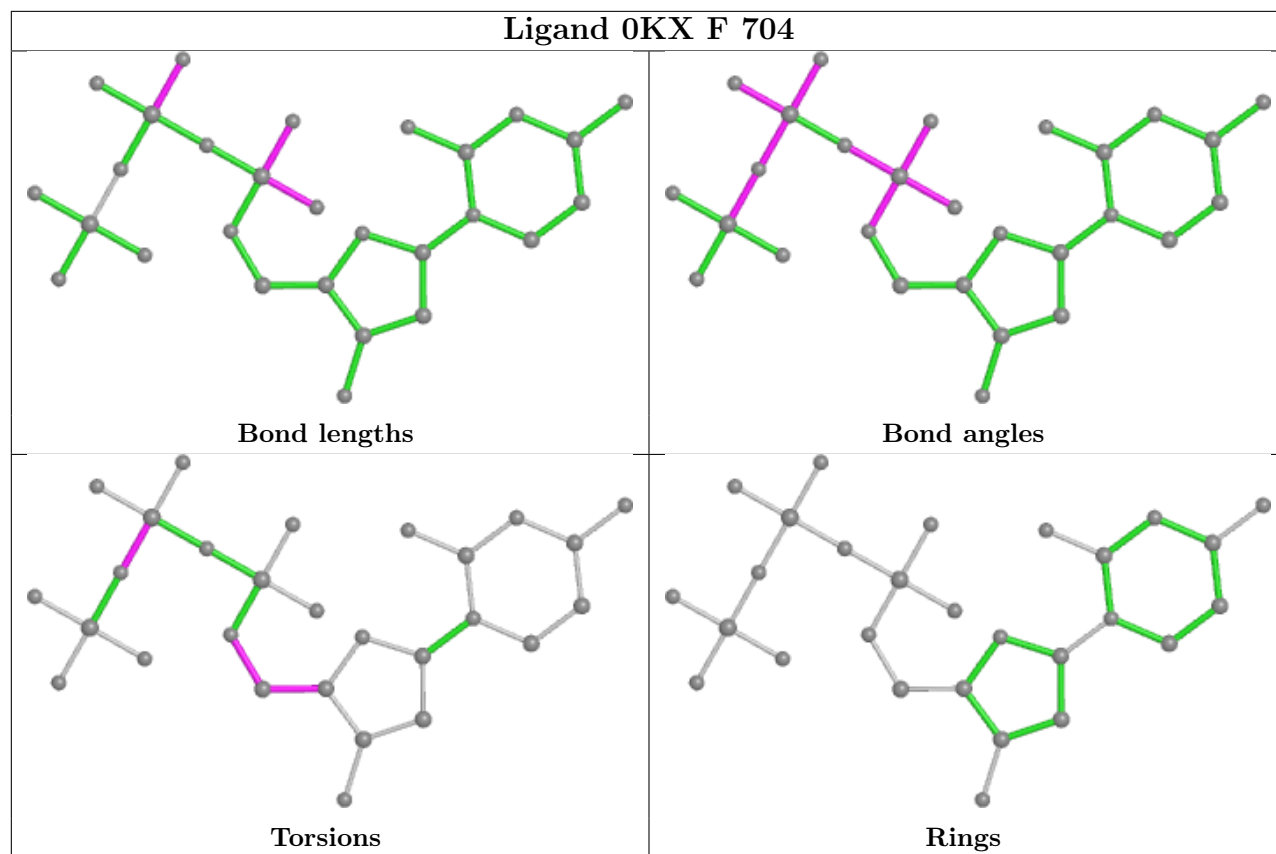


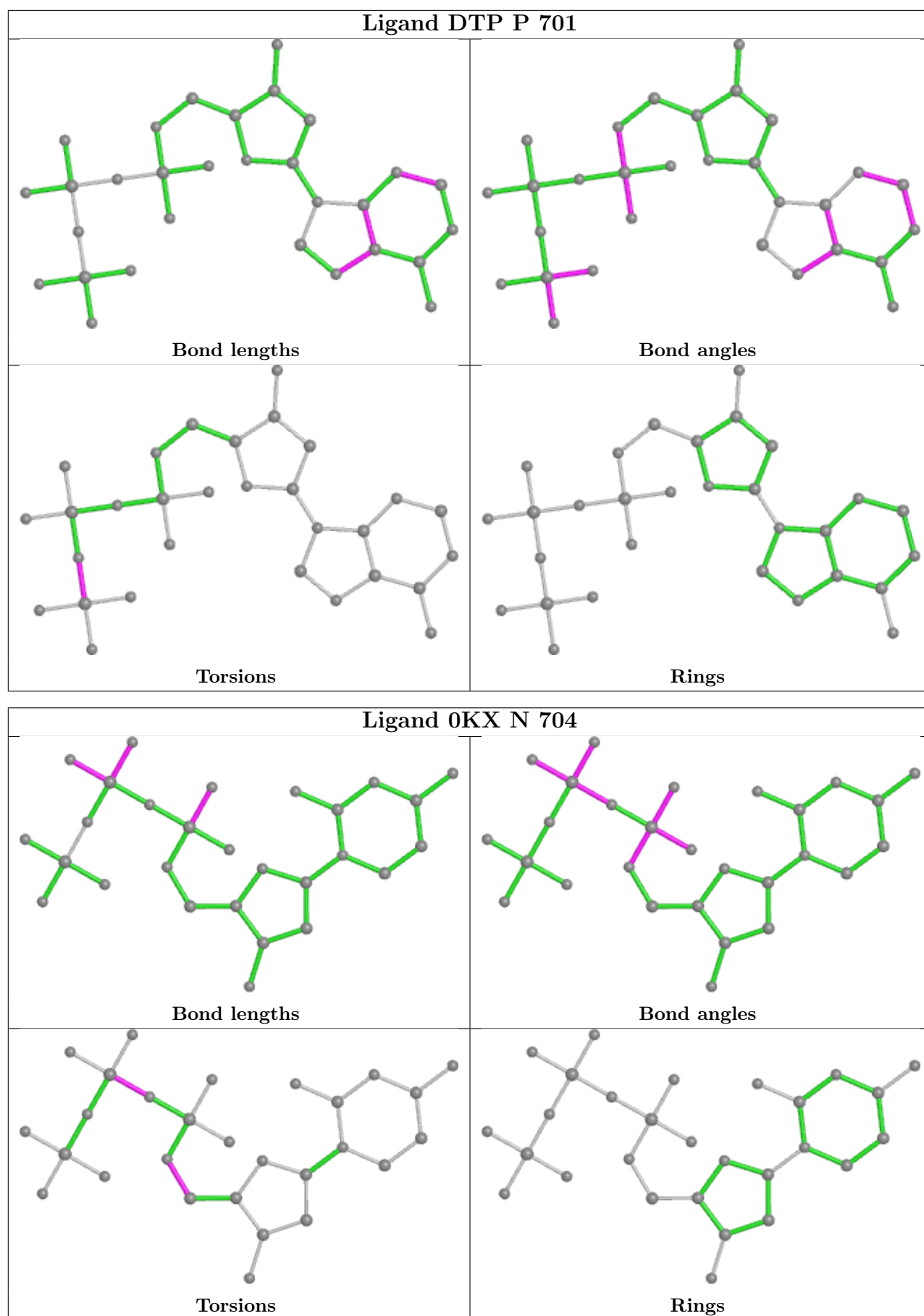


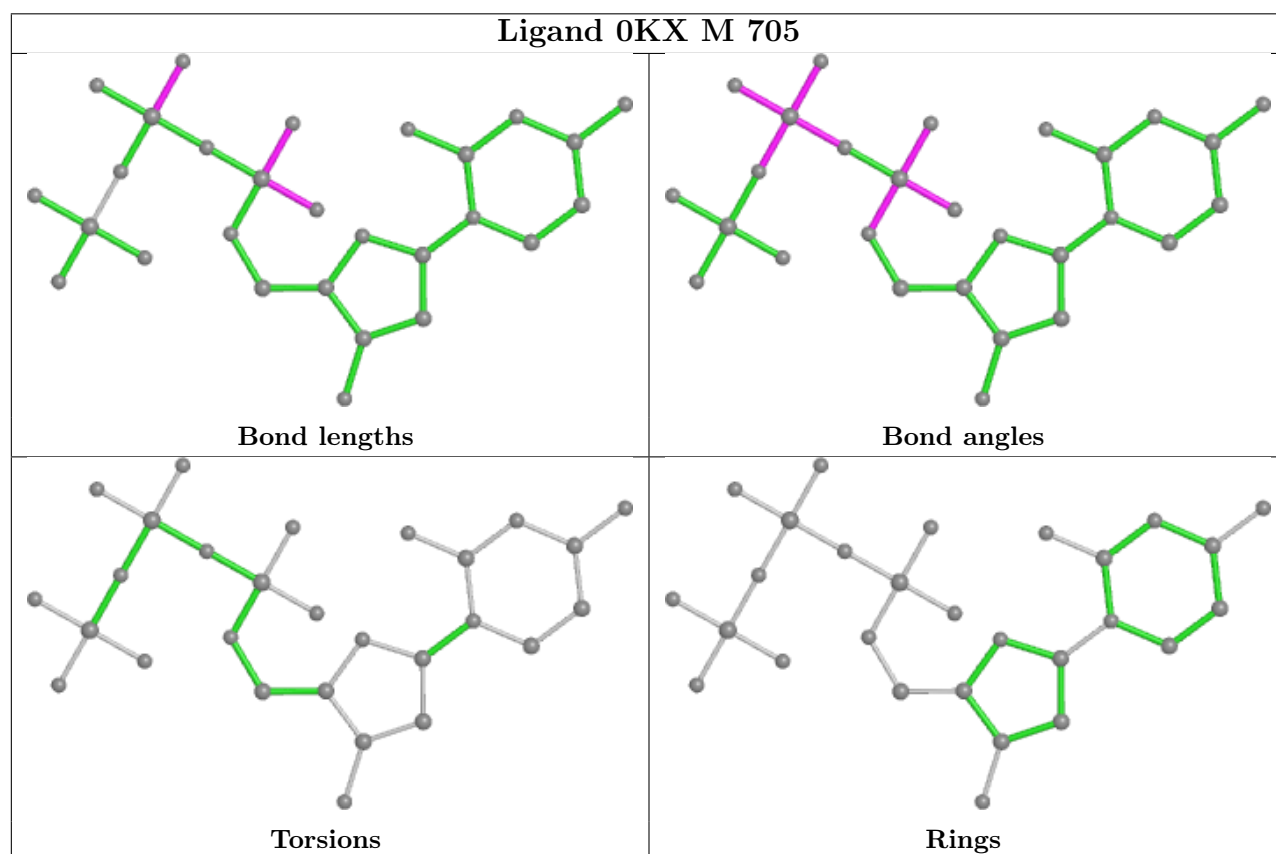
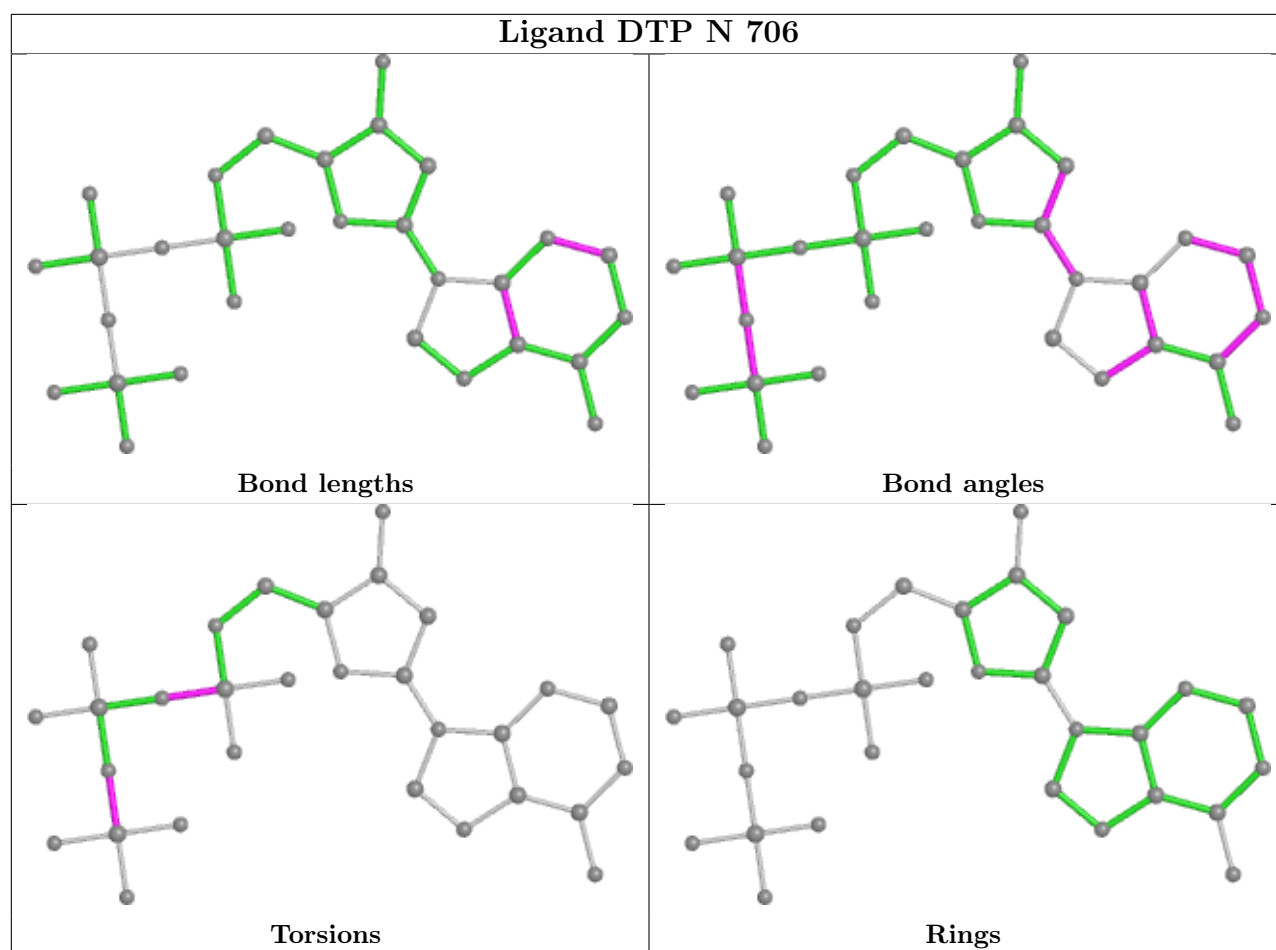


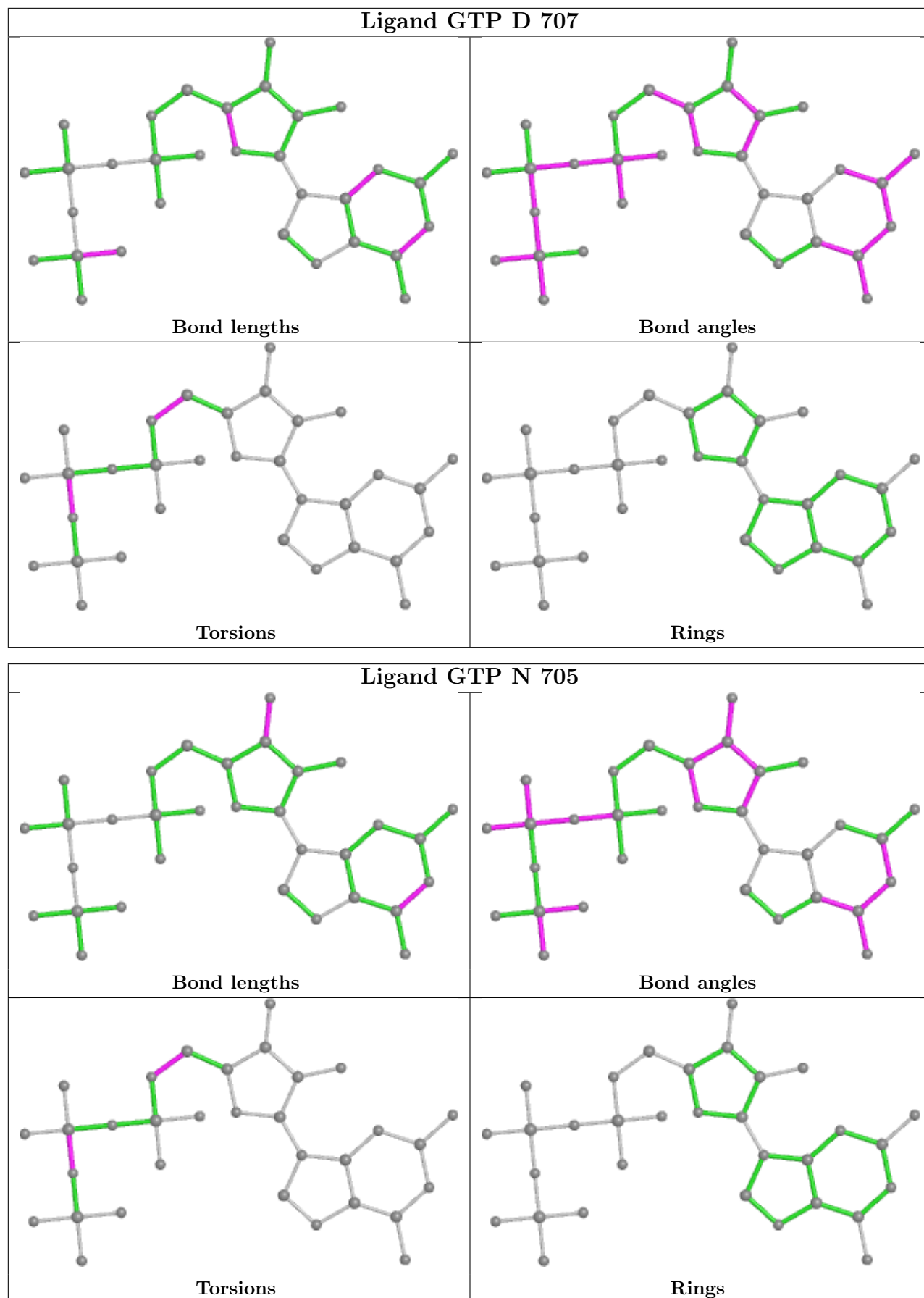


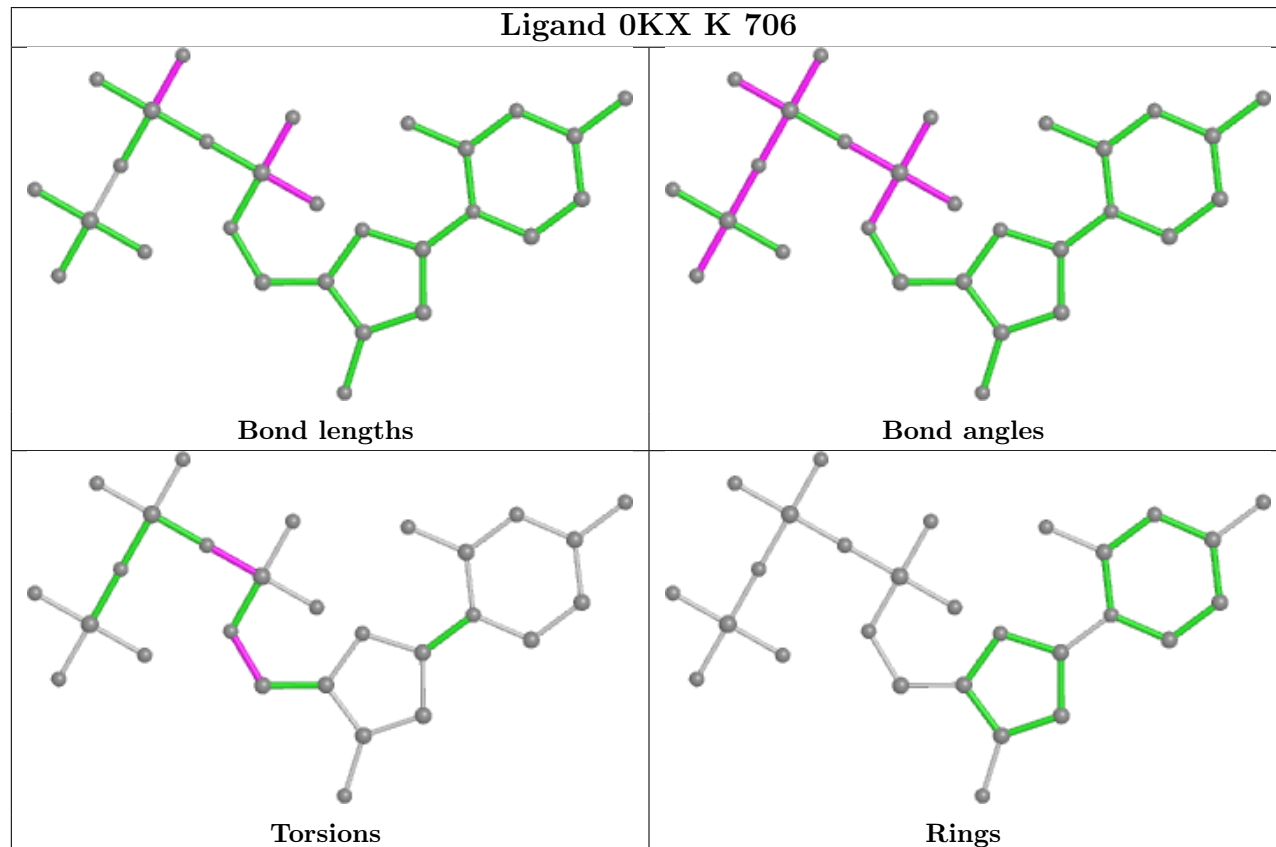
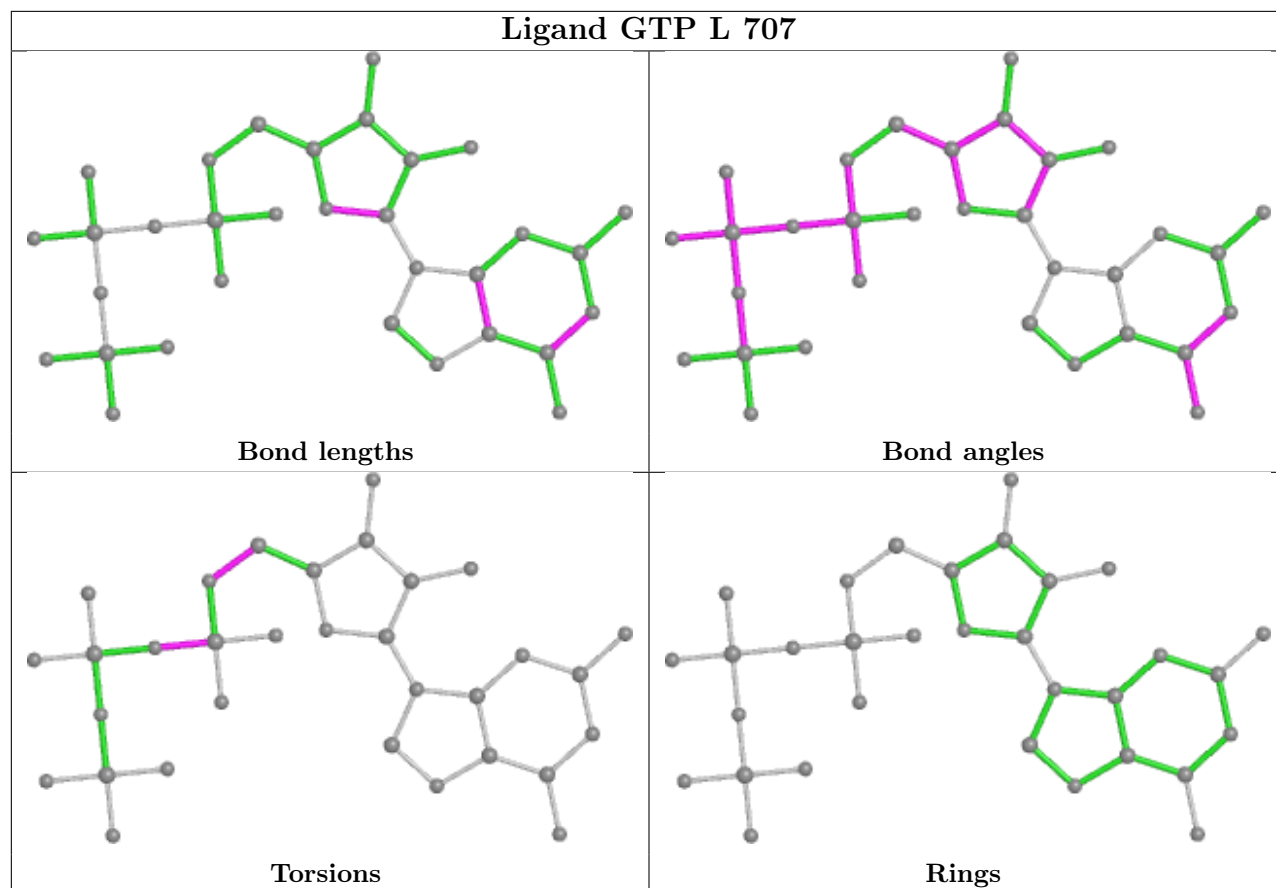


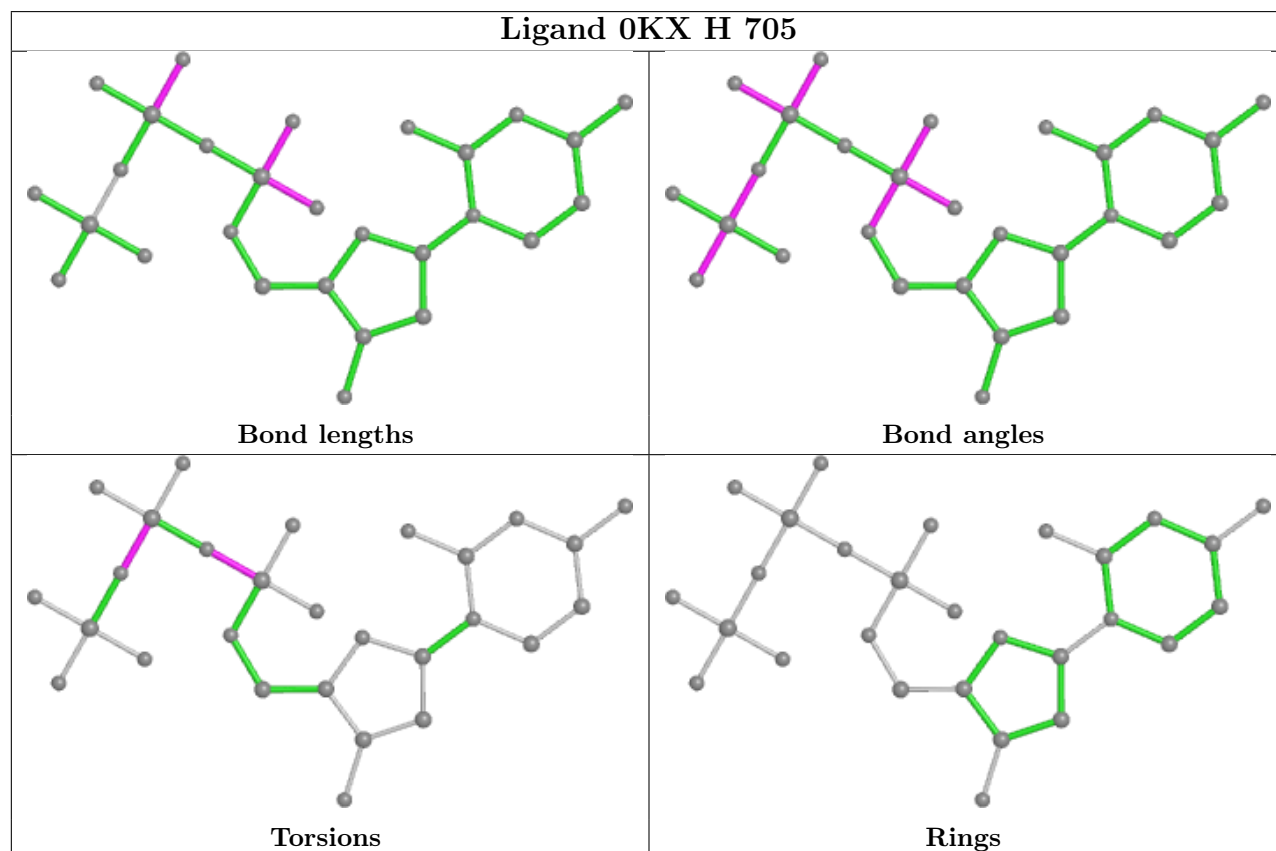
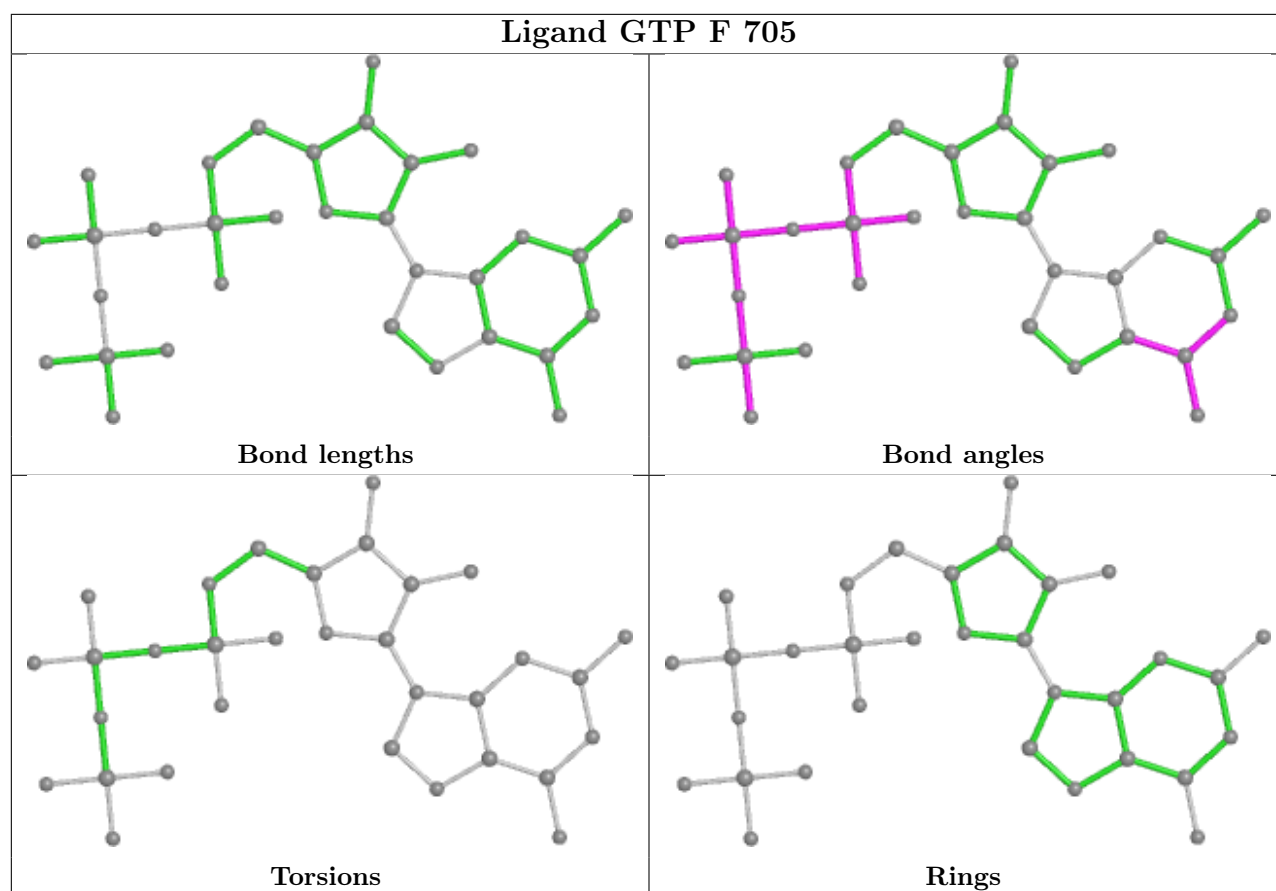


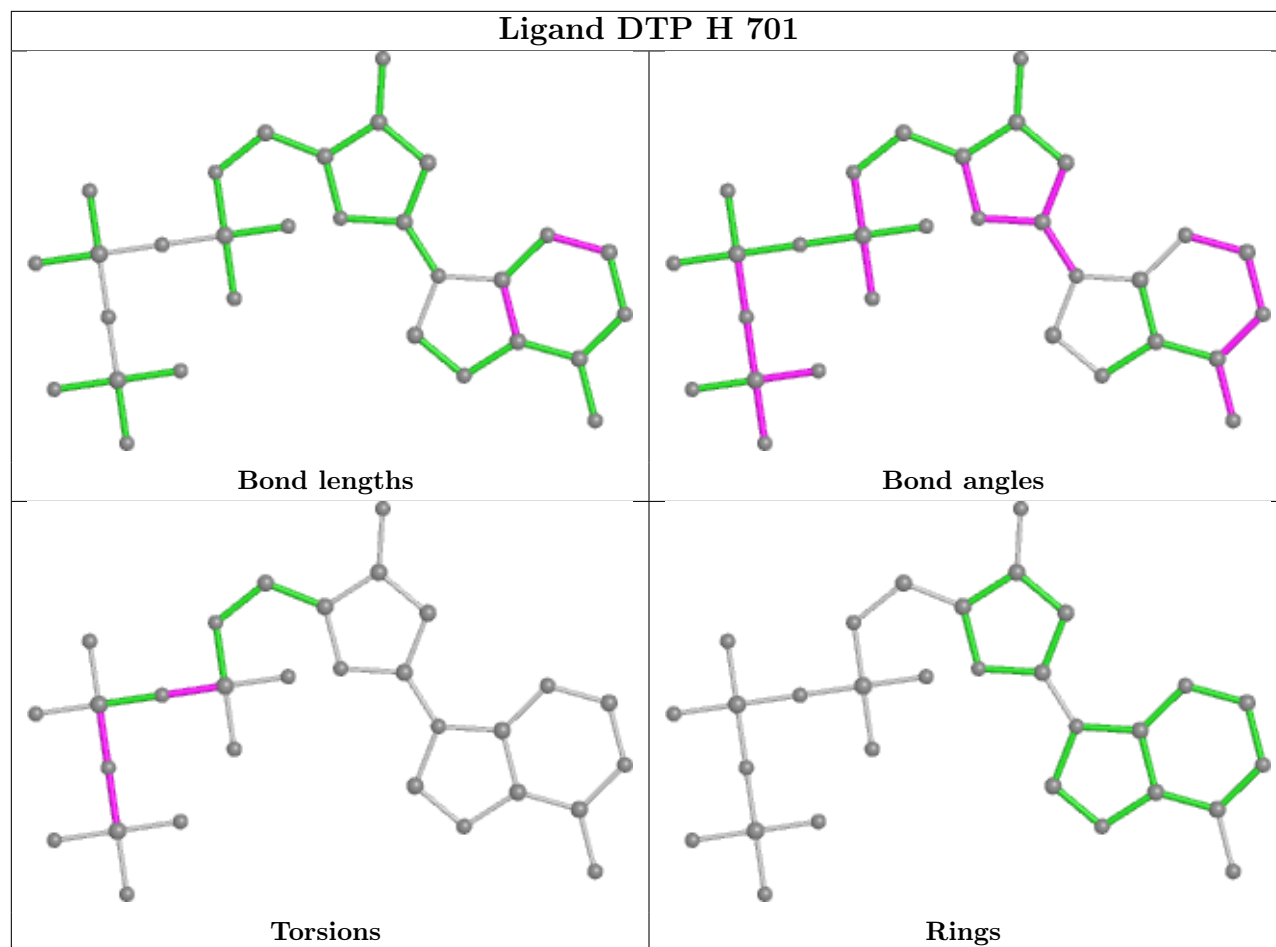


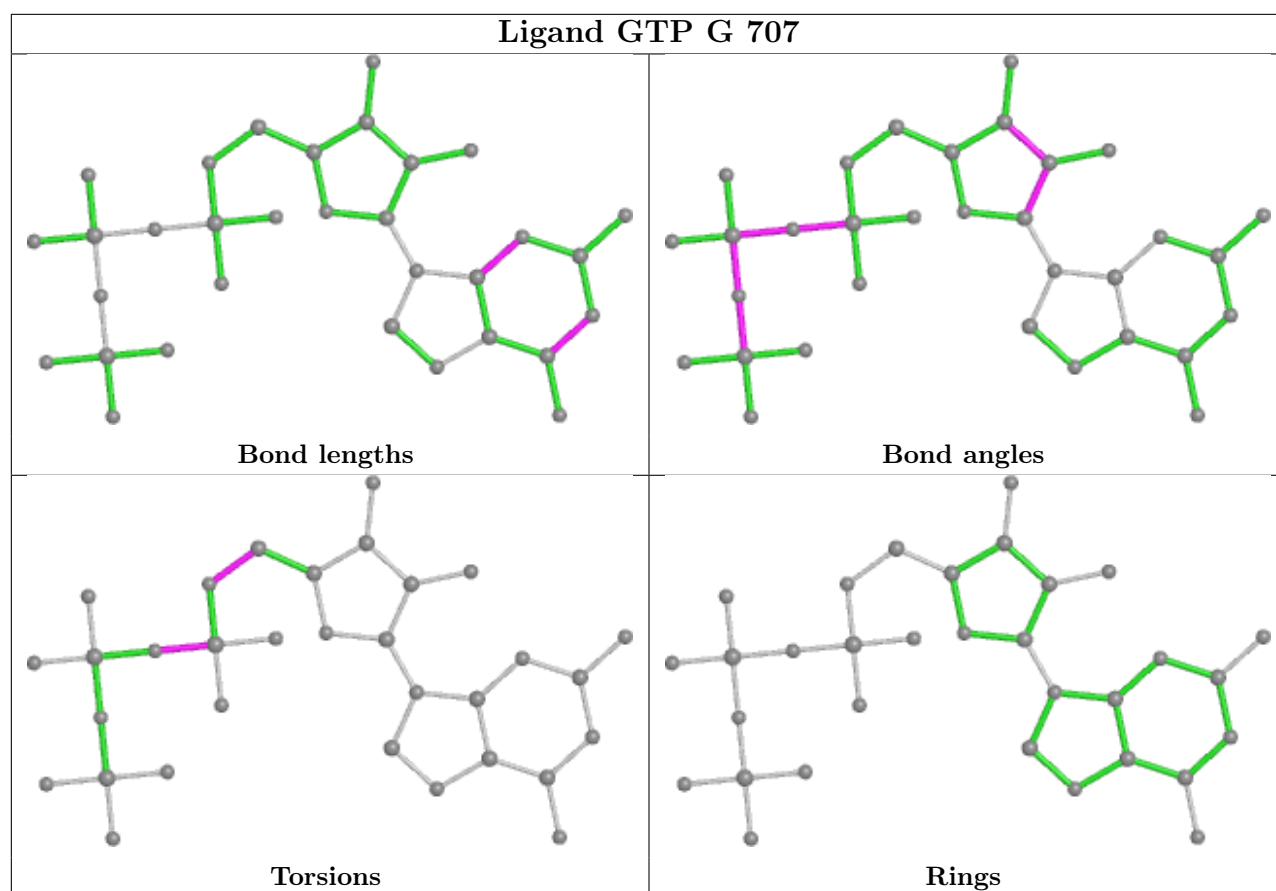












5.7 Other polymers [i](#)

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 i

6.1 Protein, DNA and RNA chains i

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

All (132) RSRZ outliers are listed below:

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

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Mol	Chain	Res	Type	RSRZ
1	E	568	TYR	3.7
1	M	359	LEU	3.6
1	G	388	ASP	3.6
1	G	328	ASN	3.5
1	M	362	MET	3.4
1	E	445	LEU	3.3
1	N	205	CYS	3.3
1	F	409	ILE	3.1
1	F	152	GLY	3.1
1	P	464	GLY	3.1
1	M	205	CYS	3.1
1	G	530	ILE	3.0
1	P	584	GLY	3.0
1	P	452	ASN	3.0
1	E	465	GLN	2.9
1	M	328	ASN	2.8
1	F	363	PHE	2.8
1	O	570	VAL	2.8
1	P	367	ASN	2.7
1	O	540	LEU	2.7
1	O	280	VAL	2.7
1	L	231	TRP	2.7
1	N	498	PHE	2.6
1	M	403	GLY	2.6
1	I	115	MET	2.6
1	O	515	ILE	2.6
1	G	471	GLU	2.6
1	F	482	SER	2.6
1	M	238	VAL	2.6
1	E	400	THR	2.6
1	G	460	THR	2.6
1	O	177	CYS	2.6
1	P	444	ILE	2.5
1	H	328	ASN	2.5
1	N	434	THR	2.5
1	M	426	ILE	2.5
1	F	549	LEU	2.5
1	G	441	ALA	2.5
1	E	498	PHE	2.5
1	O	591	ILE	2.5
1	G	329	PHE	2.4
1	M	550	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	O	573	CYS	2.4
1	M	330	ASP	2.4
1	M	503	ILE	2.4
1	M	241	PHE	2.4
1	M	367	ASN	2.4
1	E	476	LEU	2.4
1	O	136	ILE	2.4
1	O	360	TYR	2.4
1	N	364	HIS	2.4
1	N	386	ILE	2.4
1	L	453	LEU	2.4
1	O	448	ILE	2.4
1	M	501	ASP	2.4
1	M	522	CYS	2.4
1	M	400	THR	2.4
1	O	537	VAL	2.3
1	F	324	GLY	2.3
1	E	128	LEU	2.3
1	M	214	SER	2.3
1	O	593	PRO	2.3
1	L	488	LEU	2.3
1	E	599	ASN	2.3
1	F	448	ILE	2.3
1	B	114	THR	2.3
1	P	482	SER	2.3
1	P	360	TYR	2.3
1	G	577	ASN	2.3
1	P	583	ASP	2.3
1	H	347	LEU	2.3
1	M	584	GLY	2.3
1	O	115	MET	2.3
1	M	353	ASP	2.2
1	B	589	PRO	2.2
1	P	441	ALA	2.2
1	G	476	LEU	2.2
1	O	228	GLU	2.2
1	G	468	ILE	2.2
1	G	569	PHE	2.2
1	M	331	TYR	2.2
1	M	150	LEU	2.2
1	M	184	GLU	2.2
1	G	224	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	598	TRP	2.1
1	G	472	ASP	2.1
1	G	345	ASN	2.1
1	N	215	HIS	2.1
1	N	323	LEU	2.1
1	O	569	PHE	2.1
1	E	163	ASN	2.1
1	M	436	PRO	2.1
1	F	441	ALA	2.1
1	O	495	ALA	2.1
1	E	593	PRO	2.1
1	H	599	ASN	2.1
1	H	329	PHE	2.1
1	N	208	LEU	2.1
1	O	473	TYR	2.1
1	P	413	ILE	2.1
1	M	117	VAL	2.1
1	M	345	ASN	2.1
1	E	390	PHE	2.1
1	G	562	LEU	2.1
1	E	409	ILE	2.1
1	G	473	TYR	2.1
1	P	553	TYR	2.1
1	F	379	GLY	2.1
1	M	513	ASN	2.1
1	N	310	VAL	2.1
1	N	367	ASN	2.1
1	P	498	PHE	2.1
1	F	553	TYR	2.0
1	N	331	TYR	2.0
1	O	387	THR	2.0
1	O	117	VAL	2.0
1	F	572	TRP	2.0
1	M	502	VAL	2.0
1	F	431	LEU	2.0
1	G	327	ASN	2.0
1	O	456	TYR	2.0
1	L	329	PHE	2.0
1	O	465	GLN	2.0
1	N	390	PHE	2.0
1	F	590	LEU	2.0
1	O	169	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	452	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(Å ²)	Q<0.9
3	MG	I	702	1/1	0.81	0.15	55,55,55,55	0
6	SO4	I	707	5/5	0.81	0.15	92,93,97,97	0
3	MG	G	703	1/1	0.86	0.13	52,52,52,52	0
3	MG	N	702	1/1	0.89	0.15	40,40,40,40	0
3	MG	B	702	1/1	0.89	0.31	61,61,61,61	0
6	SO4	L	708	5/5	0.89	0.17	72,75,77,80	0
3	MG	K	703	1/1	0.90	0.31	68,68,68,68	0
6	SO4	B	707	5/5	0.90	0.16	67,68,70,71	0
3	MG	N	703	1/1	0.91	0.11	40,40,40,40	0
6	SO4	A	707	5/5	0.92	0.17	83,84,84,85	0
6	SO4	J	706	5/5	0.92	0.14	70,72,73,74	0
3	MG	H	704	1/1	0.92	0.08	37,37,37,37	0
3	MG	M	702	1/1	0.93	0.21	59,59,59,59	0
3	MG	E	702	1/1	0.93	0.23	32,32,32,32	0
3	MG	K	705	1/1	0.93	0.08	30,30,30,30	0
3	MG	P	703	1/1	0.93	0.09	39,39,39,39	0
4	OKX	M	705	28/28	0.93	0.17	52,56,59,61	0
6	SO4	M	707	5/5	0.93	0.15	88,89,90,92	0
3	MG	M	703	1/1	0.94	0.18	46,46,46,46	0
3	MG	H	703	1/1	0.94	0.17	25,25,25,25	0
6	SO4	H	707	5/5	0.94	0.14	94,94,94,95	0
3	MG	L	703	1/1	0.94	0.19	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	L	704	1/1	0.94	0.17	20,20,20,20	0
3	MG	D	703	1/1	0.94	0.15	32,32,32,32	0
5	GTP	F	705	32/32	0.94	0.16	44,48,53,55	0
4	OKX	G	706	28/28	0.95	0.15	40,45,47,49	0
3	MG	F	703	1/1	0.95	0.09	44,44,44,44	0
6	SO4	D	708	5/5	0.95	0.11	69,71,72,73	0
3	MG	G	704	1/1	0.95	0.21	33,33,33,33	0
5	GTP	H	706	32/32	0.95	0.13	36,39,43,45	0
5	GTP	M	706	32/32	0.95	0.17	48,51,56,56	0
5	GTP	N	705	32/32	0.95	0.15	50,52,54,54	0
5	GTP	O	706	32/32	0.95	0.15	45,50,58,61	0
3	MG	I	703	1/1	0.96	0.17	20,20,20,20	0
3	MG	P	705	1/1	0.96	0.08	43,43,43,43	0
3	MG	C	703	1/1	0.96	0.16	32,32,32,32	0
3	MG	F	702	1/1	0.96	0.25	35,35,35,35	0
4	OKX	N	704	28/28	0.96	0.16	51,54,55,55	0
5	GTP	O	707	32/32	0.96	0.14	37,41,47,48	0
4	OKX	O	705	28/28	0.96	0.17	48,51,56,59	0
7	DTP	E	706	30/30	0.96	0.14	28,29,34,34	0
7	DTP	F	706	30/30	0.96	0.15	36,39,45,47	0
7	DTP	G	701	30/30	0.96	0.17	41,44,52,54	0
7	DTP	P	701	30/30	0.96	0.16	44,45,49,51	0
5	GTP	A	706	32/32	0.97	0.14	21,23,27,29	0
5	GTP	E	705	32/32	0.97	0.12	45,49,55,57	0
3	MG	D	704	1/1	0.97	0.21	13,13,13,13	0
5	GTP	G	707	32/32	0.97	0.12	30,31,32,33	0
3	MG	K	704	1/1	0.97	0.14	19,19,19,19	0
5	GTP	I	706	32/32	0.97	0.16	26,29,37,38	0
5	GTP	J	705	32/32	0.97	0.12	21,23,25,26	0
5	GTP	K	707	32/32	0.97	0.15	36,40,44,46	0
5	GTP	L	707	32/32	0.97	0.14	21,24,26,27	0
3	MG	D	705	1/1	0.97	0.11	23,23,23,23	0
2	FE	I	701	1/1	0.97	0.10	25,25,25,25	0
4	OKX	A	705	28/28	0.97	0.14	23,29,32,33	0
4	OKX	C	706	28/28	0.97	0.14	19,21,26,27	0
4	OKX	D	706	28/28	0.97	0.15	21,23,27,30	0
4	OKX	E	704	28/28	0.97	0.13	42,45,48,50	0
6	SO4	C	708	5/5	0.97	0.11	57,57,59,60	0
4	OKX	F	704	28/28	0.97	0.15	42,47,50,52	0
3	MG	E	703	1/1	0.97	0.09	52,52,52,52	0
4	OKX	H	705	28/28	0.97	0.14	38,40,42,44	0
4	OKX	I	705	28/28	0.97	0.14	28,31,33,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	OKX	J	704	28/28	0.97	0.16	23,26,28,29	0
4	OKX	L	706	28/28	0.97	0.13	31,35,39,41	0
7	DTP	A	708	30/30	0.97	0.17	21,25,26,28	0
7	DTP	D	701	30/30	0.97	0.15	20,25,28,30	0
3	MG	L	705	1/1	0.97	0.13	22,22,22,22	0
2	FE	P	702	1/1	0.97	0.12	30,30,30,30	0
3	MG	A	702	1/1	0.97	0.15	48,48,48,48	0
7	DTP	H	701	30/30	0.97	0.15	39,43,49,52	0
7	DTP	I	708	30/30	0.97	0.16	30,33,38,39	0
7	DTP	J	707	30/30	0.97	0.17	19,21,23,23	0
7	DTP	L	701	30/30	0.97	0.15	26,28,31,32	0
7	DTP	M	708	30/30	0.97	0.18	41,45,58,59	0
7	DTP	N	706	30/30	0.97	0.18	38,43,48,50	0
7	DTP	O	701	30/30	0.97	0.15	44,46,49,49	0
4	OKX	P	706	28/28	0.97	0.18	40,43,50,53	0
5	GTP	C	707	32/32	0.98	0.14	21,23,26,27	0
5	GTP	D	707	32/32	0.98	0.13	16,17,19,20	0
3	MG	B	704	1/1	0.98	0.12	20,20,20,20	0
2	FE	N	701	1/1	0.98	0.09	38,38,38,38	0
3	MG	C	704	1/1	0.98	0.21	13,13,13,13	0
3	MG	A	704	1/1	0.98	0.08	20,20,20,20	0
7	DTP	B	708	30/30	0.98	0.15	15,16,19,19	0
7	DTP	C	701	30/30	0.98	0.14	16,18,23,24	0
3	MG	I	704	1/1	0.98	0.09	23,23,23,23	0
3	MG	J	702	1/1	0.98	0.09	17,17,17,17	0
3	MG	J	703	1/1	0.98	0.12	18,18,18,18	0
3	MG	O	703	1/1	0.98	0.13	31,31,31,31	0
4	OKX	K	706	28/28	0.98	0.16	31,34,38,40	0
3	MG	O	704	1/1	0.98	0.06	43,43,43,43	0
2	FE	G	702	1/1	0.98	0.10	30,30,30,30	0
7	DTP	K	701	30/30	0.98	0.14	25,28,30,30	0
3	MG	P	704	1/1	0.98	0.24	28,28,28,28	0
3	MG	B	703	1/1	0.98	0.15	13,13,13,13	0
3	MG	G	705	1/1	0.98	0.07	25,25,25,25	0
4	OKX	B	705	28/28	0.98	0.14	19,22,24,25	0
5	GTP	B	706	32/32	0.98	0.14	20,22,26,27	0
3	MG	M	704	1/1	0.99	0.05	49,49,49,49	0
2	FE	O	702	1/1	0.99	0.09	39,39,39,39	0
2	FE	E	701	1/1	0.99	0.09	42,42,42,42	0
2	FE	A	701	1/1	0.99	0.12	22,22,22,22	0
3	MG	A	703	1/1	0.99	0.23	16,16,16,16	0
2	FE	H	702	1/1	0.99	0.08	26,26,26,26	0

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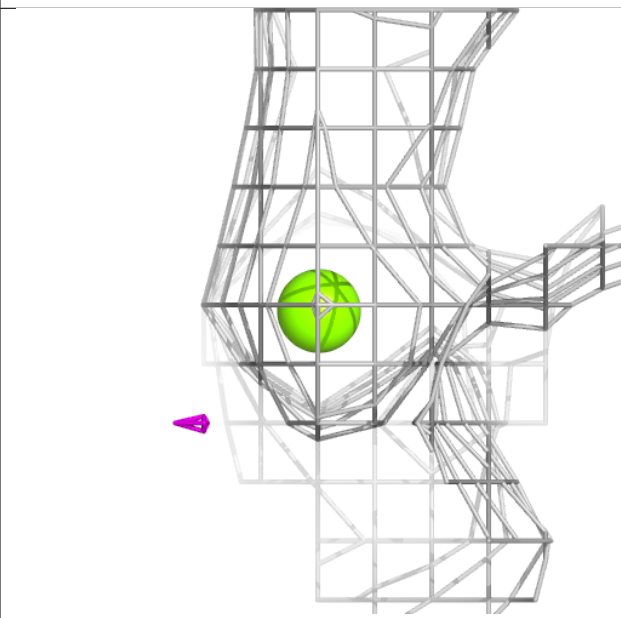
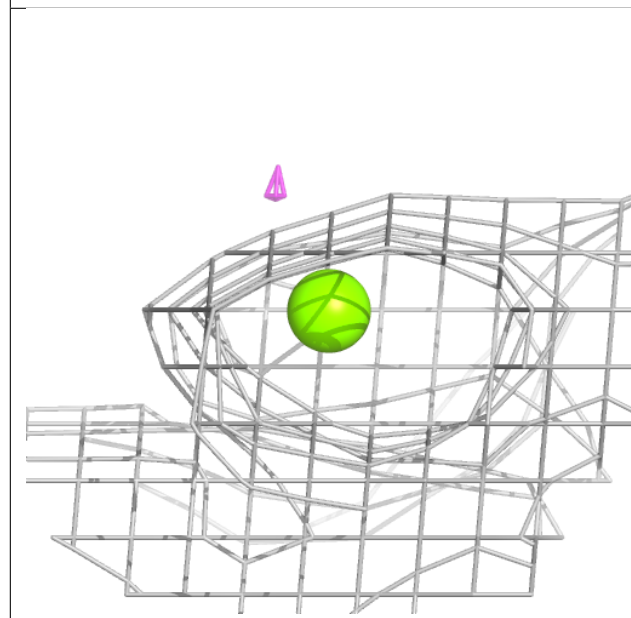
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FE	B	701	1/1	0.99	0.12	16,16,16,16	0
2	FE	J	701	1/1	0.99	0.11	18,18,18,18	0
2	FE	K	702	1/1	0.99	0.10	28,28,28,28	0
2	FE	L	702	1/1	0.99	0.10	25,25,25,25	0
2	FE	M	701	1/1	0.99	0.08	44,44,44,44	0
3	MG	C	705	1/1	0.99	0.04	24,24,24,24	0
2	FE	D	702	1/1	0.99	0.14	14,14,14,14	0
2	FE	F	701	1/1	1.00	0.10	33,33,33,33	0
2	FE	C	702	1/1	1.00	0.09	17,17,17,17	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.

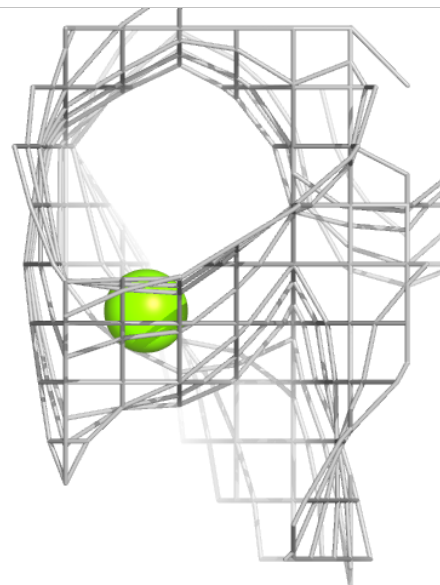
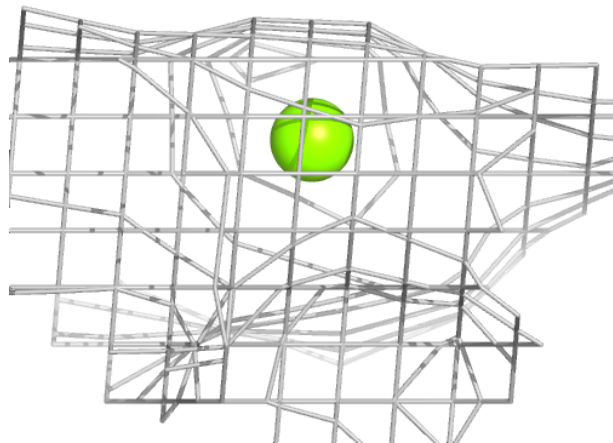
Electron density around MG I 702:

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



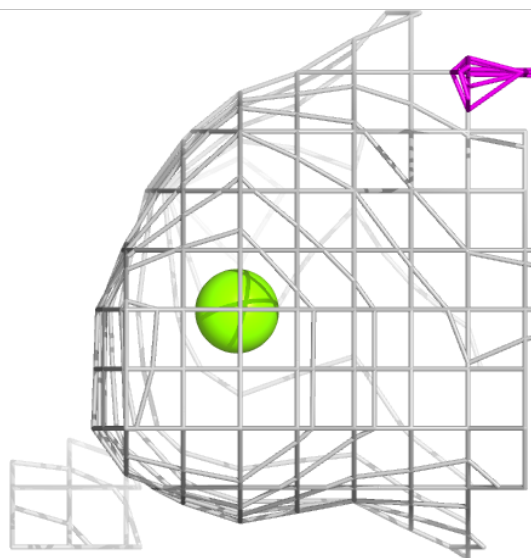
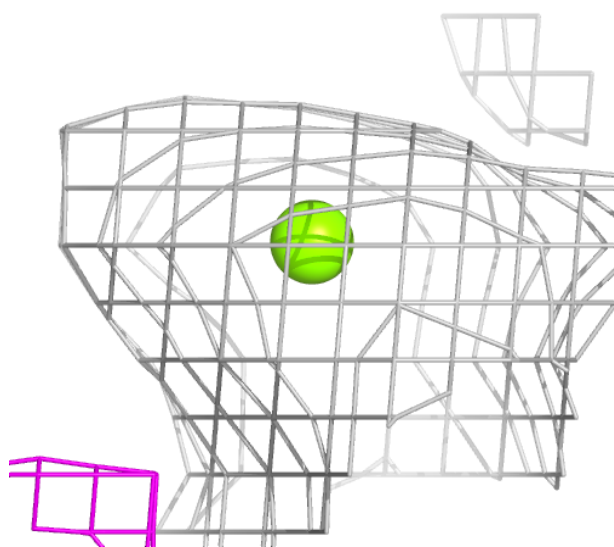
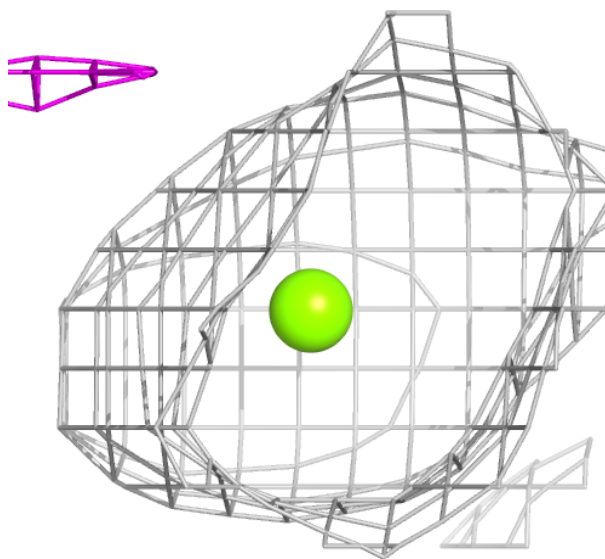
Electron density around MG G 703:

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



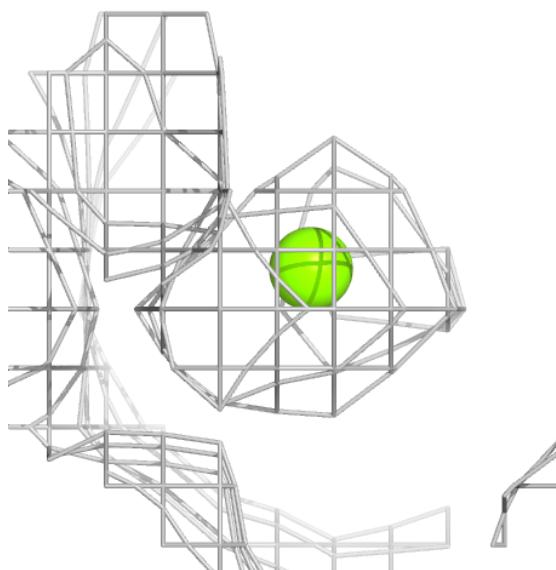
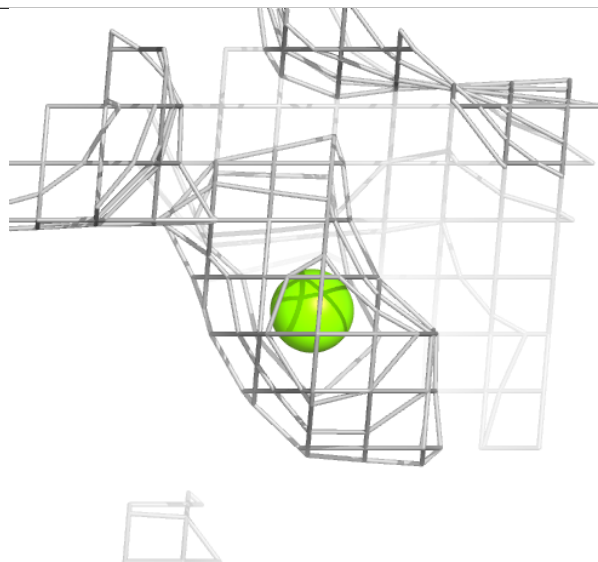
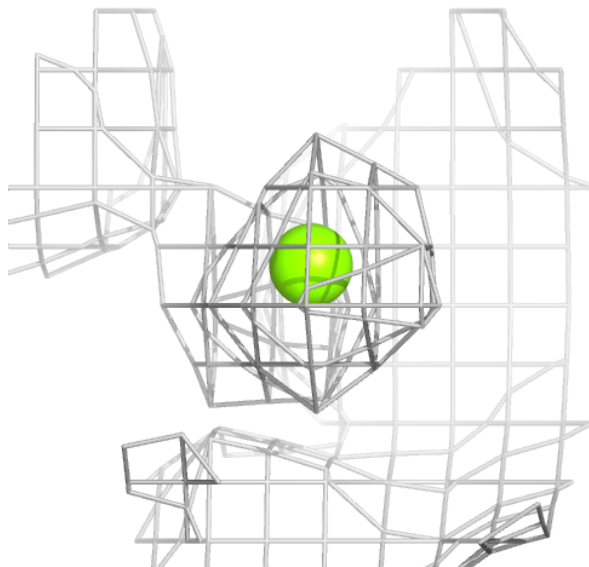
Electron density around MG N 702:

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and green (positive)



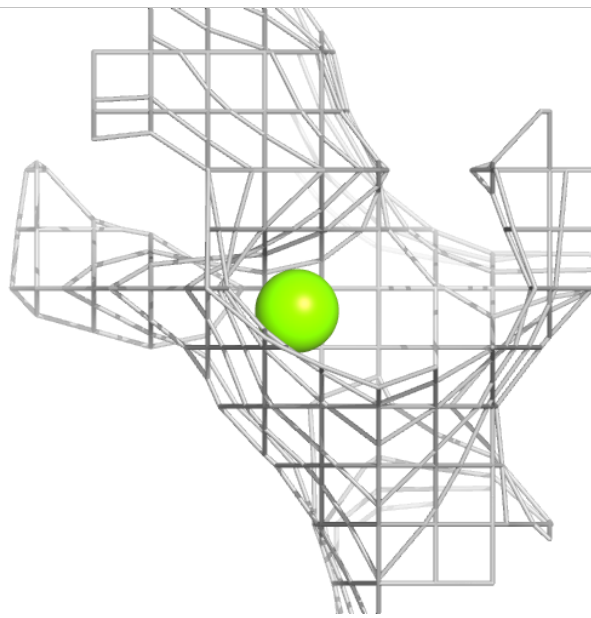
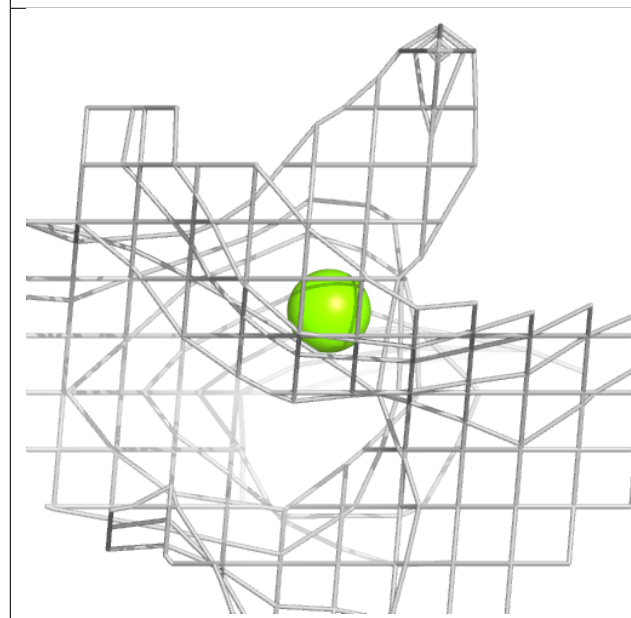
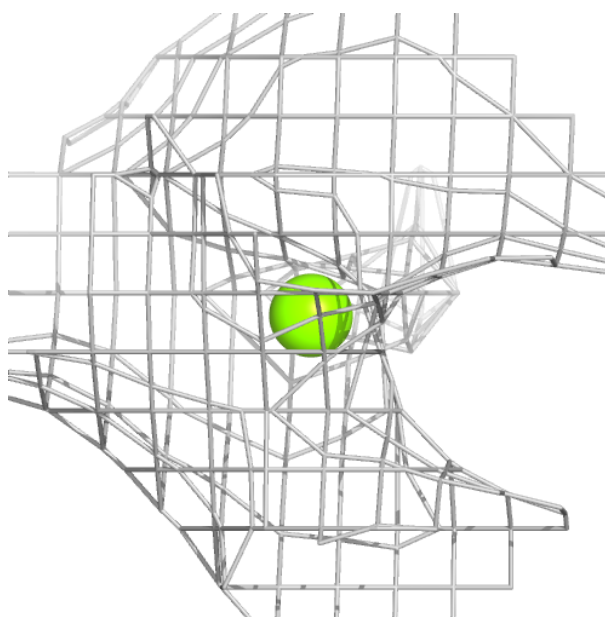
Electron density around MG B 702:

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



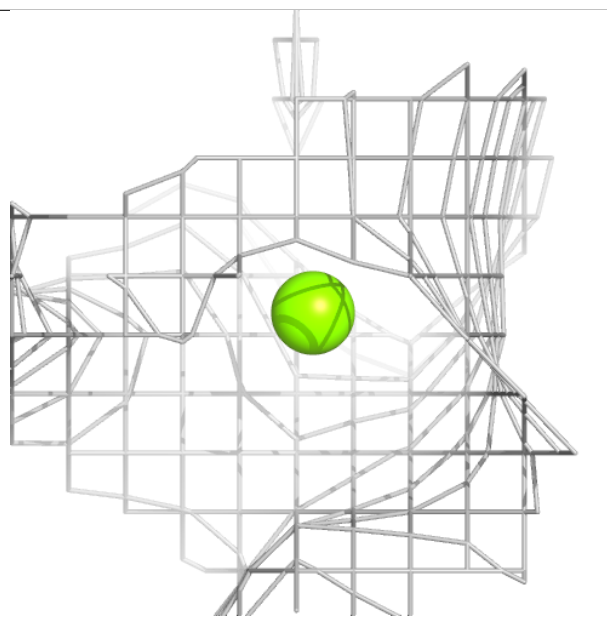
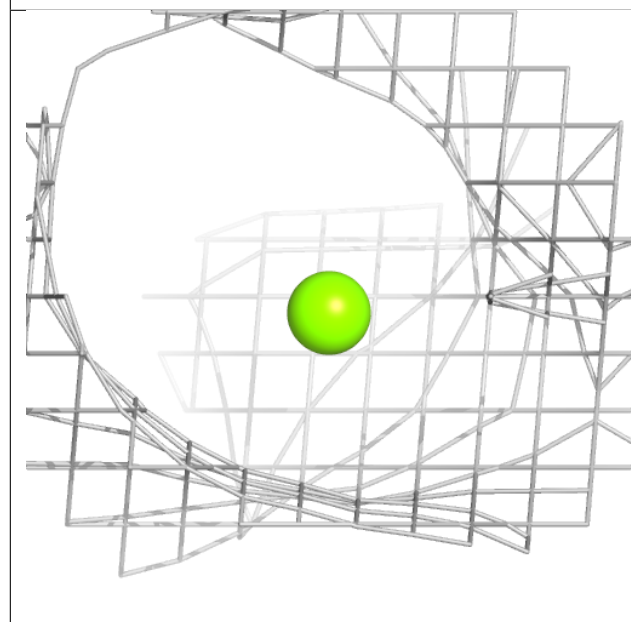
Electron density around MG K 703:

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



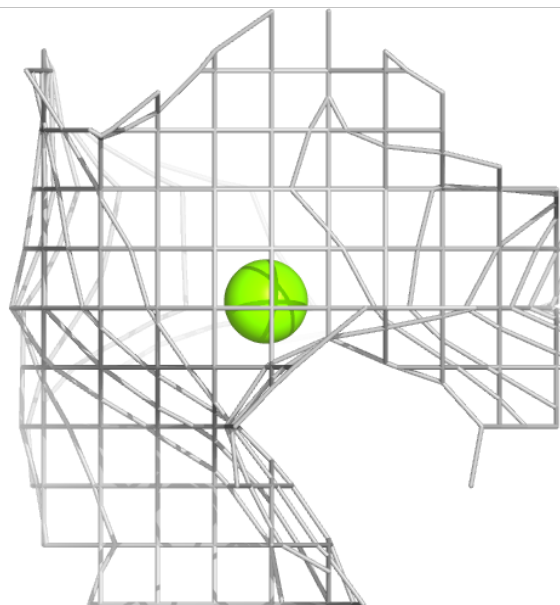
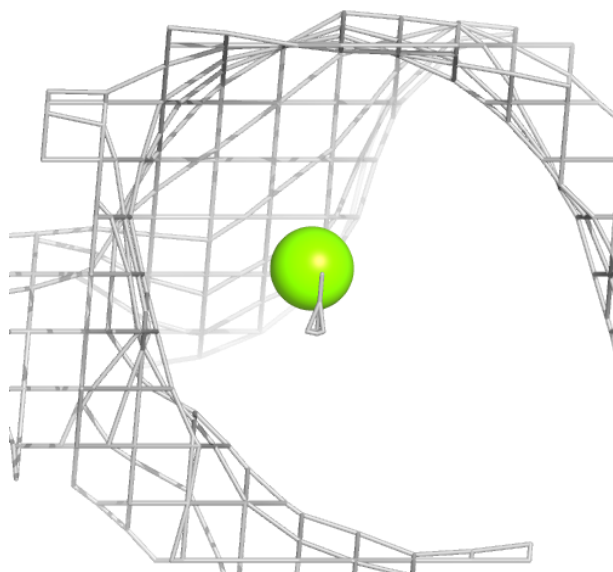
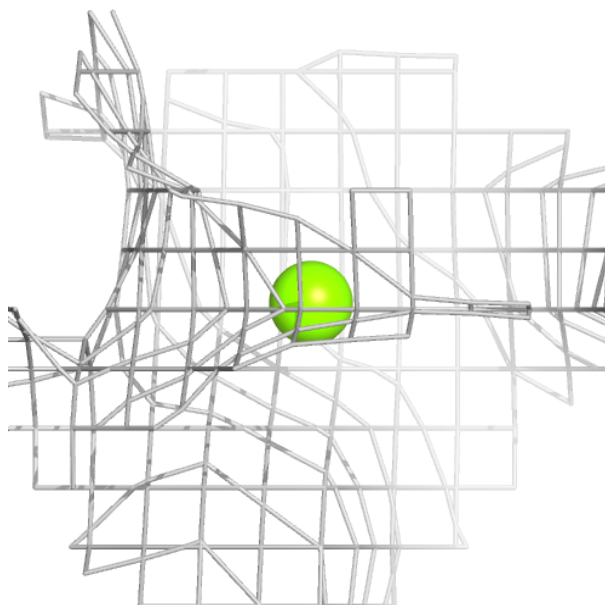
Electron density around MG N 703:

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



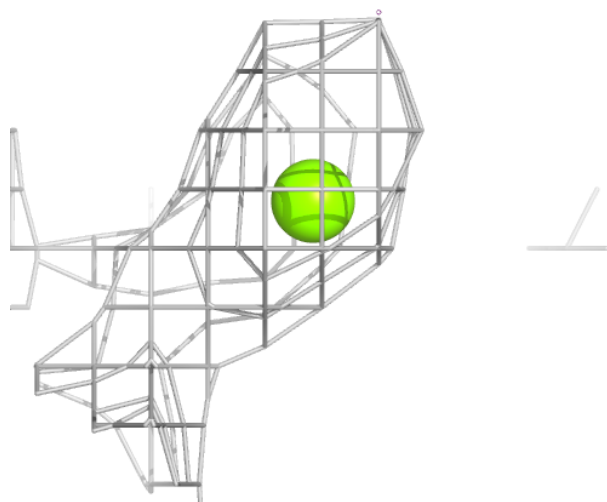
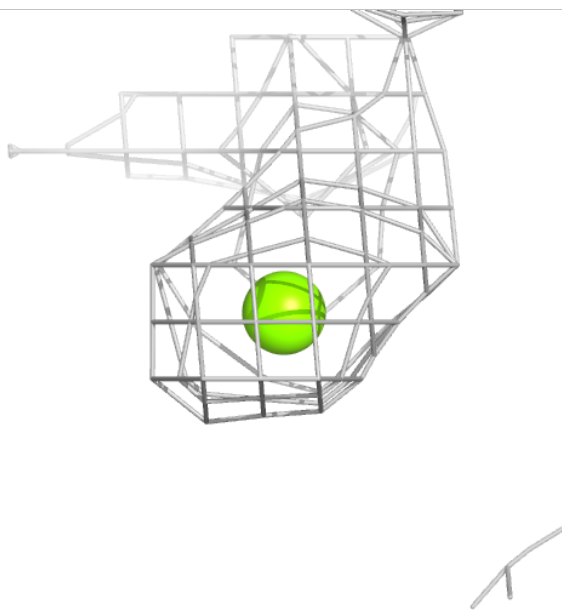
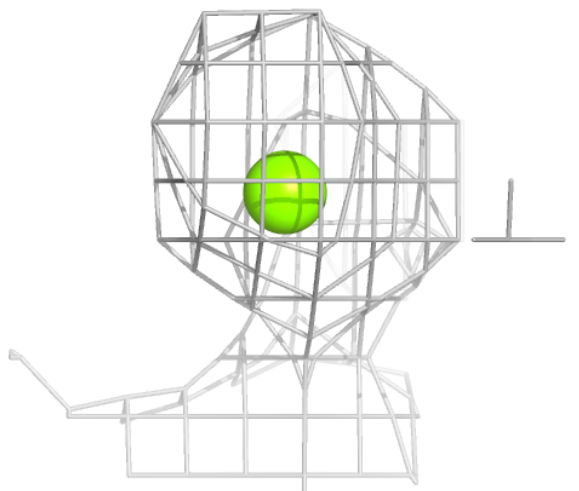
Electron density around MG H 704:

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



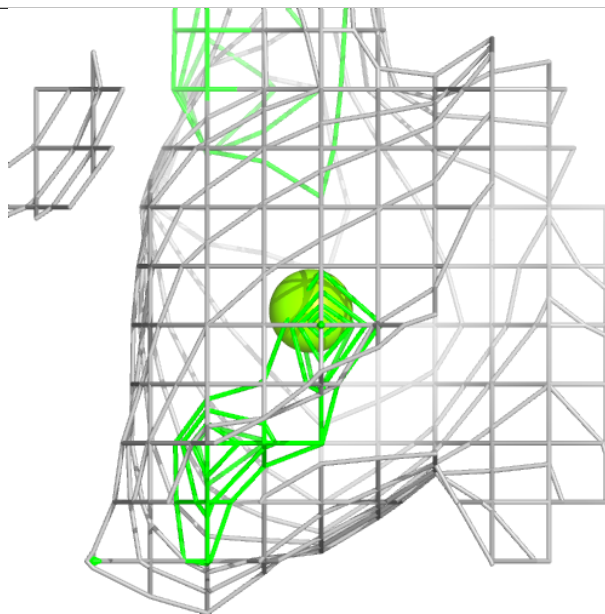
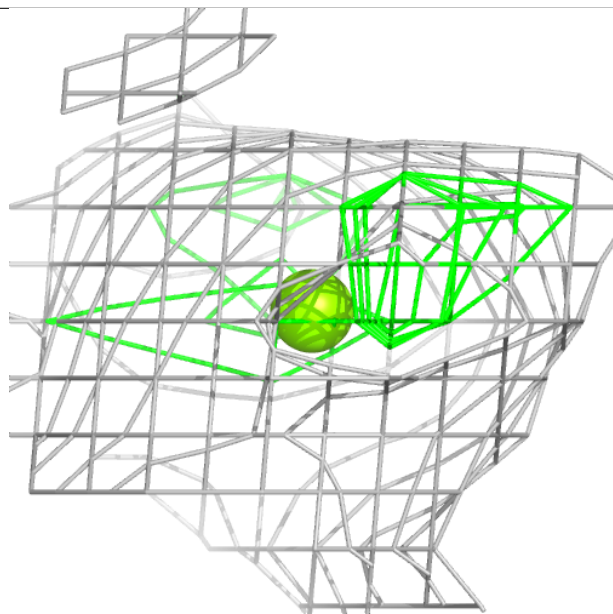
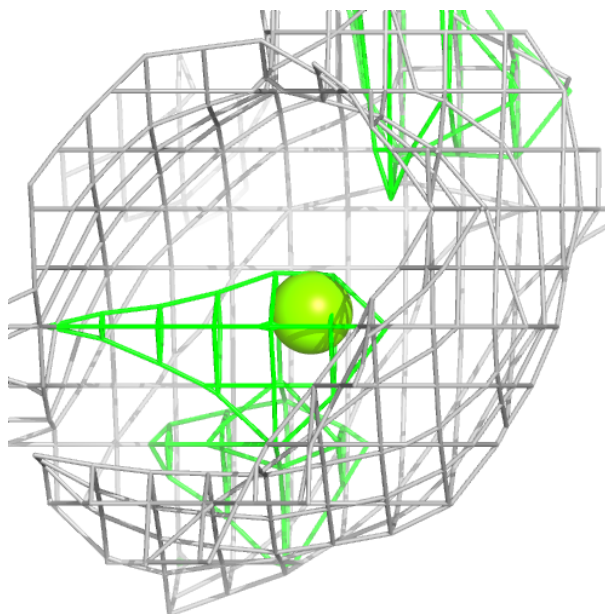
Electron density around MG M 702:

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



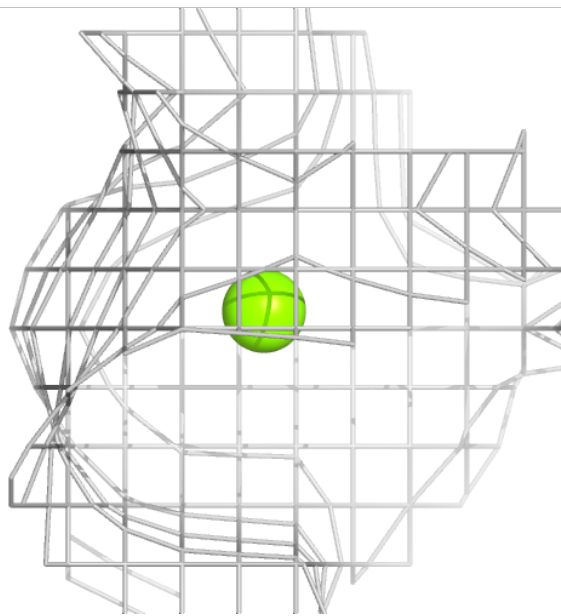
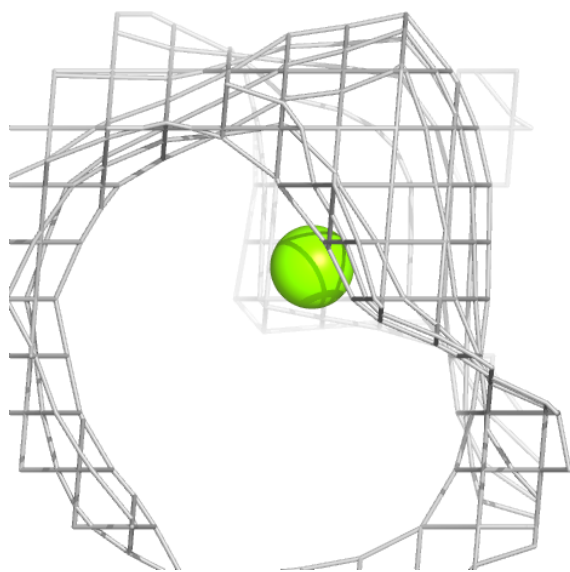
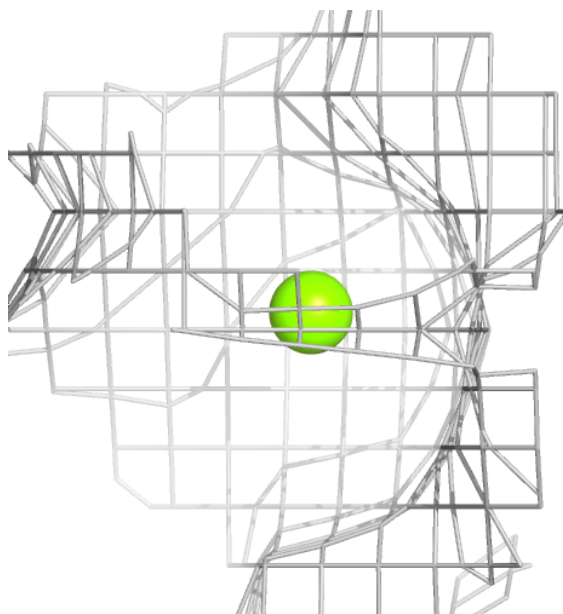
Electron density around MG E 702:

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



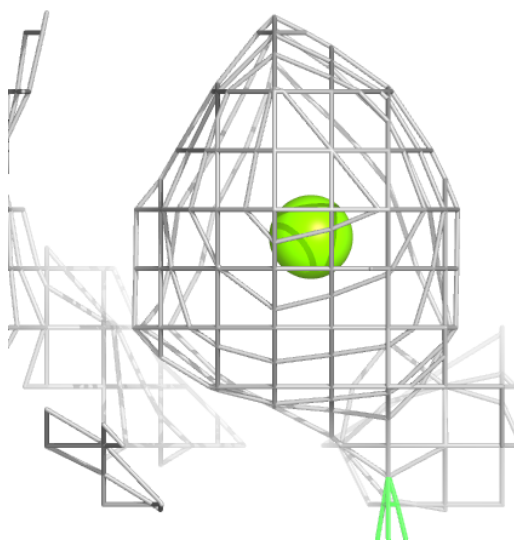
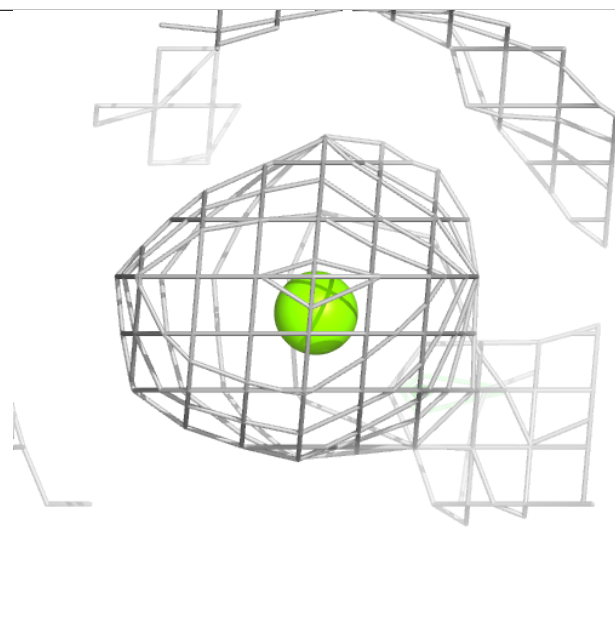
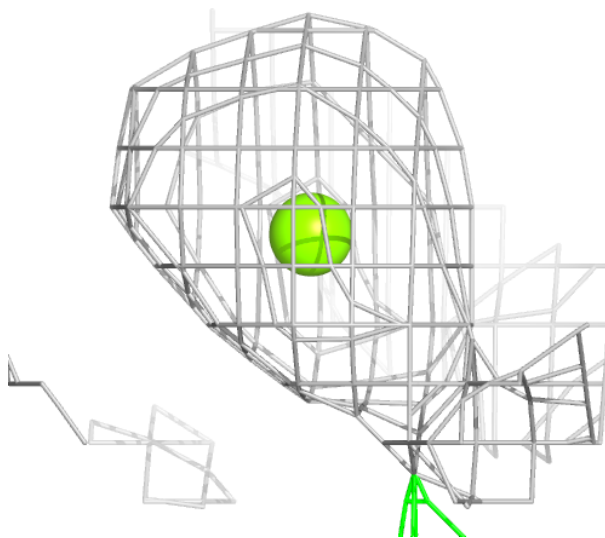
Electron density around MG K 705:

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and green (positive)



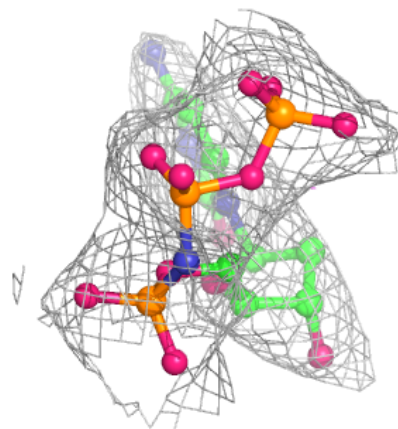
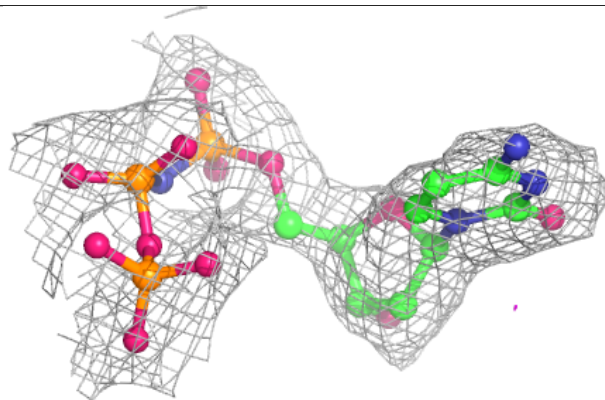
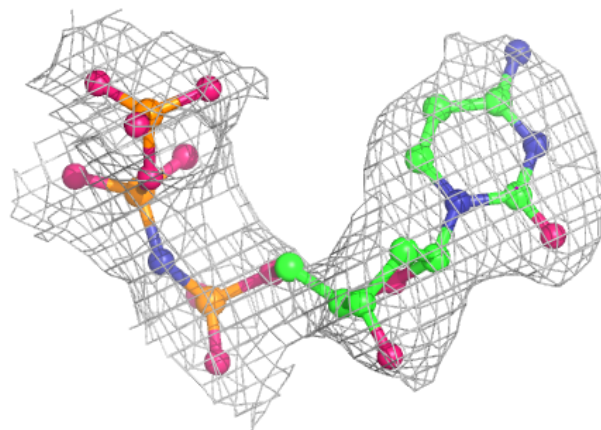
Electron density around MG P 703:

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and green (positive)



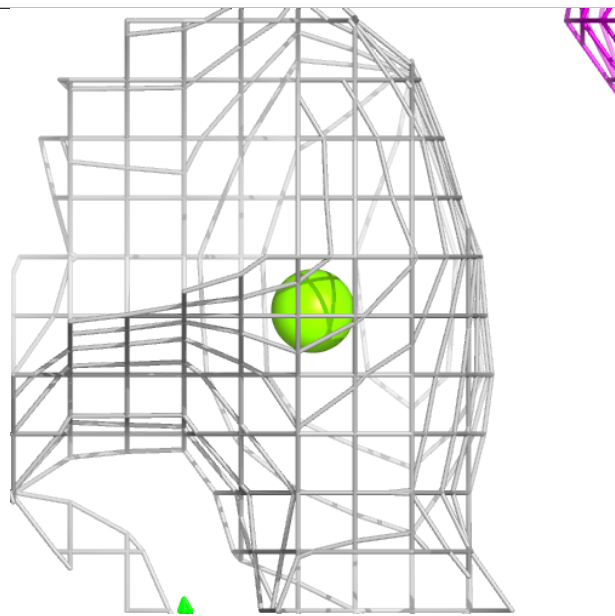
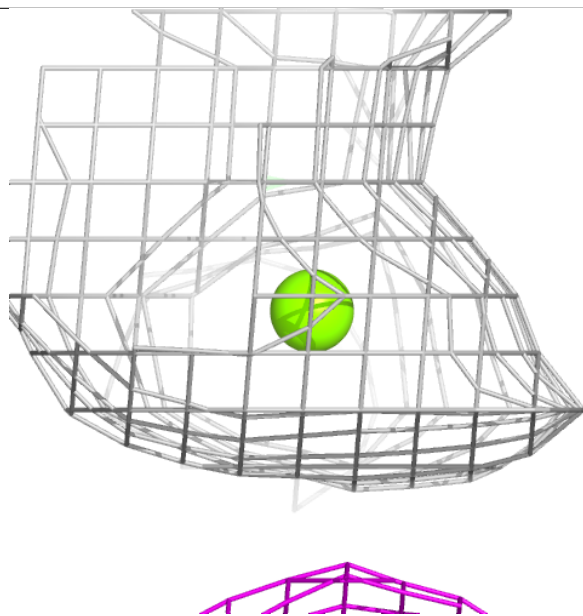
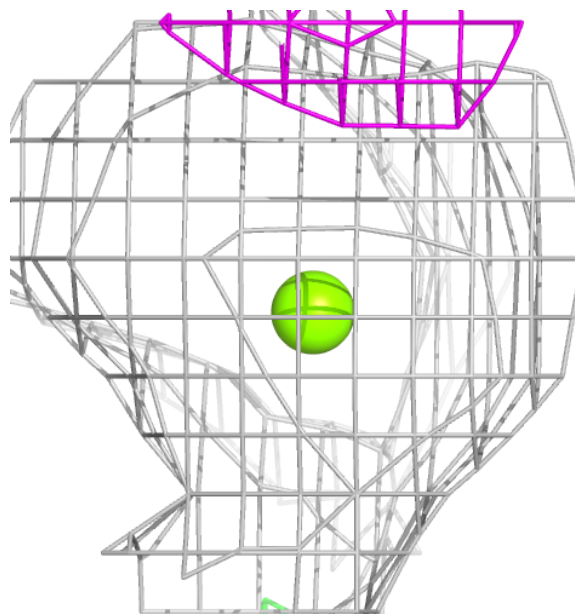
Electron density around 0KX M 705:

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



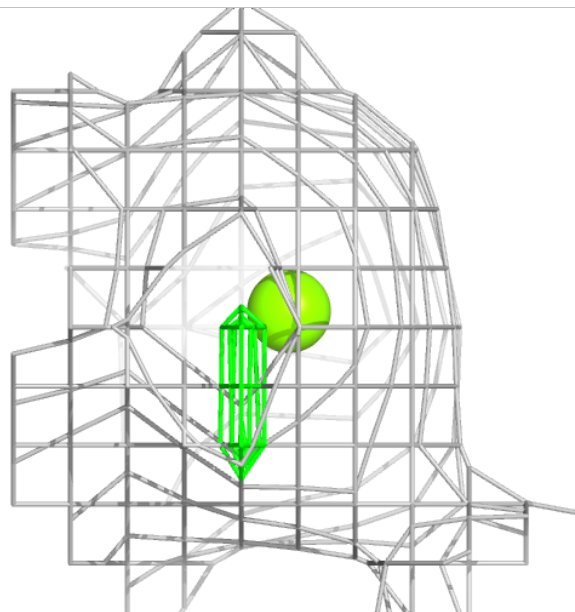
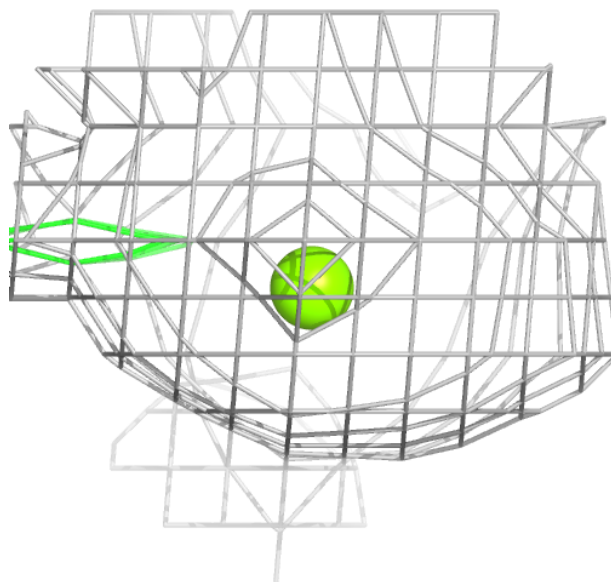
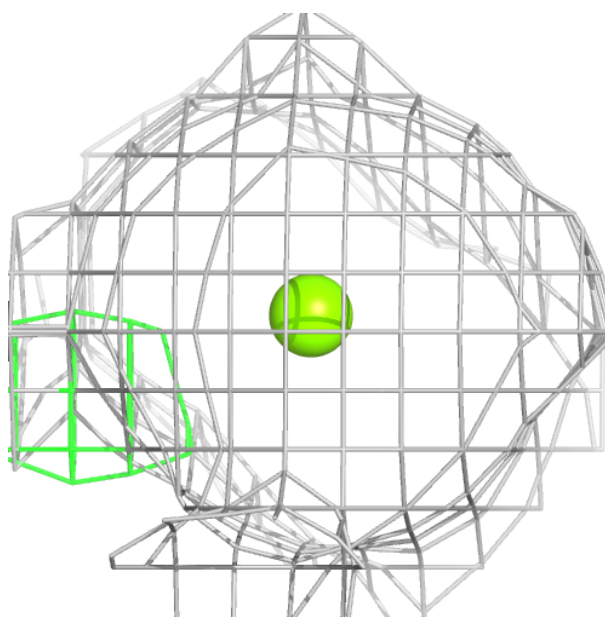
Electron density around MG M 703:

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



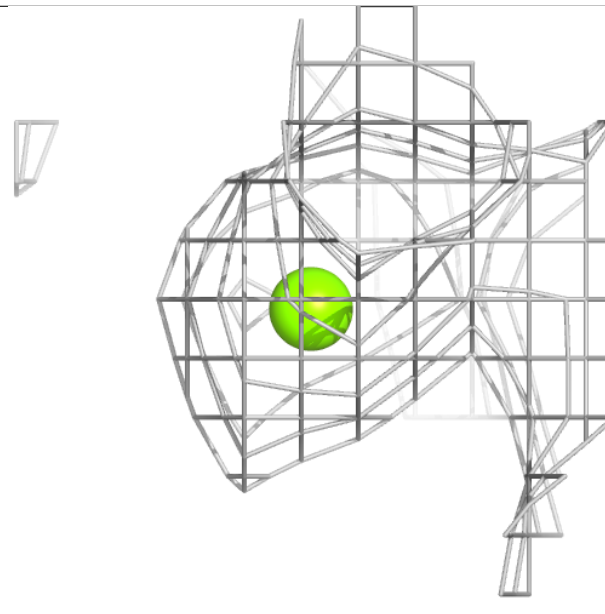
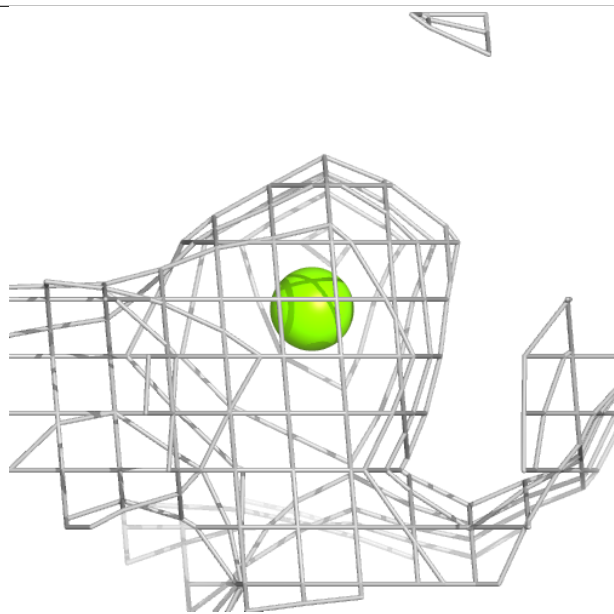
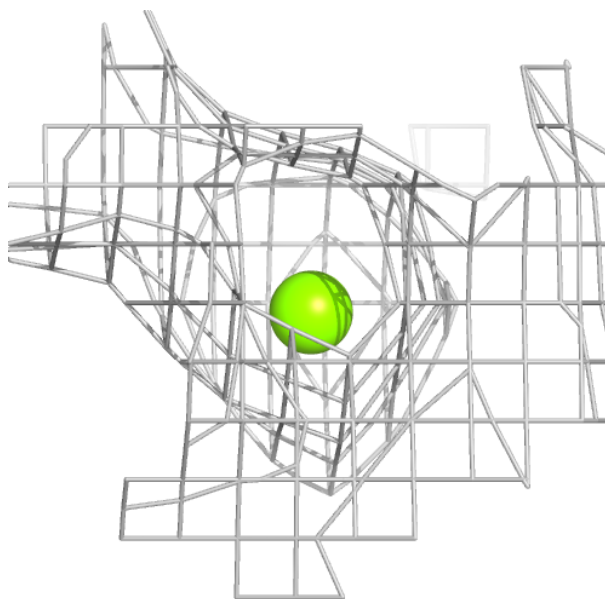
Electron density around MG H 703:

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



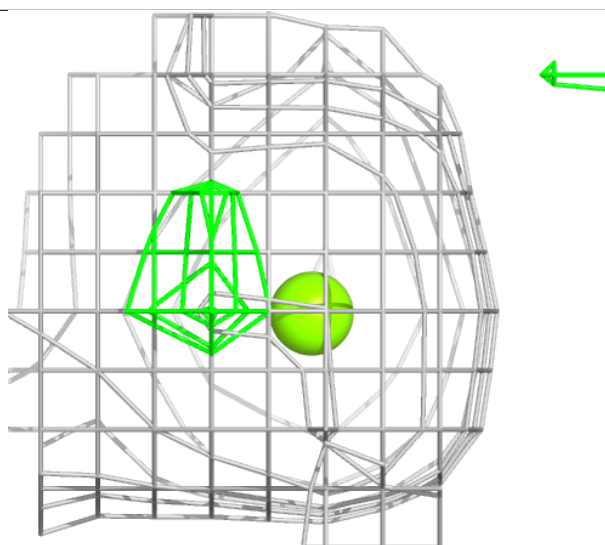
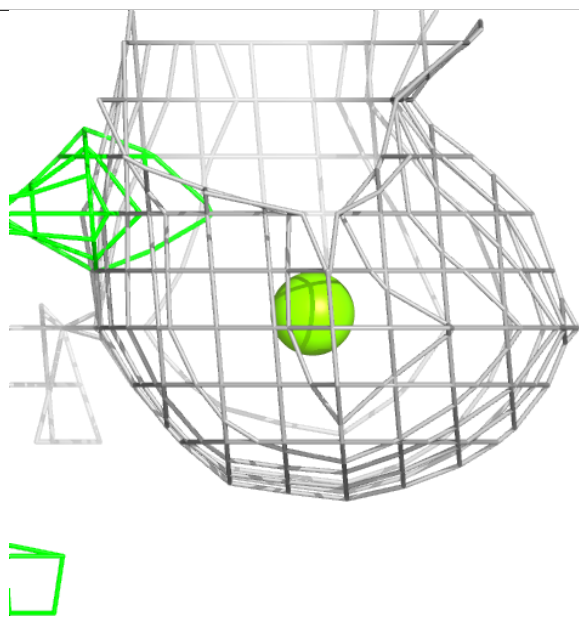
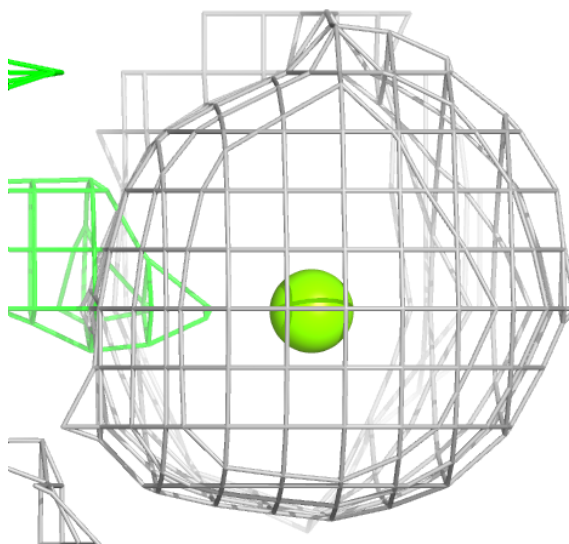
Electron density around MG L 703:

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and green (positive)



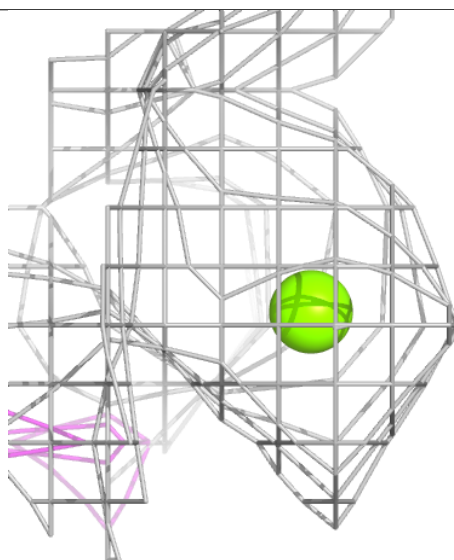
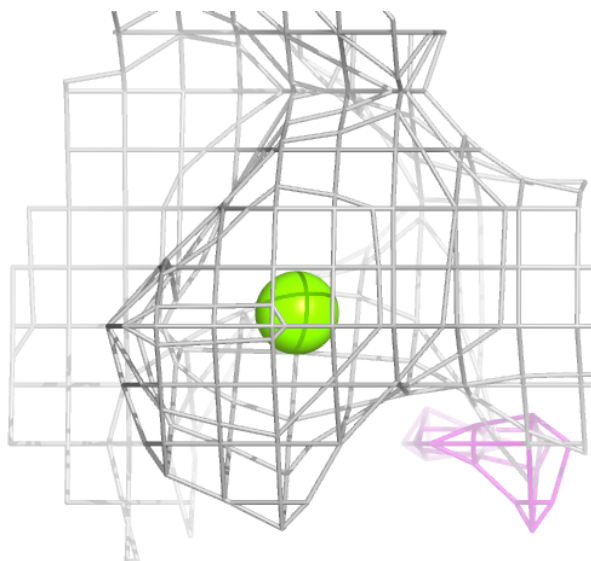
Electron density around MG L 704:

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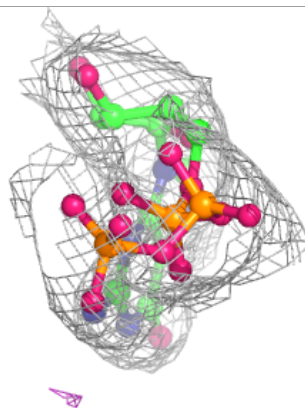
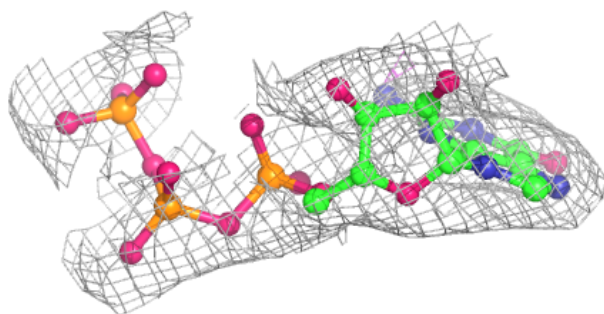
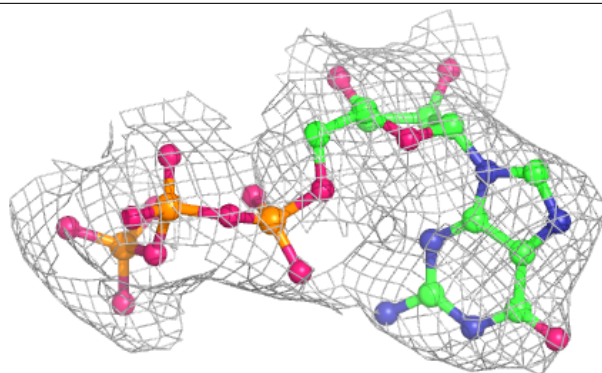
Electron density around MG D 703:

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and green (positive)



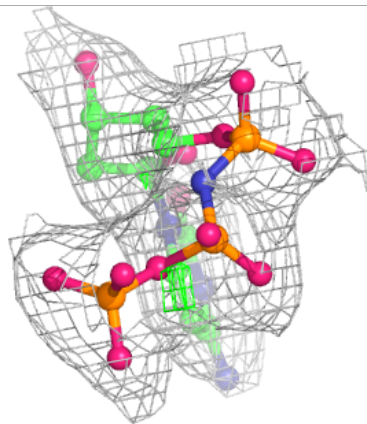
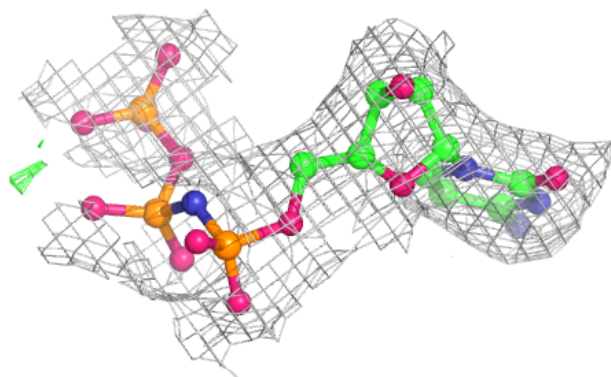
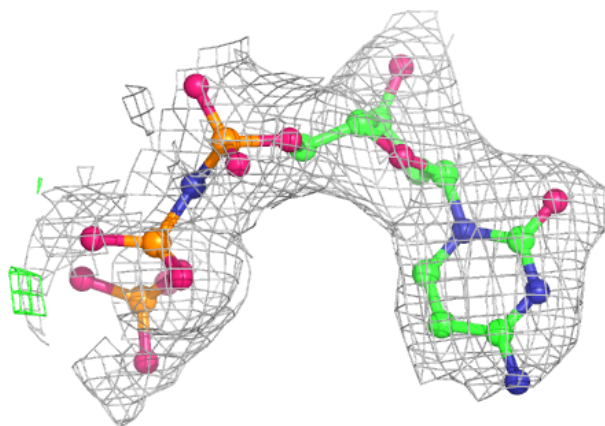
Electron density around GTP F 705:

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



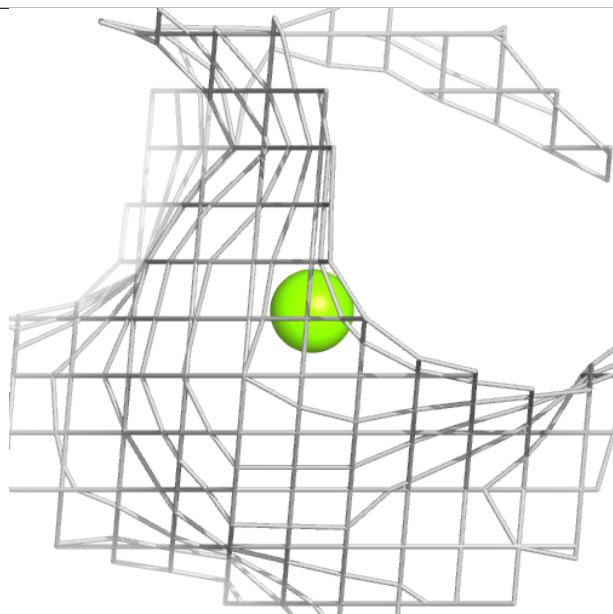
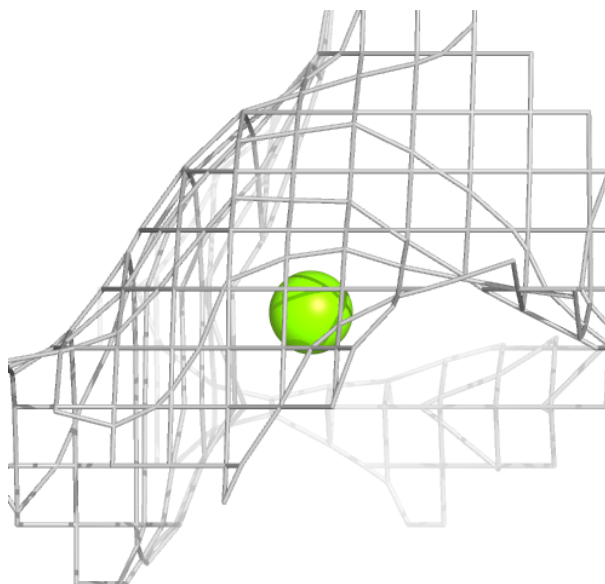
Electron density around 0KX G 706:

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



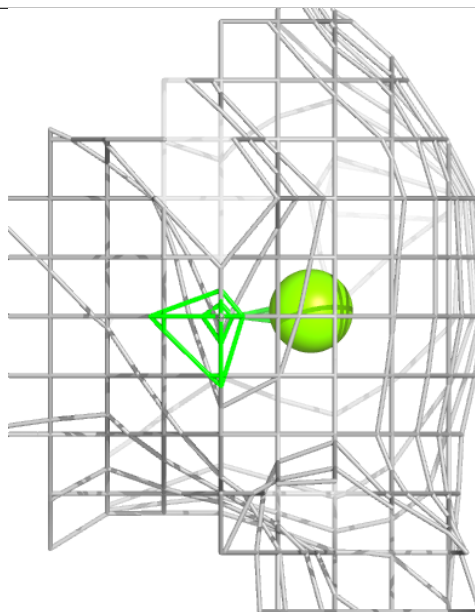
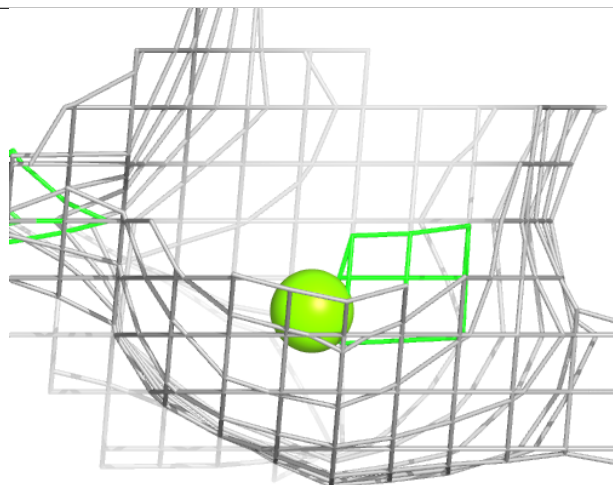
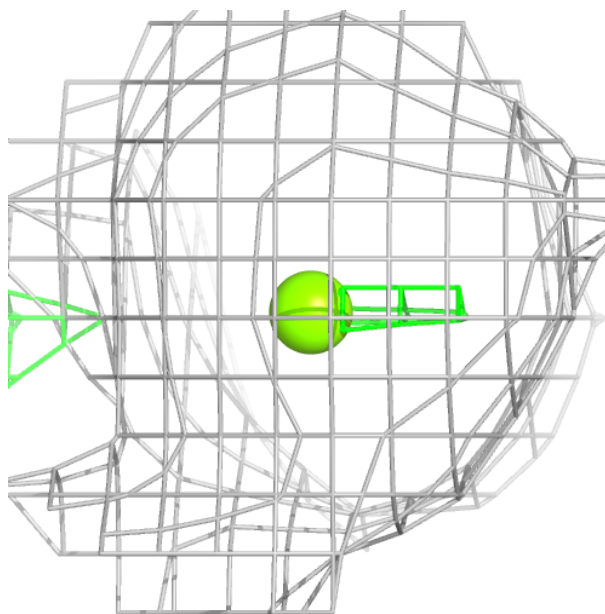
Electron density around MG F 703:

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



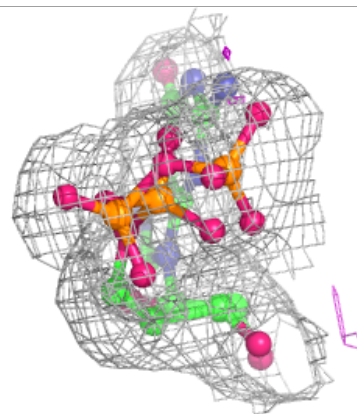
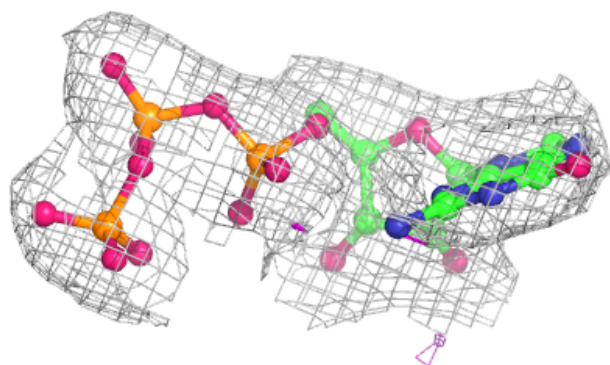
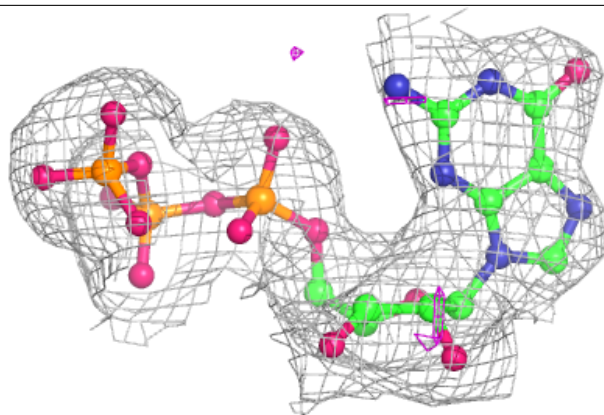
Electron density around MG G 704:

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

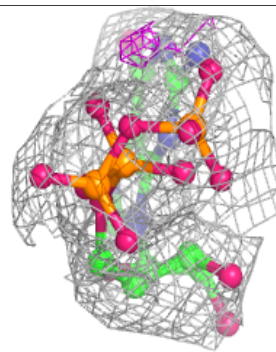
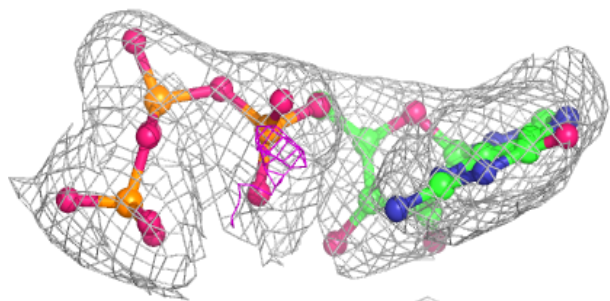
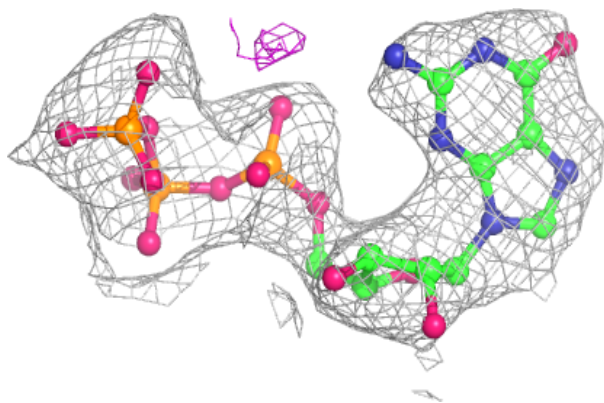


Electron density around GTP H 706:

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

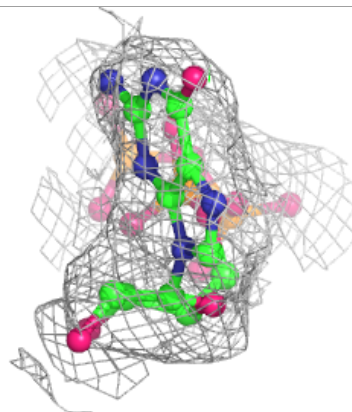
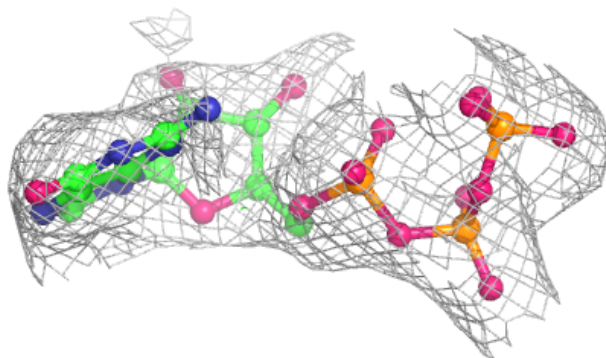
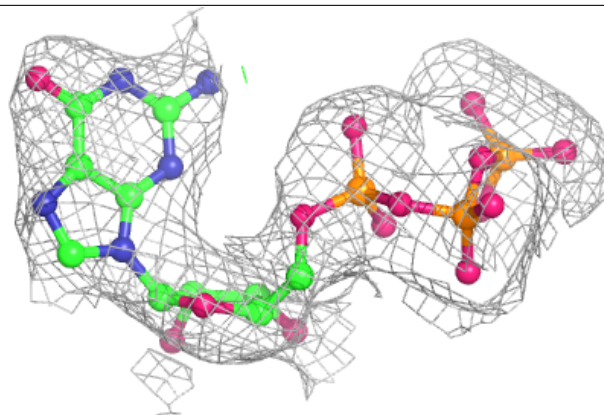
**Electron density around GTP M 706:**

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

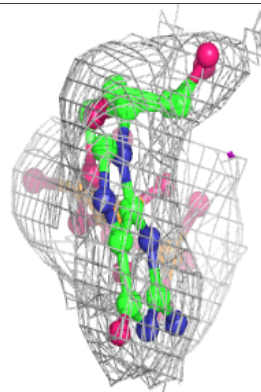
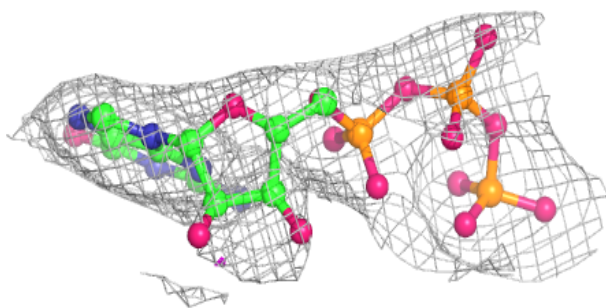
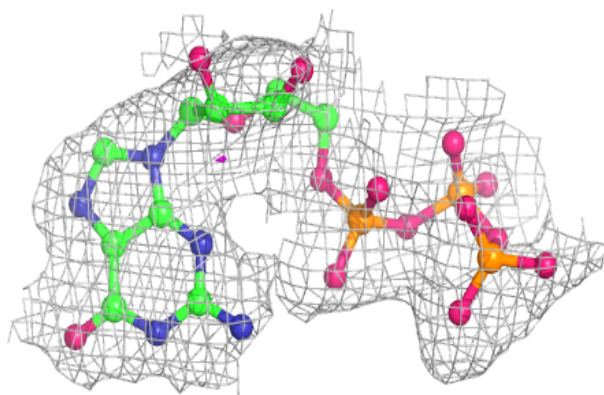


Electron density around GTP N 705:

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

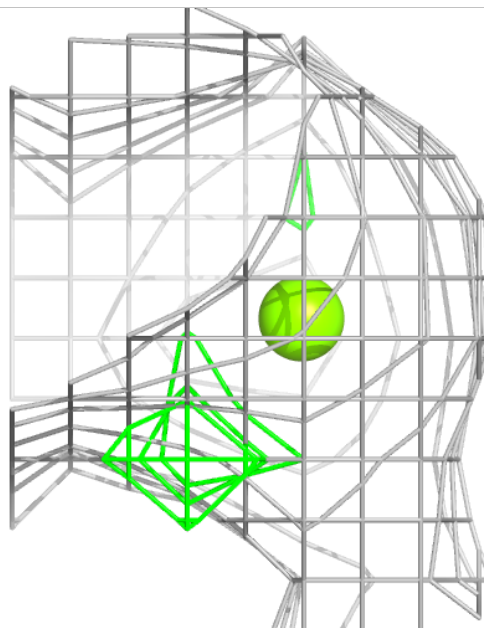
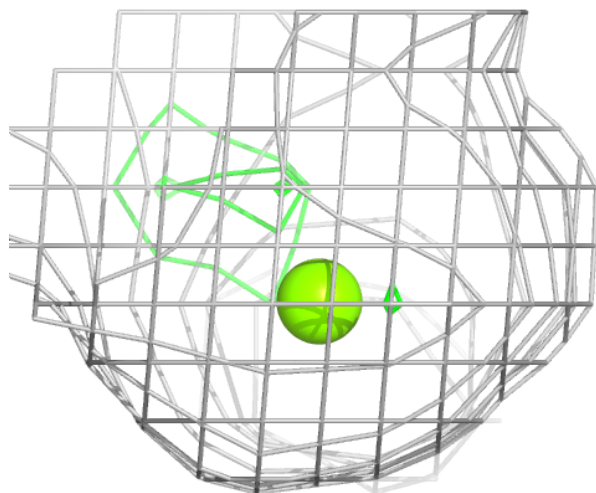
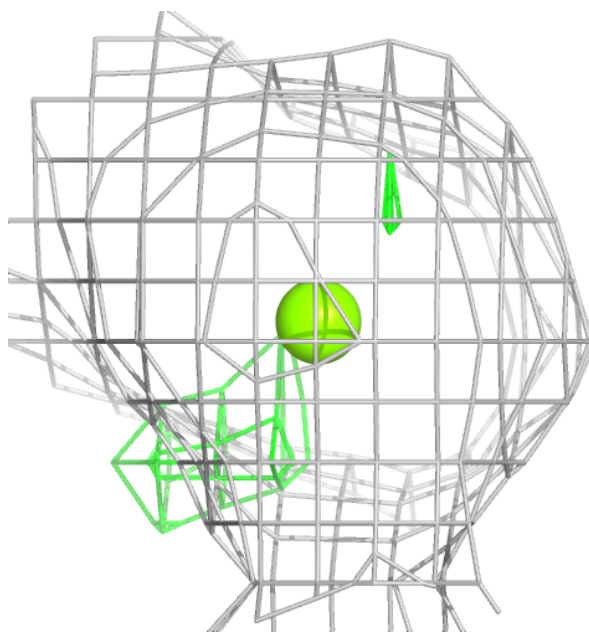
**Electron density around GTP O 706:**

