



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 15, 2024 – 10:51 pm GMT

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

This is a 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)
Xtrriage (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

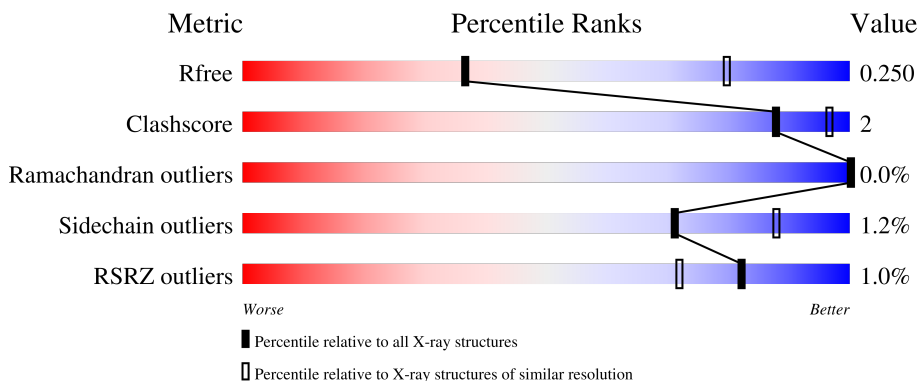
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 Å.

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













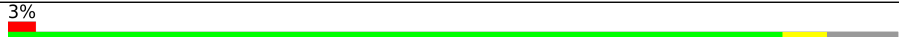

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	86% 6% 8%
1	B	520	87% 5% 8%
1	C	520	87% 5% 8%
1	D	520	87% 5% 8%

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

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 62675 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	480	Total 3862	C 2472	N 666	O 704	S 20	0	0	0
1	B	479	Total 3841	C 2458	N 663	O 700	S 20	0	0	0
1	C	480	Total 3839	C 2459	N 662	O 698	S 20	0	0	0
1	D	481	Total 3852	C 2465	N 666	O 701	S 20	0	0	0
1	E	479	Total 3845	C 2461	N 664	O 700	S 20	0	0	0
1	F	478	Total 3831	C 2452	N 658	O 701	S 20	0	0	0
1	G	479	Total 3826	C 2447	N 658	O 701	S 20	0	0	0
1	H	480	Total 3862	C 2473	N 667	O 702	S 20	0	0	0
1	I	477	Total 3824	C 2448	N 658	O 698	S 20	0	0	0
1	J	478	Total 3823	C 2448	N 660	O 695	S 20	0	0	0
1	K	478	Total 3824	C 2448	N 658	O 698	S 20	0	0	0
1	L	478	Total 3785	C 2422	N 646	O 697	S 20	0	0	0
1	M	475	Total 3744	C 2398	N 636	O 690	S 20	0	0	0
1	N	477	Total 3812	C 2442	N 652	O 698	S 20	0	0	0
1	O	481	Total 3818	C 2441	N 654	O 703	S 20	0	0	0
1	P	474	Total 3728	C 2391	N 635	O 682	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).

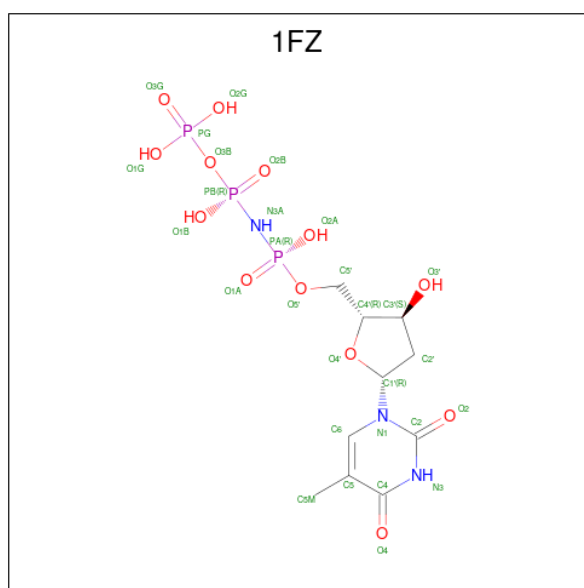
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mg 2 2	0	0
3	B	2	Total Mg 2 2	0	0
3	C	2	Total Mg 2 2	0	0
3	D	2	Total Mg 2 2	0	0
3	E	2	Total Mg 2 2	0	0

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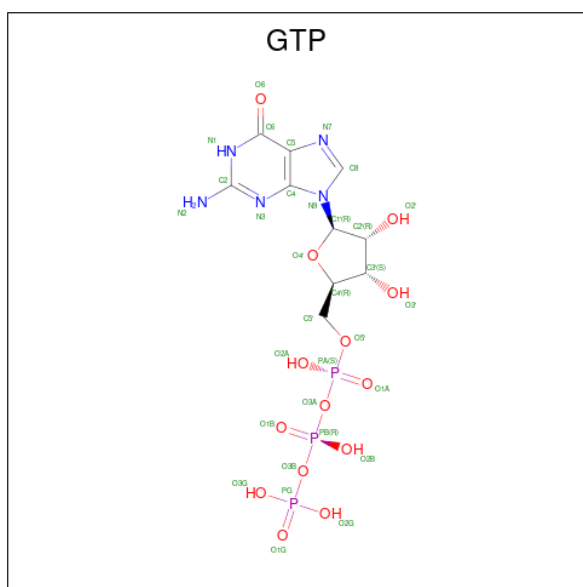
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	2	Total Mg 2 2	0	0
3	G	2	Total Mg 2 2	0	0
3	H	2	Total Mg 2 2	0	0
3	I	2	Total Mg 2 2	0	0
3	J	2	Total Mg 2 2	0	0
3	K	2	Total Mg 2 2	0	0
3	L	2	Total Mg 2 2	0	0
3	M	2	Total Mg 2 2	0	0
3	N	2	Total Mg 2 2	0	0
3	O	2	Total Mg 2 2	0	0
3	P	2	Total Mg 2 2	0	0

- Molecule 4 is 5'-O-[(R)-hydroxy{[(R)-hydroxy(phosphonooxy)phosphoryl]amino}phosphoryl]thymidine (three-letter code: 1FZ) (formula: C₁₀H₁₈N₃O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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

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



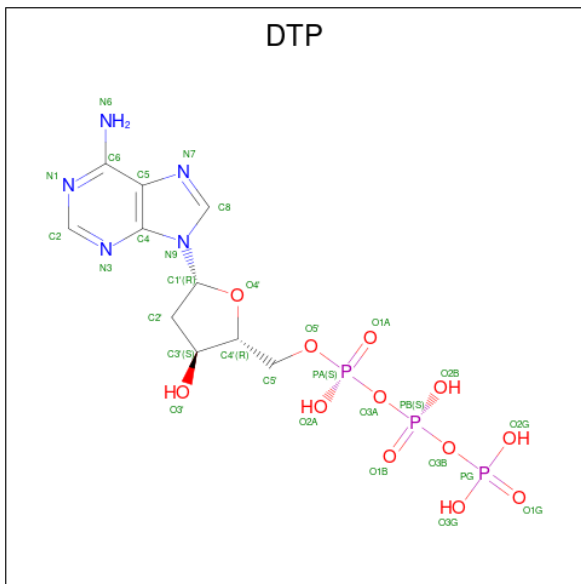
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	E	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	F	1	Total	C	N	O	P	0	0
		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

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

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



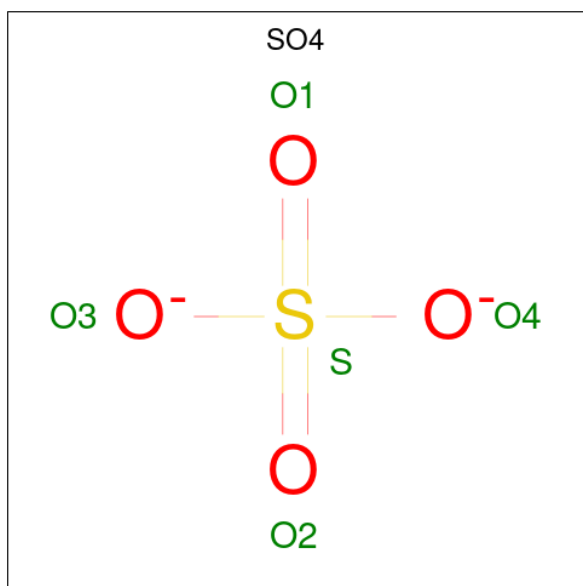
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
6	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
6	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
6	C	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
6	D	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
6	E	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
6	F	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
6	G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

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

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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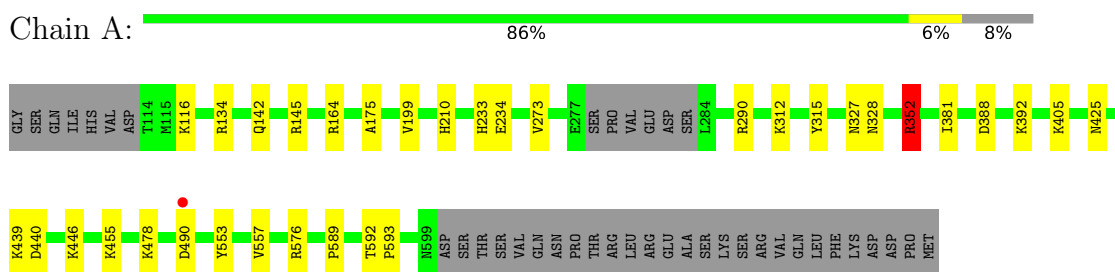
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	F	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	I	1	Total	O	S	0	0
			5	4	1		
7	J	1	Total	O	S	0	0
			5	4	1		
7	K	1	Total	O	S	0	0
			5	4	1		
7	N	1	Total	O	S	0	0
			5	4	1		
7	O	1	Total	O	S	0	0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

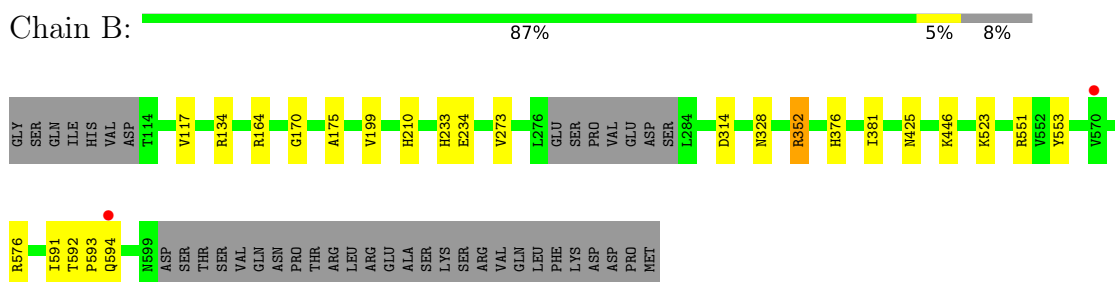
3 Residue-property plots [i](#)

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

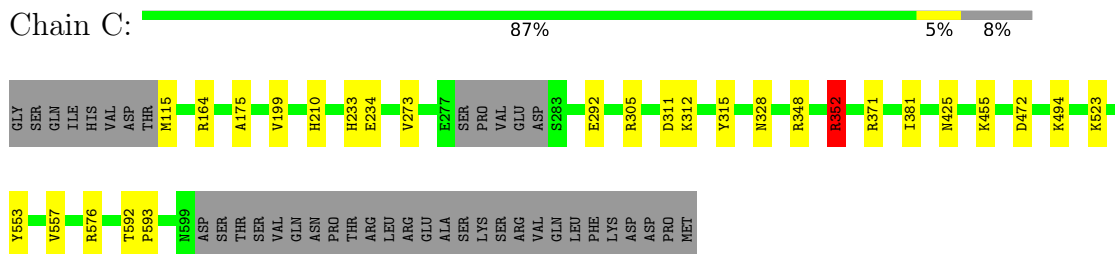
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



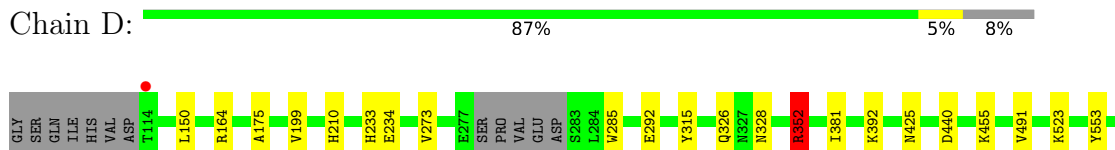
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

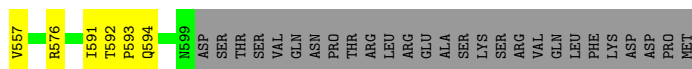


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



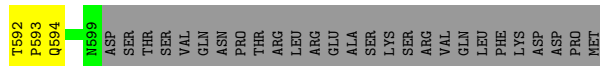
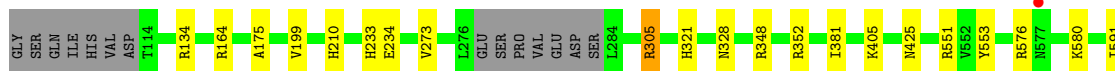
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





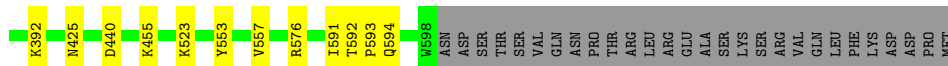
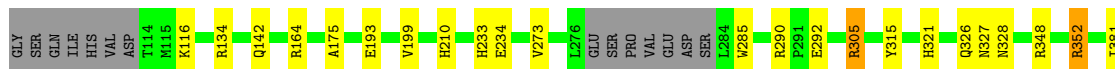
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain E: 88% 8%



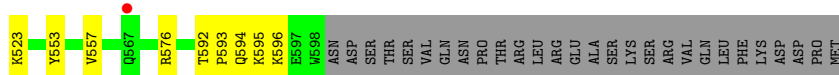
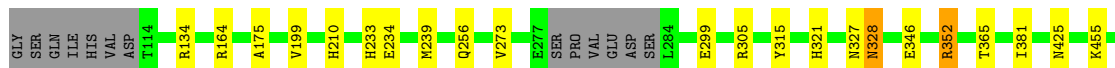
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain F: 85% 6% 8%



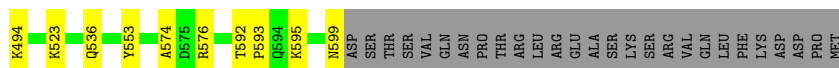
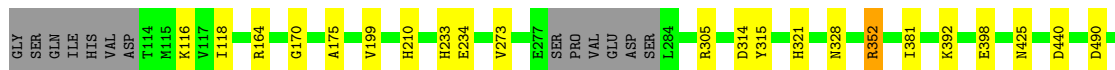
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain G: 86% 6% 8%



- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain H: 86% 6% 8%

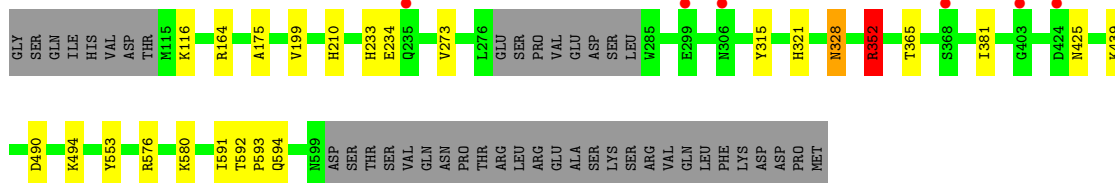
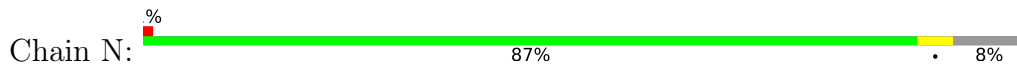


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

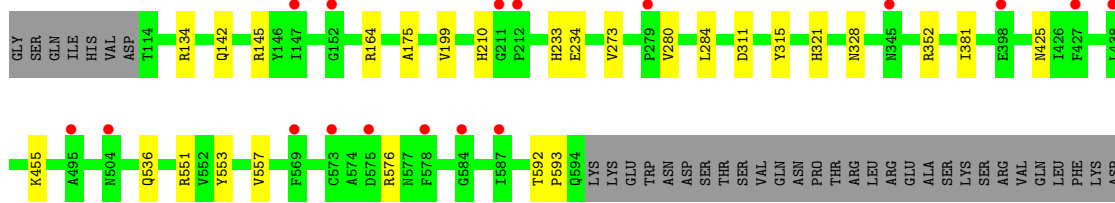
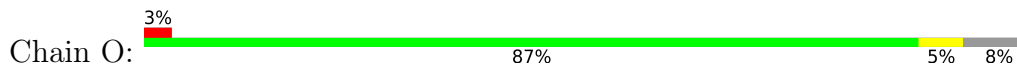
Chain I: 86% 5% 8%

SER
LYS
GLN
SER
ARG
VAL
GLN
LEU
PHE
LYS
ASP
ASP
PRO
MET

● Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

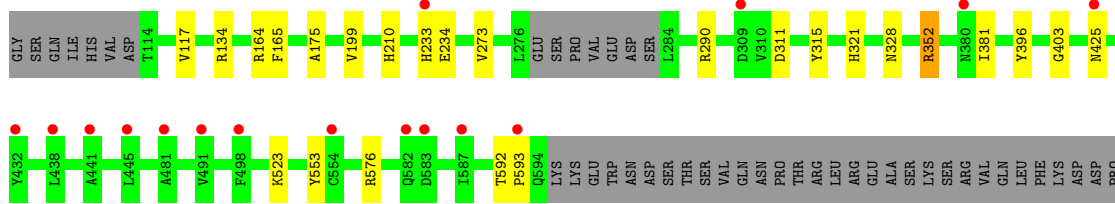
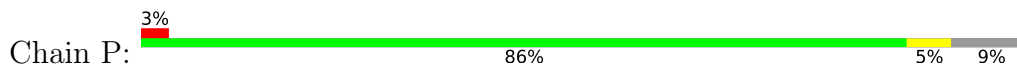


● Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



ASP
PRO
MET

● Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



MET

4 Data and refinement statistics

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

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

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: SO4, DTP, MG, 1FZ, GTP, FE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.53	0/3955	0.75	5/5356 (0.1%)
1	B	0.51	0/3934	0.72	4/5332 (0.1%)
1	C	0.51	1/3932 (0.0%)	0.71	4/5328 (0.1%)
1	D	0.51	0/3945	0.74	3/5346 (0.1%)
1	E	0.49	0/3938	0.71	5/5336 (0.1%)
1	F	0.50	1/3924 (0.0%)	0.72	4/5320 (0.1%)
1	G	0.53	0/3919	0.73	4/5317 (0.1%)
1	H	0.52	1/3955 (0.0%)	0.75	3/5355 (0.1%)
1	I	0.47	0/3917	0.71	4/5308 (0.1%)
1	J	0.48	0/3916	0.74	3/5309 (0.1%)
1	K	0.49	0/3917	0.72	5/5311 (0.1%)
1	L	0.52	1/3878 (0.0%)	0.75	2/5268 (0.0%)
1	M	0.48	0/3837	0.69	2/5216 (0.0%)
1	N	0.50	0/3905	0.74	3/5294 (0.1%)
1	O	0.49	0/3911	0.70	4/5310 (0.1%)
1	P	0.48	0/3819	0.74	3/5189 (0.1%)
All	All	0.50	4/62602 (0.0%)	0.73	58/84895 (0.1%)

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

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

All (4) bond length outliers are listed below:

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

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

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	164	ARG	NE-CZ-NH1	14.86	127.73	120.30
1	D	164	ARG	NE-CZ-NH1	14.57	127.58	120.30
1	H	164	ARG	NE-CZ-NH2	-14.55	113.03	120.30
1	P	164	ARG	NE-CZ-NH1	14.51	127.56	120.30
1	N	164	ARG	NE-CZ-NH2	-14.46	113.07	120.30
1	H	164	ARG	NE-CZ-NH1	14.28	127.44	120.30
1	L	164	ARG	NE-CZ-NH2	-14.17	113.21	120.30
1	J	164	ARG	NE-CZ-NH2	-14.17	113.22	120.30
1	J	164	ARG	NE-CZ-NH1	14.10	127.35	120.30
1	P	164	ARG	NE-CZ-NH2	-14.01	113.30	120.30
1	D	164	ARG	NE-CZ-NH2	-13.97	113.32	120.30
1	N	164	ARG	NE-CZ-NH1	13.81	127.21	120.30
1	A	352	ARG	NE-CZ-NH1	-8.76	115.92	120.30
1	I	164	ARG	NE-CZ-NH1	-8.56	116.02	120.30
1	O	164	ARG	NE-CZ-NH2	8.55	124.57	120.30
1	G	164	ARG	NE-CZ-NH2	8.53	124.56	120.30
1	O	164	ARG	NE-CZ-NH1	-8.42	116.09	120.30
1	M	164	ARG	NE-CZ-NH2	8.37	124.49	120.30
1	M	164	ARG	NE-CZ-NH1	-8.34	116.13	120.30
1	E	164	ARG	NE-CZ-NH1	-8.32	116.14	120.30
1	F	164	ARG	NE-CZ-NH2	8.32	124.46	120.30
1	K	164	ARG	NE-CZ-NH2	8.31	124.46	120.30
1	I	164	ARG	NE-CZ-NH2	8.29	124.45	120.30
1	C	164	ARG	NE-CZ-NH2	8.28	124.44	120.30
1	A	164	ARG	NE-CZ-NH1	-8.26	116.17	120.30
1	F	290	ARG	NE-CZ-NH2	8.21	124.40	120.30
1	F	164	ARG	NE-CZ-NH1	-8.12	116.24	120.30
1	K	164	ARG	NE-CZ-NH1	-8.06	116.27	120.30
1	G	164	ARG	NE-CZ-NH1	-8.06	116.27	120.30
1	K	290	ARG	NE-CZ-NH2	8.01	124.30	120.30
1	A	164	ARG	NE-CZ-NH2	8.00	124.30	120.30
1	B	164	ARG	NE-CZ-NH2	7.96	124.28	120.30
1	P	290	ARG	NE-CZ-NH2	7.93	124.26	120.30
1	I	490	ASP	CB-CG-OD2	-7.93	111.17	118.30
1	C	164	ARG	NE-CZ-NH1	-7.89	116.35	120.30
1	B	164	ARG	NE-CZ-NH1	-7.85	116.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	164	ARG	NE-CZ-NH2	7.80	124.20	120.30
1	A	290	ARG	NE-CZ-NH2	7.73	124.16	120.30
1	K	415	ASP	CB-CG-OD1	6.65	124.29	118.30
1	C	371	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	H	599	ASN	CA-C-O	6.28	133.28	120.10
1	E	551	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	B	551	ARG	NE-CZ-NH1	-5.81	117.39	120.30
1	B	551	ARG	NE-CZ-NH2	5.75	123.17	120.30
1	I	388	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	O	551	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	G	596	LYS	CA-C-O	5.55	131.76	120.10
1	K	305	ARG	NE-CZ-NH2	5.49	123.05	120.30
1	F	305	ARG	CG-CD-NE	-5.49	100.28	111.80
1	C	352	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	388	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	O	551	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	E	305	ARG	CG-CD-NE	-5.23	100.82	111.80
1	E	551	ARG	NE-CZ-NH2	5.21	122.90	120.30
1	D	352	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	J	239	MET	CG-SD-CE	5.06	108.30	100.20
1	N	352	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	G	239	MET	CG-SD-CE	5.01	108.22	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	595	LYS	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3862	0	3766	18	0
1	B	3841	0	3729	14	0
1	C	3839	0	3730	15	1
1	D	3852	0	3743	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3845	0	3740	13	0
1	F	3831	0	3711	20	0
1	G	3826	0	3685	18	0
1	H	3862	0	3773	17	0
1	I	3824	0	3709	17	2
1	J	3823	0	3703	23	0
1	K	3824	0	3700	18	0
1	L	3785	0	3608	17	3
1	M	3744	0	3554	24	0
1	N	3812	0	3687	14	0
1	O	3818	0	3675	15	0
1	P	3728	0	3568	14	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
3	M	2	0	0	0	0
3	N	2	0	0	0	0

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	K	30	0	12	2	0
6	L	30	0	12	3	0
6	M	60	0	24	4	0
6	N	60	0	24	2	0
7	B	5	0	0	0	0
7	C	5	0	0	0	0
7	D	5	0	0	0	0
7	E	5	0	0	1	0
7	F	5	0	0	0	0
7	H	5	0	0	1	0
7	I	5	0	0	0	0
7	J	5	0	0	0	0
7	K	5	0	0	0	0
7	N	5	0	0	0	0
7	O	5	0	0	0	0
All	All	62675	0	59689	245	4

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

All (245) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:305:ARG:NH1	1:K:348:ARG:HD3	1.55	1.22
1:J:488:LEU:HA	1:M:488:LEU:HB2	1.30	1.13
1:J:488:LEU:CA	1:M:488:LEU:HB2	1.90	1.00
1:K:305:ARG:HH11	1:K:348:ARG:HD3	1.22	0.90
1:J:488:LEU:HB2	1:M:488:LEU:N	1.94	0.83
1:J:488:LEU:HD13	1:M:488:LEU:HA	1.61	0.81
1:M:523:LYS:NZ	5:O:705:GTP:O3G	2.16	0.79
1:A:490:ASP:OD2	1:I:263:GLU:OE1	2.00	0.78
1:I:328:ASN:HB2	1:L:328:ASN:HB2	1.65	0.77
6:E:707:DTP:O1B	5:G:706:GTP:O3'	2.04	0.74
6:M:706:DTP:O2G	1:P:352:ARG:NH2	2.19	0.72
1:A:328:ASN:HB2	1:D:328:ASN:HB2	1.73	0.71
1:E:425:ASN:OD1	1:F:425:ASN:ND2	2.24	0.70
1:K:305:ARG:NH1	1:K:348:ARG:CD	2.45	0.70
1:O:425:ASN:OD1	1:P:425:ASN:ND2	2.24	0.69
1:M:425:ASN:ND2	1:N:425:ASN:OD1	2.28	0.66
6:I:708:DTP:O1B	5:K:706:GTP:O3'	2.12	0.64
6:E:707:DTP:O1G	5:G:706:GTP:O1B	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:328:ASN:HB2	1:P:328:ASN:HB2	1.80	0.64
1:B:328:ASN:HB2	1:C:328:ASN:HB2	1.81	0.63
5:B:705:GTP:O1B	6:D:701:DTP:O1G	2.17	0.63
1:D:491:VAL:HG13	1:G:256:GLN:O	1.99	0.62
1:J:328:ASN:HB2	1:K:328:ASN:HB2	1.78	0.62
1:G:425:ASN:ND2	1:H:425:ASN:OD1	2.33	0.62
1:E:328:ASN:HB2	1:H:328:ASN:HB2	1.81	0.62
1:D:150:LEU:O	4:D:706:1FZ:H2	2.00	0.62
1:J:488:LEU:N	1:M:488:LEU:HB2	2.17	0.59
1:N:352:ARG:NH2	6:N:708:DTP:O2G	2.36	0.58
1:C:352:ARG:NH2	6:C:701:DTP:O2G	2.35	0.57
1:N:328:ASN:ND2	1:N:365:THR:OG1	2.38	0.57
5:A:705:GTP:O3G	1:C:523:LYS:NZ	2.38	0.57
1:J:488:LEU:HA	1:M:488:LEU:CB	2.20	0.56
1:J:488:LEU:HB2	1:M:488:LEU:CA	2.34	0.56
1:G:328:ASN:ND2	1:G:365:THR:OG1	2.39	0.56
1:D:352:ARG:NH2	6:D:701:DTP:O2G	2.38	0.56
1:J:488:LEU:CD1	1:M:488:LEU:HA	2.31	0.56
1:L:455:LYS:HE3	1:L:557:VAL:HG13	1.88	0.55
1:I:425:ASN:OD1	1:J:425:ASN:ND2	2.40	0.55
1:D:150:LEU:HA	4:D:706:1FZ:H1	1.88	0.55
1:K:425:ASN:ND2	1:L:425:ASN:OD1	2.40	0.55
1:D:392:LYS:HD3	1:D:440:ASP:HB3	1.89	0.55
1:H:392:LYS:HD3	1:H:440:ASP:HB3	1.90	0.54
1:J:455:LYS:HE3	1:J:557:VAL:HG13	1.89	0.54
1:G:455:LYS:HE3	1:G:557:VAL:HG13	1.89	0.54
1:A:392:LYS:HD3	1:A:440:ASP:HB3	1.90	0.54
5:I:705:GTP:H5''	6:K:701:DTP:O1B	2.08	0.54
1:F:392:LYS:HD3	1:F:440:ASP:HB3	1.90	0.53
1:M:352:ARG:NH2	6:M:707:DTP:O2G	2.40	0.53
6:M:707:DTP:O2B	5:O:705:GTP:H5'	2.08	0.53
1:A:381:ILE:HD13	1:A:553:TYR:CG	2.44	0.53
1:J:381:ILE:HD13	1:J:553:TYR:CG	2.44	0.53
1:K:352:ARG:NH2	6:K:701:DTP:O2G	2.42	0.53
1:C:381:ILE:HD13	1:C:553:TYR:CG	2.45	0.52
1:M:381:ILE:HD13	1:M:553:TYR:CG	2.44	0.52
1:I:381:ILE:HD13	1:I:553:TYR:CG	2.45	0.52
1:B:117:VAL:O	5:B:705:GTP:O2'	2.24	0.52
1:D:381:ILE:HD13	1:D:553:TYR:CG	2.45	0.52
1:F:381:ILE:HD13	1:F:553:TYR:CG	2.45	0.52
1:M:392:LYS:HD3	1:M:440:ASP:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:381:ILE:HD13	1:E:553:TYR:CG	2.46	0.51
1:P:381:ILE:HD13	1:P:553:TYR:CG	2.45	0.51
1:L:381:ILE:HD13	1:L:553:TYR:CG	2.45	0.51
1:O:381:ILE:HD13	1:O:553:TYR:CG	2.45	0.51
1:H:381:ILE:HD13	1:H:553:TYR:CG	2.45	0.51
1:N:381:ILE:HD13	1:N:553:TYR:CG	2.45	0.51
1:K:381:ILE:HD13	1:K:553:TYR:CG	2.45	0.51
1:B:381:ILE:HD13	1:B:553:TYR:CG	2.45	0.51
1:C:455:LYS:HE3	1:C:557:VAL:HG13	1.93	0.50
1:F:234:GLU:HB3	1:F:273:VAL:HG12	1.94	0.50
1:E:305:ARG:HD3	7:E:706:SO4:O3	2.11	0.50
1:O:234:GLU:HB3	1:O:273:VAL:HG12	1.94	0.50
1:N:234:GLU:HB3	1:N:273:VAL:HG12	1.93	0.50
1:L:234:GLU:HB3	1:L:273:VAL:HG12	1.93	0.50
1:A:425:ASN:ND2	1:B:425:ASN:OD1	2.44	0.50
1:D:455:LYS:HE2	1:D:557:VAL:HG13	1.93	0.50
1:G:234:GLU:HB3	1:G:273:VAL:HG12	1.94	0.50
1:G:381:ILE:HD13	1:G:553:TYR:CG	2.46	0.50
1:A:589:PRO:HG3	1:I:255:GLU:HB3	1.93	0.50
1:P:234:GLU:HB3	1:P:273:VAL:HG12	1.93	0.49
1:G:299:GLU:OE2	1:G:305:ARG:HD2	2.12	0.49
1:L:215:HIS:NE2	4:L:705:1FZ:H12	2.27	0.49
1:I:234:GLU:HB3	1:I:273:VAL:HG12	1.95	0.49
1:M:234:GLU:HB3	1:M:273:VAL:HG12	1.94	0.49
1:E:234:GLU:HB3	1:E:273:VAL:HG12	1.95	0.49
1:K:312:LYS:NZ	4:K:705:1FZ:O2G	2.42	0.49
1:A:175:ALA:HB1	1:A:199:VAL:HG12	1.95	0.49
1:H:234:GLU:HB3	1:H:273:VAL:HG12	1.93	0.49
6:B:707:DTP:O1B	5:D:707:GTP:H5'	2.13	0.48
1:F:175:ALA:HB1	1:F:199:VAL:HG12	1.96	0.48
1:J:175:ALA:HB1	1:J:199:VAL:HG12	1.95	0.48
1:H:175:ALA:HB1	1:H:199:VAL:HG12	1.95	0.48
1:J:234:GLU:HB3	1:J:273:VAL:HG12	1.94	0.48
1:K:234:GLU:HB3	1:K:273:VAL:HG12	1.96	0.48
1:K:591:ILE:O	1:K:594:GLN:HB3	2.13	0.48
1:N:175:ALA:HB1	1:N:199:VAL:HG12	1.96	0.48
1:D:234:GLU:HB3	1:D:273:VAL:HG12	1.96	0.48
1:L:175:ALA:HB1	1:L:199:VAL:HG12	1.95	0.48
1:O:311:ASP:OD2	4:O:704:1FZ:N3A	2.47	0.48
1:P:175:ALA:HB1	1:P:199:VAL:HG12	1.95	0.48
1:A:234:GLU:HB3	1:A:273:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:175:ALA:HB1	1:I:199:VAL:HG12	1.95	0.47
1:B:175:ALA:HB1	1:B:199:VAL:HG12	1.96	0.47
1:G:352:ARG:NH2	6:G:701:DTP:O2G	2.43	0.47
1:J:591:ILE:O	1:J:594:GLN:HB3	2.15	0.47
1:N:591:ILE:O	1:N:594:GLN:HB3	2.15	0.47
1:A:116:LYS:NZ	5:A:705:GTP:O1G	2.45	0.47
1:E:305:ARG:CZ	1:E:348:ARG:HD3	2.45	0.47
1:E:580:LYS:HE2	1:H:536:GLN:NE2	2.29	0.47
1:E:591:ILE:O	1:E:594:GLN:HB3	2.15	0.47
1:O:145:ARG:NH2	5:O:705:GTP:N7	2.63	0.47
1:J:233:HIS:NE2	4:J:704:1FZ:O2A	2.48	0.47
1:M:175:ALA:HB1	1:M:199:VAL:HG12	1.96	0.47
1:D:591:ILE:O	1:D:594:GLN:HB3	2.15	0.47
1:E:175:ALA:HB1	1:E:199:VAL:HG12	1.95	0.47
1:O:175:ALA:HB1	1:O:199:VAL:HG12	1.95	0.47
1:D:175:ALA:HB1	1:D:199:VAL:HG12	1.96	0.47
1:H:592:THR:N	1:H:593:PRO:HD2	2.30	0.46
1:A:455:LYS:HE3	1:A:557:VAL:HG13	1.98	0.46
1:B:170:GLY:HA3	1:B:314:ASP:OD2	2.15	0.46
1:G:592:THR:N	1:G:593:PRO:HD2	2.30	0.46
1:N:580:LYS:HE2	1:O:536:GLN:NE2	2.30	0.46
1:P:117:VAL:O	5:P:705:GTP:O2'	2.31	0.46
1:F:142:GLN:NE2	5:F:705:GTP:O6	2.47	0.46
1:G:175:ALA:HB1	1:G:199:VAL:HG12	1.95	0.46
1:H:170:GLY:HA3	1:H:314:ASP:OD2	2.16	0.46
1:L:488:LEU:HG	1:L:488:LEU:O	2.14	0.46
1:M:591:ILE:O	1:M:594:GLN:HB3	2.14	0.46
1:B:234:GLU:HB3	1:B:273:VAL:HG12	1.96	0.46
1:C:175:ALA:HB1	1:C:199:VAL:HG12	1.96	0.46
1:F:591:ILE:O	1:F:594:GLN:HB3	2.15	0.46
1:K:175:ALA:HB1	1:K:199:VAL:HG12	1.96	0.46
1:A:142:GLN:NE2	5:A:705:GTP:O6	2.40	0.46
1:F:455:LYS:HE3	1:F:557:VAL:HG13	1.98	0.46
1:K:312:LYS:HE3	4:K:705:1FZ:O1G	2.16	0.46
1:B:591:ILE:O	1:B:594:GLN:HB3	2.15	0.45
1:F:116:LYS:HE2	5:F:705:GTP:O2A	2.16	0.45
5:I:707:GTP:H5'	6:L:701:DTP:O1B	2.16	0.45
1:L:150:LEU:O	4:L:705:1FZ:H2	2.17	0.45
1:B:352:ARG:NH2	6:B:707:DTP:O2G	2.49	0.45
1:J:580:LYS:HE2	1:K:536:GLN:NE2	2.31	0.45
1:M:592:THR:N	1:M:593:PRO:HD2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:170:GLY:HA3	1:I:314:ASP:OD2	2.16	0.45
1:I:157:PHE:CE2	6:L:701:DTP:H1'	2.52	0.45
6:N:708:DTP:O1B	5:P:705:GTP:O3'	2.28	0.45
1:A:352:ARG:NH1	6:A:706:DTP:O2G	2.42	0.45
1:M:381:ILE:HD13	1:M:553:TYR:CD2	2.52	0.45
1:C:234:GLU:HB3	1:C:273:VAL:HG12	1.98	0.44
1:C:381:ILE:HD13	1:C:553:TYR:CD2	2.52	0.44
1:O:381:ILE:HD13	1:O:553:TYR:CD2	2.53	0.44
1:B:376:HIS:NE2	6:C:701:DTP:O2A	2.32	0.44
1:H:116:LYS:HE2	5:H:706:GTP:O2A	2.18	0.44
1:A:327:ASN:O	1:D:326:GLN:CB	2.65	0.44
1:D:592:THR:N	1:D:593:PRO:HD2	2.33	0.44
1:G:305:ARG:NH2	1:G:346:GLU:OE2	2.50	0.44
1:M:210:HIS:CE1	1:M:233:HIS:CG	3.05	0.44
1:C:210:HIS:CE1	1:C:233:HIS:CG	3.05	0.44
1:F:210:HIS:CE1	1:F:233:HIS:CG	3.06	0.44
1:F:305:ARG:CZ	1:F:348:ARG:HD3	2.47	0.44
1:F:381:ILE:HD13	1:F:553:TYR:CD2	2.52	0.44
1:J:210:HIS:CE1	1:J:233:HIS:CG	3.05	0.44
1:J:381:ILE:HD13	1:J:553:TYR:CD2	2.53	0.44
1:D:381:ILE:HD13	1:D:553:TYR:CD2	2.53	0.44
1:E:321:HIS:CE1	1:F:321:HIS:CE1	3.05	0.44
1:F:326:GLN:HG2	1:G:327:ASN:O	2.18	0.44
1:H:381:ILE:HD13	1:H:553:TYR:CD2	2.53	0.44
1:I:381:ILE:HD13	1:I:553:TYR:CD2	2.53	0.44
5:I:707:GTP:O3G	1:L:523:LYS:NZ	2.50	0.44
1:L:210:HIS:CE1	1:L:233:HIS:CG	3.05	0.44
1:N:210:HIS:CE1	1:N:233:HIS:CG	3.06	0.44
1:P:381:ILE:HD13	1:P:553:TYR:CD2	2.53	0.44
1:F:592:THR:N	1:F:593:PRO:HD2	2.33	0.44
1:G:210:HIS:CE1	1:G:233:HIS:CG	3.05	0.44
1:G:381:ILE:HD13	1:G:553:TYR:CD2	2.52	0.44
1:I:155:TYR:O	5:I:707:GTP:C8	2.70	0.44
1:L:381:ILE:HD13	1:L:553:TYR:CD2	2.53	0.44
1:A:381:ILE:HD13	1:A:553:TYR:CD2	2.52	0.44
1:J:592:THR:N	1:J:593:PRO:HD2	2.33	0.44
1:K:210:HIS:CE1	1:K:233:HIS:CG	3.06	0.44
1:P:592:THR:N	1:P:593:PRO:HD2	2.33	0.44
1:C:592:THR:N	1:C:593:PRO:HD2	2.33	0.44
1:E:210:HIS:CE1	1:E:233:HIS:CG	3.06	0.44
1:I:210:HIS:CE1	1:I:233:HIS:CG	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:165:PHE:HZ	5:P:705:GTP:O6	2.01	0.44
1:E:592:THR:N	1:E:593:PRO:HD2	2.33	0.44
1:N:116:LYS:NZ	5:N:706:GTP:O2G	2.45	0.44
1:H:210:HIS:CE1	1:H:233:HIS:CG	3.05	0.43
1:I:592:THR:N	1:I:593:PRO:HD2	2.33	0.43
1:B:592:THR:N	1:B:593:PRO:HD2	2.33	0.43
1:D:210:HIS:CE1	1:D:233:HIS:CG	3.06	0.43
1:K:592:THR:N	1:K:593:PRO:HD2	2.33	0.43
1:M:352:ARG:HH22	6:M:707:DTP:PG	2.41	0.43
1:N:381:ILE:HD13	1:N:553:TYR:CD2	2.53	0.43
1:B:381:ILE:HD13	1:B:553:TYR:CD2	2.52	0.43
1:K:381:ILE:HD13	1:K:553:TYR:CD2	2.53	0.43
1:O:284:LEU:N	1:O:284:LEU:HD12	2.32	0.43
1:A:592:THR:N	1:A:593:PRO:HD2	2.33	0.43
1:B:210:HIS:CE1	1:B:233:HIS:CG	3.06	0.43
1:K:360:TYR:CE1	1:K:515:ILE:HG21	2.53	0.43
1:P:311:ASP:OD2	4:P:704:1FZ:N3A	2.52	0.43
1:L:145:ARG:NH2	5:L:706:GTP:N7	2.66	0.43
1:L:592:THR:N	1:L:593:PRO:HD2	2.33	0.43
1:N:328:ASN:HB2	1:O:328:ASN:HB2	1.99	0.43
1:O:210:HIS:CE1	1:O:233:HIS:CG	3.05	0.43
1:J:488:LEU:HD12	1:M:488:LEU:CD1	2.49	0.43
1:N:592:THR:N	1:N:593:PRO:HD2	2.33	0.43
1:F:285:TRP:CD2	1:F:292:GLU:HG2	2.54	0.43
1:I:356:VAL:HG11	1:L:582:GLN:HE22	1.84	0.43
1:P:210:HIS:CE1	1:P:233:HIS:CG	3.05	0.43
1:A:210:HIS:CE1	1:A:233:HIS:CG	3.06	0.43
1:O:142:GLN:NE2	5:O:705:GTP:O6	2.48	0.43
1:G:321:HIS:CE1	1:H:321:HIS:CE1	3.06	0.43
1:A:312:LYS:NZ	4:A:704:1FZ:O2G	2.46	0.42
1:C:312:LYS:NZ	4:C:705:1FZ:O2G	2.46	0.42
1:I:321:HIS:CE1	1:J:321:HIS:CE1	3.08	0.42
1:O:592:THR:N	1:O:593:PRO:HD2	2.33	0.42
1:A:145:ARG:NH2	5:A:705:GTP:N7	2.67	0.42
1:C:425:ASN:OD1	1:D:425:ASN:ND2	2.53	0.42
1:E:381:ILE:HD13	1:E:553:TYR:CD2	2.53	0.42
1:F:326:GLN:HB3	1:G:327:ASN:O	2.20	0.42
1:I:352:ARG:NH1	6:I:708:DTP:O3G	2.53	0.42
1:H:118:ILE:HA	5:H:706:GTP:O2'	2.20	0.42
1:H:305:ARG:HD3	7:H:707:SO4:O4	2.20	0.42
1:H:574:ALA:HB1	1:H:595:LYS:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:326:GLN:HG3	1:F:327:ASN:N	2.35	0.41
1:M:321:HIS:CE1	1:N:321:HIS:CE1	3.08	0.41
1:O:455:LYS:HE3	1:O:557:VAL:HG13	2.00	0.41
1:G:352:ARG:NH2	1:G:523:LYS:HB2	2.35	0.41
1:M:352:ARG:NH2	1:M:523:LYS:HB2	2.36	0.41
1:L:352:ARG:NH2	1:L:523:LYS:HB2	2.36	0.41
1:B:352:ARG:NH2	1:B:523:LYS:HB2	2.35	0.41
1:K:352:ARG:NH2	1:K:523:LYS:HB2	2.35	0.41
1:L:599:ASN:O	1:L:600:ASP:CB	2.68	0.41
1:C:305:ARG:NE	1:C:348:ARG:HD3	2.36	0.41
1:F:352:ARG:NH2	1:F:523:LYS:HB2	2.36	0.41
1:F:328:ASN:HB2	1:G:328:ASN:HB2	2.03	0.41
5:I:707:GTP:H5'	6:L:701:DTP:PB	2.61	0.41
1:O:321:HIS:CE1	1:P:321:HIS:CE1	3.08	0.40
1:P:352:ARG:NH2	1:P:523:LYS:HB2	2.36	0.40
1:J:352:ARG:NH2	1:J:523:LYS:HB2	2.36	0.40
1:H:352:ARG:NH2	1:H:523:LYS:HB2	2.36	0.40
1:I:352:ARG:NH2	1:I:523:LYS:HB2	2.37	0.40
1:C:352:ARG:NH2	1:C:523:LYS:HB2	2.36	0.40
1:D:285:TRP:CD2	1:D:292:GLU:HG2	2.57	0.40
1:D:352:ARG:NH2	1:D:523:LYS:HB2	2.36	0.40
1:C:311:ASP:OD2	4:C:705:1FZ:N3A	2.55	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:472:ASP:OD1	1:P:396:TYR:OH[1_565]	1.29	0.91
1:I:475:SER:OG	1:L:436:PRO:CB[2_754]	1.70	0.50
1:I:475:SER:CB	1:L:436:PRO:CB[2_754]	2.11	0.09
1:L:190:GLN:OE1	1:P:403:GLY:N[2_654]	2.12	0.08

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

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

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	280	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	411/464 (89%)	403 (98%)	8 (2%)	57	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	407/464 (88%)	403 (99%)	4 (1%)	76	90
1	C	406/464 (88%)	401 (99%)	5 (1%)	71	88
1	D	408/464 (88%)	405 (99%)	3 (1%)	84	94
1	E	408/464 (88%)	404 (99%)	4 (1%)	76	90
1	F	406/464 (88%)	402 (99%)	4 (1%)	76	90
1	G	403/464 (87%)	397 (98%)	6 (2%)	65	85
1	H	411/464 (89%)	406 (99%)	5 (1%)	71	88
1	I	405/464 (87%)	399 (98%)	6 (2%)	65	85
1	J	403/464 (87%)	399 (99%)	4 (1%)	76	90
1	K	404/464 (87%)	399 (99%)	5 (1%)	71	88
1	L	395/464 (85%)	390 (99%)	5 (1%)	69	87
1	M	389/464 (84%)	385 (99%)	4 (1%)	76	90
1	N	403/464 (87%)	396 (98%)	7 (2%)	60	83
1	O	403/464 (87%)	399 (99%)	4 (1%)	76	90
1	P	388/464 (84%)	384 (99%)	4 (1%)	76	90
All	All	6450/7424 (87%)	6372 (99%)	78 (1%)	71	88

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	ARG
1	A	315	TYR
1	A	352	ARG
1	A	405	LYS
1	A	439	LYS
1	A	446	LYS
1	A	478	LYS
1	A	576	ARG
1	B	134	ARG
1	B	352	ARG
1	B	446	LYS
1	B	576	ARG
1	C	115	MET
1	C	315	TYR
1	C	352	ARG
1	C	494	LYS
1	C	576	ARG

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Mol	Chain	Res	Type
1	D	315	TYR
1	D	352	ARG
1	D	576	ARG
1	E	134	ARG
1	E	352	ARG
1	E	405	LYS
1	E	576	ARG
1	F	134	ARG
1	F	315	TYR
1	F	352	ARG
1	F	576	ARG
1	G	134	ARG
1	G	315	TYR
1	G	328	ASN
1	G	352	ARG
1	G	576	ARG
1	G	594	GLN
1	H	315	TYR
1	H	352	ARG
1	H	490	ASP
1	H	494	LYS
1	H	576	ARG
1	I	134	ARG
1	I	315	TYR
1	I	352	ARG
1	I	490	ASP
1	I	494	LYS
1	I	576	ARG
1	J	315	TYR
1	J	352	ARG
1	J	405	LYS
1	J	576	ARG
1	K	134	ARG
1	K	315	TYR
1	K	352	ARG
1	K	576	ARG
1	K	594	GLN
1	L	134	ARG
1	L	315	TYR
1	L	352	ARG
1	L	488	LEU
1	L	576	ARG

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Mol	Chain	Res	Type
1	M	134	ARG
1	M	315	TYR
1	M	352	ARG
1	M	576	ARG
1	N	315	TYR
1	N	328	ASN
1	N	352	ARG
1	N	439	LYS
1	N	490	ASP
1	N	494	LYS
1	N	576	ARG
1	O	134	ARG
1	O	315	TYR
1	O	352	ARG
1	O	576	ARG
1	P	134	ARG
1	P	315	TYR
1	P	352	ARG
1	P	576	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	GLN
1	A	210	HIS
1	A	271	GLN
1	A	375	GLN
1	A	380	ASN
1	A	425	ASN
1	B	271	GLN
1	B	375	GLN
1	B	380	ASN
1	B	571	GLN
1	B	594	GLN
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	375	GLN
1	D	380	ASN

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Mol	Chain	Res	Type
1	E	210	HIS
1	E	271	GLN
1	E	322	HIS
1	E	375	GLN
1	E	380	ASN
1	E	571	GLN
1	E	594	GLN
1	F	210	HIS
1	F	271	GLN
1	F	322	HIS
1	F	375	GLN
1	F	380	ASN
1	F	571	GLN
1	F	594	GLN
1	G	210	HIS
1	G	271	GLN
1	G	322	HIS
1	G	375	GLN
1	G	380	ASN
1	G	425	ASN
1	G	571	GLN
1	G	594	GLN
1	H	271	GLN
1	H	322	HIS
1	H	375	GLN
1	H	380	ASN
1	I	210	HIS
1	I	271	GLN
1	I	322	HIS
1	I	375	GLN
1	I	380	ASN
1	J	210	HIS
1	J	271	GLN
1	J	322	HIS
1	J	375	GLN
1	J	380	ASN
1	J	425	ASN
1	J	571	GLN
1	J	594	GLN
1	K	210	HIS
1	K	271	GLN
1	K	375	GLN

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Mol	Chain	Res	Type
1	K	380	ASN
1	K	425	ASN
1	K	571	GLN
1	K	594	GLN
1	L	210	HIS
1	L	233	HIS
1	L	271	GLN
1	L	375	GLN
1	L	380	ASN
1	L	582	GLN
1	M	210	HIS
1	M	271	GLN
1	M	375	GLN
1	M	380	ASN
1	M	425	ASN
1	N	271	GLN
1	N	375	GLN
1	N	380	ASN
1	N	571	GLN
1	N	594	GLN
1	O	210	HIS
1	O	271	GLN
1	O	322	HIS
1	O	375	GLN
1	O	380	ASN
1	P	210	HIS
1	P	233	HIS
1	P	271	GLN
1	P	322	HIS
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 107 ligands modelled in this entry, 48 are monoatomic - leaving 59 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	DTP	K	701	3	26,32,32	1.13	2 (7%)	30,50,50	1.62	5 (16%)
5	GTP	I	705	3	26,34,34	0.93	1 (3%)	32,54,54	1.67	8 (25%)
6	DTP	D	701	3	26,32,32	1.01	2 (7%)	30,50,50	1.77	6 (20%)
6	DTP	G	701	3	26,32,32	0.94	2 (7%)	30,50,50	1.60	5 (16%)
7	SO4	I	706	-	4,4,4	0.40	0	6,6,6	0.23	0
4	1FZ	P	704	3,2	29,30,30	1.10	4 (13%)	42,47,47	1.22	3 (7%)
4	1FZ	E	704	3,2	29,30,30	1.14	4 (13%)	42,47,47	1.12	3 (7%)
4	1FZ	B	704	3,2	29,30,30	1.12	4 (13%)	42,47,47	1.49	6 (14%)
6	DTP	L	701	3	26,32,32	0.91	0	30,50,50	1.54	7 (23%)
5	GTP	P	705	3	26,34,34	0.96	1 (3%)	32,54,54	1.18	3 (9%)
7	SO4	N	707	-	4,4,4	0.27	0	6,6,6	0.37	0
4	1FZ	J	704	3,2	29,30,30	1.25	5 (17%)	42,47,47	1.37	5 (11%)
5	GTP	D	702	3	26,34,34	0.97	1 (3%)	32,54,54	1.21	1 (3%)
5	GTP	D	707	3	26,34,34	1.02	1 (3%)	32,54,54	1.28	6 (18%)
5	GTP	H	706	3	26,34,34	0.88	1 (3%)	32,54,54	1.43	3 (9%)
5	GTP	F	705	3	26,34,34	1.11	1 (3%)	32,54,54	1.43	4 (12%)
6	DTP	I	708	3	26,32,32	0.97	2 (7%)	30,50,50	1.49	6 (20%)
6	DTP	M	707	3	26,32,32	0.96	2 (7%)	30,50,50	1.47	4 (13%)
7	SO4	E	706	-	4,4,4	0.49	0	6,6,6	0.39	0
6	DTP	E	707	3	26,32,32	1.00	2 (7%)	30,50,50	1.84	7 (23%)
4	1FZ	L	705	3	29,30,30	1.09	4 (13%)	42,47,47	1.37	4 (9%)
4	1FZ	O	704	3,2	29,30,30	1.14	4 (13%)	42,47,47	1.39	3 (7%)
5	GTP	G	706	3	26,34,34	1.06	1 (3%)	32,54,54	1.41	3 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GTP	B	705	3	26,34,34	1.08	1 (3%)	32,54,54	1.31	4 (12%)
5	GTP	A	705	3	26,34,34	1.04	1 (3%)	32,54,54	1.32	6 (18%)
5	GTP	K	706	3	26,34,34	0.86	0	32,54,54	1.30	4 (12%)
6	DTP	C	701	3	26,32,32	1.04	2 (7%)	30,50,50	1.54	7 (23%)
5	GTP	L	706	3	26,34,34	1.02	1 (3%)	32,54,54	1.20	3 (9%)
4	1FZ	M	704	3,2	29,30,30	1.04	4 (13%)	42,47,47	1.34	5 (11%)
6	DTP	J	706	3	26,32,32	0.90	1 (3%)	30,50,50	1.77	5 (16%)
6	DTP	N	701	3	26,32,32	1.06	3 (11%)	30,50,50	1.60	4 (13%)
7	SO4	C	706	-	4,4,4	0.35	0	6,6,6	0.33	0
4	1FZ	C	705	3,2	29,30,30	1.17	2 (6%)	42,47,47	1.29	4 (9%)
4	1FZ	N	705	3,2	29,30,30	1.05	4 (13%)	42,47,47	1.45	5 (11%)
7	SO4	K	707	-	4,4,4	0.30	0	6,6,6	0.38	0
5	GTP	O	705	3	26,34,34	1.10	3 (11%)	32,54,54	1.26	2 (6%)
4	1FZ	G	705	3,2	29,30,30	1.20	5 (17%)	42,47,47	1.31	3 (7%)
6	DTP	N	708	3	26,32,32	0.96	1 (3%)	30,50,50	1.76	7 (23%)
5	GTP	I	707	3	26,34,34	1.22	2 (7%)	32,54,54	1.62	8 (25%)
7	SO4	O	706	-	4,4,4	0.40	0	6,6,6	0.33	0
6	DTP	F	707	3	26,32,32	0.82	0	30,50,50	1.55	7 (23%)
6	DTP	B	707	3	26,32,32	1.02	2 (7%)	30,50,50	1.38	4 (13%)
4	1FZ	K	705	3,2	29,30,30	1.06	4 (13%)	42,47,47	1.27	3 (7%)
7	SO4	H	707	-	4,4,4	0.44	0	6,6,6	0.30	0
7	SO4	D	708	-	4,4,4	0.47	0	6,6,6	0.55	0
7	SO4	J	705	-	4,4,4	0.31	0	6,6,6	0.36	0
5	GTP	E	705	3	26,34,34	0.97	1 (3%)	32,54,54	1.77	7 (21%)
6	DTP	H	701	3	26,32,32	0.98	2 (7%)	30,50,50	1.46	4 (13%)
4	1FZ	H	705	3,2	29,30,30	1.17	4 (13%)	42,47,47	1.38	5 (11%)
6	DTP	M	706	3	26,32,32	1.08	2 (7%)	30,50,50	1.54	7 (23%)
5	GTP	N	706	3	26,34,34	1.14	1 (3%)	32,54,54	1.37	6 (18%)
6	DTP	A	706	3	26,32,32	0.96	1 (3%)	30,50,50	1.85	8 (26%)
7	SO4	B	706	-	4,4,4	0.39	0	6,6,6	0.29	0
5	GTP	M	705	3	26,34,34	0.86	1 (3%)	32,54,54	1.52	4 (12%)
4	1FZ	F	704	3,2	29,30,30	1.15	4 (13%)	42,47,47	1.24	4 (9%)
4	1FZ	I	704	3,2	29,30,30	1.17	4 (13%)	42,47,47	1.27	4 (9%)
4	1FZ	A	704	3,2	29,30,30	1.20	3 (10%)	42,47,47	1.28	5 (11%)
4	1FZ	D	706	3,2	29,30,30	1.30	4 (13%)	42,47,47	1.23	4 (9%)
7	SO4	F	706	-	4,4,4	0.41	0	6,6,6	0.21	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	DTP	K	701	3	-	2/18/34/34	0/3/3/3
5	GTP	I	705	3	-	4/18/38/38	0/3/3/3
6	DTP	D	701	3	-	1/18/34/34	0/3/3/3
6	DTP	G	701	3	-	2/18/34/34	0/3/3/3
4	1FZ	P	704	3,2	-	7/19/34/34	0/2/2/2
4	1FZ	E	704	3,2	-	6/19/34/34	0/2/2/2
4	1FZ	B	704	3,2	-	6/19/34/34	0/2/2/2
6	DTP	L	701	3	-	2/18/34/34	0/3/3/3
5	GTP	P	705	3	-	4/18/38/38	0/3/3/3
4	1FZ	J	704	3,2	-	10/19/34/34	0/2/2/2
5	GTP	D	702	3	-	5/18/38/38	0/3/3/3
5	GTP	D	707	3	-	5/18/38/38	0/3/3/3
5	GTP	H	706	3	-	0/18/38/38	0/3/3/3
5	GTP	F	705	3	-	2/18/38/38	0/3/3/3
6	DTP	I	708	3	-	3/18/34/34	0/3/3/3
6	DTP	M	707	3	-	6/18/34/34	0/3/3/3
6	DTP	E	707	3	-	2/18/34/34	0/3/3/3
4	1FZ	L	705	3	-	12/19/34/34	0/2/2/2
4	1FZ	O	704	3,2	-	9/19/34/34	0/2/2/2
5	GTP	G	706	3	-	1/18/38/38	0/3/3/3
5	GTP	B	705	3	-	2/18/38/38	0/3/3/3
5	GTP	A	705	3	-	7/18/38/38	0/3/3/3
5	GTP	K	706	3	-	1/18/38/38	0/3/3/3
6	DTP	C	701	3	-	2/18/34/34	0/3/3/3
5	GTP	L	706	3	-	7/18/38/38	0/3/3/3
4	1FZ	M	704	3,2	-	5/19/34/34	0/2/2/2
6	DTP	J	706	3	-	3/18/34/34	0/3/3/3
6	DTP	N	701	3	-	4/18/34/34	0/3/3/3
4	1FZ	C	705	3,2	-	6/19/34/34	0/2/2/2
4	1FZ	N	705	3,2	-	8/19/34/34	0/2/2/2
5	GTP	O	705	3	-	6/18/38/38	0/3/3/3
4	1FZ	G	705	3,2	-	11/19/34/34	0/2/2/2

