



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 14, 2024 – 02:53 am GMT

PDB ID : 6XU1  
Title : Crystal structure of tetrameric human H215A-SAMHD1 (residues 109-626) with GTP, dAMPNPP and Mg  
Authors : Morris, E.R.; Kunzelmann, S.; Caswell, S.J.; Arnold, L.H.; Purkiss, A.G.; Kelly, G.; Taylor, I.A.  
Deposited on : 2020-01-17  
Resolution : 2.20 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

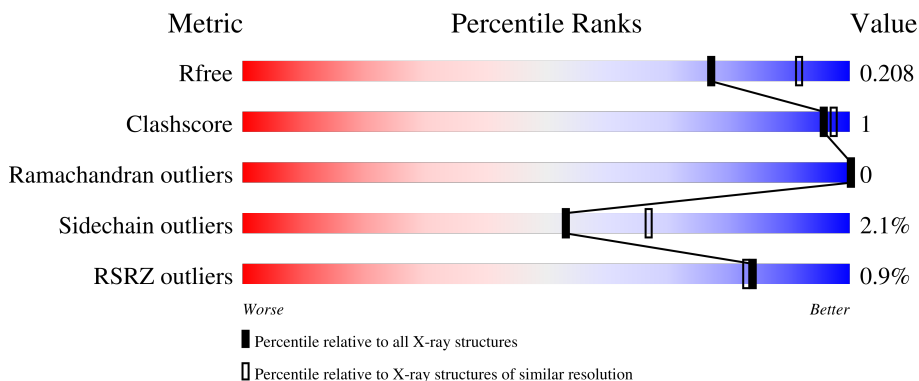
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


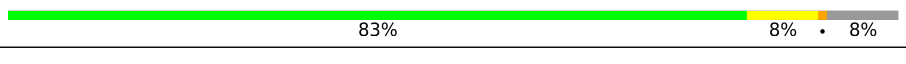
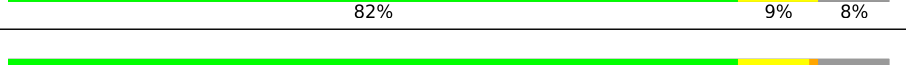

The reported resolution of this entry is 2.20 Å.

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.



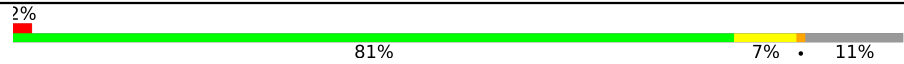



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	520	 86% 6% • 8%
1	B	520	 83% 8% • 8%
1	C	520	 82% 9% 8%
1	D	520	 82% 8% • 8%

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Mol	Chain	Length	Quality of chain
1	E	520	 2% 81% 7% 11%
1	F	520	 82% 10% 8%
1	G	520	 % 84% 8% 8%
1	H	520	 2% 85% 7% 8%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 32438 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	3882	2485	672	705	20	0	0	0
1	B	479	3882	2487	673	702	20	0	0	0
1	C	478	3864	2475	668	701	20	0	0	0
1	D	478	3868	2479	668	701	20	0	0	0
1	E	464	3757	2404	651	682	20	0	0	0
1	F	480	3894	2494	676	704	20	0	0	0
1	G	479	3882	2486	674	702	20	0	0	0
1	H	478	3844	2467	667	690	20	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	GLY	-	expression tag	UNP Q9Y3Z3
A	108	SER	-	expression tag	UNP Q9Y3Z3
A	215	ALA	HIS	engineered mutation	UNP Q9Y3Z3
B	107	GLY	-	expression tag	UNP Q9Y3Z3
B	108	SER	-	expression tag	UNP Q9Y3Z3
B	215	ALA	HIS	engineered mutation	UNP Q9Y3Z3
C	107	GLY	-	expression tag	UNP Q9Y3Z3
C	108	SER	-	expression tag	UNP Q9Y3Z3
C	215	ALA	HIS	engineered mutation	UNP Q9Y3Z3
D	107	GLY	-	expression tag	UNP Q9Y3Z3
D	108	SER	-	expression tag	UNP Q9Y3Z3
D	215	ALA	HIS	engineered mutation	UNP Q9Y3Z3
E	107	GLY	-	expression tag	UNP Q9Y3Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	108	SER	-	expression tag	UNP Q9Y3Z3
E	215	ALA	HIS	engineered mutation	UNP Q9Y3Z3
F	107	GLY	-	expression tag	UNP Q9Y3Z3
F	108	SER	-	expression tag	UNP Q9Y3Z3
F	215	ALA	HIS	engineered mutation	UNP Q9Y3Z3
G	107	GLY	-	expression tag	UNP Q9Y3Z3
G	108	SER	-	expression tag	UNP Q9Y3Z3
G	215	ALA	HIS	engineered mutation	UNP Q9Y3Z3
H	107	GLY	-	expression tag	UNP Q9Y3Z3
H	108	SER	-	expression tag	UNP Q9Y3Z3
H	215	ALA	HIS	engineered mutation	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
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

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

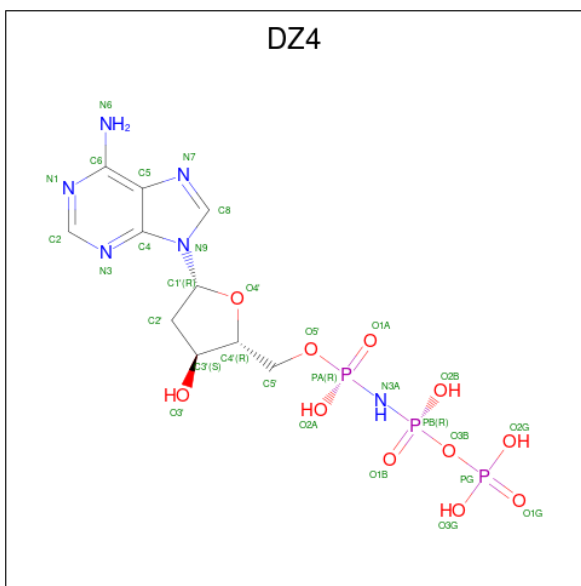
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Mg 3 3	0	0
3	B	3	Total Mg 3 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	3	Total 3	Mg 3	0	0
3	D	4	Total 4	Mg 4	0	0
3	E	3	Total 3	Mg 3	0	0
3	F	3	Total 3	Mg 3	0	0
3	G	3	Total 3	Mg 3	0	0
3	H	3	Total 3	Mg 3	0	0