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



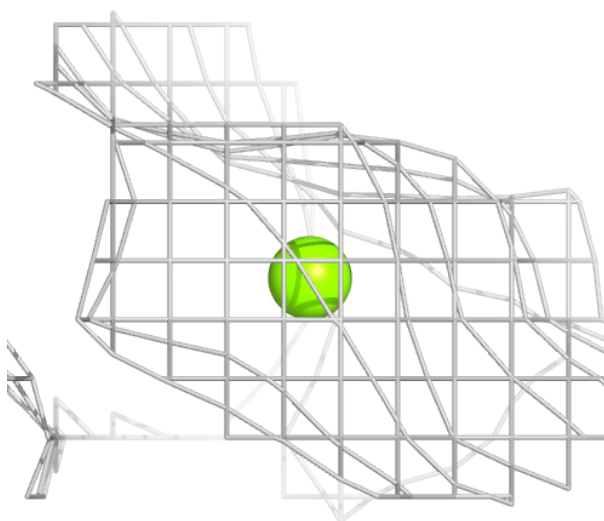
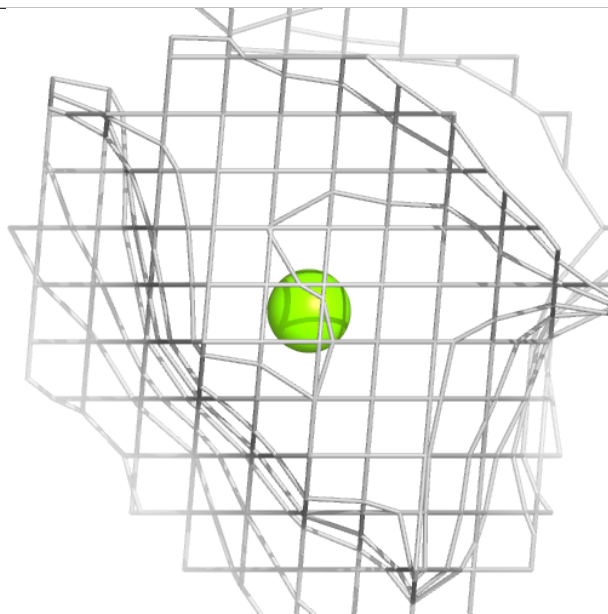
Electron density around MG I 703:

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



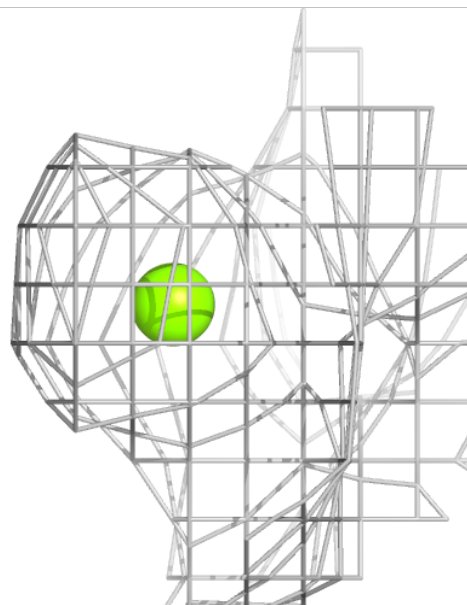
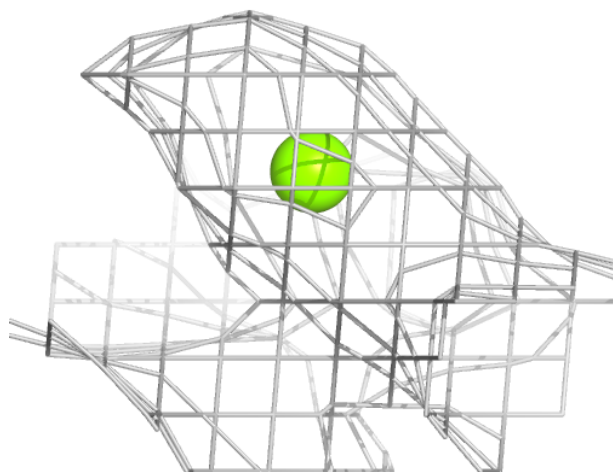
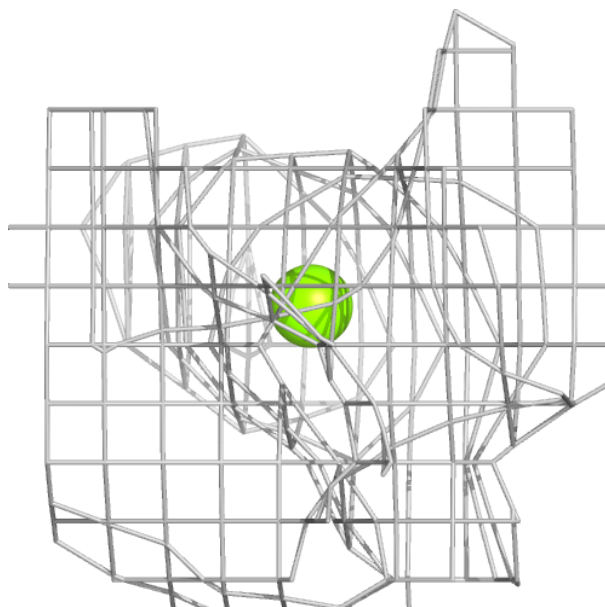
Electron density around MG P 705:

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



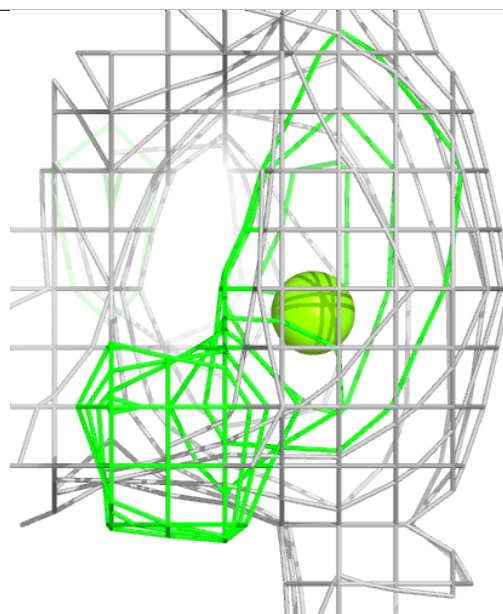
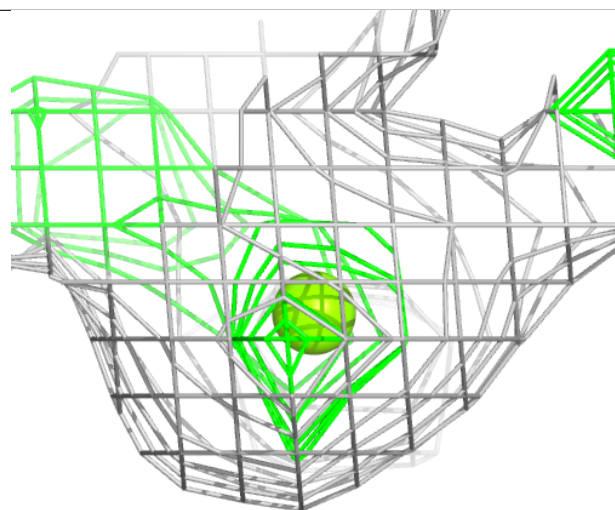
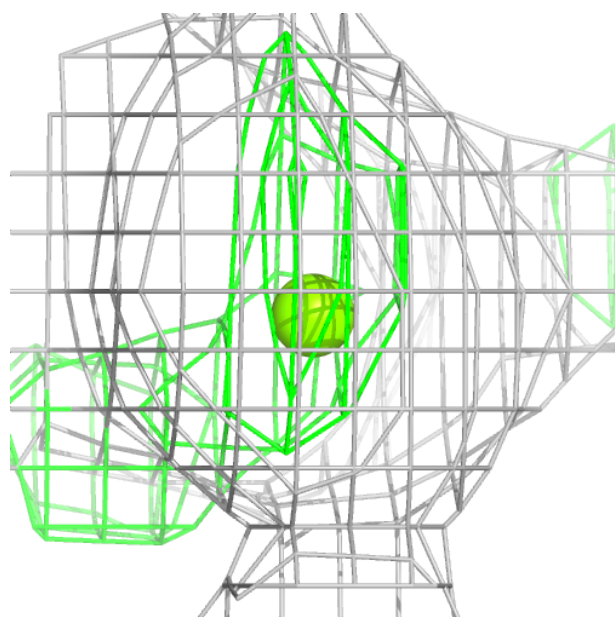
Electron density around MG C 703:

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



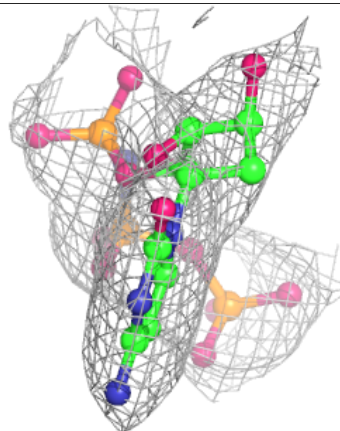
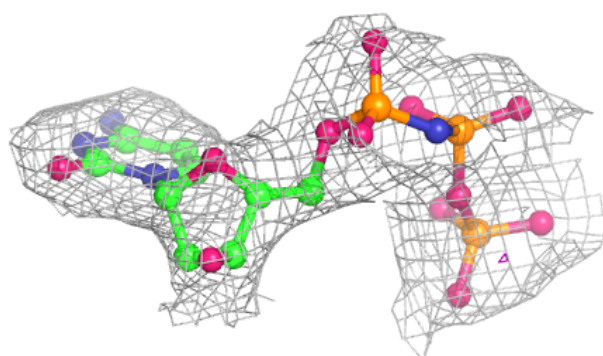
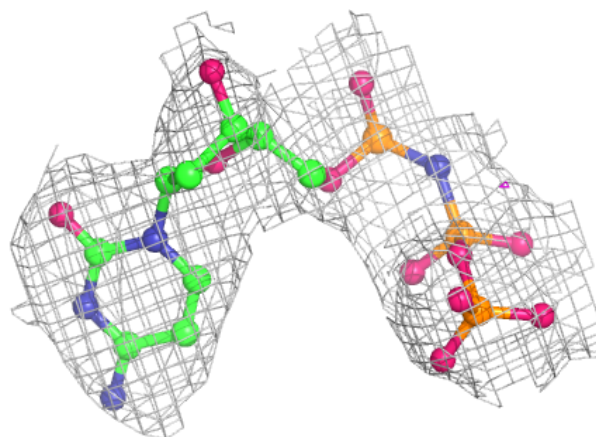
Electron density around MG F 702:

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

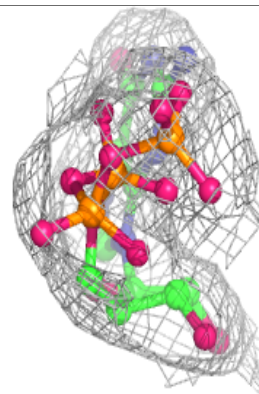
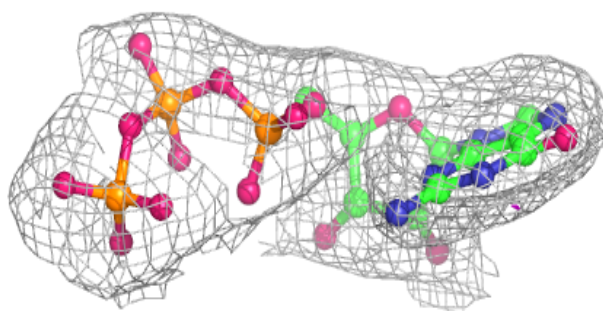
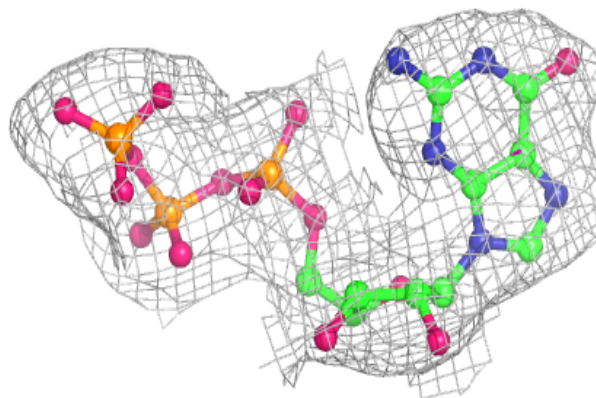


Electron density around 0KX N 704:

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

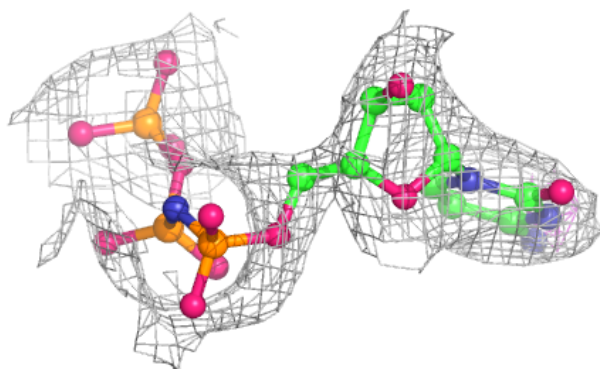
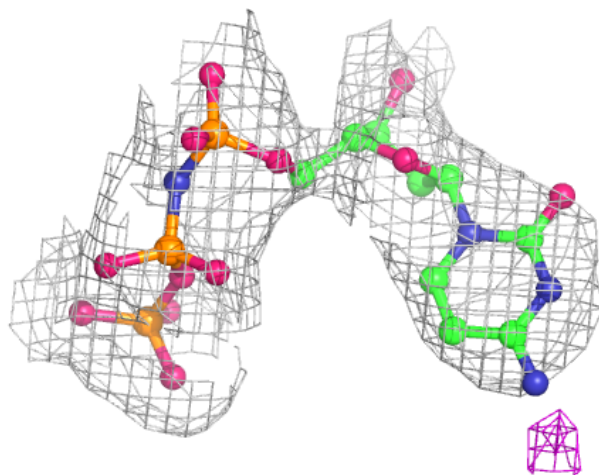
**Electron density around GTP O 707:**

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



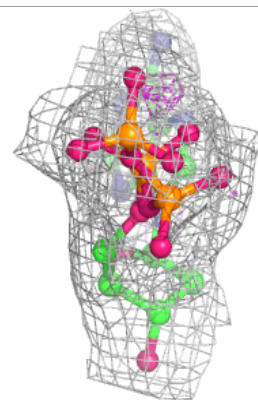
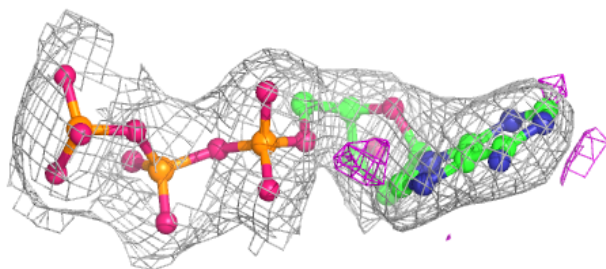
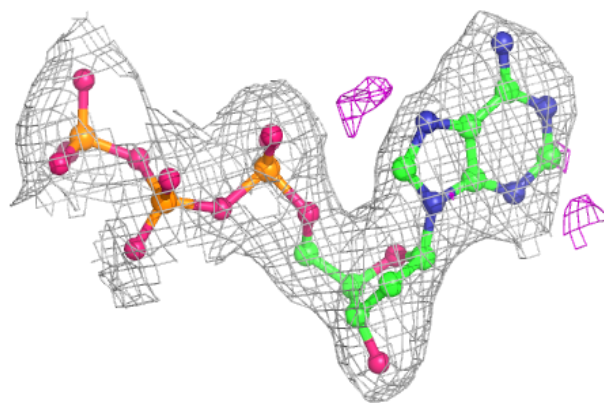
Electron density around 0KX O 705:

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

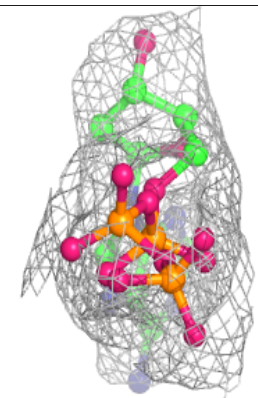
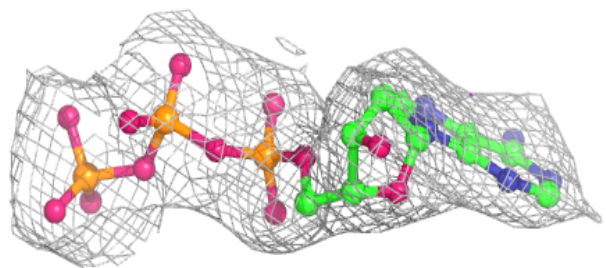
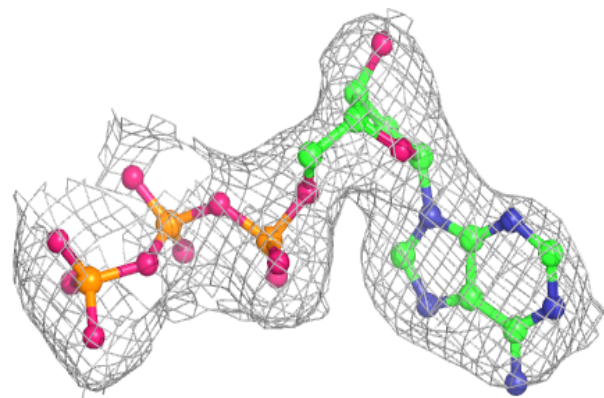


Electron density around DTP E 706:

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

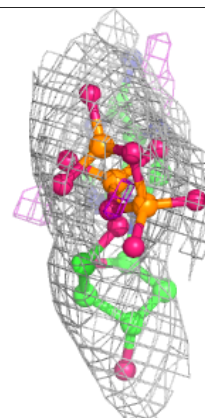
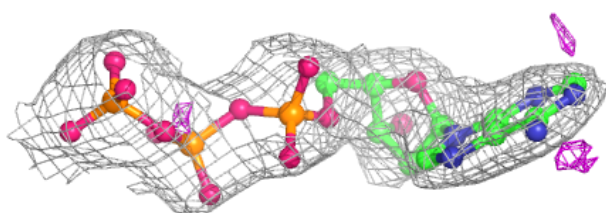
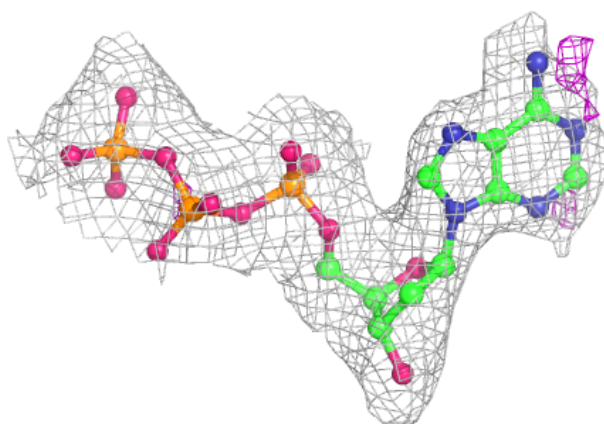
**Electron density around DTP F 706:**

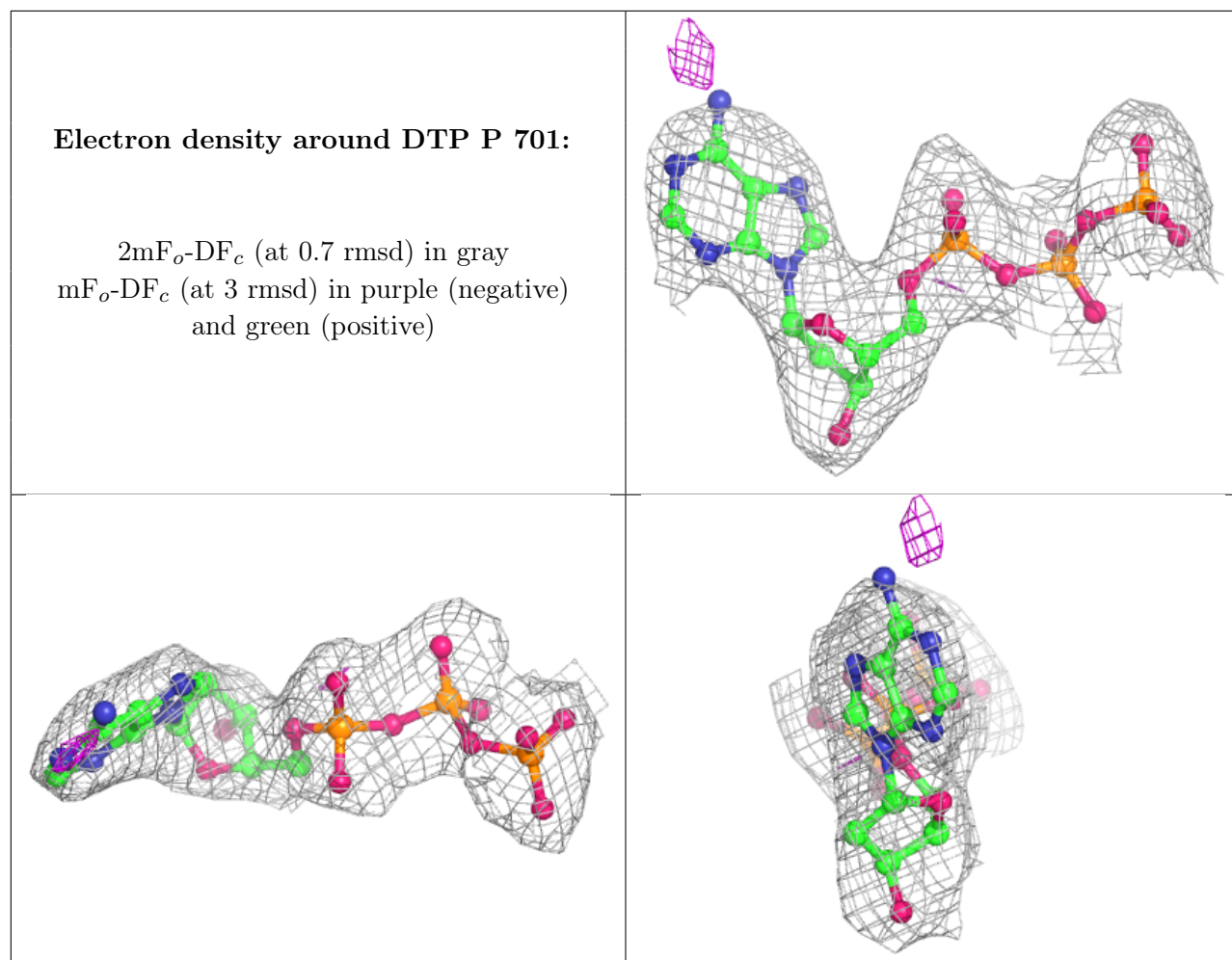
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around DTP G 701:

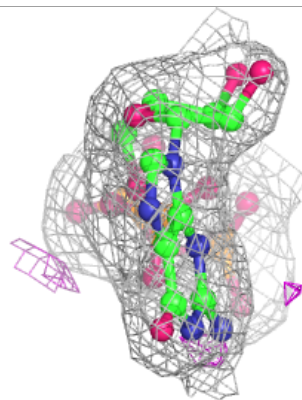
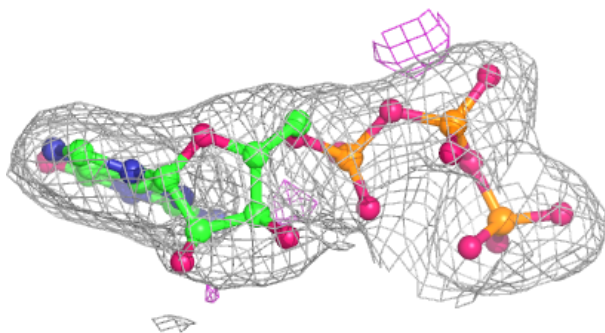
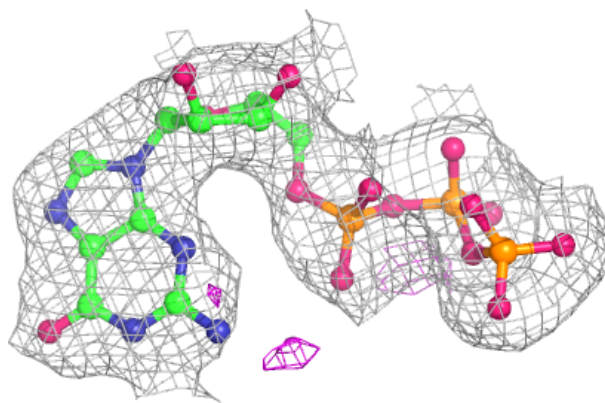
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



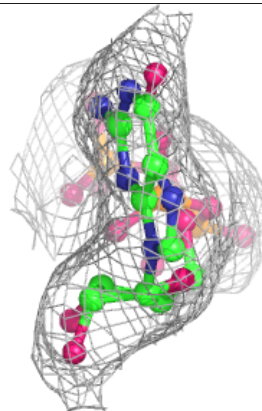
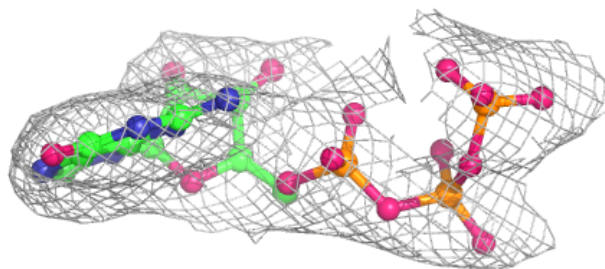
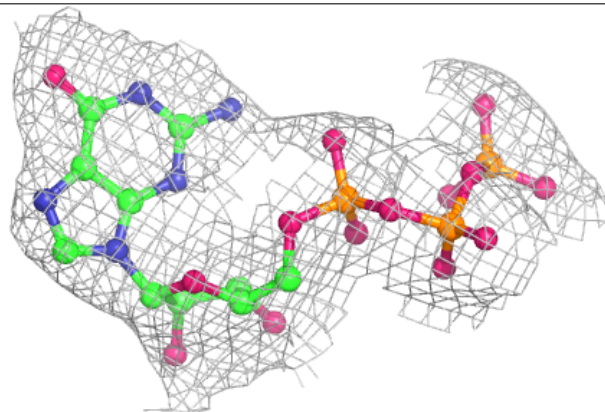


Electron density around GTP A 706:

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

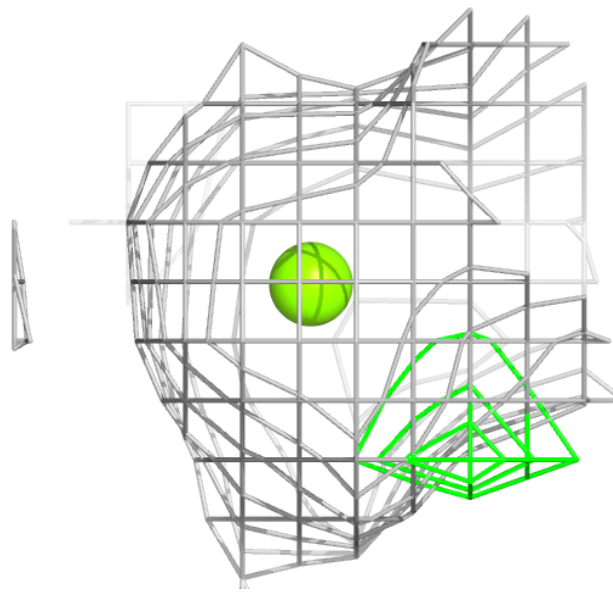
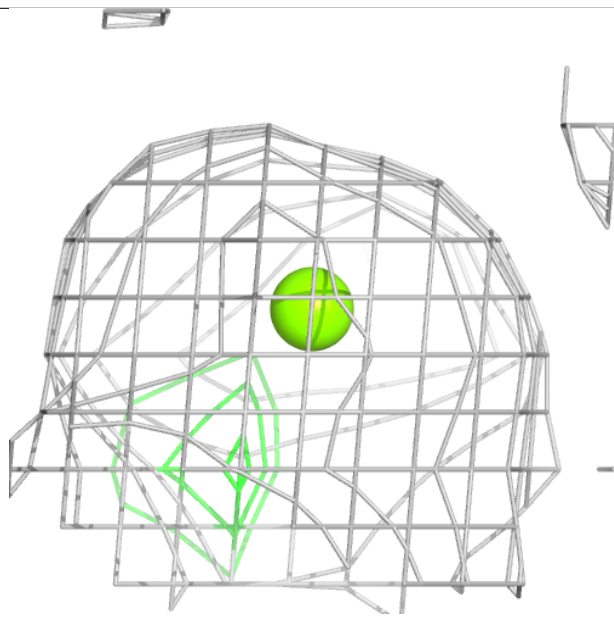
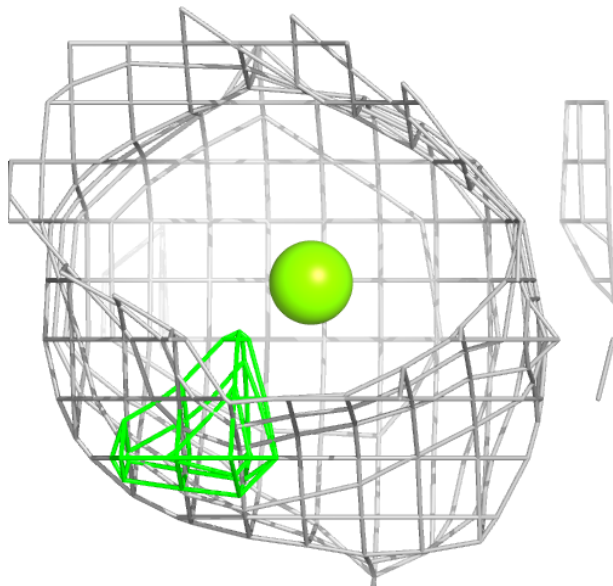
**Electron density around GTP E 705:**

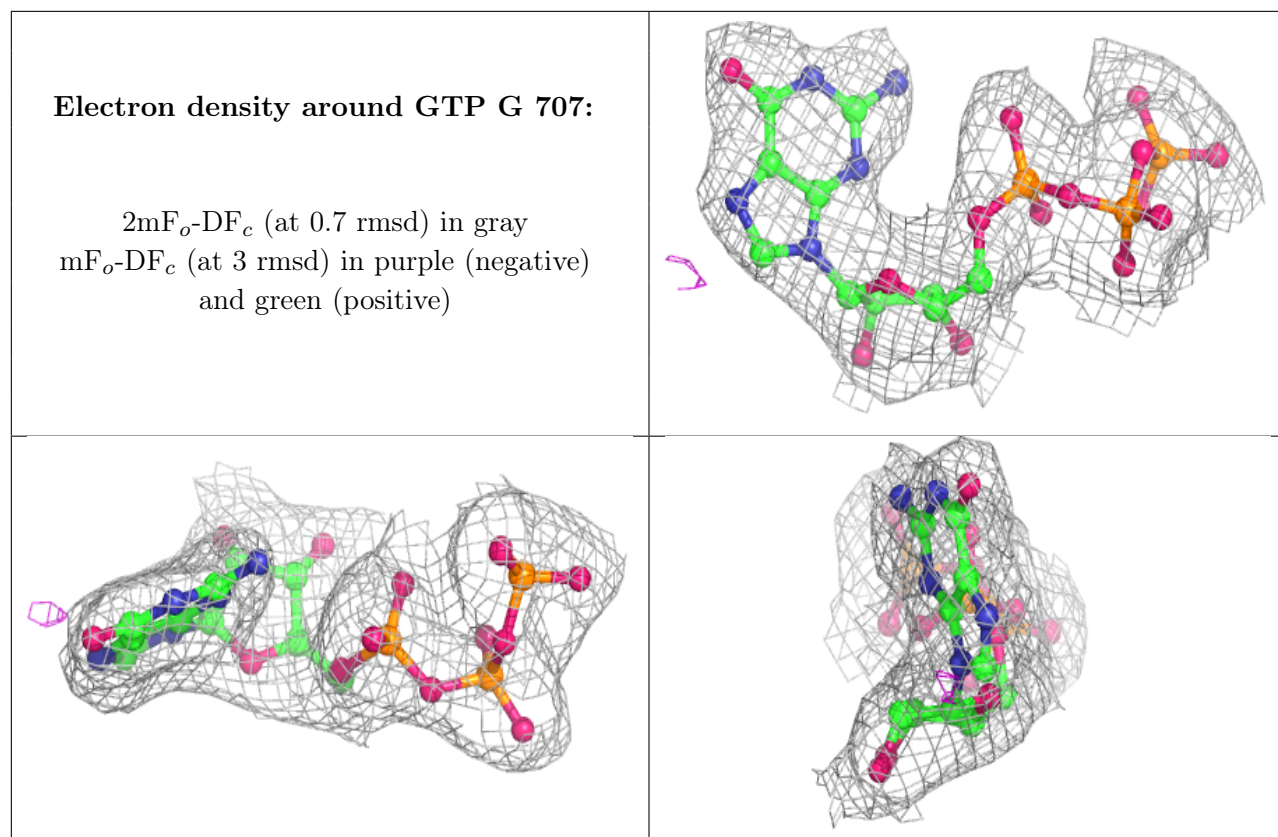
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG D 704:

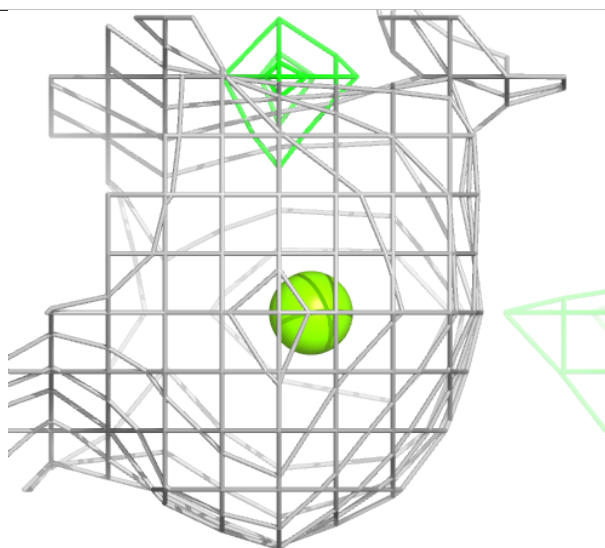
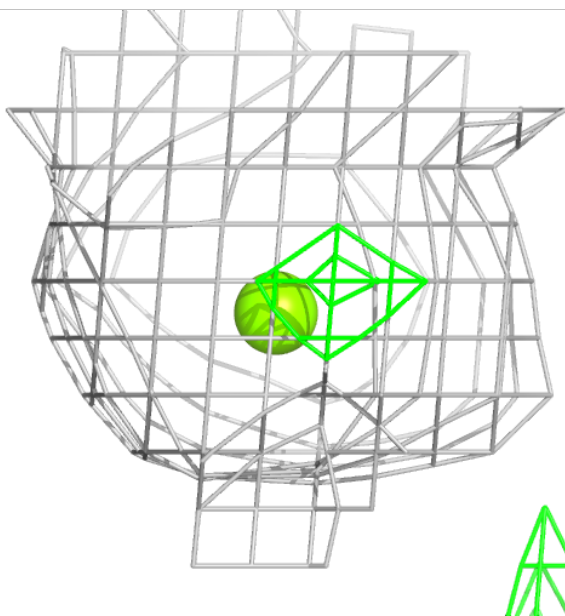
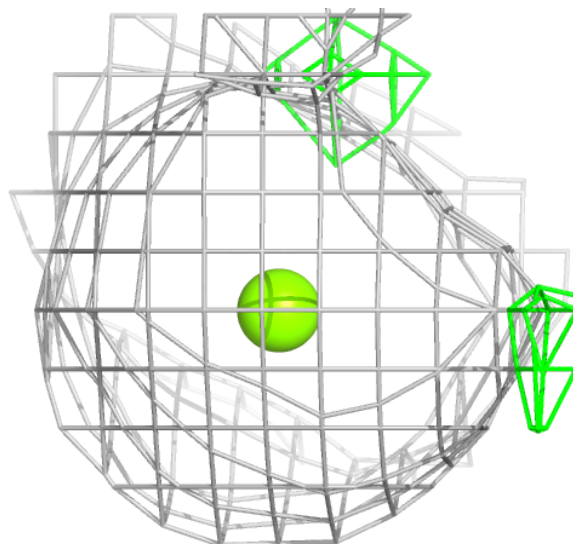
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





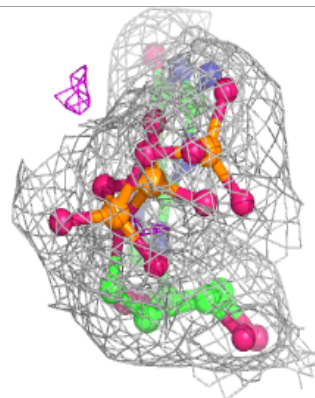
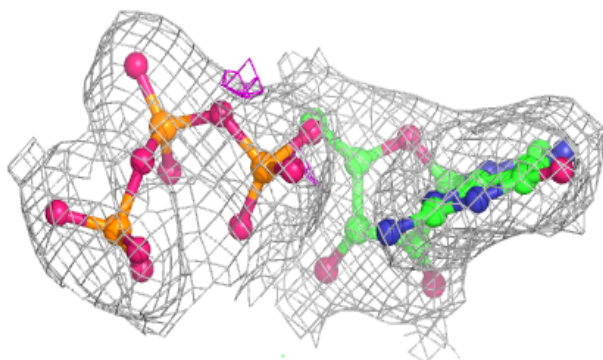
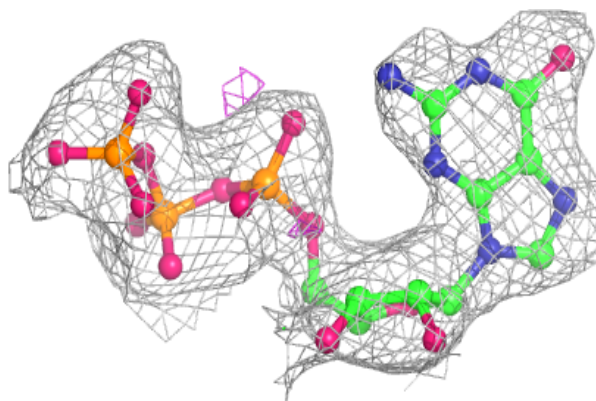
Electron density around MG K 704:

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

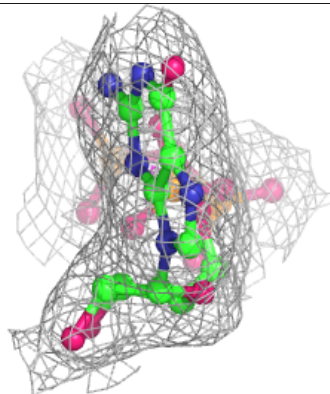
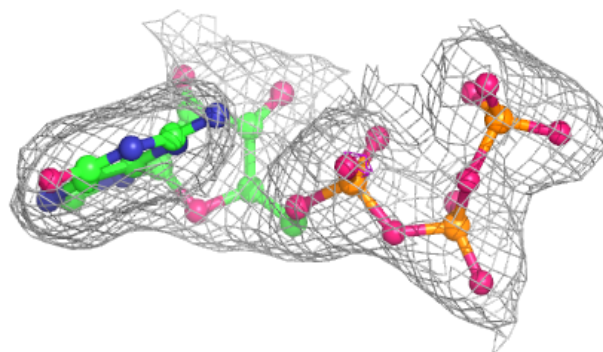
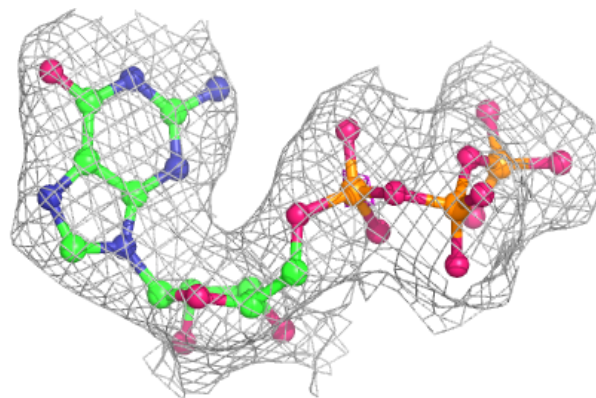


Electron density around GTP I 706:

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

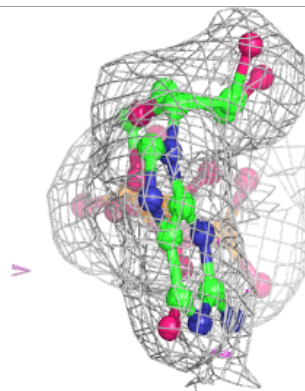
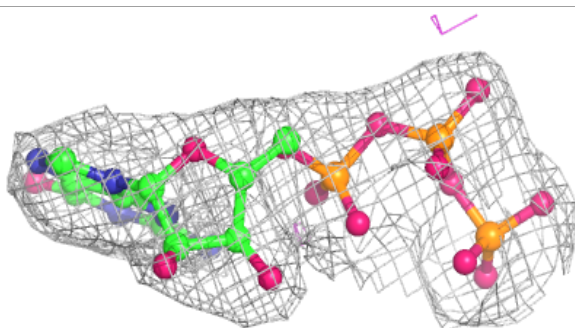
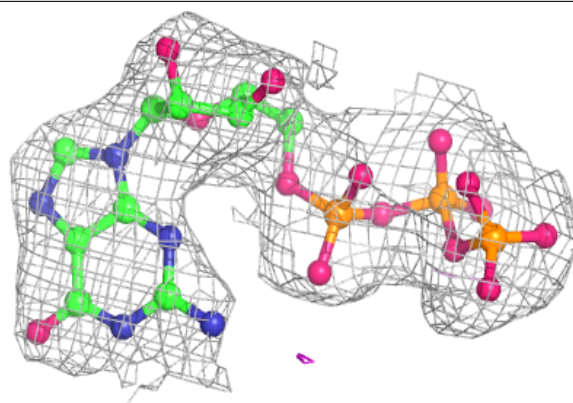
**Electron density around GTP J 705:**