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

All (107) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	707	GTP	C6-N1	-4.43	1.31	1.37
4	H	705	1FZ	PB-O2B	4.06	1.52	1.46
4	I	704	1FZ	PB-O2B	4.02	1.52	1.46
4	D	706	1FZ	PB-O2B	3.99	1.52	1.46
4	A	704	1FZ	PB-O2B	3.95	1.52	1.46
4	J	704	1FZ	PB-O2B	3.93	1.52	1.46
4	C	705	1FZ	PB-O2B	3.92	1.52	1.46
4	G	705	1FZ	PB-O2B	3.73	1.52	1.46
4	B	704	1FZ	PB-O2B	3.69	1.52	1.46
4	O	704	1FZ	PB-O2B	3.67	1.52	1.46
4	F	704	1FZ	PB-O2B	3.63	1.51	1.46
5	A	705	GTP	C6-N1	-3.61	1.32	1.37
4	E	704	1FZ	PB-O2B	3.59	1.51	1.46
4	L	705	1FZ	PB-O2B	3.54	1.51	1.46
5	F	705	GTP	C6-N1	-3.44	1.32	1.37
5	N	706	GTP	C6-N1	-3.42	1.32	1.37
4	K	705	1FZ	PB-O2B	3.41	1.51	1.46
4	A	704	1FZ	PA-O1A	3.35	1.51	1.46
5	G	706	GTP	C6-N1	-3.34	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	704	1FZ	PB-O2B	3.33	1.51	1.46
4	C	705	1FZ	PA-O1A	3.31	1.51	1.46
4	P	704	1FZ	PB-O2B	3.26	1.51	1.46
5	L	706	GTP	C6-N1	-3.21	1.33	1.37
5	D	707	GTP	C6-N1	-3.18	1.33	1.37
4	N	705	1FZ	PB-O2B	3.13	1.51	1.46
4	B	704	1FZ	PA-O1A	3.13	1.51	1.46
4	O	704	1FZ	PA-O1A	3.11	1.51	1.46
5	E	705	GTP	C6-N1	-3.11	1.33	1.37
4	D	706	1FZ	PA-O1A	3.05	1.51	1.46
6	K	701	DTP	C2-N3	3.04	1.37	1.32
5	P	705	GTP	C6-N1	-3.03	1.33	1.37
4	P	704	1FZ	PA-O1A	2.99	1.50	1.46
4	G	705	1FZ	PA-O1A	2.90	1.50	1.46
6	B	707	DTP	C2-N3	2.89	1.36	1.32
6	M	706	DTP	C5-C4	2.85	1.48	1.40
4	F	704	1FZ	PA-O1A	2.83	1.50	1.46
4	K	705	1FZ	PA-O1A	2.81	1.50	1.46
4	J	704	1FZ	PA-O1A	2.75	1.50	1.46
4	H	705	1FZ	PA-O1A	2.74	1.50	1.46
5	O	705	GTP	C6-N1	-2.67	1.33	1.37
4	E	704	1FZ	PA-O1A	2.64	1.50	1.46
4	M	704	1FZ	PA-O1A	2.64	1.50	1.46
5	M	705	GTP	C6-N1	-2.63	1.33	1.37
6	K	701	DTP	C5-C4	2.63	1.47	1.40
6	H	701	DTP	C5-C4	2.60	1.47	1.40
6	E	707	DTP	C5-C4	2.58	1.47	1.40
6	I	708	DTP	C5-C4	2.58	1.47	1.40
4	N	705	1FZ	PB-O1B	-2.56	1.49	1.56
5	B	705	GTP	C6-N1	-2.56	1.34	1.37
5	I	705	GTP	C6-N1	-2.55	1.34	1.37
4	L	705	1FZ	PA-O1A	2.54	1.50	1.46
4	I	704	1FZ	PA-O1A	2.53	1.50	1.46
6	C	701	DTP	C2-N3	2.53	1.36	1.32
6	D	701	DTP	C2-N3	2.53	1.36	1.32
6	N	701	DTP	C5-C4	2.52	1.47	1.40
6	A	706	DTP	C5-C4	2.52	1.47	1.40
6	E	707	DTP	C2-N3	2.50	1.36	1.32
6	H	701	DTP	C2-N3	2.50	1.36	1.32
4	N	705	1FZ	PA-O1A	2.50	1.50	1.46
4	D	706	1FZ	PB-O3B	2.49	1.62	1.59
6	C	701	DTP	C5-C4	2.48	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	707	DTP	C5-C4	2.48	1.47	1.40
4	H	705	1FZ	PA-O2A	-2.45	1.50	1.56
6	G	701	DTP	C5-C4	2.45	1.47	1.40
6	J	706	DTP	C5-C4	2.45	1.47	1.40
4	J	704	1FZ	PA-O2A	-2.44	1.50	1.56
4	M	704	1FZ	PA-O2A	-2.44	1.50	1.56
6	D	701	DTP	C5-C4	2.44	1.47	1.40
4	I	704	1FZ	PA-O2A	-2.39	1.50	1.56
6	G	701	DTP	C2-N3	2.36	1.35	1.32
4	E	704	1FZ	PA-O2A	-2.35	1.50	1.56
6	M	707	DTP	C5-C4	2.35	1.47	1.40
6	M	707	DTP	C2-N3	2.32	1.35	1.32
6	I	708	DTP	C2-N3	2.30	1.35	1.32
5	I	707	GTP	C4-N3	-2.29	1.31	1.37
6	N	708	DTP	C5-C4	2.26	1.46	1.40
4	D	706	1FZ	PA-O2A	-2.26	1.50	1.56
4	P	704	1FZ	PB-O1B	-2.25	1.50	1.56
4	K	705	1FZ	PA-O2A	-2.24	1.50	1.56
4	L	705	1FZ	PA-O2A	-2.22	1.50	1.56
4	F	704	1FZ	PA-O2A	-2.22	1.50	1.56
4	N	705	1FZ	PA-O2A	-2.22	1.50	1.56
4	K	705	1FZ	PB-O1B	-2.21	1.50	1.56
4	G	705	1FZ	PB-O3B	2.20	1.61	1.59
6	N	701	DTP	C2-N3	2.20	1.35	1.32
4	B	704	1FZ	PB-O1B	-2.20	1.50	1.56
4	P	704	1FZ	PA-O2A	-2.20	1.50	1.56
6	N	701	DTP	C4-N3	2.19	1.38	1.35
6	M	706	DTP	C2-N3	2.14	1.35	1.32
4	A	704	1FZ	PB-O1B	-2.13	1.51	1.56
4	F	704	1FZ	PB-O1B	-2.13	1.51	1.56
4	E	704	1FZ	PB-O1B	-2.12	1.51	1.56
5	H	706	GTP	C6-N1	-2.11	1.34	1.37
4	J	704	1FZ	PB-O1B	-2.11	1.51	1.56
4	G	705	1FZ	PA-O2A	-2.11	1.51	1.56
5	D	702	GTP	C6-N1	-2.10	1.34	1.37
4	B	704	1FZ	PA-O2A	-2.10	1.51	1.56
5	O	705	GTP	C5-C4	2.09	1.48	1.43
4	L	705	1FZ	PB-O1B	-2.09	1.51	1.56
4	J	704	1FZ	PB-O3B	2.09	1.61	1.59
4	I	704	1FZ	PB-O1B	-2.08	1.51	1.56
4	H	705	1FZ	PB-O1B	-2.07	1.51	1.56
4	M	704	1FZ	PB-O1B	-2.07	1.51	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	704	1FZ	PB-O1B	-2.06	1.51	1.56
4	O	704	1FZ	PA-O2A	-2.06	1.51	1.56
4	G	705	1FZ	PB-O1B	-2.03	1.51	1.56
5	O	705	GTP	C2'-C1'	-2.02	1.50	1.53

All (231) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	705	GTP	PA-O3A-PB	-5.40	114.29	132.83
4	K	705	1FZ	O1B-PB-O2B	5.06	120.54	109.92
6	N	708	DTP	N3-C2-N1	-5.02	120.84	128.68
5	F	705	GTP	PA-O3A-PB	-5.00	115.66	132.83
6	K	701	DTP	N3-C2-N1	-4.96	120.93	128.68
6	N	701	DTP	N3-C2-N1	-4.85	121.09	128.68
5	H	706	GTP	PA-O3A-PB	-4.84	116.20	132.83
5	I	705	GTP	PA-O3A-PB	-4.82	116.28	132.83
6	L	701	DTP	N3-C2-N1	-4.68	121.37	128.68
4	D	706	1FZ	O1B-PB-O2B	4.62	119.61	109.92
4	F	704	1FZ	O1B-PB-O2B	4.60	119.57	109.92
4	A	704	1FZ	O1B-PB-O2B	4.59	119.54	109.92
4	C	705	1FZ	O1B-PB-O2B	4.57	119.50	109.92
6	D	701	DTP	PB-O3B-PG	-4.55	117.21	132.83
4	O	704	1FZ	O1B-PB-O2B	4.54	119.45	109.92
6	G	701	DTP	N3-C2-N1	-4.54	121.58	128.68
4	M	704	1FZ	O1B-PB-O2B	4.53	119.41	109.92
6	J	706	DTP	N3-C2-N1	-4.49	121.66	128.68
4	J	704	1FZ	O1B-PB-O2B	4.47	119.30	109.92
4	B	704	1FZ	O2A-PA-O1A	4.44	119.23	109.92
4	G	705	1FZ	O2A-PA-O1A	4.40	119.15	109.92
5	E	705	GTP	PB-O3B-PG	-4.33	117.95	132.83
4	E	704	1FZ	O1B-PB-O2B	4.33	119.00	109.92
4	C	705	1FZ	O2A-PA-O1A	4.26	118.86	109.92
6	E	707	DTP	PA-O3A-PB	-4.26	118.22	132.83
6	E	707	DTP	N3-C2-N1	-4.26	122.02	128.68
4	N	705	1FZ	O1B-PB-O2B	4.25	118.83	109.92
4	L	705	1FZ	O2A-PA-O1A	4.24	118.81	109.92
4	H	705	1FZ	O2A-PA-O1A	4.20	118.72	109.92
6	F	707	DTP	N3-C2-N1	-4.19	122.14	128.68
4	I	704	1FZ	O1B-PB-O2B	4.18	118.69	109.92
4	B	704	1FZ	O1B-PB-O2B	4.17	118.67	109.92
4	G	705	1FZ	O1B-PB-O2B	4.16	118.65	109.92
4	P	704	1FZ	O2A-PA-O1A	4.15	118.63	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	705	GTP	PA-O3A-PB	-4.15	118.58	132.83
4	L	705	1FZ	O1B-PB-O2B	4.13	118.58	109.92
6	A	706	DTP	N3-C2-N1	-4.13	122.22	128.68
4	B	704	1FZ	O2B-PB-N3A	4.13	117.85	111.77
6	J	706	DTP	PB-O3B-PG	-4.13	118.67	132.83
6	E	707	DTP	O3G-PG-O2G	4.10	123.32	107.64
4	H	705	1FZ	O1B-PB-O2B	4.10	118.51	109.92
4	P	704	1FZ	O1B-PB-O2B	4.09	118.50	109.92
4	N	705	1FZ	O2A-PA-O1A	4.02	118.36	109.92
4	F	704	1FZ	O2A-PA-O1A	3.99	118.30	109.92
4	M	704	1FZ	O2A-PA-O1A	3.92	118.13	109.92
4	O	704	1FZ	O3B-PB-N3A	-3.90	95.78	106.59
6	M	707	DTP	N3-C2-N1	-3.86	122.65	128.68
6	G	701	DTP	PB-O3B-PG	-3.85	119.61	132.83
6	N	701	DTP	PB-O3B-PG	-3.83	119.67	132.83
6	I	708	DTP	N3-C2-N1	-3.83	122.69	128.68
6	C	701	DTP	PB-O3B-PG	-3.73	120.02	132.83
4	K	705	1FZ	O2A-PA-O1A	3.68	117.64	109.92
4	I	704	1FZ	O2A-PA-O1A	3.65	117.58	109.92
5	I	707	GTP	PA-O3A-PB	-3.64	120.34	132.83
5	G	706	GTP	PA-O3A-PB	-3.63	120.38	132.83
4	J	704	1FZ	O5'-PA-O1A	-3.62	100.31	114.24
6	D	701	DTP	N3-C2-N1	-3.61	123.03	128.68
4	N	705	1FZ	O5'-PA-O1A	-3.61	100.34	114.24
4	M	704	1FZ	O3B-PB-N3A	-3.59	96.63	106.59
4	J	704	1FZ	O2A-PA-O1A	3.57	117.40	109.92
4	O	704	1FZ	O2A-PA-O1A	3.56	117.39	109.92
6	M	706	DTP	N3-C2-N1	-3.56	123.11	128.68
6	A	706	DTP	O2G-PG-O3B	-3.53	92.79	104.64
5	B	705	GTP	PA-O3A-PB	-3.51	120.78	132.83
6	B	707	DTP	N3-C2-N1	-3.50	123.21	128.68
5	I	707	GTP	C3'-C2'-C1'	3.49	106.24	100.98
6	H	701	DTP	PB-O3B-PG	-3.48	120.90	132.83
4	D	706	1FZ	O2A-PA-O1A	3.44	117.14	109.92
6	H	701	DTP	N3-C2-N1	-3.41	123.34	128.68
4	A	704	1FZ	O2A-PA-O1A	3.41	117.07	109.92
6	E	707	DTP	O2G-PG-O3B	-3.40	93.23	104.64
4	E	704	1FZ	O2A-PA-O1A	3.35	116.95	109.92
6	J	706	DTP	C2-N1-C6	3.34	124.47	118.75
5	M	705	GTP	PB-O3B-PG	-3.33	121.41	132.83
5	K	706	GTP	PA-O3A-PB	-3.30	121.49	132.83
6	J	706	DTP	PA-O3A-PB	-3.29	121.52	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	701	DTP	N3-C2-N1	-3.29	123.54	128.68
4	B	704	1FZ	O1A-PA-N3A	-3.25	106.98	111.77
6	D	701	DTP	N6-C6-N1	3.21	125.24	118.57
6	M	706	DTP	C2-N1-C6	3.17	124.17	118.75
4	G	705	1FZ	O5'-PA-O1A	-3.15	102.14	114.24
5	N	706	GTP	PA-O3A-PB	-3.13	122.08	132.83
4	H	705	1FZ	O5'-PA-O1A	-3.12	102.25	114.24
4	L	705	1FZ	O3B-PB-N3A	-3.06	98.11	106.59
6	D	701	DTP	O2G-PG-O3B	-3.06	94.38	104.64
6	A	706	DTP	O3G-PG-O2G	3.05	119.31	107.64
5	N	706	GTP	C3'-C2'-C1'	3.05	105.57	100.98
5	D	702	GTP	PA-O3A-PB	-3.05	122.36	132.83
6	A	706	DTP	C4-C5-N7	-2.99	106.29	109.40
4	P	704	1FZ	O3B-PB-N3A	-2.98	98.31	106.59
4	H	705	1FZ	O3B-PB-N3A	-2.97	98.34	106.59
6	N	708	DTP	C2-N1-C6	2.96	123.83	118.75
5	B	705	GTP	C5-C6-N1	2.96	119.17	113.95
5	D	707	GTP	C5-C6-N1	2.94	119.15	113.95
5	F	705	GTP	C8-N7-C5	2.93	108.58	102.99
6	K	701	DTP	PB-O3B-PG	-2.90	122.86	132.83
6	F	707	DTP	O3G-PG-O2G	2.89	118.70	107.64
5	P	705	GTP	PA-O3A-PB	-2.89	122.90	132.83
6	F	707	DTP	O2G-PG-O3B	-2.87	95.00	104.64
4	J	704	1FZ	O2B-PB-N3A	2.86	115.99	111.77
6	K	701	DTP	O2G-PG-O3B	-2.86	95.04	104.64
4	A	704	1FZ	O5'-PA-O1A	-2.86	103.25	114.24
5	P	705	GTP	C5-C6-N1	2.85	118.99	113.95
4	A	704	1FZ	O2B-PB-N3A	2.85	115.97	111.77
4	B	704	1FZ	O3B-PB-N3A	-2.82	98.76	106.59
5	I	705	GTP	PB-O3B-PG	-2.81	123.17	132.83
6	F	707	DTP	PA-O3A-PB	-2.81	123.18	132.83
6	D	701	DTP	O3G-PG-O2G	2.81	118.36	107.64
6	J	706	DTP	N6-C6-N1	2.79	124.37	118.57
6	A	706	DTP	C2-N1-C6	2.77	123.50	118.75
5	E	705	GTP	C5-C6-N1	2.71	118.74	113.95
6	N	708	DTP	PA-O3A-PB	-2.68	123.63	132.83
5	G	706	GTP	C5-C6-N1	2.68	118.68	113.95
6	G	701	DTP	PA-O3A-PB	-2.68	123.64	132.83
5	I	705	GTP	C3'-C2'-C1'	2.67	105.00	100.98
6	E	707	DTP	N6-C6-N1	2.67	124.12	118.57
5	B	705	GTP	PB-O3B-PG	-2.65	123.73	132.83
6	M	707	DTP	C4-C5-N7	-2.65	106.64	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	708	DTP	C4-C5-N7	-2.64	106.64	109.40
4	K	705	1FZ	O1B-PB-O3B	-2.64	95.84	104.64
6	L	701	DTP	O2G-PG-O3B	-2.63	95.80	104.64
4	N	705	1FZ	O2B-PB-N3A	2.63	115.64	111.77
5	A	705	GTP	PB-O3B-PG	-2.62	123.83	132.83
6	N	708	DTP	O4'-C1'-C2'	2.59	111.14	106.25
4	I	704	1FZ	O3B-PB-N3A	-2.59	99.42	106.59
6	H	701	DTP	PA-O3A-PB	-2.58	123.97	132.83
6	M	707	DTP	O3G-PG-O2G	2.57	117.46	107.64
5	A	705	GTP	C5-C6-N1	2.57	118.48	113.95
5	L	706	GTP	C5-C6-N1	2.57	118.48	113.95
5	N	706	GTP	C5-C6-N1	2.56	118.48	113.95
5	I	707	GTP	C5'-C4'-C3'	-2.55	105.61	115.18
6	L	701	DTP	O3G-PG-O2G	2.54	117.35	107.64
5	K	706	GTP	O6-C6-C5	-2.54	119.42	124.37
6	C	701	DTP	N6-C6-N1	2.53	123.83	118.57
5	E	705	GTP	C3'-C2'-C1'	2.52	104.78	100.98
6	I	708	DTP	O3G-PG-O2G	2.51	117.21	107.64
5	E	705	GTP	C8-N7-C5	2.50	107.76	102.99
5	A	705	GTP	PA-O3A-PB	-2.50	124.23	132.83
6	G	701	DTP	O3G-PG-O2G	2.49	117.16	107.64
6	A	706	DTP	PB-O3B-PG	-2.45	124.43	132.83
5	A	705	GTP	C8-N7-C5	2.42	107.60	102.99
5	M	705	GTP	C5-C6-N1	2.42	118.23	113.95
5	D	707	GTP	O6-C6-N1	-2.42	117.80	120.65
4	M	704	1FZ	O1A-PA-N3A	-2.41	108.22	111.77
6	A	706	DTP	O4'-C4'-C3'	-2.40	100.07	105.67
6	N	708	DTP	N6-C6-N1	2.40	123.55	118.57
4	N	705	1FZ	O1B-PB-O3B	-2.39	96.66	104.64
6	M	707	DTP	PB-O3B-PG	-2.39	124.62	132.83
6	M	706	DTP	C5-C6-N1	-2.39	114.94	120.35
5	K	706	GTP	C5-C6-N1	2.39	118.17	113.95
6	C	701	DTP	O2G-PG-O1G	2.39	120.02	110.68
5	D	707	GTP	PA-O3A-PB	-2.38	124.65	132.83
5	D	707	GTP	C8-N7-C5	2.38	107.52	102.99
5	I	705	GTP	O2G-PG-O1G	2.38	119.99	110.68
6	F	707	DTP	C4-C5-N7	-2.37	106.93	109.40
6	N	701	DTP	C2-N1-C6	2.37	122.81	118.75
4	C	705	1FZ	O3B-PB-N3A	-2.36	100.03	106.59
5	O	705	GTP	PA-O3A-PB	-2.36	124.72	132.83
6	M	706	DTP	O5'-C5'-C4'	2.36	117.11	108.99
6	I	708	DTP	PA-O3A-PB	-2.36	124.73	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	706	GTP	C8-N7-C5	2.36	107.48	102.99
6	A	706	DTP	C2'-C1'-N9	2.35	119.70	114.27
6	N	708	DTP	PB-O3B-PG	-2.35	124.76	132.83
6	M	706	DTP	C4-C5-N7	-2.35	106.95	109.40
6	M	706	DTP	N6-C6-N1	2.35	123.45	118.57
4	H	705	1FZ	O4'-C1'-N1	2.34	112.05	107.86
5	I	705	GTP	O3G-PG-O3B	2.34	112.47	104.64
5	I	707	GTP	O5'-PA-O1A	-2.34	99.94	109.07
6	D	701	DTP	C2-N1-C6	2.33	122.74	118.75
6	H	701	DTP	N6-C6-N1	2.32	123.39	118.57
5	B	705	GTP	C2-N1-C6	-2.32	120.83	125.10
5	I	705	GTP	O3B-PG-O1G	-2.32	98.35	111.19
6	N	701	DTP	PA-O3A-PB	-2.31	124.90	132.83
6	F	707	DTP	PB-O3B-PG	-2.30	124.94	132.83
4	I	704	1FZ	O1A-PA-N3A	-2.28	108.41	111.77
5	M	705	GTP	O6-C6-C5	-2.27	119.94	124.37
5	I	707	GTP	C2-N1-C6	-2.26	120.94	125.10
5	D	707	GTP	C3'-C2'-C1'	2.24	104.35	100.98
6	M	706	DTP	PB-O3B-PG	-2.23	125.17	132.83
5	I	705	GTP	C5-C6-N1	2.23	117.89	113.95
6	B	707	DTP	N6-C6-N1	2.22	123.19	118.57
5	H	706	GTP	O2A-PA-O1A	2.22	123.22	112.24
5	N	706	GTP	C8-N7-C5	2.22	107.22	102.99
5	L	706	GTP	PA-O3A-PB	-2.22	125.21	132.83
5	E	705	GTP	C2'-C3'-C4'	-2.22	98.33	102.64
6	I	708	DTP	C2-N1-C6	2.21	122.53	118.75
6	L	701	DTP	C4-C5-N7	-2.21	107.10	109.40
6	I	708	DTP	O2G-PG-O3B	-2.20	97.26	104.64
6	N	708	DTP	C3'-C2'-C1'	-2.19	97.04	102.54
4	E	704	1FZ	O5'-PA-O1A	-2.19	105.83	114.24
4	B	704	1FZ	O5'-PA-O1A	-2.18	105.87	114.24
6	C	701	DTP	C4-C5-N7	-2.18	107.13	109.40
4	J	704	1FZ	O3B-PB-N3A	-2.17	100.56	106.59
5	E	705	GTP	O6-C6-N1	-2.16	118.09	120.65
4	F	704	1FZ	PB-O3B-PG	-2.15	125.03	132.62
4	M	704	1FZ	O5'-PA-O1A	-2.15	105.97	114.24
5	F	705	GTP	PB-O3B-PG	-2.15	125.46	132.83
5	P	705	GTP	C3'-C2'-C1'	2.14	104.20	100.98
6	L	701	DTP	PB-O3B-PG	-2.13	125.51	132.83
4	D	706	1FZ	O2G-PG-O1G	2.13	115.77	107.64
4	C	705	1FZ	O2G-PG-O1G	2.12	115.75	107.64
5	N	706	GTP	C2-N1-C6	-2.12	121.19	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	707	GTP	O4'-C4'-C3'	2.12	109.31	105.11
5	N	706	GTP	O6-C6-N1	-2.11	118.16	120.65
5	I	707	GTP	C5-C6-N1	2.11	117.68	113.95
5	F	705	GTP	O3G-PG-O2G	2.11	115.69	107.64
4	L	705	1FZ	O5'-PA-O1A	-2.10	106.16	114.24
6	C	701	DTP	O2B-PB-O1B	2.09	122.56	112.24
5	I	707	GTP	PB-O3B-PG	-2.08	125.70	132.83
5	I	705	GTP	C8-N7-C5	2.08	106.94	102.99
5	L	706	GTP	C3'-C2'-C1'	2.07	104.10	100.98
6	G	701	DTP	C2-N1-C6	2.07	122.29	118.75
6	E	707	DTP	C2-N1-C6	2.05	122.27	118.75
5	A	705	GTP	O4'-C1'-C2'	2.05	109.92	106.93
5	K	706	GTP	C3'-C2'-C1'	2.05	104.06	100.98
5	D	707	GTP	C2-N1-C6	-2.04	121.33	125.10
6	L	701	DTP	O2B-PB-O1B	2.04	122.32	112.24
6	E	707	DTP	PB-O3B-PG	-2.04	125.83	132.83
6	K	701	DTP	O3G-PG-O2G	2.04	115.43	107.64
6	C	701	DTP	C2-N1-C6	2.03	122.23	118.75
5	A	705	GTP	C3'-C2'-C1'	2.03	104.04	100.98
4	F	704	1FZ	O5'-PA-O1A	-2.02	106.45	114.24
6	K	701	DTP	O2B-PB-O1B	2.02	122.25	112.24
6	B	707	DTP	O3G-PG-O3B	2.02	111.40	104.64
4	A	704	1FZ	O2G-PG-O1G	2.02	115.35	107.64
5	O	705	GTP	O5'-PA-O1A	-2.02	101.19	109.07
6	F	707	DTP	O2B-PB-O1B	2.02	122.21	112.24
5	G	706	GTP	PB-O3B-PG	-2.01	125.93	132.83
4	D	706	1FZ	O5'-PA-O1A	-2.01	106.52	114.24
6	B	707	DTP	O2G-PG-O3B	-2.00	97.92	104.64
6	L	701	DTP	C2-N1-C6	2.00	122.18	118.75

There are no chirality outliers.

All (224) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	704	1FZ	O4'-C1'-N1-C2
4	A	704	1FZ	PA-N3A-PB-O2B
4	A	704	1FZ	PG-O3B-PB-O2B
4	B	704	1FZ	O4'-C1'-N1-C2
4	B	704	1FZ	PA-N3A-PB-O2B
4	B	704	1FZ	PG-O3B-PB-O2B
4	C	705	1FZ	PA-N3A-PB-O2B
4	D	706	1FZ	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
4	D	706	1FZ	PB-N3A-PA-O1A
4	D	706	1FZ	PA-N3A-PB-O2B
4	D	706	1FZ	PG-O3B-PB-O1B
4	D	706	1FZ	PG-O3B-PB-O2B
4	D	706	1FZ	PB-O3B-PG-O2G
4	E	704	1FZ	PA-N3A-PB-O2B
4	E	704	1FZ	PG-O3B-PB-O1B
4	E	704	1FZ	PG-O3B-PB-O2B
4	F	704	1FZ	PA-N3A-PB-O2B
4	F	704	1FZ	PG-O3B-PB-O2B
4	G	705	1FZ	PA-N3A-PB-O2B
4	G	705	1FZ	PG-O3B-PB-O1B
4	G	705	1FZ	PG-O3B-PB-O2B
4	G	705	1FZ	PB-O3B-PG-O1G
4	G	705	1FZ	PB-O3B-PG-O2G
4	H	705	1FZ	O4'-C1'-N1-C2
4	H	705	1FZ	PB-N3A-PA-O1A
4	H	705	1FZ	PA-N3A-PB-O2B
4	H	705	1FZ	PG-O3B-PB-O1B
4	H	705	1FZ	PG-O3B-PB-O2B
4	H	705	1FZ	PB-O3B-PG-O1G
4	H	705	1FZ	PB-O3B-PG-O2G
4	I	704	1FZ	PA-N3A-PB-O2B
4	I	704	1FZ	PG-O3B-PB-O1B
4	I	704	1FZ	PG-O3B-PB-O2B
4	J	704	1FZ	C5'-O5'-PA-O1A
4	J	704	1FZ	C5'-O5'-PA-O2A
4	J	704	1FZ	C5'-O5'-PA-N3A
4	J	704	1FZ	PB-N3A-PA-O5'
4	J	704	1FZ	PA-N3A-PB-O2B
4	J	704	1FZ	PG-O3B-PB-O1B
4	J	704	1FZ	PG-O3B-PB-O2B
4	K	705	1FZ	O4'-C1'-N1-C6
4	K	705	1FZ	O4'-C1'-N1-C2
4	K	705	1FZ	PA-N3A-PB-O2B
4	K	705	1FZ	PB-O3B-PG-O1G
4	K	705	1FZ	PB-O3B-PG-O2G
4	L	705	1FZ	PB-N3A-PA-O1A
4	L	705	1FZ	PA-N3A-PB-O2B
4	L	705	1FZ	PG-O3B-PB-O1B
4	L	705	1FZ	PG-O3B-PB-O2B
4	L	705	1FZ	PB-O3B-PG-O2G

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Mol	Chain	Res	Type	Atoms
4	M	704	1FZ	PA-N3A-PB-O2B
4	N	705	1FZ	O4'-C1'-N1-C2
4	N	705	1FZ	C5'-O5'-PA-O2A
4	N	705	1FZ	C5'-O5'-PA-N3A
4	N	705	1FZ	PB-N3A-PA-O1A
4	N	705	1FZ	PA-N3A-PB-O2B
4	O	704	1FZ	O4'-C1'-N1-C2
4	O	704	1FZ	PG-O3B-PB-O2B
4	O	704	1FZ	PB-O3B-PG-O2G
4	P	704	1FZ	PA-N3A-PB-O2B
5	D	707	GTP	PB-O3B-PG-O3G
5	I	705	GTP	PB-O3B-PG-O3G
5	I	707	GTP	C5'-O5'-PA-O1A
5	I	707	GTP	C5'-O5'-PA-O2A
5	I	707	GTP	O4'-C4'-C5'-O5'
5	I	707	GTP	C3'-C4'-C5'-O5'
5	O	705	GTP	C5'-O5'-PA-O2A
5	O	705	GTP	O4'-C4'-C5'-O5'
5	P	705	GTP	PB-O3B-PG-O3G
6	H	701	DTP	PB-O3B-PG-O2G
6	H	701	DTP	PB-O3B-PG-O3G
6	I	708	DTP	PB-O3A-PA-O5'
6	M	707	DTP	C5'-O5'-PA-O1A
6	M	707	DTP	C5'-O5'-PA-O3A
6	N	708	DTP	PB-O3B-PG-O2G
4	A	704	1FZ	O4'-C1'-N1-C6
4	B	704	1FZ	O4'-C1'-N1-C6
4	D	706	1FZ	O4'-C1'-N1-C6
4	H	705	1FZ	O4'-C1'-N1-C6
4	N	705	1FZ	O4'-C1'-N1-C6
4	E	704	1FZ	O4'-C1'-N1-C2
4	L	705	1FZ	C3'-C4'-C5'-O5'
4	L	705	1FZ	O4'-C4'-C5'-O5'
5	O	705	GTP	C3'-C4'-C5'-O5'
4	E	704	1FZ	O4'-C1'-N1-C6
4	O	704	1FZ	O4'-C1'-N1-C6
5	A	705	GTP	O4'-C4'-C5'-O5'
4	F	704	1FZ	O4'-C1'-N1-C6
4	I	704	1FZ	O4'-C1'-N1-C6
4	J	704	1FZ	O4'-C1'-N1-C6
4	M	704	1FZ	O4'-C1'-N1-C6
4	I	704	1FZ	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
4	J	704	1FZ	O4'-C1'-N1-C2
4	C	705	1FZ	O4'-C1'-N1-C6
4	F	704	1FZ	O4'-C1'-N1-C2
4	C	705	1FZ	C3'-C4'-C5'-O5'
5	A	705	GTP	C3'-C4'-C5'-O5'
4	G	705	1FZ	O4'-C1'-N1-C6
4	P	704	1FZ	O4'-C1'-N1-C6
4	M	704	1FZ	O4'-C1'-N1-C2
4	L	705	1FZ	C2'-C1'-N1-C2
4	J	704	1FZ	C3'-C4'-C5'-O5'
4	C	705	1FZ	O4'-C1'-N1-C2
4	P	704	1FZ	O4'-C1'-N1-C2
4	N	705	1FZ	C5'-O5'-PA-O1A
4	L	705	1FZ	O4'-C1'-N1-C6
4	G	705	1FZ	O4'-C1'-N1-C2
5	D	702	GTP	PB-O3A-PA-O1A
6	M	707	DTP	PB-O3A-PA-O1A
4	L	705	1FZ	C2'-C1'-N1-C6
5	P	705	GTP	C4'-C5'-O5'-PA
6	H	701	DTP	PB-O3A-PA-O5'
6	J	706	DTP	PB-O3A-PA-O5'
4	I	704	1FZ	PB-O3B-PG-O3G
5	L	706	GTP	PB-O3B-PG-O1G
4	G	705	1FZ	C2'-C1'-N1-C2
4	L	705	1FZ	O4'-C1'-N1-C2
5	D	702	GTP	PB-O3B-PG-O3G
6	I	708	DTP	PB-O3B-PG-O3G
6	N	708	DTP	PB-O3B-PG-O3G
5	O	705	GTP	C5'-O5'-PA-O3A
6	F	707	DTP	C5'-O5'-PA-O3A
5	A	705	GTP	PG-O3B-PB-O1B
5	A	705	GTP	PB-O3A-PA-O1A
5	I	705	GTP	PB-O3A-PA-O2A
5	L	706	GTP	PB-O3A-PA-O2A
6	C	701	DTP	PA-O3A-PB-O2B
6	E	707	DTP	PA-O3A-PB-O2B
6	F	707	DTP	PA-O3A-PB-O2B
6	J	706	DTP	PA-O3A-PB-O2B
6	N	701	DTP	PB-O3A-PA-O1A
5	O	705	GTP	C5'-O5'-PA-O1A
6	M	707	DTP	C5'-O5'-PA-O2A
4	P	704	1FZ	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
4	G	705	1FZ	PB-N3A-PA-O5'
4	I	704	1FZ	PB-N3A-PA-O5'
4	K	705	1FZ	PB-N3A-PA-O5'
4	G	705	1FZ	C3'-C4'-C5'-O5'
4	C	705	1FZ	C2'-C1'-N1-C2
4	O	704	1FZ	PB-O3B-PG-O3G
5	P	705	GTP	PB-O3B-PG-O1G
5	G	706	GTP	C4'-C5'-O5'-PA
4	G	705	1FZ	C2'-C1'-N1-C6
4	P	704	1FZ	C2'-C1'-N1-C6
4	A	704	1FZ	C4'-C5'-O5'-PA
4	F	704	1FZ	C4'-C5'-O5'-PA
4	O	704	1FZ	C4'-C5'-O5'-PA
5	D	702	GTP	PB-O3A-PA-O2A
5	I	705	GTP	PB-O3A-PA-O1A
5	P	705	GTP	PB-O3A-PA-O2A
6	A	706	DTP	PA-O3A-PB-O2B
6	B	707	DTP	PA-O3A-PB-O2B
6	G	701	DTP	PA-O3A-PB-O2B
6	K	701	DTP	PB-O3A-PA-O2A
6	M	706	DTP	PB-O3A-PA-O2A
6	M	707	DTP	PB-O3A-PA-O2A
5	L	706	GTP	C4'-C5'-O5'-PA
4	M	704	1FZ	C2'-C1'-N1-C2
4	C	705	1FZ	C4'-C5'-O5'-PA
4	P	704	1FZ	C4'-C5'-O5'-PA
4	N	705	1FZ	C3'-C4'-C5'-O5'
5	B	705	GTP	C4'-C5'-O5'-PA
5	K	706	GTP	C4'-C5'-O5'-PA
4	O	704	1FZ	PA-N3A-PB-O2B
5	D	702	GTP	C4'-C5'-O5'-PA
4	M	704	1FZ	C4'-C5'-O5'-PA
4	A	704	1FZ	PG-O3B-PB-O1B
4	B	704	1FZ	PG-O3B-PB-O1B
4	F	704	1FZ	PG-O3B-PB-O1B
4	O	704	1FZ	PG-O3B-PB-O1B
5	D	707	GTP	PB-O3A-PA-O1A
5	O	705	GTP	PB-O3A-PA-O2A
6	A	706	DTP	PA-O3A-PB-O1B
6	C	701	DTP	PA-O3A-PB-O1B
6	E	707	DTP	PA-O3A-PB-O1B
6	F	707	DTP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
6	J	706	DTP	PA-O3A-PB-O1B
6	L	701	DTP	PA-O3A-PB-O1B
6	M	706	DTP	PB-O3A-PA-O1A
6	N	701	DTP	PA-O3A-PB-O1B
6	N	701	DTP	PA-O3A-PB-O2B
6	N	708	DTP	PA-O3A-PB-O1B
6	N	708	DTP	PA-O3A-PB-O2B
4	B	704	1FZ	C4'-C5'-O5'-PA
5	D	707	GTP	O4'-C4'-C5'-O5'
4	K	705	1FZ	C5'-O5'-PA-O2A
4	P	704	1FZ	C3'-C4'-C5'-O5'
4	L	705	1FZ	PB-O3B-PG-O3G
5	D	702	GTP	PB-O3B-PG-O1G
5	I	705	GTP	PB-O3B-PG-O1G
4	D	706	1FZ	PB-O3B-PG-O1G
5	F	705	GTP	PB-O3B-PG-O2G
5	L	706	GTP	PB-O3B-PG-O2G
5	L	706	GTP	PB-O3B-PG-O3G
5	N	706	GTP	PB-O3B-PG-O2G
6	B	707	DTP	PB-O3B-PG-O2G
6	I	708	DTP	PB-O3B-PG-O2G
5	I	707	GTP	C5'-O5'-PA-O3A
5	M	705	GTP	C4'-C5'-O5'-PA
4	I	704	1FZ	C3'-C4'-C5'-O5'
5	D	707	GTP	C3'-C4'-C5'-O5'
5	A	705	GTP	PB-O3A-PA-O2A
5	B	705	GTP	PB-O3A-PA-O2A
5	D	707	GTP	PB-O3A-PA-O2A
5	F	705	GTP	PB-O3A-PA-O1A
5	L	706	GTP	PG-O3B-PB-O2B
5	L	706	GTP	PB-O3A-PA-O1A
5	N	706	GTP	PB-O3A-PA-O2A
6	B	707	DTP	PA-O3A-PB-O1B
6	G	701	DTP	PA-O3A-PB-O1B
6	H	701	DTP	PA-O3A-PB-O2B
6	K	701	DTP	PB-O3A-PA-O1A
6	L	701	DTP	PA-O3A-PB-O2B
6	M	707	DTP	PG-O3B-PB-O2B
6	N	701	DTP	PB-O3A-PA-O2A
5	A	705	GTP	C4'-C5'-O5'-PA
4	E	704	1FZ	C4'-C5'-O5'-PA
5	A	705	GTP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
6	A	706	DTP	C5'-O5'-PA-O1A
6	D	701	DTP	C5'-O5'-PA-O1A
6	F	707	DTP	C5'-O5'-PA-O1A
4	O	704	1FZ	PA-N3A-PB-O3B
4	H	705	1FZ	C5'-O5'-PA-N3A
4	K	705	1FZ	C5'-O5'-PA-N3A

There are no ring outliers.

35 monomers are involved in 55 short contacts:

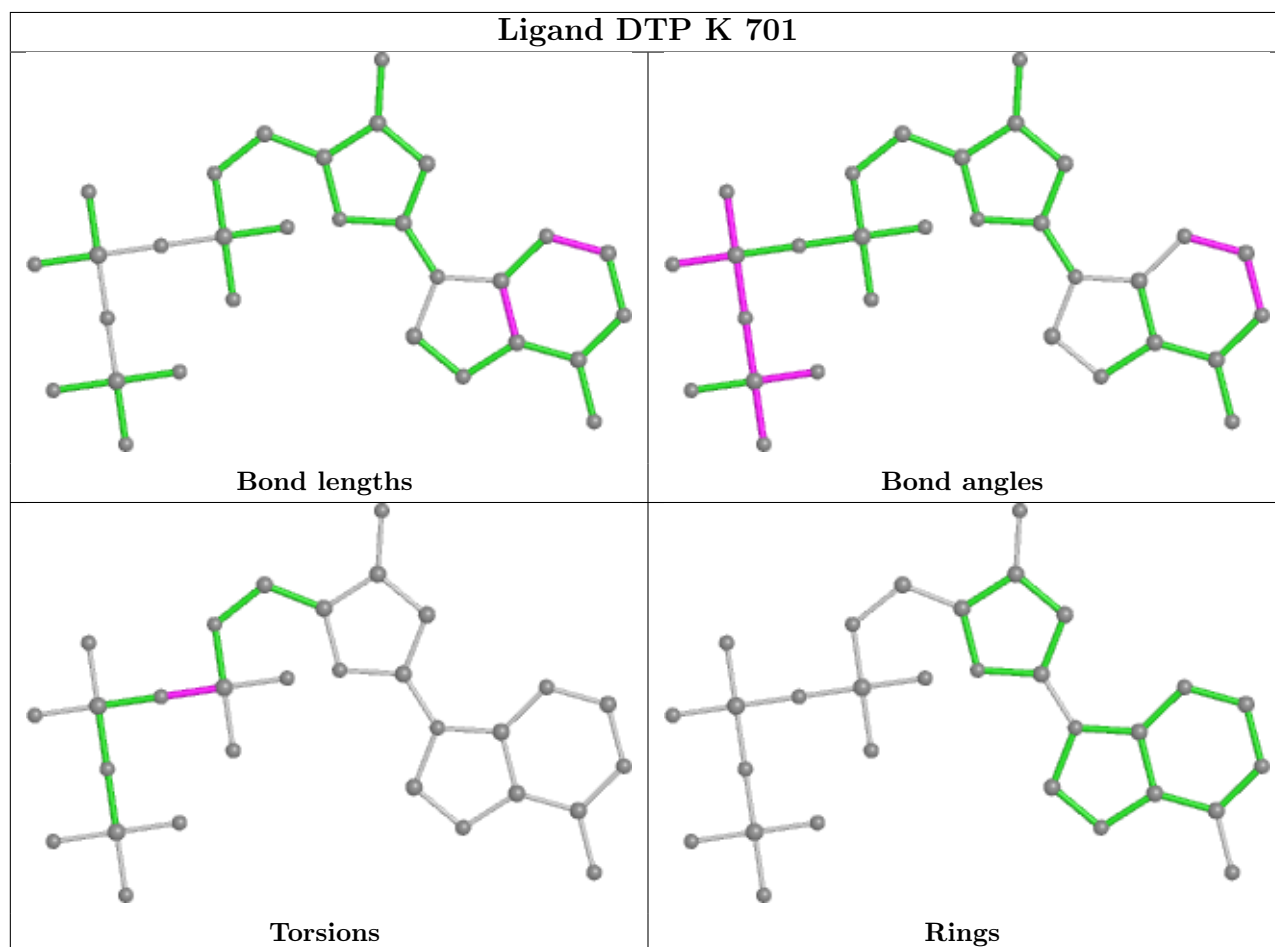
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	701	DTP	2	0
5	I	705	GTP	1	0
6	D	701	DTP	2	0
6	G	701	DTP	1	0
4	P	704	1FZ	1	0
6	L	701	DTP	3	0
5	P	705	GTP	3	0
4	J	704	1FZ	1	0
5	D	707	GTP	1	0
5	H	706	GTP	2	0
5	F	705	GTP	2	0
6	I	708	DTP	2	0
6	M	707	DTP	3	0
7	E	706	SO4	1	0
6	E	707	DTP	2	0
4	L	705	1FZ	2	0
4	O	704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

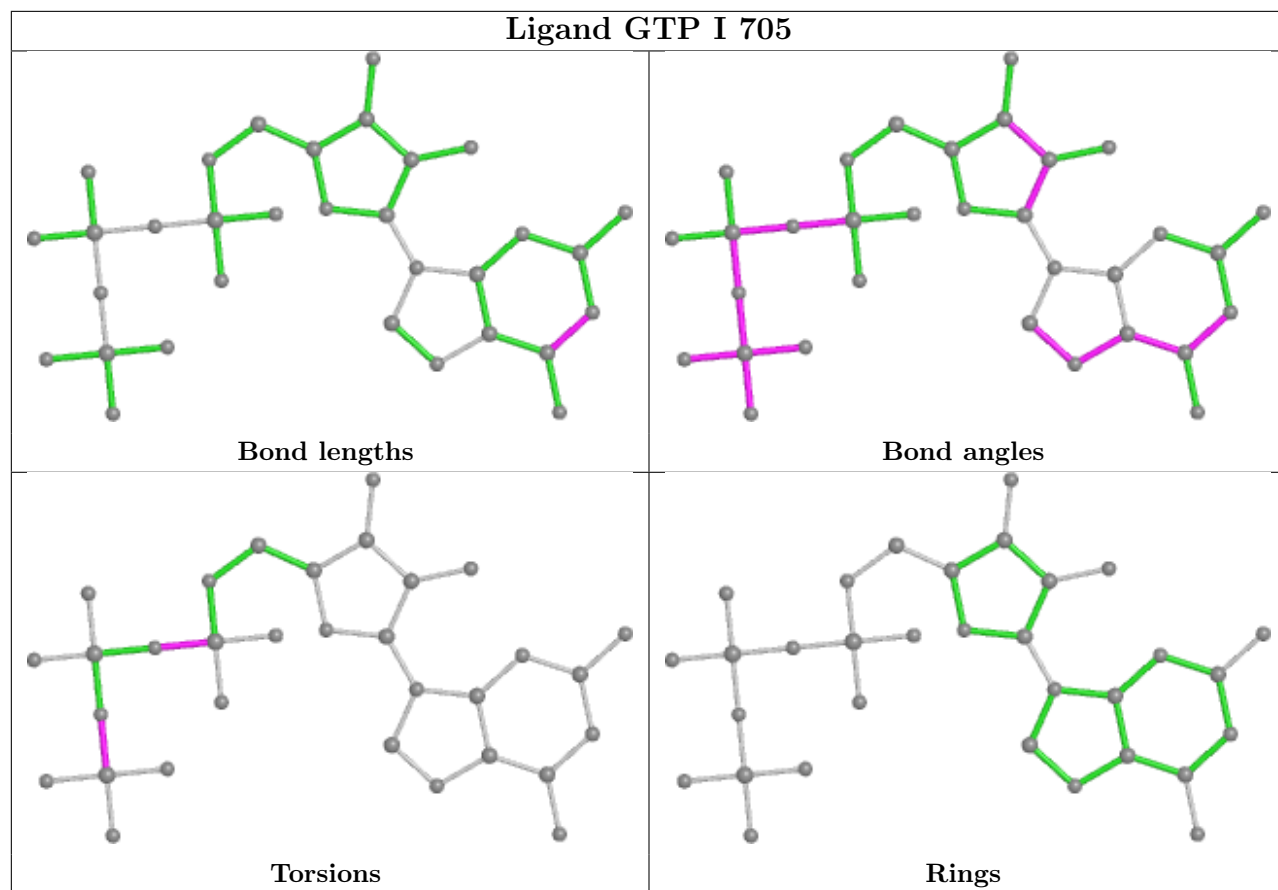
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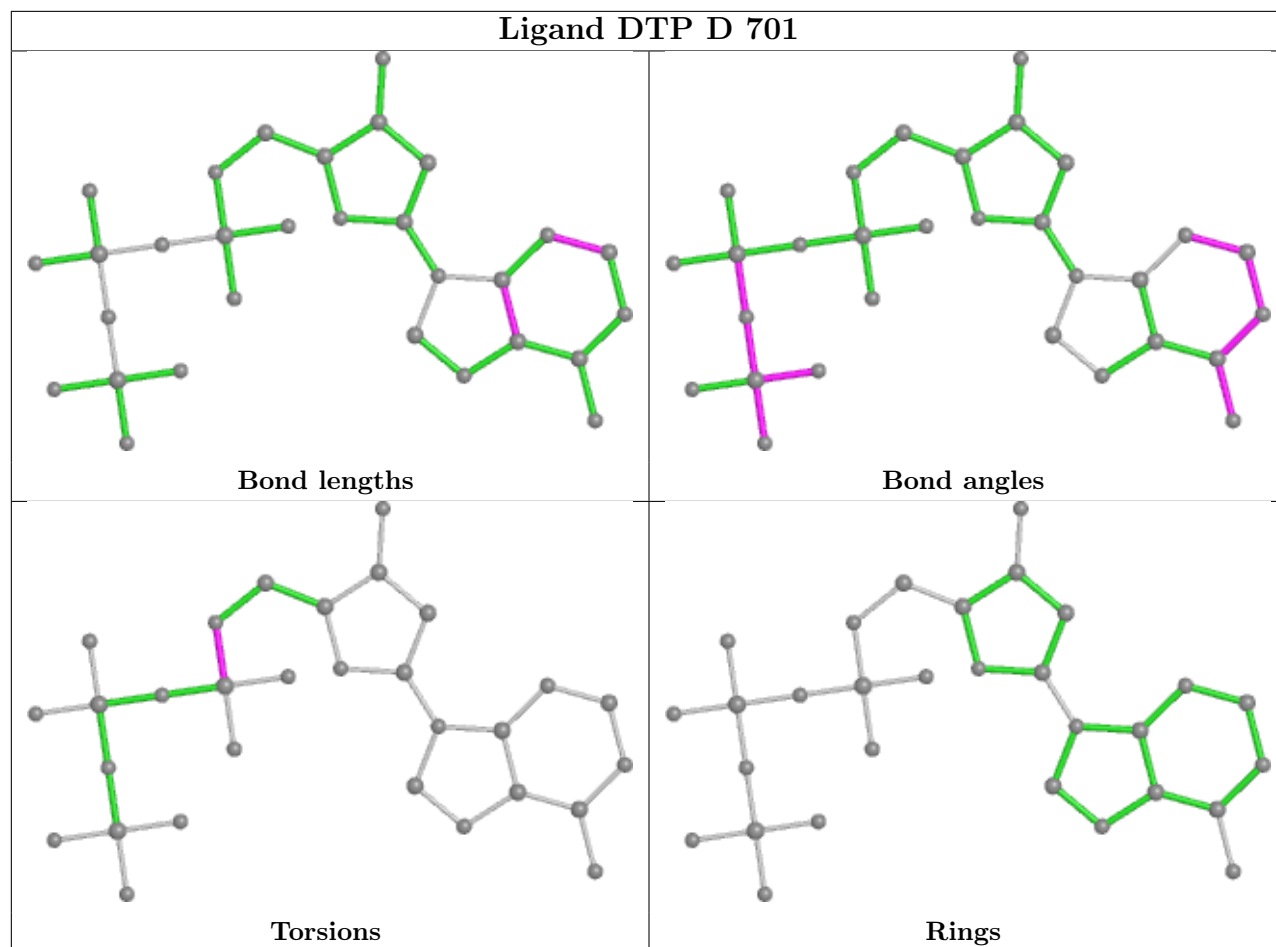
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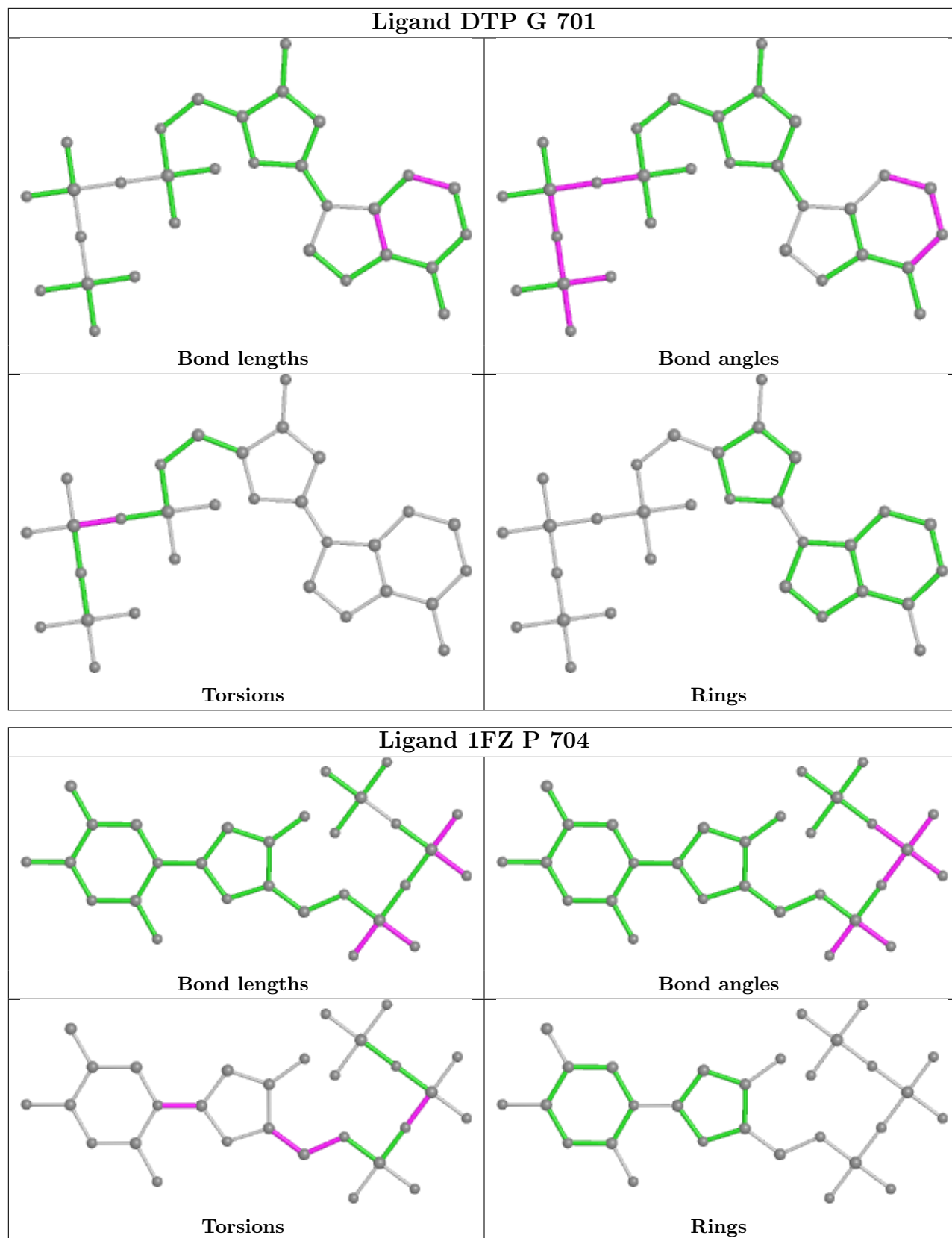
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	N	706	GTP	1	0
6	A	706	DTP	1	0
4	A	704	1FZ	1	0
4	D	706	1FZ	2	0

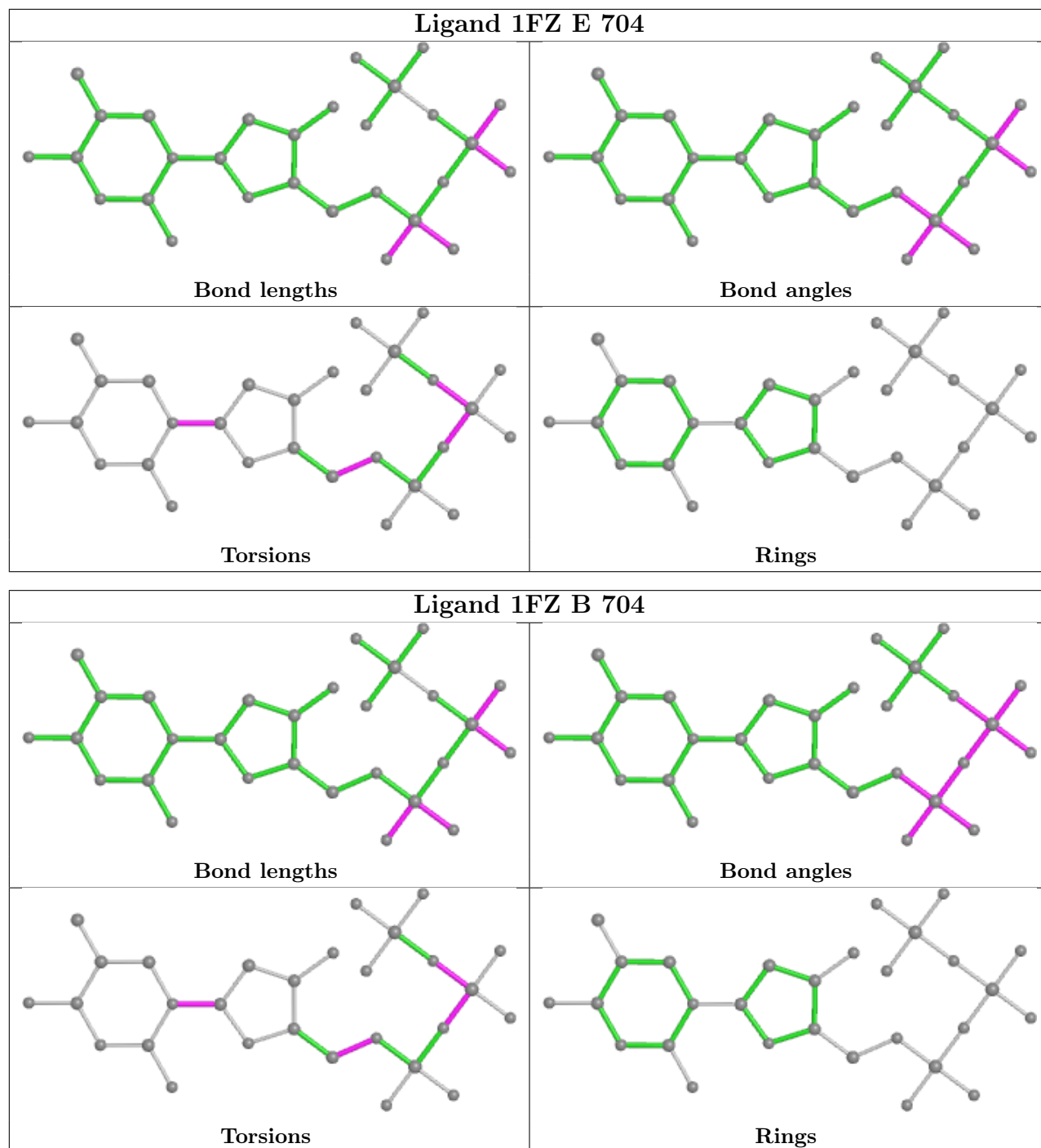
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