- Molecule 4 is 2'-deoxy-5'-O-[(R)-hydroxy{(R)-hydroxy(phosphonoxy)phosphoryl}amino]phosphoryl]adenosine (three-letter code: DZ4) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>11</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



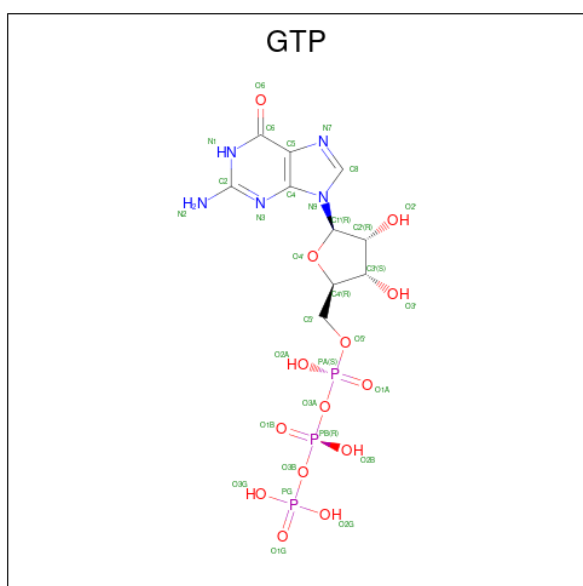
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 30	C 10	N 6	O 11	P 3	0	0
4	A	1	Total 30	C 10	N 6	O 11	P 3	0	0
4	B	1	Total 30	C 10	N 6	O 11	P 3	0	0
4	C	1	Total 30	C 10	N 6	O 11	P 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			30	10	6	11	3		
4	C	1	Total	C	N	O	P	0	0
			30	10	6	11	3		
4	D	1	Total	C	N	O	P	0	0
			30	10	6	11	3		
4	D	1	Total	C	N	O	P	0	0
			30	10	6	11	3		
4	E	1	Total	C	N	O	P	0	0
			30	10	6	11	3		
4	E	1	Total	C	N	O	P	0	0
			30	10	6	11	3		
4	F	1	Total	C	N	O	P	0	0
			30	10	6	11	3		
4	F	1	Total	C	N	O	P	0	0
			30	10	6	11	3		
4	G	1	Total	C	N	O	P	0	0
			30	10	6	11	3		
4	G	1	Total	C	N	O	P	0	0
			30	10	6	11	3		
4	H	1	Total	C	N	O	P	0	0
			30	10	6	11	3		
4	H	1	Total	C	N	O	P	0	0
			30	10	6	11	3		

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



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

- Molecule 6 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	99	Total	O	0	0
			99	99		
6	B	113	Total	O	0	0
			113	113		
6	C	116	Total	O	0	0
			116	116		
6	D	99	Total	O	0	0
			99	99		
6	E	71	Total	O	0	0
			71	71		
6	F	124	Total	O	0	0
			124	124		
6	G	115	Total	O	0	0
			115	115		
6	H	59	Total	O	0	0
			59	59		

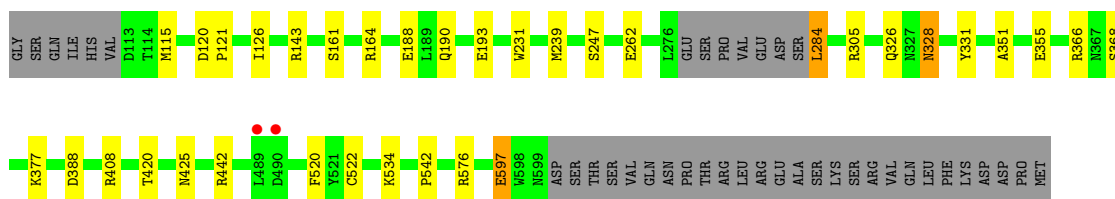


### 3 Residue-property plots [i](#)


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

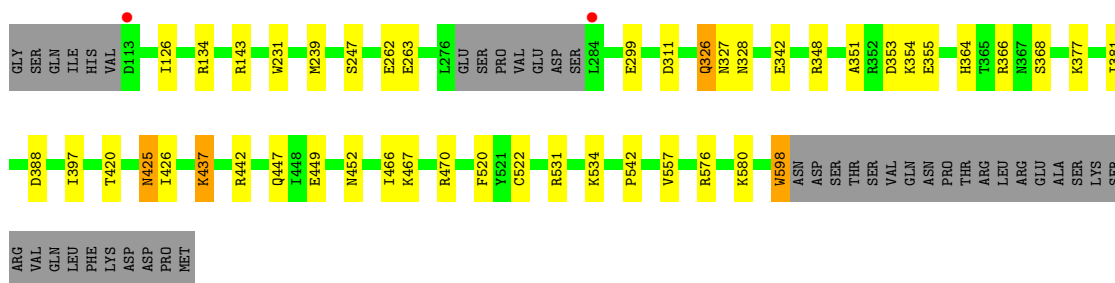
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain A: 




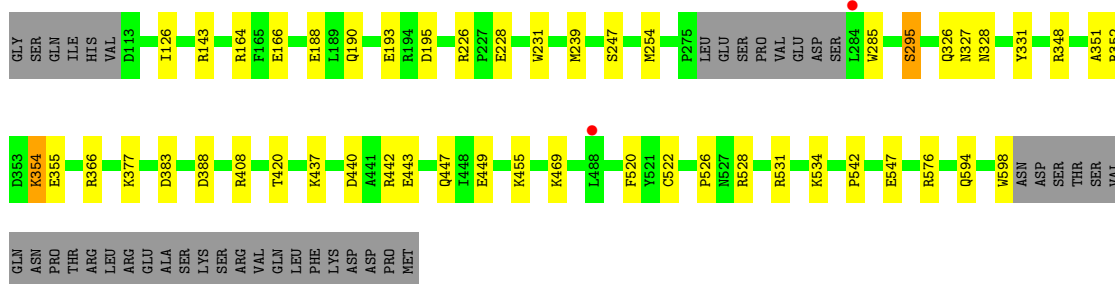
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain B: 