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

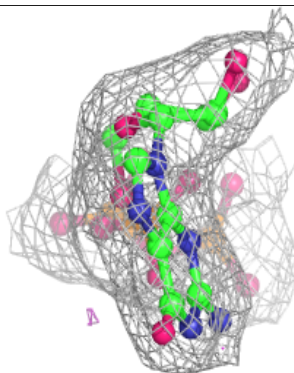
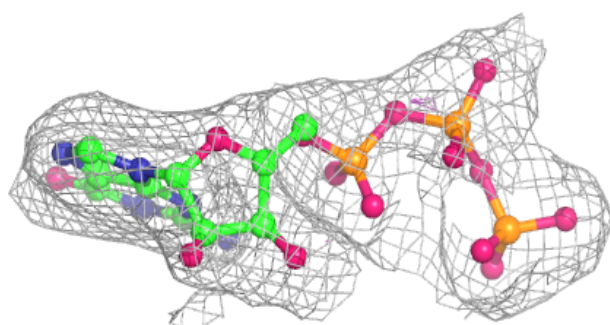
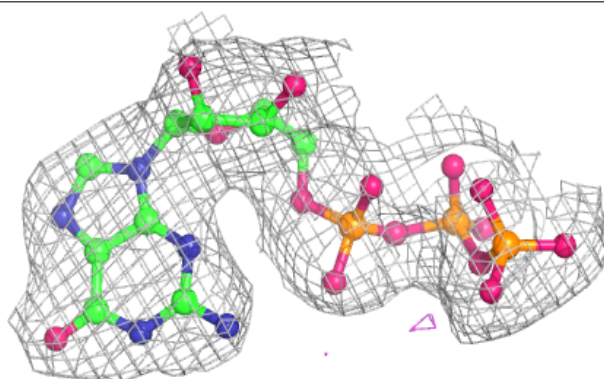


Electron density around GTP K 707:

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

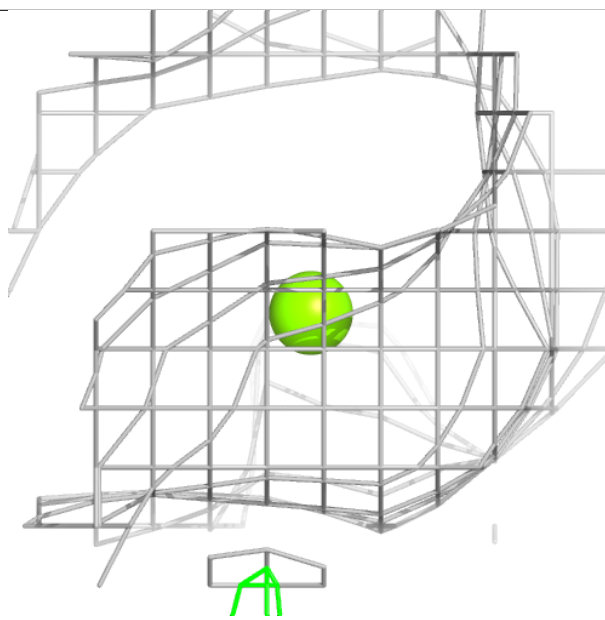
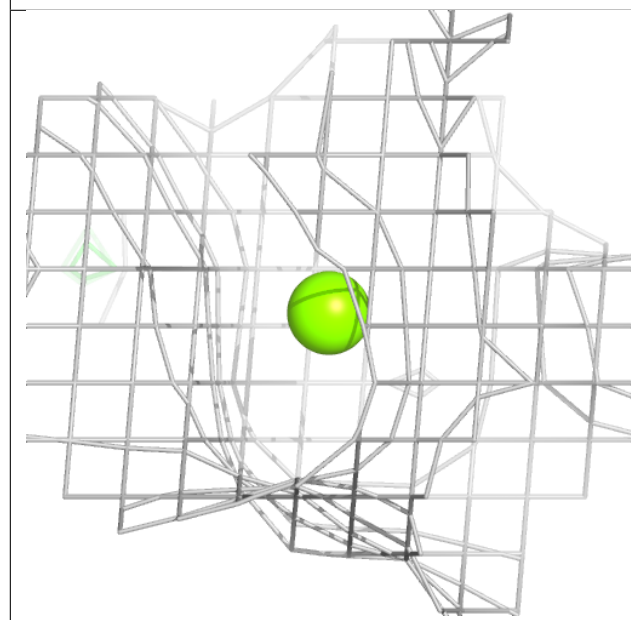
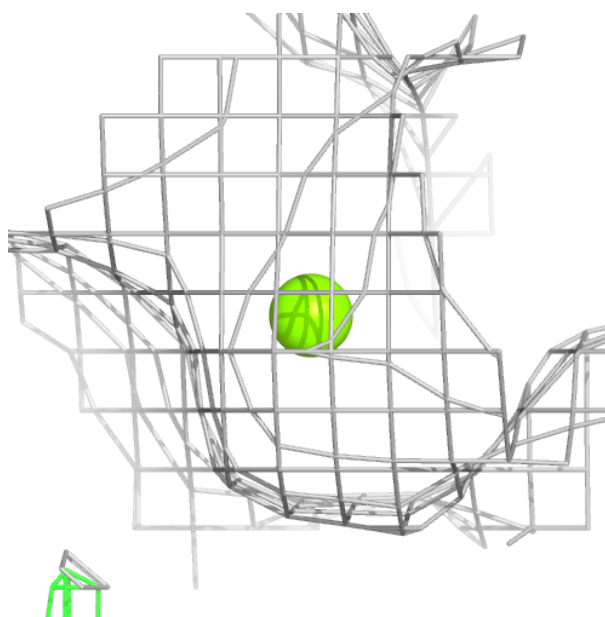
**Electron density around GTP L 707:**

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



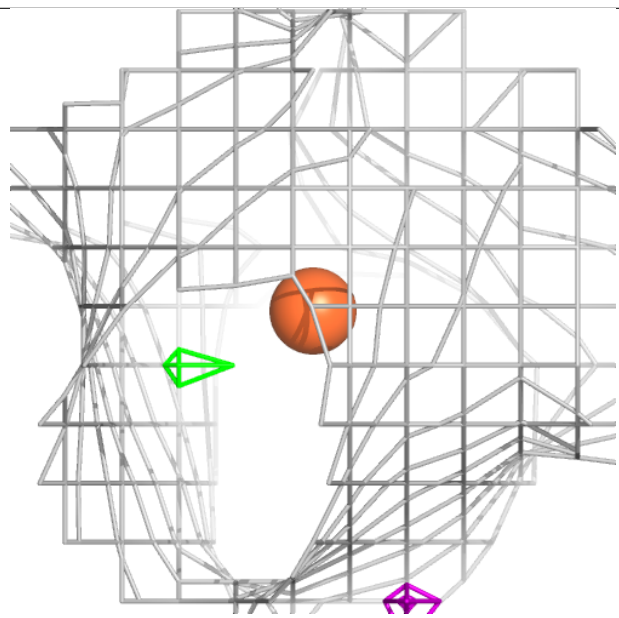
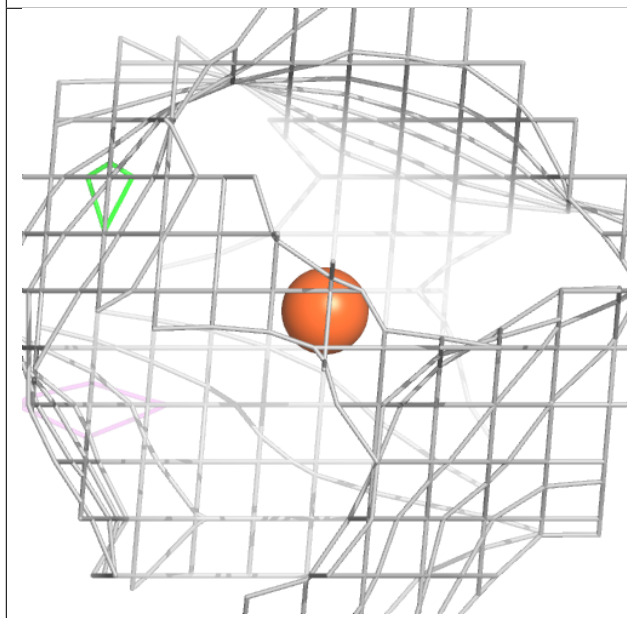
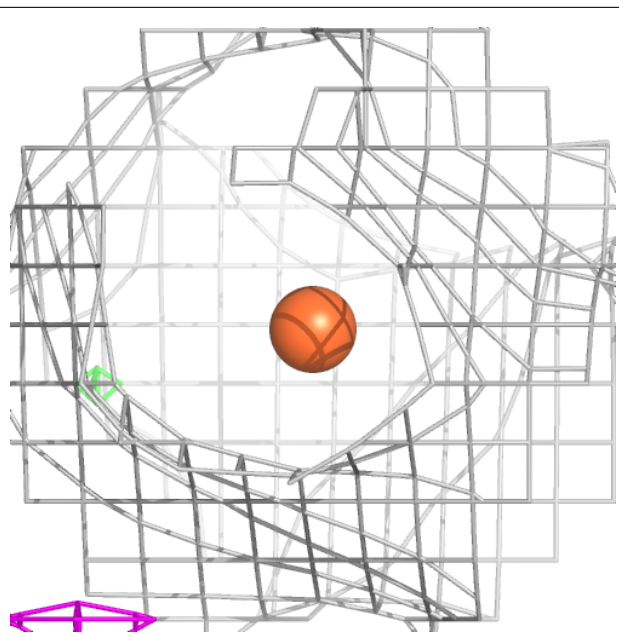
Electron density around MG D 705:

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



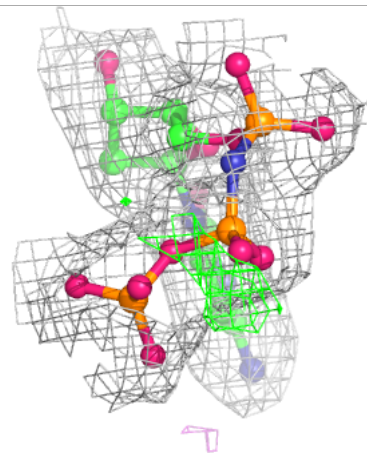
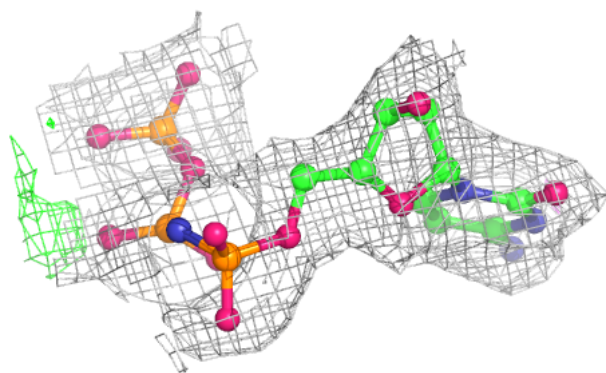
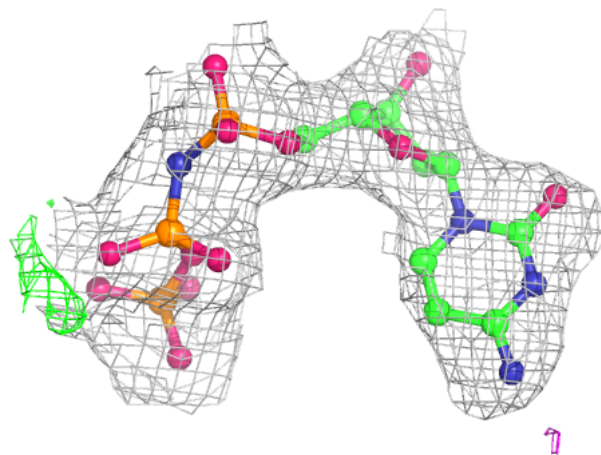
Electron density around FE I 701:

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



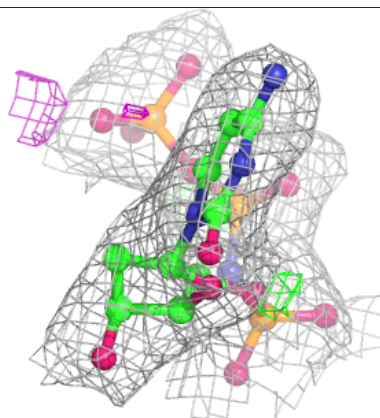
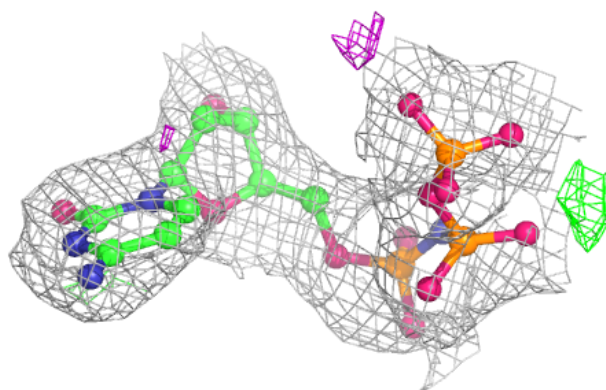
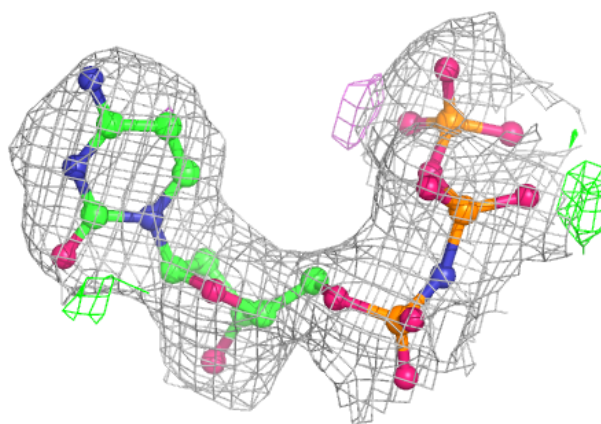
Electron density around 0KX A 705:

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



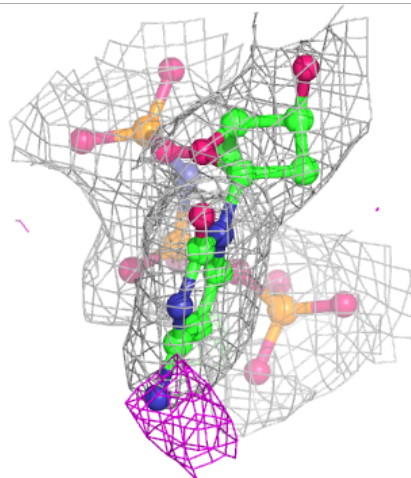
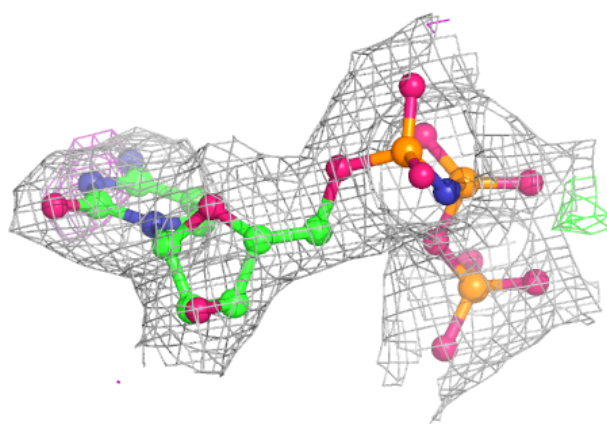
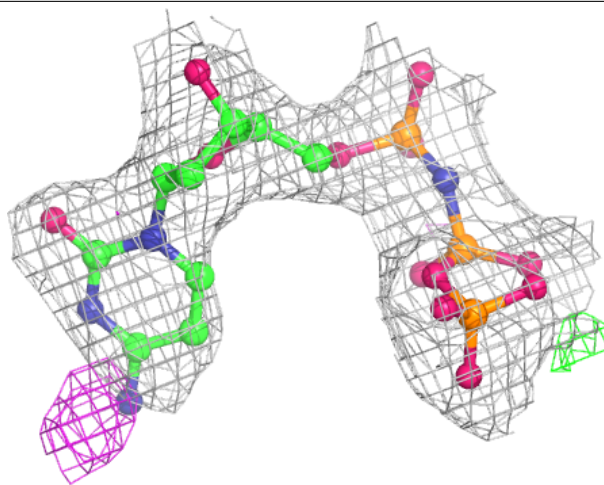
Electron density around 0KX C 706:

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



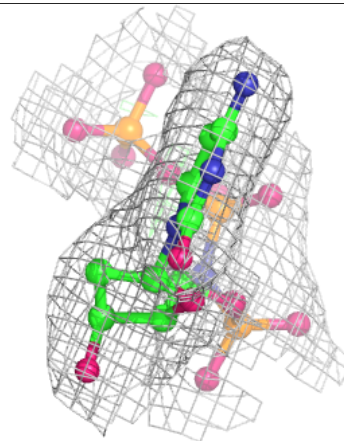
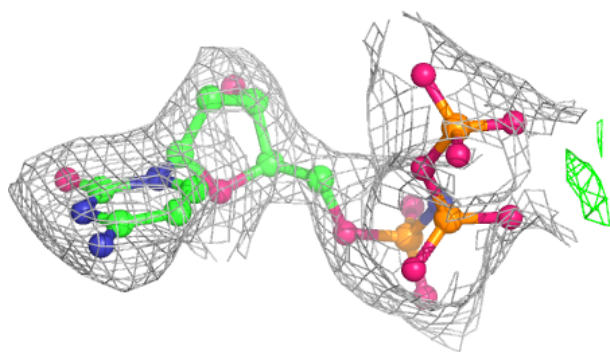
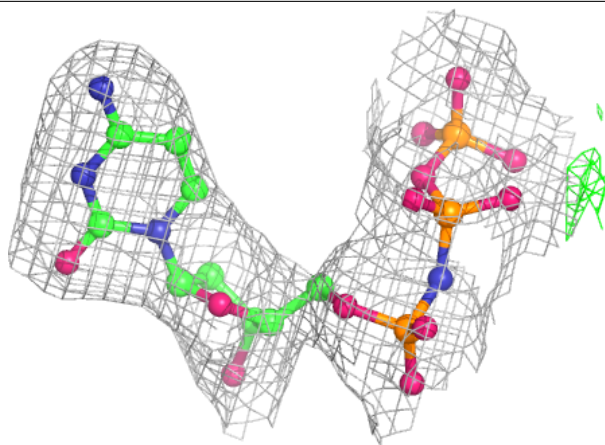
Electron density around 0KX D 706:

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



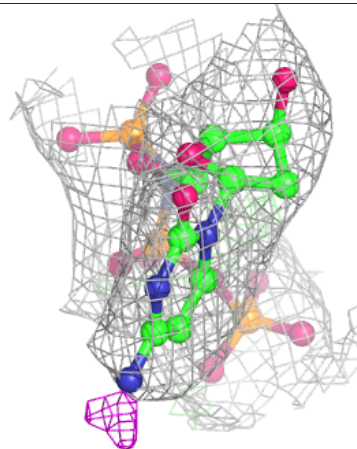
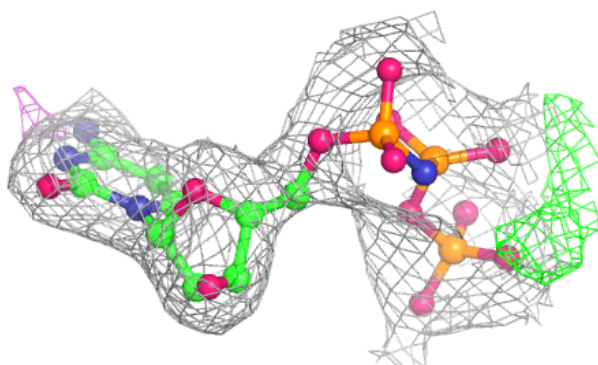
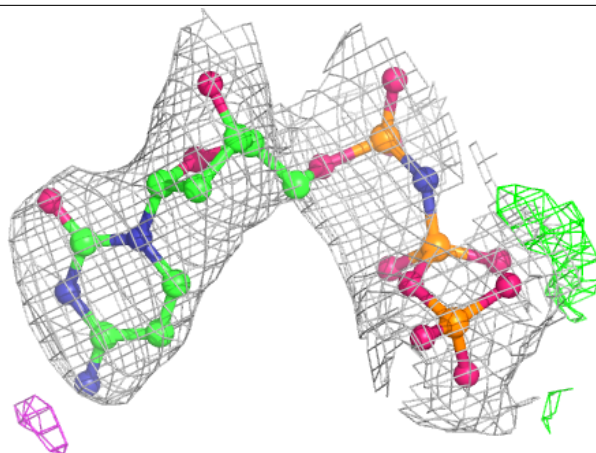
Electron density around 0KX E 704:

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



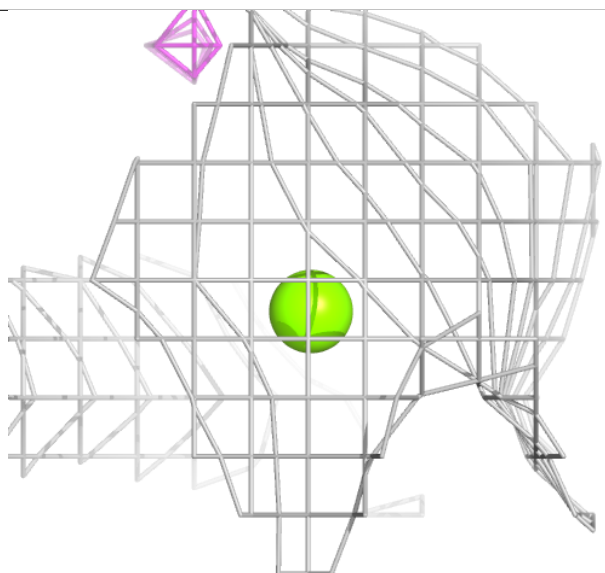
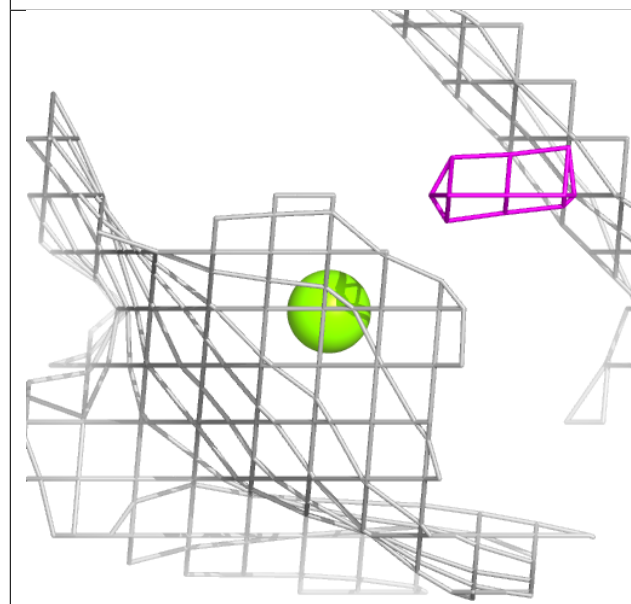
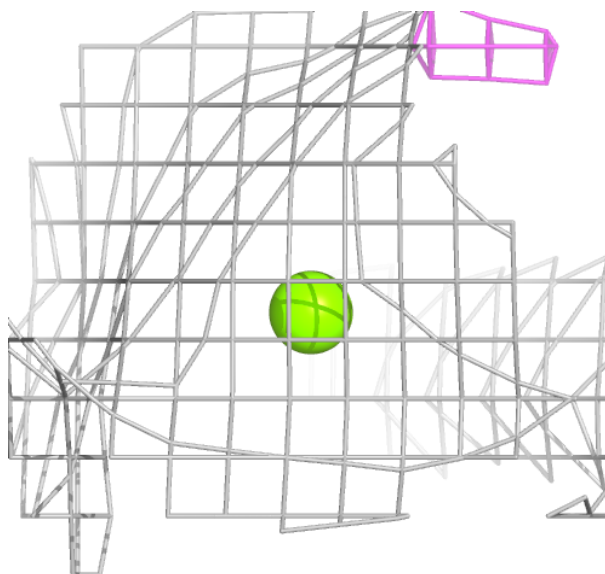
Electron density around 0KX F 704:

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



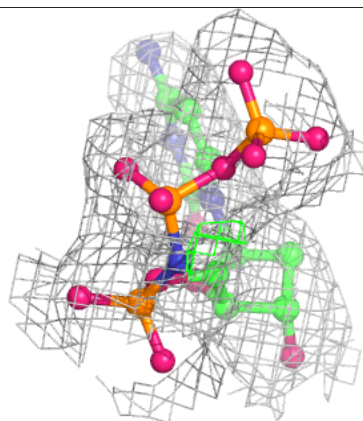
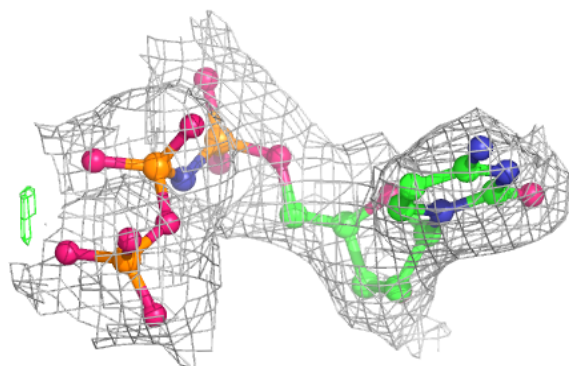
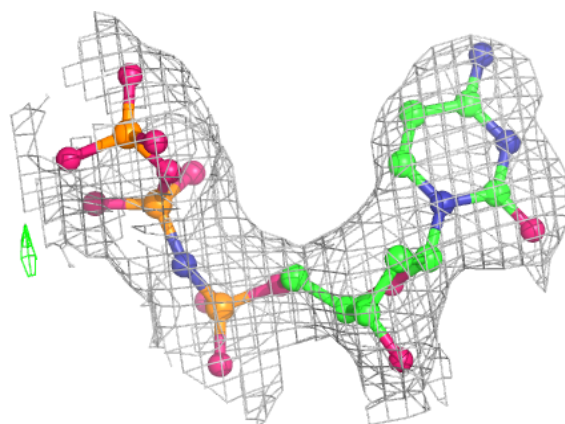
Electron density around MG E 703:

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

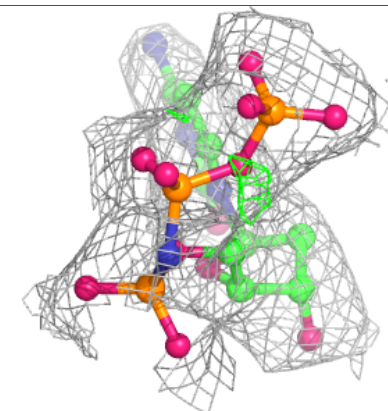
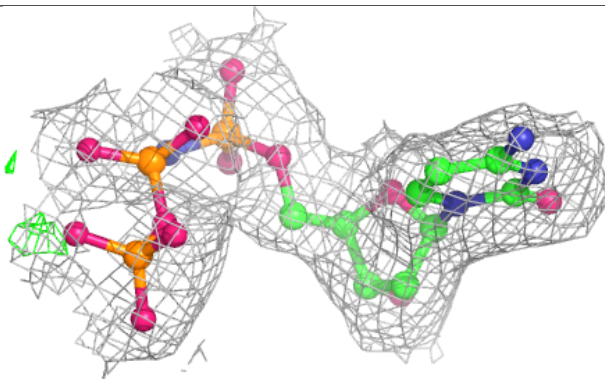
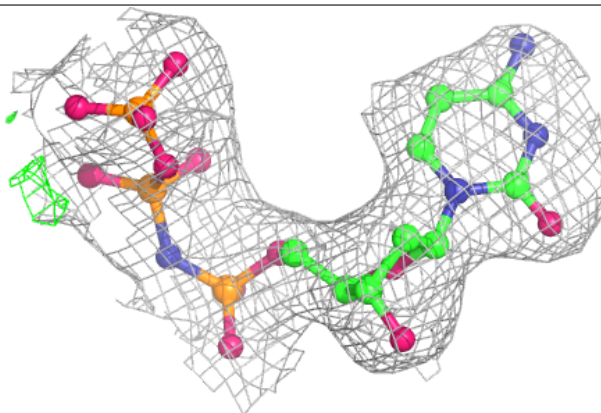


Electron density around 0KX H 705:

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

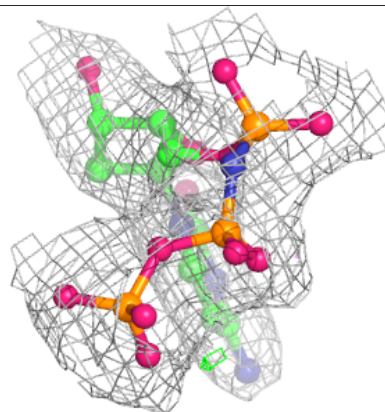
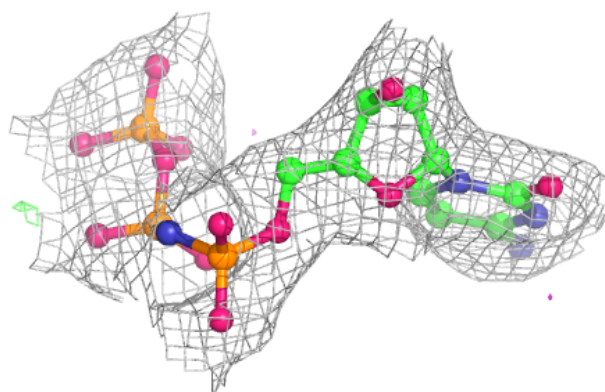
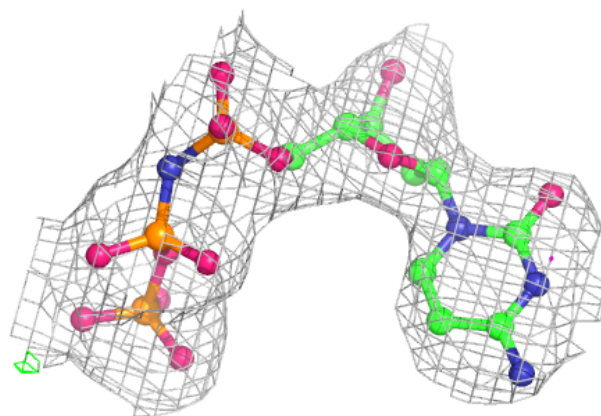
**Electron density around 0KX I 705:**

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

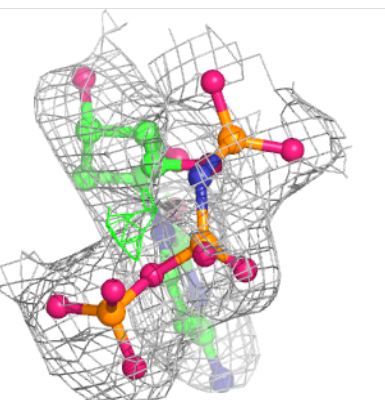
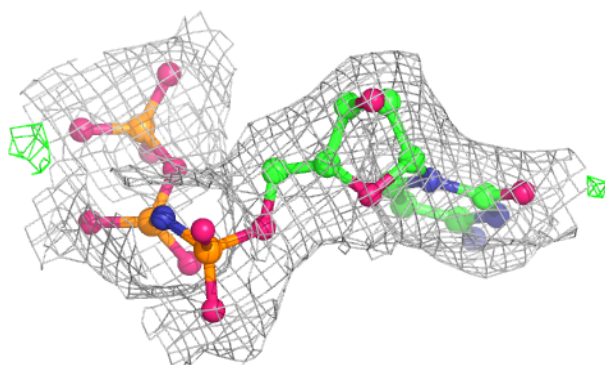
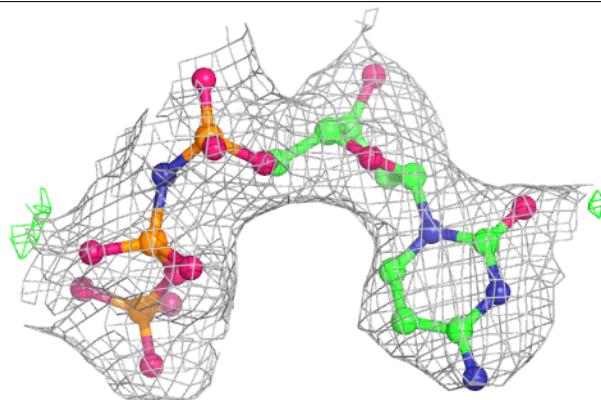


Electron density around 0KX J 704:

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

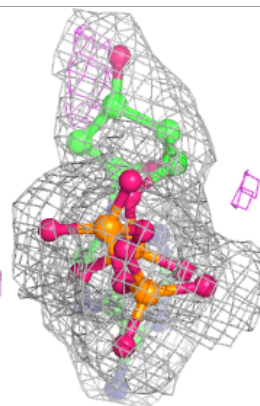
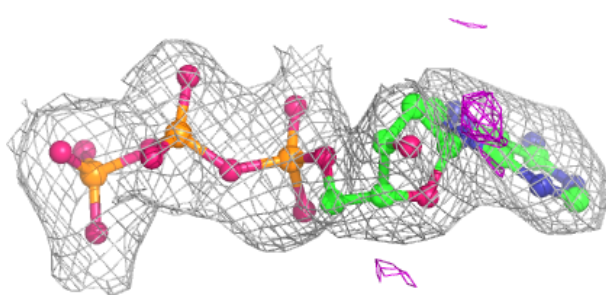
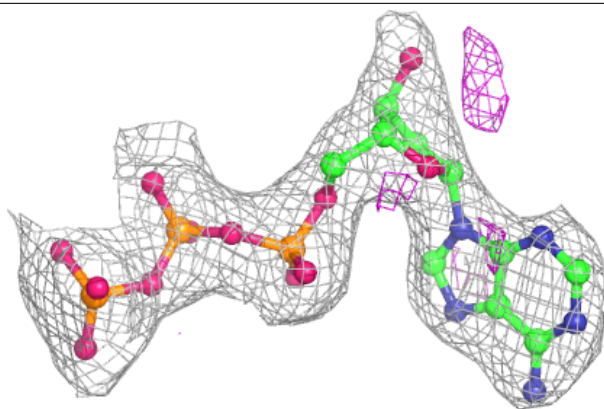
**Electron density around 0KX L 706:**

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

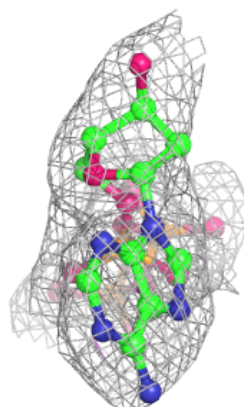
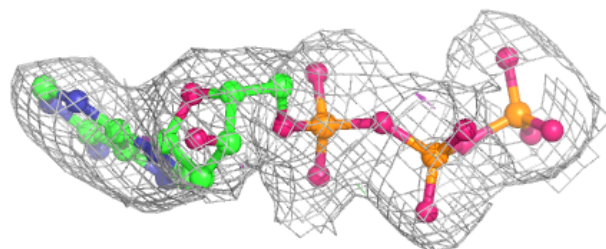
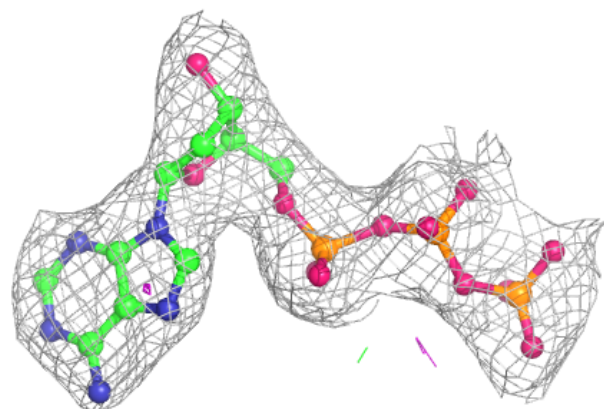


Electron density around DTP A 708:

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

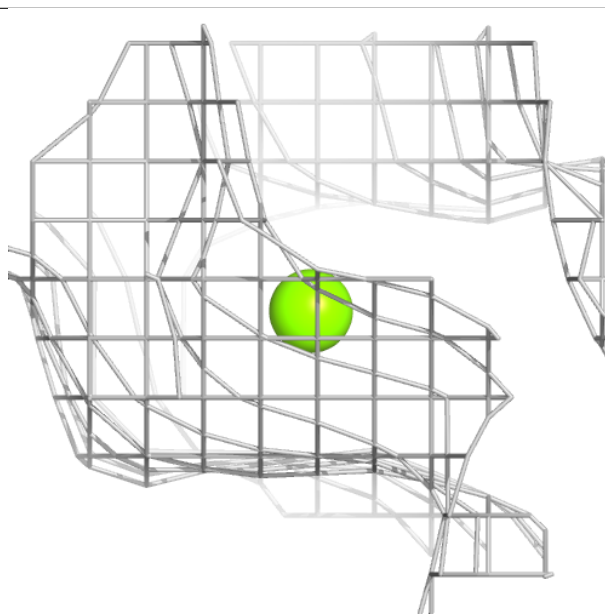
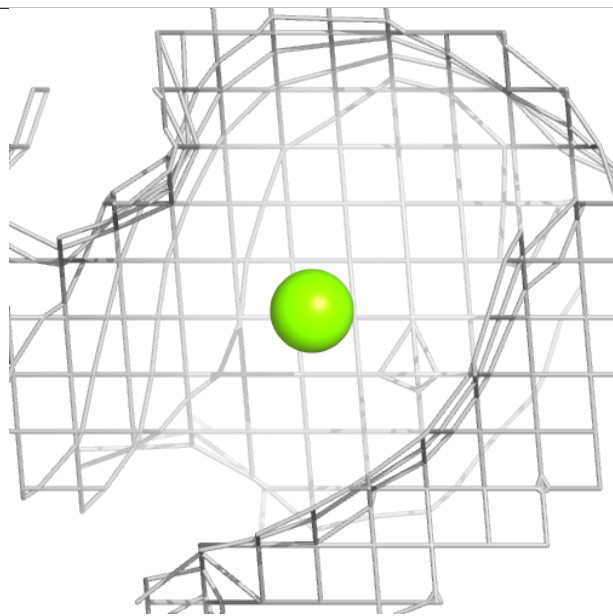
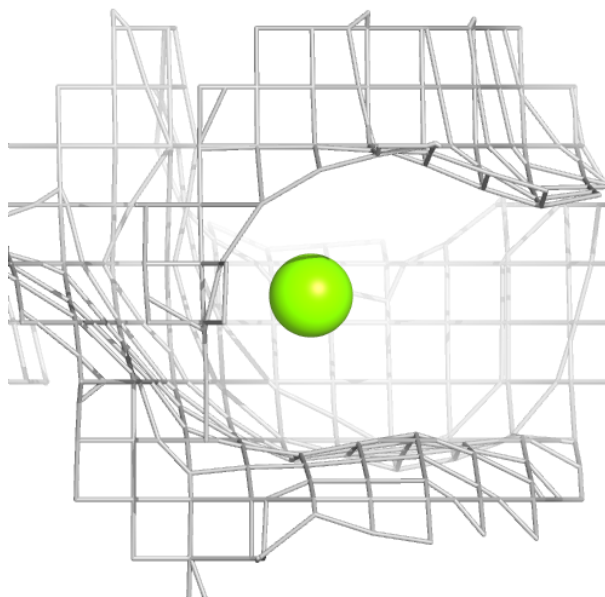
**Electron density around DTP D 701:**

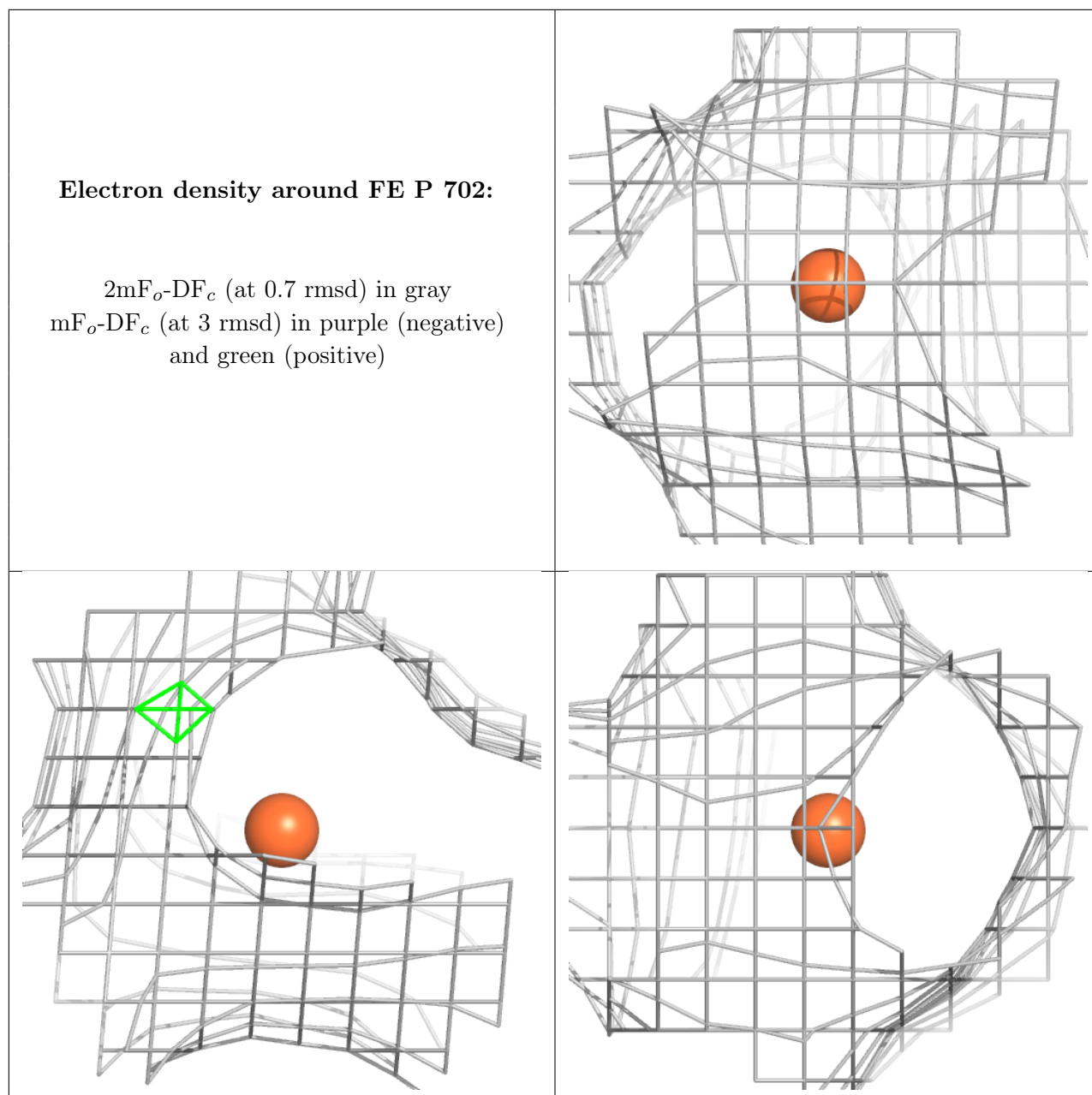
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG L 705:

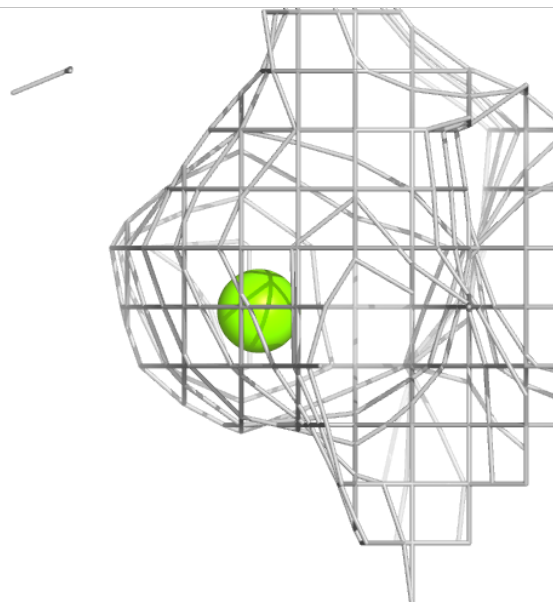
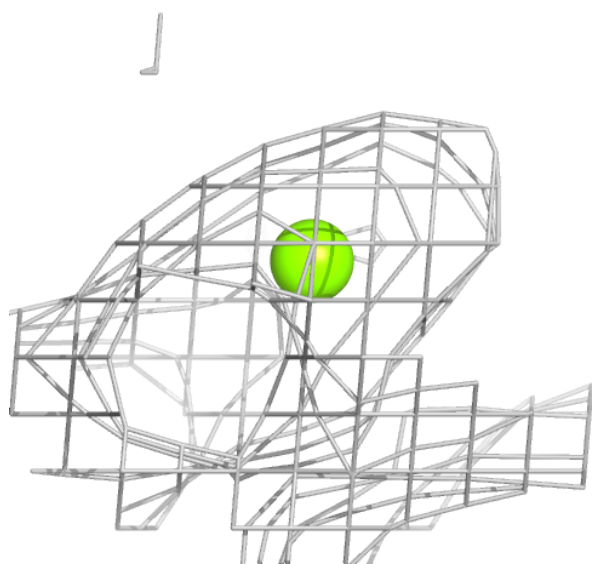
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





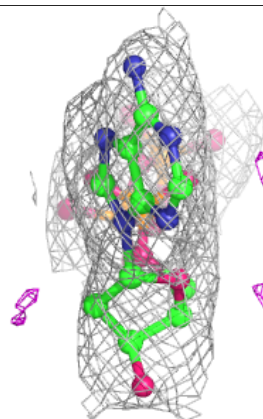
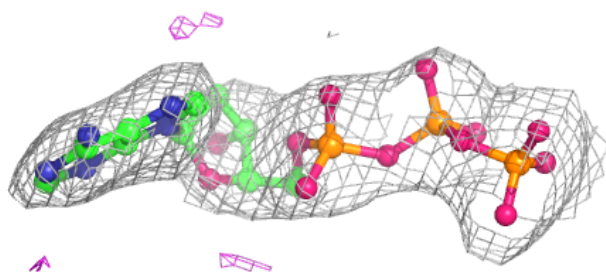
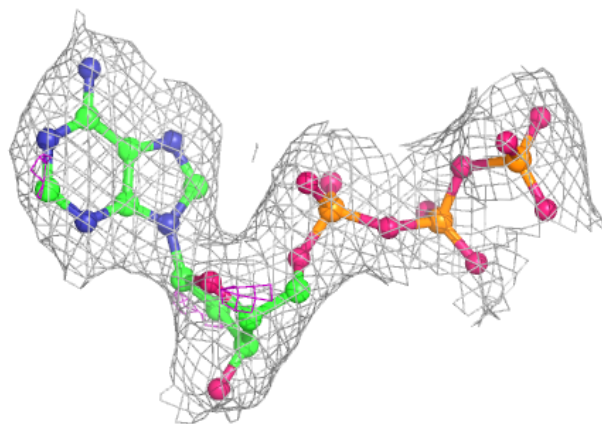
Electron density around MG A 702:

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

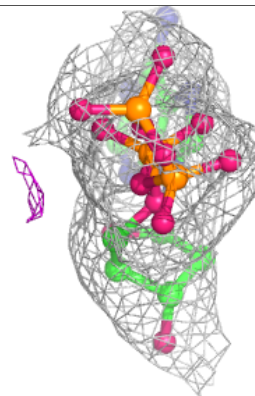
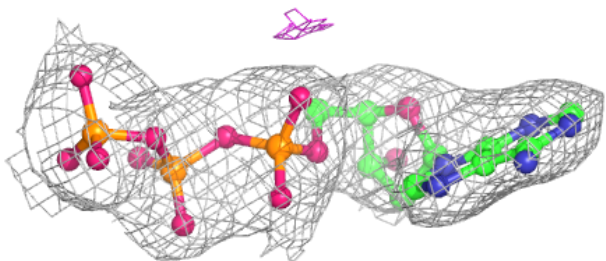
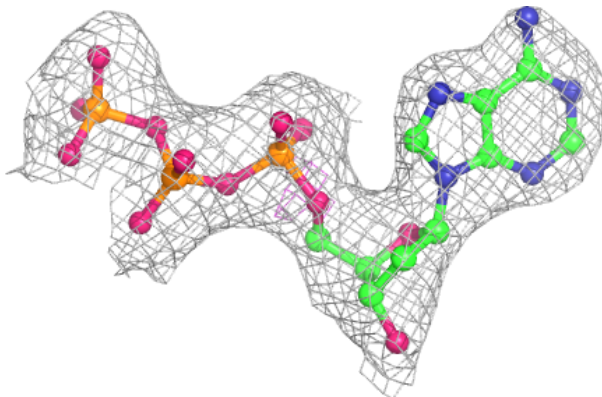


Electron density around DTP H 701:

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

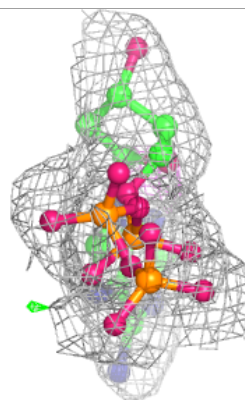
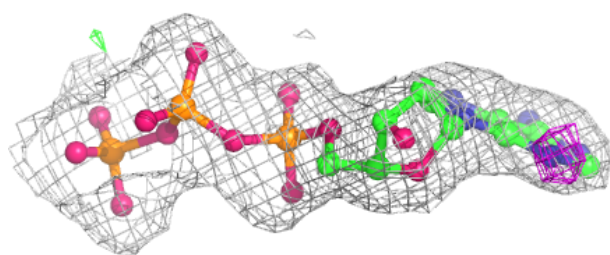
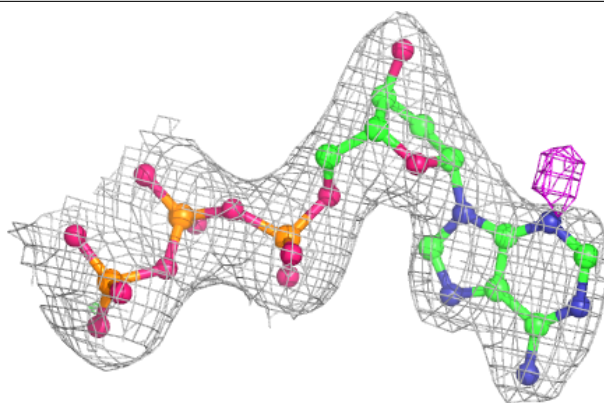
**Electron density around DTP I 708:**

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

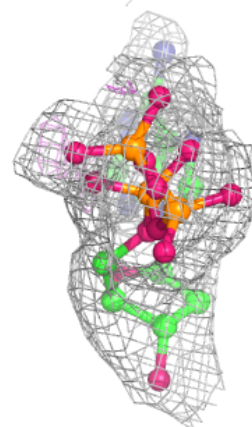
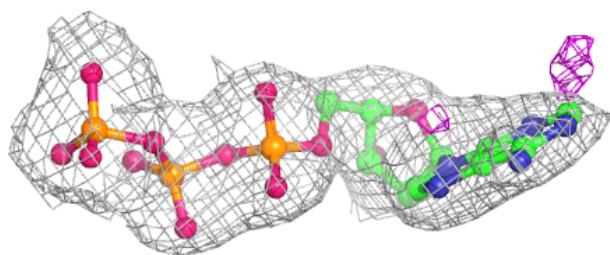
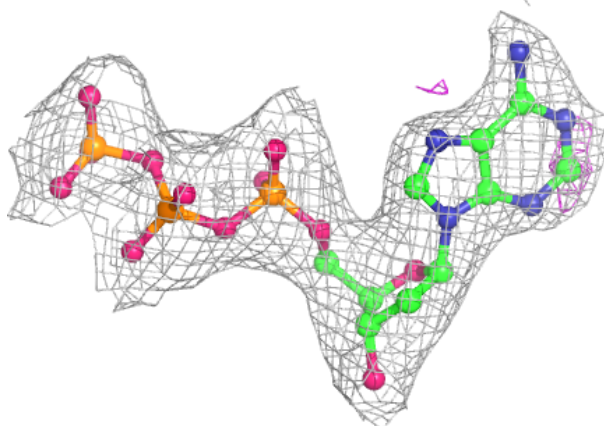


Electron density around DTP J 707:

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

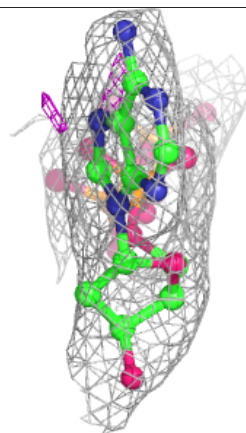
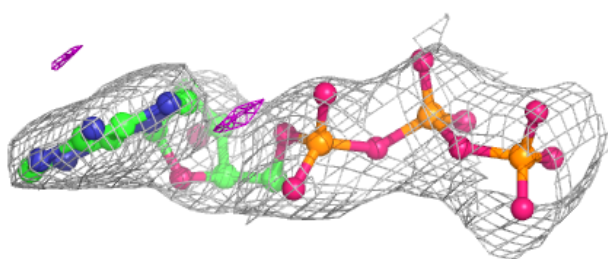
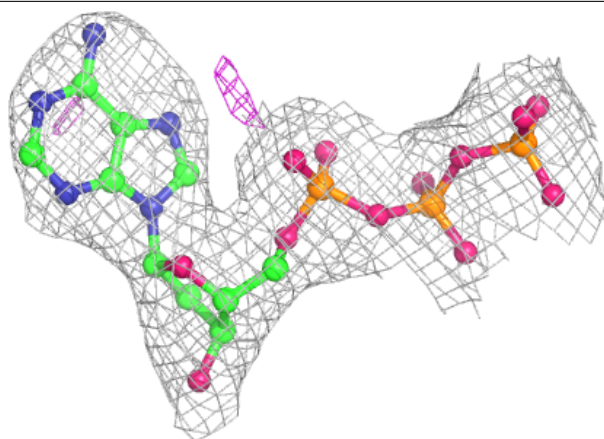
**Electron density around DTP L 701:**

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

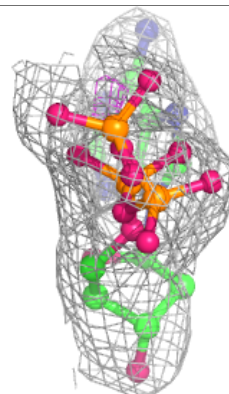
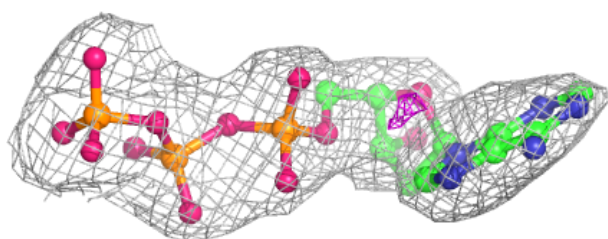
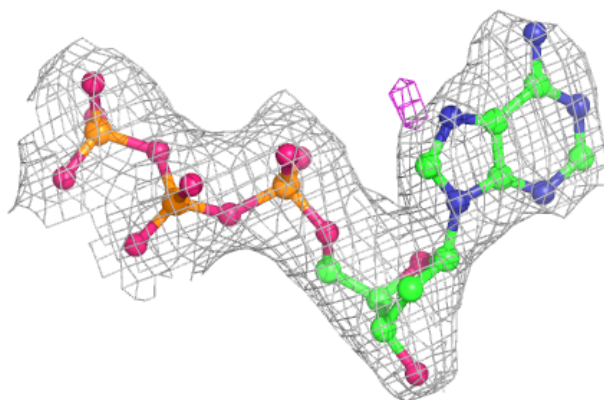


Electron density around DTP M 708:

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

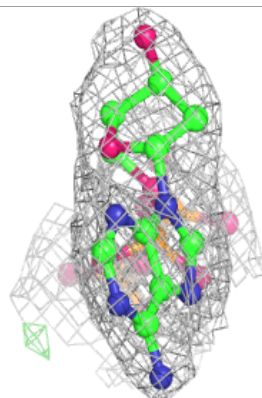
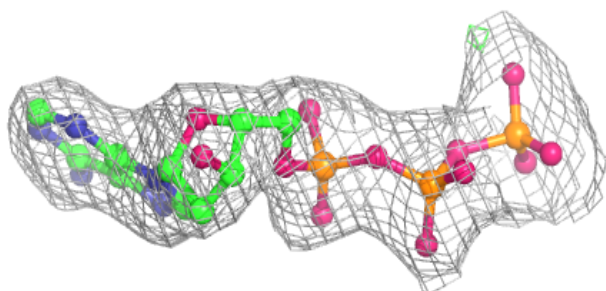
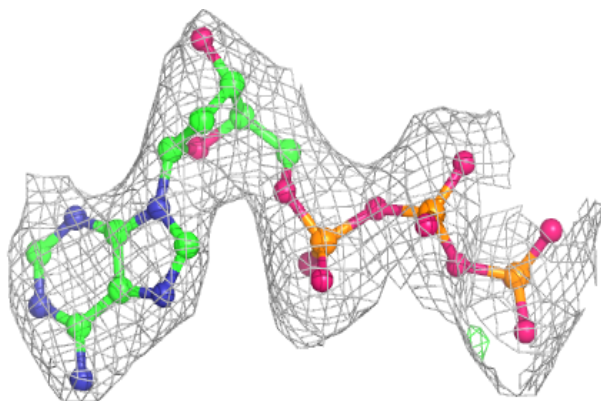
**Electron density around DTP N 706:**

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

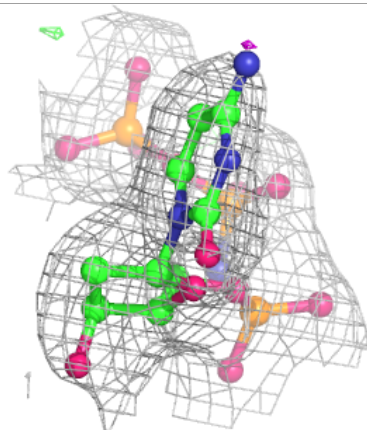
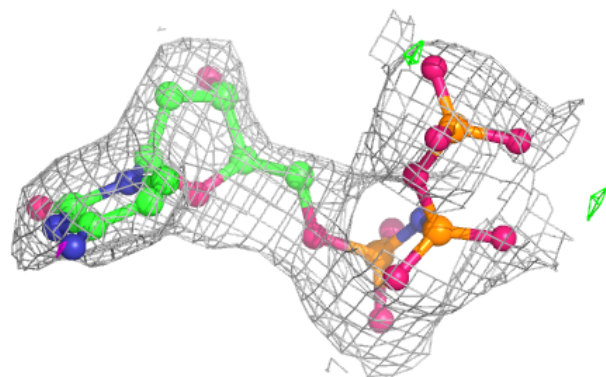
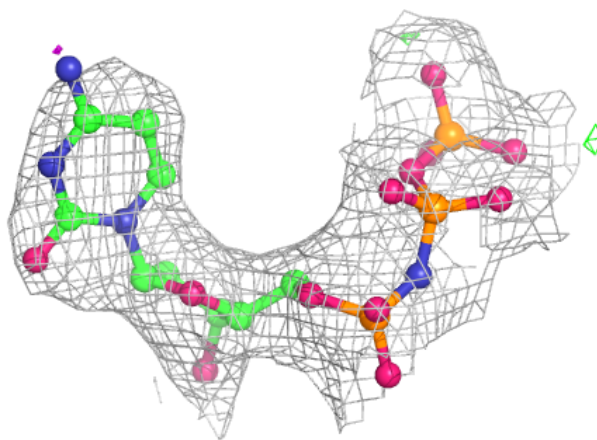


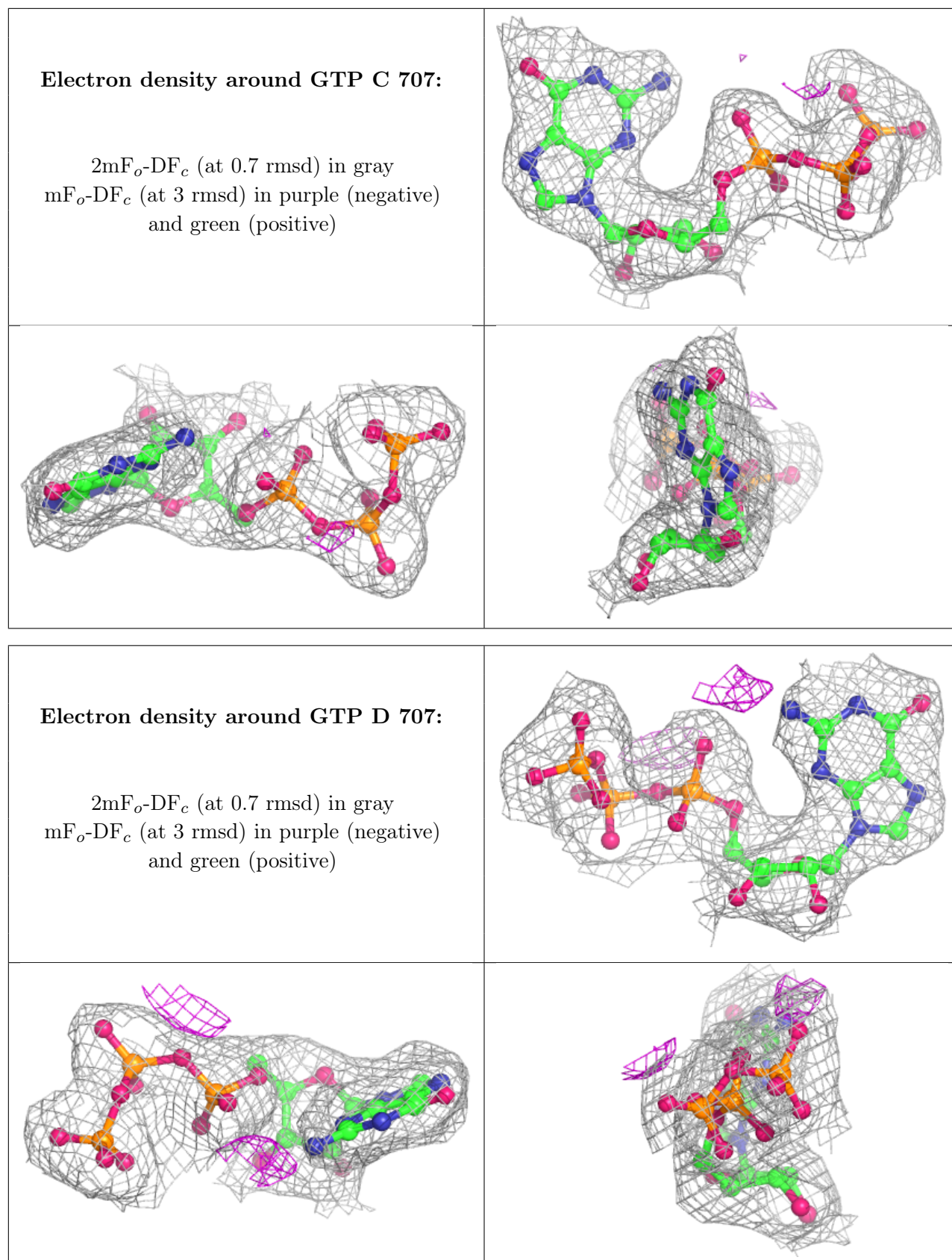
Electron density around DTP O 701:

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

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

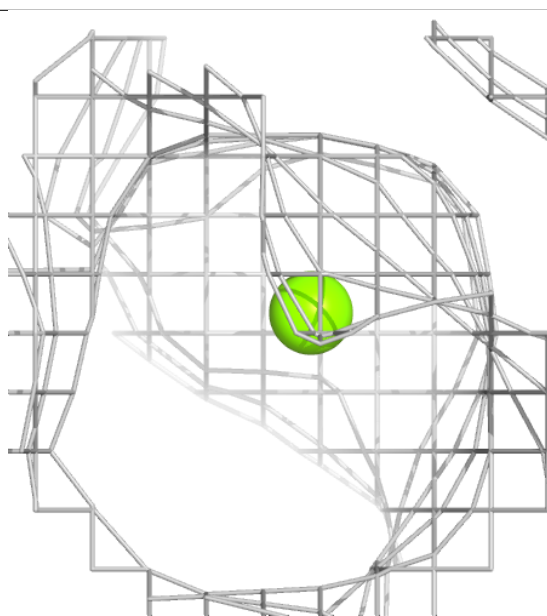
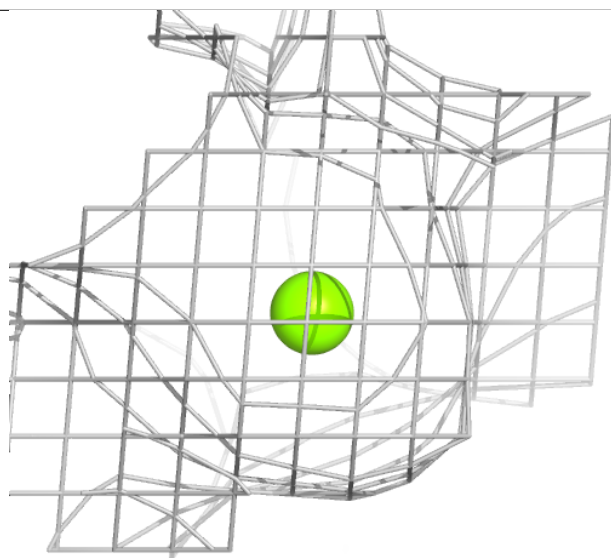
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





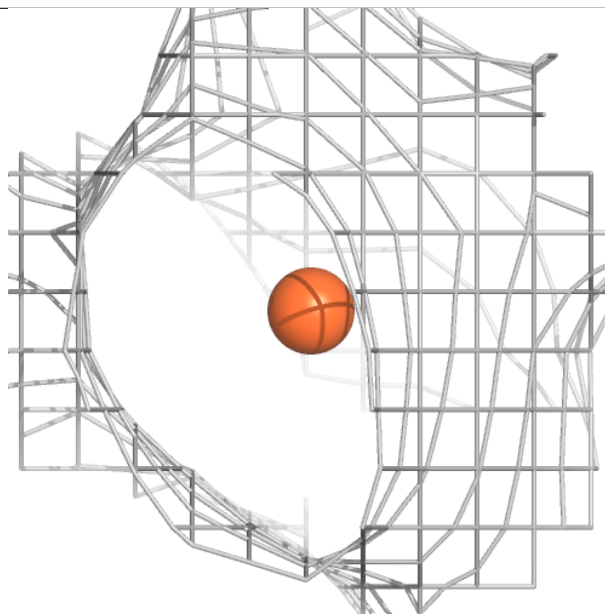
Electron density around MG B 704:

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



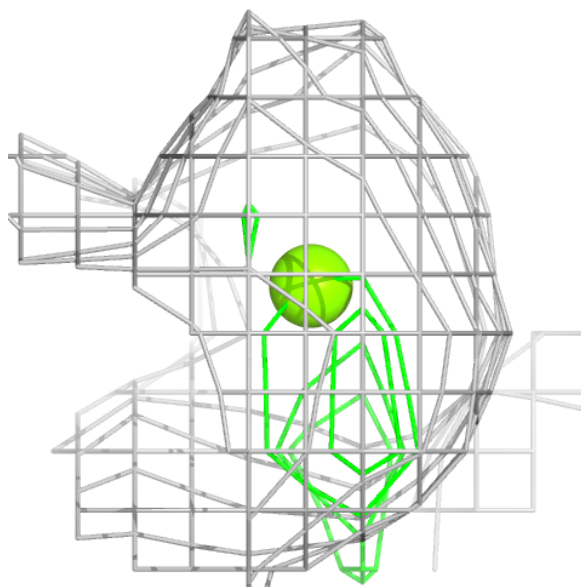
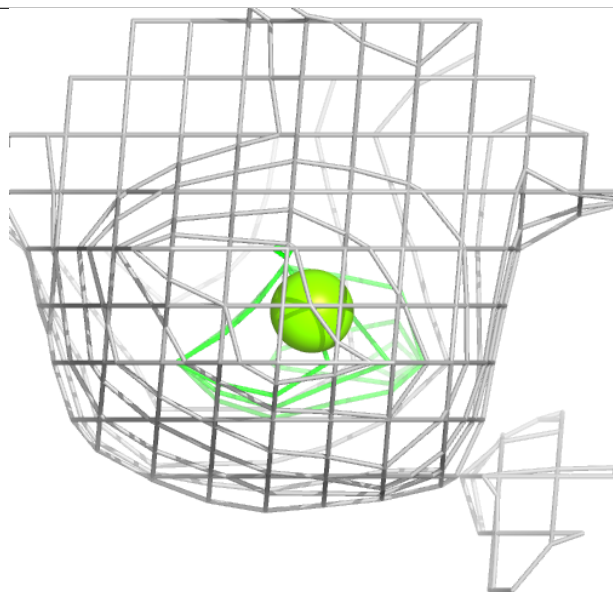
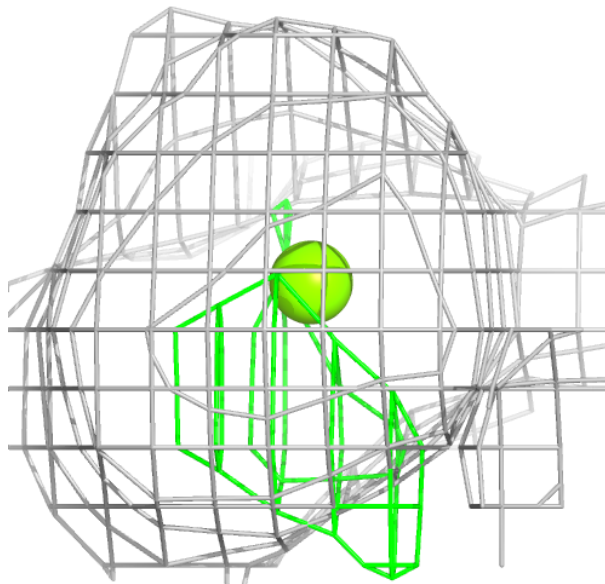
Electron density around FE N 701:

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



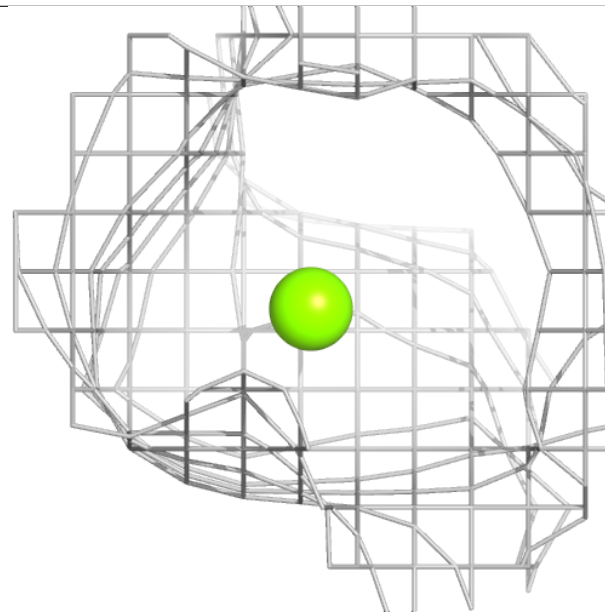
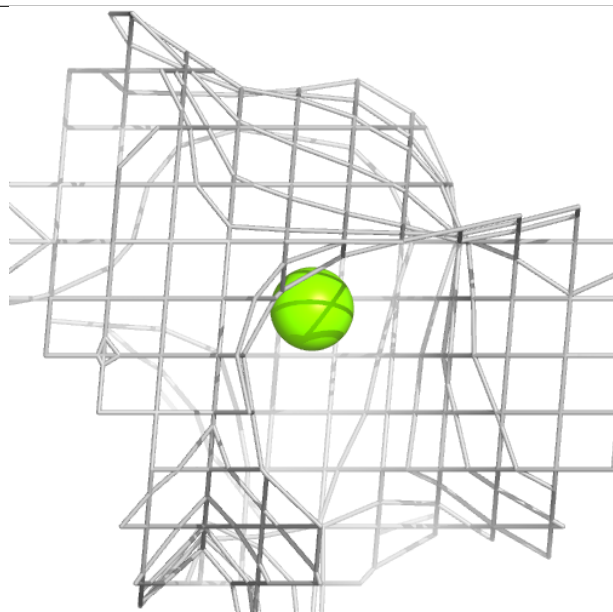
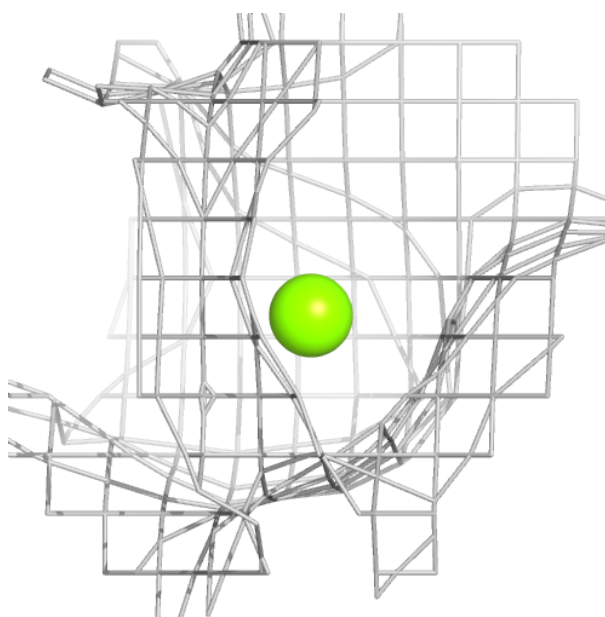
Electron density around MG C 704:

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



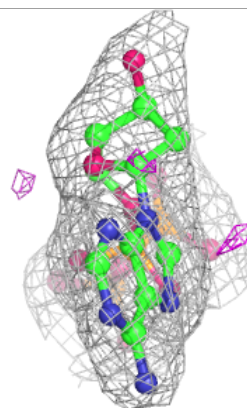
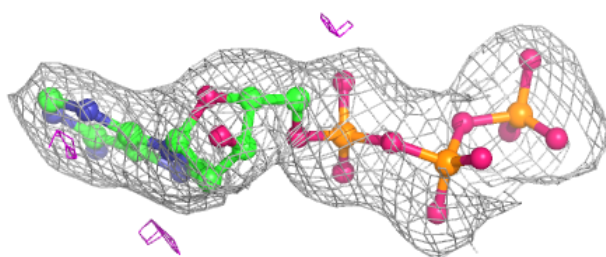
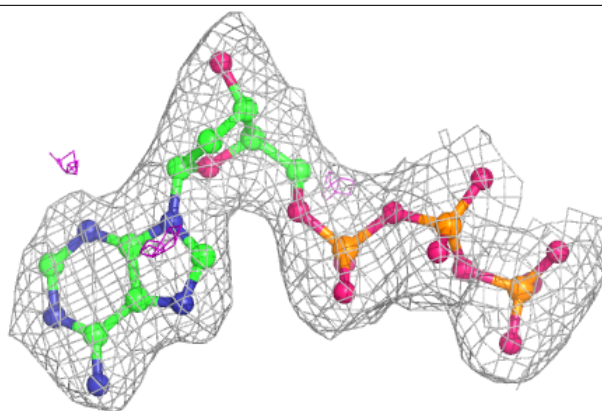
Electron density around MG A 704:

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

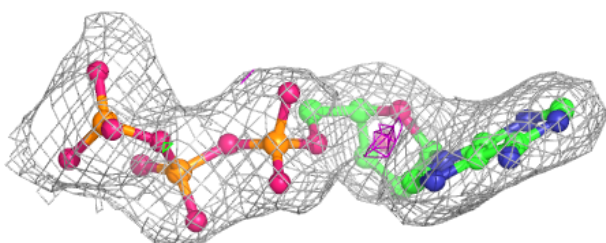
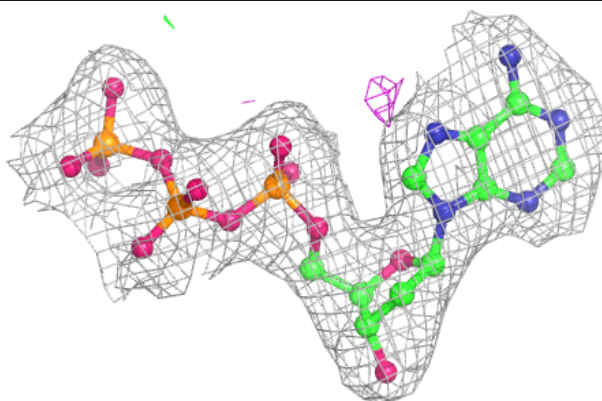


Electron density around DTP B 708:

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

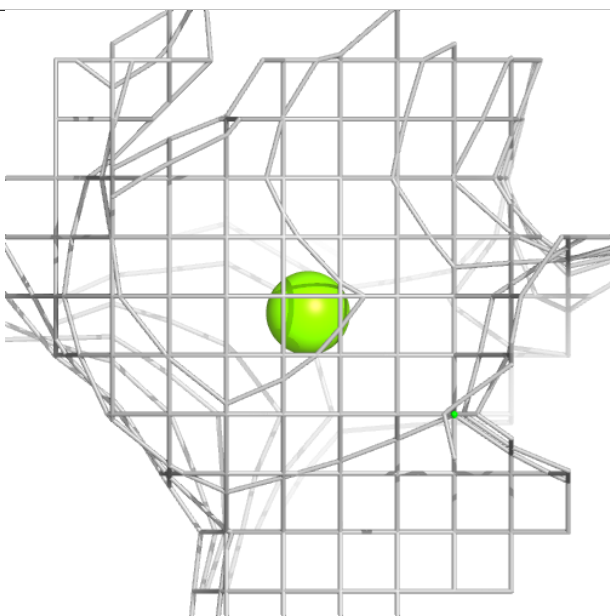
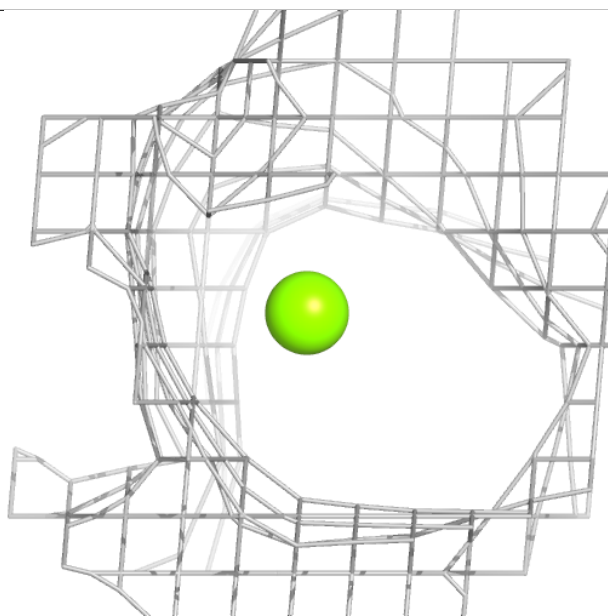
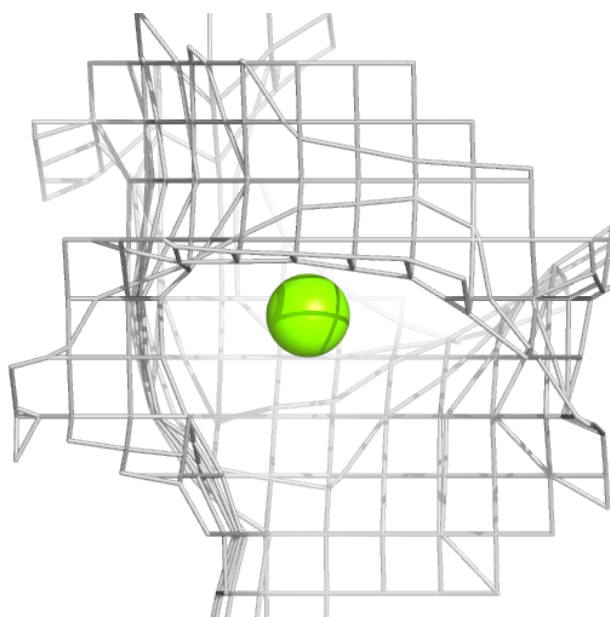
**Electron density around DTP C 701:**

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



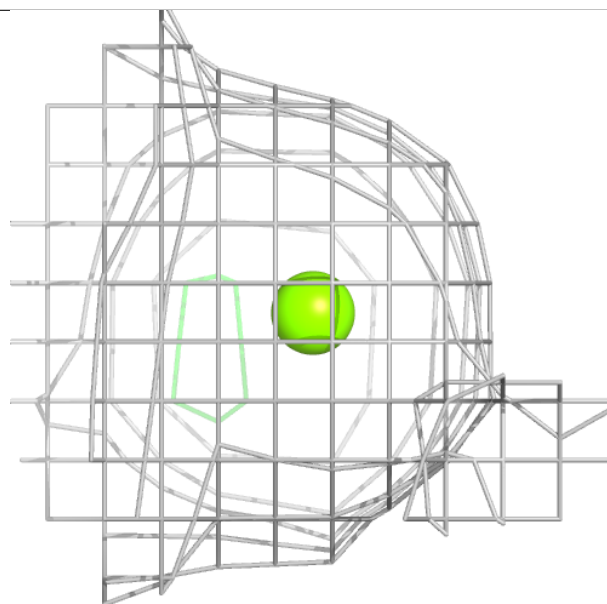
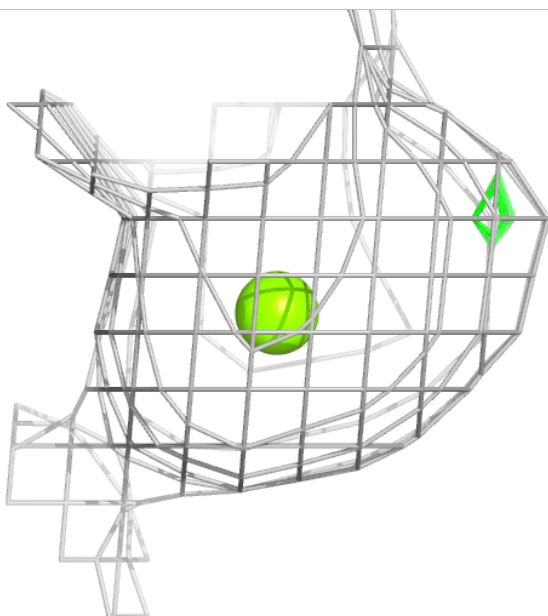
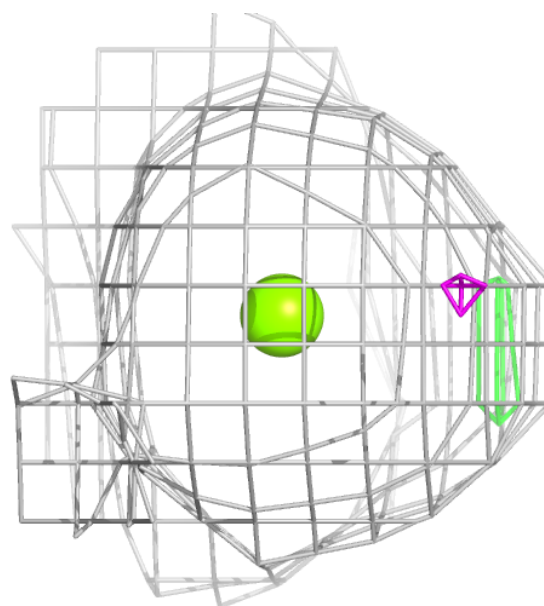
Electron density around MG I 704:

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



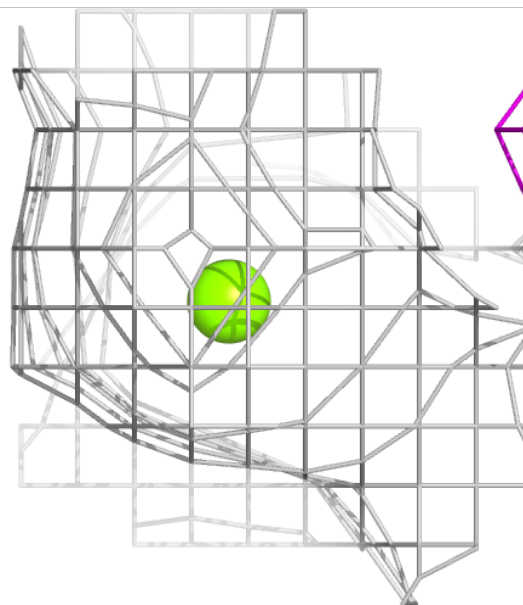
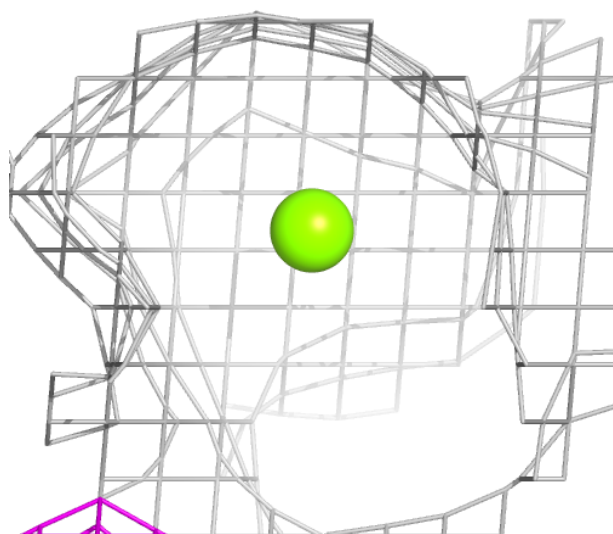
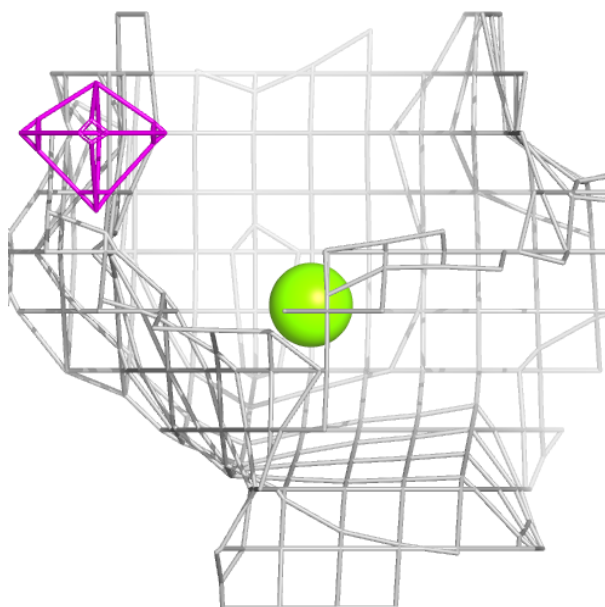
Electron density around MG J 702:

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



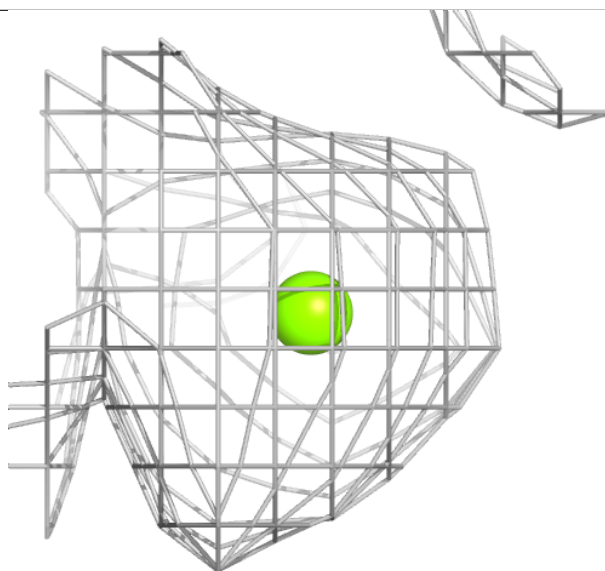
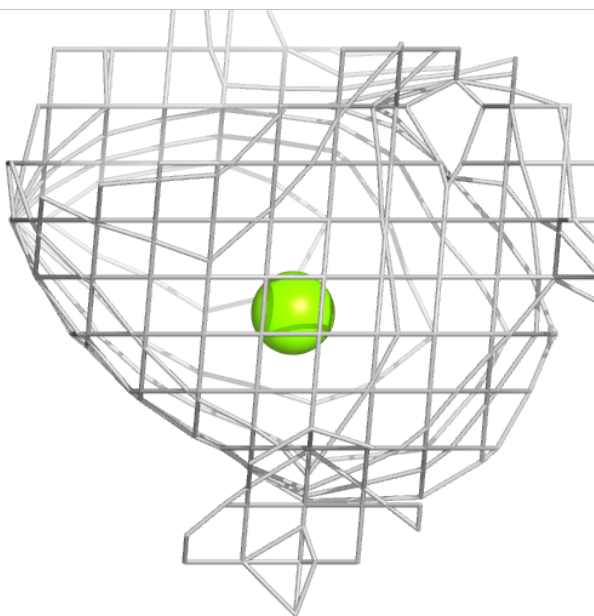
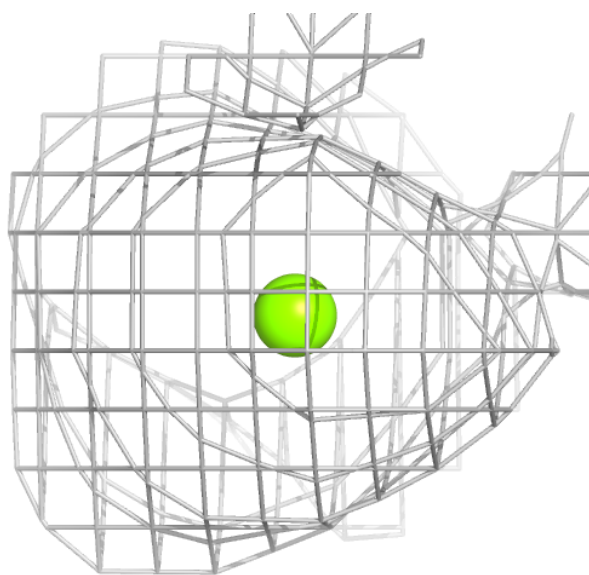
Electron density around MG J 703:

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



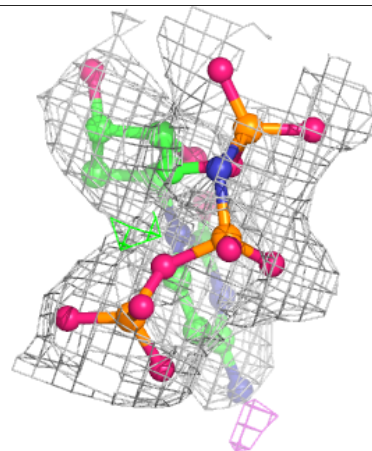
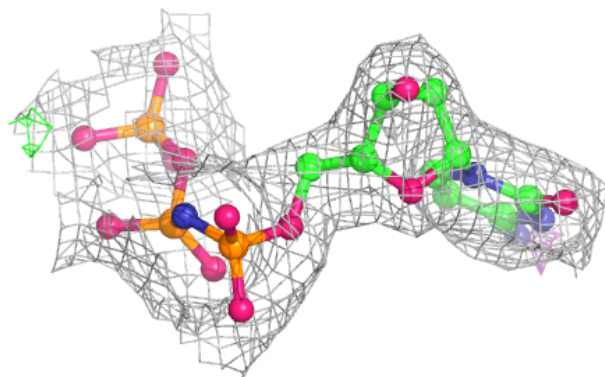
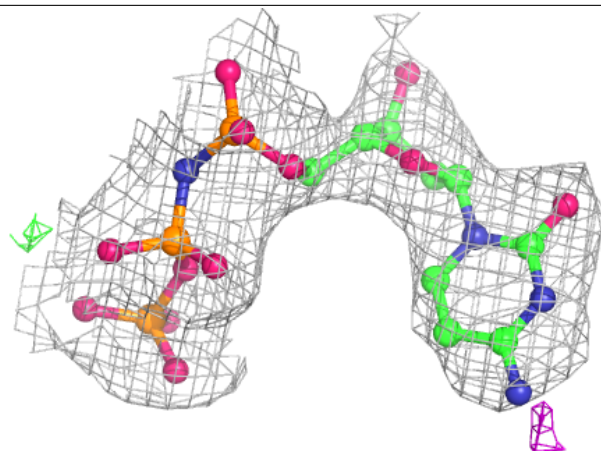
Electron density around MG O 703:

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



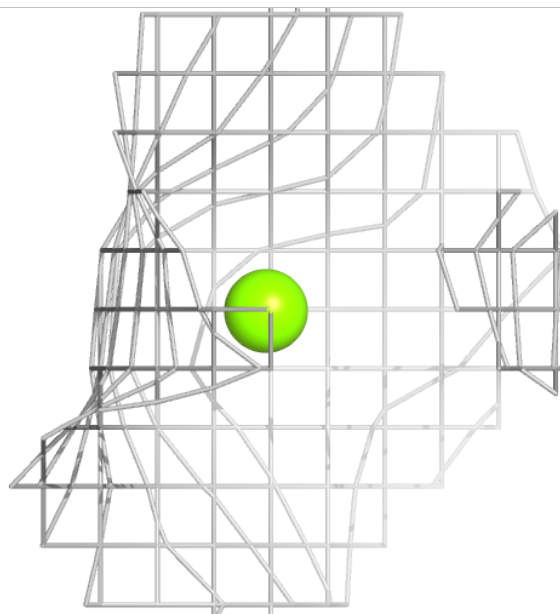
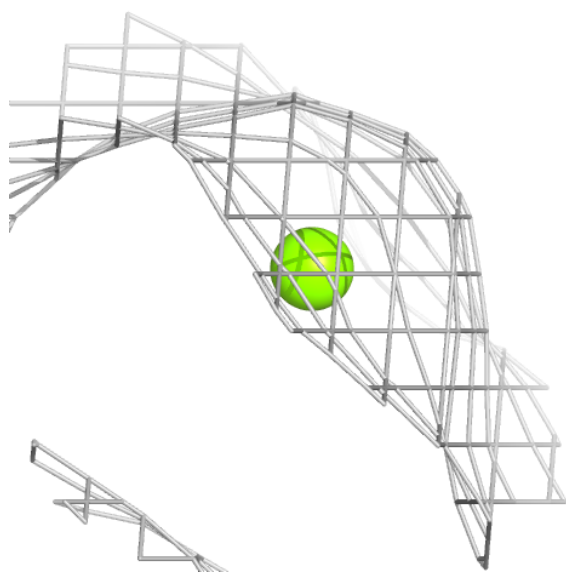
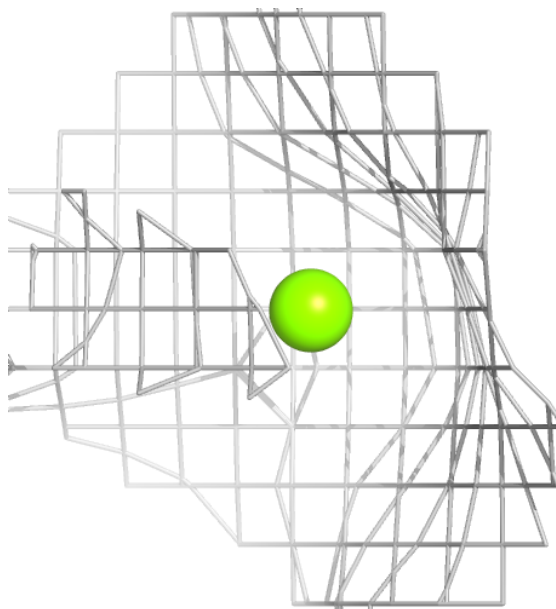
Electron density around 0KX K 706:

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



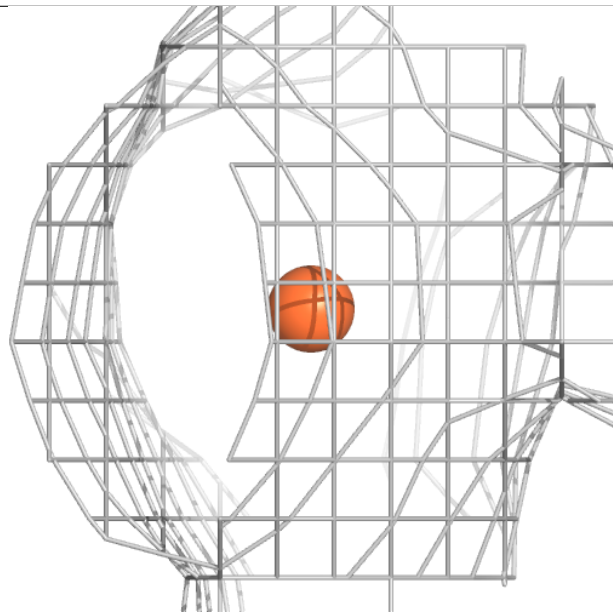
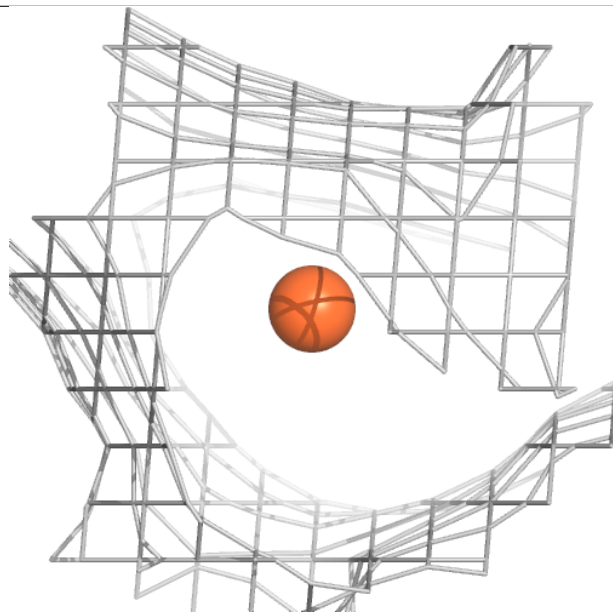
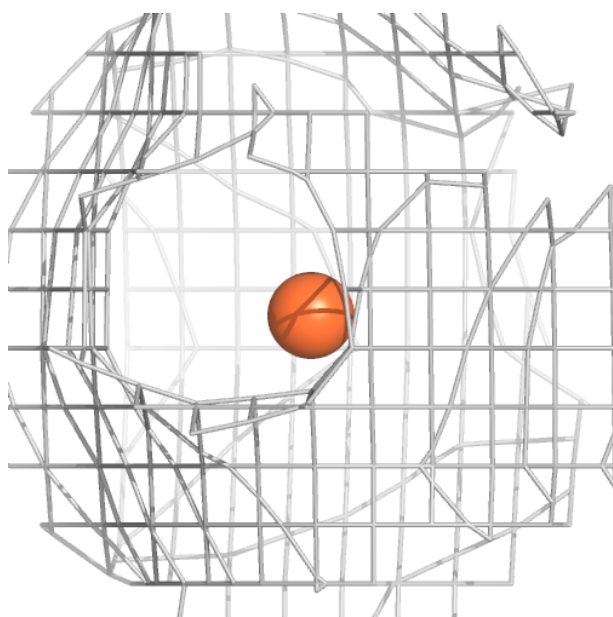
Electron density around MG O 704:

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



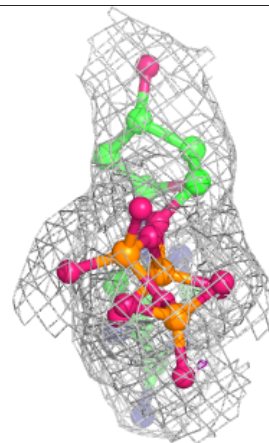
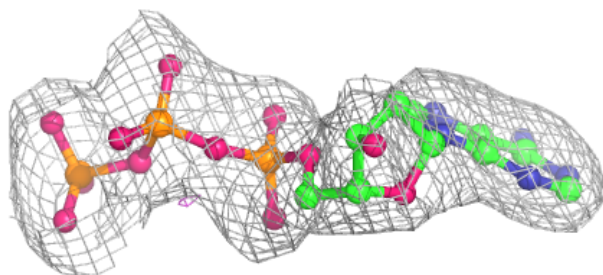
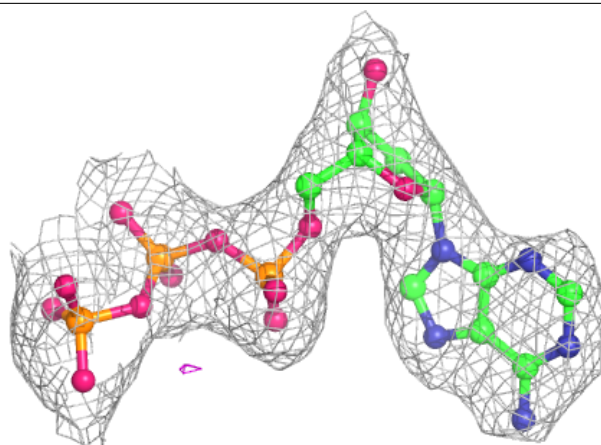
Electron density around FE G 702:

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



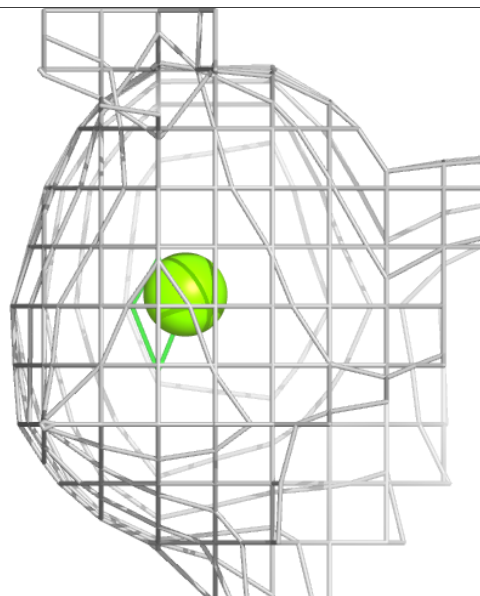
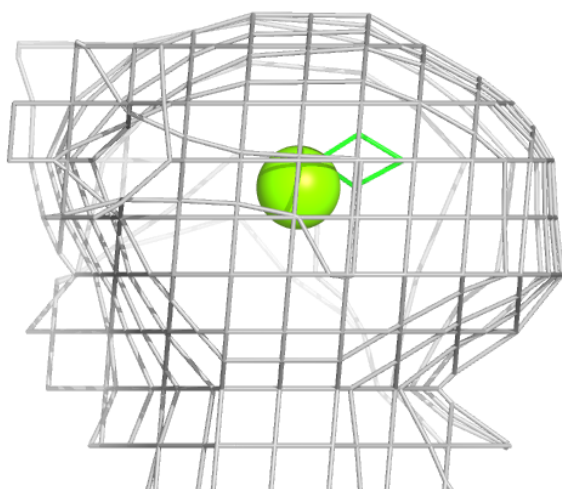
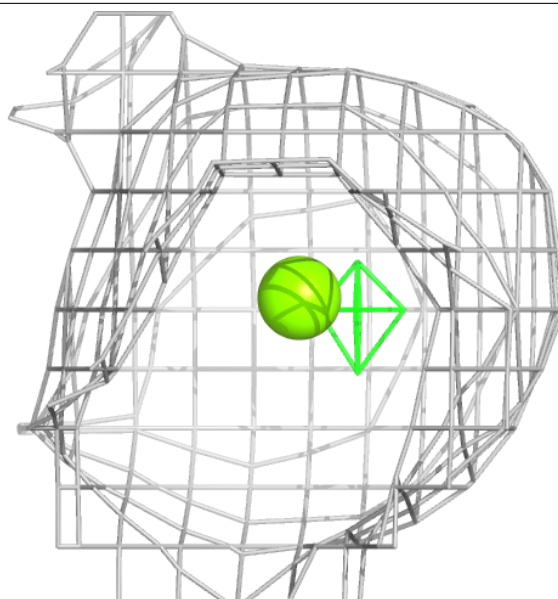
Electron density around DTP K 701:

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



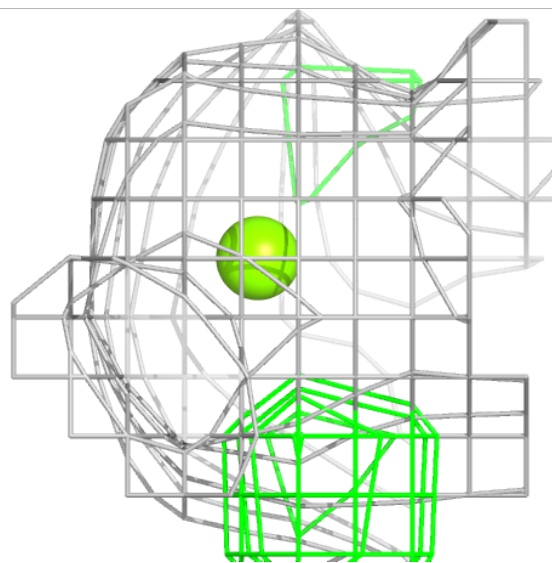
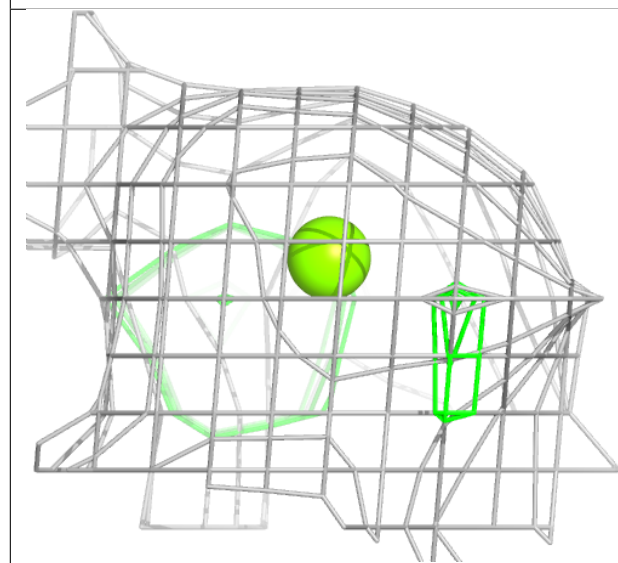
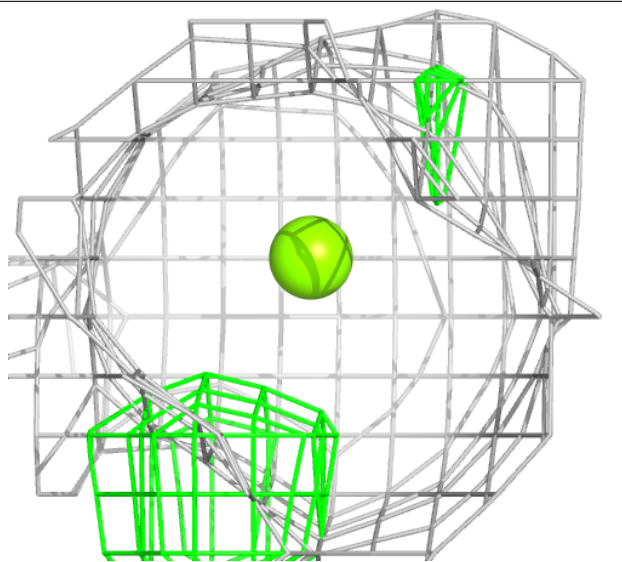
Electron density around MG P 704:

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



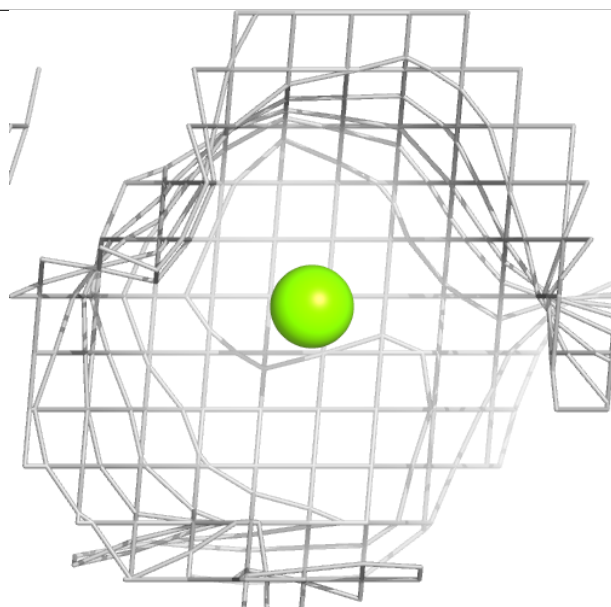
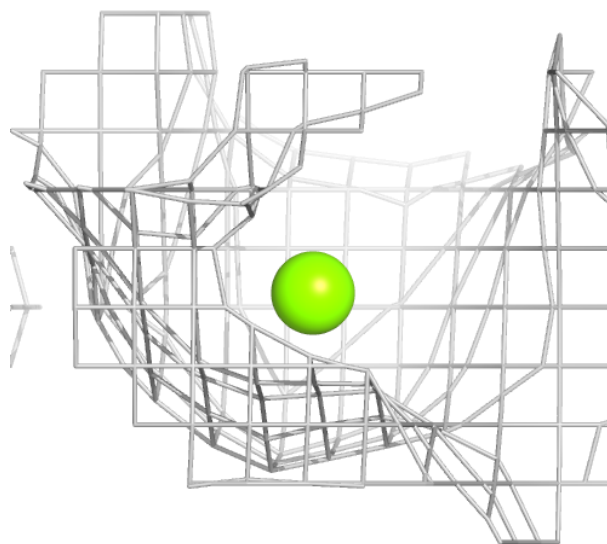
Electron density around MG B 703:

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



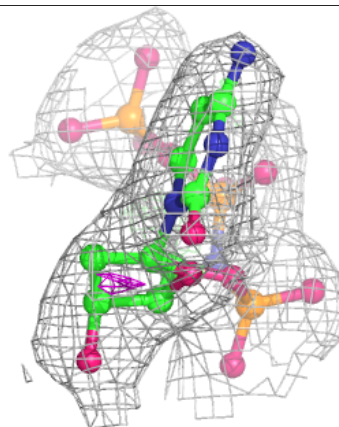
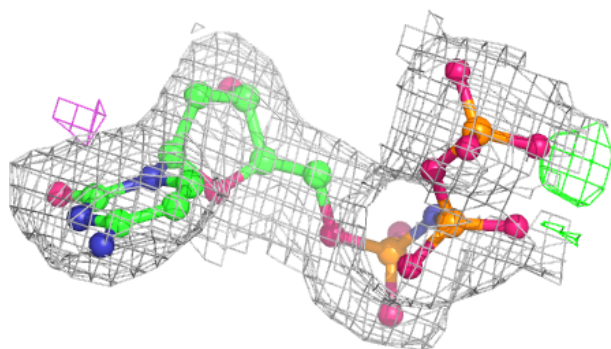
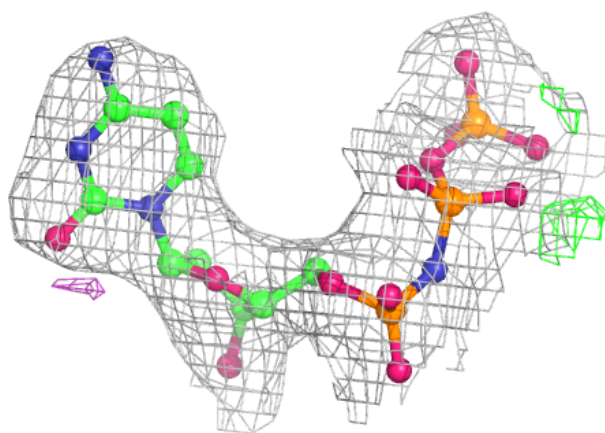
Electron density around MG G 705:

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

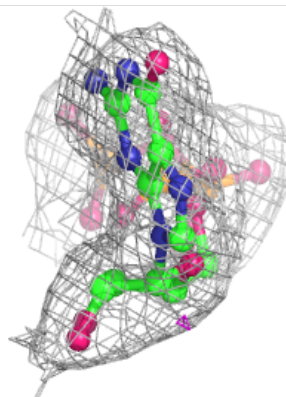
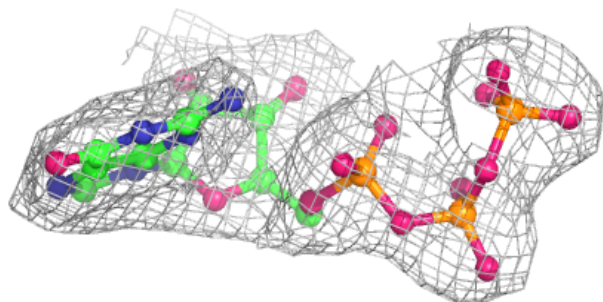
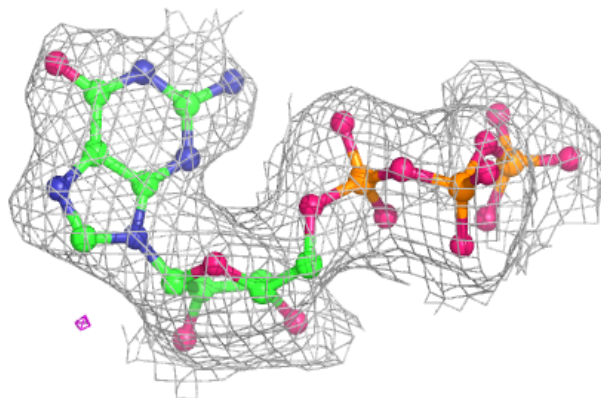


Electron density around 0KX B 705:

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

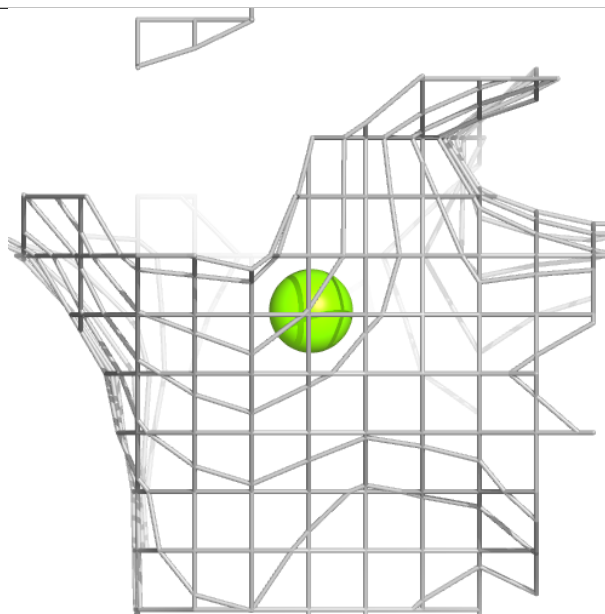
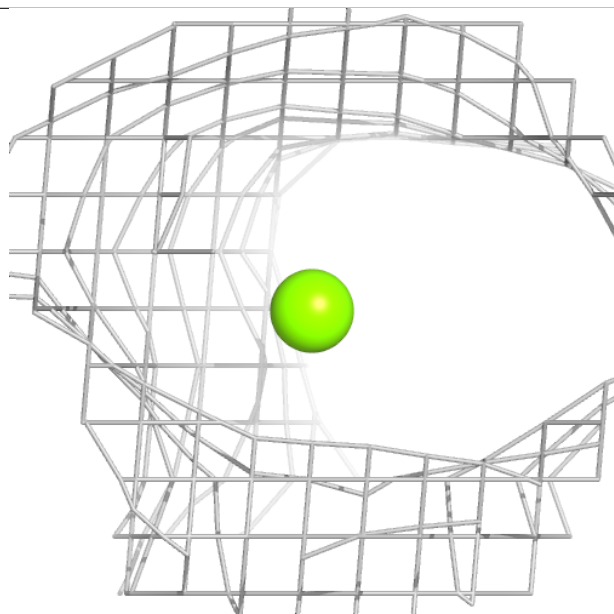
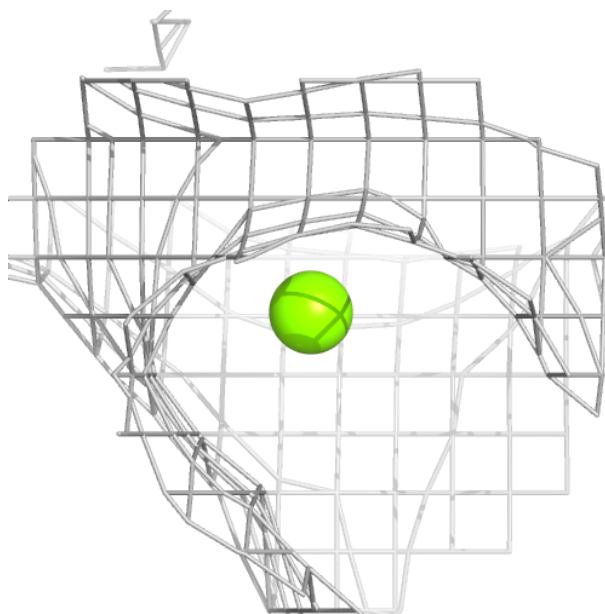
**Electron density around GTP B 706:**

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



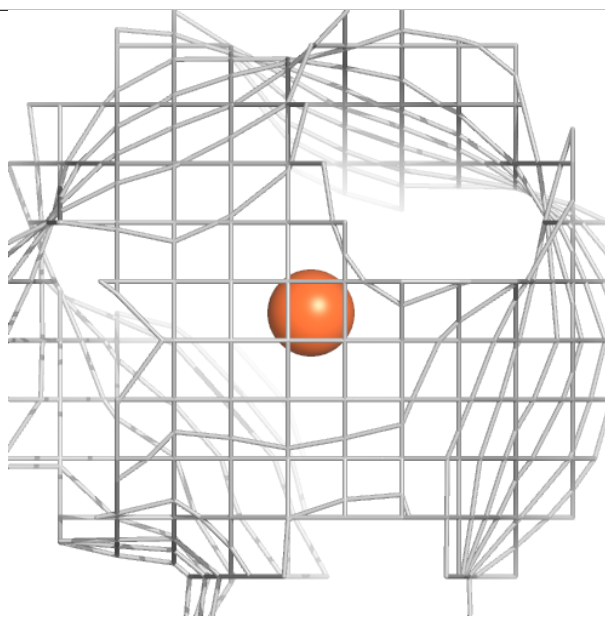
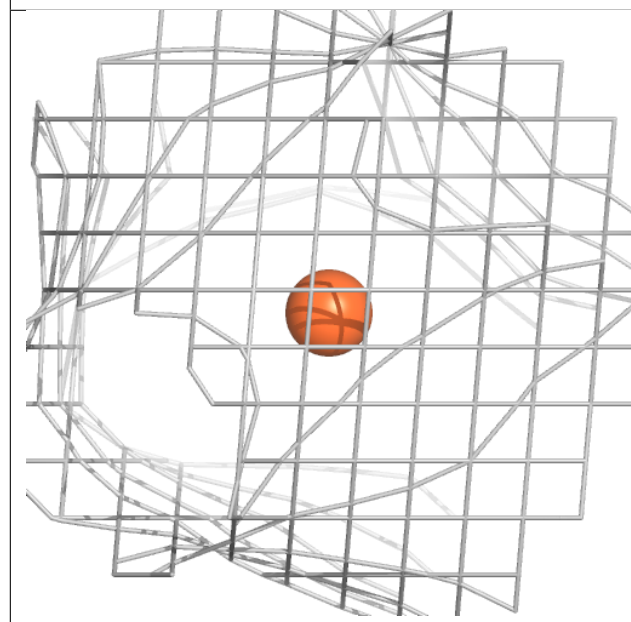
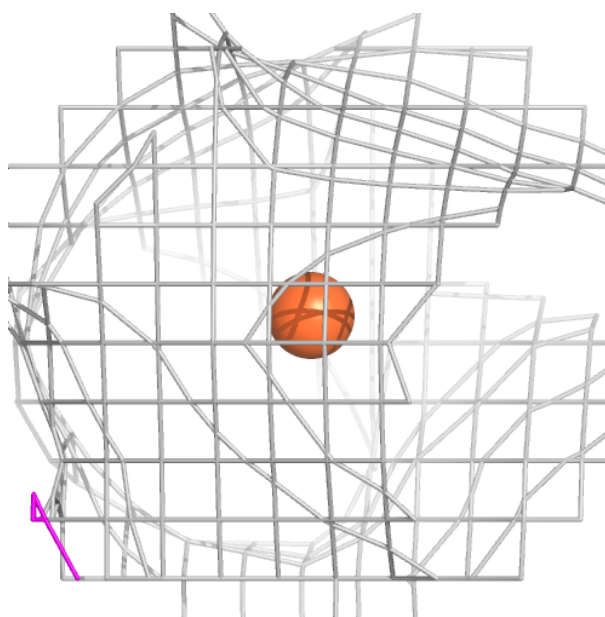
Electron density around MG M 704:

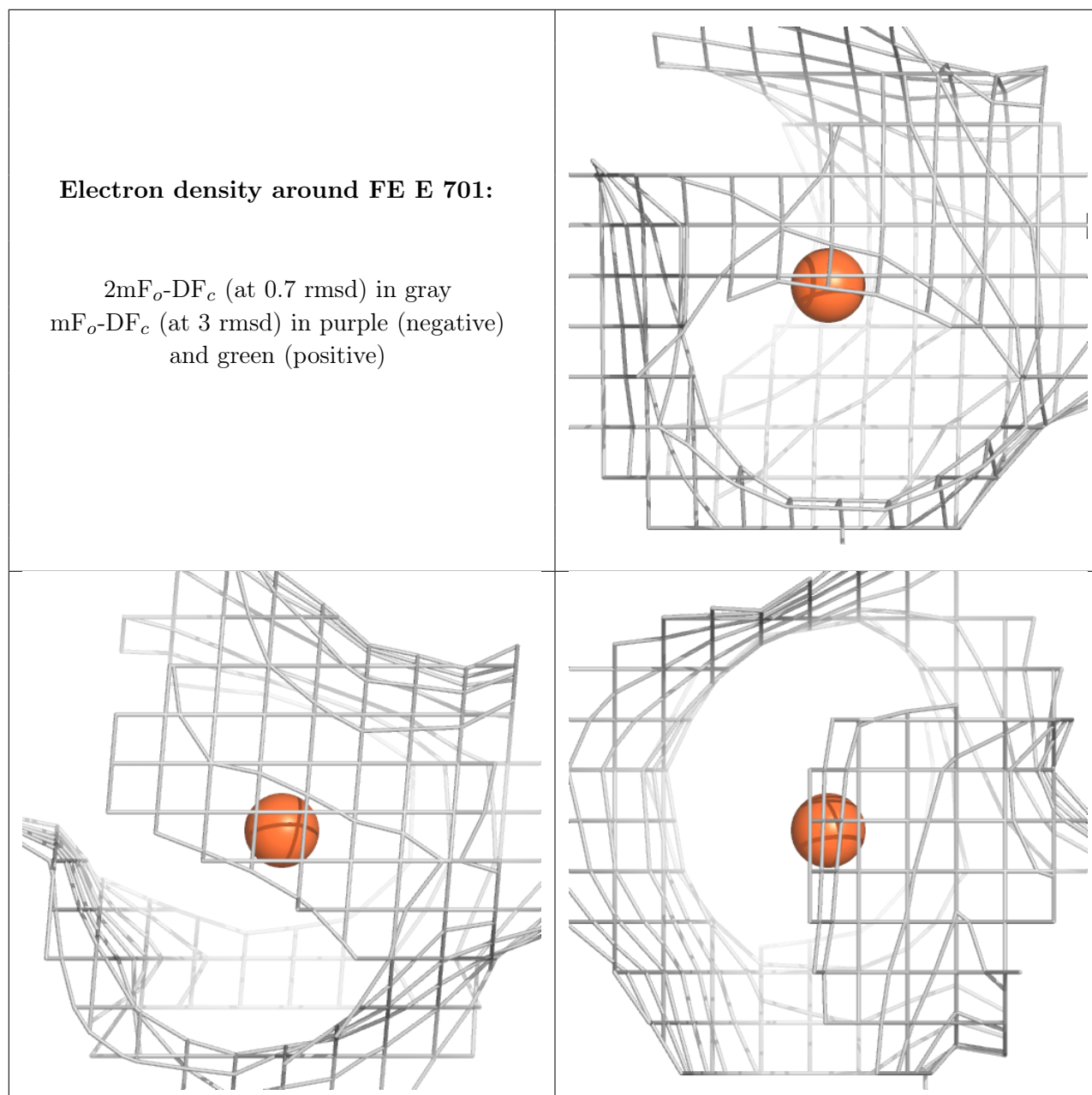
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE O 702:

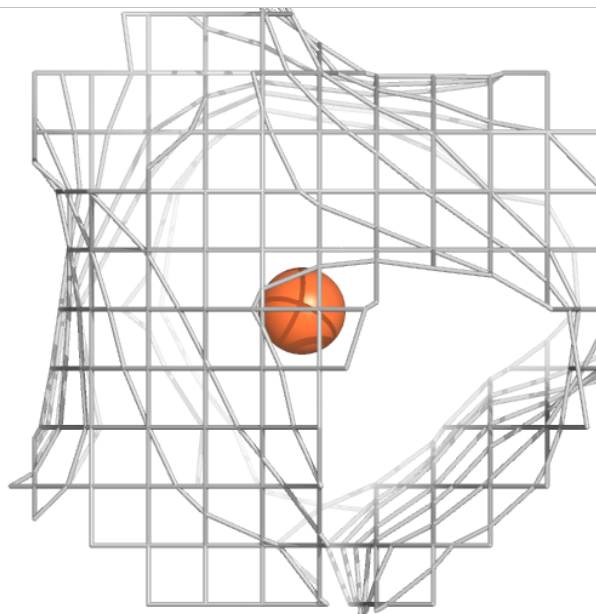
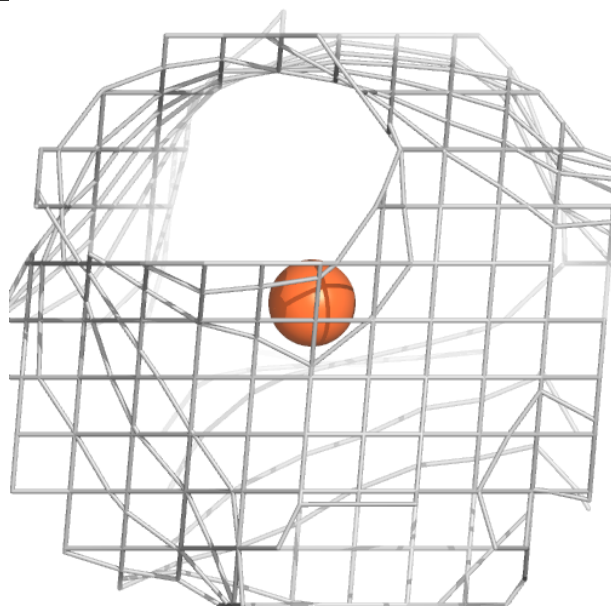
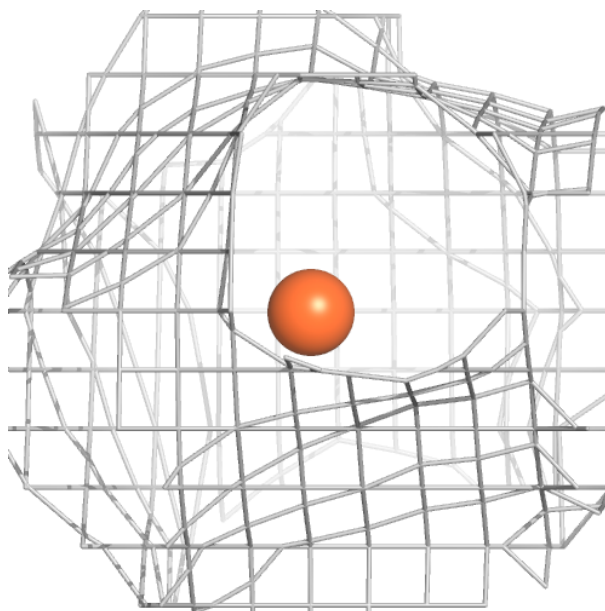
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





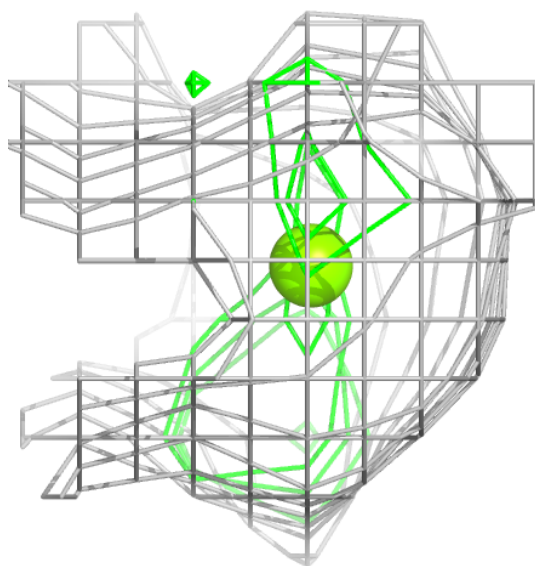
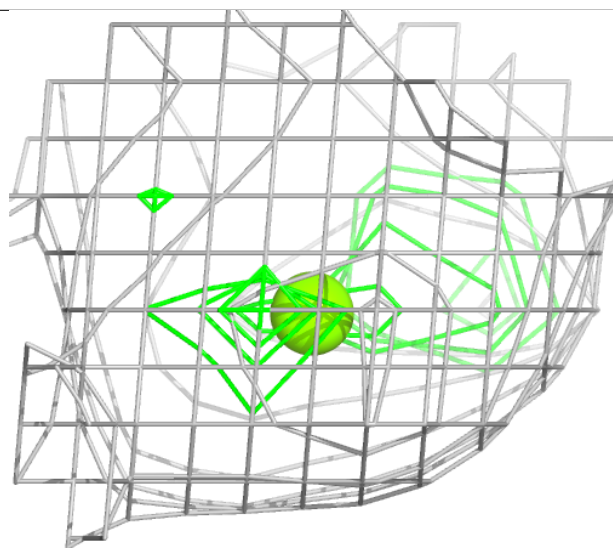
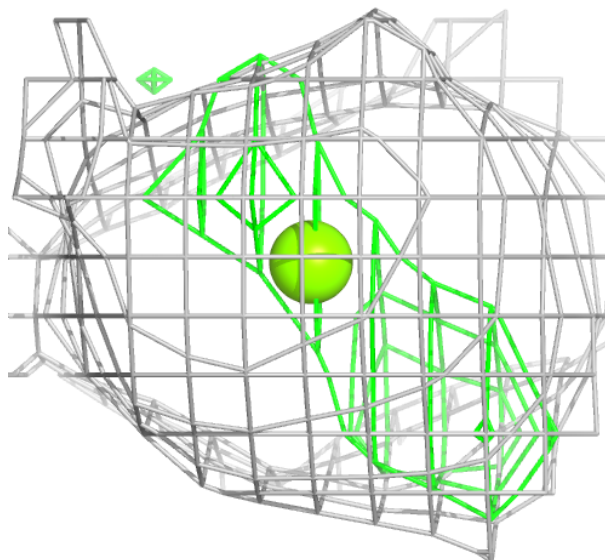
Electron density around FE A 701:

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



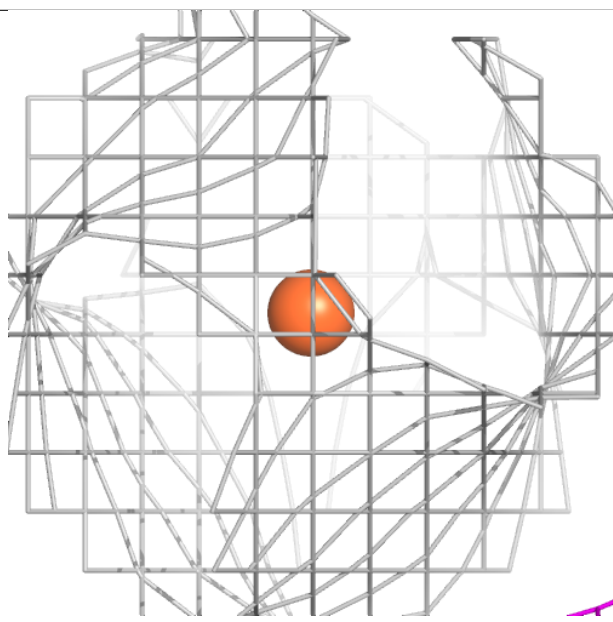
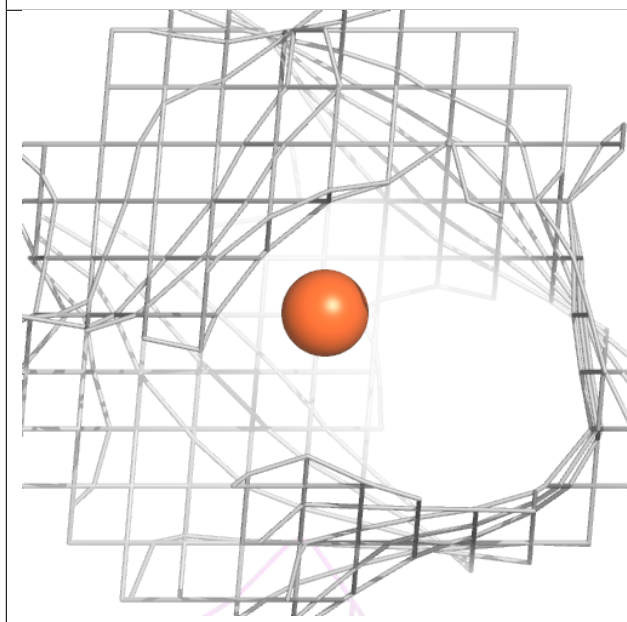
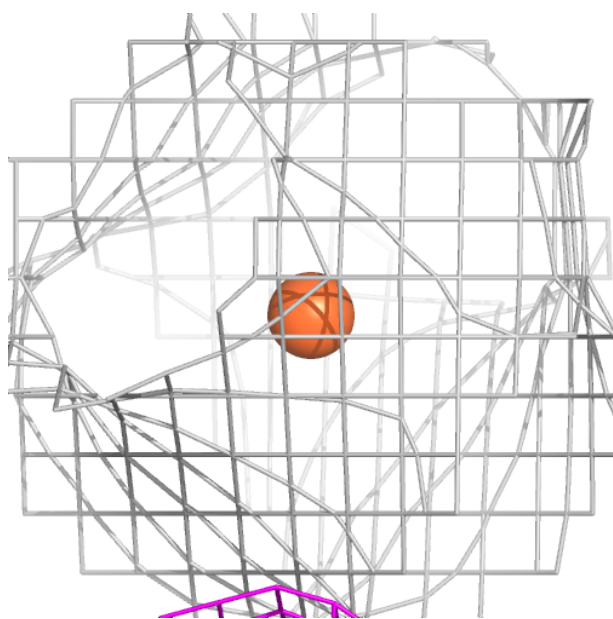
Electron density around MG A 703:

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



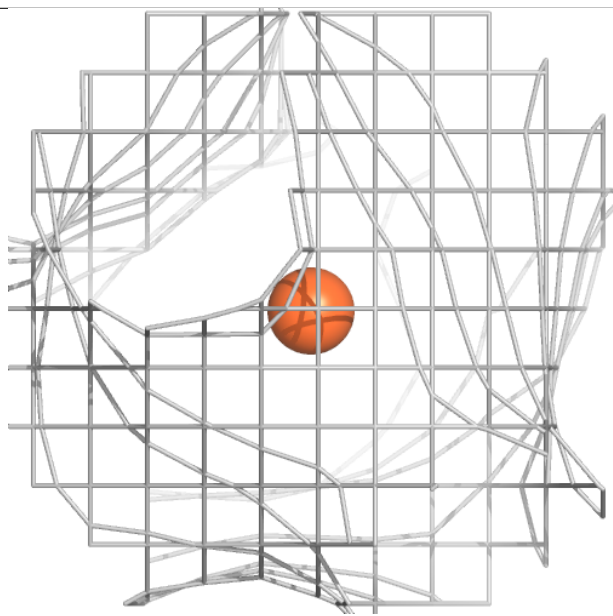
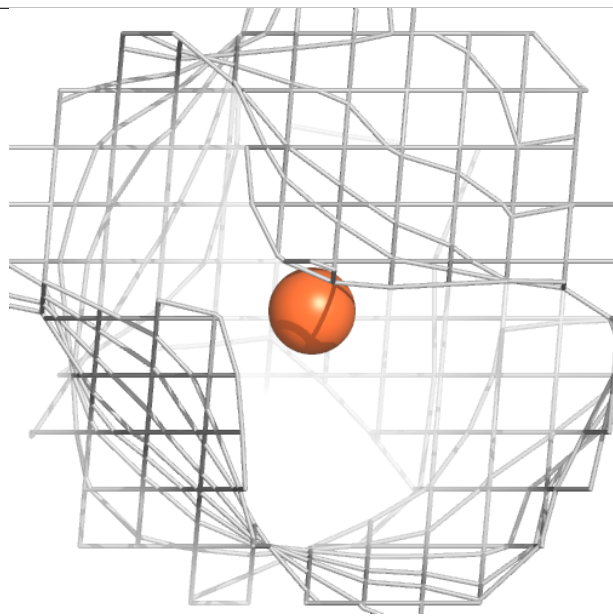
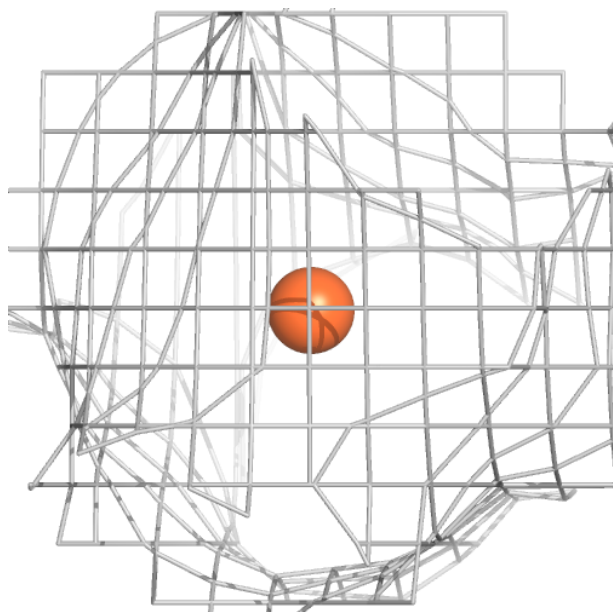
Electron density around FE H 702:

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



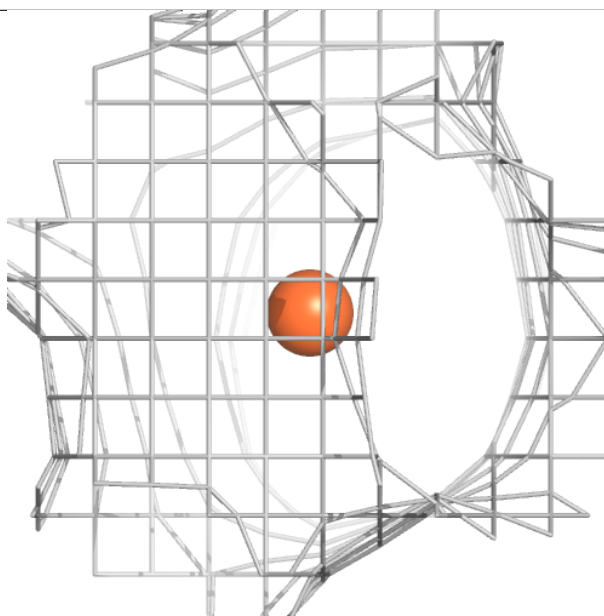
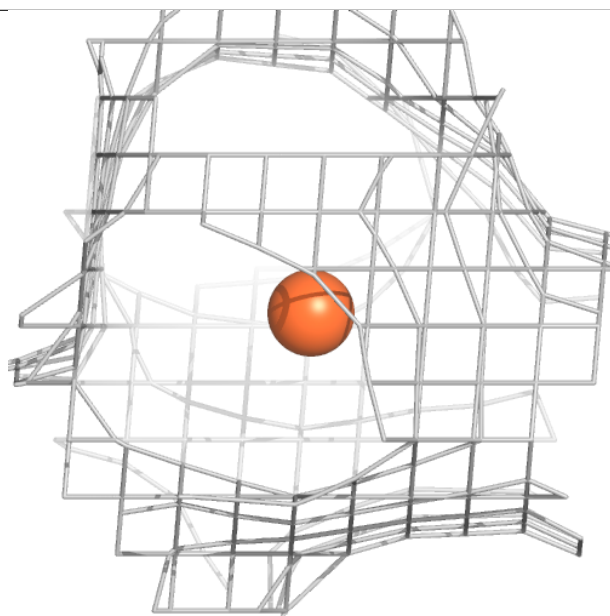
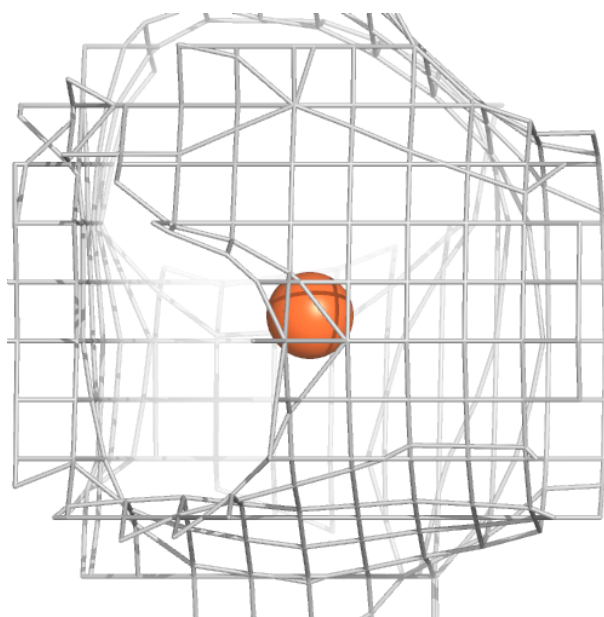
Electron density around FE B 701:

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



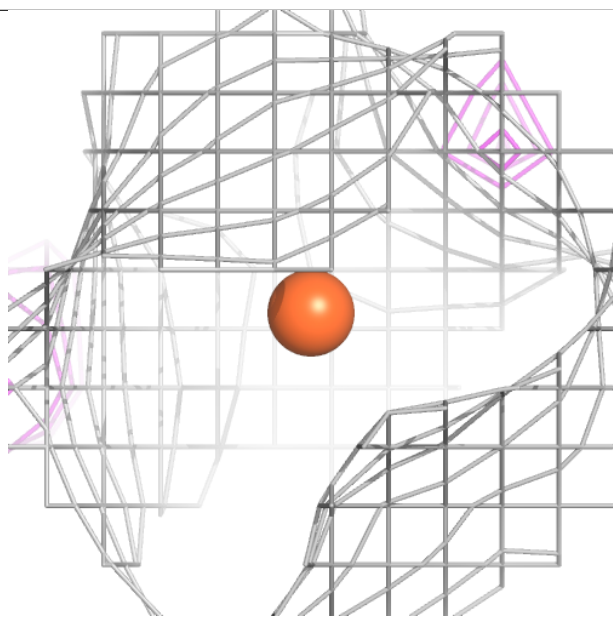
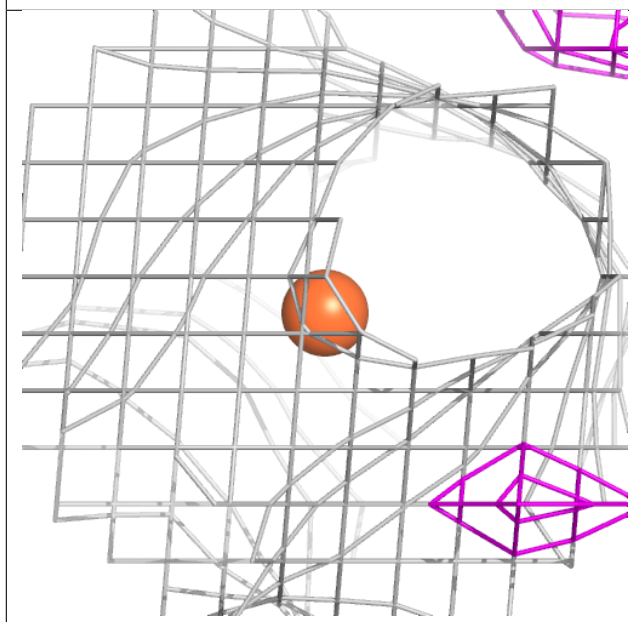
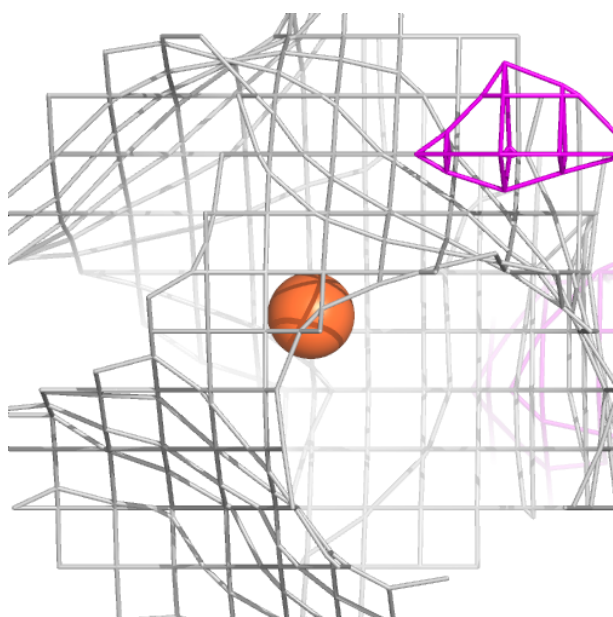
Electron density around FE J 701:

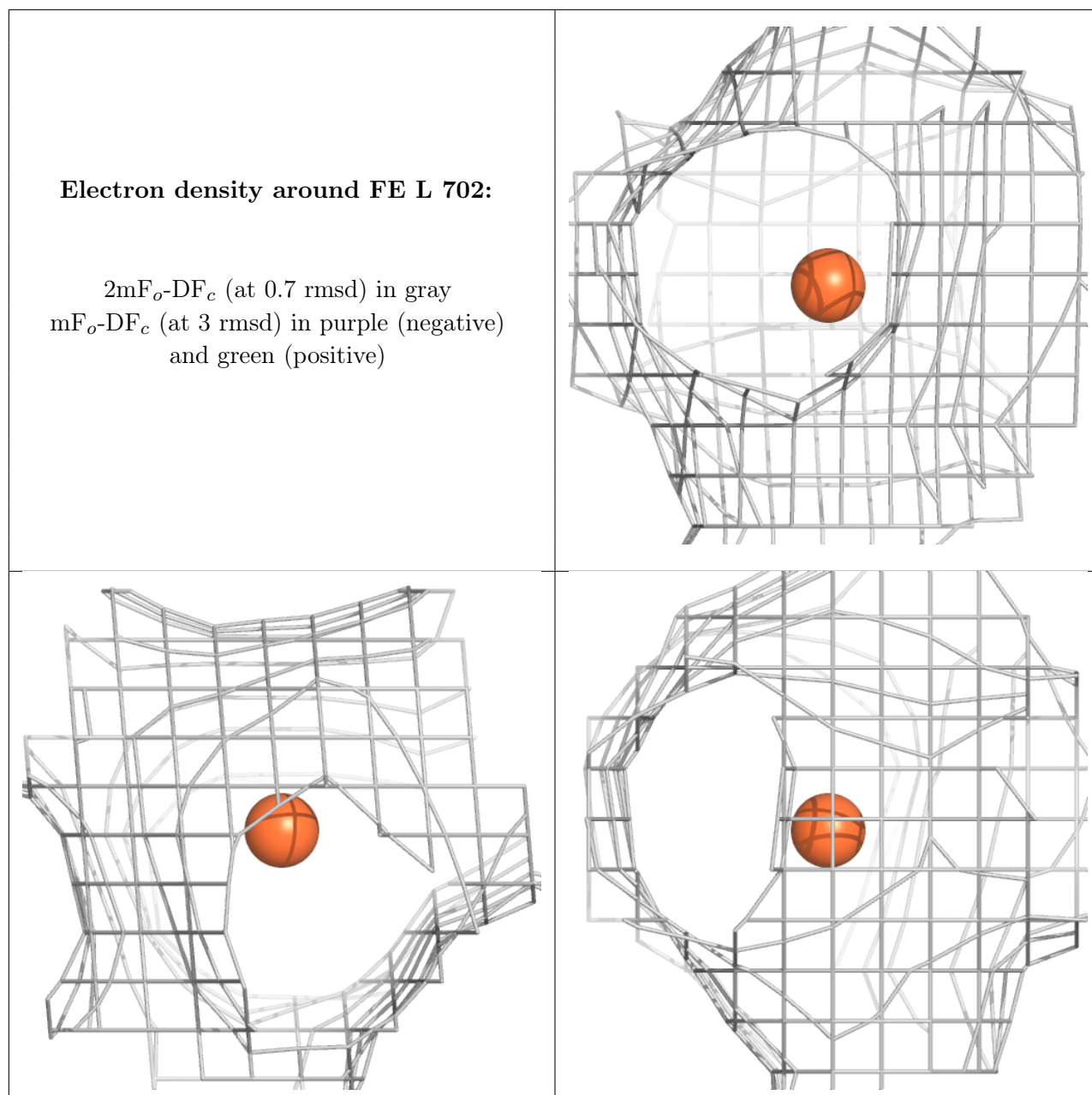
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE K 702:

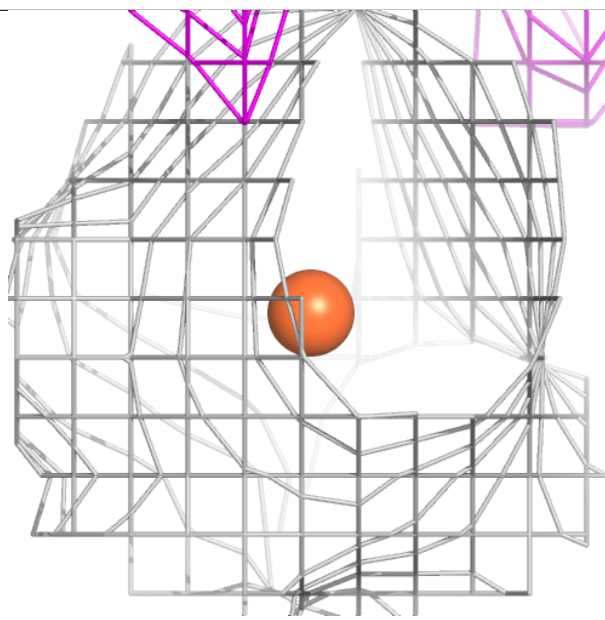
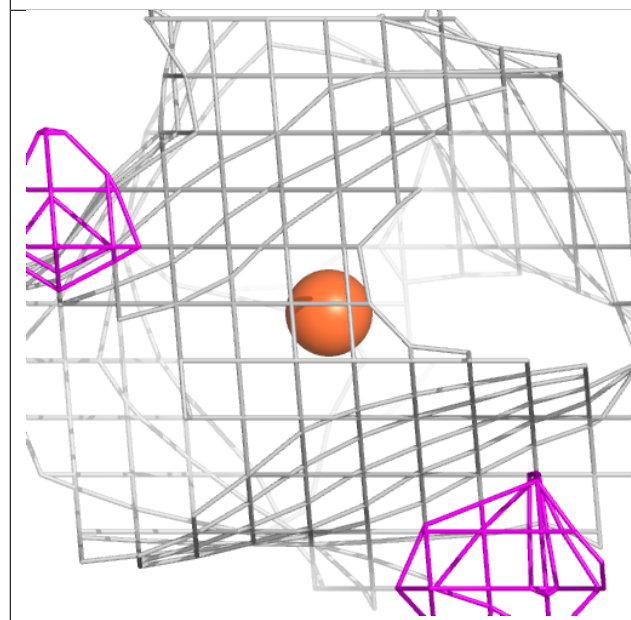
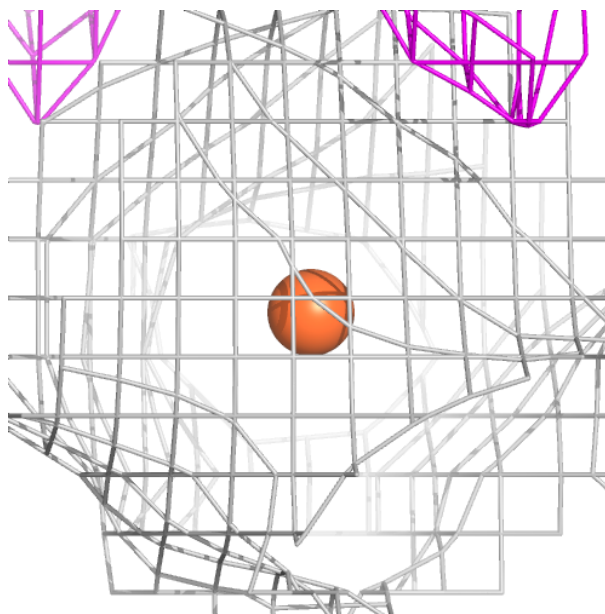
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





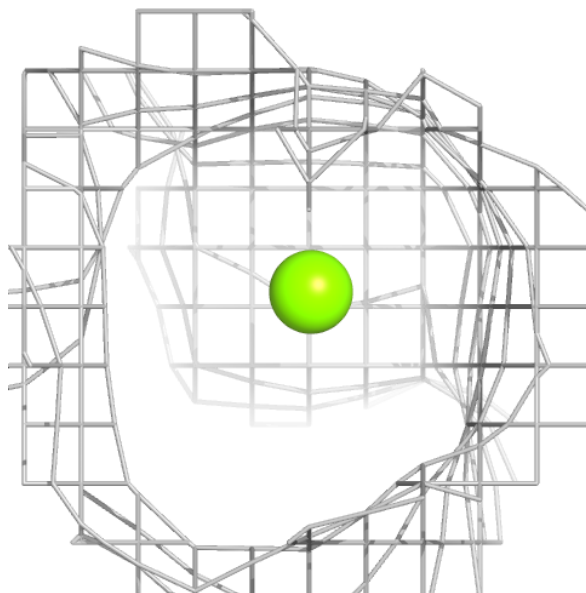
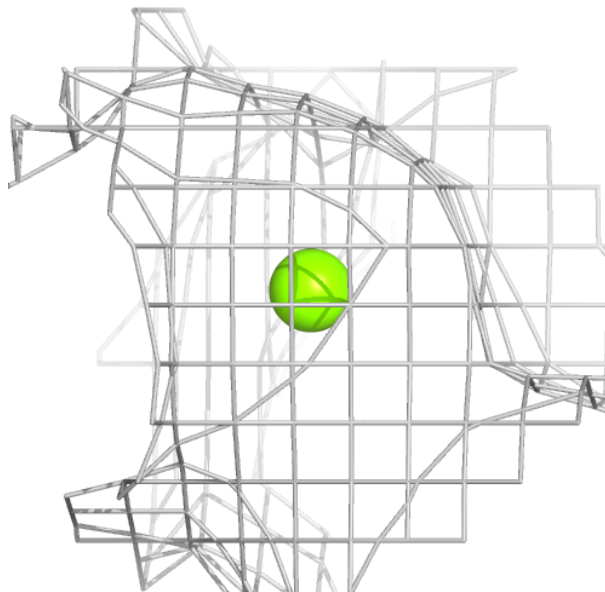
Electron density around FE M 701:

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



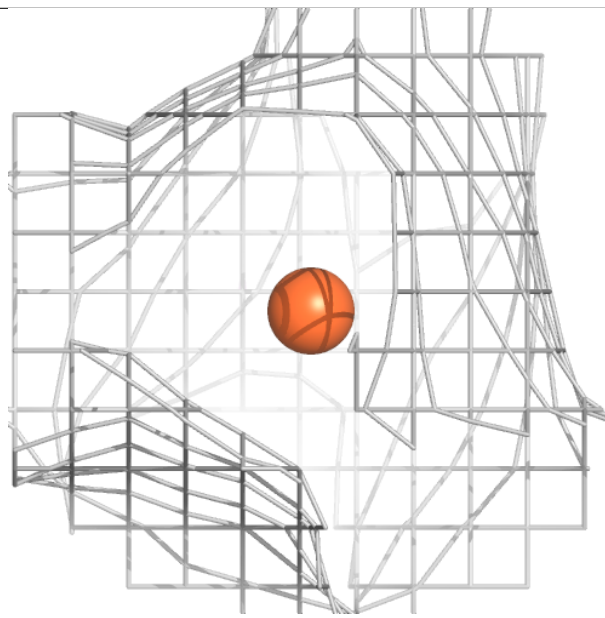
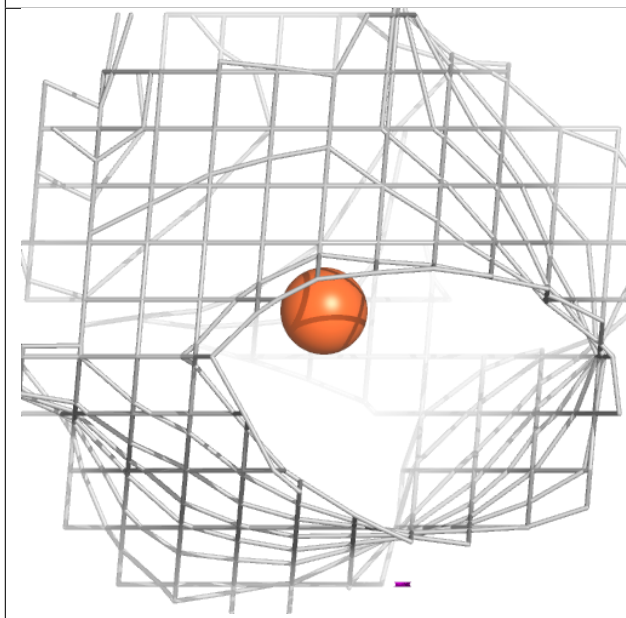
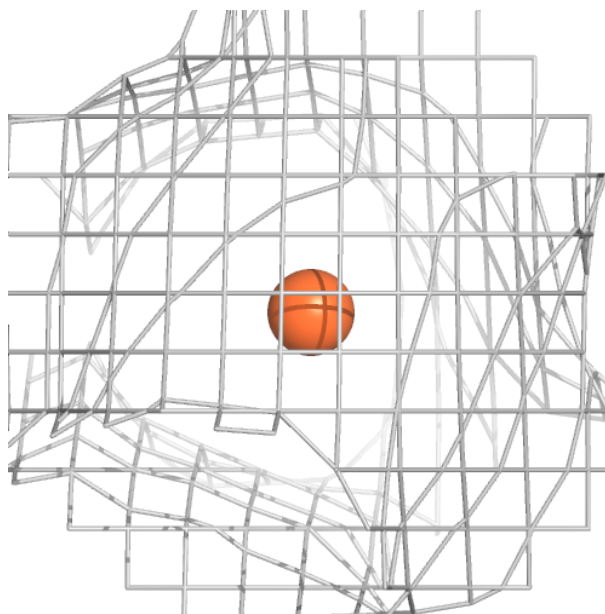
Electron density around MG C 705:

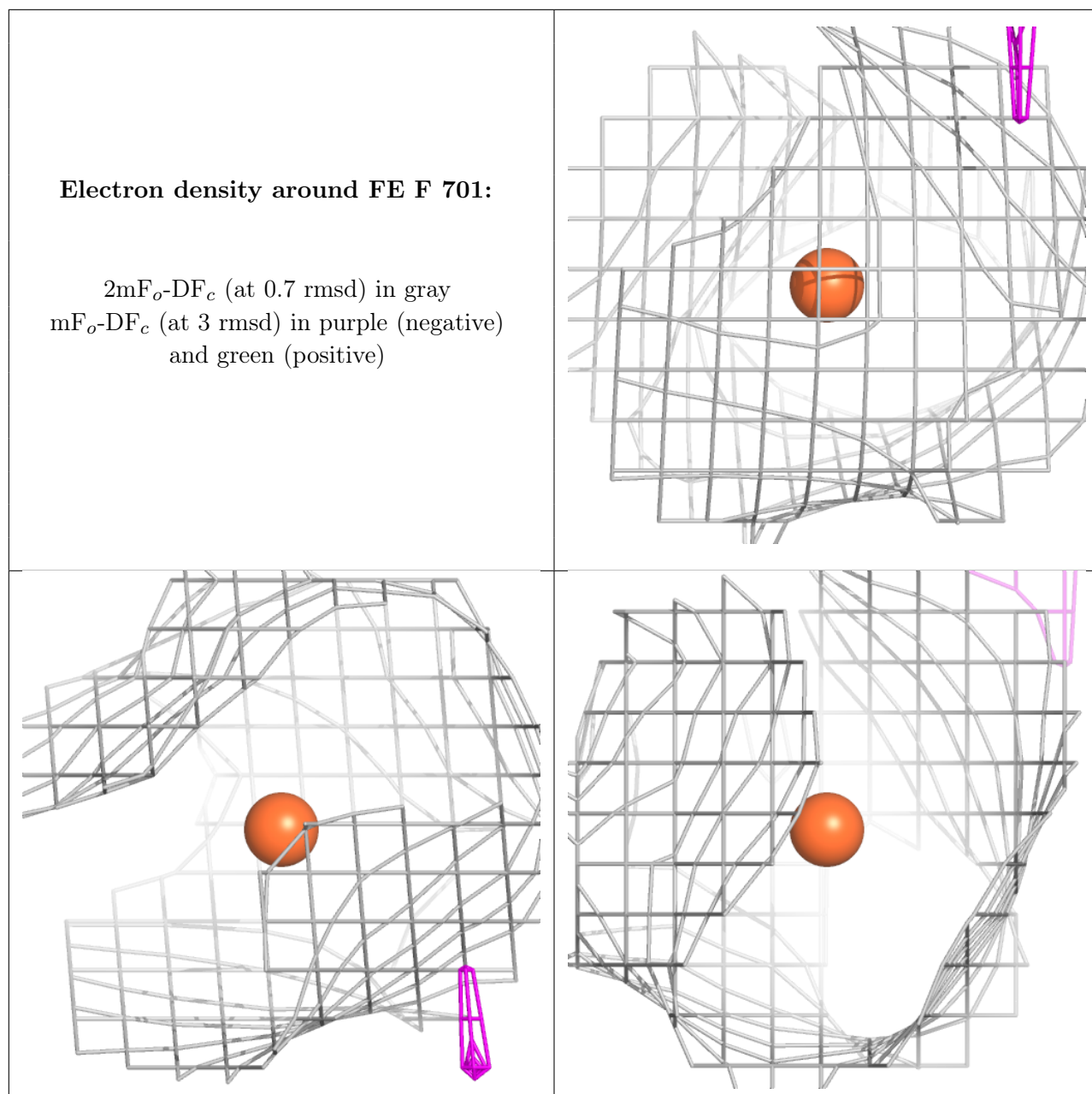
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

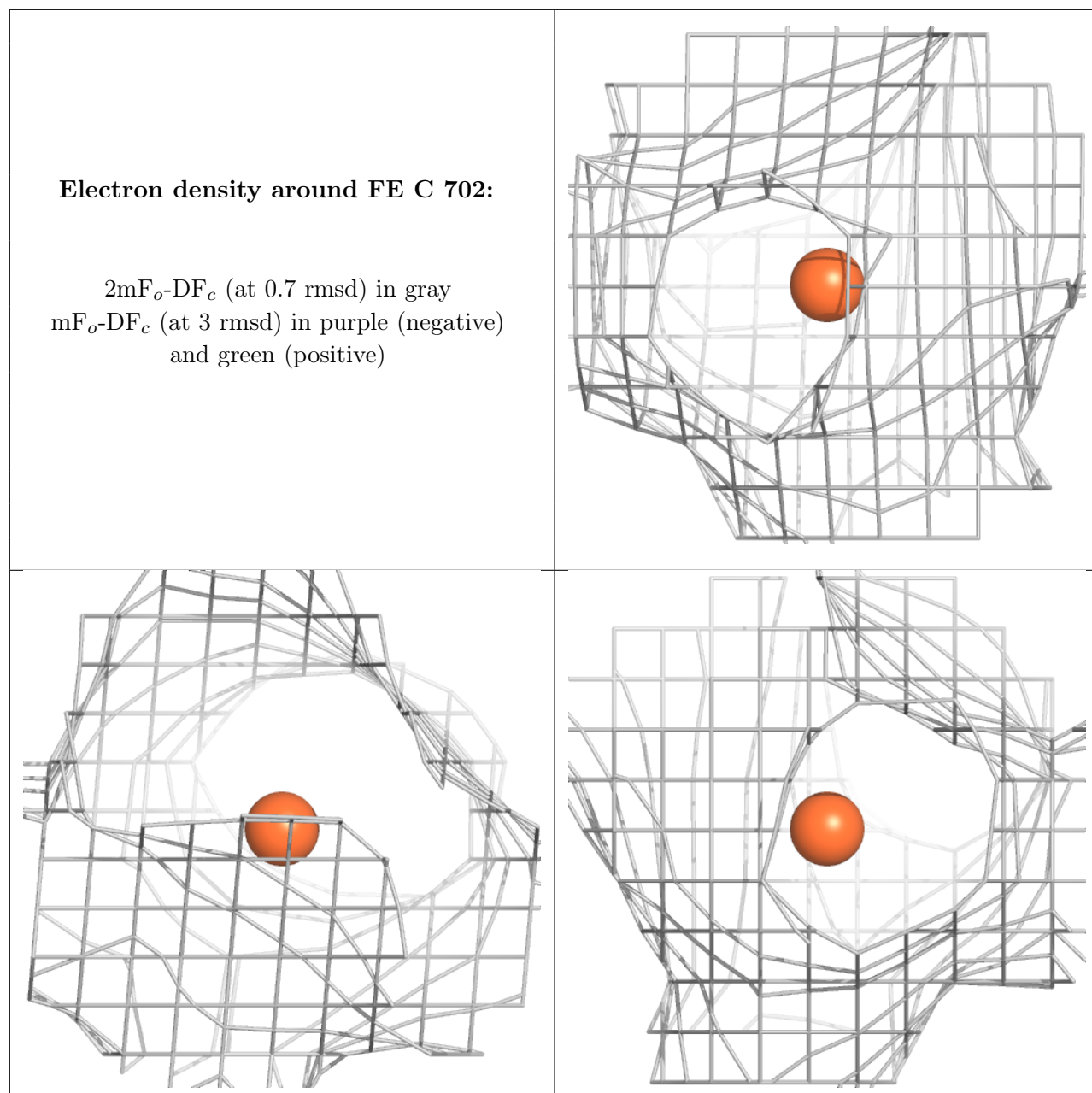


Electron density around FE D 702:

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







6.5 Other polymers [i](#)

There are no such residues in this entry.