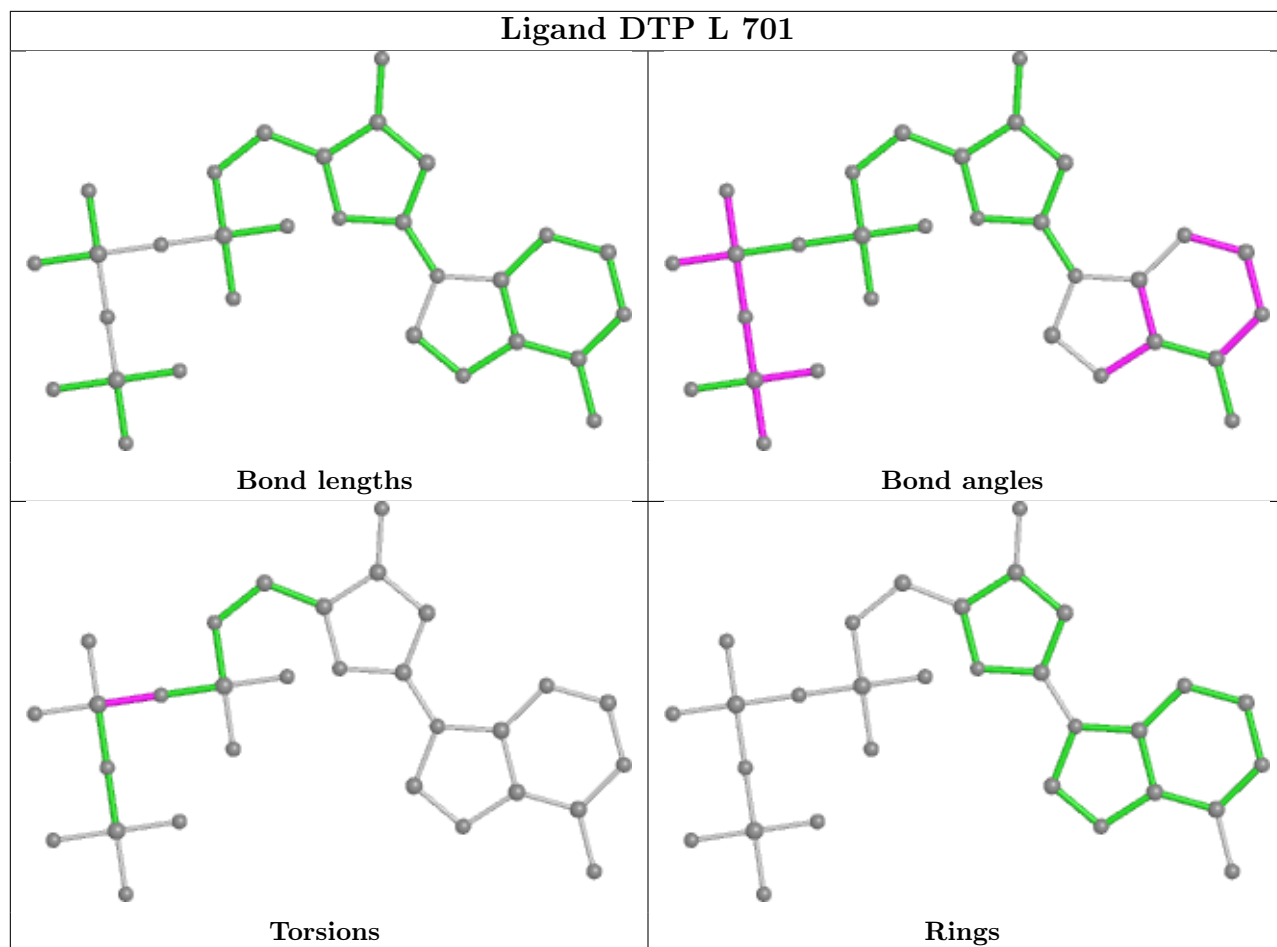


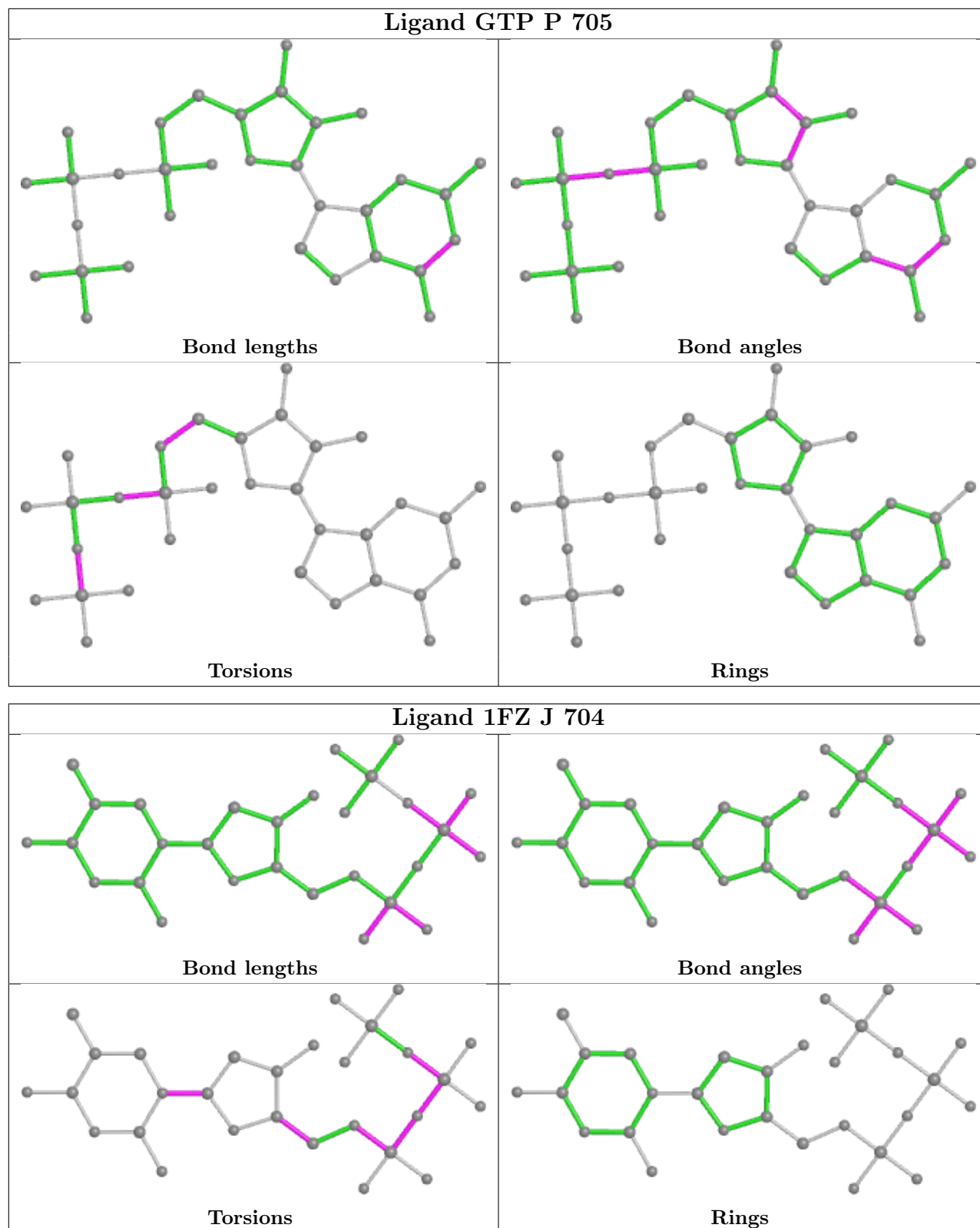


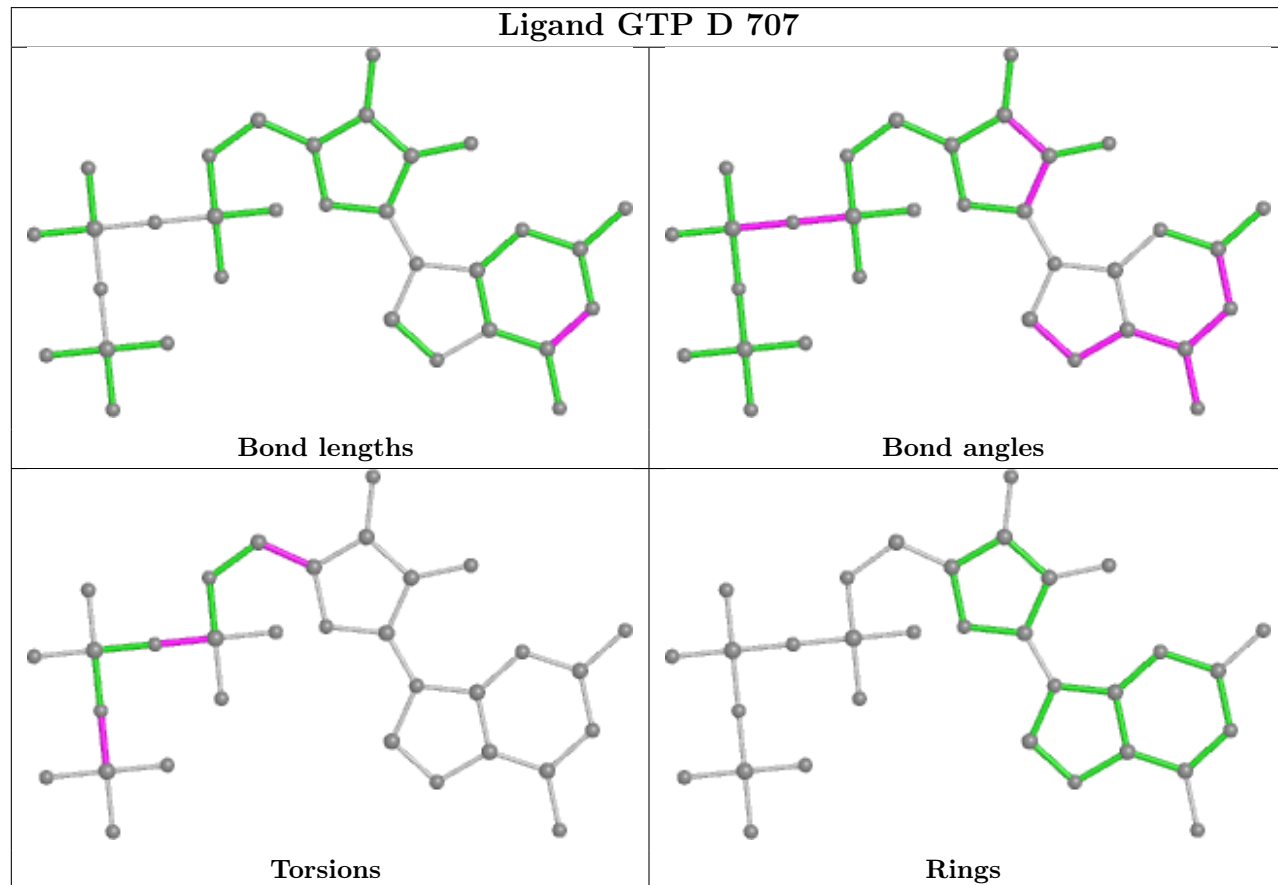
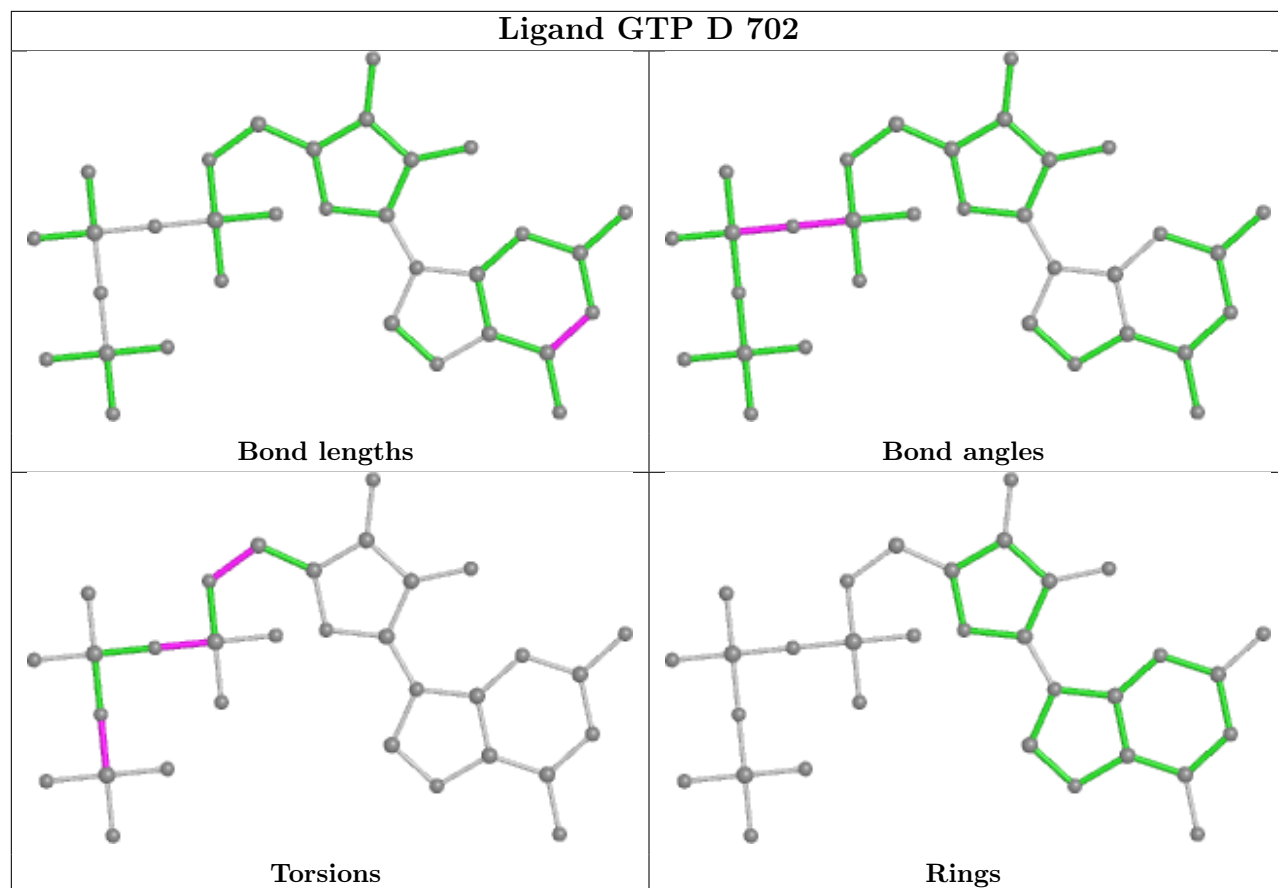