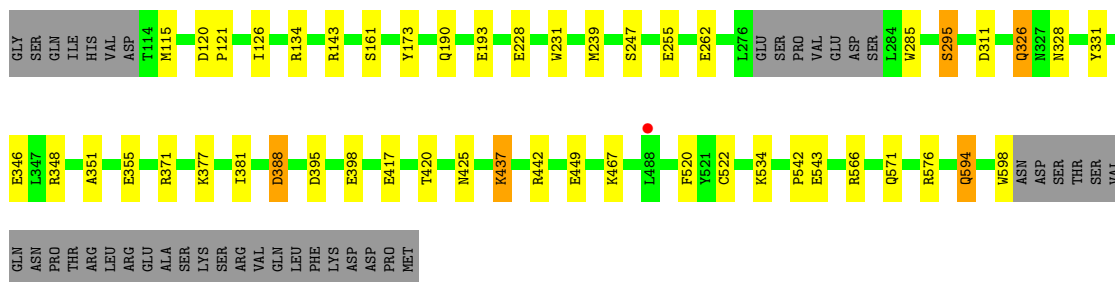
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain C: 




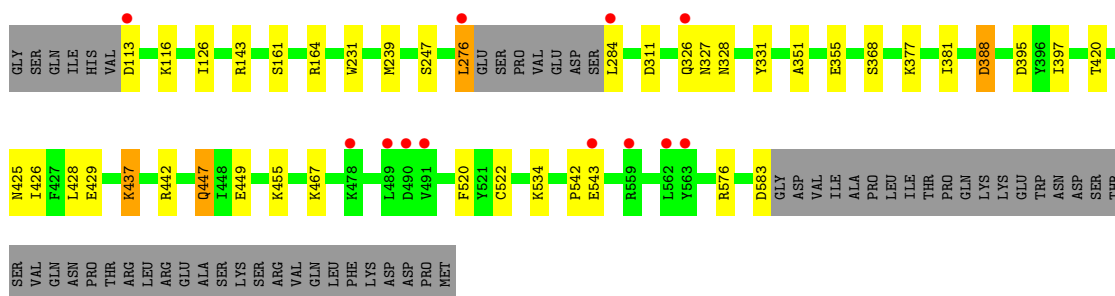
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain D: 




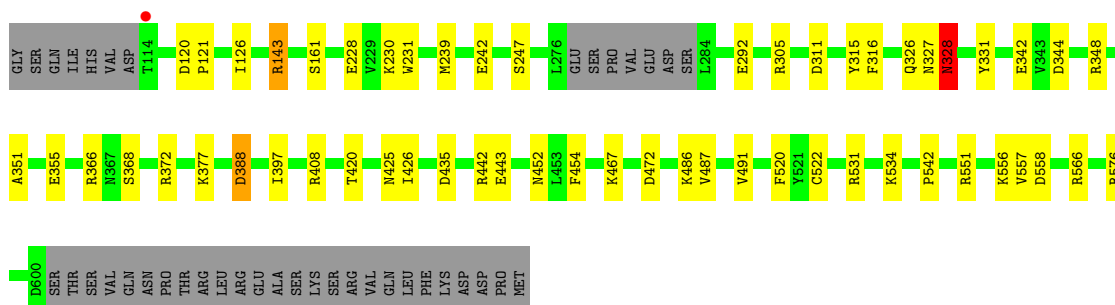
● Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain E: 




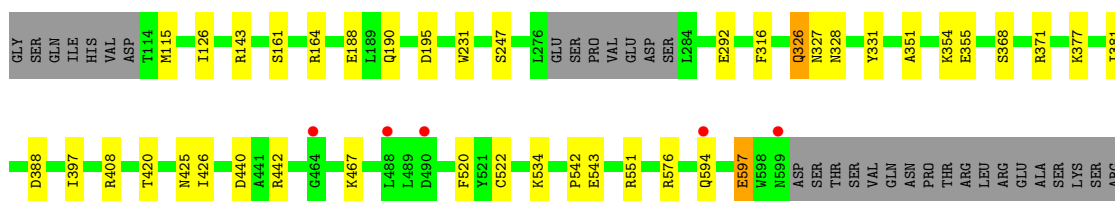
● Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain F: 




● Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain G: 



VAL  
GLN  
LEU  
PHE  
LYS  
ASP  
ASP  
PRO  
MET

● Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain H:  2% 85% 7% 8%

GLY  
SER  
GLN  
ILE  
HIS  
VAL  
ASP  
T114  
M115  
I126  
R143  
S161  
Q190  
E193  
R220  
W231  
M239  
S247  
L276  
GLU  
SER  
PRO  
VAL  
GLU  
ASP  
SER  
L284  
S295  
Q326  
N327  
N328  
Y331  
N345  
R348  
A351  
E355  
R366  
Y367  
S368  
R372

K377  
D388  
I397  
E403  
T420  
N425  
I426  
E429  
R442  
Q447  
K467  
L488  
V491  
F520  
F521  
C522  
K534  
F542  
R559  
K560  
S561  
R576  
L590  
V598  
ASN  
ASP  
SER  
THR  
SER  
VAL  
GLN  
ASN  
PRO  
THR  
ARG  
LEU  
ARG  
GLU  
ALA  
SER  
LYS  
SER

ARG  
VAL  
GLN  
LEU  
PHE  
LYS  
ASP  
ASP  
PRO  
MET

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.37Å 171.86Å 179.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	107.30 – 2.20 107.30 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.6 (107.30-2.20) 98.6 (107.30-2.20)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.176 , 0.202 0.183 , 0.208	Depositor DCC
$R_{free}$ test set	10526 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.4	Xtrriage
Anisotropy	0.268	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 39.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.008 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	32438	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, DZ4, MG, 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	1.13	11/3974 (0.3%)	1.07	15/5375 (0.3%)
1	B	1.11	12/3974 (0.3%)	1.07	20/5372 (0.4%)
1	C	1.11	18/3956 (0.5%)	1.06	21/5350 (0.4%)
1	D	1.09	16/3960 (0.4%)	1.03	19/5355 (0.4%)
1	E	1.02	10/3845 (0.3%)	1.05	16/5197 (0.3%)
1	F	1.17	16/3986 (0.4%)	1.11	28/5387 (0.5%)
1	G	1.07	10/3974 (0.3%)	1.02	16/5373 (0.3%)
1	H	0.99	12/3936 (0.3%)	0.98	12/5325 (0.2%)
All	All	1.09	105/31605 (0.3%)	1.05	147/42734 (0.3%)

All (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	SER	CB-OG	13.29	1.59	1.42
1	G	355	GLU	CD-OE1	12.10	1.39	1.25
1	B	355	GLU	CD-OE1	12.03	1.38	1.25
1	C	355	GLU	CD-OE1	11.73	1.38	1.25
1	F	355	GLU	CD-OE1	10.79	1.37	1.25
1	D	355	GLU	CD-OE1	10.22	1.36	1.25
1	E	449	GLU	CD-OE2	10.08	1.36	1.25
1	F	228	GLU	CD-OE2	9.79	1.36	1.25
1	A	355	GLU	CD-OE1	9.48	1.36	1.25
1	B	449	GLU	CD-OE2	9.27	1.35	1.25
1	E	355	GLU	CD-OE1	8.81	1.35	1.25
1	H	355	GLU	CD-OE1	8.79	1.35	1.25
1	E	247	SER	CB-OG	-8.70	1.30	1.42
1	F	368	SER	CB-OG	-8.49	1.31	1.42
1	F	161	SER	CB-OG	8.08	1.52	1.42
1	C	449	GLU	CD-OE2	7.76	1.34	1.25
1	A	262	GLU	CG-CD	7.75	1.63	1.51
1	A	247	SER	CB-OG	-7.75	1.32	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	161	SER	CB-OG	7.73	1.52	1.42
1	B	368	SER	CB-OG	-7.65	1.32	1.42
1	D	247	SER	CB-OG	-7.51	1.32	1.42
1	F	342	GLU	CD-OE1	7.41	1.33	1.25
1	G	161	SER	CB-OG	7.38	1.51	1.42
1	C	547	GLU	CD-OE2	7.11	1.33	1.25
1	G	292	GLU	CG-CD	7.00	1.62	1.51
1	H	231	TRP	CE3-CZ3	-6.89	1.26	1.38
1	D	598	TRP	CB-CG	6.87	1.62	1.50
1	C	443	GLU	CD-OE2	6.78	1.33	1.25
1	D	255	GLU	CG-CD	6.76	1.62	1.51
1	A	368	SER	CB-OG	-6.75	1.33	1.42
1	F	228	GLU	CD-OE1	6.67	1.32	1.25
1	D	398	GLU	CG-CD	6.67	1.61	1.51
1	H	161	SER	CB-OG	6.65	1.50	1.42
1	A	231	TRP	CE3-CZ3	-6.65	1.27	1.38
1	C	188	GLU	CD-OE1	6.63	1.32	1.25
1	B	447	GLN	CG-CD	6.62	1.66	1.51
1	B	262	GLU	CG-CD	6.61	1.61	1.51
1	G	368	SER	CB-OG	-6.56	1.33	1.42
1	E	368	SER	CB-OG	-6.54	1.33	1.42
1	D	228	GLU	CD-OE2	6.52	1.32	1.25
1	H	247	SER	CB-OG	-6.51	1.33	1.42
1	C	247	SER	CB-OG	-6.48	1.33	1.42
1	B	247	SER	CB-OG	-6.48	1.33	1.42
1	F	342	GLU	CD-OE2	6.38	1.32	1.25
1	C	331	TYR	CZ-OH	6.34	1.48	1.37
1	F	247	SER	CB-OG	-6.30	1.34	1.42
1	F	372	ARG	CZ-NH2	6.26	1.41	1.33
1	C	295	SER	CB-OG	-6.25	1.34	1.42
1	H	355	GLU	CD-OE2	6.24	1.32	1.25
1	A	193	GLU	CG-CD	6.21	1.61	1.51
1	G	231	TRP	CE3-CZ3	-6.16	1.27	1.38
1	E	231	TRP	CE3-CZ3	-6.09	1.28	1.38
1	B	425	ASN	CG-ND2	6.01	1.47	1.32
1	G	188	GLU	CD-OE1	5.97	1.32	1.25
1	C	447	GLN	CG-CD	5.93	1.64	1.51
1	G	247	SER	CB-OG	-5.93	1.34	1.42
1	H	429	GLU	CD-OE1	5.92	1.32	1.25
1	E	355	GLU	CG-CD	5.91	1.60	1.51
1	D	425	ASN	CG-ND2	5.89	1.47	1.32
1	D	262	GLU	CG-CD	5.89	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	326	GLN	CG-CD	5.88	1.64	1.51
1	C	443	GLU	CD-OE1	5.86	1.32	1.25
1	C	231	TRP	CE3-CZ3	-5.86	1.28	1.38
1	H	295	SER	CB-OG	-5.84	1.34	1.42
1	B	598	TRP	CB-CG	5.82	1.60	1.50
1	F	372	ARG	CZ-NH1	5.81	1.40	1.33
1	D	449	GLU	CG-CD	5.81	1.60	1.51
1	C	449	GLU	CD-OE1	5.72	1.31	1.25
1	C	598	TRP	CB-CG	5.70	1.60	1.50
1	F	331	TYR	CZ-OH	5.67	1.47	1.37
1	C	228	GLU	CD-OE2	5.67	1.31	1.25
1	F	231	TRP	CE3-CZ3	-5.66	1.28	1.38
1	A	328	ASN	CG-ND2	5.66	1.47	1.32
1	D	417	GLU	CD-OE1	5.63	1.31	1.25
1	H	368	SER	CB-OG	-5.63	1.34	1.42
1	D	193	GLU	CG-CD	5.58	1.60	1.51
1	H	598	TRP	CB-CG	5.57	1.60	1.50
1	F	292	GLU	CD-OE2	-5.56	1.19	1.25
1	F	443	GLU	CD-OE1	5.55	1.31	1.25
1	C	193	GLU	CD-OE2	5.54	1.31	1.25
1	A	188	GLU	CD-OE1	5.52	1.31	1.25
1	F	242	GLU	CD-OE1	5.46	1.31	1.25
1	E	447	GLN	CG-CD	5.44	1.63	1.51
1	C	383	ASP	CB-CG	5.41	1.63	1.51
1	F	491	VAL	C-O	-5.32	1.13	1.23
1	H	193	GLU	CG-CD	5.32	1.59	1.51
1	D	295	SER	CB-OG	-5.31	1.35	1.42
1	C	193	GLU	CG-CD	5.25	1.59	1.51
1	B	342	GLU	CD-OE2	5.17	1.31	1.25
1	B	231	TRP	CE3-CZ3	-5.17	1.29	1.38
1	H	331	TYR	CZ-OH	5.16	1.46	1.37
1	D	173	TYR	CE1-CZ	5.14	1.45	1.38
1	C	166	GLU	CG-CD	5.11	1.59	1.51
1	H	355	GLU	CG-CD	5.10	1.59	1.51
1	A	305	ARG	CZ-NH2	5.09	1.39	1.33
1	D	449	GLU	CD-OE1	5.08	1.31	1.25
1	G	543	GLU	CG-CD	5.08	1.59	1.51
1	D	231	TRP	CE3-CZ3	-5.04	1.29	1.38
1	E	331	TYR	CZ-OH	5.04	1.46	1.37
1	G	331	TYR	CZ-OH	5.03	1.46	1.37
1	A	193	GLU	CD-OE2	5.03	1.31	1.25
1	E	429	GLU	CD-OE1	5.01	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	161	SER	CB-OG	5.01	1.48	1.42
1	B	355	GLU	CD-OE2	5.00	1.31	1.25
1	B	447	GLN	CD-NE2	5.00	1.45	1.32