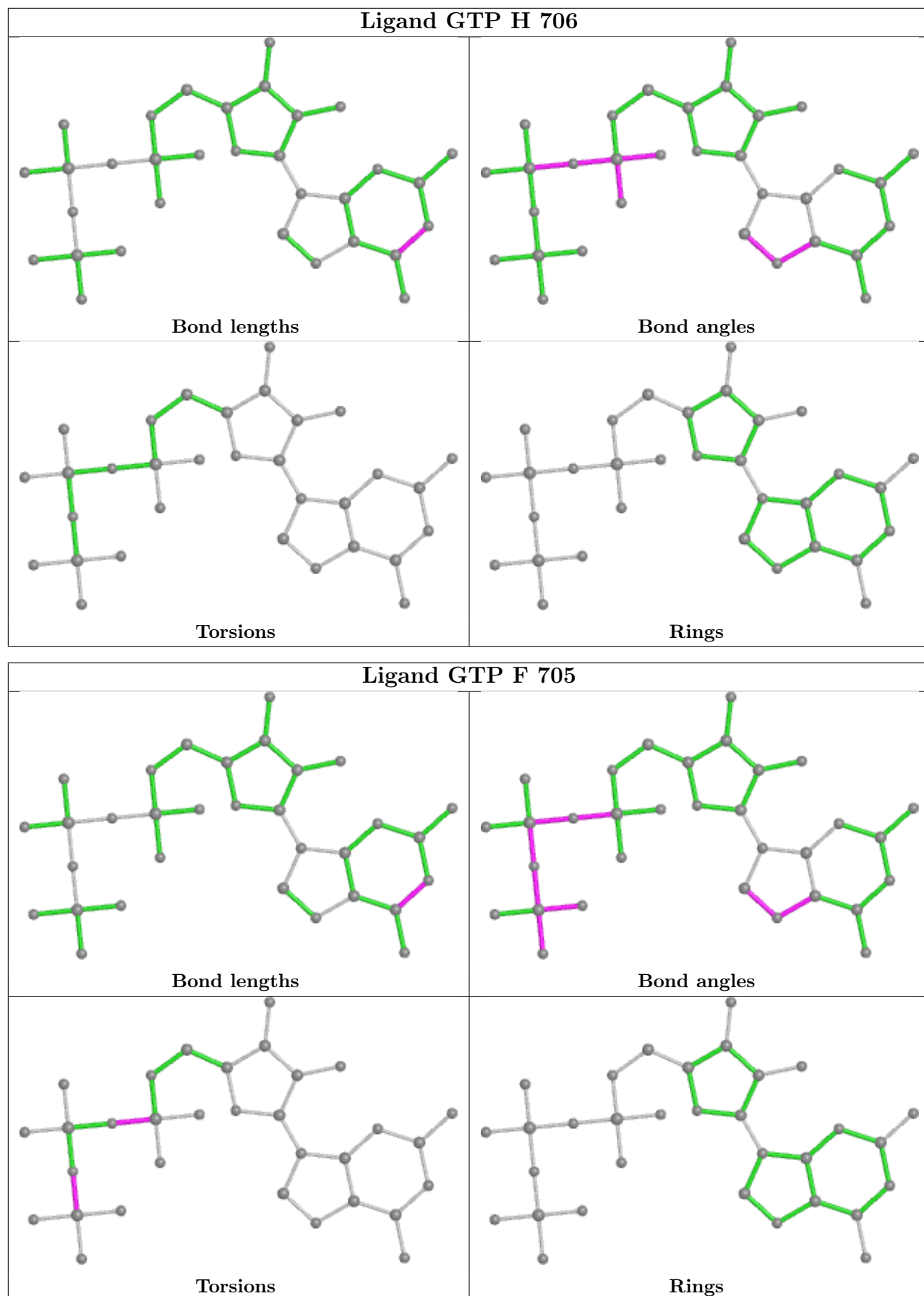


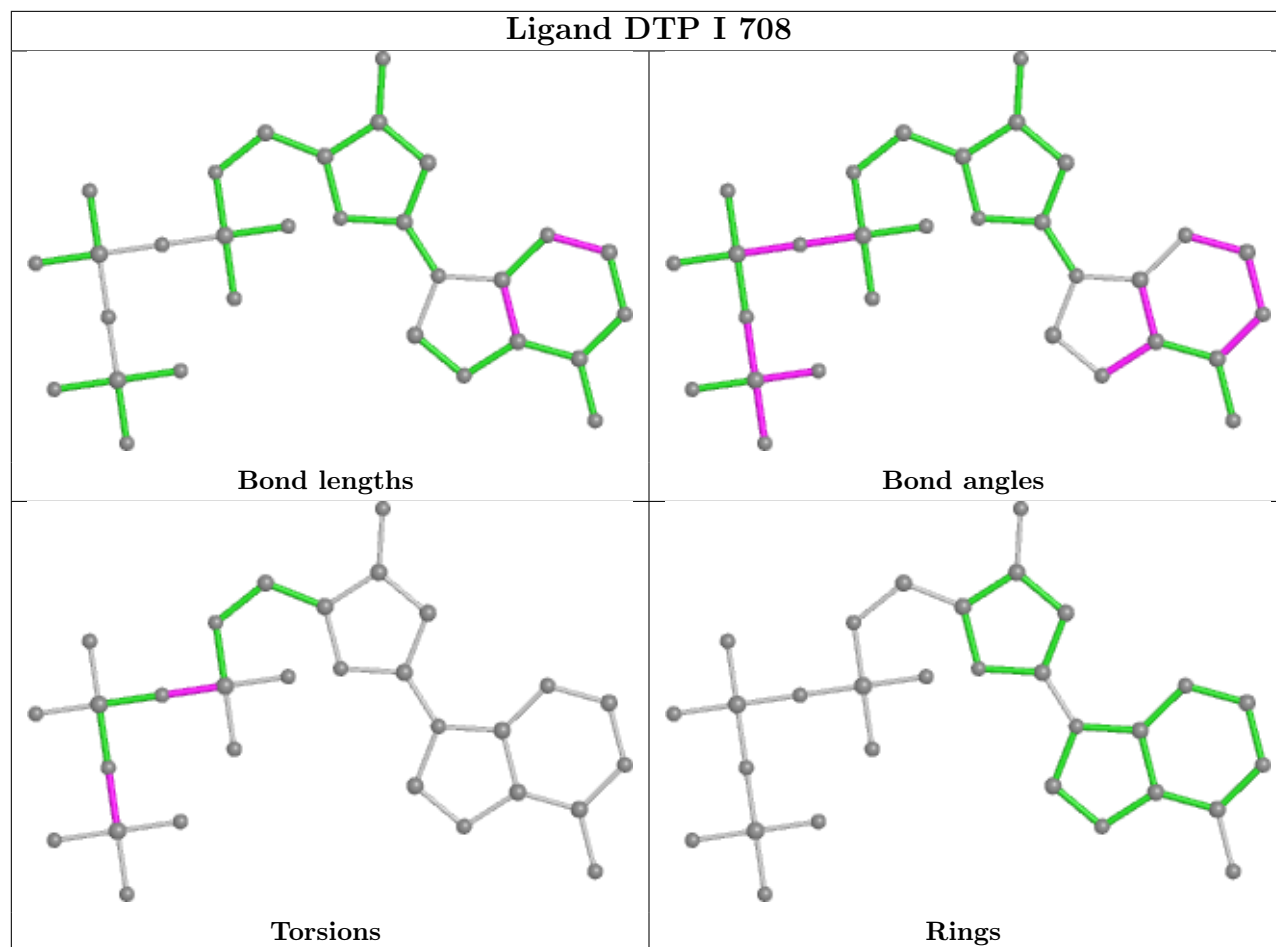


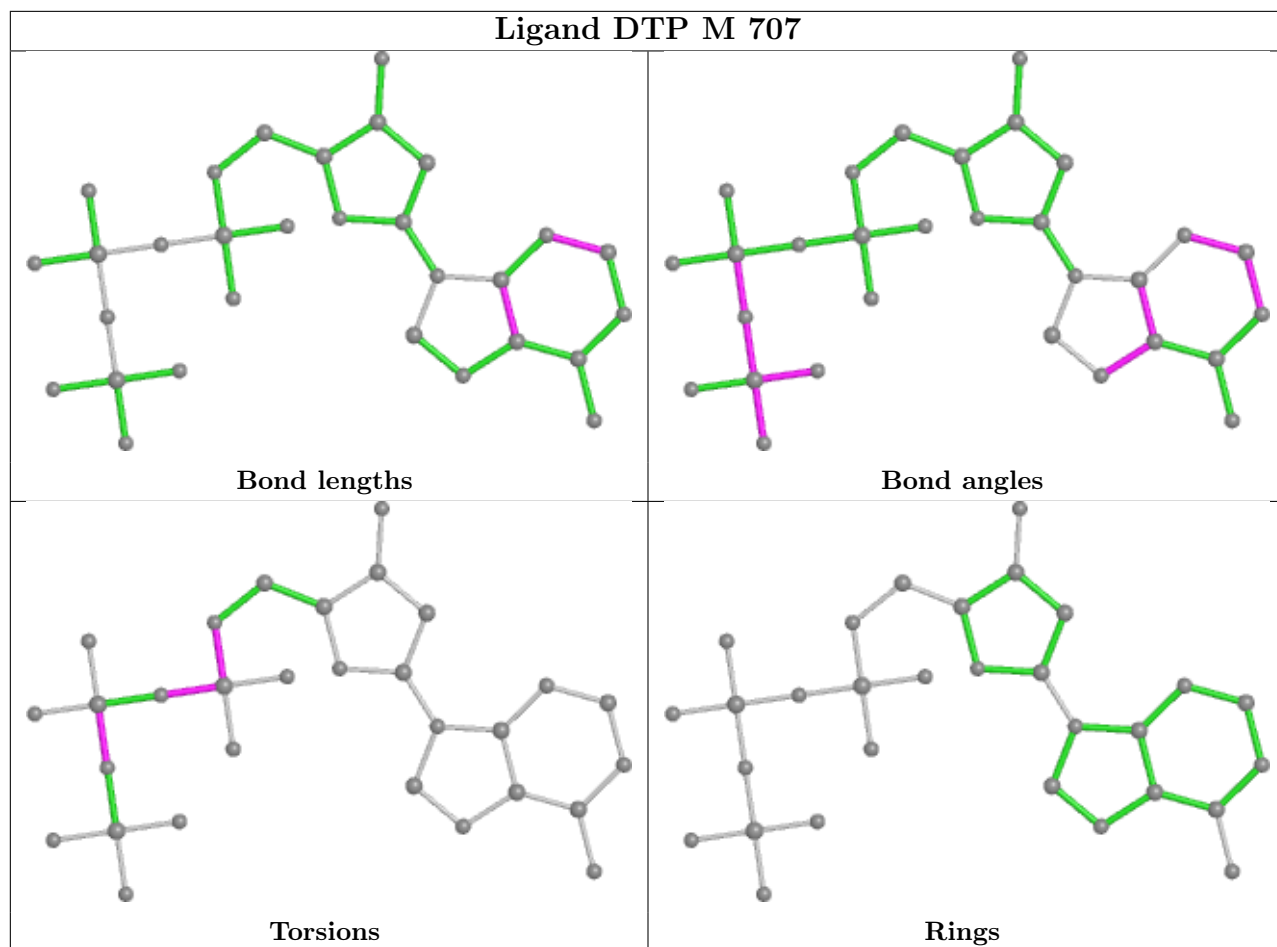


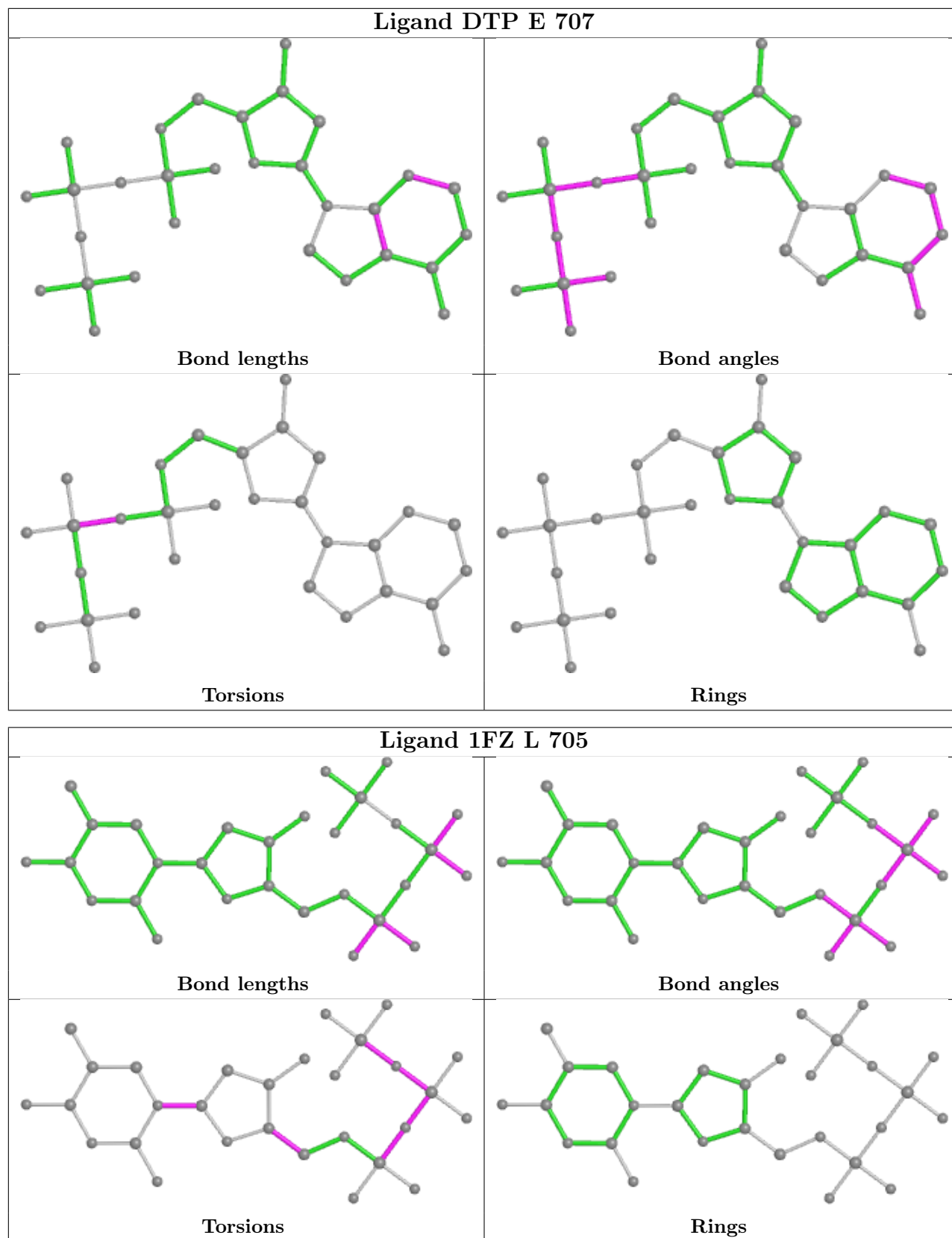


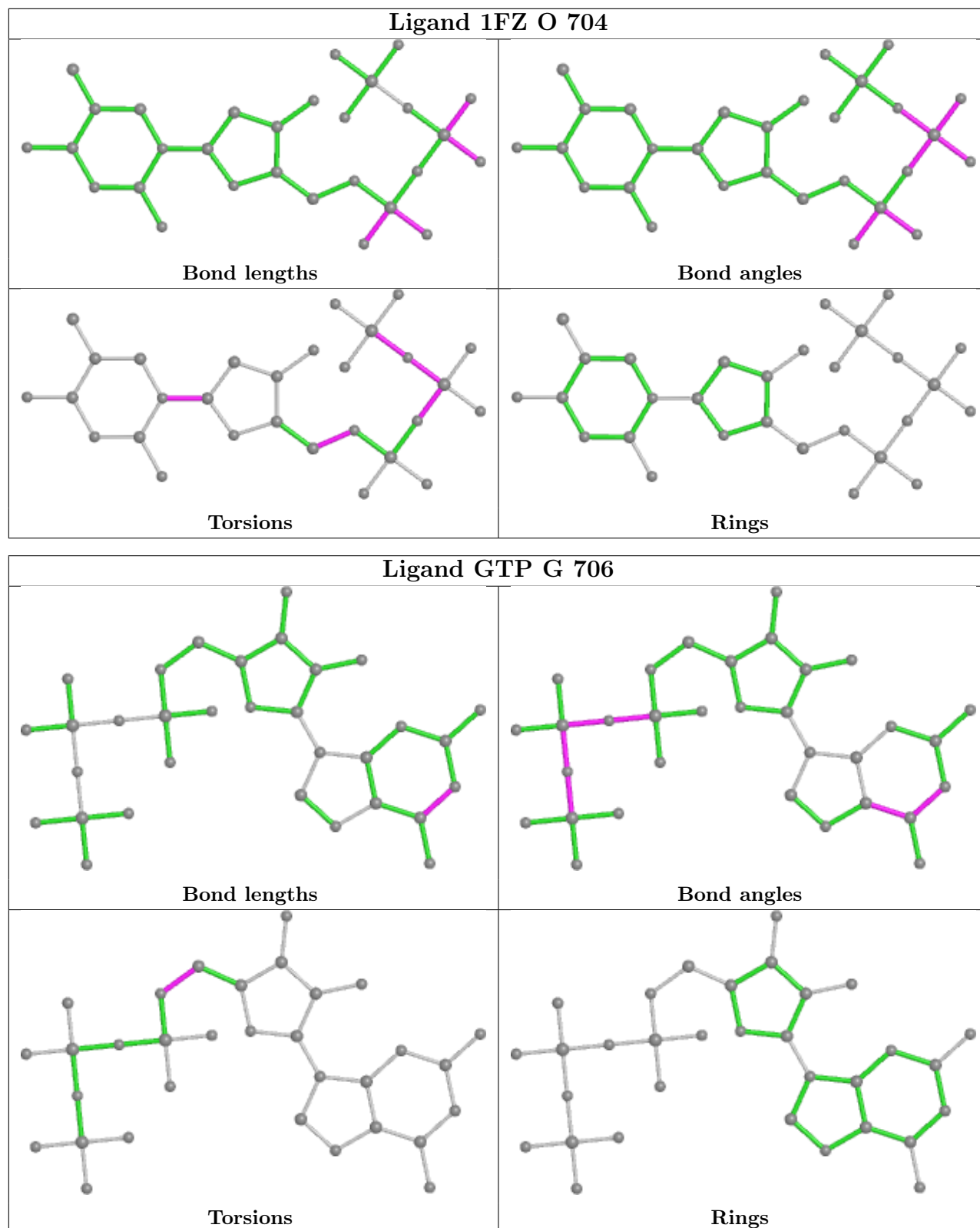


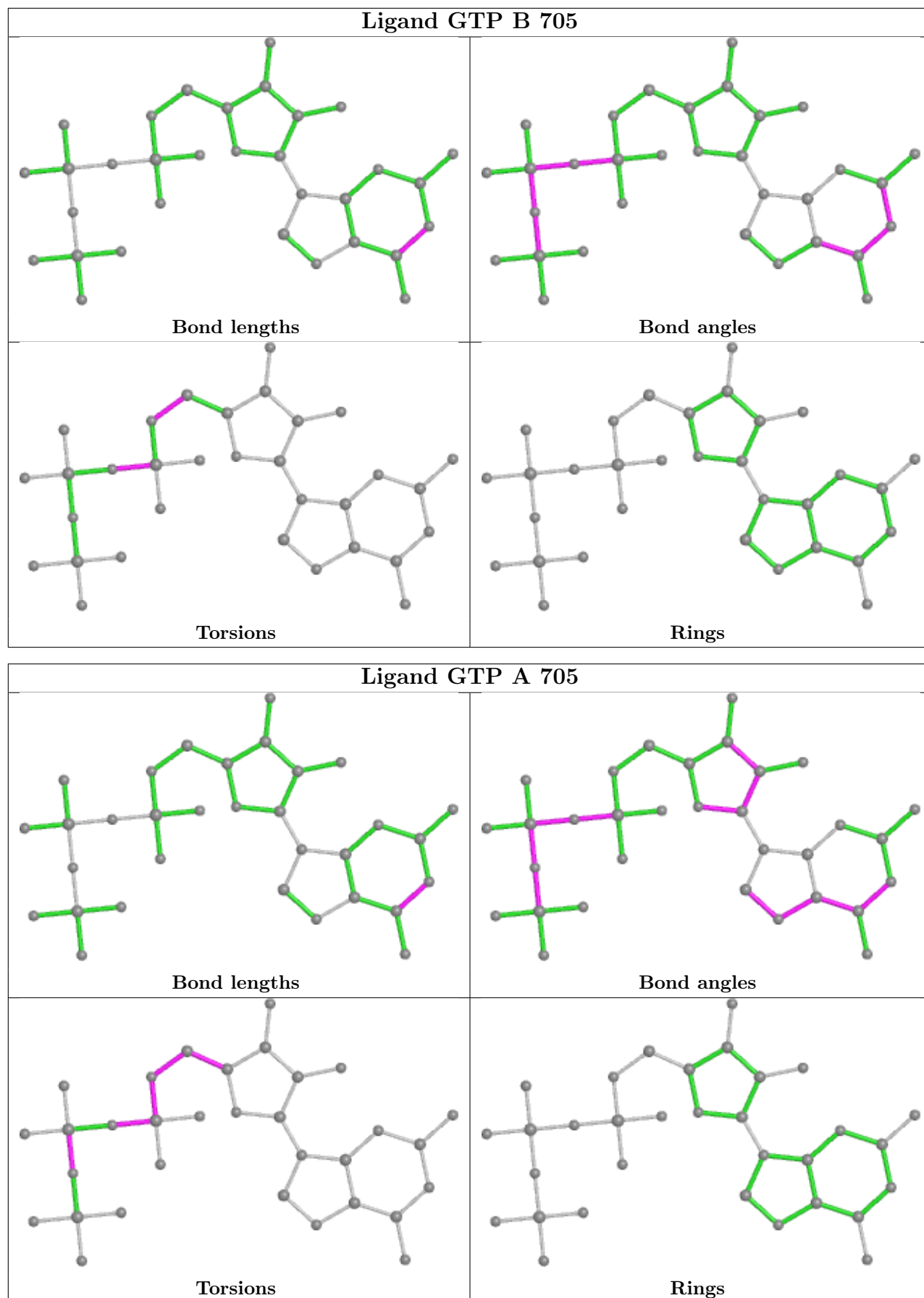


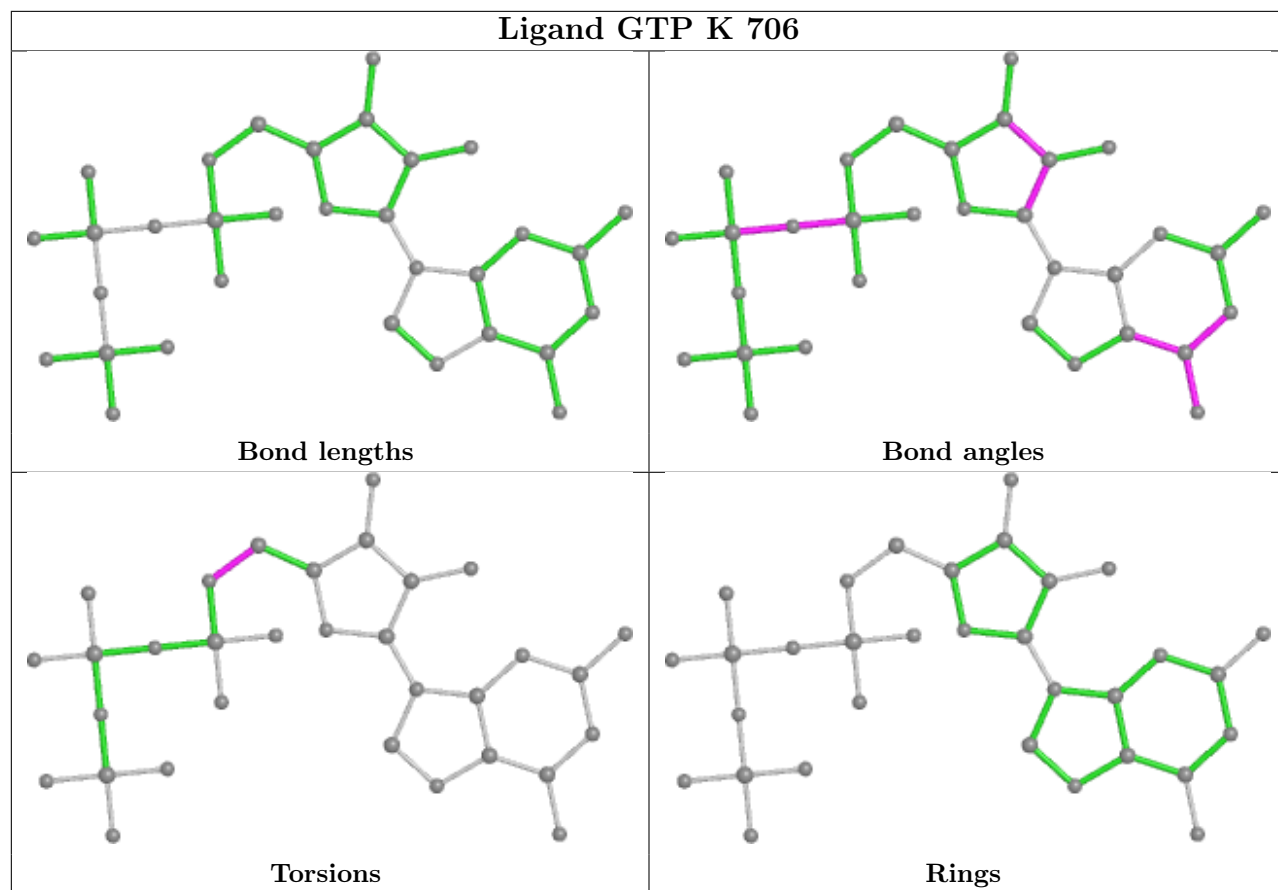


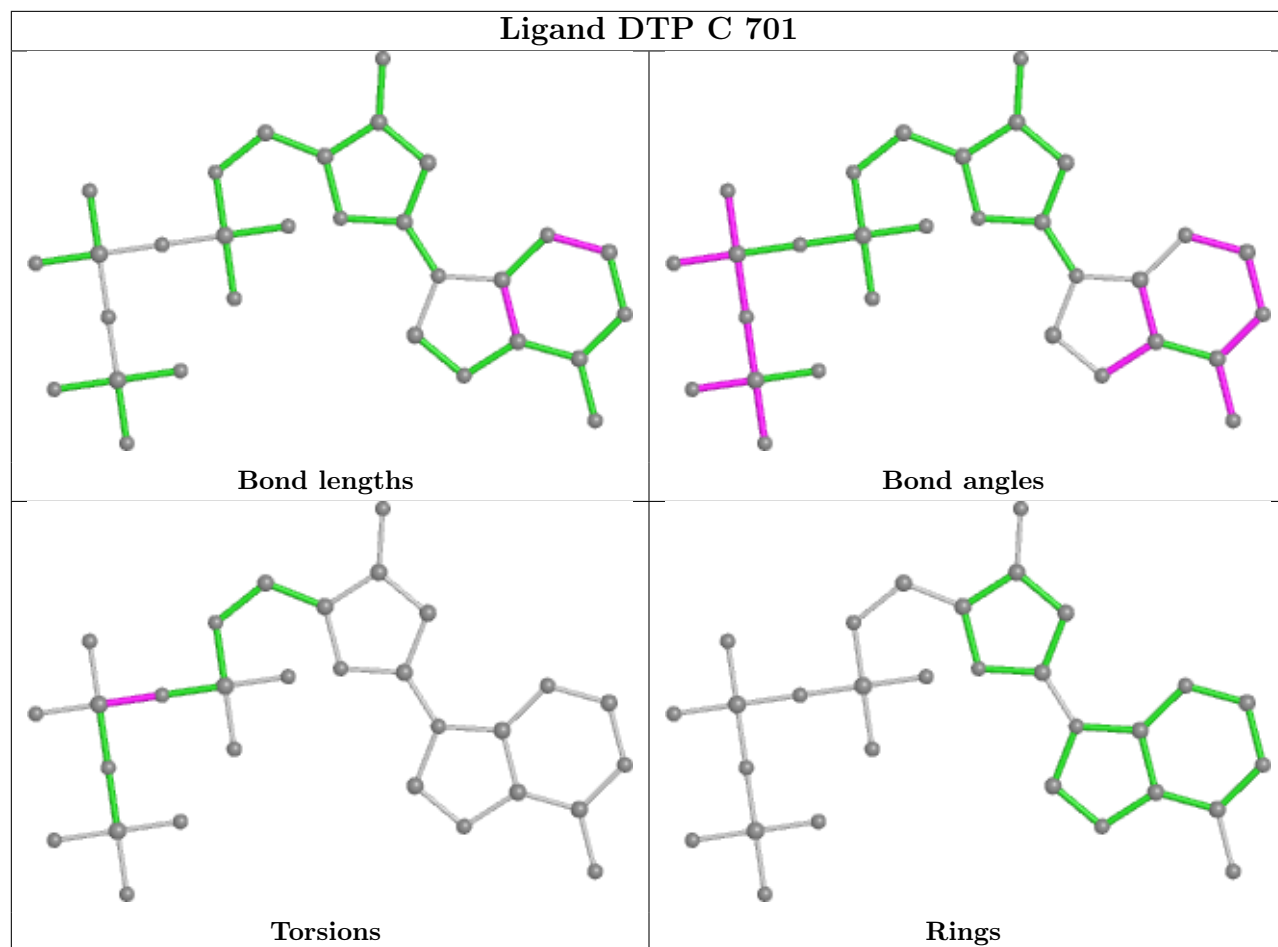


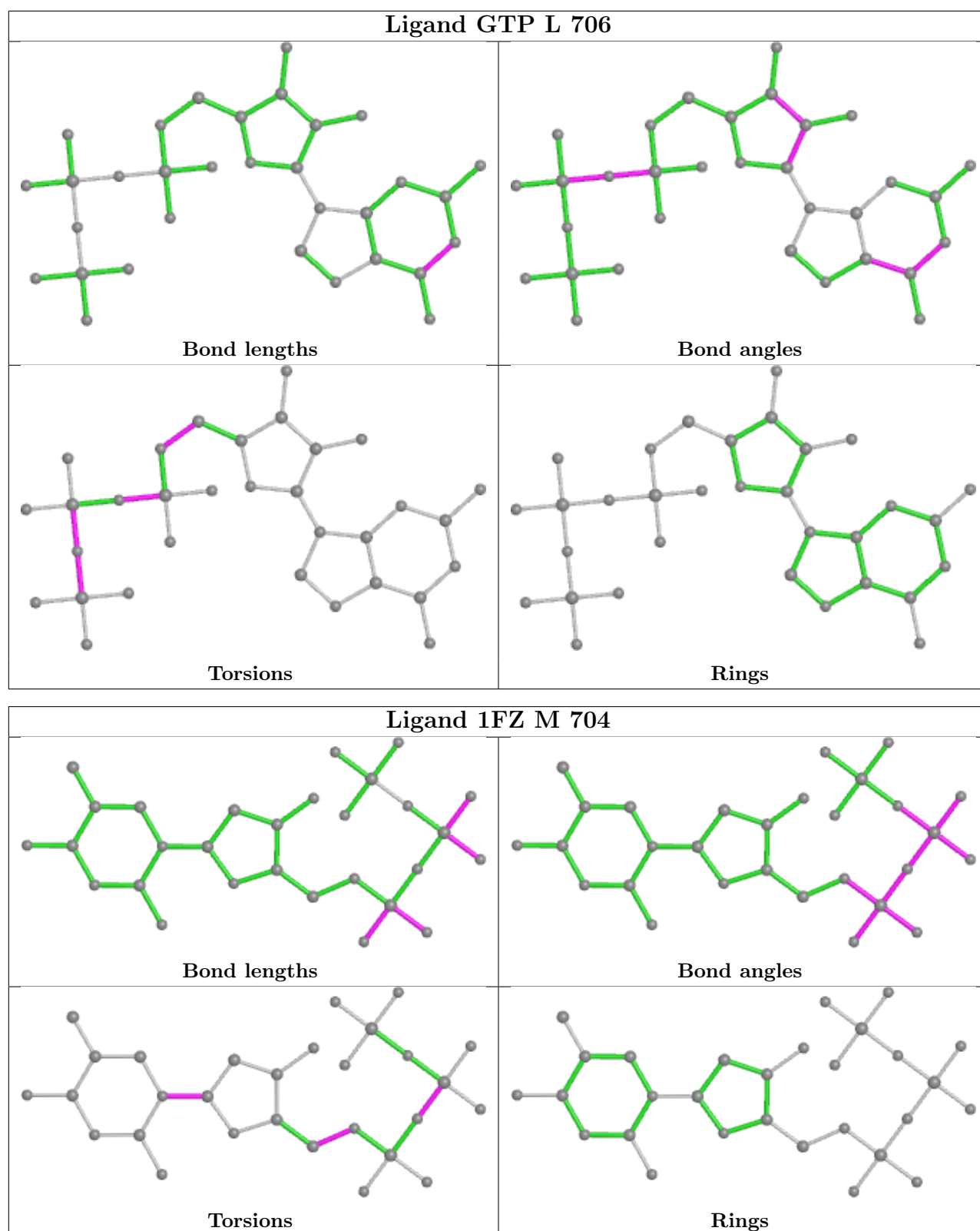


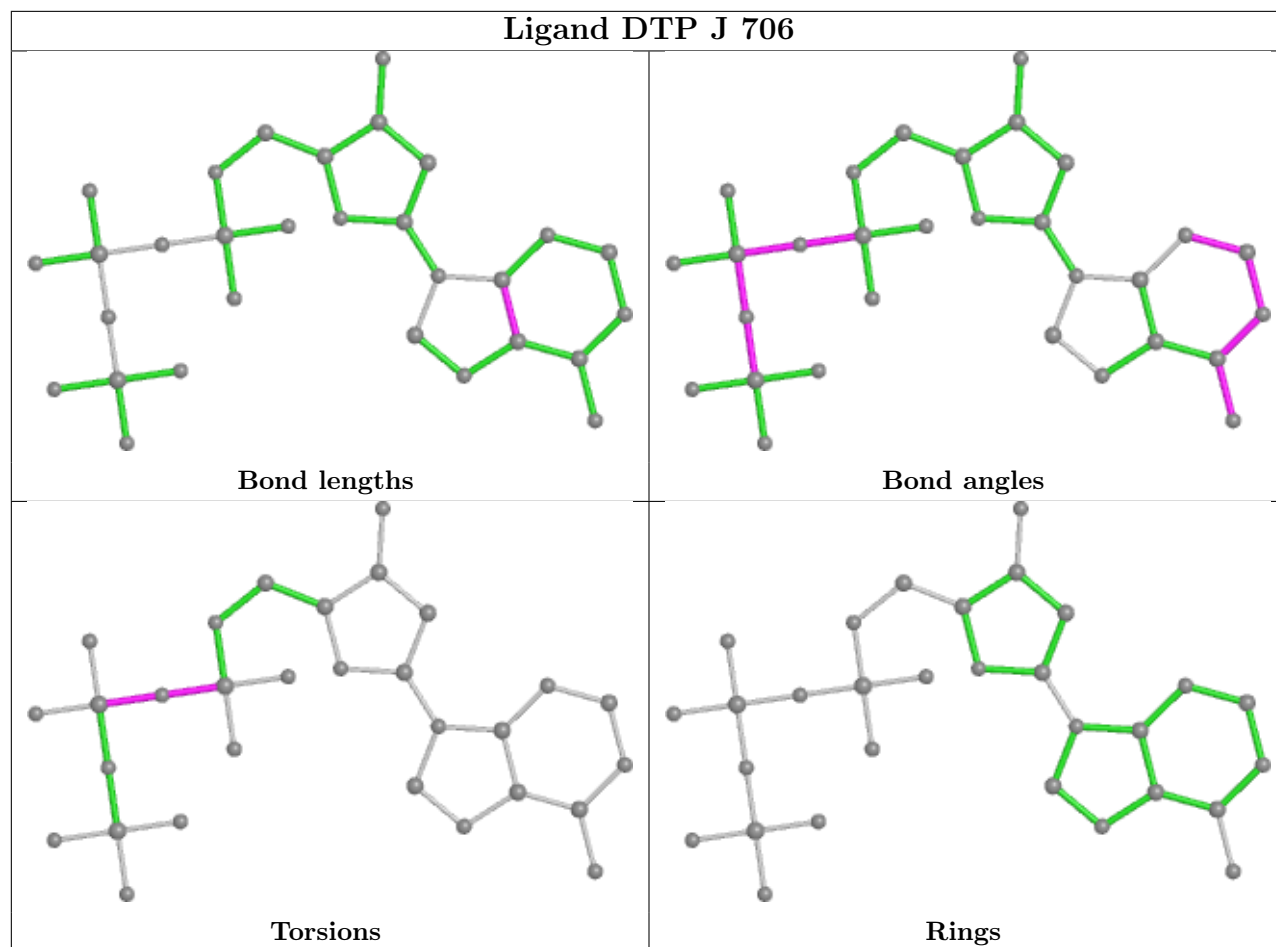


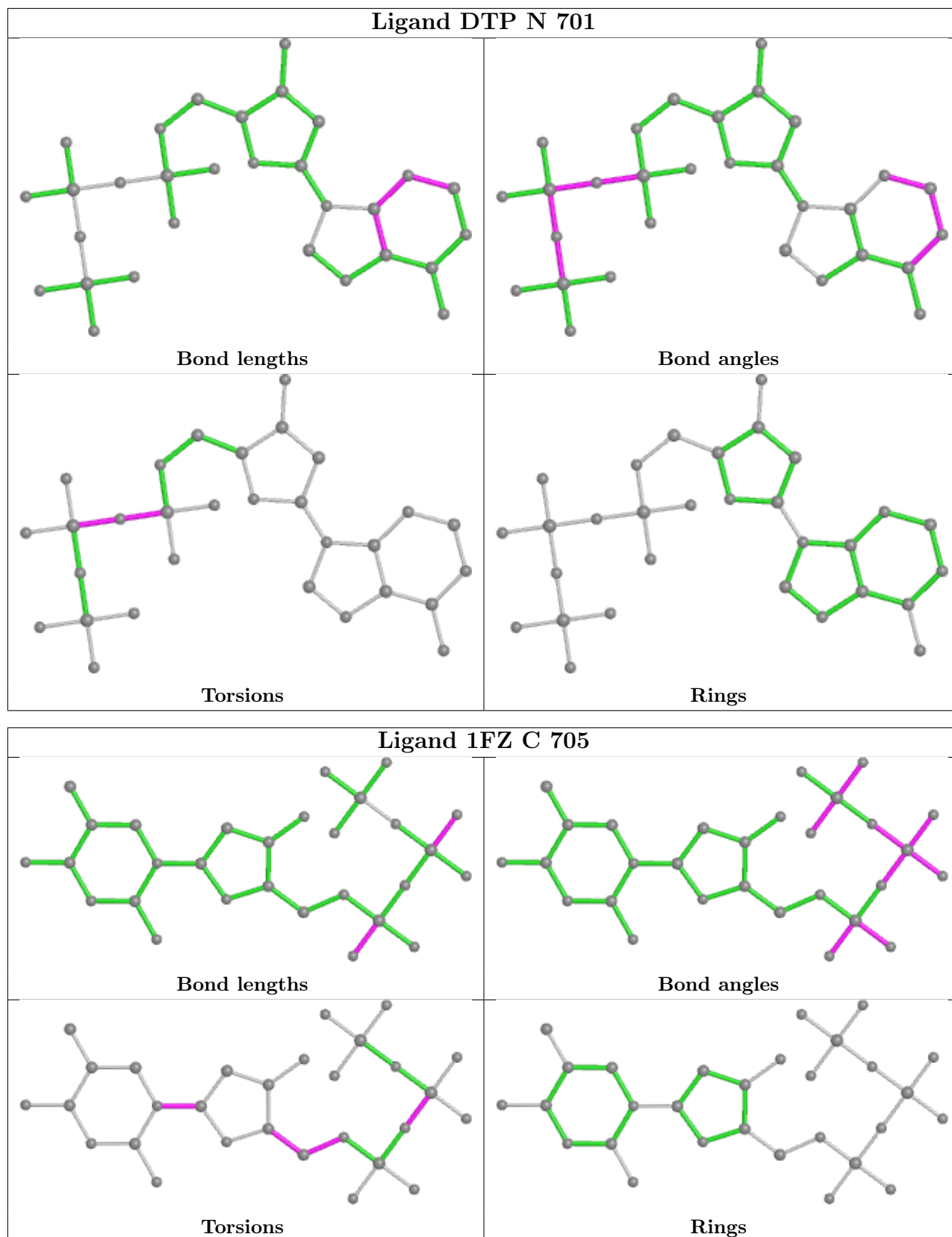


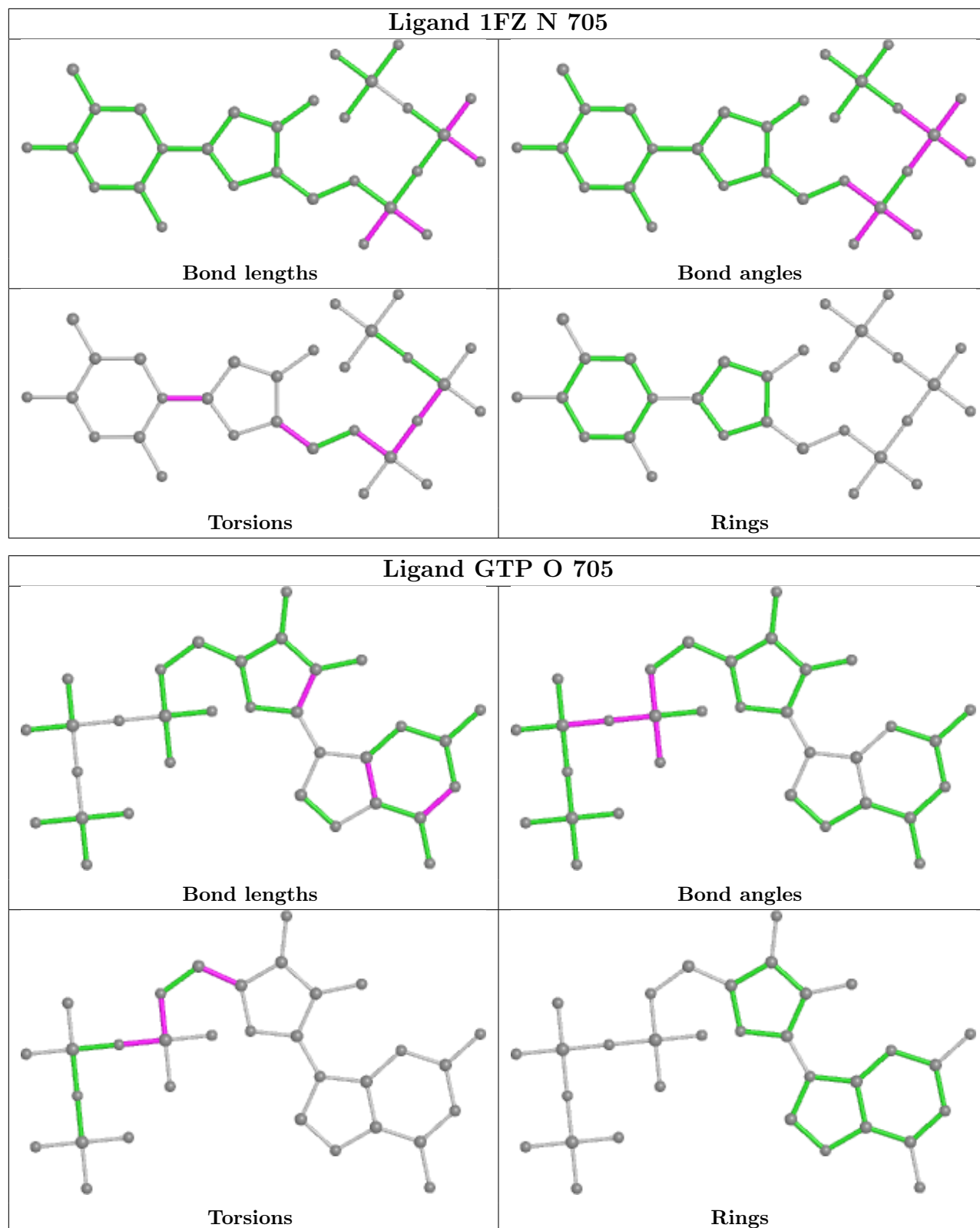


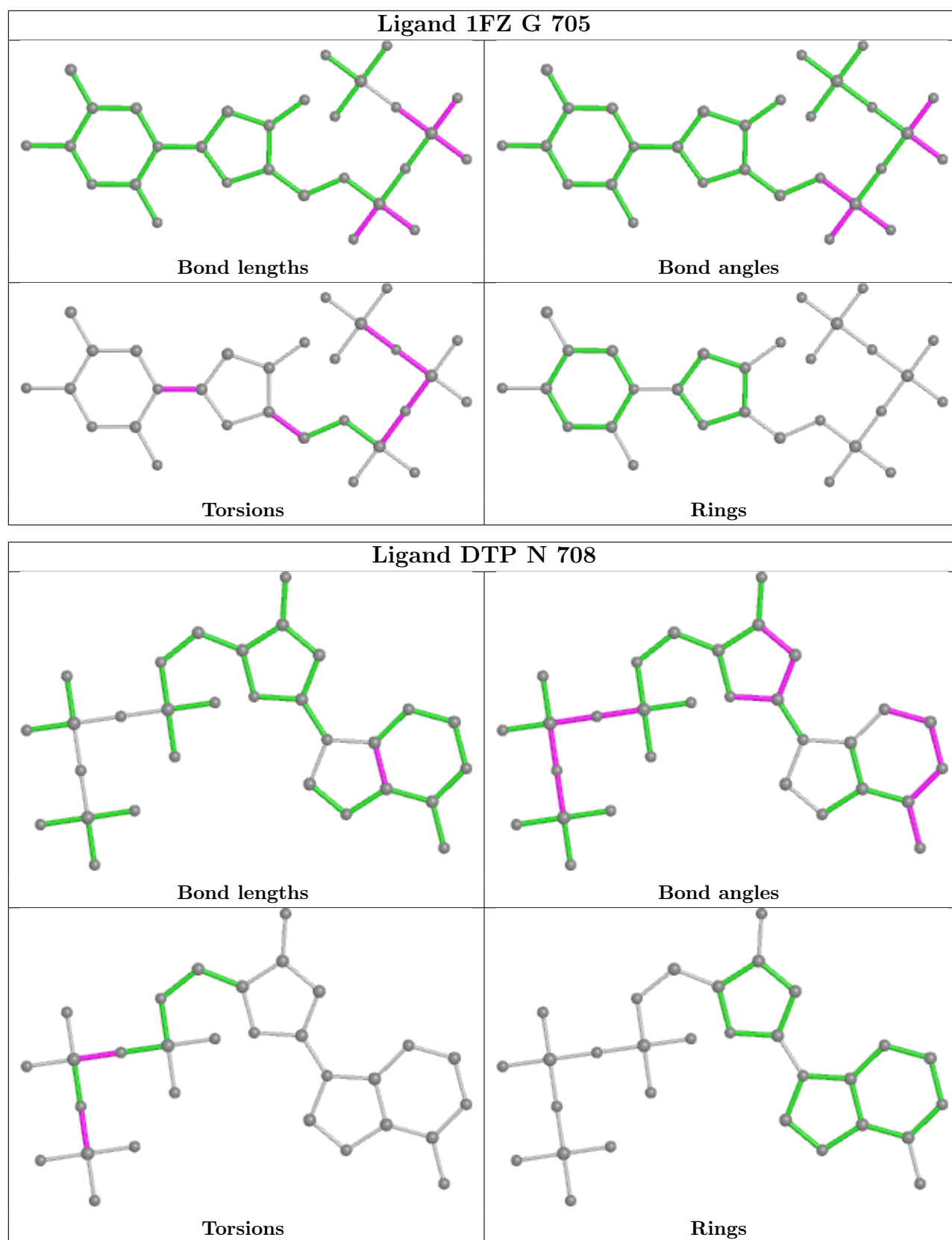


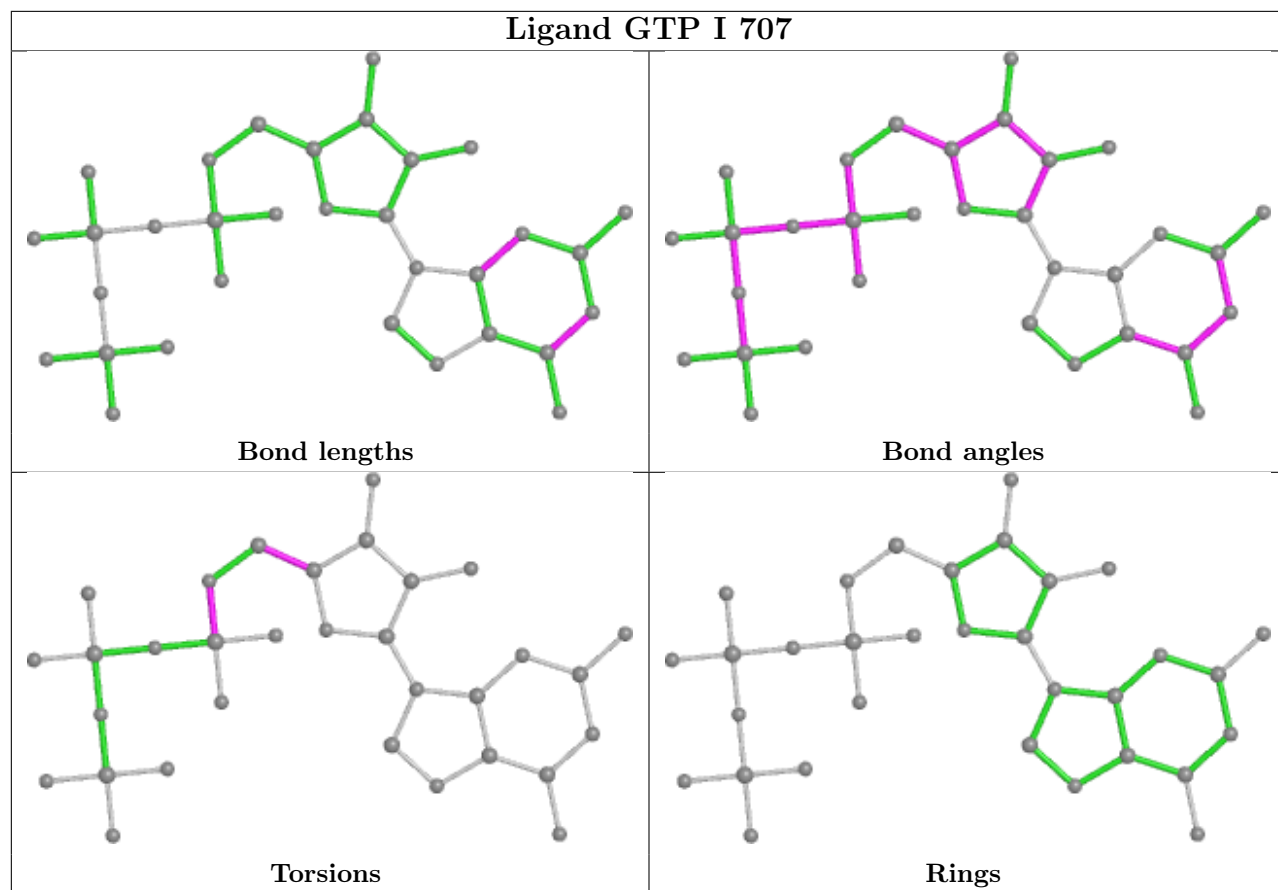


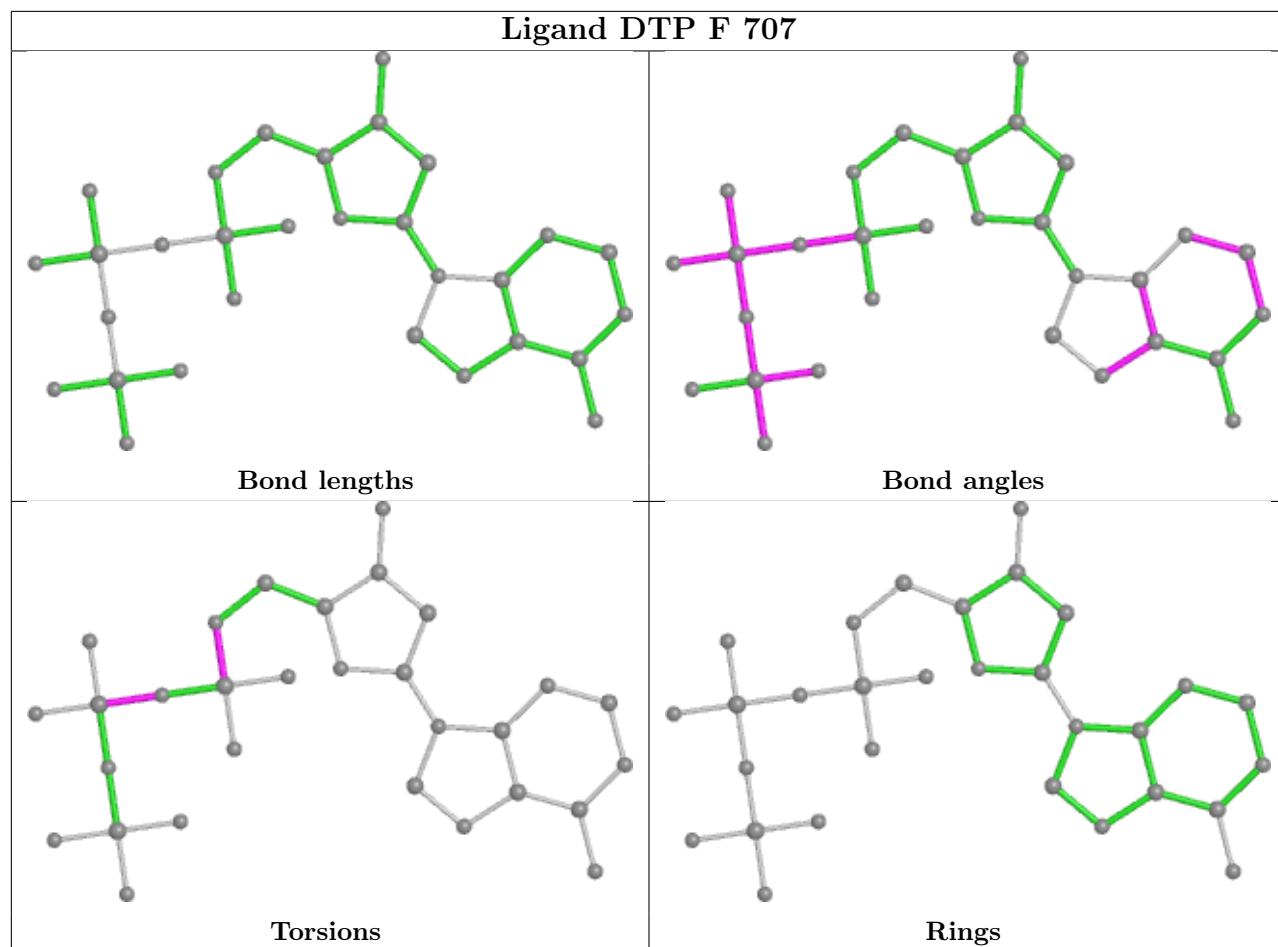


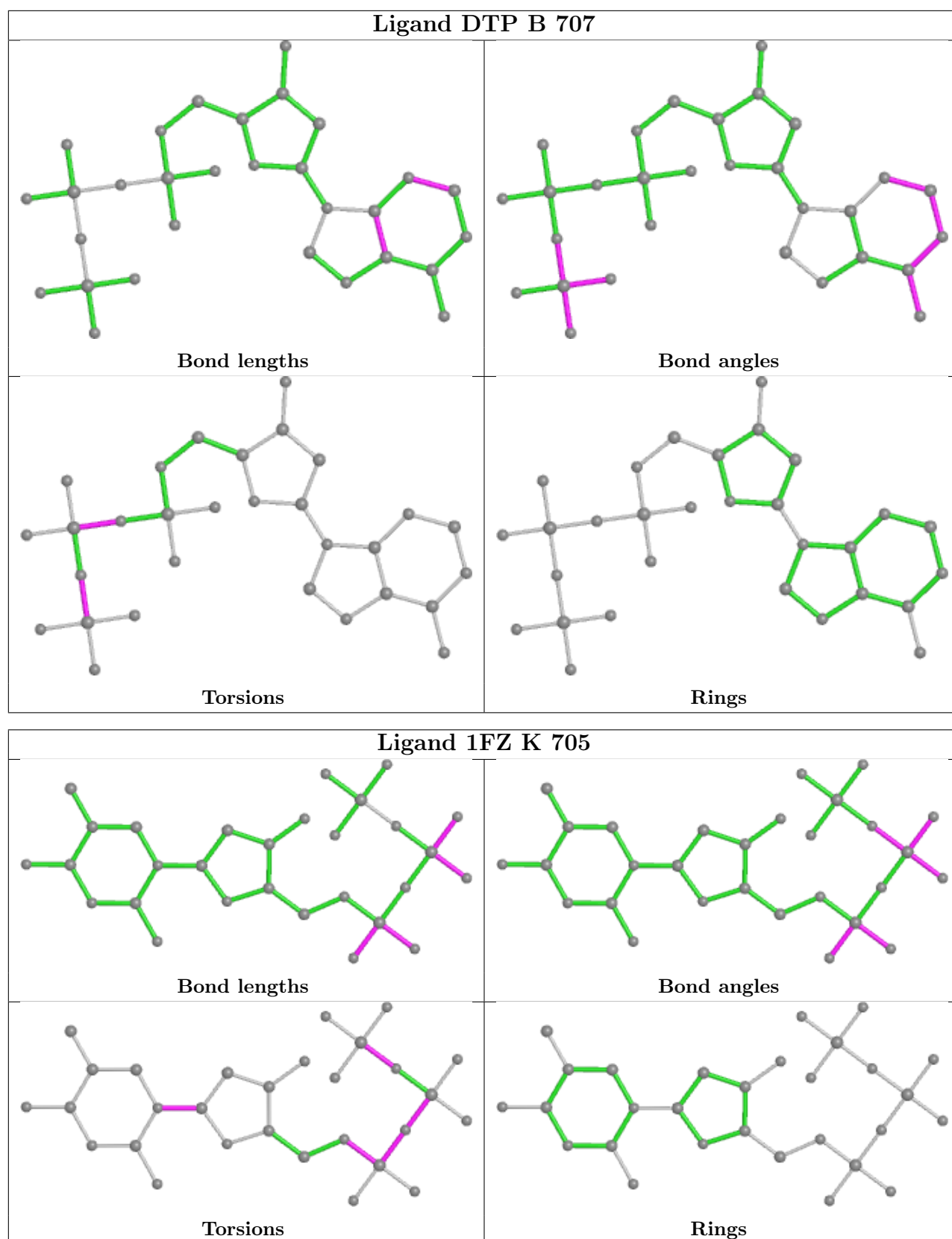


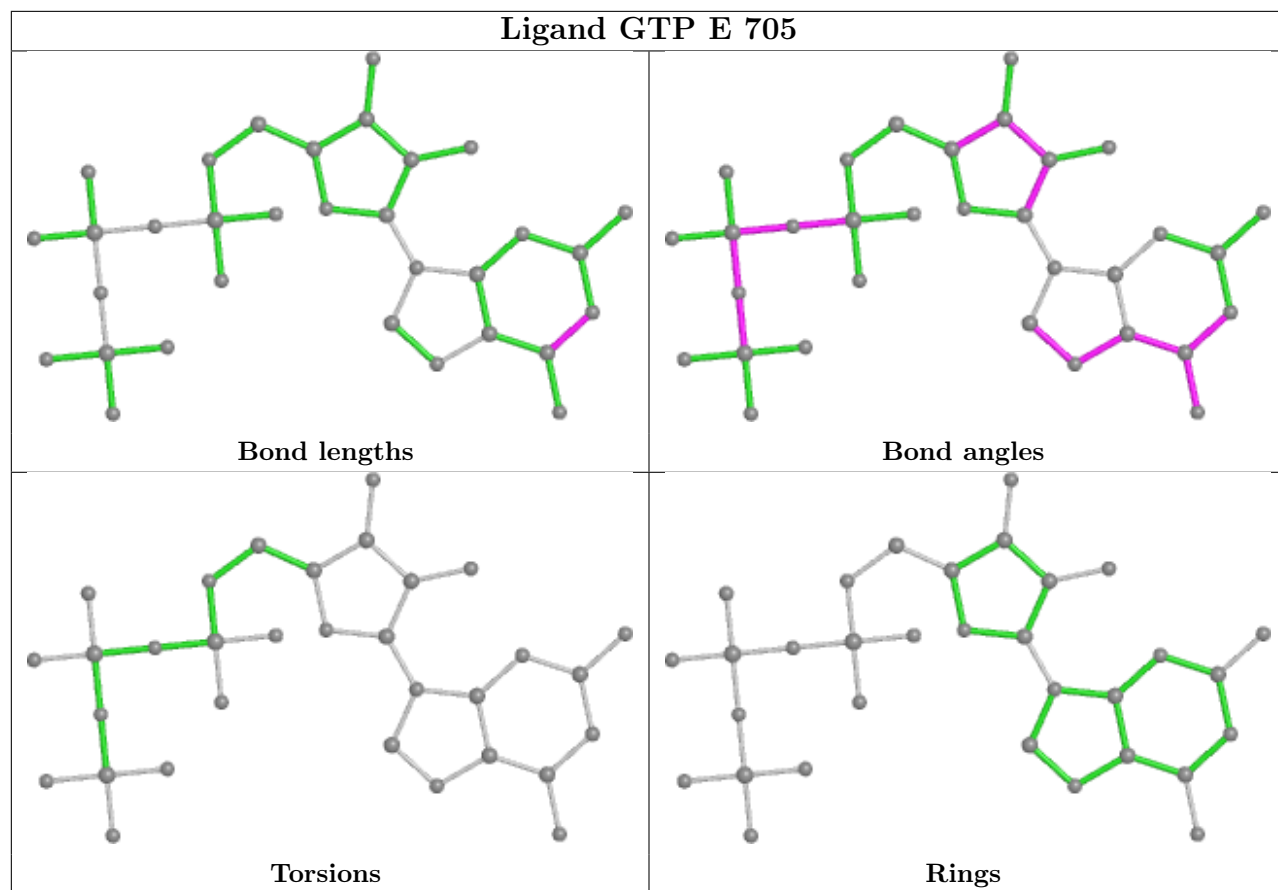


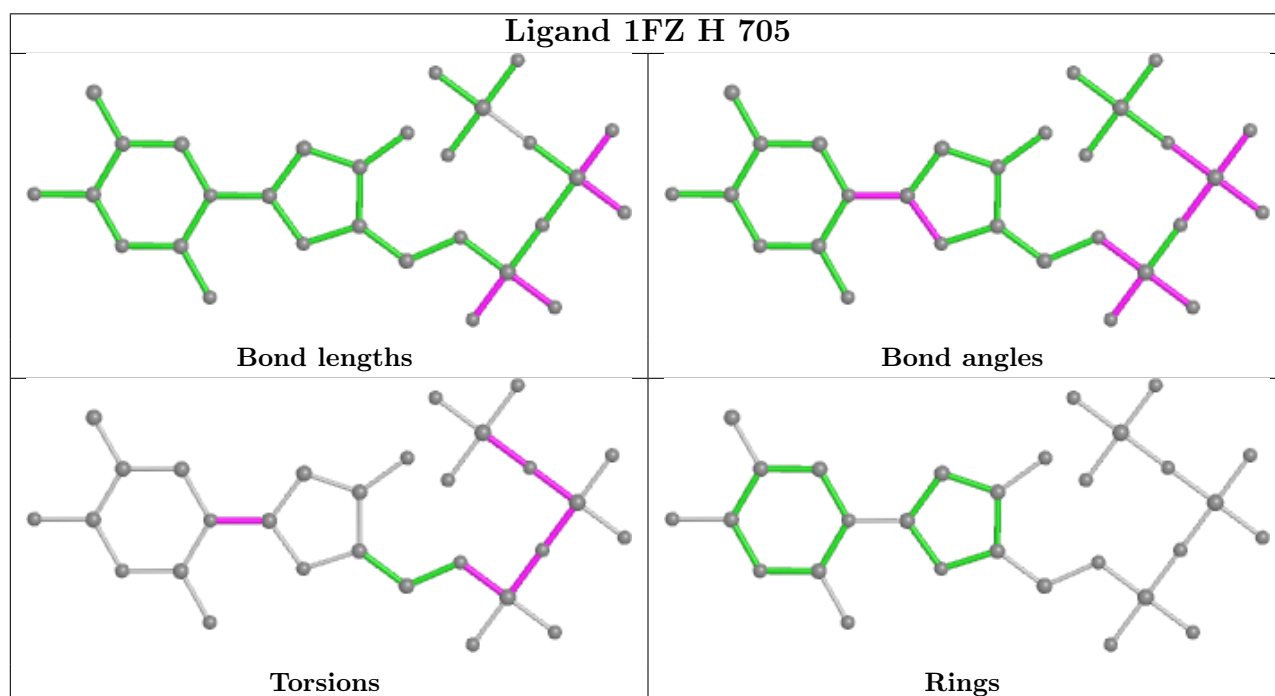
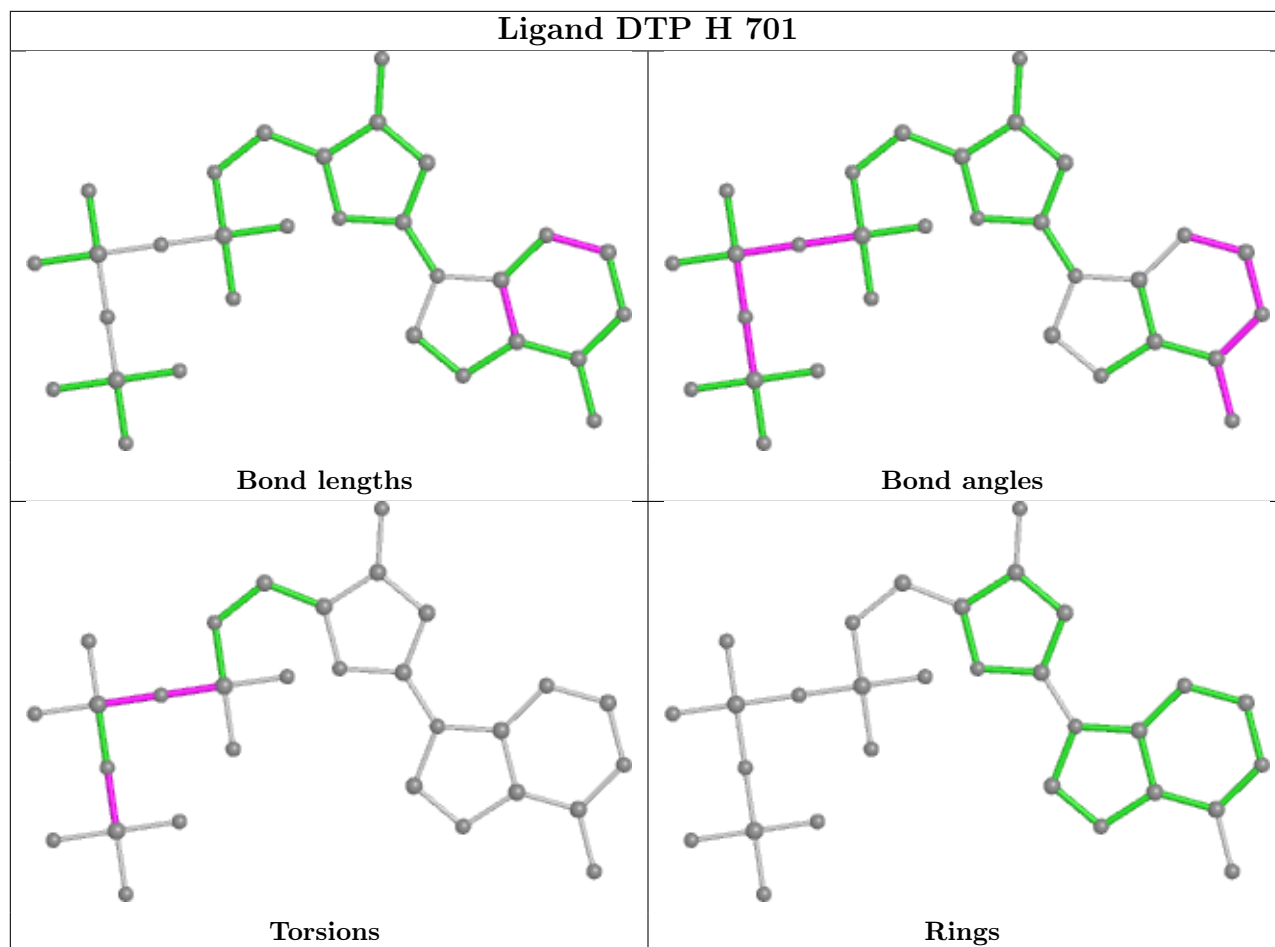


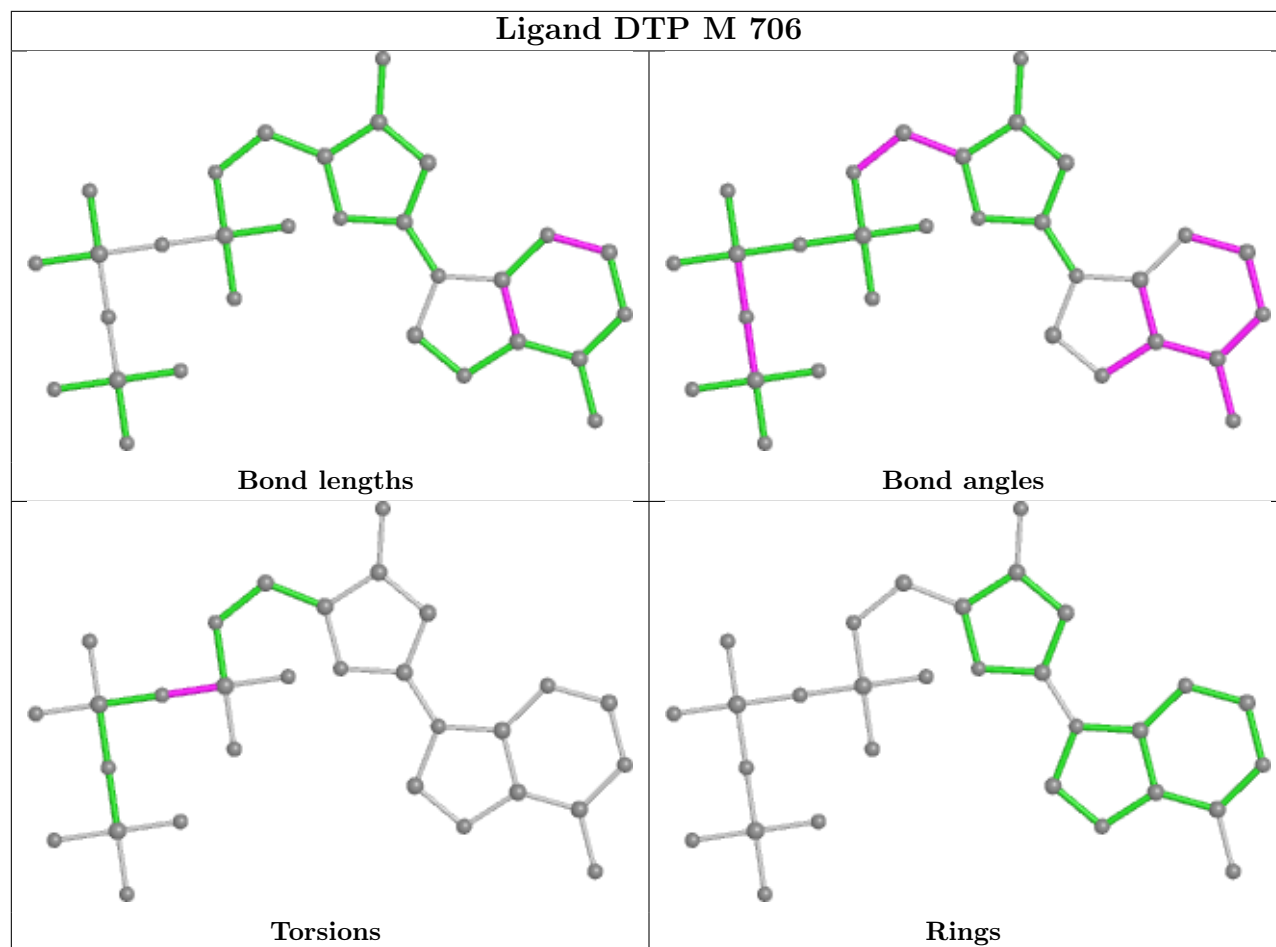


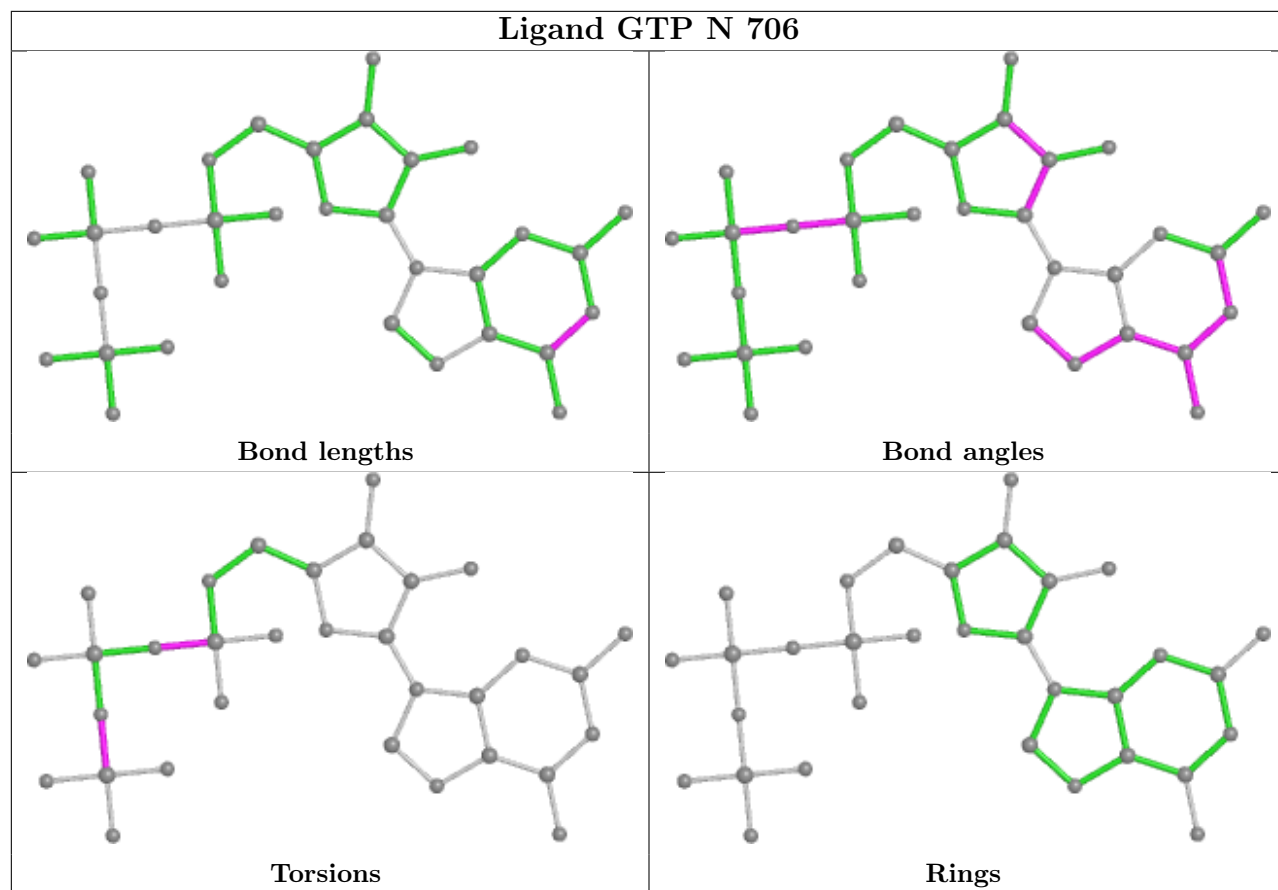


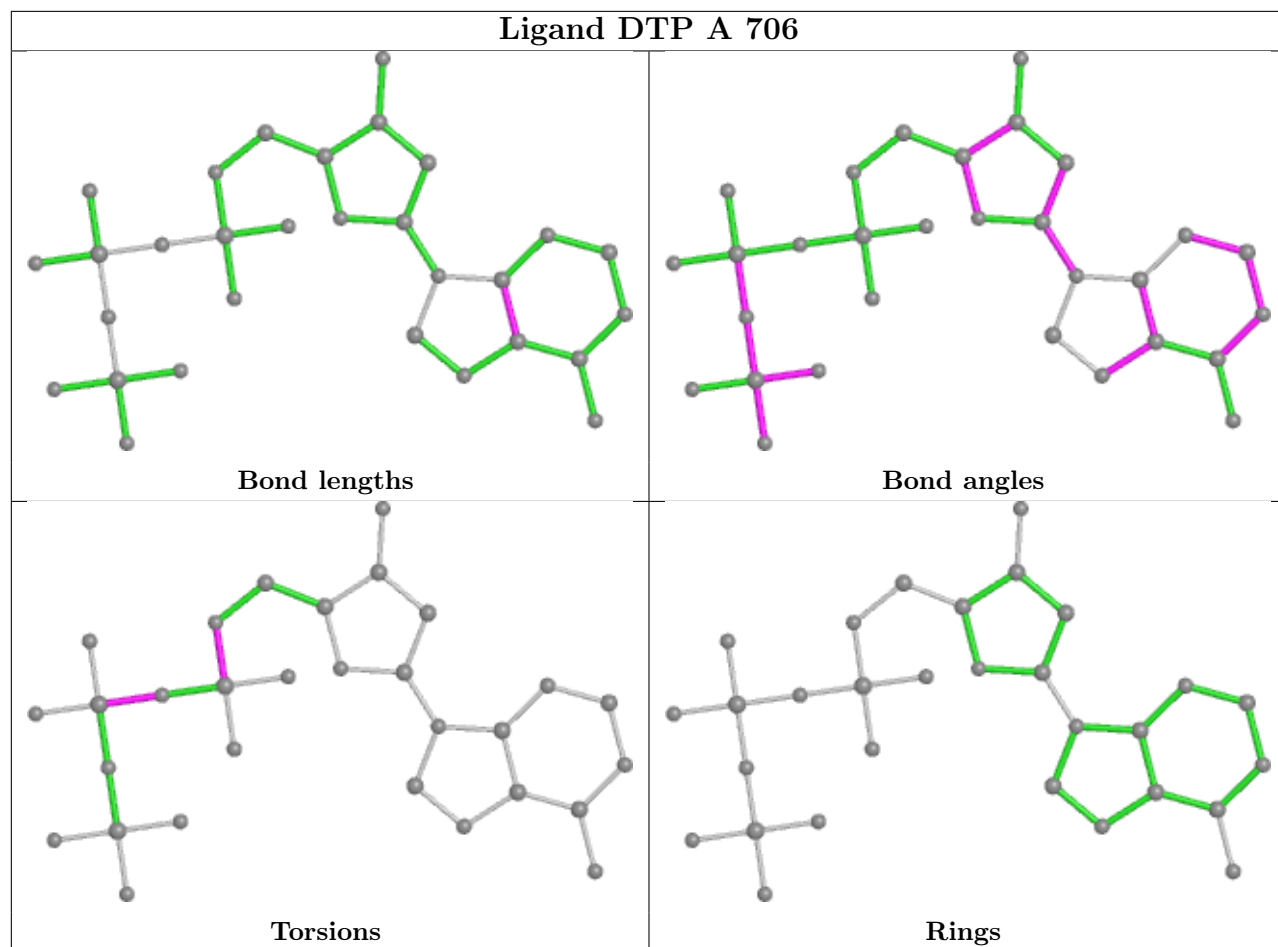


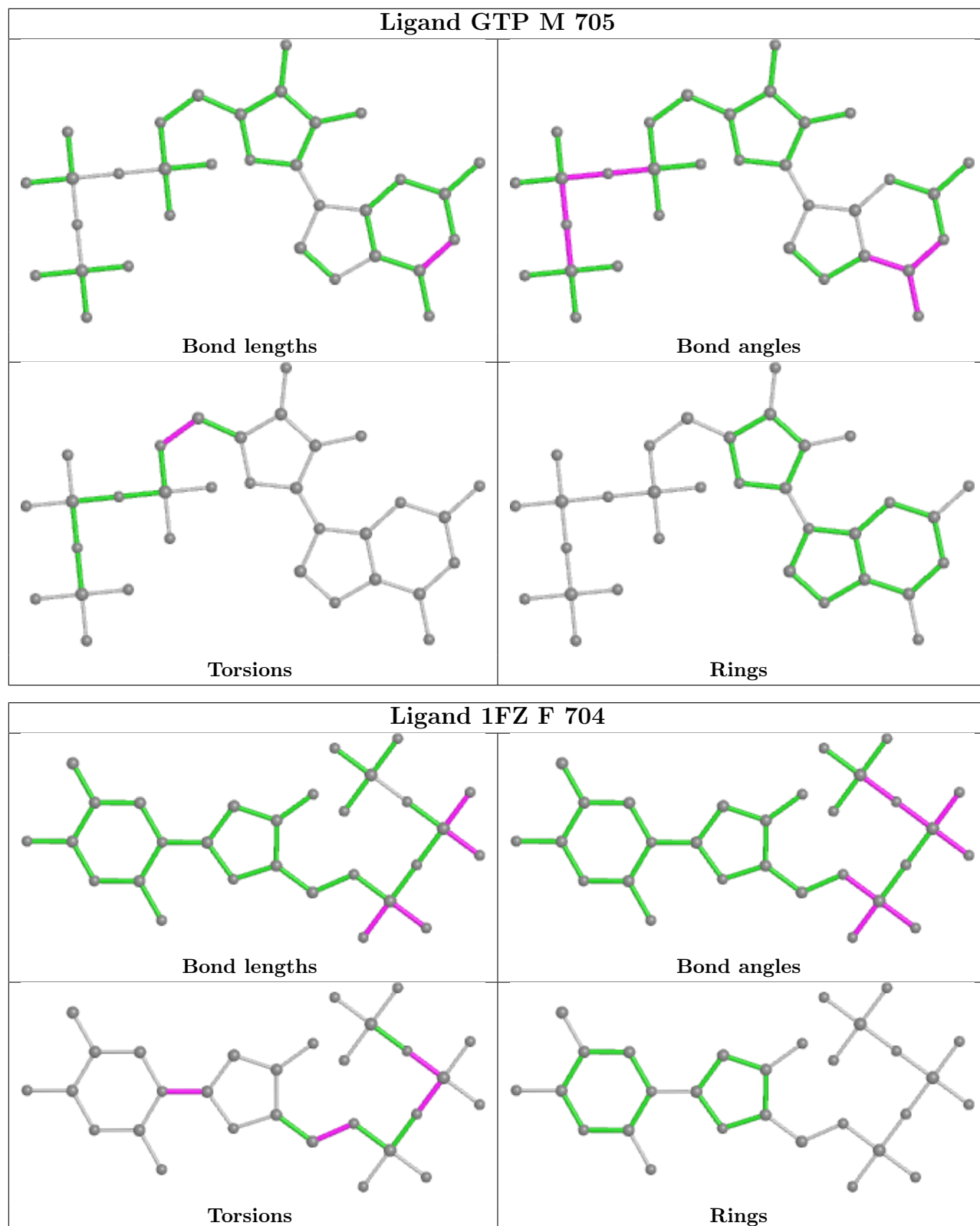


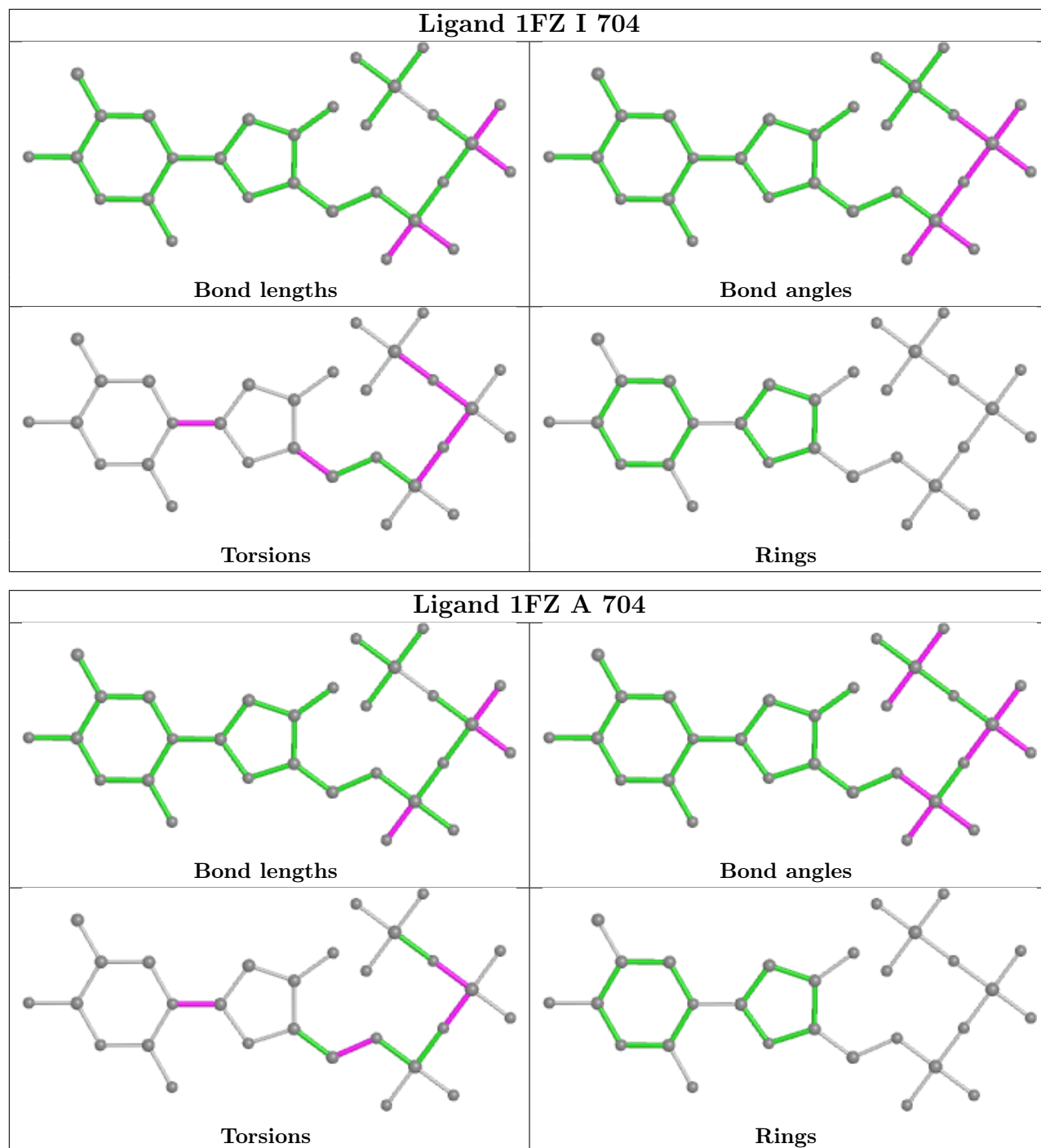


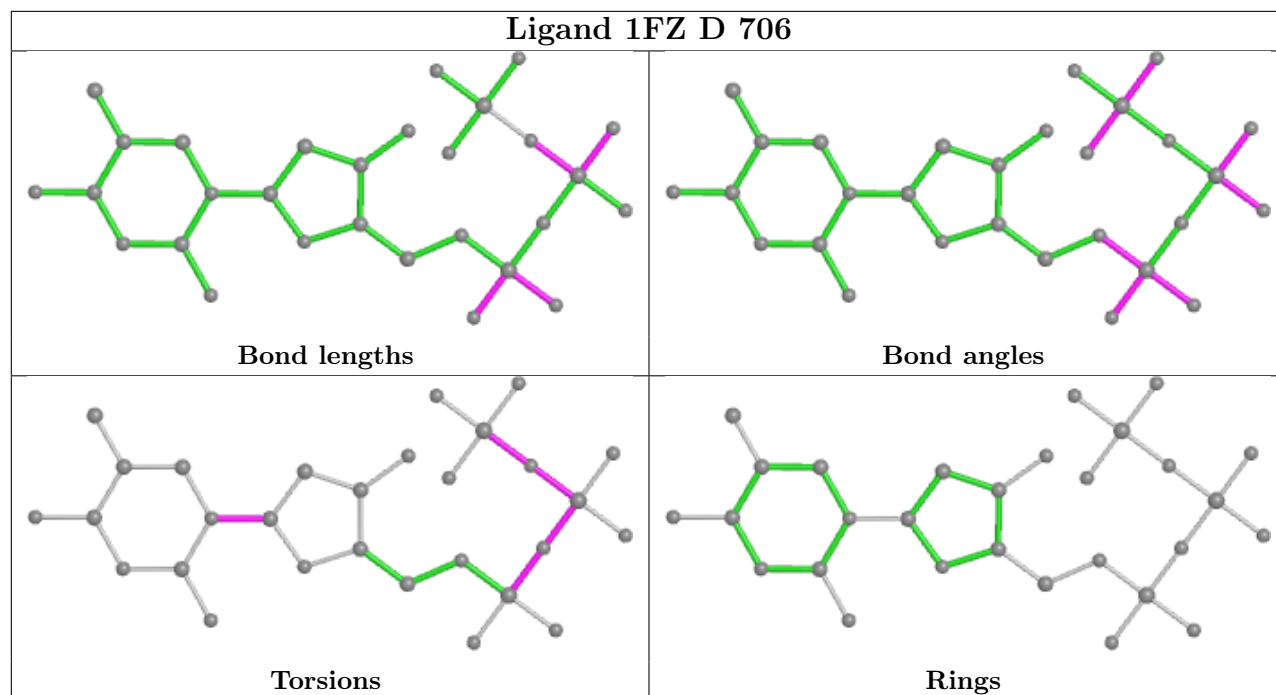












5.7 Other polymers [i](#)

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

6.1 Protein, DNA and RNA chains

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

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

All (75) RSRZ outliers are listed below:

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

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Mol	Chain	Res	Type	RSRZ
1	P	481	ALA	3.2
1	N	235	GLN	3.1
1	M	399	ILE	3.1
1	M	198	CYS	3.0
1	M	480	VAL	3.0
1	M	397	ILE	2.9
1	I	472	ASP	2.8
1	M	501	ASP	2.8
1	P	583	ASP	2.8
1	P	582	GLN	2.7
1	L	487	VAL	2.6
1	O	345	ASN	2.6
1	D	114	THR	2.6
1	O	427	PHE	2.6
1	O	152	GLY	2.6
1	M	345	ASN	2.6
1	O	398	GLU	2.6
1	K	120	ASP	2.5
1	P	309	ASP	2.5
1	N	368	SER	2.5
1	M	582	GLN	2.5
1	O	504	ASN	2.5
1	M	514	PRO	2.4
1	O	147	ILE	2.4
1	A	490	ASP	2.4
1	O	495	ALA	2.4
1	M	347	LEU	2.4
1	J	489	LEU	2.4
1	P	554	CYS	2.3
1	M	287	TYR	2.3
1	P	233	HIS	2.3
1	P	425	ASN	2.3
1	N	424	ASP	2.3
1	L	557	VAL	2.3
1	B	594	GLN	2.3
1	M	424	ASP	2.3
1	L	558	ASP	2.3
1	M	431	LEU	2.3
1	M	403	GLY	2.3
1	I	597	GLU	2.3
1	N	403	GLY	2.3
1	M	554	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	O	438	LEU	2.2
1	P	445	LEU	2.2
1	P	498	PHE	2.2
1	O	575	ASP	2.2
1	O	279	PRO	2.2
1	P	380	ASN	2.2
1	G	567	GLN	2.2
1	M	409	ILE	2.2
1	P	441	ALA	2.2
1	E	577	ASN	2.2
1	N	299	GLU	2.2
1	O	211	GLY	2.2
1	M	440	ASP	2.2
1	M	288	LYS	2.2
1	M	225	ALA	2.1
1	M	505	MET	2.1
1	P	593	PRO	2.1
1	O	587	ILE	2.1
1	O	584	GLY	2.1
1	P	432	TYR	2.1
1	M	191	ILE	2.1
1	O	578	PHE	2.0
1	O	573	CYS	2.0
1	B	570	VAL	2.0
1	O	212	PRO	2.0
1	I	306	ASN	2.0
1	P	438	LEU	2.0
1	N	306	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
7	SO4	I	706	5/5	0.77	0.23	125,126,129,131	0
7	SO4	N	707	5/5	0.81	0.30	128,128,132,134	0
7	SO4	O	706	5/5	0.84	0.22	117,121,125,126	0
3	MG	E	702	1/1	0.86	0.16	16,16,16,16	0
7	SO4	C	706	5/5	0.90	0.19	105,105,109,110	0
7	SO4	B	706	5/5	0.90	0.16	93,96,97,99	0
7	SO4	F	706	5/5	0.91	0.18	103,104,105,106	0
3	MG	O	702	1/1	0.92	0.14	19,19,19,19	0
7	SO4	K	707	5/5	0.93	0.16	89,90,91,92	0
5	GTP	N	706	32/32	0.94	0.19	66,68,76,79	0
4	1FZ	L	705	29/29	0.94	0.20	60,75,85,87	0
4	1FZ	M	704	29/29	0.95	0.21	66,74,83,90	0
4	1FZ	P	704	29/29	0.95	0.19	79,85,90,91	0
7	SO4	H	707	5/5	0.95	0.16	78,79,80,81	0
3	MG	H	704	1/1	0.95	0.09	44,44,44,44	0
7	SO4	J	705	5/5	0.95	0.14	102,103,104,105	0
5	GTP	O	705	32/32	0.95	0.17	72,76,80,81	0
6	DTP	M	707	30/30	0.95	0.18	72,74,82,83	0
3	MG	N	703	1/1	0.95	0.13	29,29,29,29	0
3	MG	M	702	1/1	0.96	0.09	20,20,20,20	0
6	DTP	N	708	30/30	0.96	0.18	54,57,80,81	0
3	MG	H	703	1/1	0.96	0.14	15,15,15,15	0
4	1FZ	N	705	29/29	0.96	0.17	54,60,66,67	0
7	SO4	D	708	5/5	0.96	0.12	77,77,79,81	0
4	1FZ	O	704	29/29	0.96	0.18	54,62,65,65	0
3	MG	G	704	1/1	0.96	0.08	18,18,18,18	0
5	GTP	E	705	32/32	0.96	0.16	46,49,54,55	0
5	GTP	K	706	32/32	0.96	0.18	55,58,65,66	0
4	1FZ	G	705	29/29	0.96	0.17	37,40,53,56	0
4	1FZ	K	705	29/29	0.96	0.18	45,47,49,49	0
6	DTP	M	706	30/30	0.96	0.17	65,71,76,77	0
5	GTP	F	705	32/32	0.97	0.16	46,47,50,52	0
5	GTP	H	706	32/32	0.97	0.18	39,42,46,47	0
5	GTP	I	705	32/32	0.97	0.16	46,48,52,52	0
5	GTP	I	707	32/32	0.97	0.15	37,42,48,49	0
4	1FZ	B	704	29/29	0.97	0.17	41,47,54,59	0
5	GTP	L	706	32/32	0.97	0.15	35,38,41,42	0
5	GTP	M	705	32/32	0.97	0.14	51,56,65,67	0
4	1FZ	D	706	29/29	0.97	0.17	27,31,40,41	0
4	1FZ	E	704	29/29	0.97	0.18	37,45,63,69	0
5	GTP	P	705	32/32	0.97	0.17	62,68,72,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	DTP	F	707	30/30	0.97	0.16	48,50,53,54	0
6	DTP	G	701	30/30	0.97	0.17	49,52,56,57	0
6	DTP	H	701	30/30	0.97	0.17	49,51,54,54	0
6	DTP	L	701	30/30	0.97	0.17	39,45,49,50	0
4	1FZ	F	704	29/29	0.97	0.16	44,50,65,67	0
3	MG	D	704	1/1	0.97	0.18	15,15,15,15	0
4	1FZ	H	705	29/29	0.97	0.18	32,39,48,53	0
4	1FZ	I	704	29/29	0.97	0.17	39,45,62,62	0
3	MG	I	702	1/1	0.97	0.18	17,17,17,17	0
3	MG	B	703	1/1	0.97	0.08	16,16,16,16	0
7	SO4	E	706	5/5	0.97	0.12	68,68,69,70	0
3	MG	C	703	1/1	0.97	0.15	16,16,16,16	0
3	MG	C	704	1/1	0.97	0.12	16,16,16,16	0
3	MG	O	703	1/1	0.97	0.15	61,61,61,61	0
3	MG	P	702	1/1	0.97	0.08	19,19,19,19	0
5	GTP	B	705	32/32	0.97	0.16	31,33,35,36	0
5	GTP	D	707	32/32	0.97	0.16	40,44,48,48	0
4	1FZ	A	704	29/29	0.97	0.15	31,35,39,41	0
6	DTP	B	707	30/30	0.98	0.16	29,31,34,35	0
6	DTP	D	701	30/30	0.98	0.15	26,27,32,33	0
6	DTP	E	707	30/30	0.98	0.17	32,33,35,35	0
3	MG	K	703	1/1	0.98	0.10	17,17,17,17	0
5	GTP	A	705	32/32	0.98	0.15	35,38,40,41	0
4	1FZ	C	705	29/29	0.98	0.16	34,37,44,46	0
6	DTP	I	708	30/30	0.98	0.17	36,41,50,50	0
6	DTP	J	706	30/30	0.98	0.17	25,26,30,31	0
6	DTP	K	701	30/30	0.98	0.15	41,42,50,51	0
5	GTP	D	702	32/32	0.98	0.16	27,31,33,34	0
3	MG	K	704	1/1	0.98	0.13	54,54,54,54	0
3	MG	L	703	1/1	0.98	0.16	17,17,17,17	0
6	DTP	N	701	30/30	0.98	0.17	53,56,60,61	0
3	MG	B	702	1/1	0.98	0.16	16,16,16,16	0
5	GTP	G	706	32/32	0.98	0.15	33,38,52,54	0
3	MG	M	703	1/1	0.98	0.09	50,50,50,50	0
3	MG	A	702	1/1	0.98	0.11	15,15,15,15	0
3	MG	N	704	1/1	0.98	0.06	73,73,73,73	0
4	1FZ	J	704	29/29	0.98	0.15	34,37,41,41	0
3	MG	A	703	1/1	0.98	0.07	22,22,22,22	0
3	MG	G	703	1/1	0.98	0.12	16,16,16,16	0
3	MG	J	702	1/1	0.98	0.18	15,15,15,15	0
3	MG	P	703	1/1	0.98	0.05	30,30,30,30	0
3	MG	J	703	1/1	0.98	0.08	30,30,30,30	0

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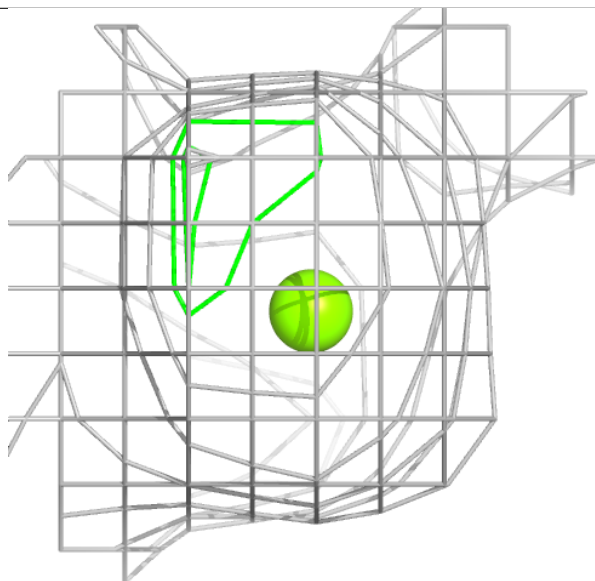
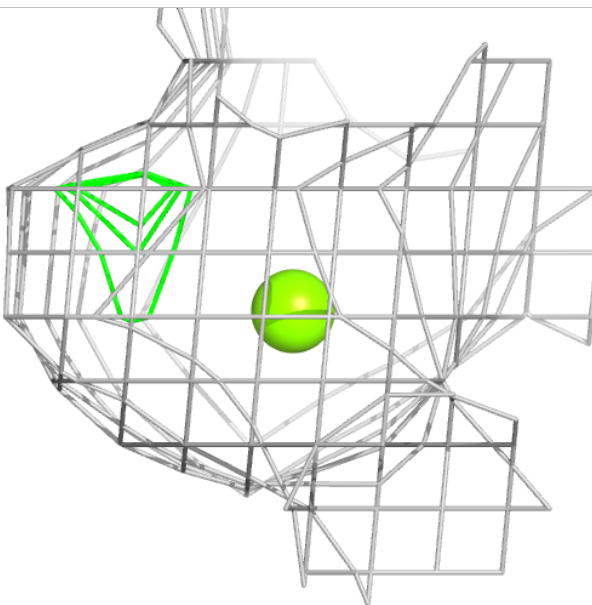
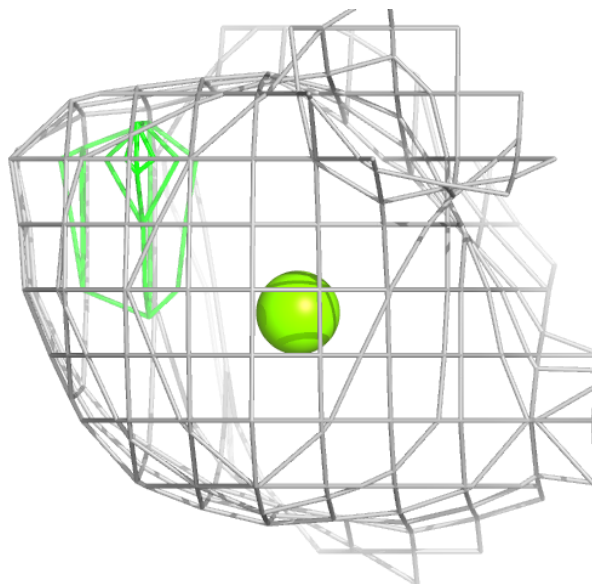
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	DTP	A	706	30/30	0.98	0.16	30,32,38,39	0
2	FE	O	701	1/1	0.99	0.09	45,45,45,45	0
3	MG	D	705	1/1	0.99	0.08	24,24,24,24	0
2	FE	P	701	1/1	0.99	0.11	44,44,44,44	0
3	MG	E	703	1/1	0.99	0.08	24,24,24,24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

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

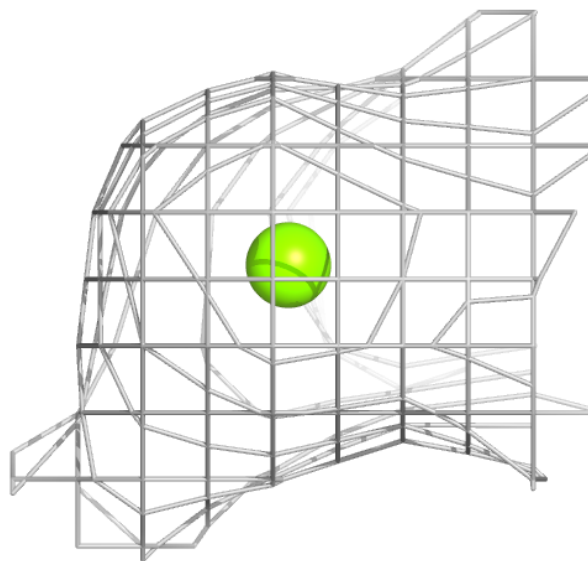
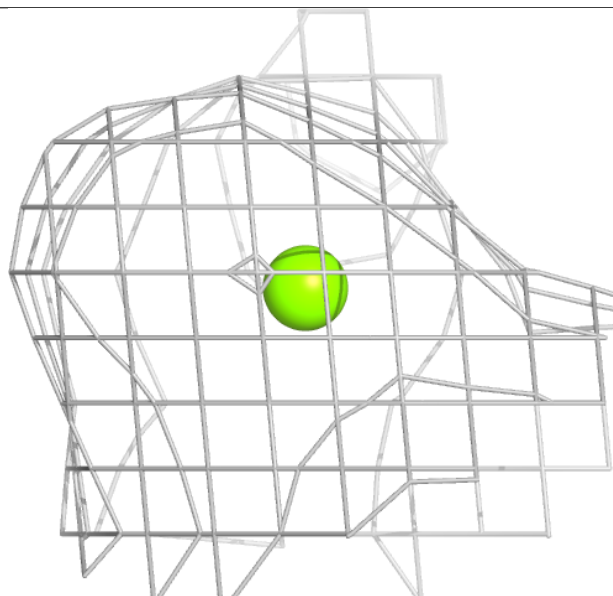
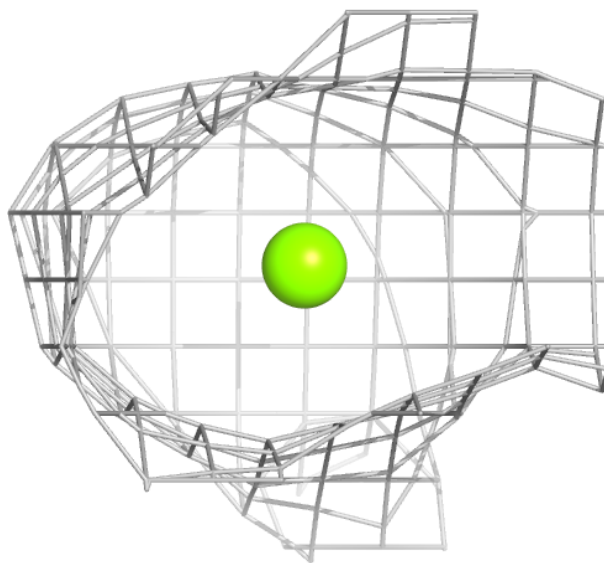
Electron density around MG E 702:

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



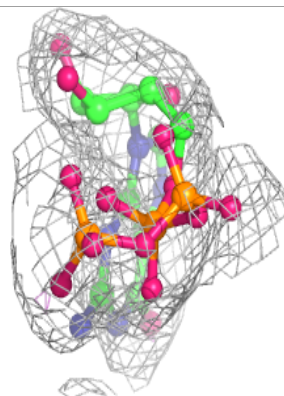
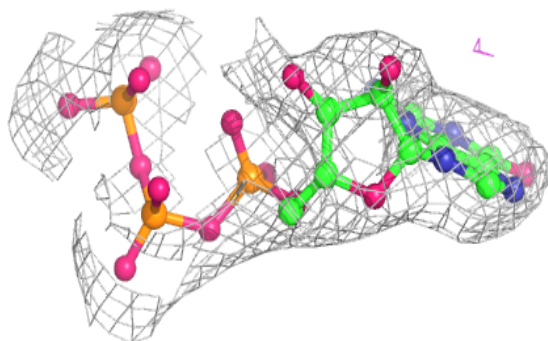
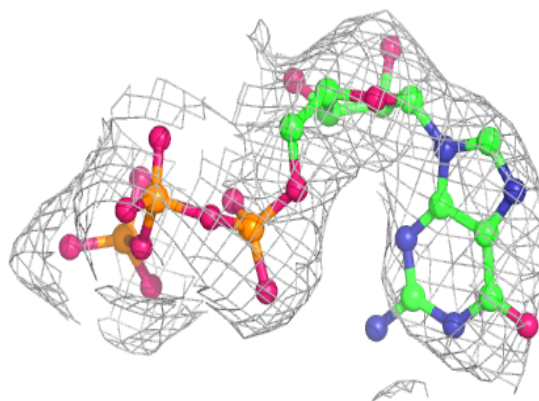
Electron density around MG O 702:

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

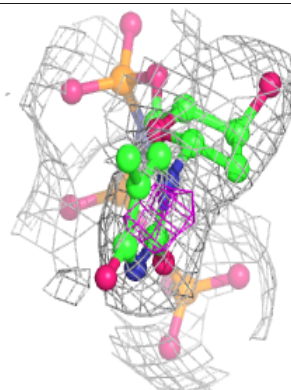
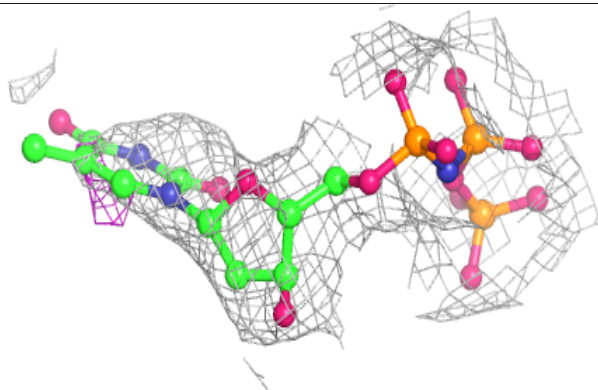
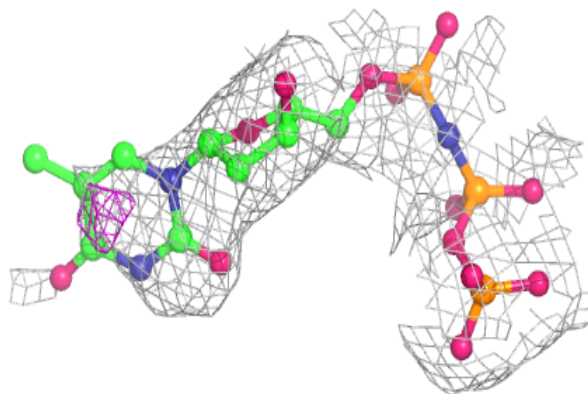


Electron density around GTP N 706:

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

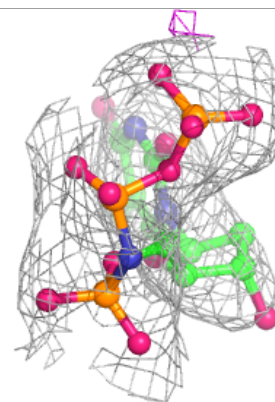
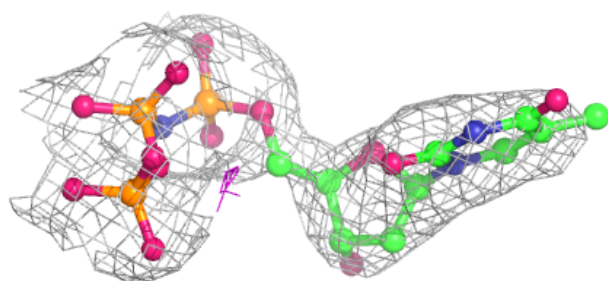
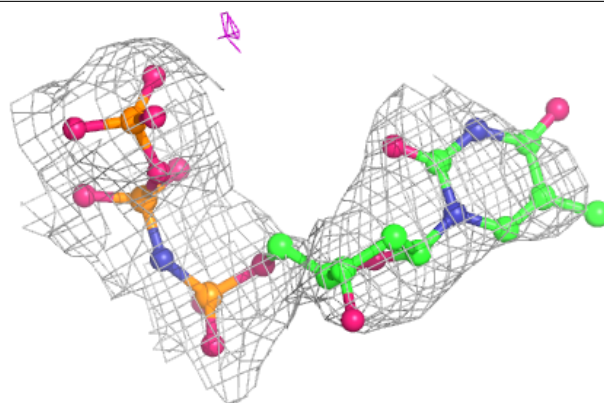
**Electron density around 1FZ L 705:**

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

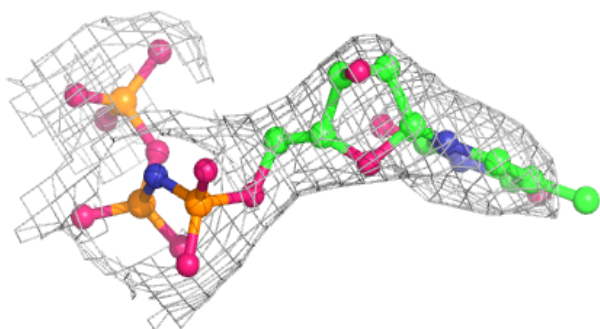
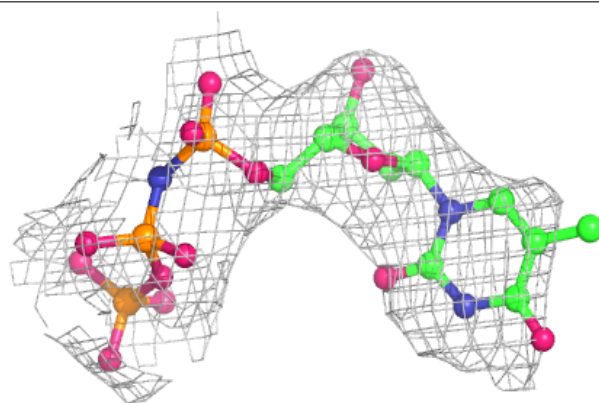


Electron density around 1FZ M 704:

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

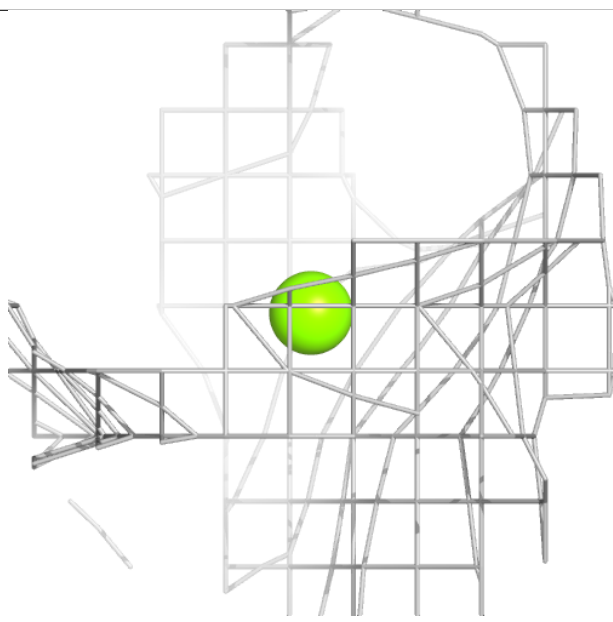
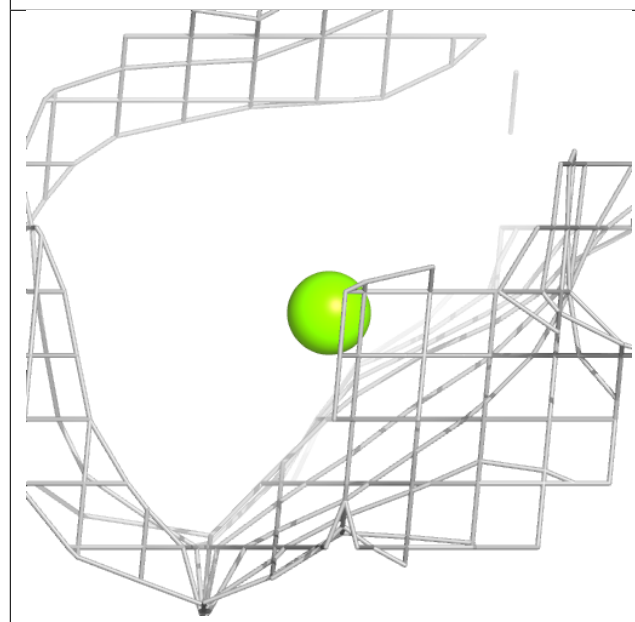
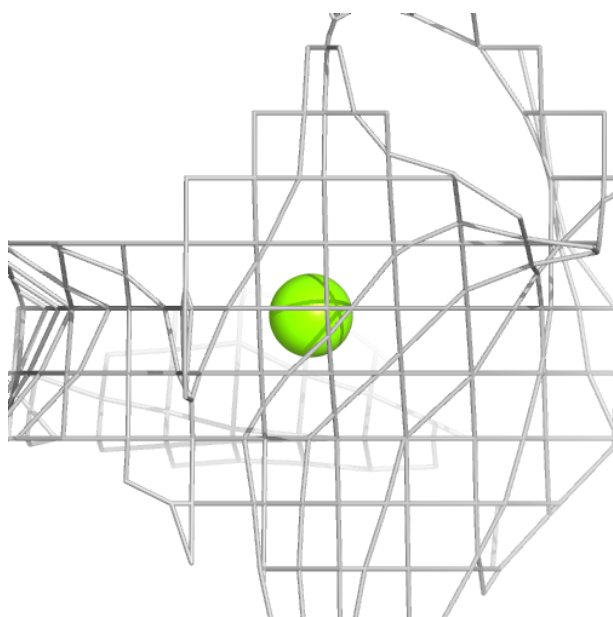
**Electron density around 1FZ P 704:**

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



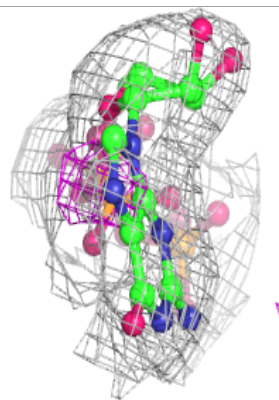
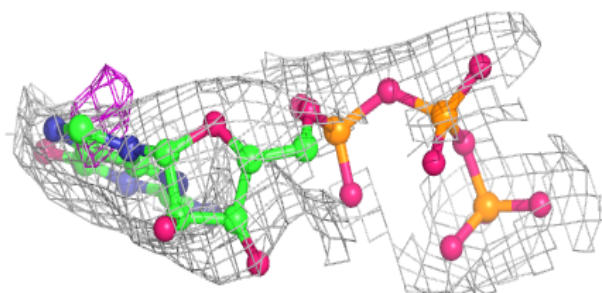
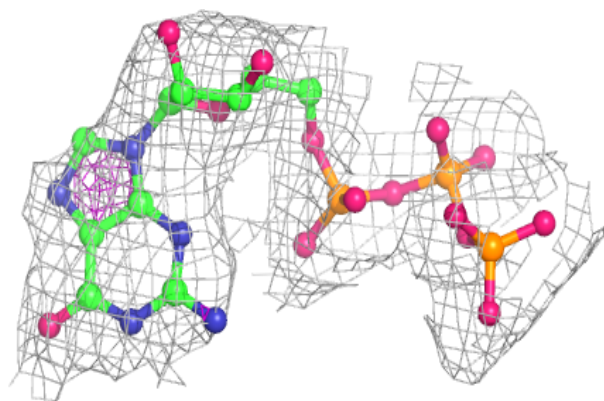
Electron density around MG H 704:

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

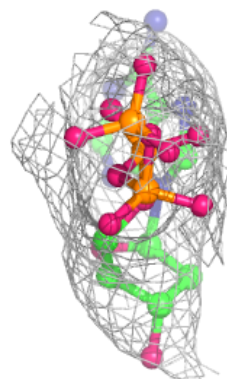
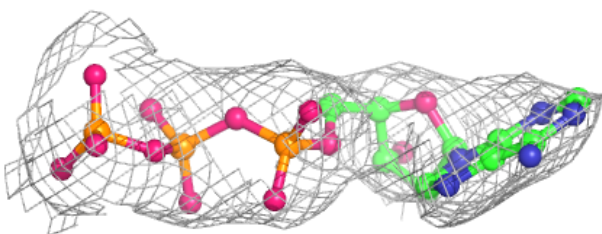
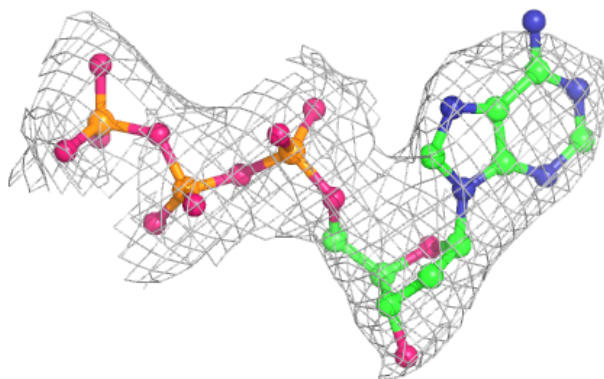


Electron density around GTP O 705:

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

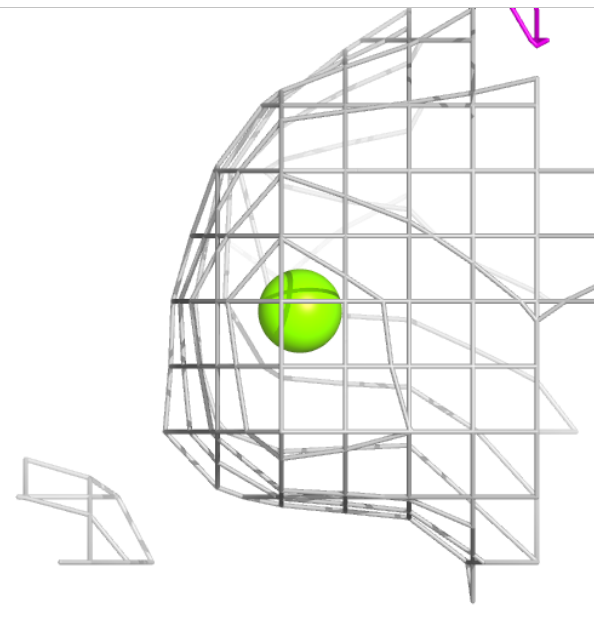
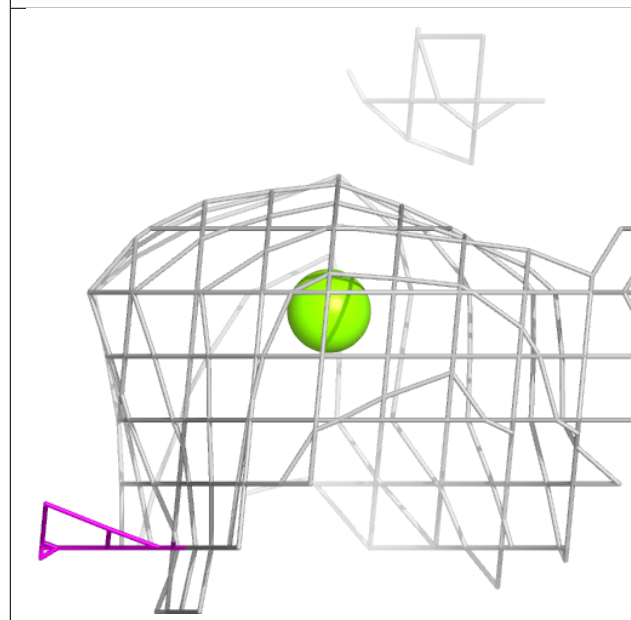
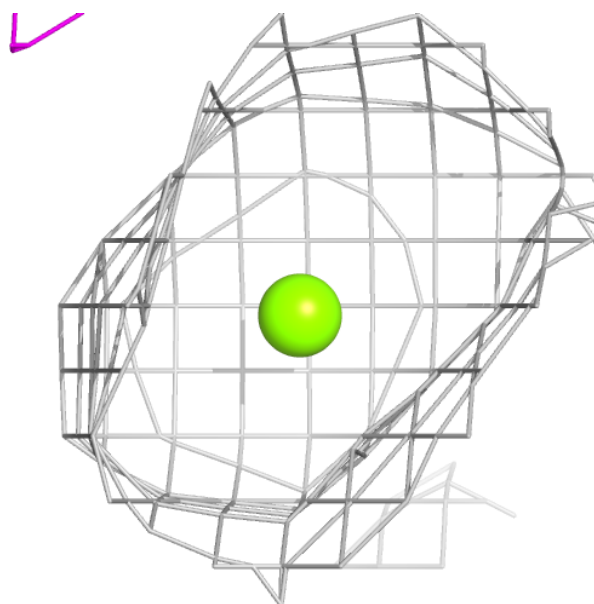
**Electron density around DTP M 707:**

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



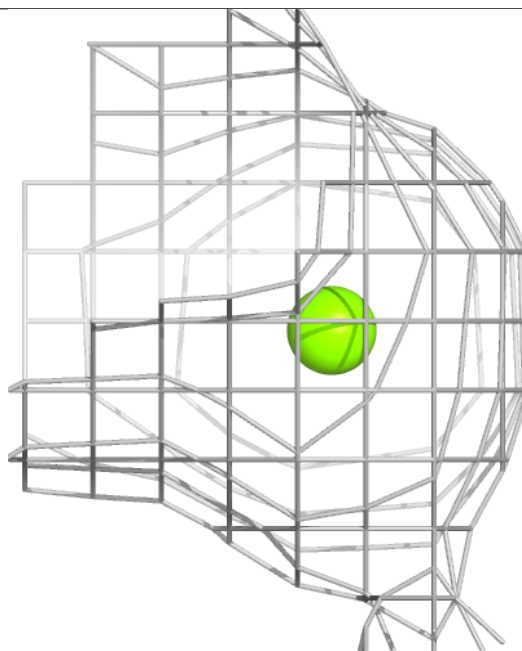
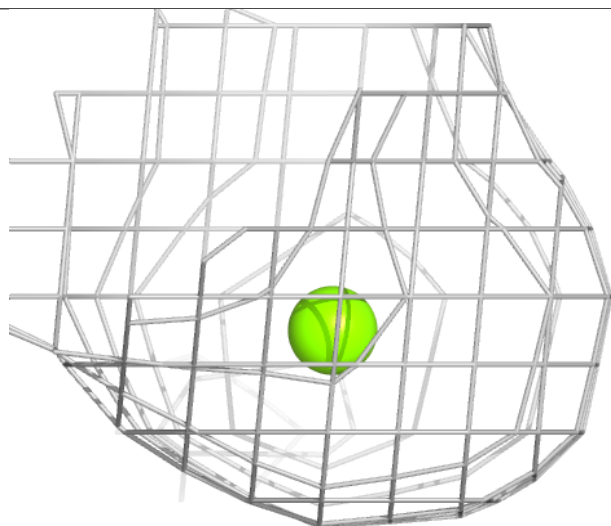
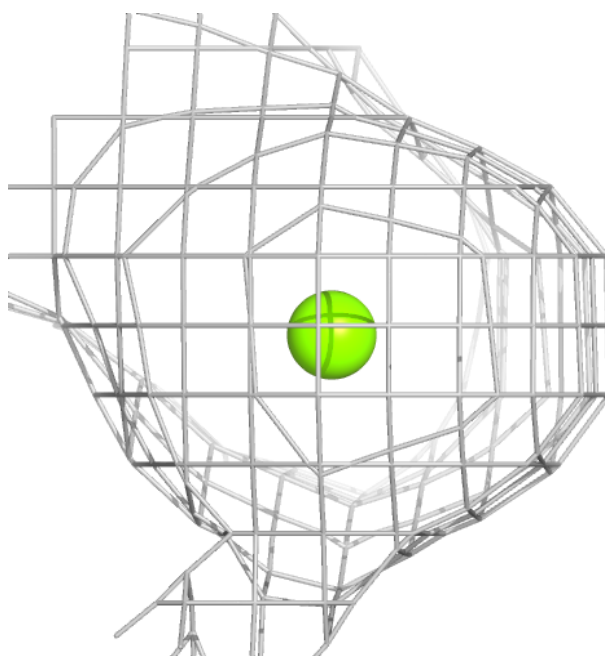
Electron density around MG N 703:

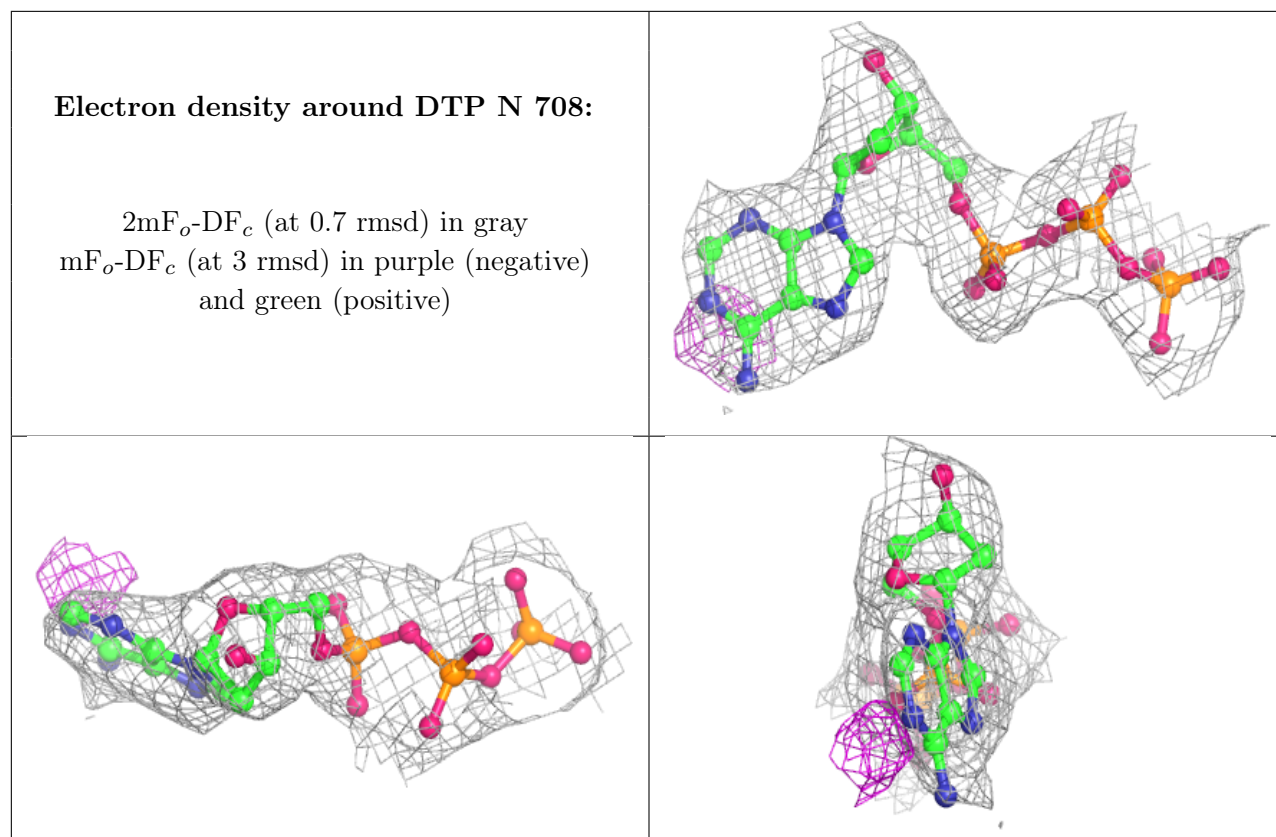
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG M 702:

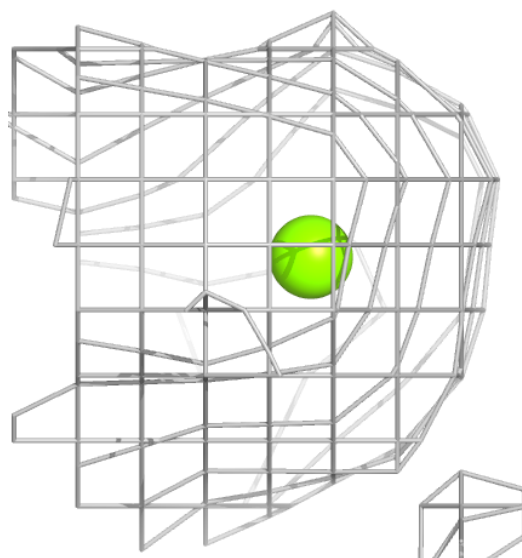
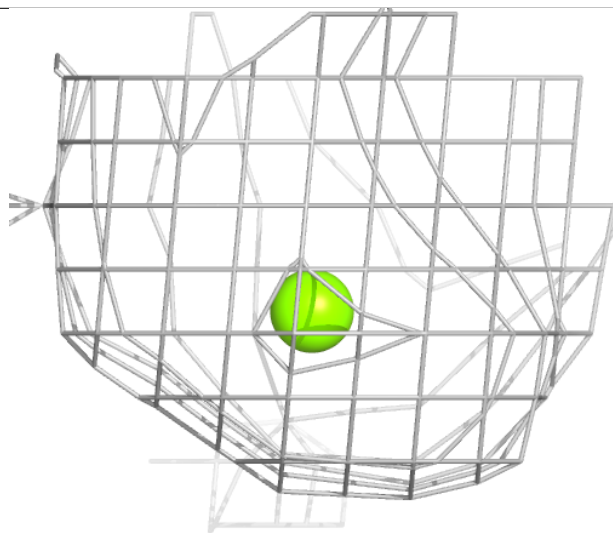
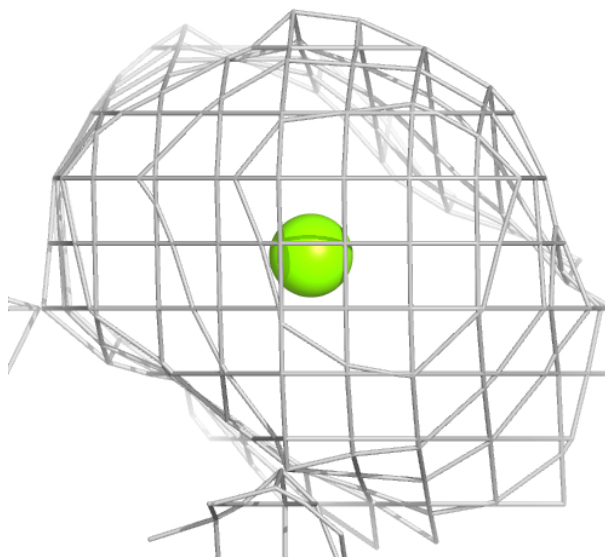
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





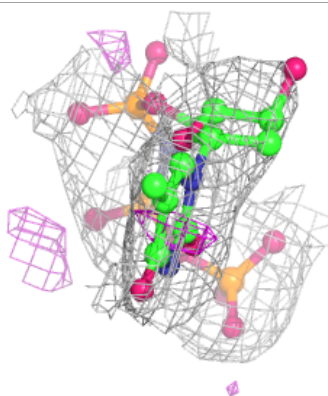
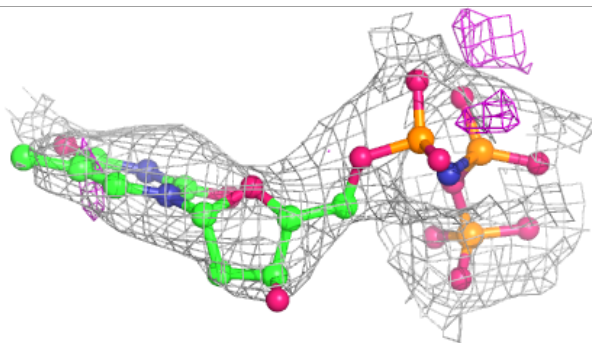
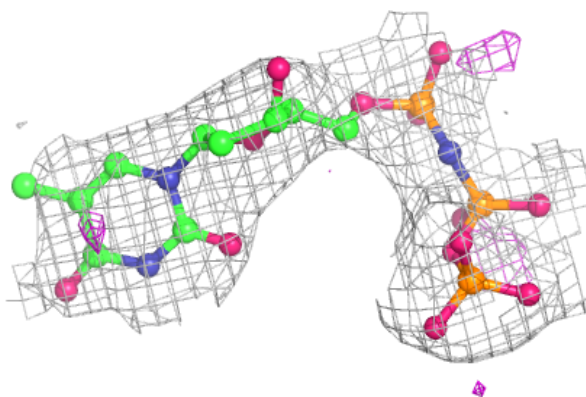
Electron density around MG H 703:

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

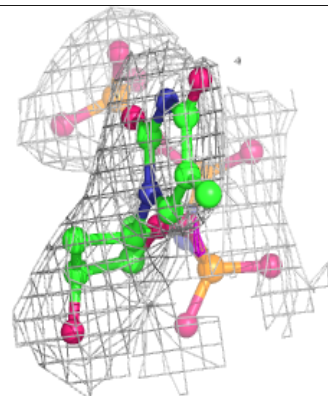
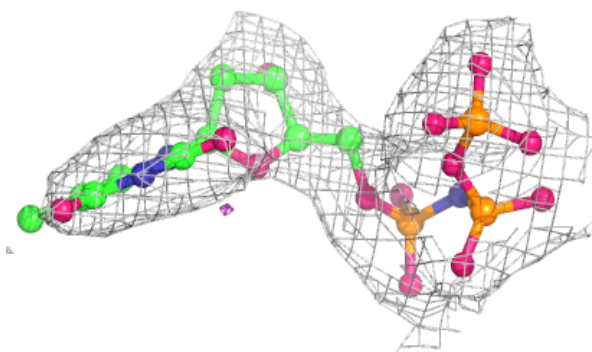
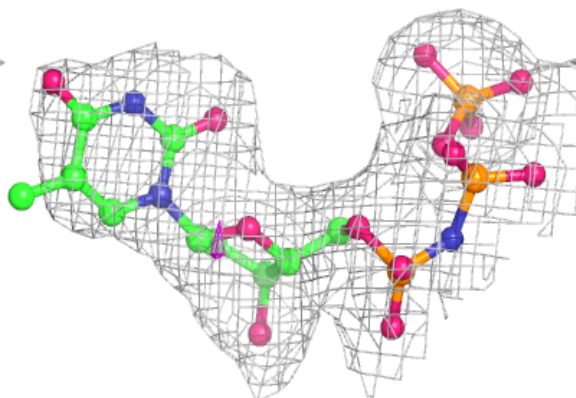


Electron density around 1FZ N 705:

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

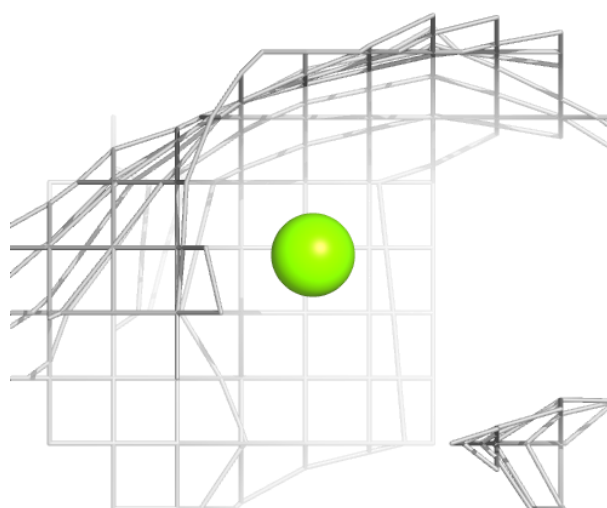
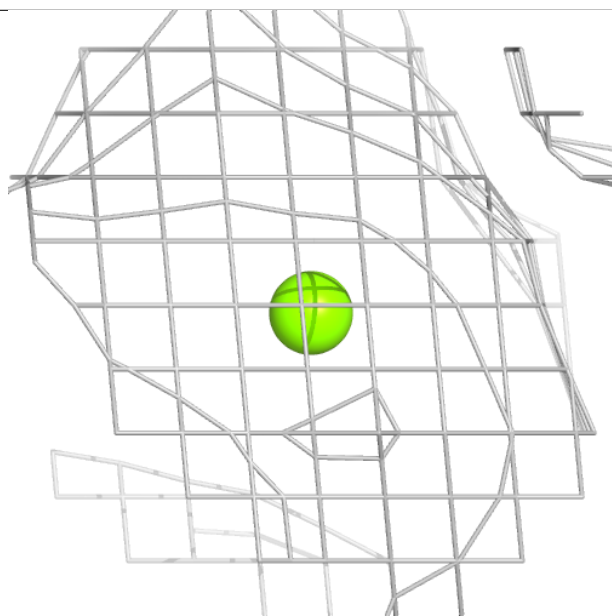
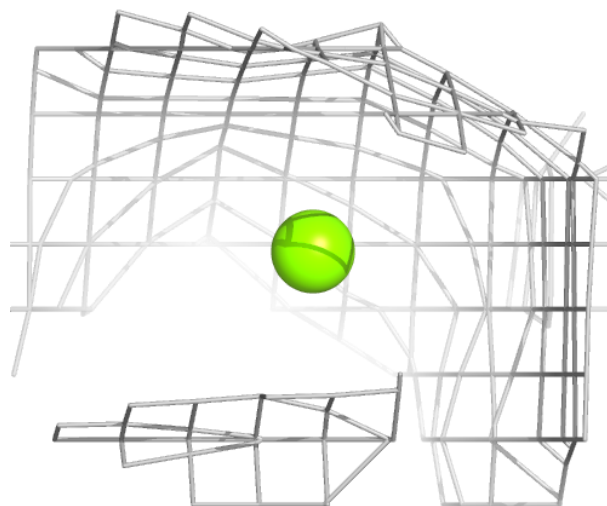
**Electron density around 1FZ O 704:**

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



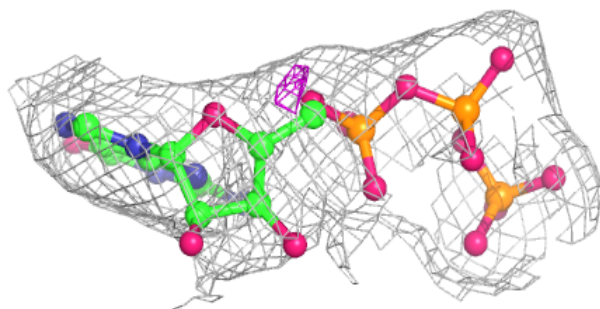
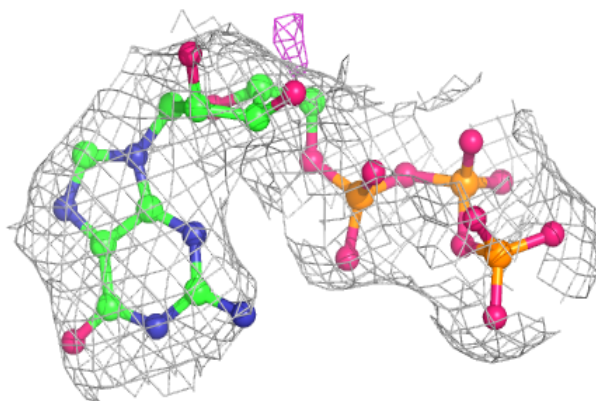
Electron density around MG G 704:

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

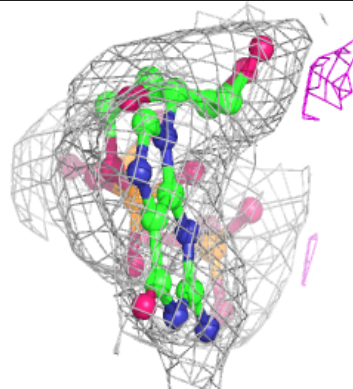
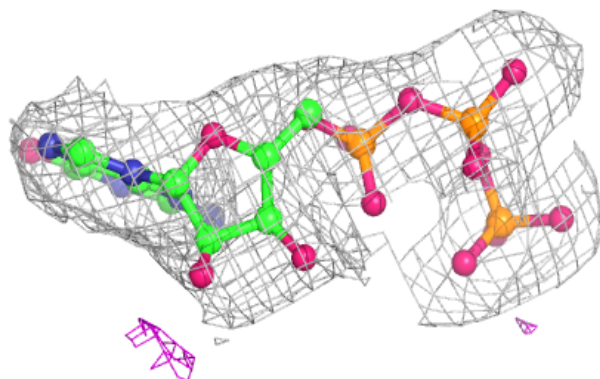
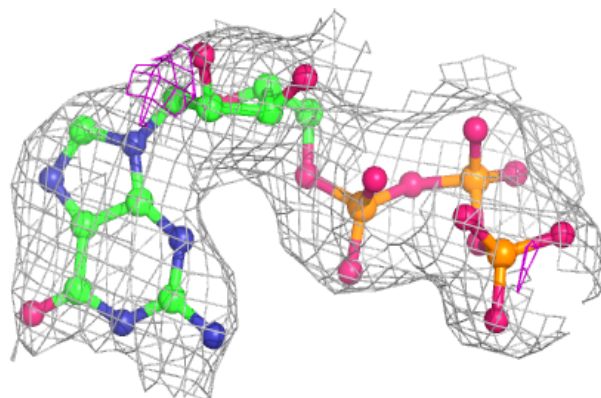


Electron density around GTP E 705:

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

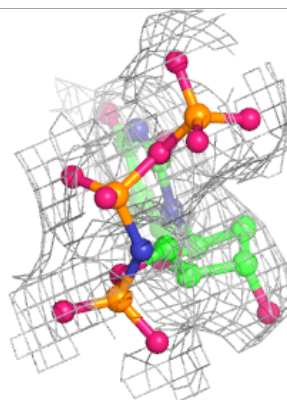
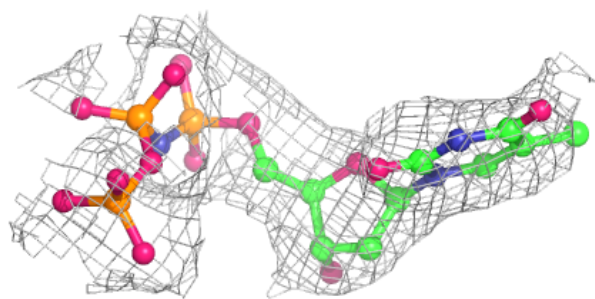
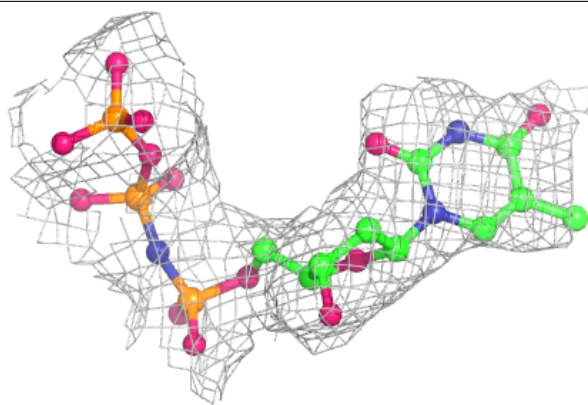
**Electron density around GTP K 706:**

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

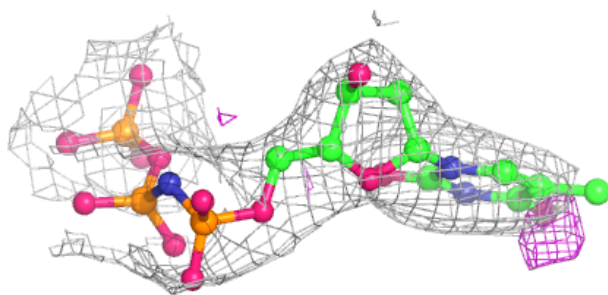
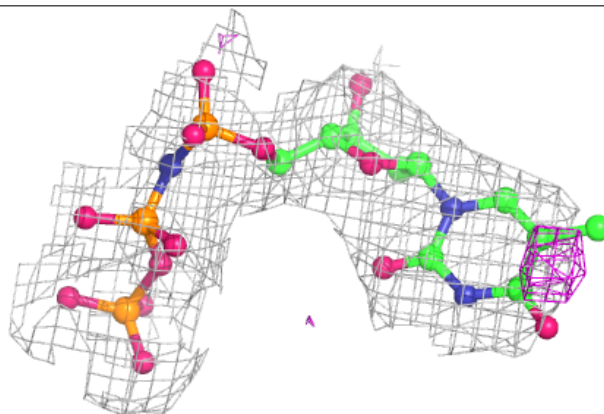


Electron density around 1FZ G 705:

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

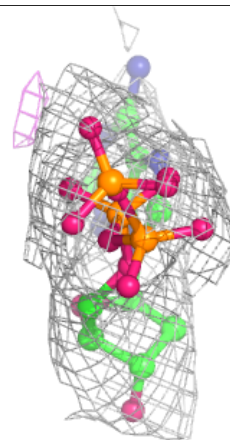
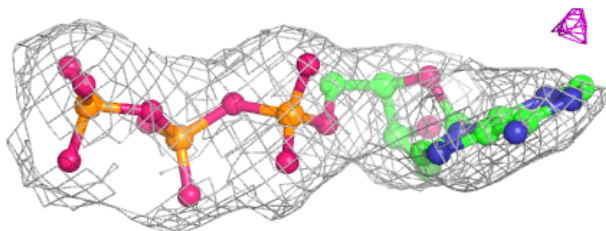
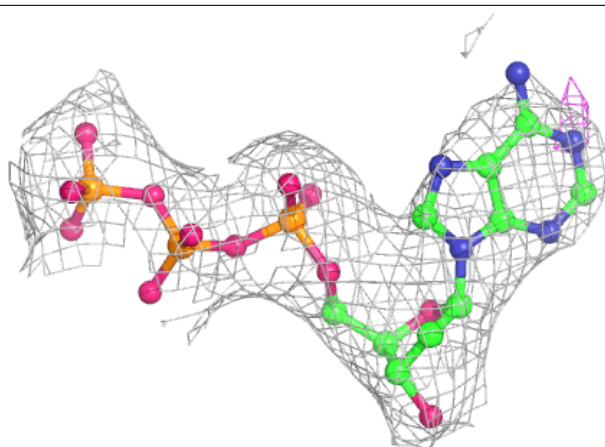
**Electron density around 1FZ K 705:**

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

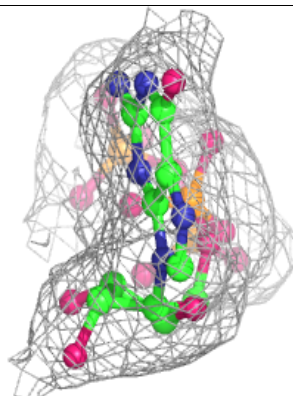
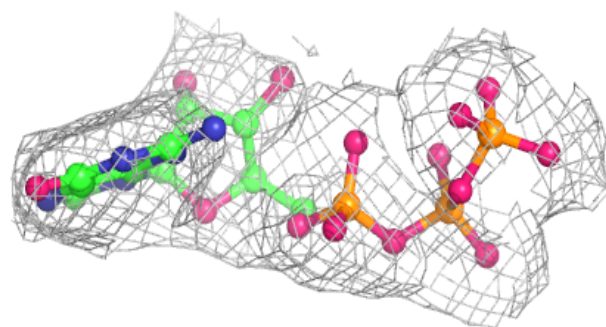
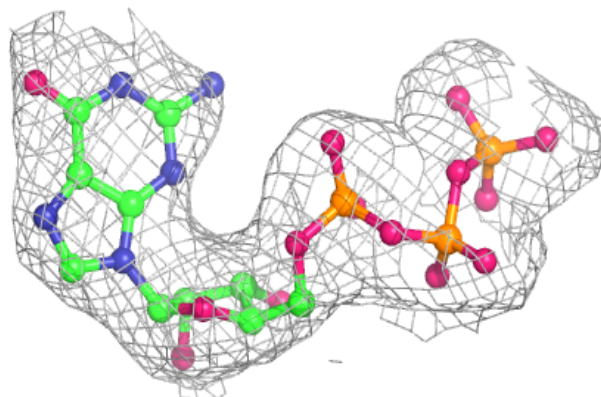


Electron density around DTP M 706:

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

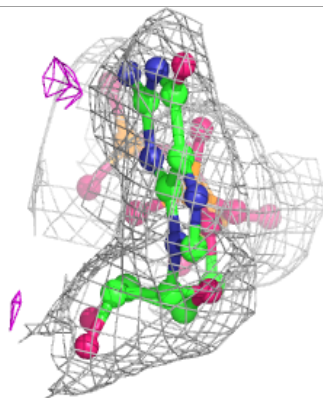
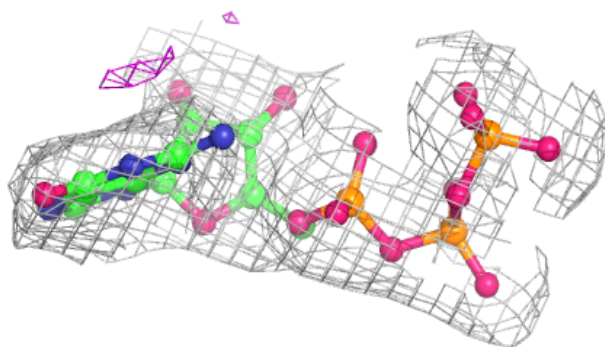
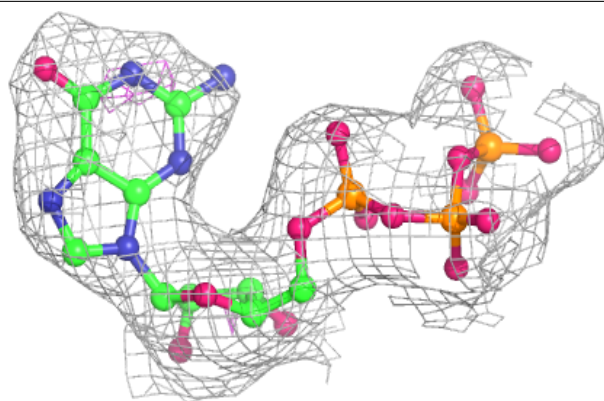
**Electron density around GTP F 705:**

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

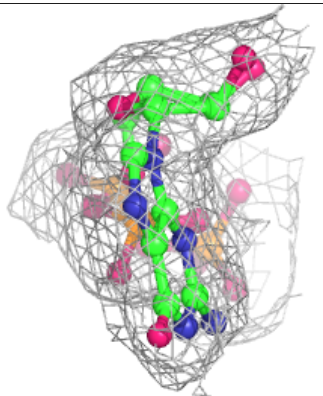
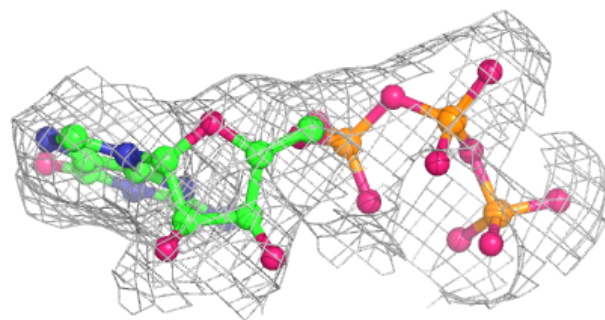
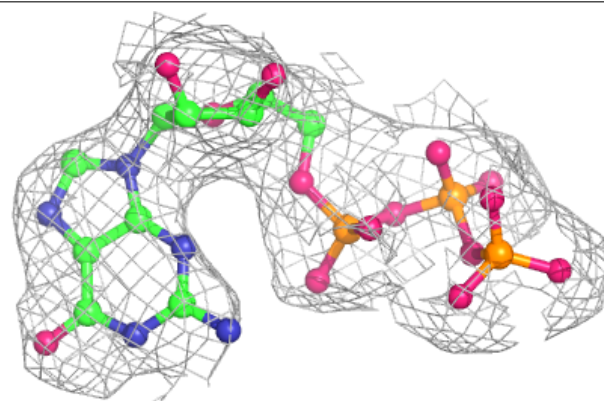


Electron density around GTP H 706:

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

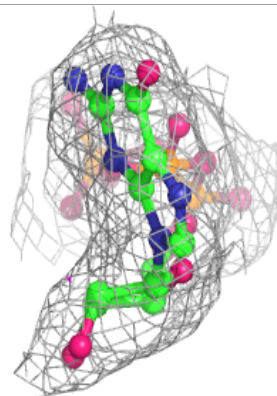
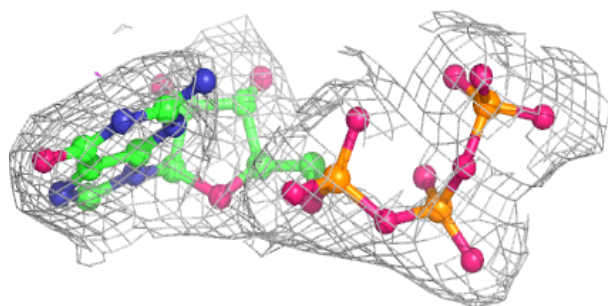
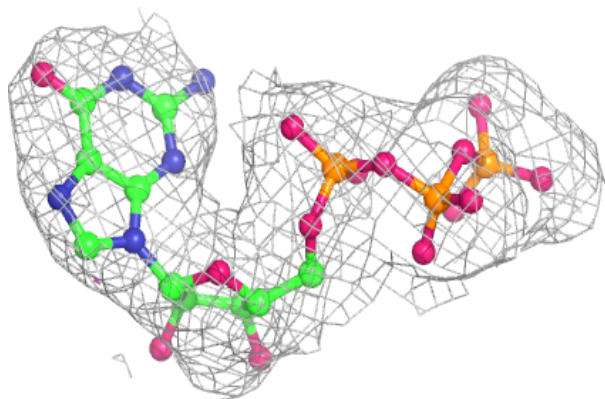
**Electron density around GTP I 705:**

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

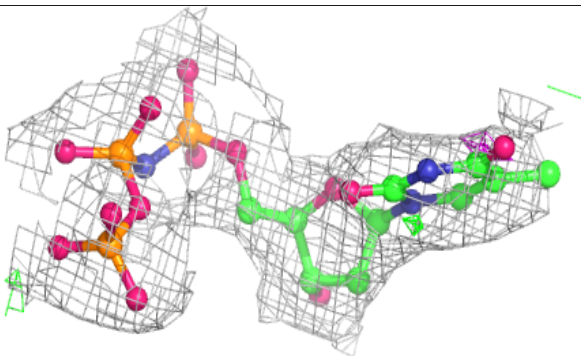
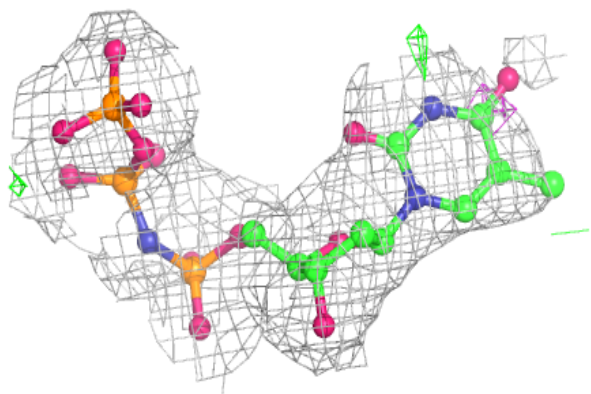


Electron density around GTP I 707:

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

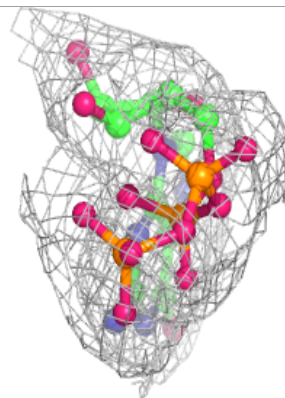
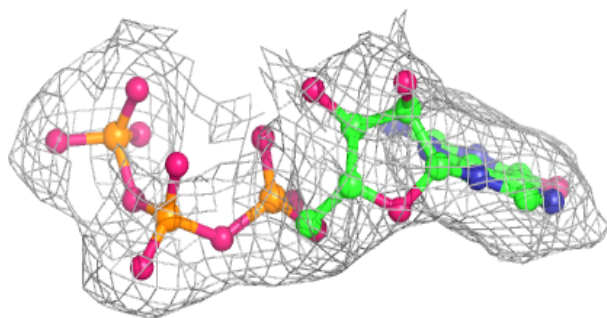
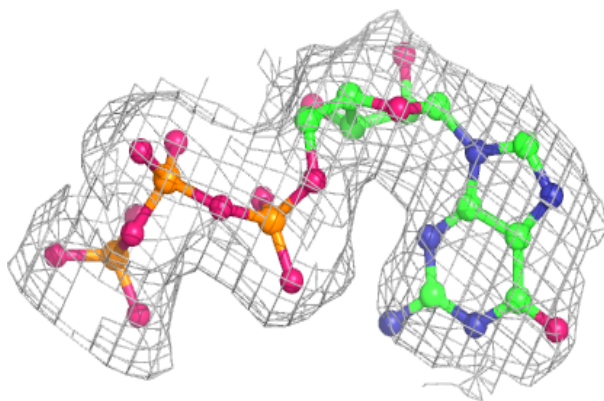
**Electron density around 1FZ B 704:**

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

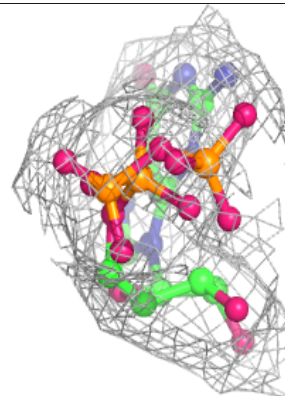
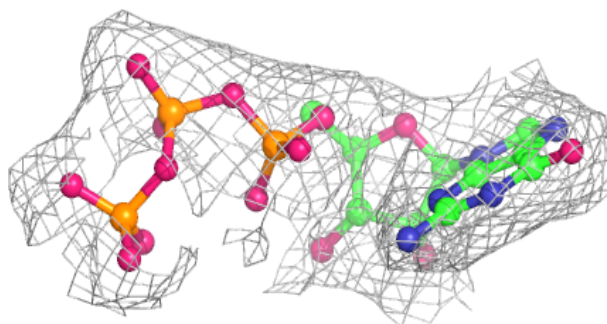
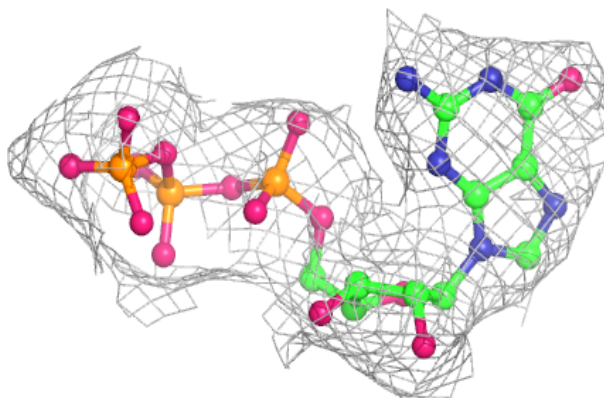


Electron density around GTP L 706:

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

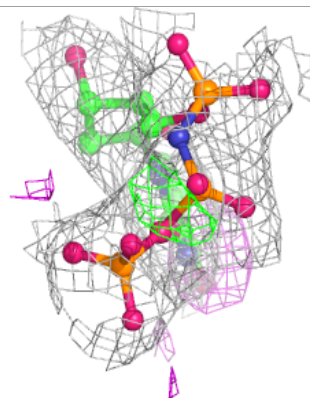
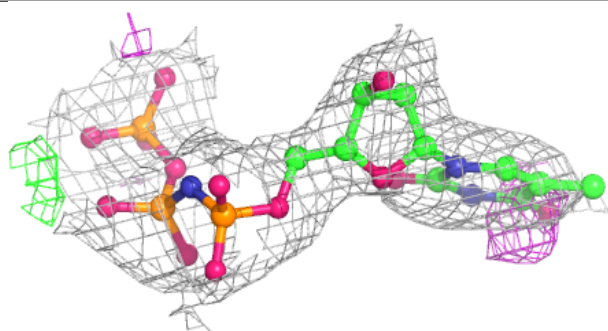
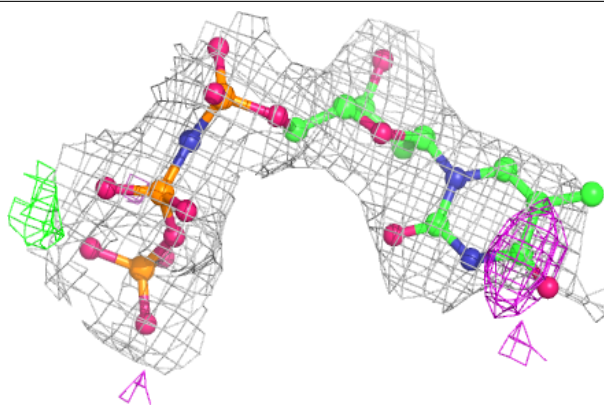
**Electron density around GTP M 705:**

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

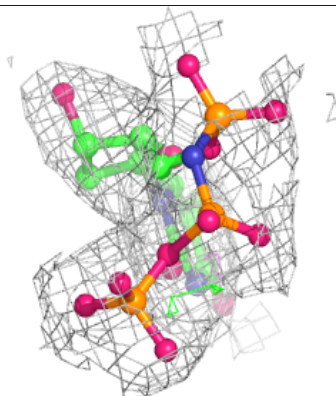
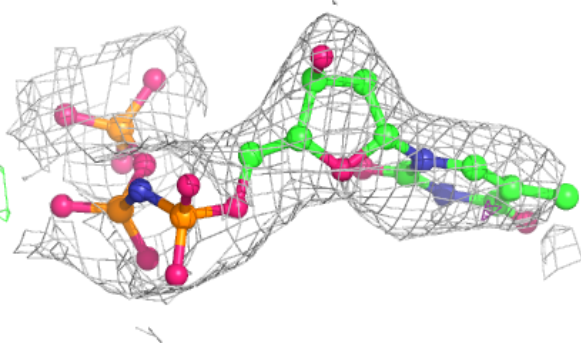
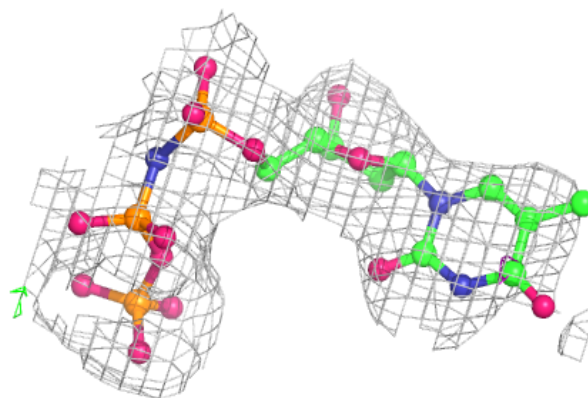


Electron density around 1FZ D 706:

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

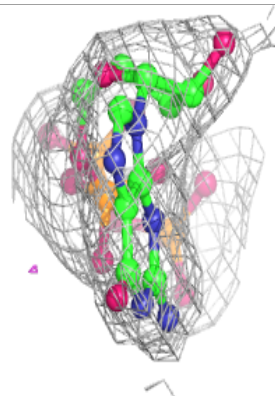
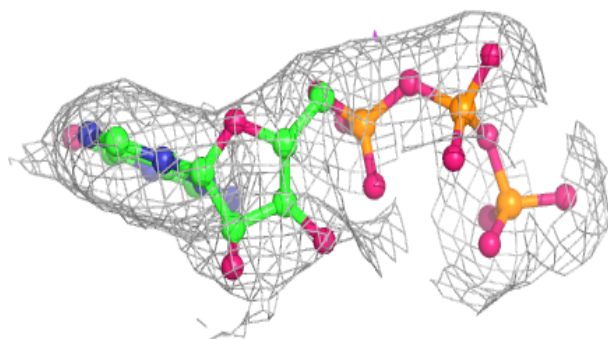
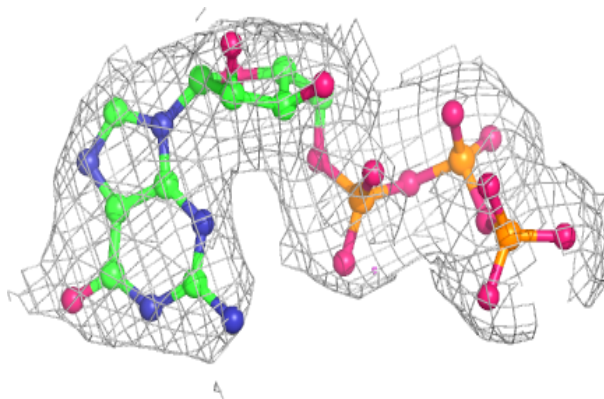
**Electron density around 1FZ E 704:**

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

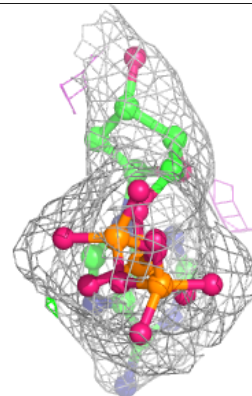
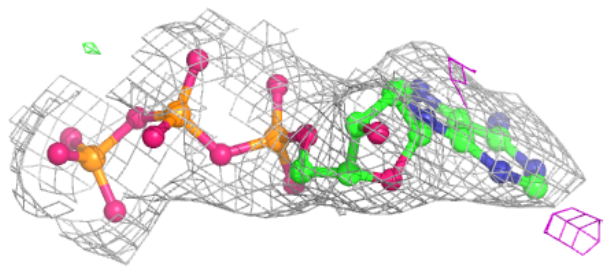
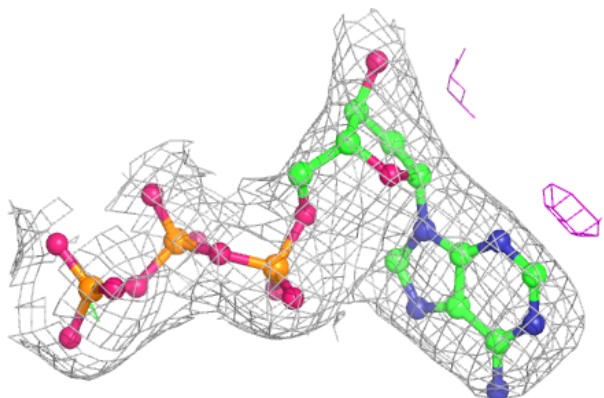