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	395	ASP	CB-CG-OD2	10.52	127.77	118.30
1	E	442	ARG	NE-CZ-NH1	9.37	124.99	120.30
1	E	164	ARG	NE-CZ-NH2	9.22	124.91	120.30
1	C	354	LYS	CD-CE-NZ	8.94	132.26	111.70
1	F	348	ARG	NE-CZ-NH2	8.94	124.77	120.30
1	F	388	ASP	CB-CG-OD2	-8.75	110.42	118.30
1	C	442	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	F	372	ARG	NE-CZ-NH2	-8.51	116.05	120.30
1	G	576	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	E	388	ASP	CB-CG-OD2	-8.34	110.80	118.30
1	B	449	GLU	OE1-CD-OE2	8.18	133.12	123.30
1	E	576	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	A	164	ARG	NE-CZ-NH2	8.01	124.31	120.30
1	B	299	GLU	OE1-CD-OE2	-7.82	113.92	123.30
1	F	442	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	D	388	ASP	CB-CG-OD2	-7.78	111.30	118.30
1	D	134	ARG	NE-CZ-NH1	-7.75	116.42	120.30
1	C	164	ARG	NE-CZ-NH2	7.59	124.10	120.30
1	B	311	ASP	CB-CG-OD1	7.50	125.05	118.30
1	E	116	LYS	CD-CE-NZ	7.49	128.92	111.70
1	B	348	ARG	NE-CZ-NH1	-7.39	116.60	120.30
1	D	442	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	H	372	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	H	348	ARG	NE-CZ-NH1	-7.23	116.69	120.30
1	F	435	ASP	CB-CG-OD2	-7.07	111.94	118.30
1	A	239	MET	CG-SD-CE	7.05	111.48	100.20
1	E	311	ASP	CB-CG-OD2	-7.04	111.97	118.30
1	A	366	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	B	576	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	G	164	ARG	NE-CZ-NH2	7.00	123.80	120.30
1	A	442	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	E	449	GLU	OE1-CD-OE2	6.95	131.64	123.30
1	F	576	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	F	305	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	C	408	ARG	NE-CZ-NH1	-6.80	116.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	440	ASP	CB-CG-OD1	6.79	124.41	118.30
1	C	576	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	G	442	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	B	134	ARG	NE-CZ-NH1	-6.73	116.94	120.30
1	E	576	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	B	576	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	F	239	MET	CG-SD-CE	6.60	110.75	100.20
1	F	487	VAL	CG1-CB-CG2	-6.57	100.39	110.90
1	D	348	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	B	311	ASP	CB-CG-OD2	-6.53	112.43	118.30
1	F	292	GLU	CG-CD-OE2	-6.45	105.39	118.30
1	C	531	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	G	576	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	H	442	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	G	115	MET	CA-CB-CG	6.34	124.08	113.30
1	H	576	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	B	354	LYS	CD-CE-NZ	6.27	126.12	111.70
1	D	348	ARG	NE-CZ-NH2	6.23	123.42	120.30
1	C	366	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	F	454	PHE	CB-CG-CD2	-6.20	116.46	120.80
1	A	442	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	G	551	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	B	239	MET	CG-SD-CE	6.15	110.04	100.20
1	F	316	PHE	CB-CG-CD1	6.13	125.09	120.80
1	G	316	PHE	CB-CG-CD1	6.10	125.07	120.80
1	H	348	ARG	NE-CZ-NH2	6.09	123.35	120.30
1	F	472	ASP	CB-CG-OD2	6.09	123.78	118.30
1	F	292	GLU	CG-CD-OE1	6.07	130.44	118.30
1	C	437	LYS	CB-CG-CD	6.01	127.24	111.60
1	E	437	LYS	CA-CB-CG	6.00	126.60	113.40
1	F	558	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	576	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	A	331	TYR	CB-CG-CD1	-5.97	117.42	121.00
1	F	566	ARG	NE-CZ-NH2	5.95	123.28	120.30
1	C	528	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	B	470	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	C	348	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	C	440	ASP	CB-CG-OD2	-5.93	112.97	118.30
1	A	408	ARG	NE-CZ-NH1	-5.92	117.34	120.30
1	E	583	ASP	CB-CG-OD2	5.91	123.62	118.30
1	D	262	GLU	OE1-CD-OE2	-5.89	116.24	123.30
1	G	522	CYS	CA-CB-SG	-5.86	103.45	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	115	MET	CA-CB-CG	5.86	123.26	113.30
1	F	522	CYS	CA-CB-SG	-5.86	103.46	114.00
1	F	408	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	E	455	LYS	CD-CE-NZ	5.83	125.11	111.70
1	F	143	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	F	344	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	F	486	LYS	CD-CE-NZ	-5.81	98.33	111.70
1	A	522	CYS	CA-CB-SG	-5.79	103.59	114.00
1	C	522	CYS	CA-CB-SG	-5.78	103.60	114.00
1	H	239	MET	CG-SD-CE	5.77	109.43	100.20
1	H	220	ARG	NE-CZ-NH2	5.75	123.17	120.30
1	B	355	GLU	OE1-CD-OE2	5.69	130.13	123.30
1	D	566	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	B	442	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	C	331	TYR	CB-CG-CD1	-5.64	117.62	121.00
1	D	346	GLU	OE1-CD-OE2	-5.62	116.55	123.30
1	D	522	CYS	CA-CB-SG	-5.59	103.94	114.00
1	B	366	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	D	331	TYR	CB-CG-CD1	-5.54	117.67	121.00
1	C	449	GLU	OE1-CD-OE2	5.51	129.92	123.30
1	C	331	TYR	CB-CG-CD2	5.49	124.30	121.00
1	D	395	ASP	CB-CG-OD1	5.48	123.23	118.30
1	G	408	ARG	NE-CZ-NH1	-5.48	117.56	120.30
1	D	437	LYS	CB-CG-CD	5.47	125.83	111.60
1	E	583	ASP	CB-CG-OD1	-5.46	113.39	118.30
1	D	311	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	C	355	GLU	OE1-CD-OE2	5.42	129.80	123.30
1	H	115	MET	CA-CB-CG	5.42	122.51	113.30
1	H	366	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	E	522	CYS	CA-CB-SG	-5.36	104.36	114.00
1	H	193	GLU	OE1-CD-OE2	-5.35	116.89	123.30
1	B	353	ASP	CB-CG-OD1	5.34	123.11	118.30
1	D	576	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	C	443	GLU	OE1-CD-OE2	5.33	129.69	123.30
1	F	551	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	G	371	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	B	522	CYS	CA-CB-SG	-5.29	104.47	114.00
1	H	355	GLU	OE1-CD-OE2	5.27	129.63	123.30
1	H	522	CYS	CA-CB-SG	-5.26	104.53	114.00
1	C	254	MET	CG-SD-CE	5.25	108.60	100.20
1	G	597	GLU	CA-CB-CG	5.24	124.93	113.40
1	A	597	GLU	CA-CB-CG	5.24	124.93	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	239	MET	CG-SD-CE	5.23	108.57	100.20
1	B	437	LYS	CB-CG-CD	5.22	125.17	111.60
1	B	366	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	F	366	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	D	371	ARG	NE-CZ-NH2	5.19	122.90	120.30
1	B	531	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	C	226	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	C	239	MET	CG-SD-CE	5.18	108.49	100.20
1	F	311	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	G	195	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	F	531	ARG	NE-CZ-NH2	5.15	122.88	120.30
1	A	262	GLU	OE1-CD-OE2	-5.15	117.12	123.30
1	G	331	TYR	CB-CG-CD1	-5.15	117.91	121.00
1	A	284	LEU	CB-CG-CD1	5.12	119.71	111.00
1	G	354	LYS	CD-CE-NZ	5.12	123.48	111.70
1	D	239	MET	CG-SD-CE	5.12	108.39	100.20
1	A	355	GLU	OE1-CD-OE2	5.12	129.44	123.30
1	A	284	LEU	CA-CB-CG	5.11	127.06	115.30
1	F	328	ASN	N-CA-CB	-5.11	101.40	110.60
1	F	372	ARG	NH1-CZ-NH2	5.09	125.00	119.40
1	A	188	GLU	CG-CD-OE2	-5.09	108.12	118.30
1	E	284	LEU	CB-CG-CD2	5.08	119.64	111.00
1	G	440	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	D	598	TRP	N-CA-C	-5.08	97.29	111.00
1	D	355	GLU	OE1-CD-OE2	5.07	129.39	123.30
1	F	230	LYS	N-CA-C	-5.06	97.33	111.00
1	C	195	ASP	CB-CG-OD2	-5.03	113.78	118.30
1	B	342	GLU	OE1-CD-OE2	5.01	129.32	123.30