Electron density around GTP P 705:

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

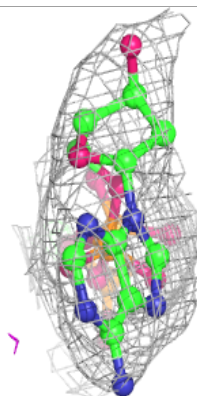
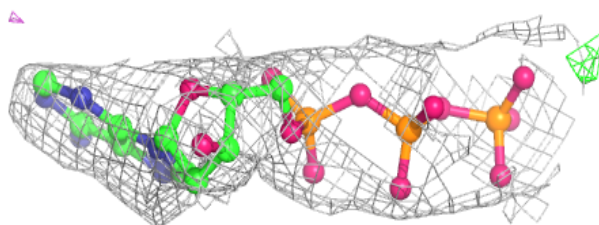
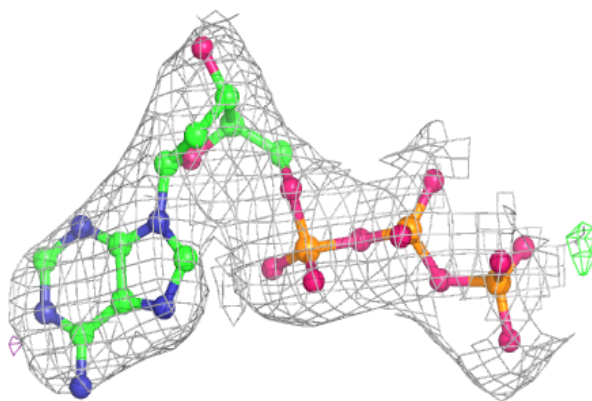
**Electron density around DTP F 707:**

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

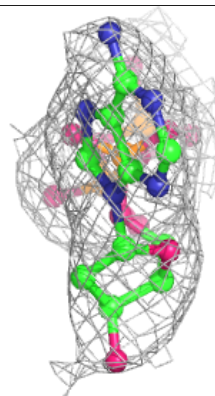
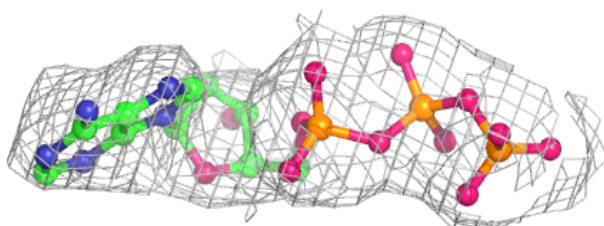
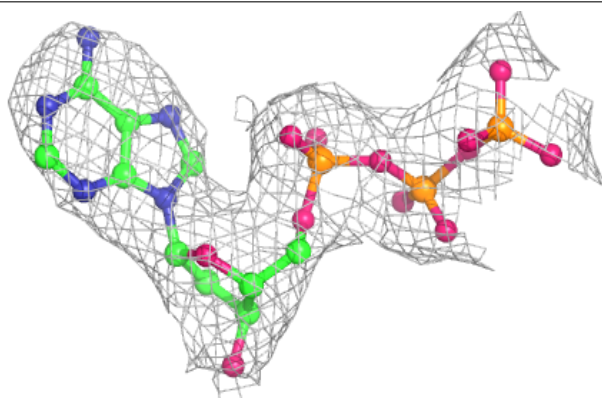


Electron density around DTP G 701:

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

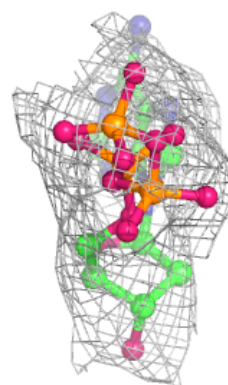
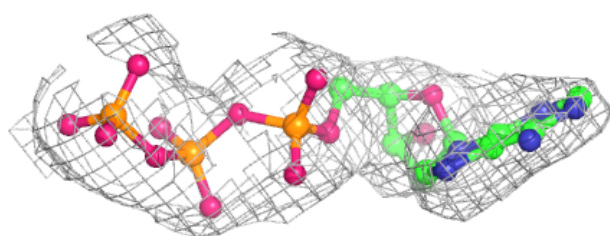
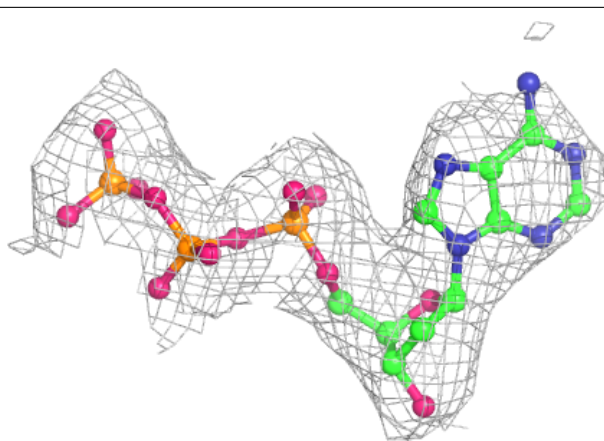
**Electron density around DTP H 701:**

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

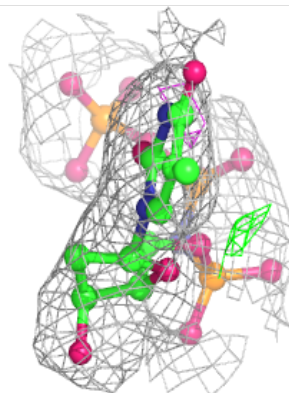
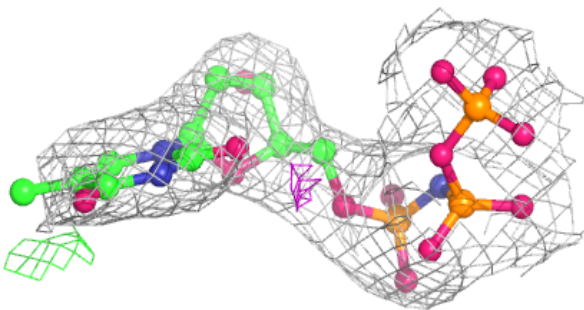
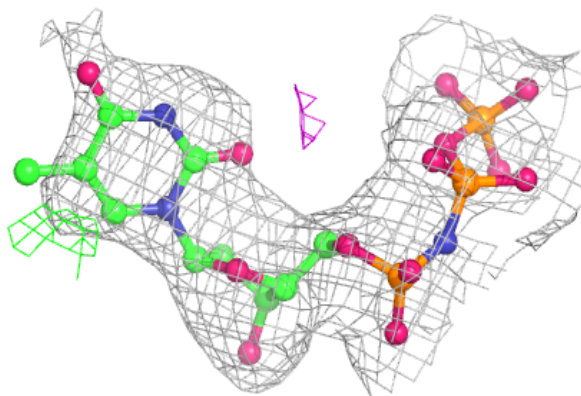


Electron density around DTP L 701:

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

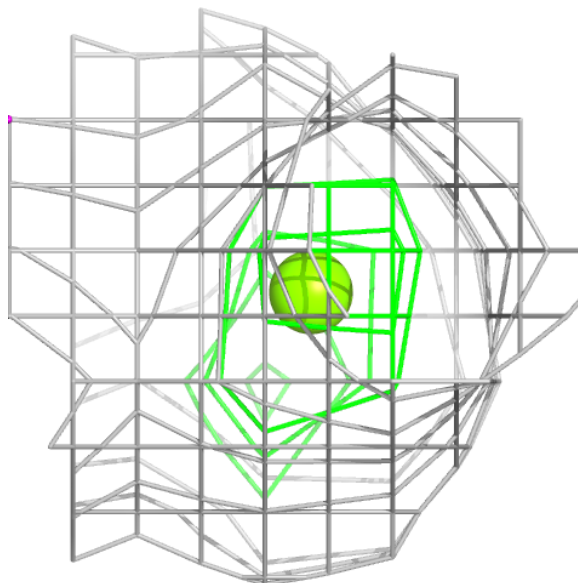
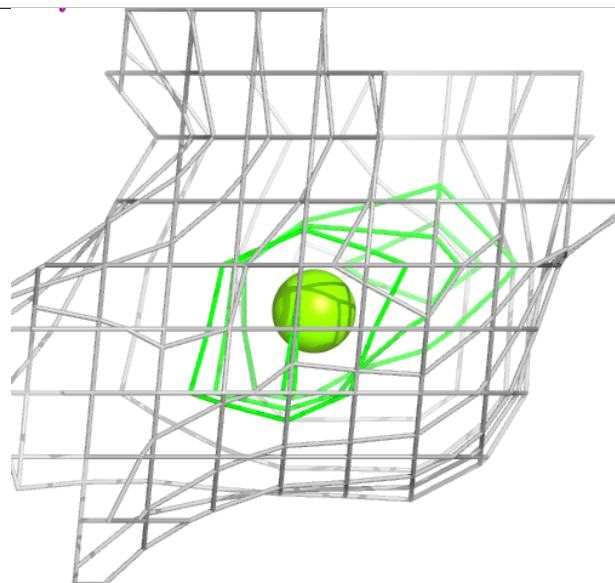
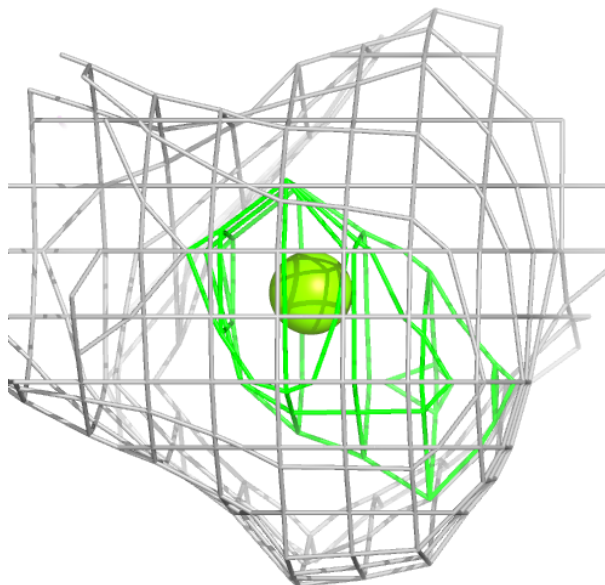
**Electron density around 1FZ F 704:**

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



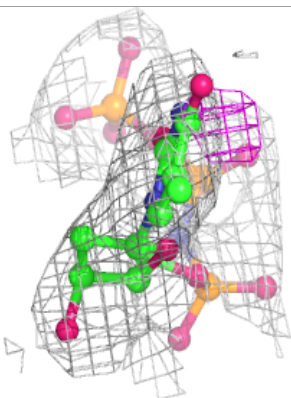
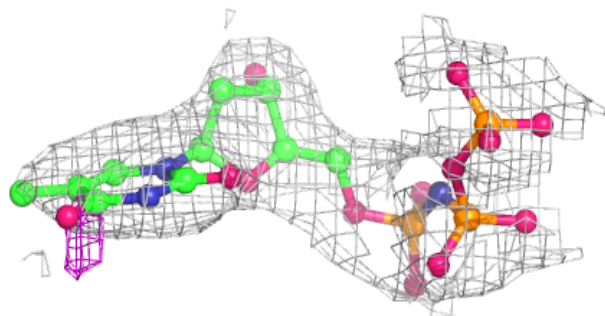
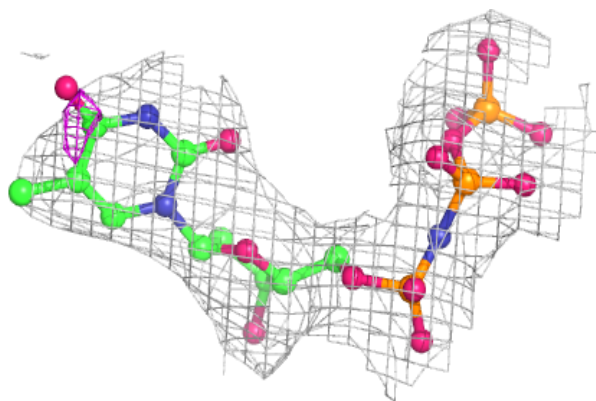
Electron density around MG D 704:

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

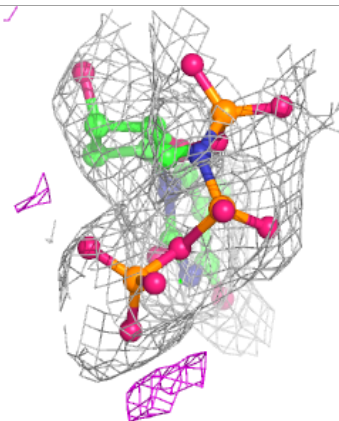
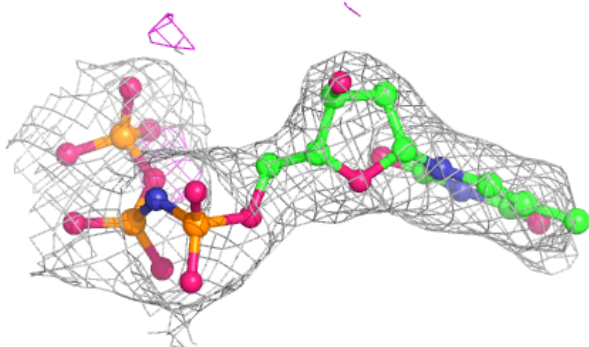
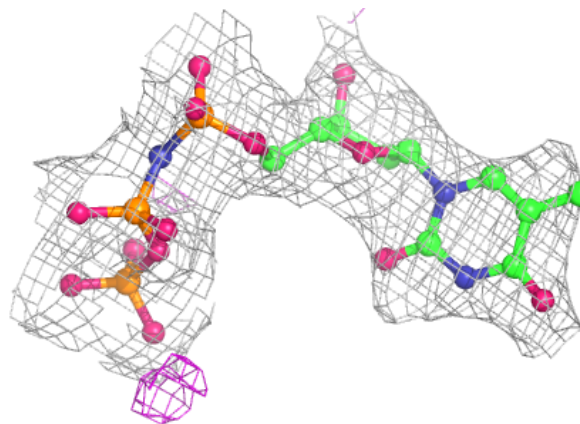


Electron density around 1FZ H 705:

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

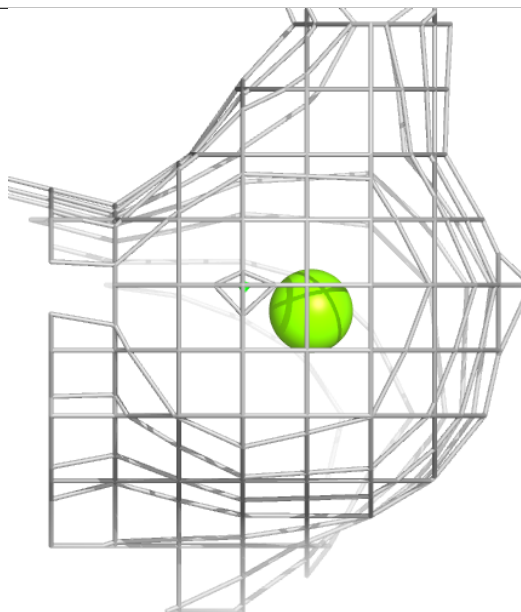
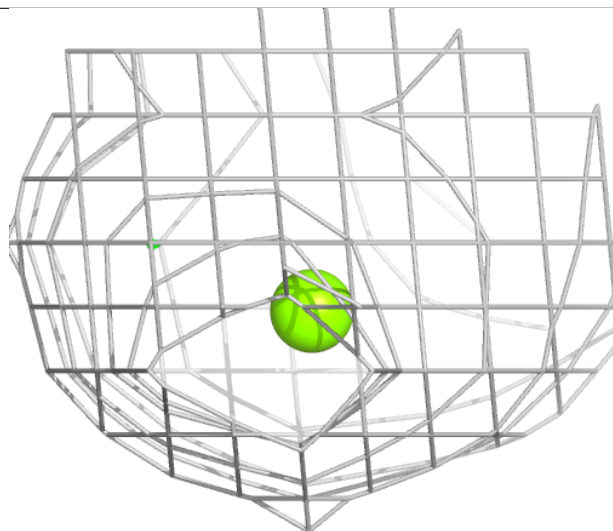
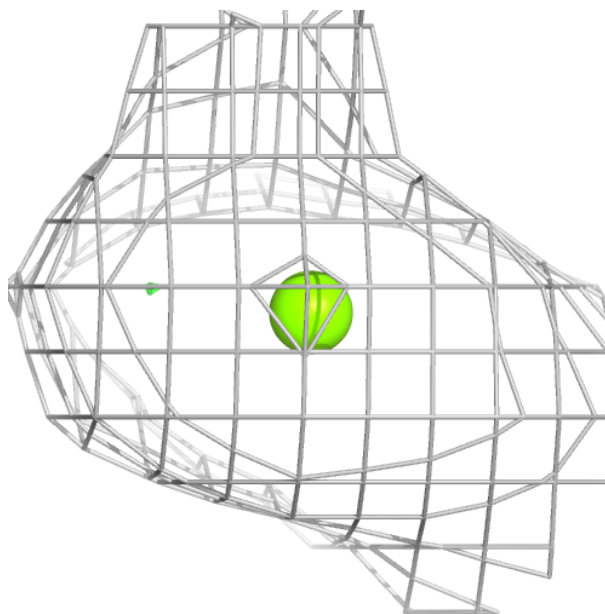
**Electron density around 1FZ I 704:**

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



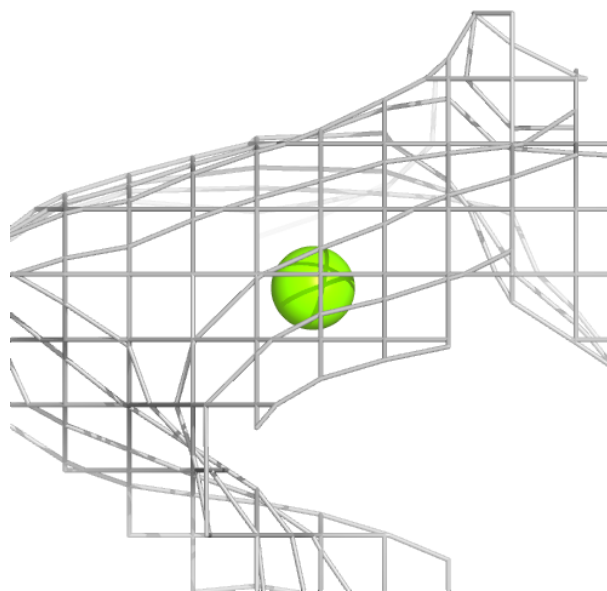
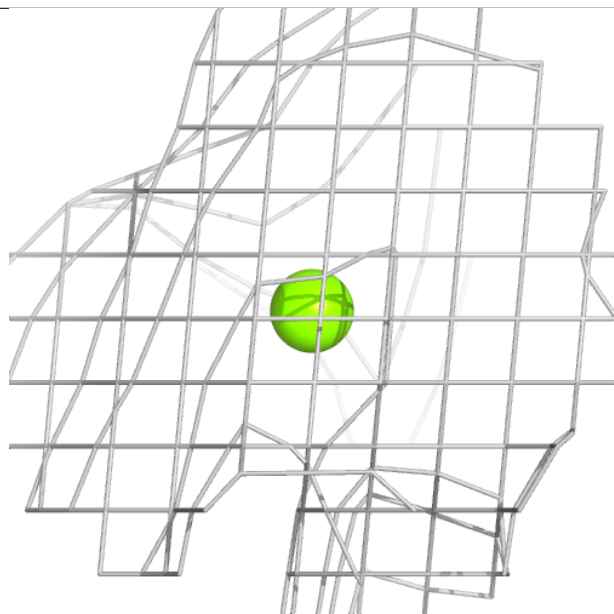
Electron density around MG I 702:

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



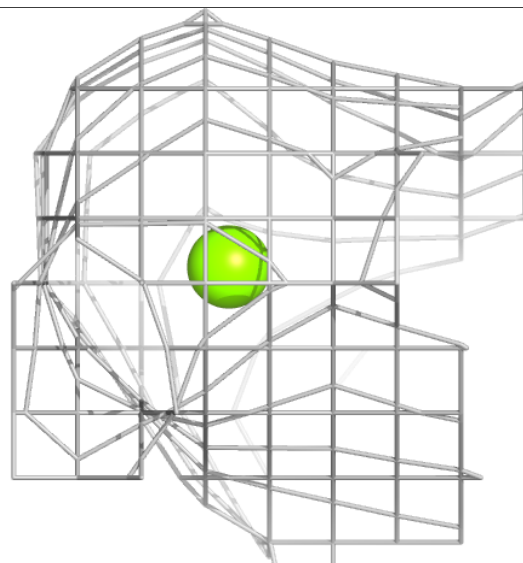
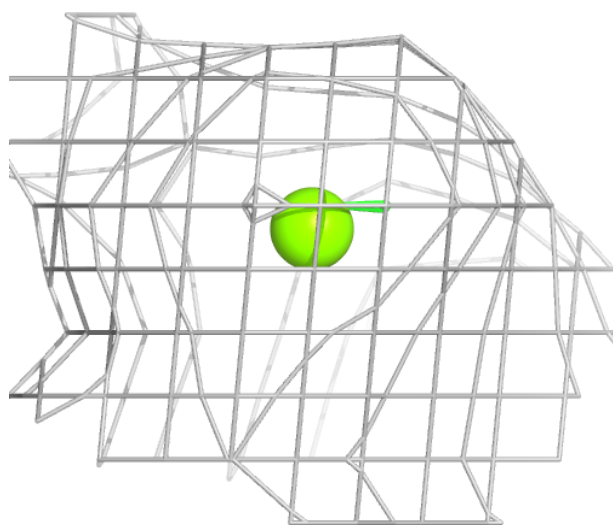
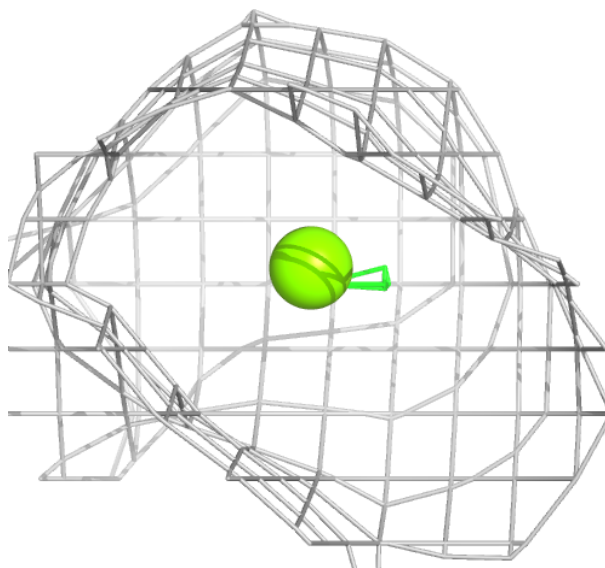
Electron density around MG B 703:

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



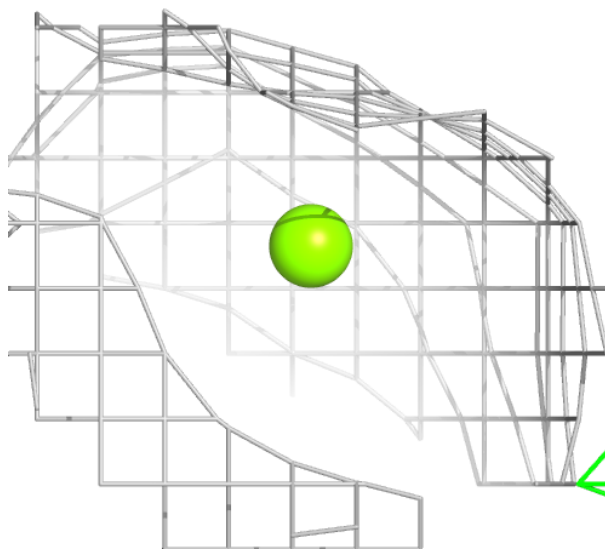
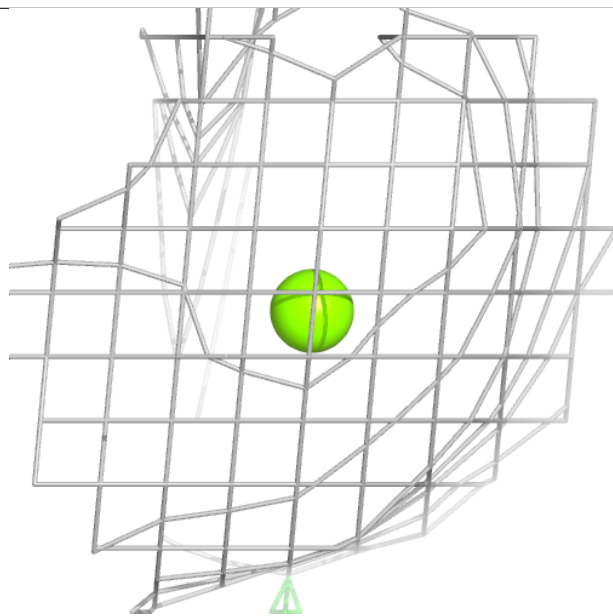
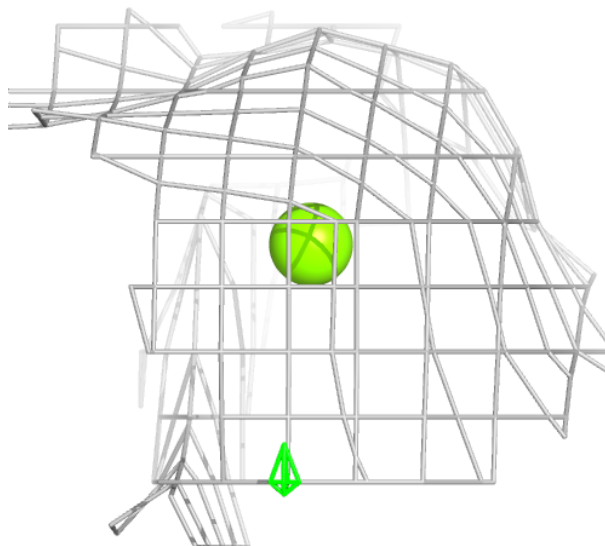
Electron density around MG C 703:

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



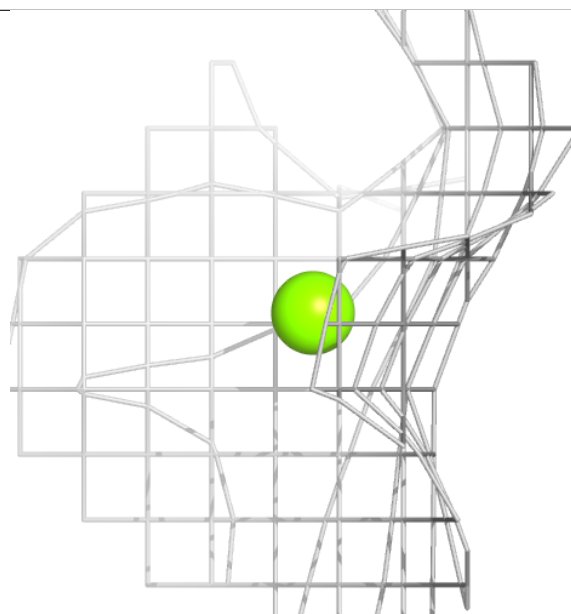
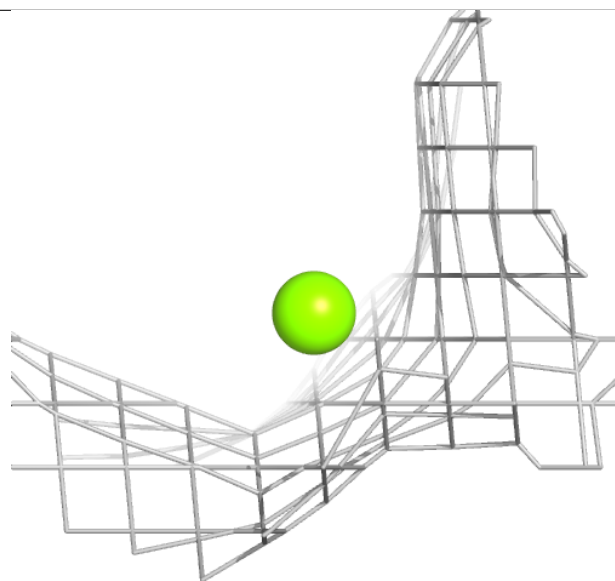
Electron density around MG C 704:

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



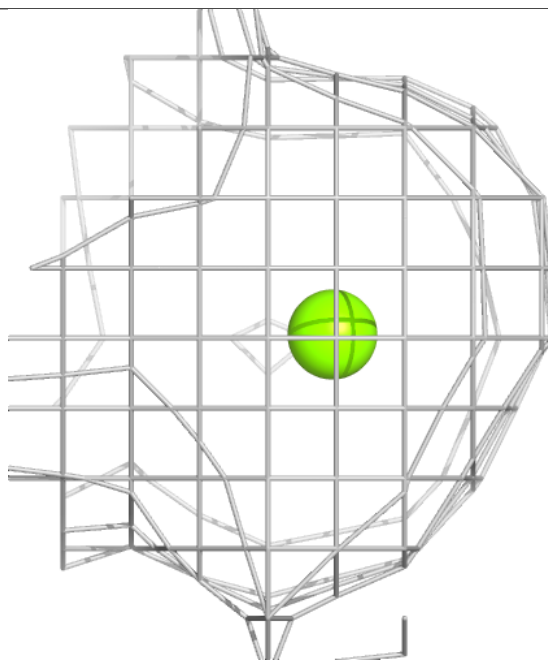
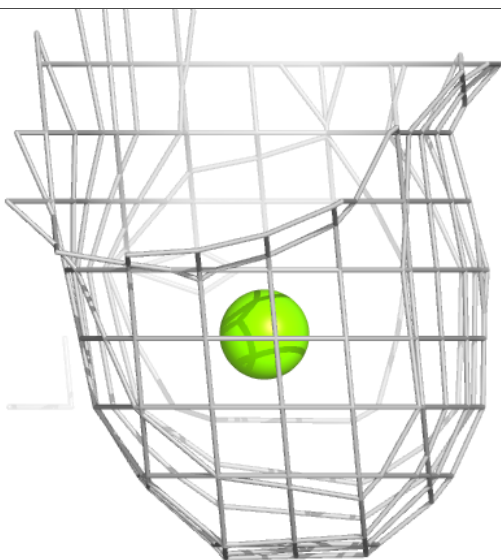
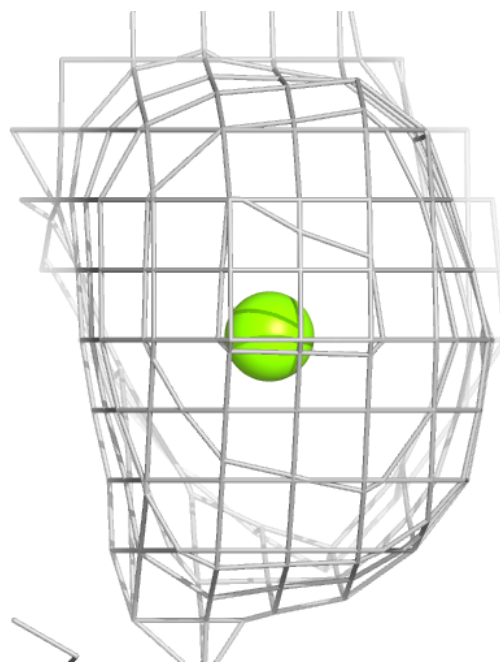
Electron density around MG O 703:

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



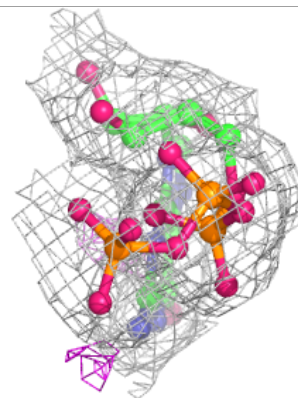
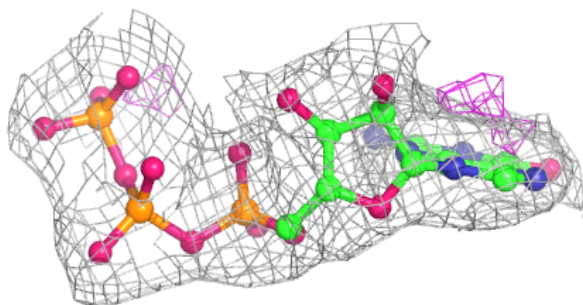
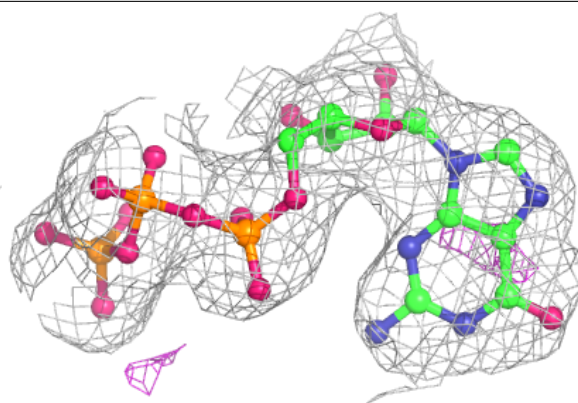
Electron density around MG P 702:

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

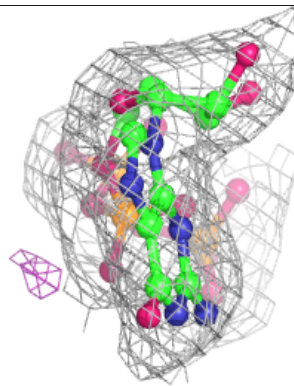
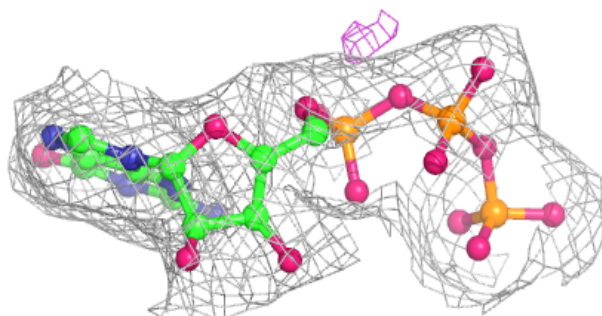
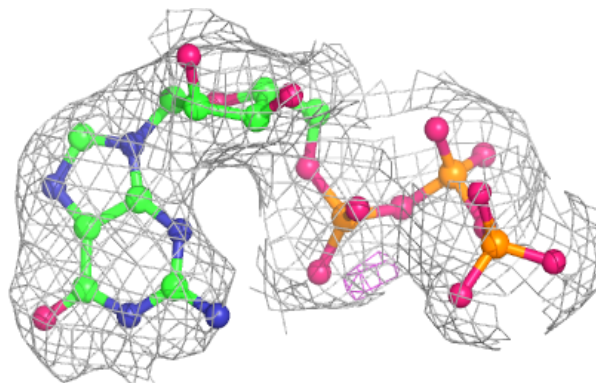


Electron density around GTP B 705:

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

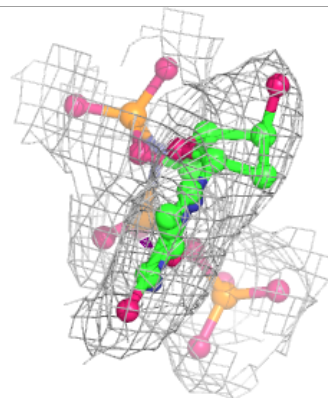
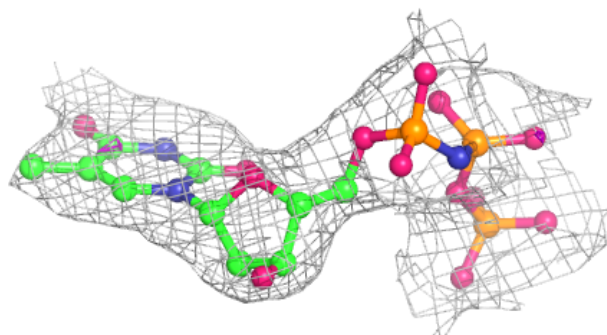
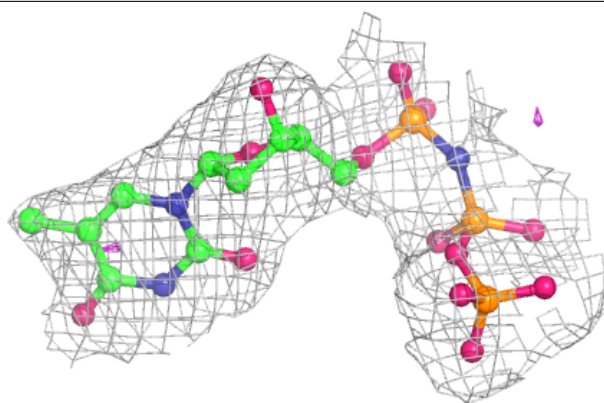
**Electron density around GTP D 707:**

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

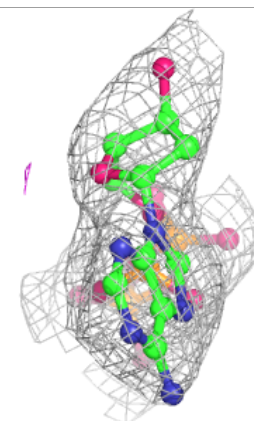
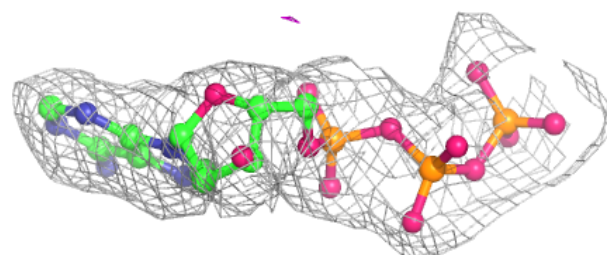
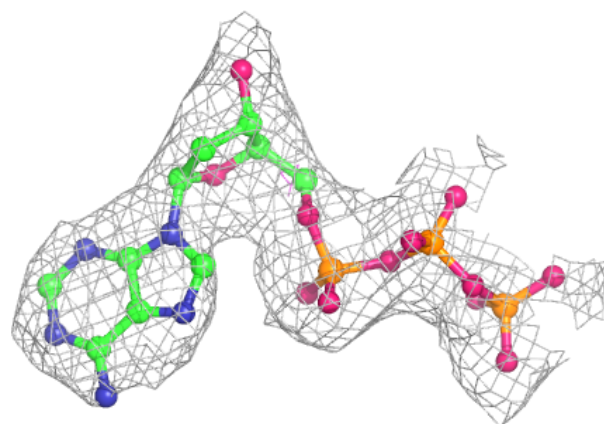


Electron density around 1FZ A 704:

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

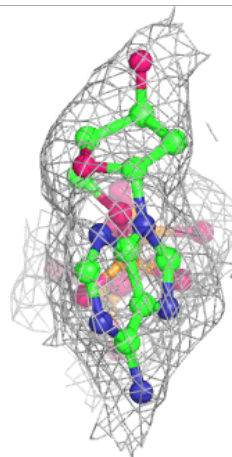
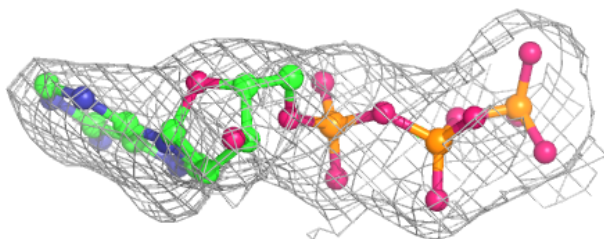
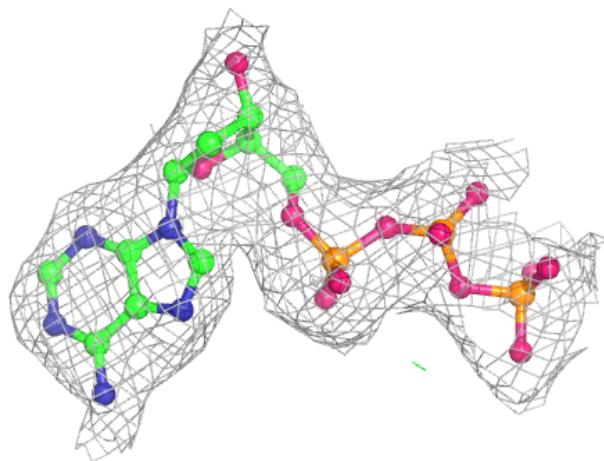
**Electron density around DTP B 707:**

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



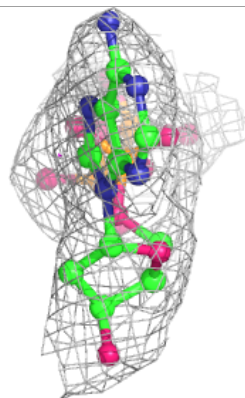
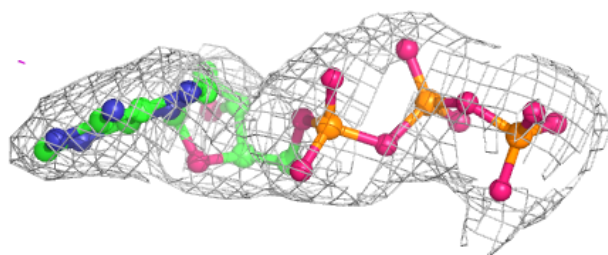
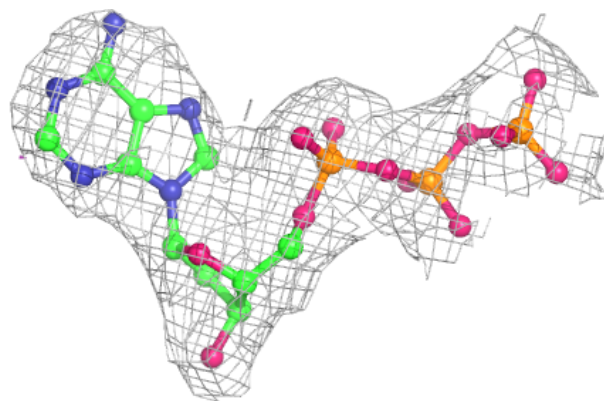
Electron density around DTP D 701:

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



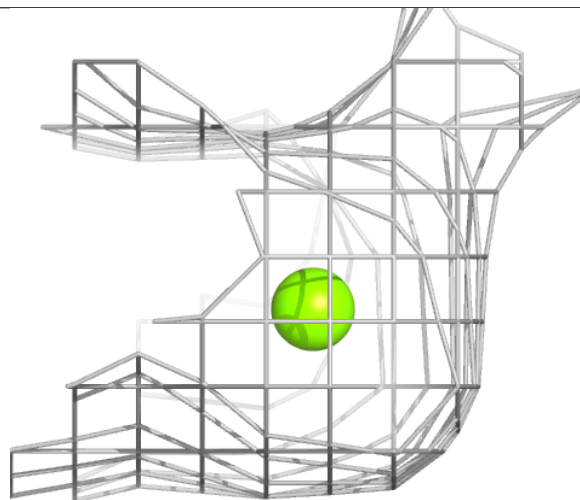
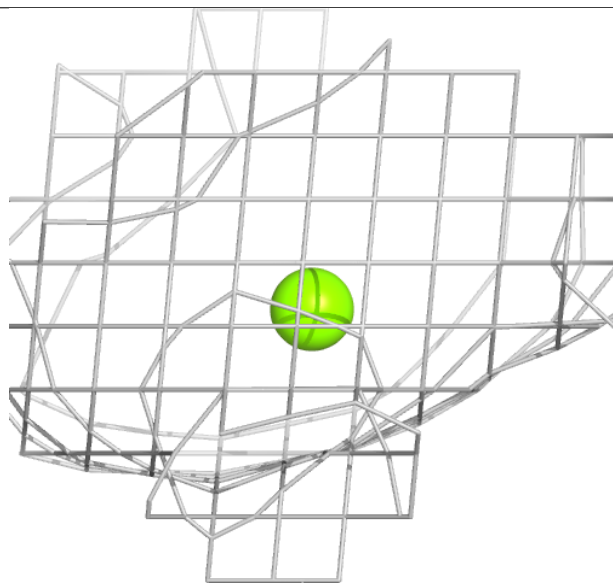
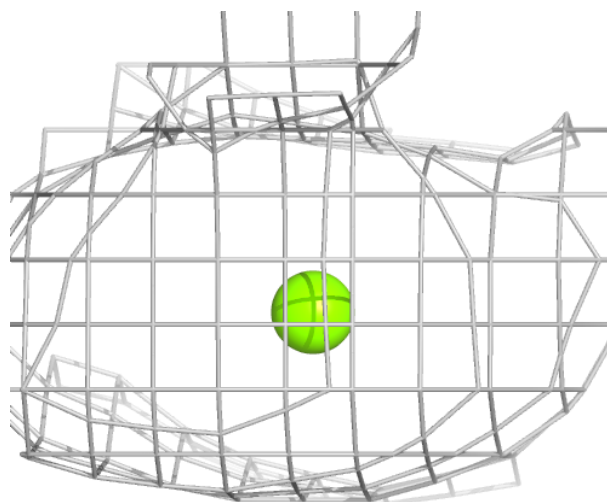
Electron density around DTP E 707:

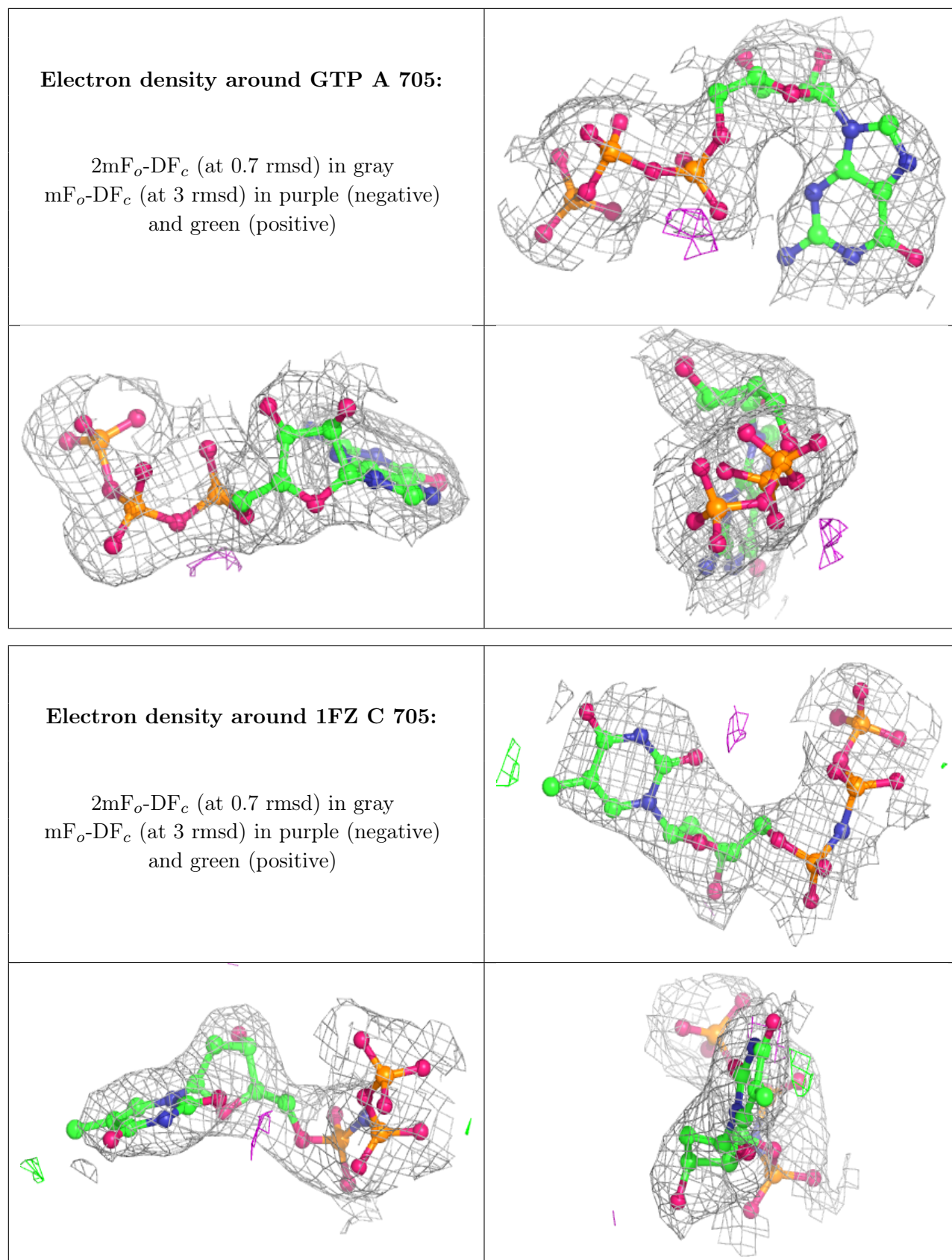
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG K 703:

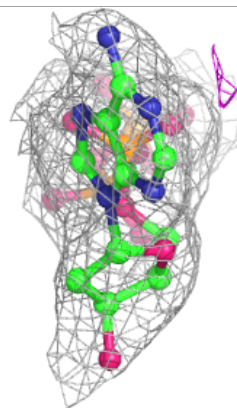
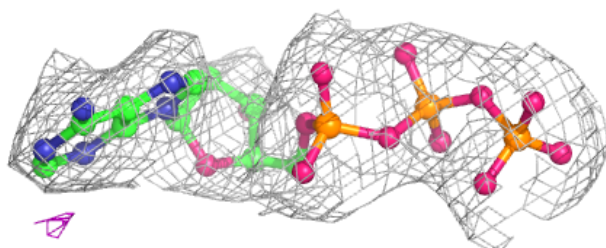
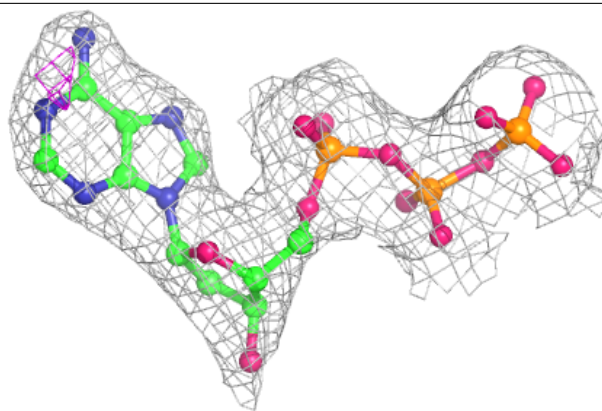
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



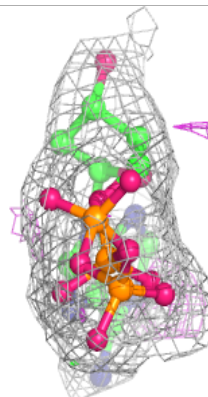
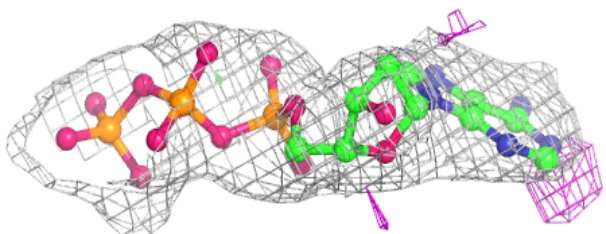
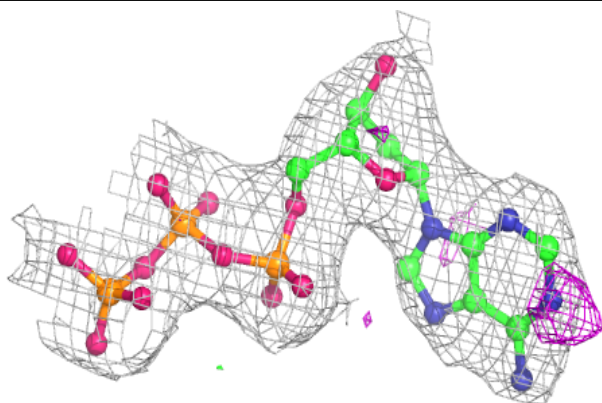


Electron density around DTP I 708:

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

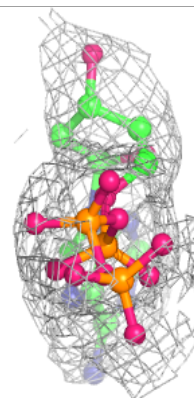
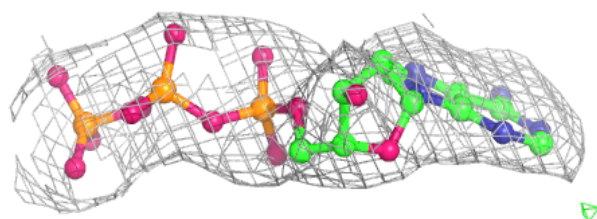
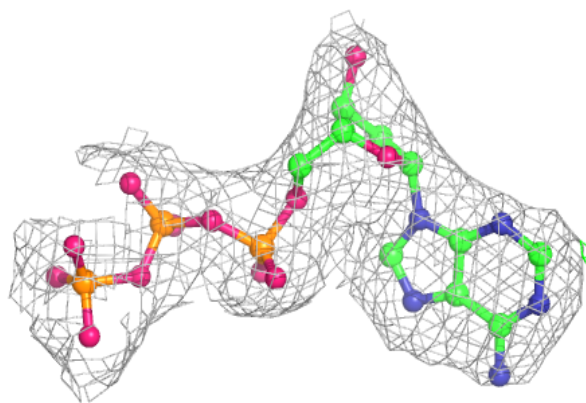
**Electron density around DTP J 706:**

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

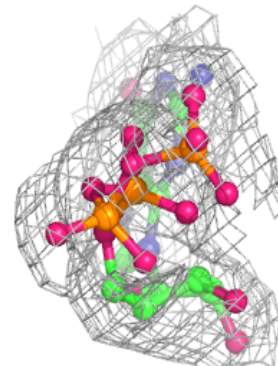
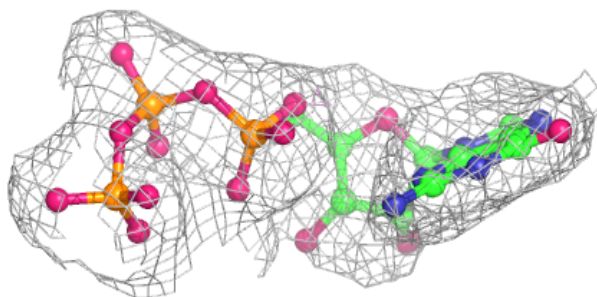
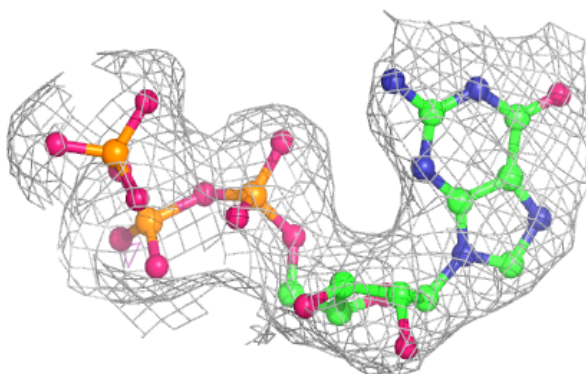


Electron density around DTP K 701:

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

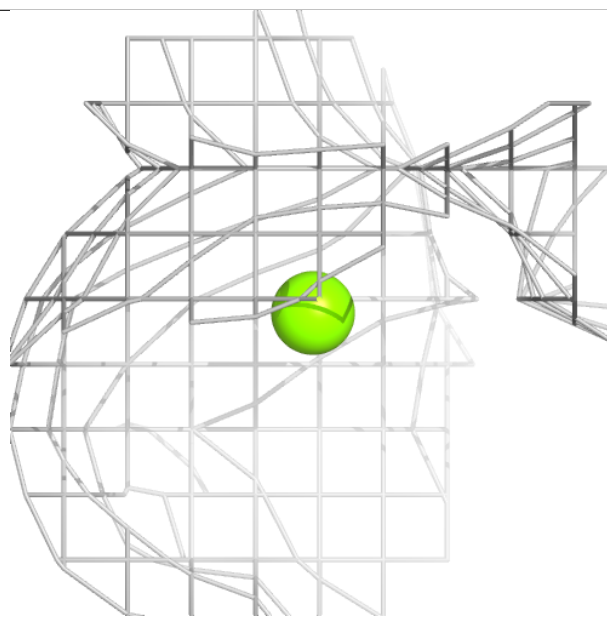
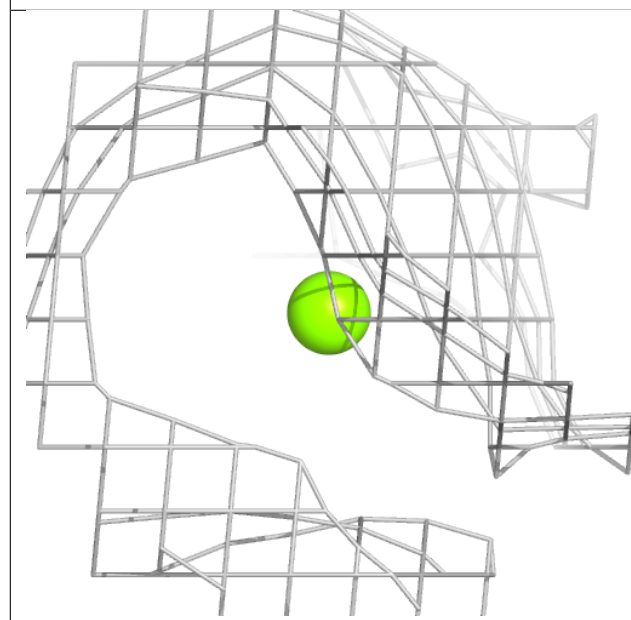
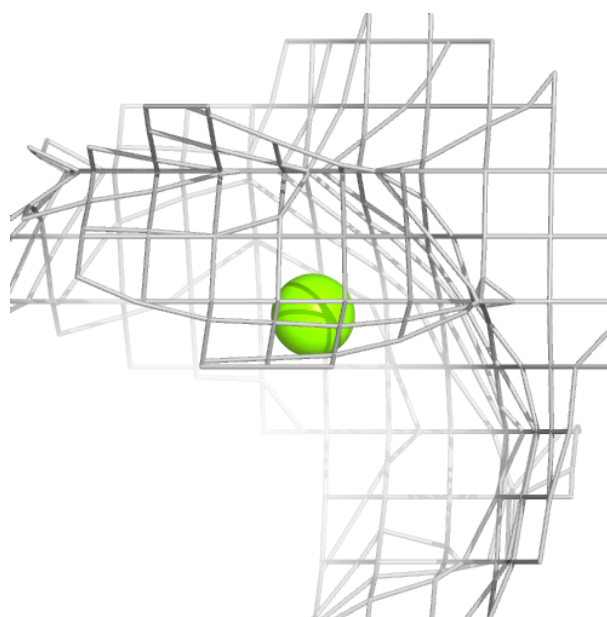
**Electron density around GTP D 702:**