There are no chirality outliers.

There are no planarity outliers.

## 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	3882	0	3823	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3882	0	3841	14	0
1	C	3864	0	3808	8	0
1	D	3868	0	3819	10	0
1	E	3757	0	3700	11	0
1	F	3894	0	3858	12	0
1	G	3882	0	3838	8	0
1	H	3844	0	3793	9	0
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
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	4	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
3	G	3	0	0	0	0
3	H	3	0	0	0	0
4	A	60	0	26	0	0
4	B	30	0	13	0	0
4	C	90	0	39	1	0
4	D	60	0	26	0	0
4	E	60	0	26	0	0
4	F	60	0	26	0	0
4	G	60	0	26	0	0
4	H	60	0	26	0	0
5	A	32	0	12	0	0
5	B	32	0	12	0	0
5	C	32	0	12	0	0
5	D	32	0	12	1	0
5	E	64	0	24	0	0
5	G	32	0	11	0	0
5	H	32	0	12	0	0
6	A	99	0	0	0	0
6	B	113	0	0	2	0
6	C	116	0	0	3	0
6	D	99	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	71	0	0	0	0
6	F	124	0	0	0	1
6	G	115	0	0	0	1
6	H	59	0	0	0	0
All	All	32438	0	30783	67	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (67) 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:F:328:ASN:N	1:F:328:ASN:OD1	2.05	0.85
1:B:437:LYS:NZ	6:B:802:HOH:O	2.26	0.68
1:E:425:ASN:OD1	1:F:425:ASN:ND2	2.28	0.66
1:A:425:ASN:OD1	1:B:425:ASN:ND2	2.26	0.61
1:D:534:LYS:HE3	1:D:542:PRO:O	2.04	0.58
1:C:534:LYS:HE3	1:C:542:PRO:O	2.04	0.56
1:B:466:ILE:HD12	6:B:854:HOH:O	2.05	0.55
1:E:326:GLN:CD	1:H:326:GLN:NE2	2.60	0.55
1:B:326:GLN:HG3	1:B:327:ASN:N	2.22	0.54
1:B:534:LYS:HE3	1:B:542:PRO:O	2.08	0.54
1:F:326:GLN:HG2	1:G:327:ASN:O	2.07	0.54
1:F:326:GLN:HG3	1:F:327:ASN:N	2.23	0.53
1:G:397:ILE:HG21	1:G:426:ILE:HD11	1.92	0.52
1:F:534:LYS:HE3	1:F:542:PRO:O	2.09	0.51
1:A:326:GLN:HB3	1:D:326:GLN:NE2	2.26	0.51
1:E:534:LYS:HE3	1:E:542:PRO:O	2.11	0.50
1:E:327:ASN:O	1:H:326:GLN:HG2	2.12	0.49
1:H:326:GLN:HG3	1:H:327:ASN:N	2.26	0.49
1:E:397:ILE:HG21	1:E:426:ILE:HD11	1.94	0.49
1:G:534:LYS:HE3	1:G:542:PRO:O	2.13	0.49
4:C:706:DZ4:PA	6:C:825:HOH:O	2.69	0.49
1:B:326:GLN:NE2	1:C:326:GLN:HB3	2.28	0.48
1:A:534:LYS:HE3	1:A:542:PRO:O	2.14	0.48
1:B:397:ILE:HG21	1:B:426:ILE:HD11	1.95	0.47
1:A:326:GLN:CG	1:D:326:GLN:HE22	2.27	0.47
1:B:326:GLN:HG2	1:C:327:ASN:O	2.14	0.47
1:H:397:ILE:HG21	1:H:426:ILE:HD11	1.97	0.47
1:E:428:LEU:HD13	1:F:425:ASN:HB2	1.96	0.47
1:E:276:LEU:HD23	1:E:276:LEU:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:143:ARG:HD2	1:F:420:THR:HA	1.98	0.45
1:C:285:TRP:CH2	1:C:295:SER:HB3	2.51	0.45
1:B:452:ASN:OD1	1:B:557:VAL:HG21	2.17	0.45
1:C:143:ARG:HD2	1:C:420:THR:HA	1.99	0.45
1:G:143:ARG:HD2	1:G:420:THR:HA	1.99	0.45
1:G:425:ASN:OD1	1:H:425:ASN:ND2	2.47	0.45
1:B:364:HIS:HE1	6:C:912:HOH:O	2.01	0.44
1:H:143:ARG:HD2	1:H:420:THR:HA	1.99	0.44
1:A:351:ALA:O	1:A:520:PHE:HA	2.18	0.44
1:F:351:ALA:O	1:F:520:PHE:HA	2.19	0.43
1:B:351:ALA:O	1:B:520:PHE:HA	2.18	0.43
1:D:285:TRP:CH2	1:D:295:SER:HB3	2.53	0.43
1:E:143:ARG:HD2	1:E:420:THR:HA	2.00	0.43
1:B:381:ILE:HD12	1:B:381:ILE:HA	1.92	0.43
1:A:143:ARG:HD2	1:A:420:THR:HA	2.00	0.42
1:B:143:ARG:HD2	1:B:420:THR:HA	2.01	0.42
1:D:351:ALA:O	1:D:520:PHE:HA	2.19	0.42
1:H:534:LYS:HE3	1:H:542:PRO:O	2.18	0.42
1:D:143:ARG:HD2	1:D:420:THR:HA	2.02	0.42
1:D:381:ILE:HD12	1:D:381:ILE:HA	1.94	0.42
1:E:326:GLN:HB3	1:H:326:GLN:NE2	2.34	0.42
1:F:452:ASN:OD1	1:F:557:VAL:HG21	2.20	0.42
1:E:351:ALA:O	1:E:520:PHE:HA	2.20	0.41
1:A:120:ASP:OD1	1:A:121:PRO:HD2	2.20	0.41
1:C:351:ALA:O	1:C:520:PHE:HA	2.20	0.41
1:F:397:ILE:HG21	1:F:426:ILE:HD11	2.02	0.41
1:G:381:ILE:HD12	1:G:381:ILE:HA	1.94	0.41
1:E:381:ILE:HD12	1:E:381:ILE:HA	1.93	0.41
1:F:120:ASP:OD1	1:F:121:PRO:HD2	2.20	0.41
1:F:326:GLN:NE2	1:G:326:GLN:HB3	2.36	0.41
1:D:120:ASP:OD1	1:D:121:PRO:HD2	2.21	0.41
1:G:351:ALA:O	1:G:520:PHE:HA	2.20	0.41
1:C:455:LYS:NZ	5:D:707:GTP:O2G	2.54	0.41
1:D:571:GLN:NE2	1:D:594:GLN:OE1	2.48	0.41
1:H:351:ALA:O	1:H:520:PHE:HA	2.20	0.41
1:B:580:LYS:HD2	1:B:598:TRP:HB3	2.03	0.40
1:A:326:GLN:HB3	1:D:326:GLN:HE22	1.87	0.40
1:C:354:LYS:NZ	6:C:807:HOH:O	2.54	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:923:HOH:O	6:G:912:HOH:O[3_655]	2.08	0.12