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



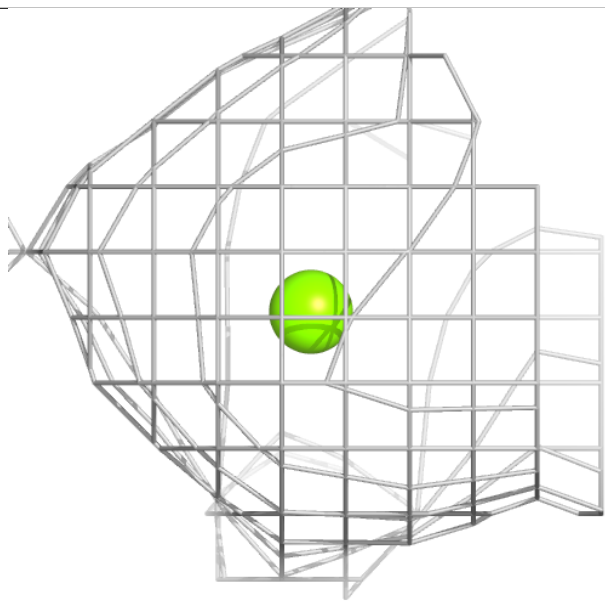
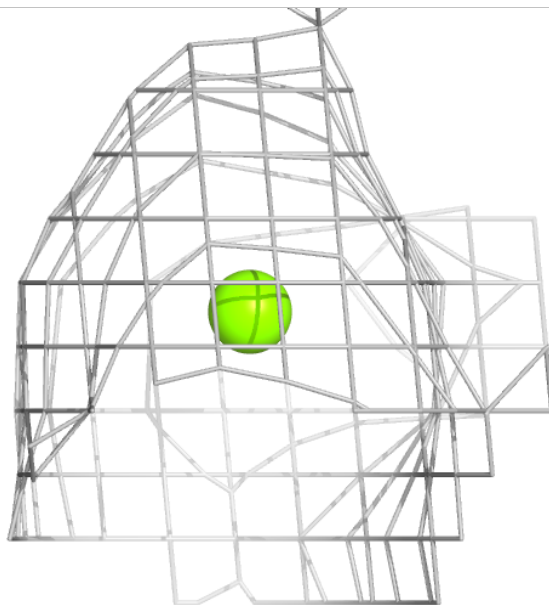
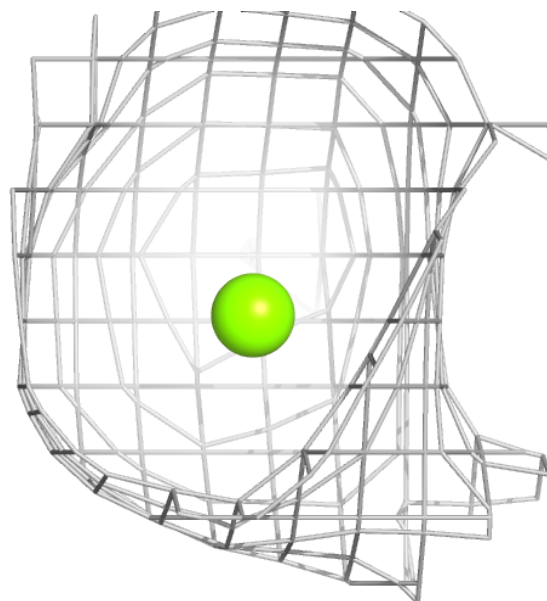
Electron density around MG K 704:

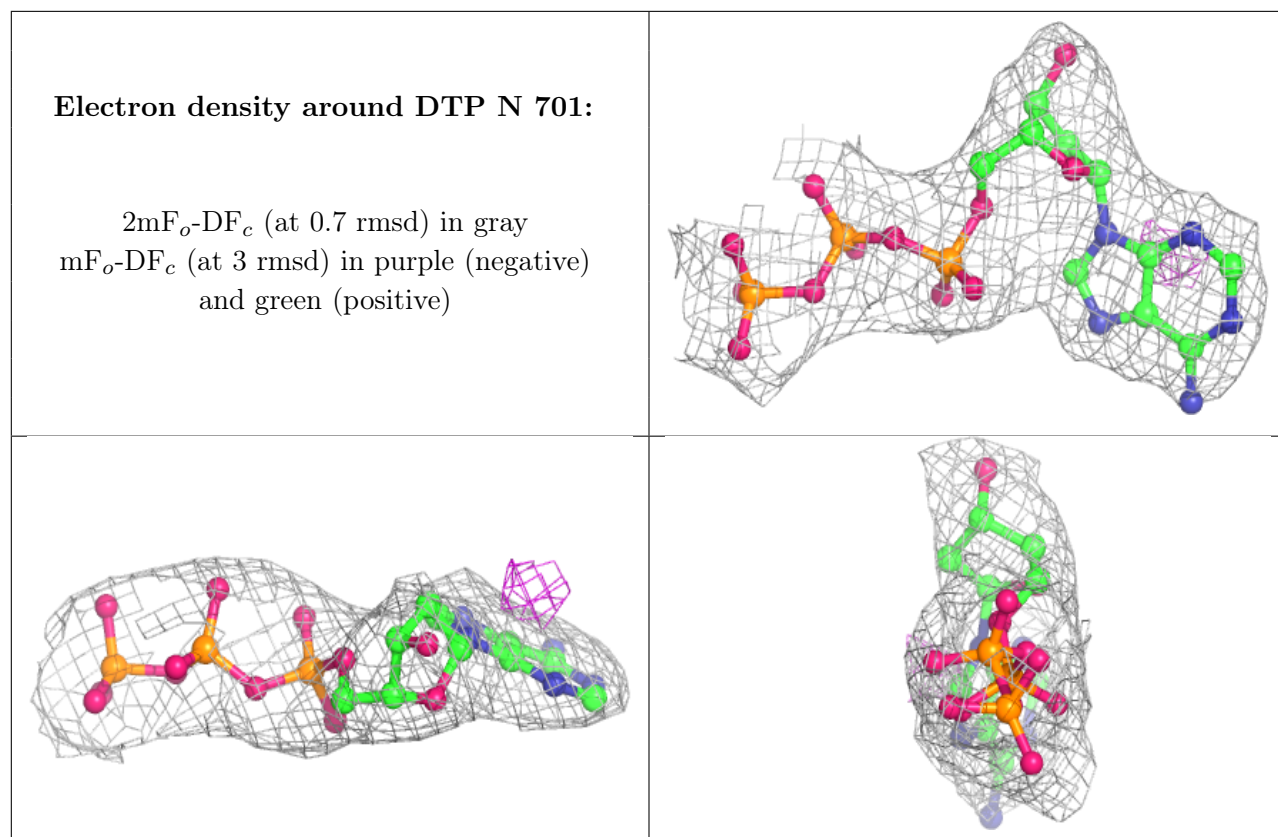
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG L 703:

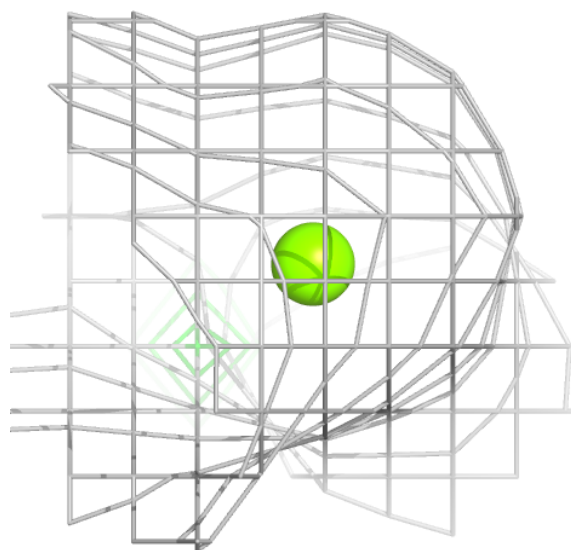
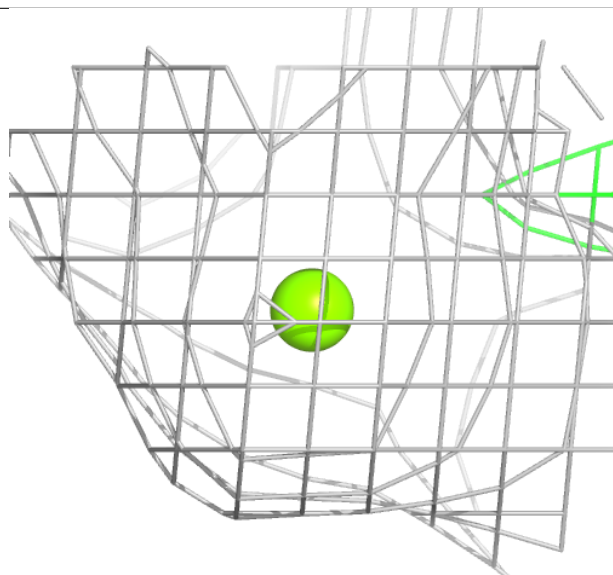
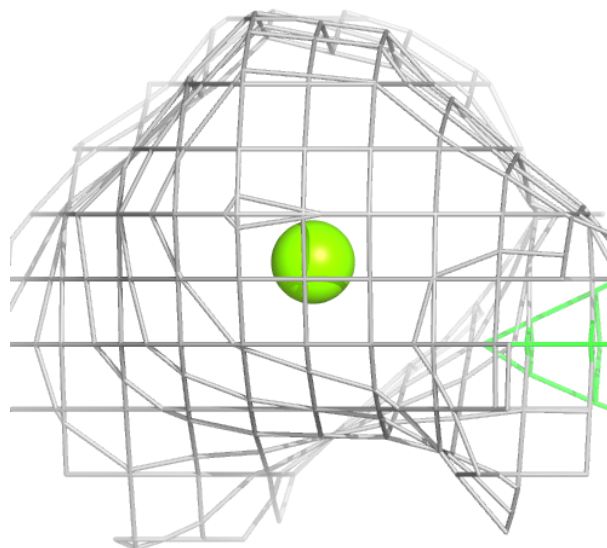
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





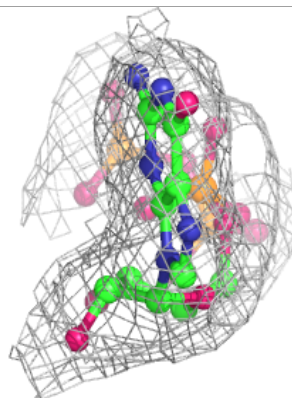
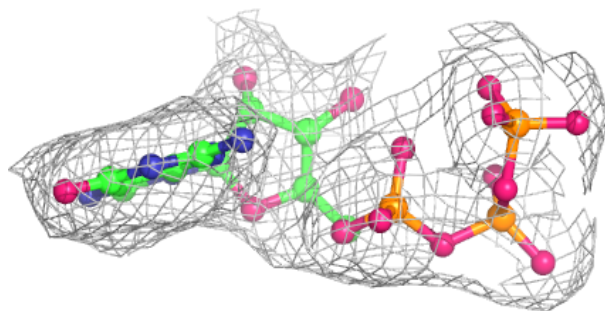
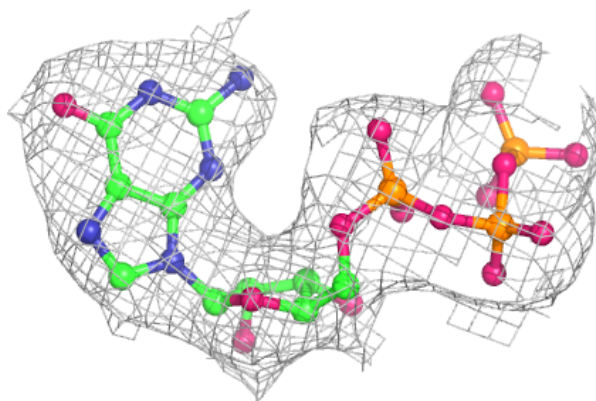
Electron density around MG B 702:

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



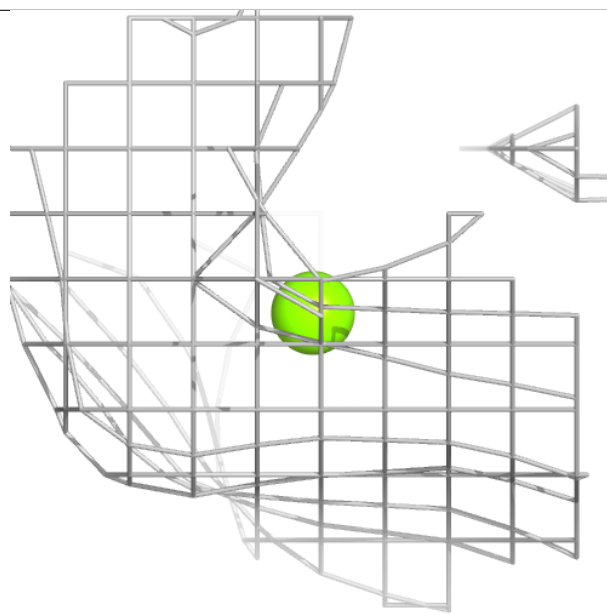
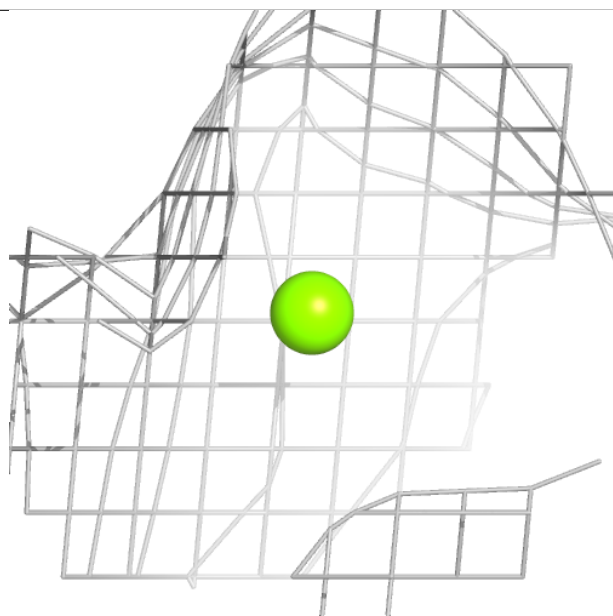
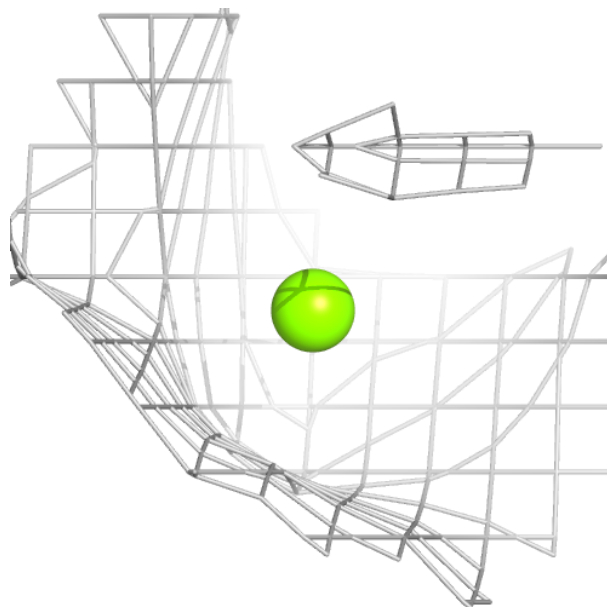
Electron density around GTP G 706:

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



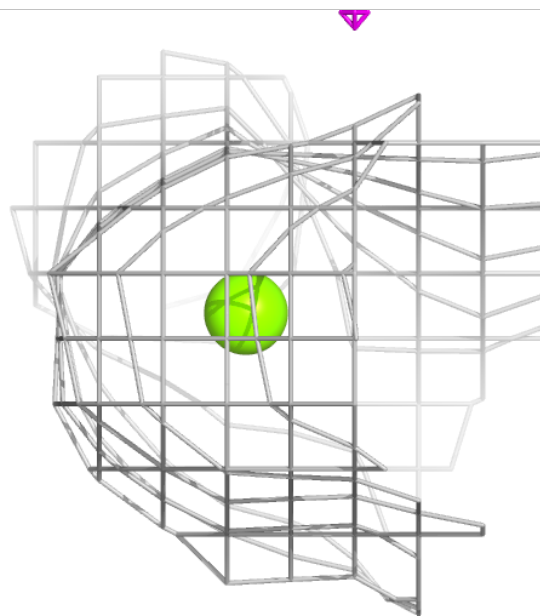
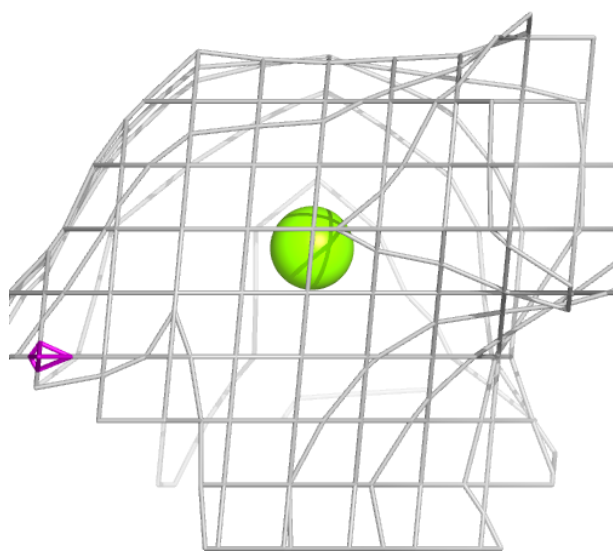
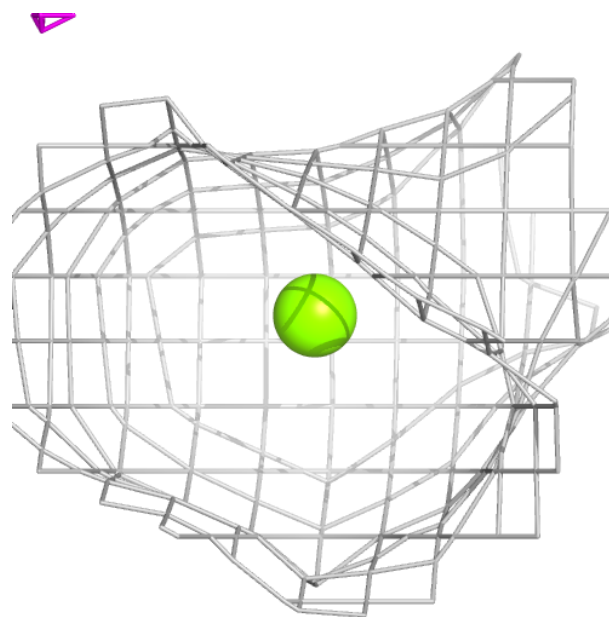
Electron density around MG M 703:

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



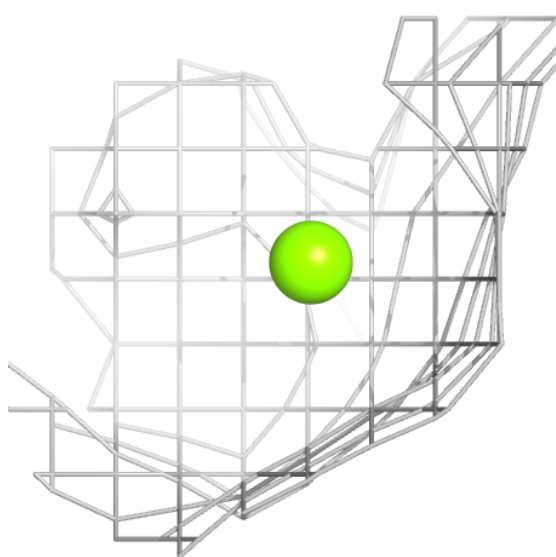
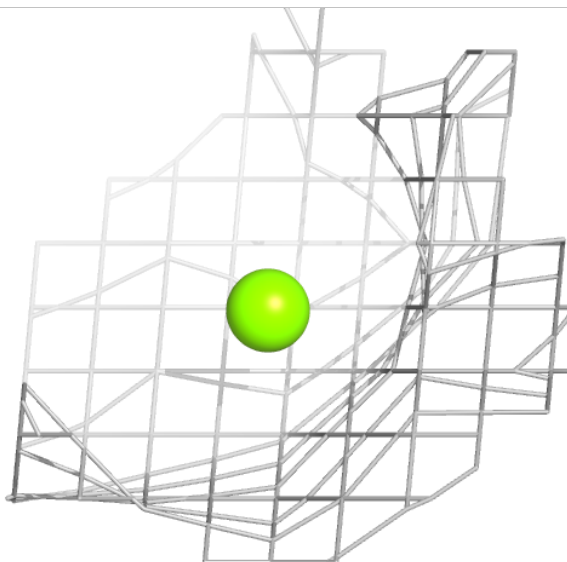
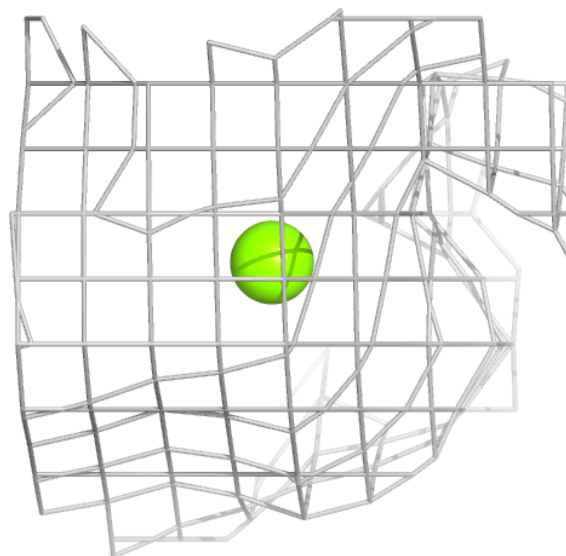
Electron density around MG A 702:

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



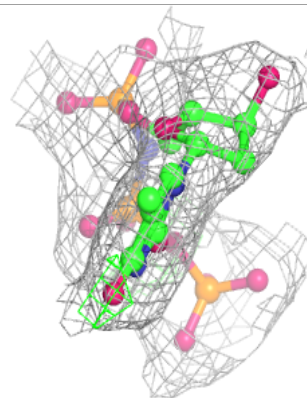
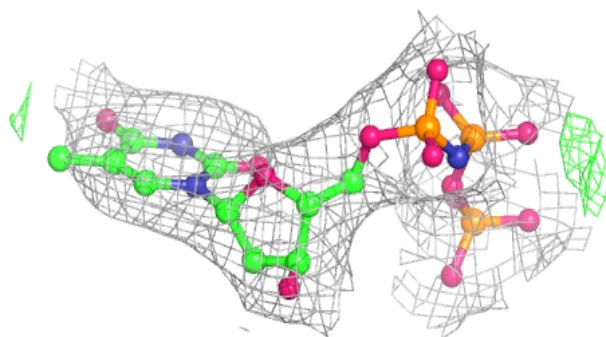
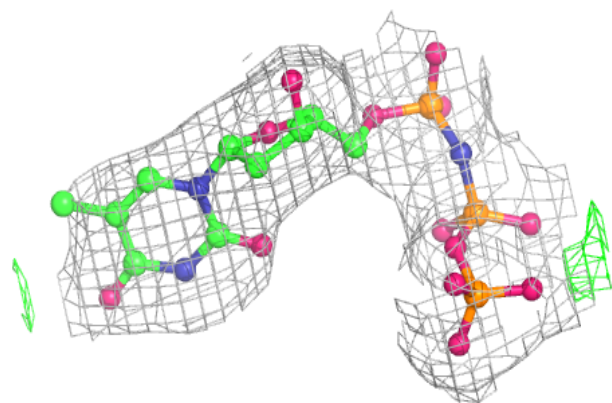
Electron density around MG N 704:

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



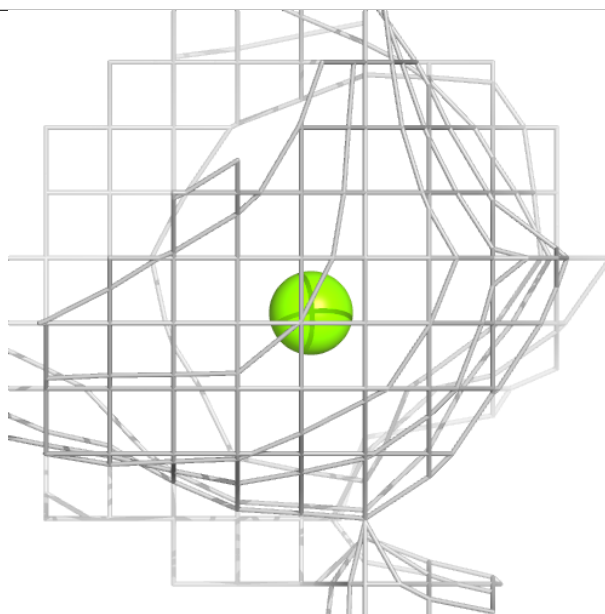
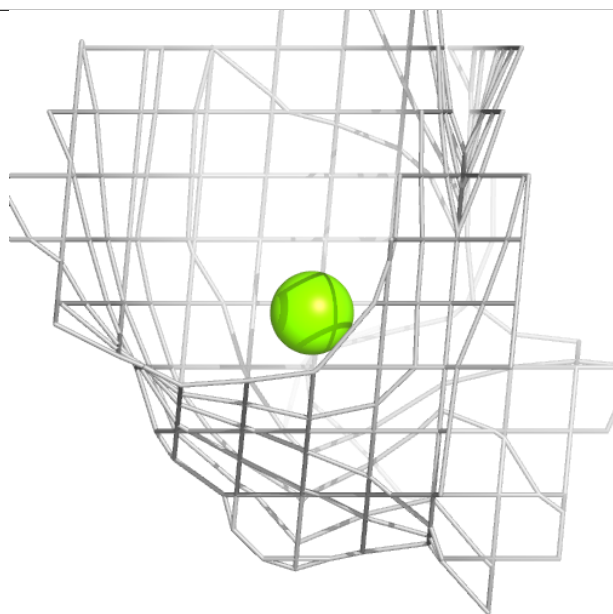
Electron density around 1FZ J 704:

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



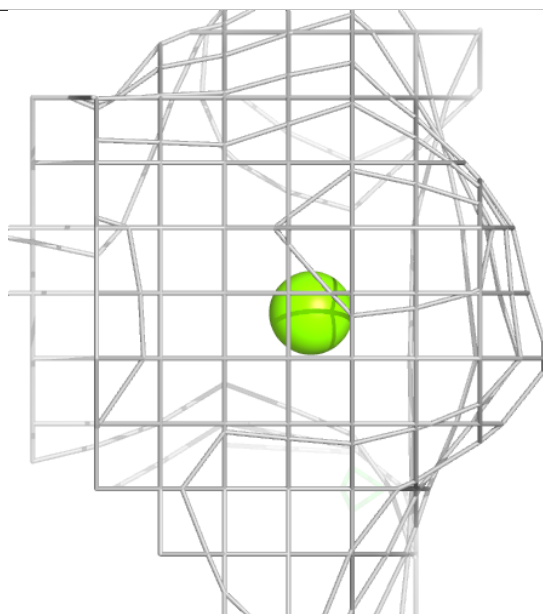
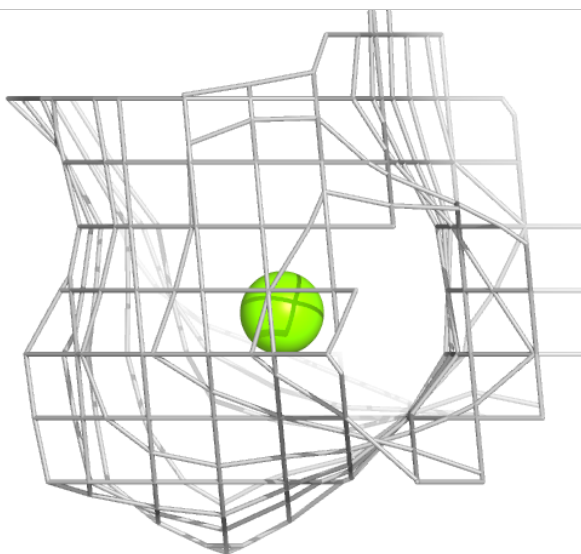
Electron density around MG A 703:

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



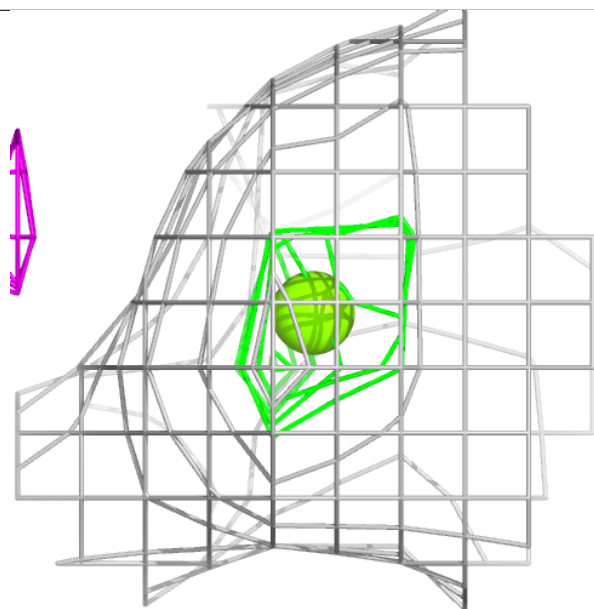
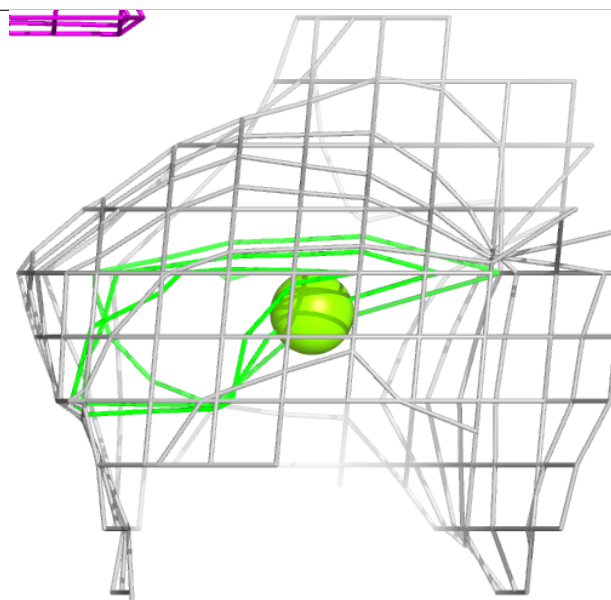
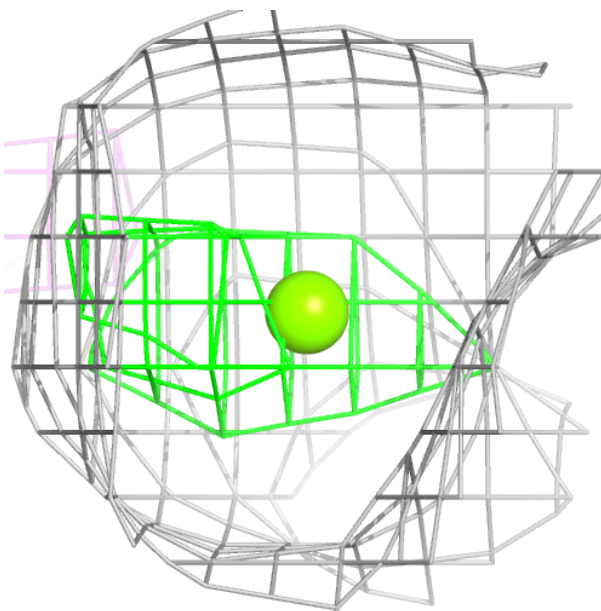
Electron density around MG G 703:

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



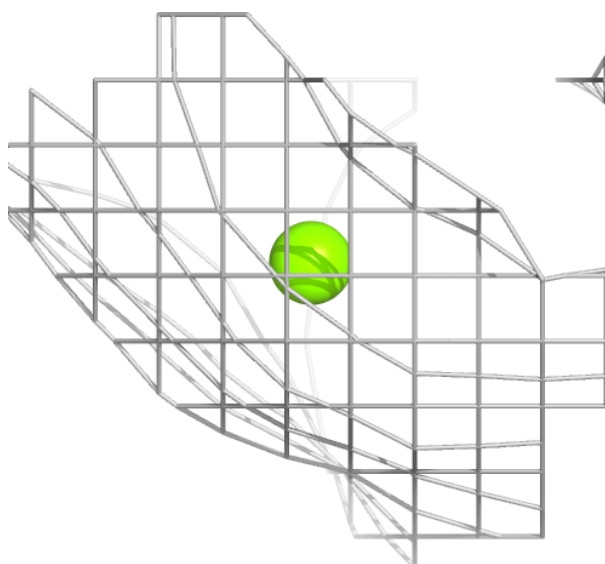
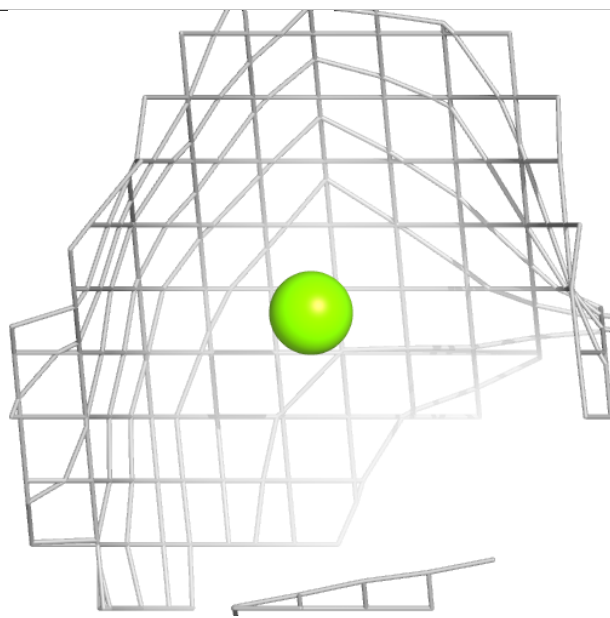
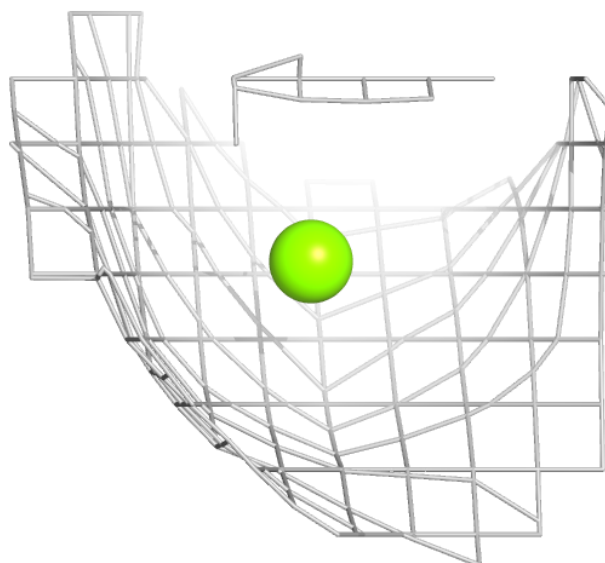
Electron density around MG J 702:

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



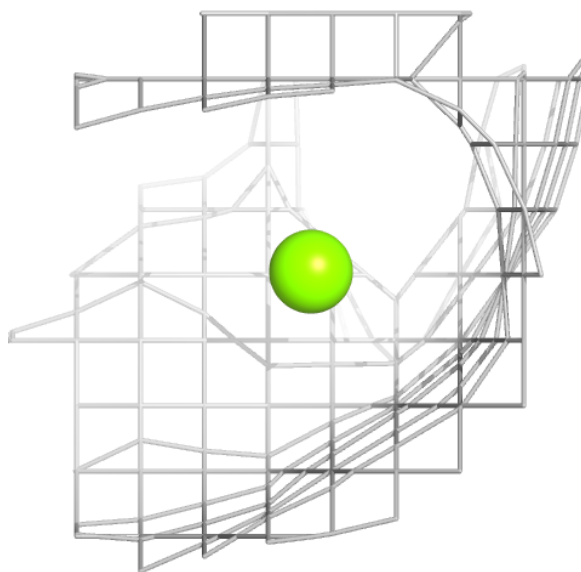
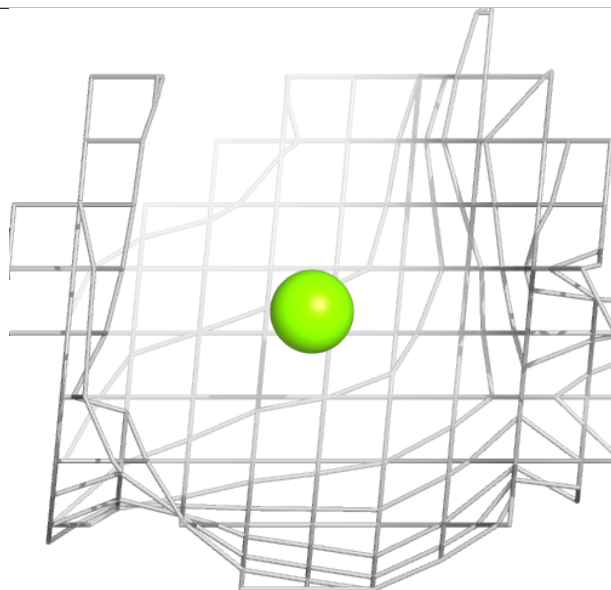
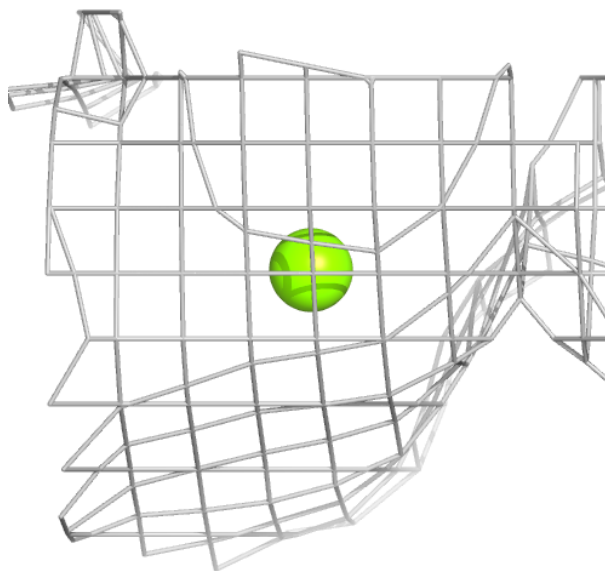
Electron density around MG P 703:

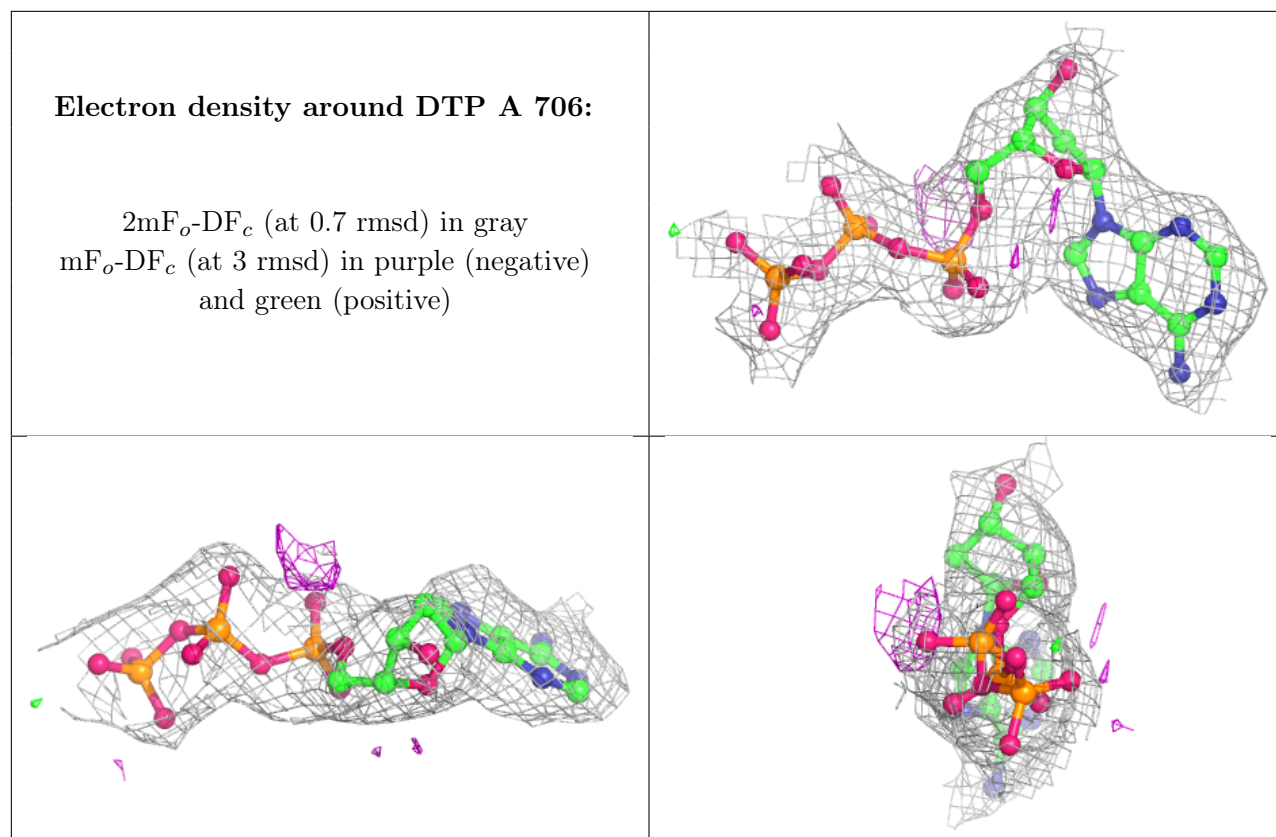
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG J 703:

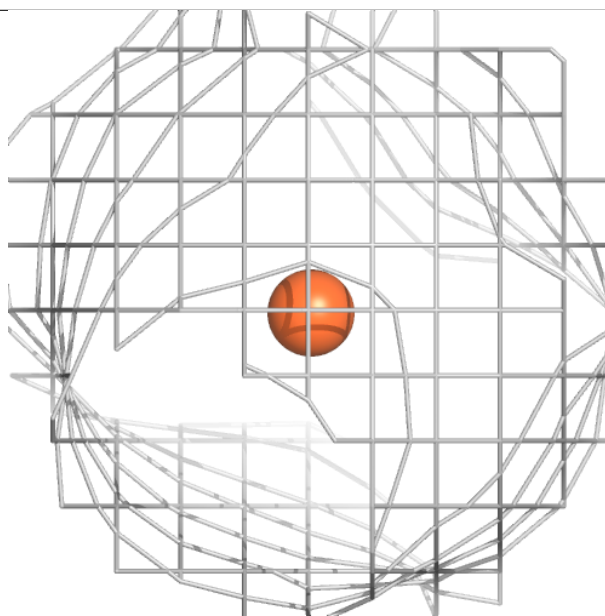
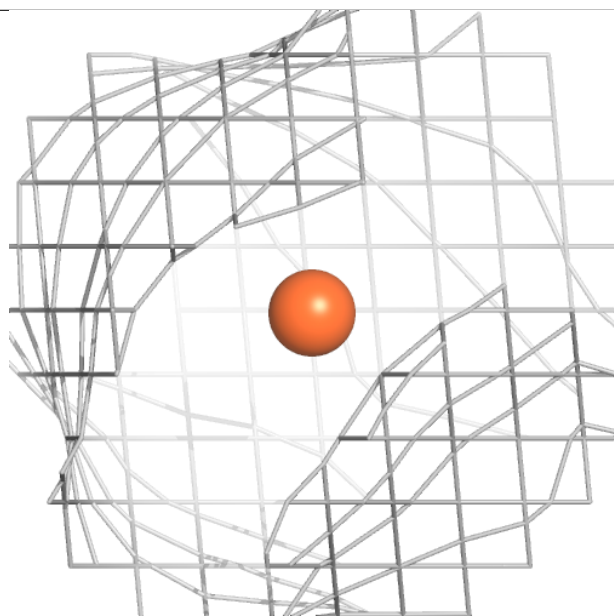
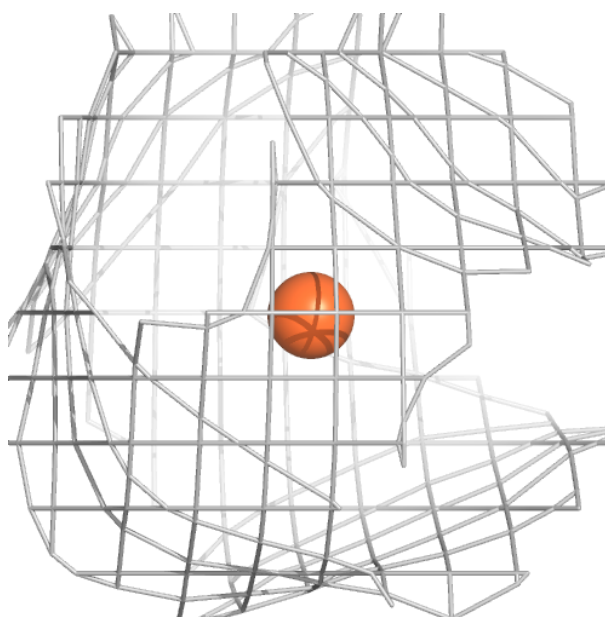
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





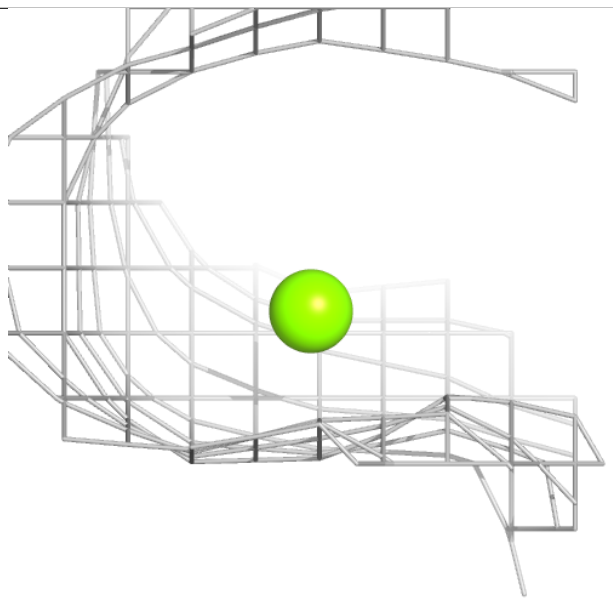
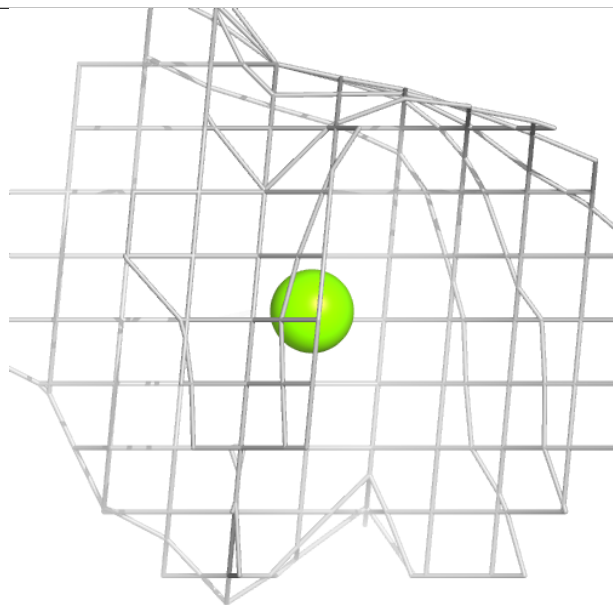
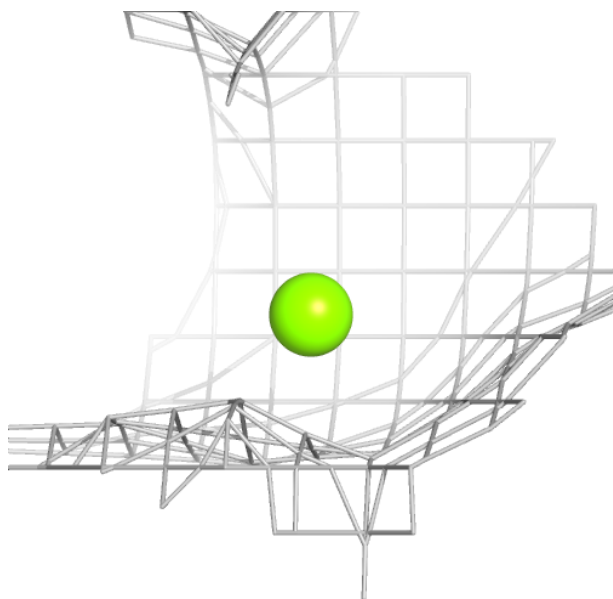
Electron density around FE O 701:

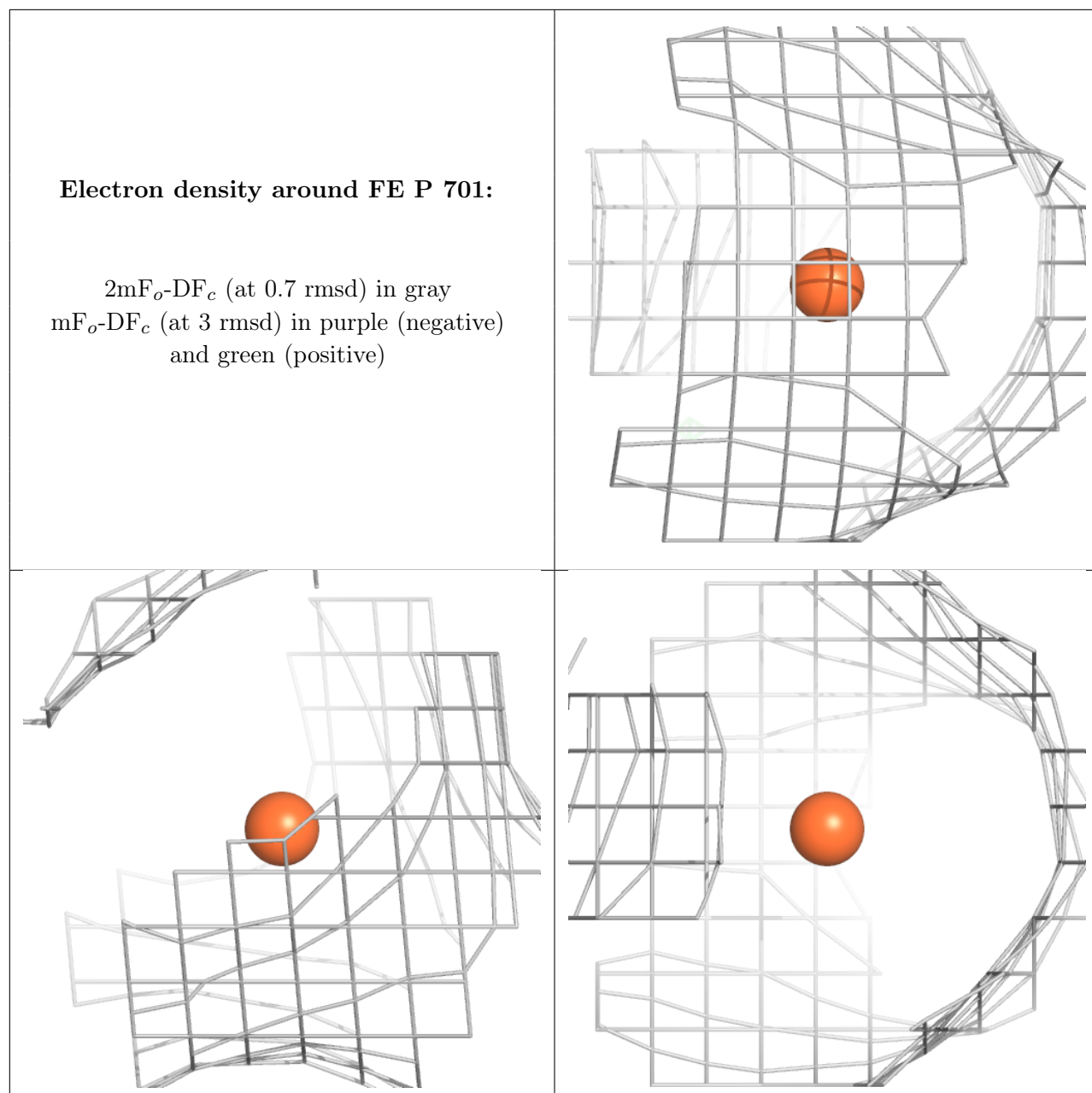
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG D 705:

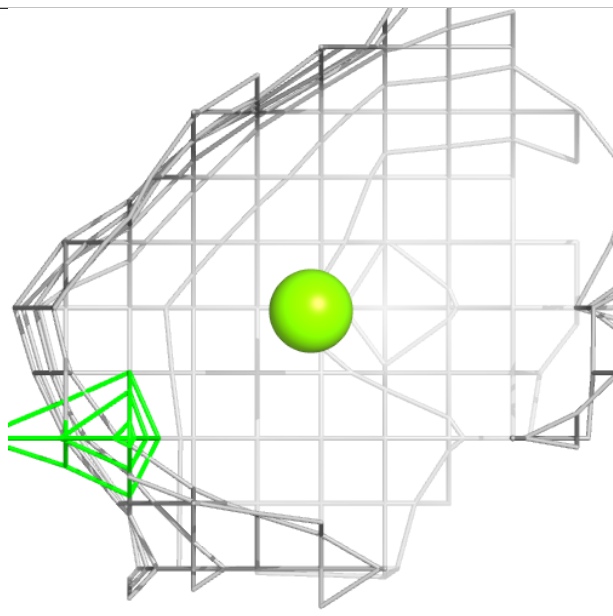
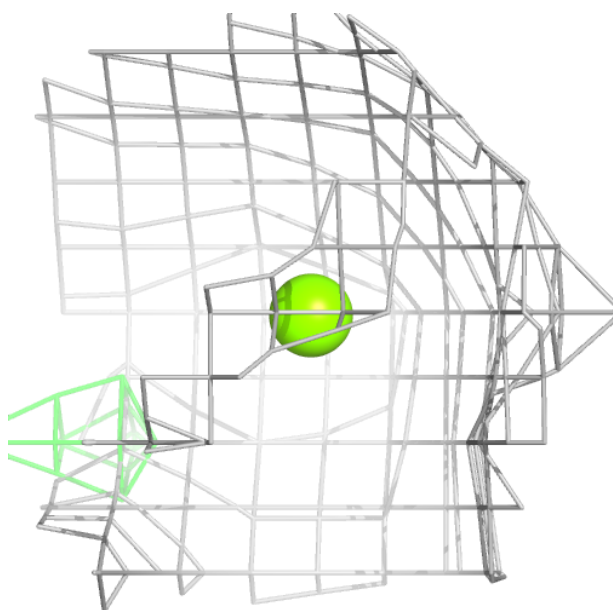
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





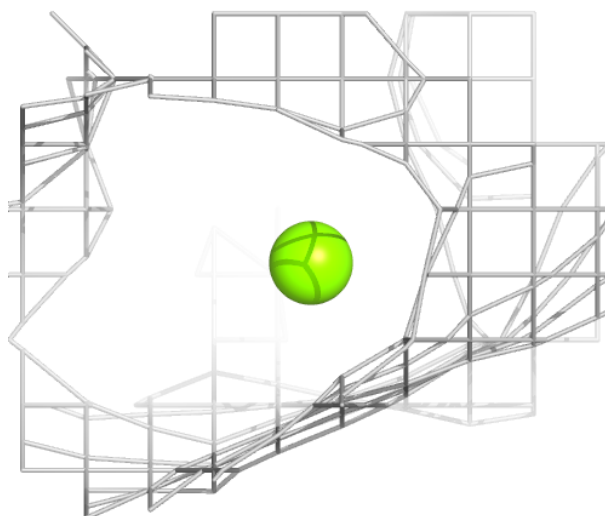
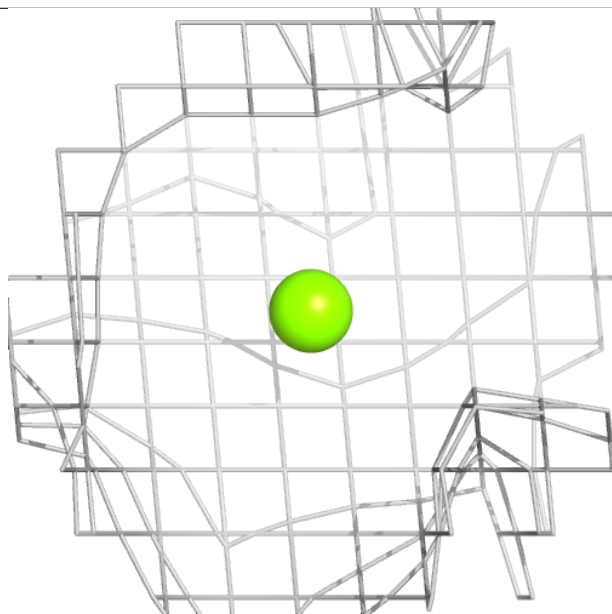
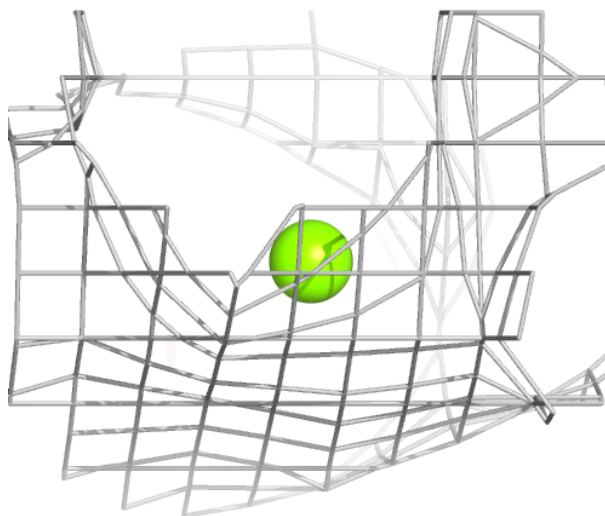
Electron density around MG E 703:

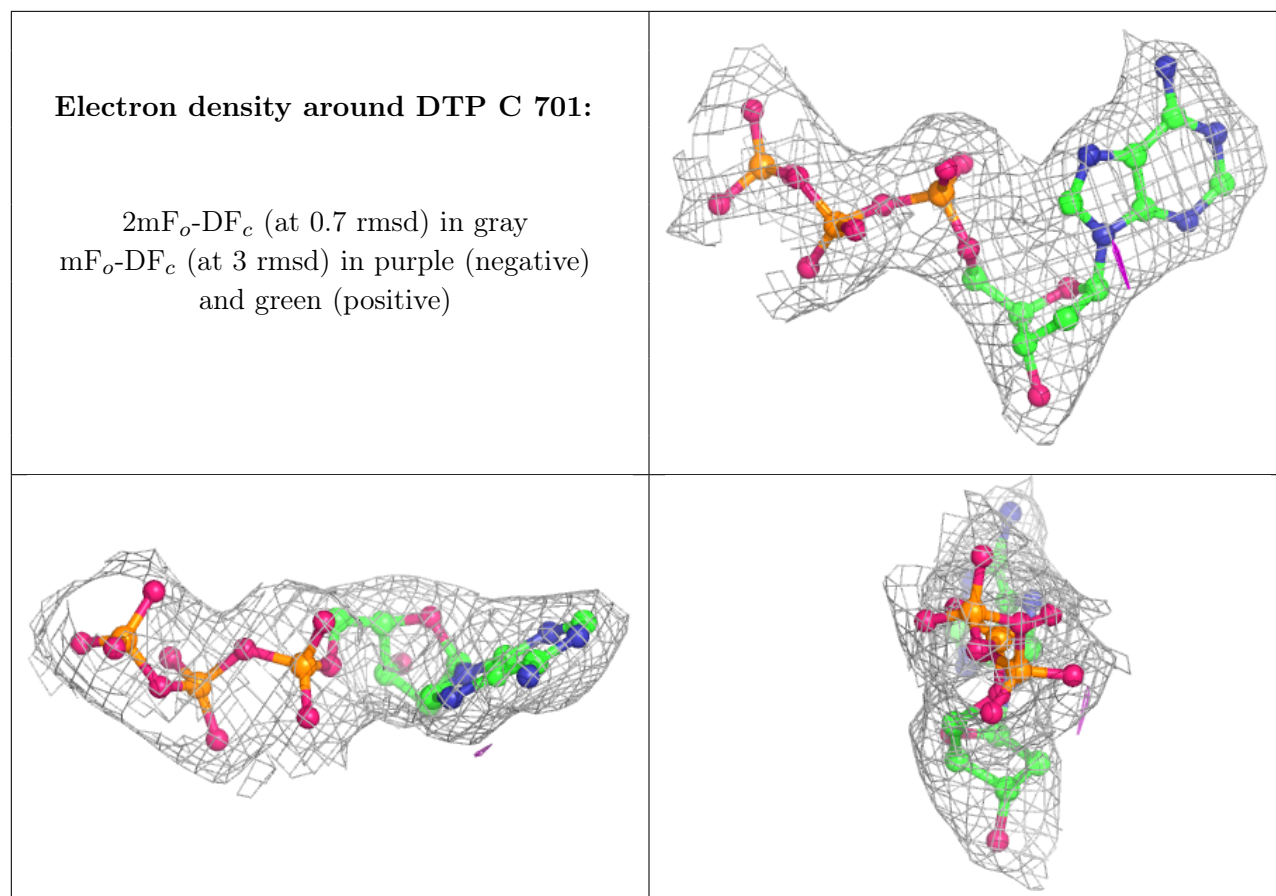
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG L 704:

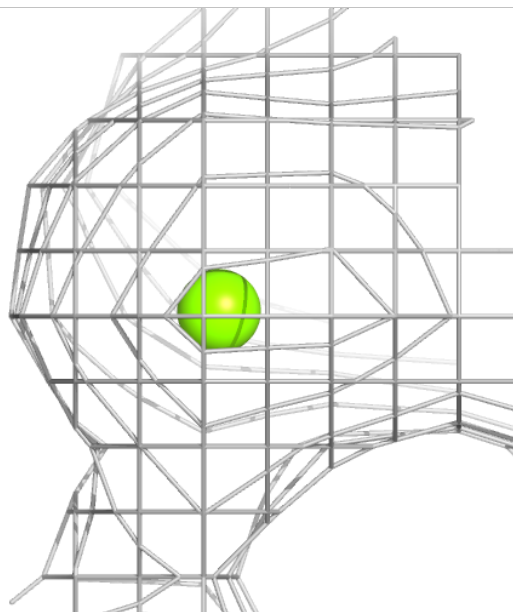
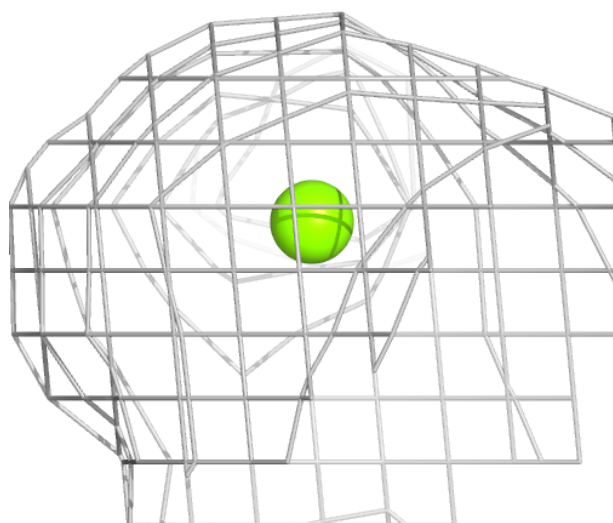
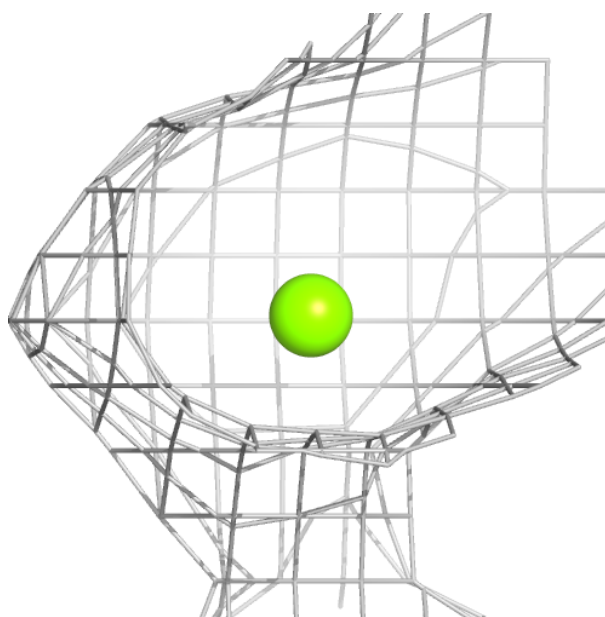
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





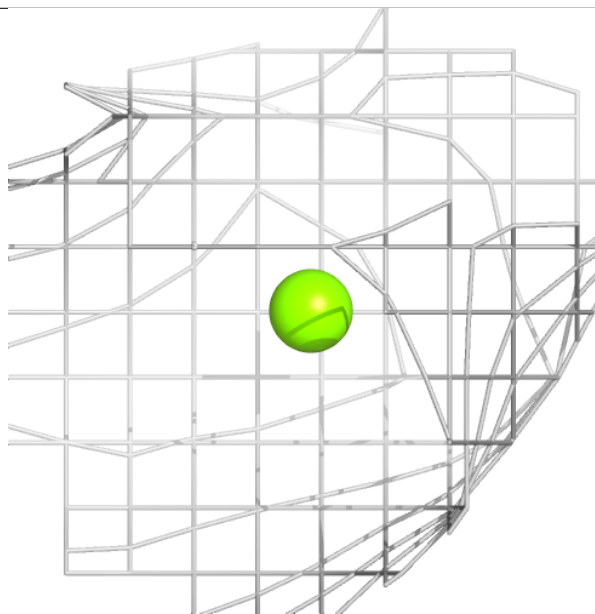
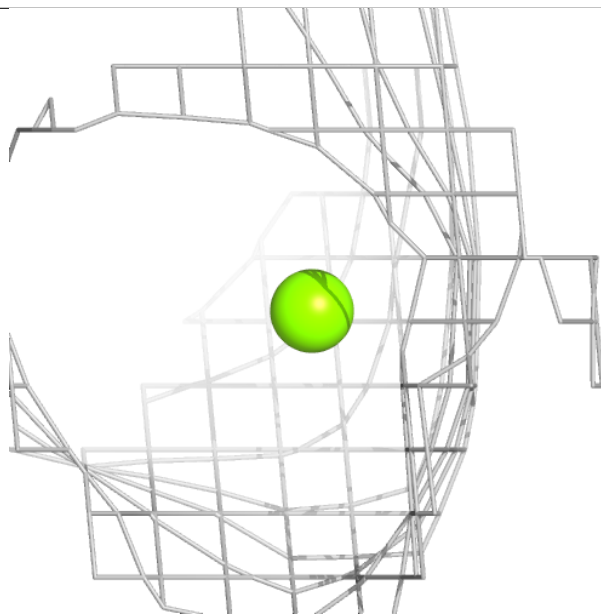
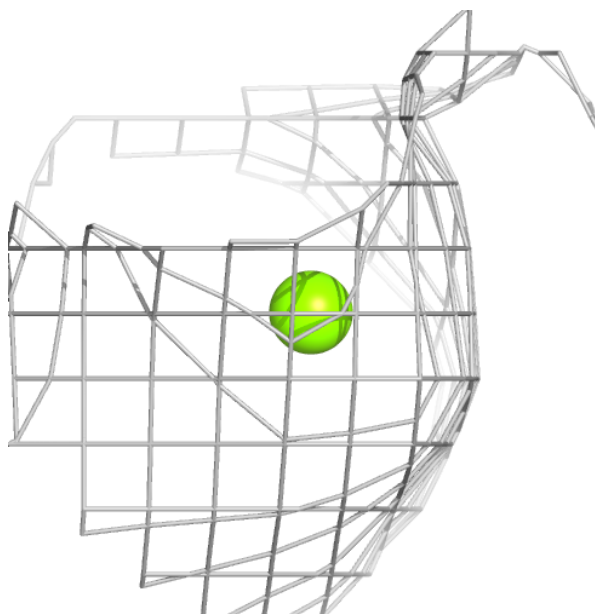
Electron density around MG F 702:

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



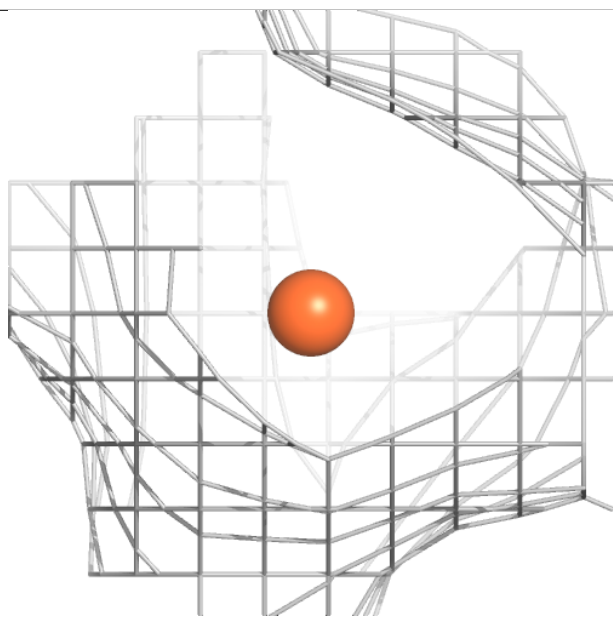
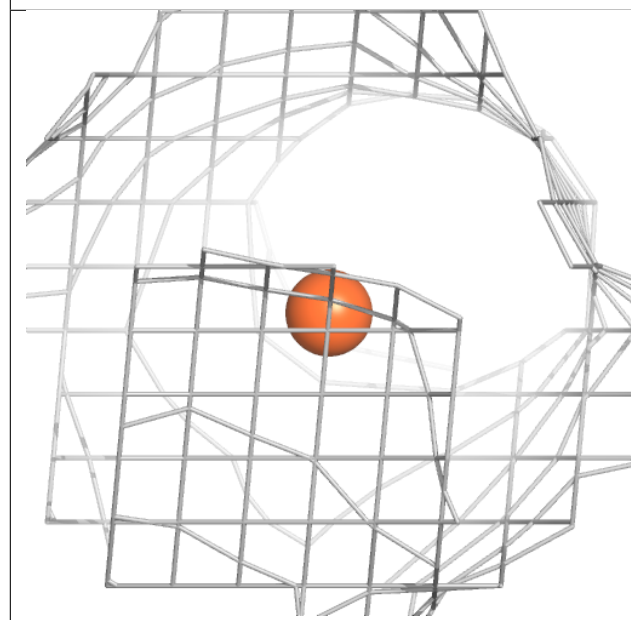
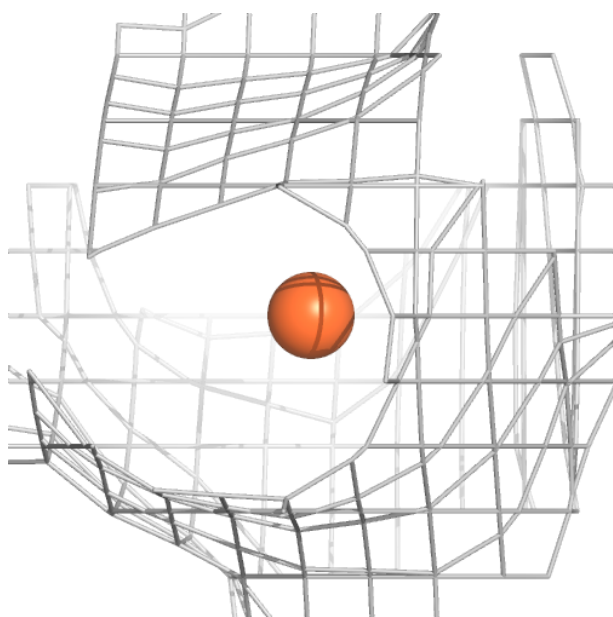
Electron density around MG F 703:

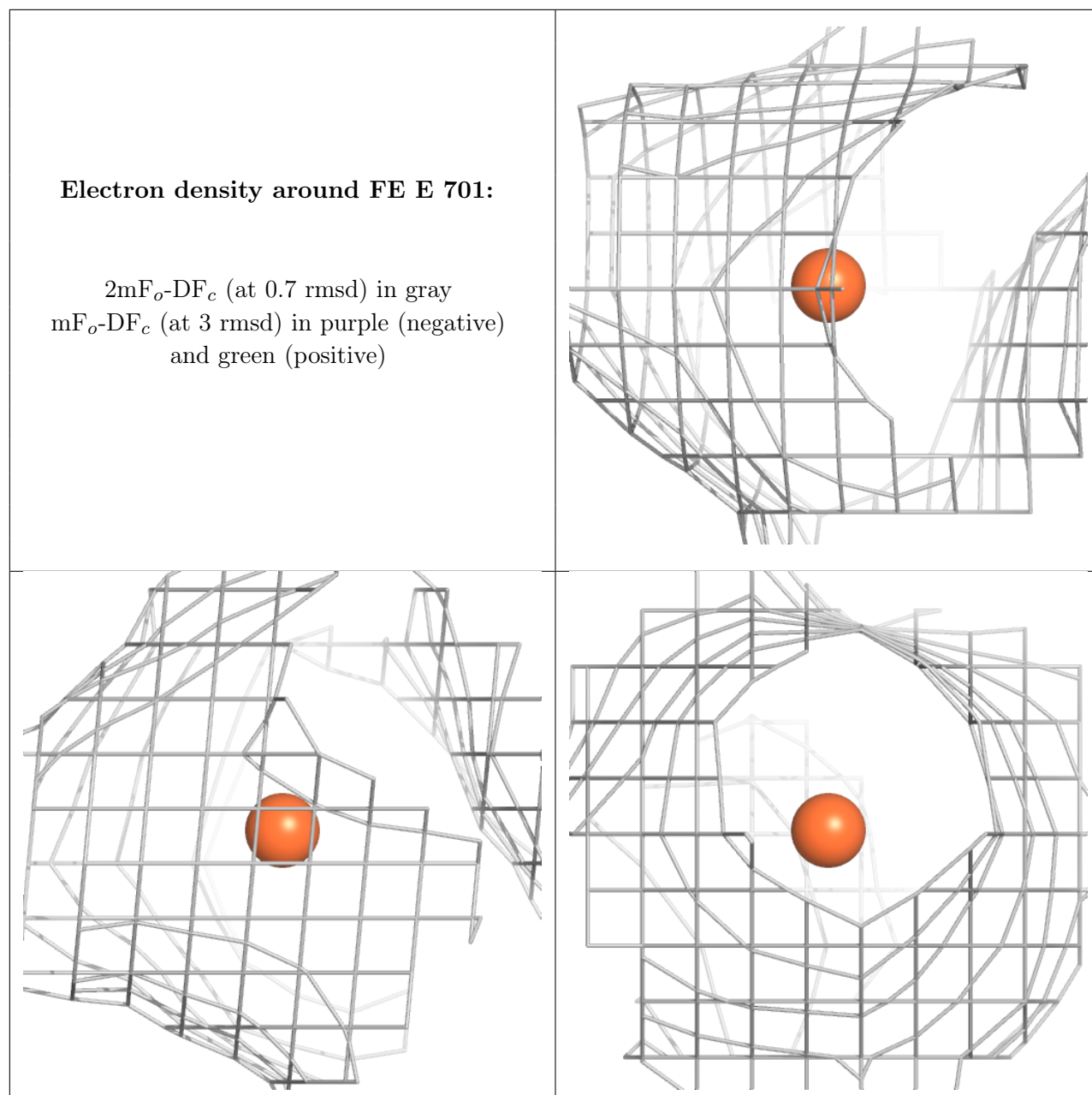
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE C 702:

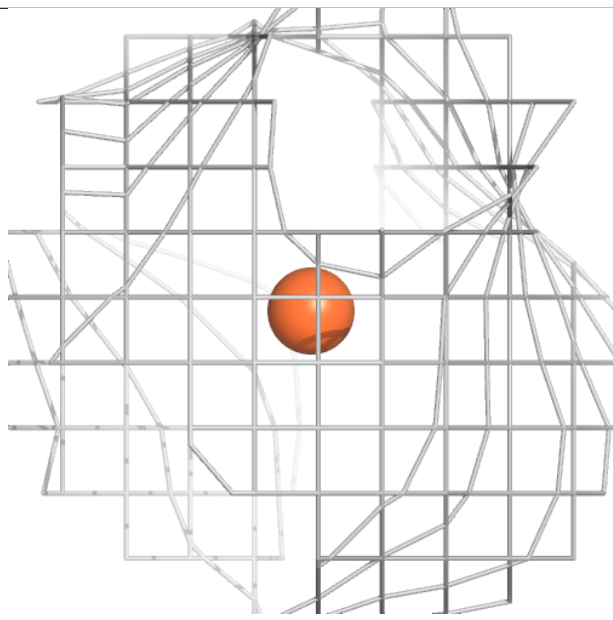
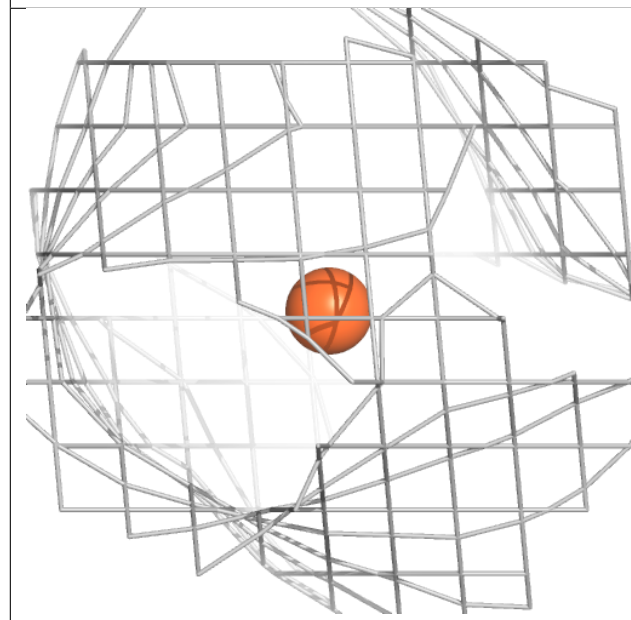
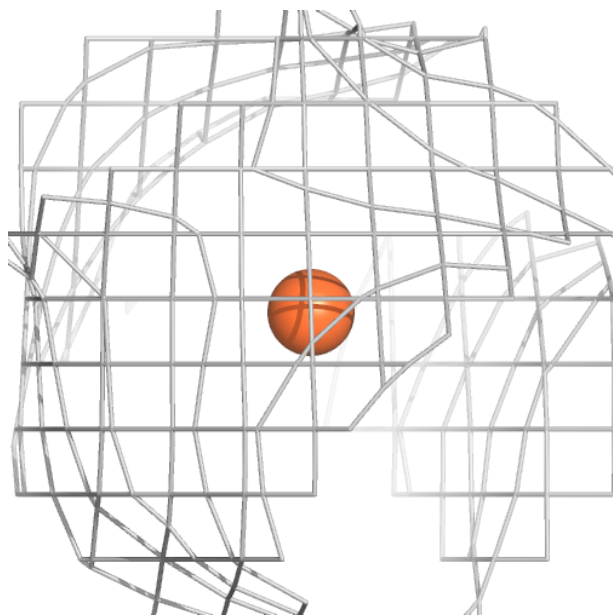
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





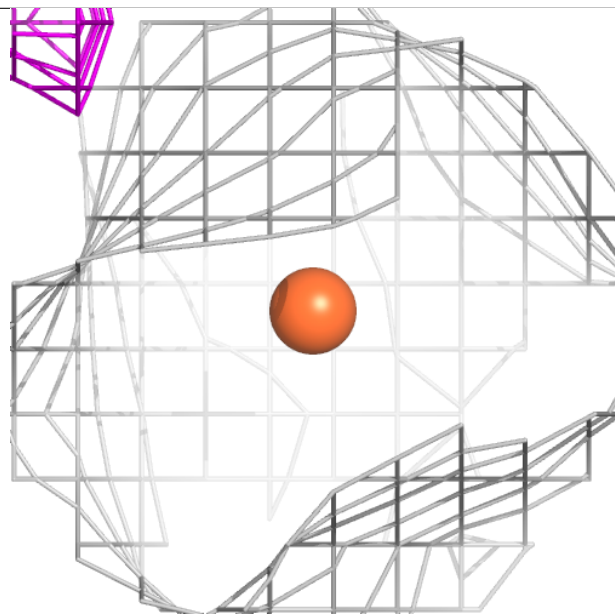
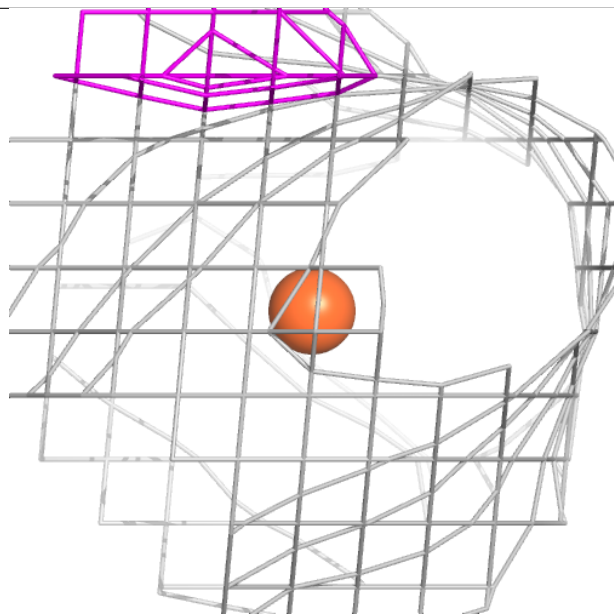
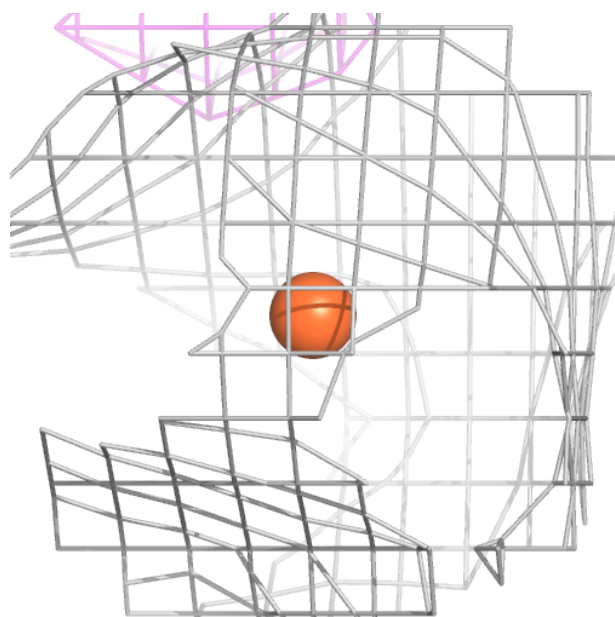
Electron density around FE I 701:

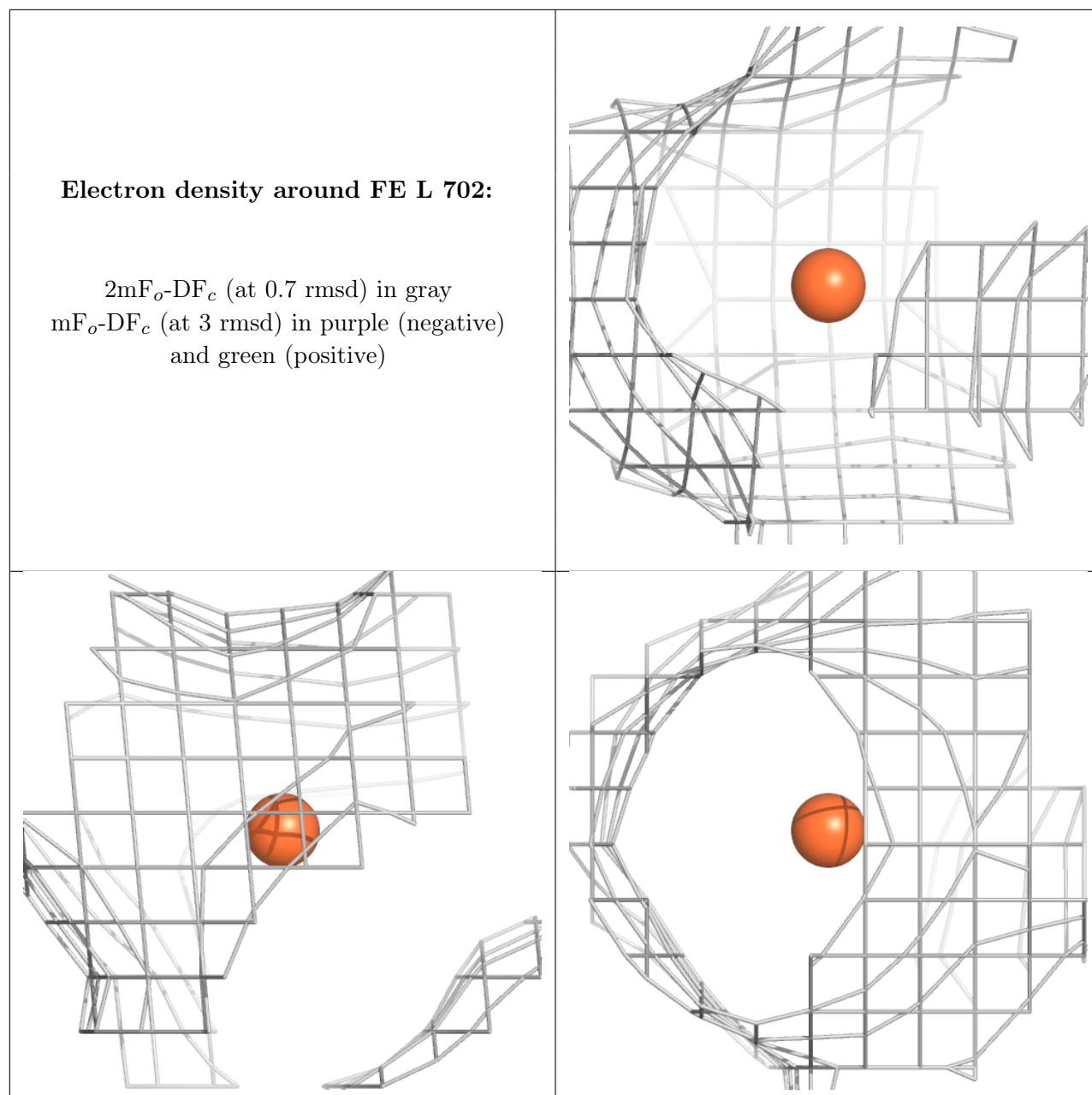
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE K 702:

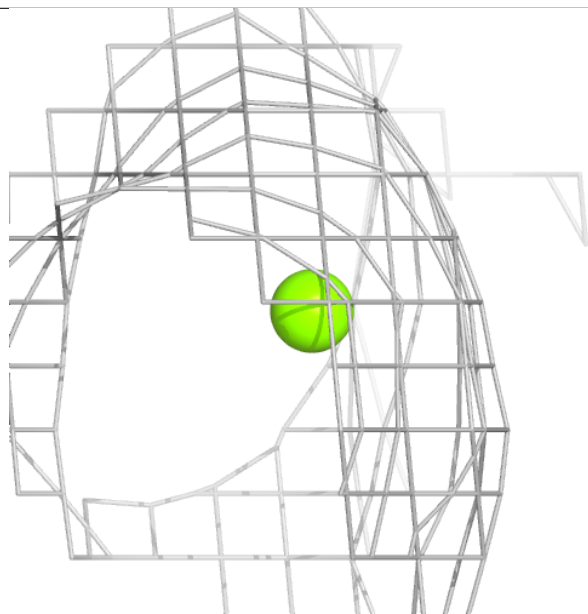
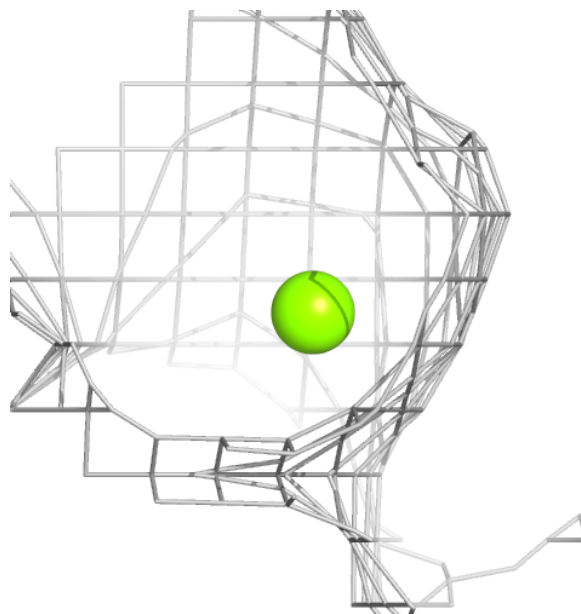
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





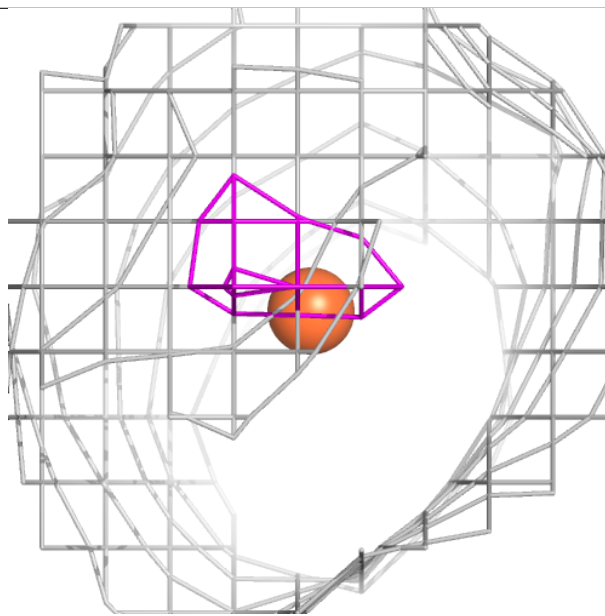
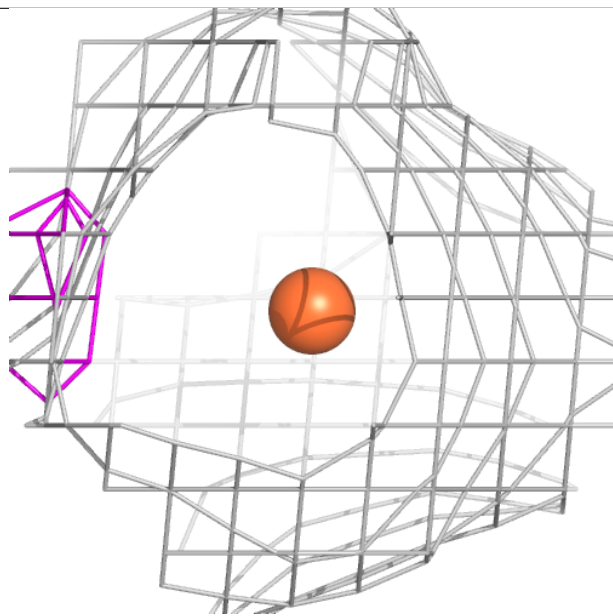
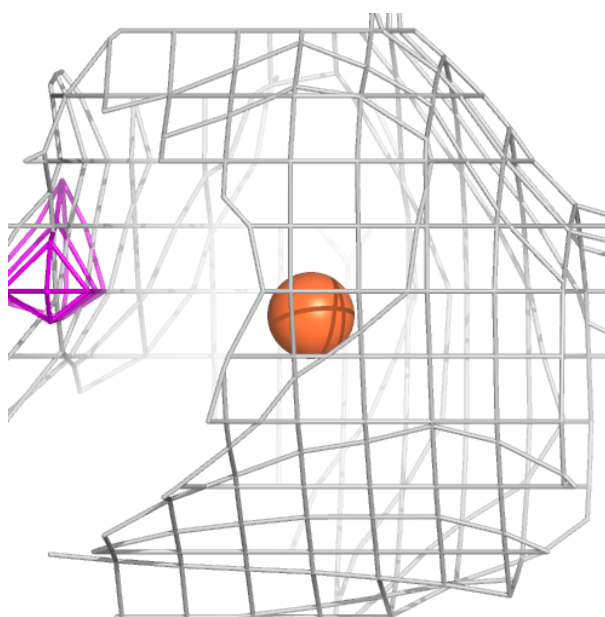
Electron density around MG I 703:

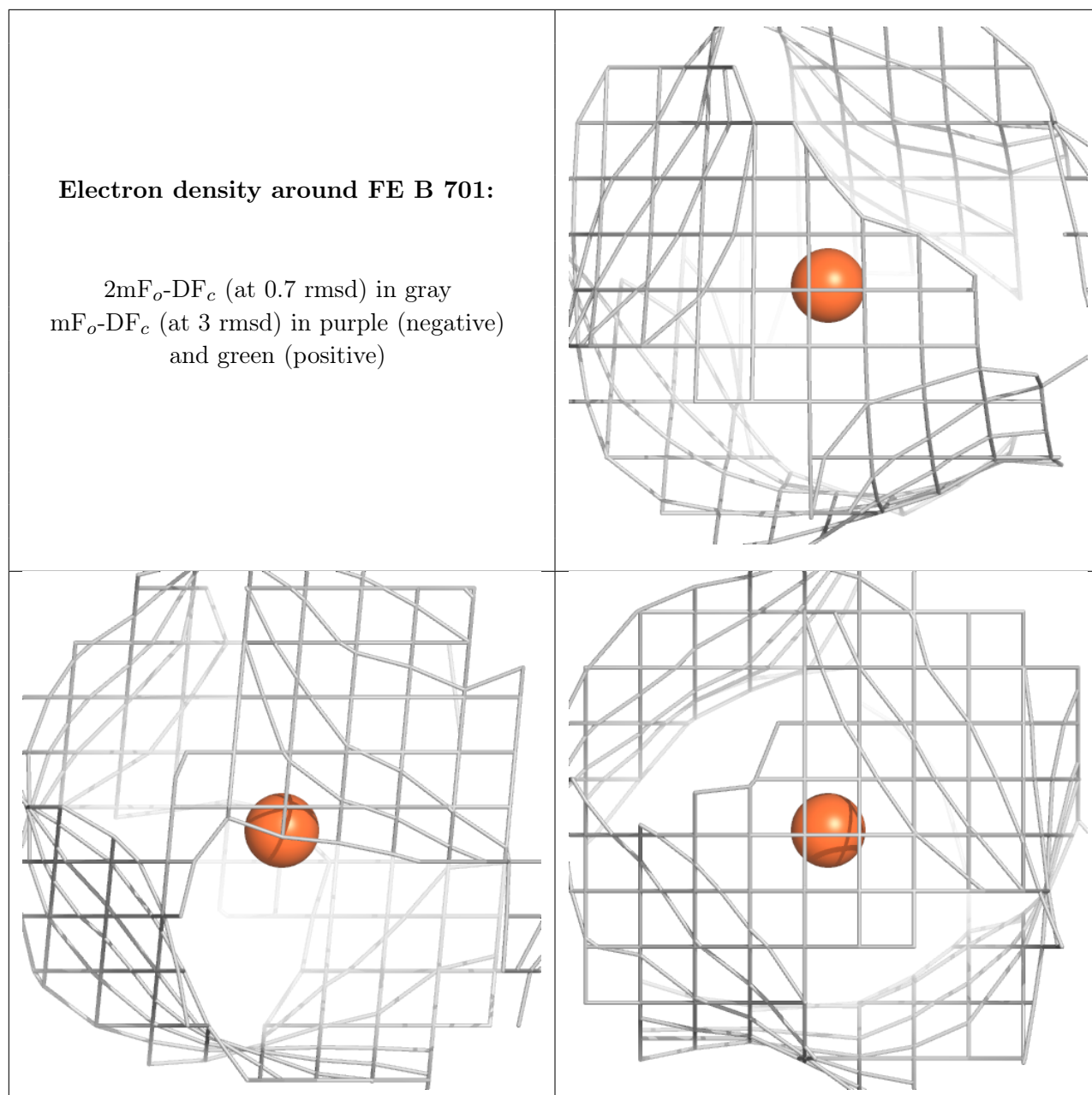
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE N 702:

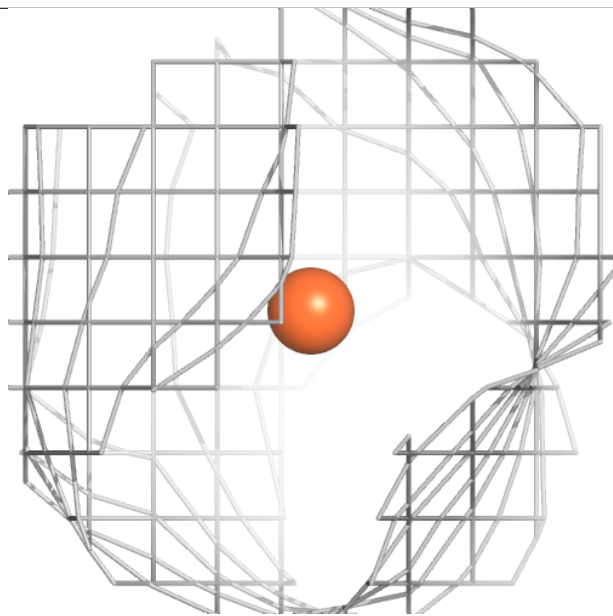
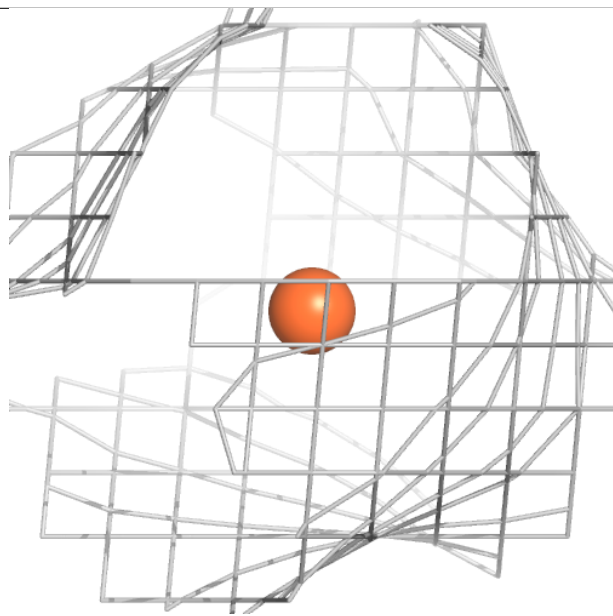
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

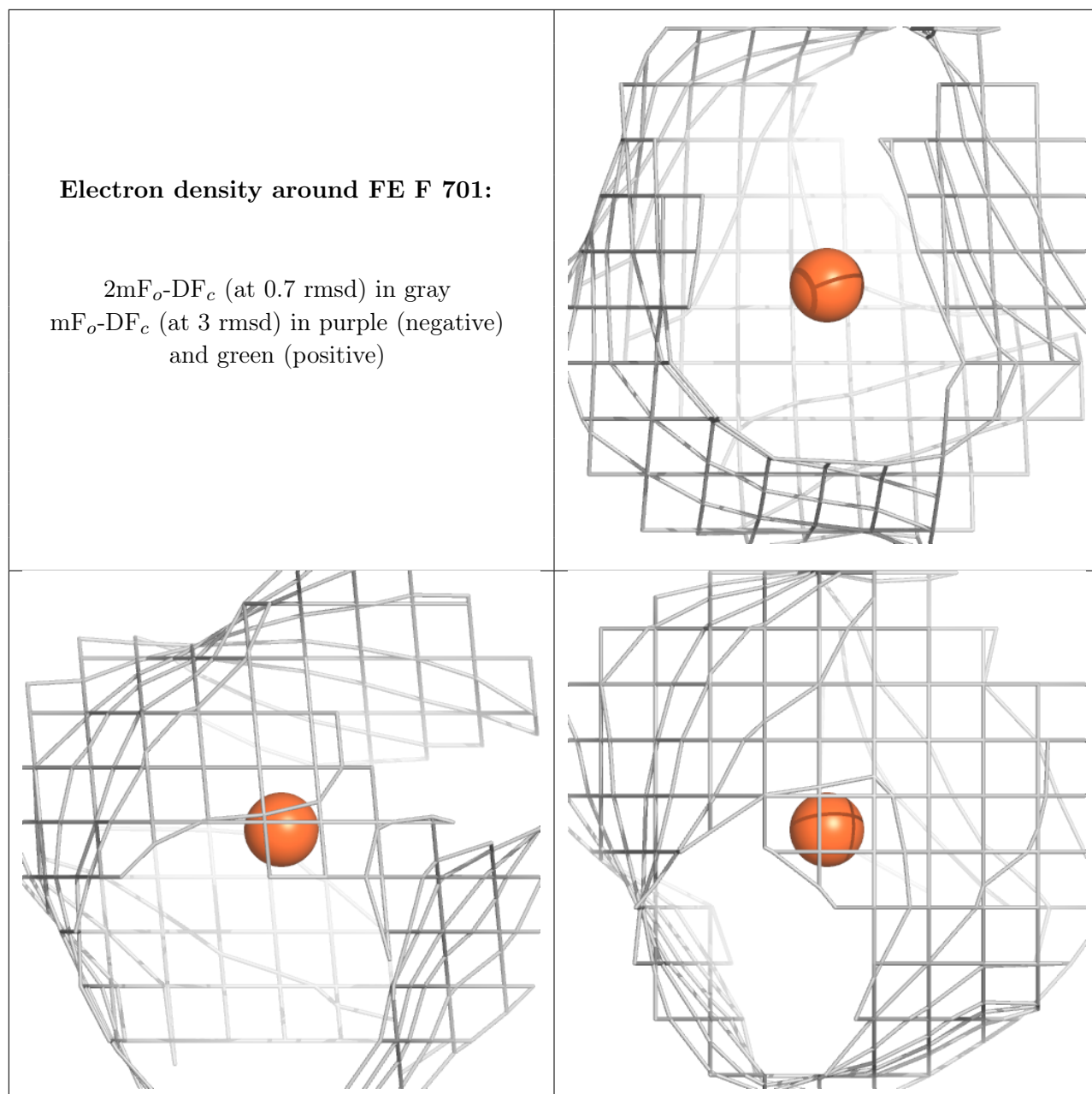




Electron density around FE M 701:

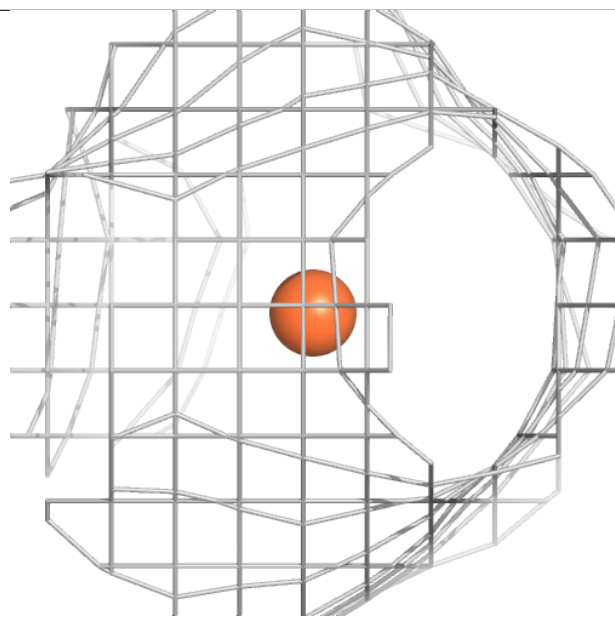
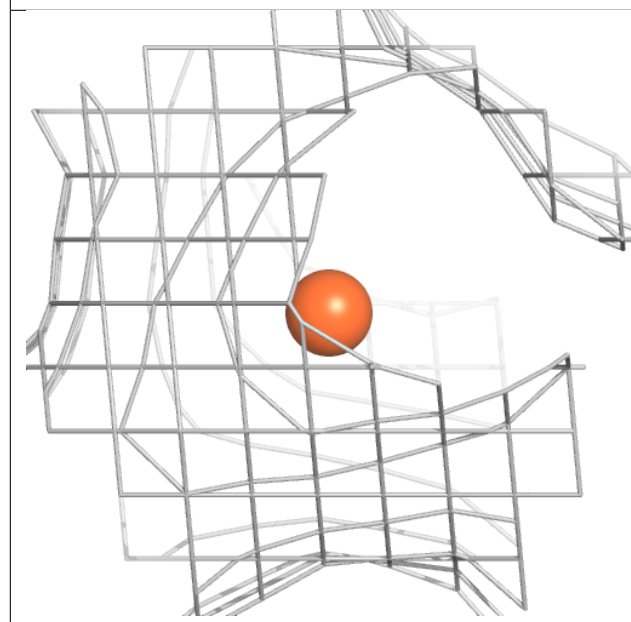
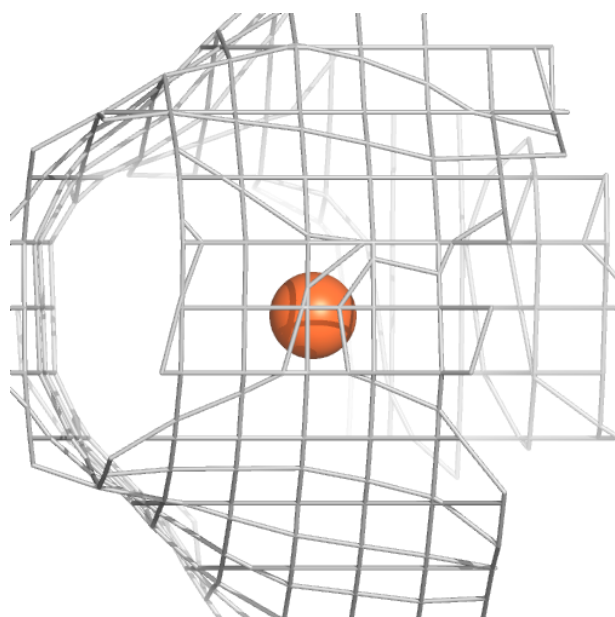
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

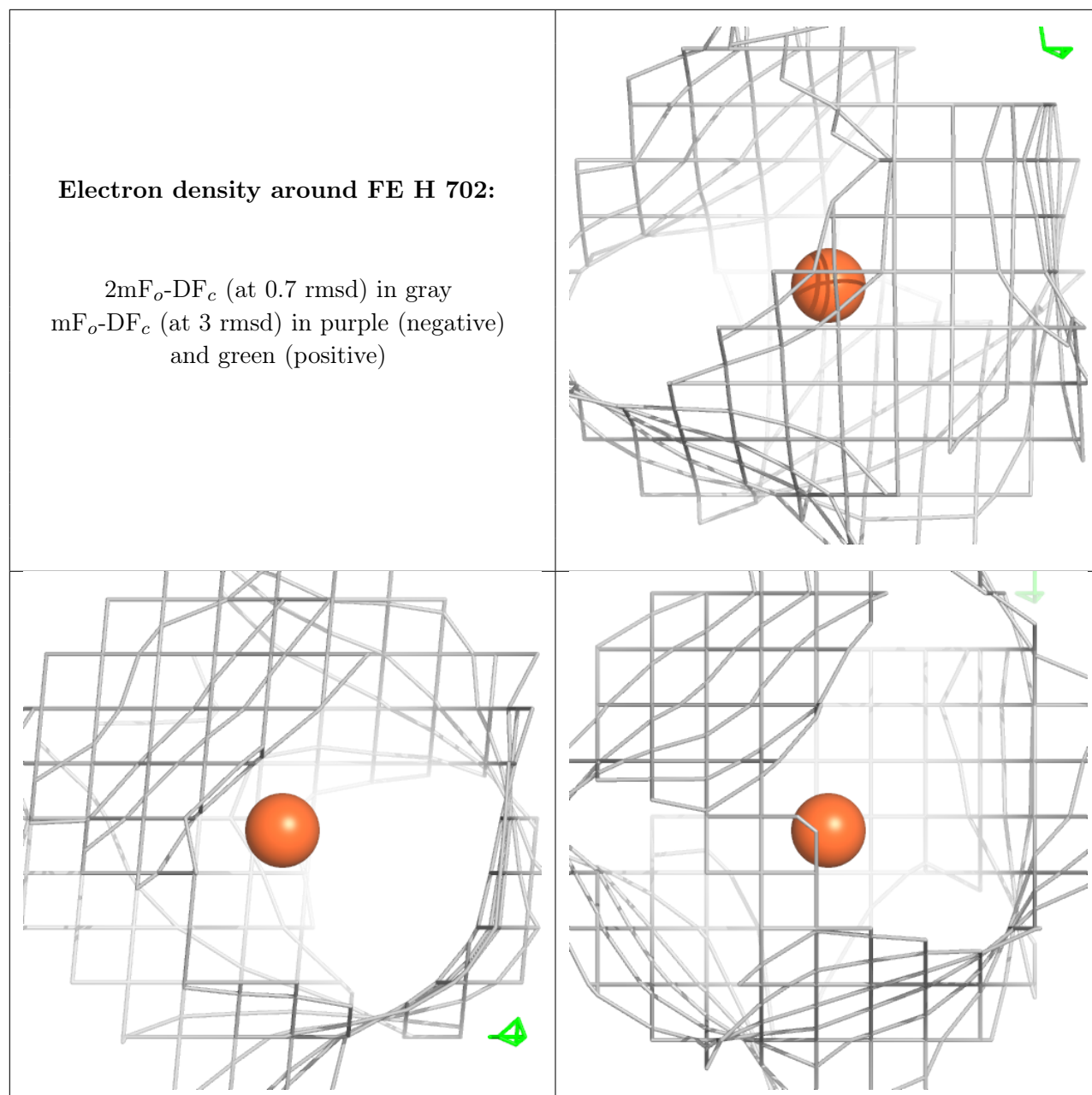




Electron density around FE G 702:

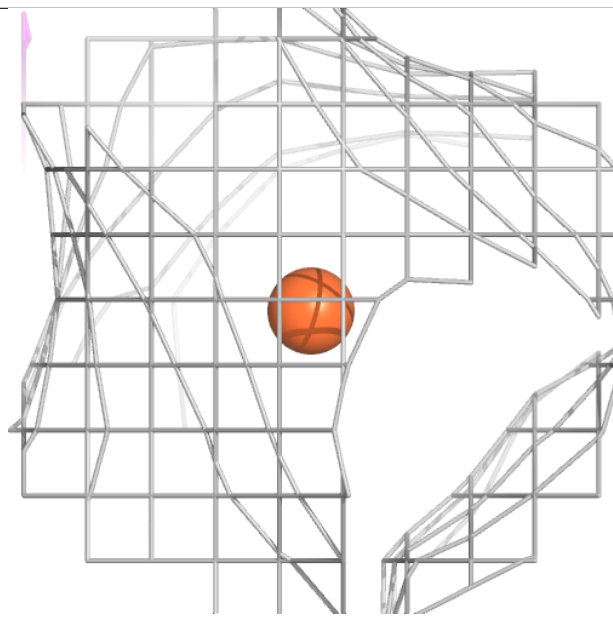
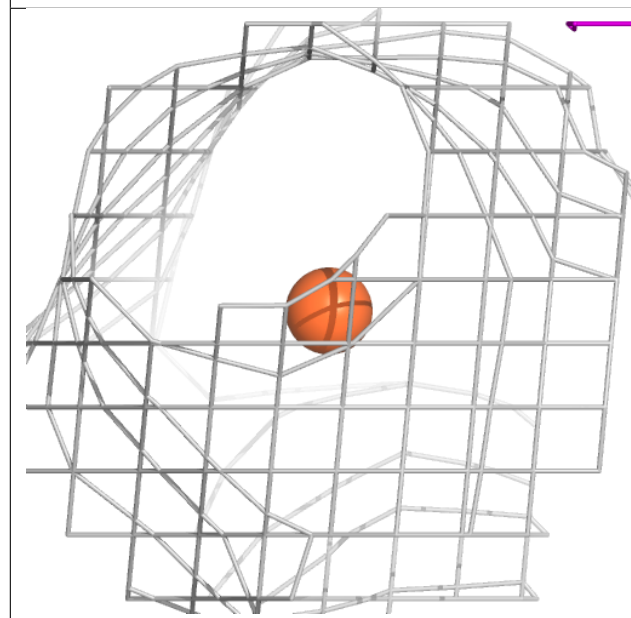
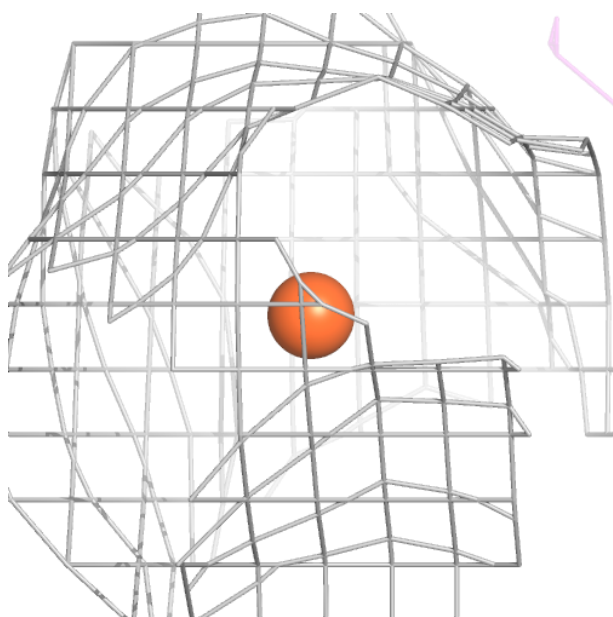
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





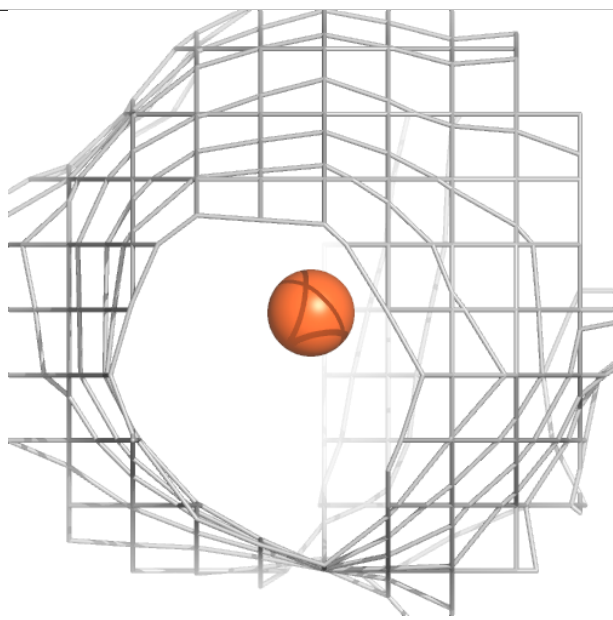
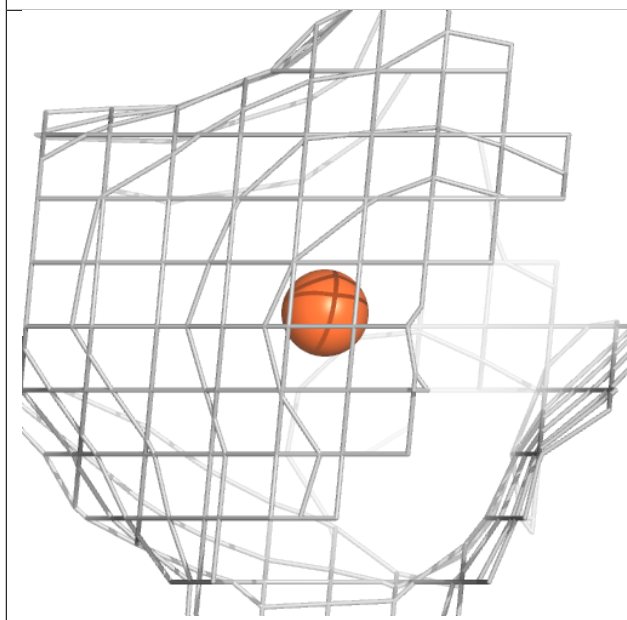
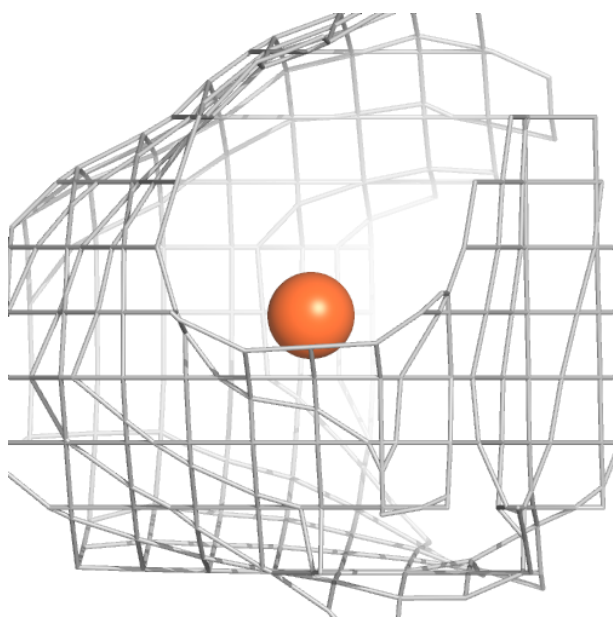
Electron density around FE A 701:

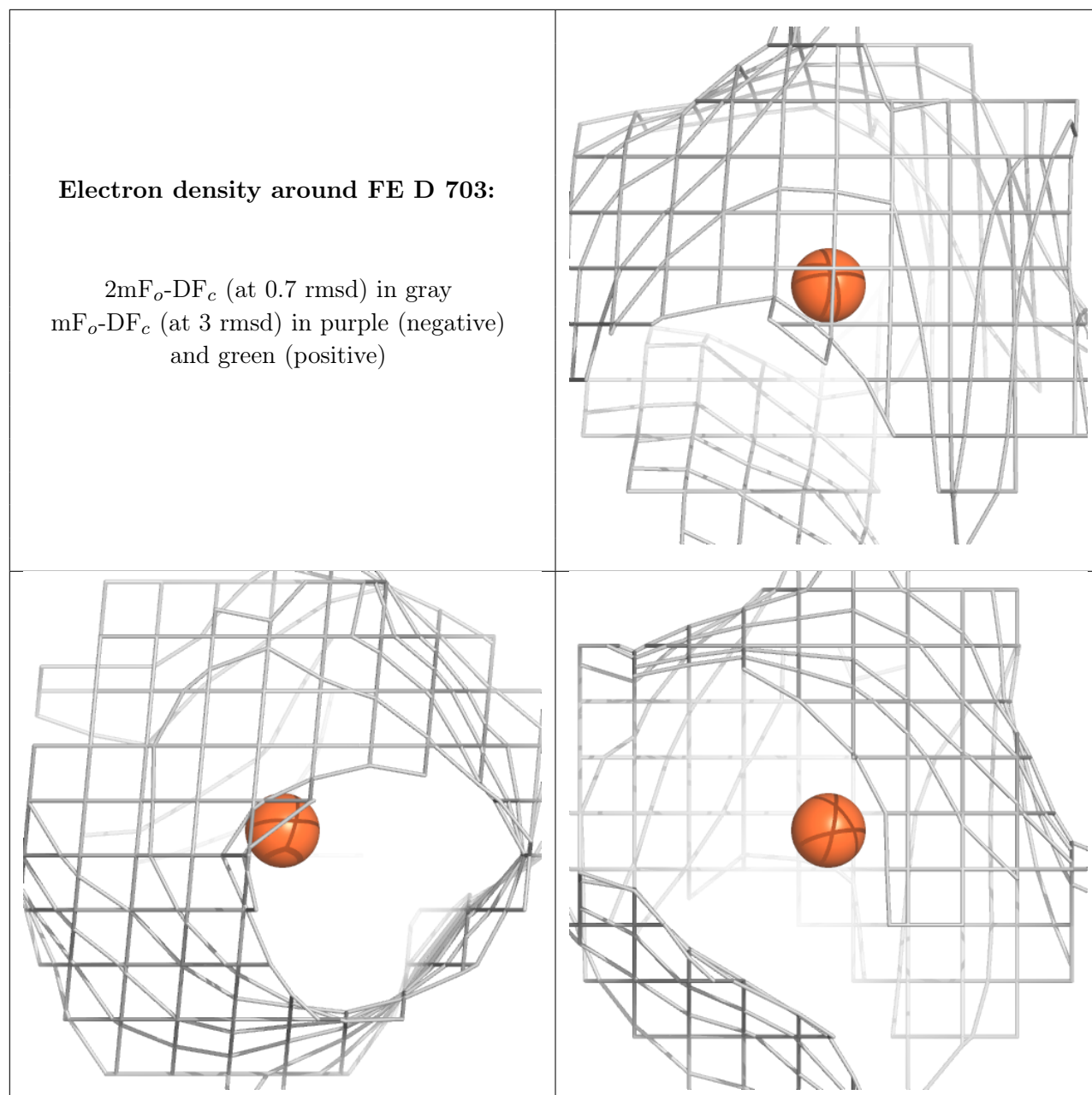
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE J 701:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.