### 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%)	466 (98%)	10 (2%)	0	100	100
1	B	475/520 (91%)	468 (98%)	7 (2%)	0	100	100
1	C	474/520 (91%)	464 (98%)	10 (2%)	0	100	100
1	D	474/520 (91%)	466 (98%)	8 (2%)	0	100	100
1	E	460/520 (88%)	452 (98%)	8 (2%)	0	100	100
1	F	476/520 (92%)	470 (99%)	6 (1%)	0	100	100
1	G	475/520 (91%)	466 (98%)	9 (2%)	0	100	100
1	H	474/520 (91%)	466 (98%)	8 (2%)	0	100	100
All	All	3784/4160 (91%)	3718 (98%)	66 (2%)	0	100	100

There are no Ramachandran outliers to report.

#### 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	416/463 (90%)	408 (98%)	8 (2%)	57	71
1	B	417/463 (90%)	410 (98%)	7 (2%)	60	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	414/463 (89%)	405 (98%)	9 (2%)	52	65
1	D	415/463 (90%)	405 (98%)	10 (2%)	49	62
1	E	403/463 (87%)	393 (98%)	10 (2%)	47	60
1	F	419/463 (90%)	412 (98%)	7 (2%)	60	74
1	G	417/463 (90%)	409 (98%)	8 (2%)	57	71
1	H	409/463 (88%)	400 (98%)	9 (2%)	52	65
All	All	3310/3704 (89%)	3242 (98%)	68 (2%)	53	67

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	MET
1	A	126	ILE
1	A	190	GLN
1	A	284	LEU
1	A	328	ASN
1	A	377	LYS
1	A	388	ASP
1	A	597	GLU
1	B	126	ILE
1	B	263	GLU
1	B	326	GLN
1	B	328	ASN
1	B	377	LYS
1	B	388	ASP
1	B	467	LYS
1	C	126	ILE
1	C	190	GLN
1	C	328	ASN
1	C	352	ARG
1	C	377	LYS
1	C	388	ASP
1	C	469	LYS
1	C	526	PRO
1	C	594	GLN
1	D	126	ILE
1	D	190	GLN
1	D	326	GLN
1	D	328	ASN
1	D	377	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	388	ASP
1	D	437	LYS
1	D	467	LYS
1	D	543	GLU
1	D	594	GLN
1	E	113	ASP
1	E	126	ILE
1	E	276	LEU
1	E	328	ASN
1	E	377	LYS
1	E	388	ASP
1	E	437	LYS
1	E	447	GLN
1	E	467	LYS
1	E	543	GLU
1	F	126	ILE
1	F	315	TYR
1	F	328	ASN
1	F	377	LYS
1	F	388	ASP
1	F	467	LYS
1	F	556	LYS
1	G	126	ILE
1	G	190	GLN
1	G	328	ASN
1	G	377	LYS
1	G	388	ASP
1	G	467	LYS
1	G	594	GLN
1	G	597	GLU
1	H	114	THR
1	H	126	ILE
1	H	190	GLN
1	H	326	GLN
1	H	328	ASN
1	H	377	LYS
1	H	388	ASP
1	H	447	GLN
1	H	467	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	328	ASN
1	A	375	GLN
1	A	380	ASN
1	B	326	GLN
1	B	328	ASN
1	B	364	HIS
1	B	375	GLN
1	B	380	ASN
1	B	517	HIS
1	C	190	GLN
1	C	328	ASN
1	C	375	GLN
1	C	380	ASN
1	D	326	GLN
1	D	328	ASN
1	D	364	HIS
1	D	375	GLN
1	D	380	ASN
1	E	328	ASN
1	E	375	GLN
1	E	380	ASN
1	E	425	ASN
1	F	326	GLN
1	F	364	HIS
1	F	375	GLN
1	F	380	ASN
1	F	425	ASN
1	G	190	GLN
1	G	328	ASN
1	G	375	GLN
1	G	380	ASN
1	G	425	ASN
1	G	571	GLN
1	G	594	GLN
1	H	326	GLN
1	H	328	ASN
1	H	375	GLN
1	H	380	ASN
1	H	425	ASN

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 57 ligands modelled in this entry, 33 are monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	DZ4	G	701	3	29,32,32	1.56	5 (17%)	33,50,50	2.12	5 (15%)
4	DZ4	F	706	3	29,32,32	1.36	5 (17%)	33,50,50	2.16	6 (18%)
4	DZ4	F	705	3,2	29,32,32	1.94	5 (17%)	33,50,50	1.64	5 (15%)
5	GTP	B	706	3	26,34,34	1.82	5 (19%)	32,54,54	1.76	9 (28%)
4	DZ4	G	706	3,2	29,32,32	1.60	4 (13%)	33,50,50	1.47	4 (12%)
4	DZ4	A	705	3,2	29,32,32	1.89	3 (10%)	33,50,50	1.49	4 (12%)
4	DZ4	C	706	3,2	29,32,32	1.50	4 (13%)	33,50,50	1.82	5 (15%)
5	GTP	E	707	3	26,34,34	1.23	1 (3%)	32,54,54	1.49	6 (18%)
4	DZ4	D	701	3	29,32,32	1.47	5 (17%)	33,50,50	1.90	6 (18%)
4	DZ4	H	706	3,2	29,32,32	2.95	7 (24%)	33,50,50	1.75	6 (18%)
4	DZ4	A	707	3	29,32,32	1.41	3 (10%)	33,50,50	1.81	4 (12%)
5	GTP	A	706	3	26,34,34	1.32	4 (15%)	32,54,54	1.78	10 (31%)
4	DZ4	C	701	3	29,32,32	1.24	5 (17%)	33,50,50	1.96	5 (15%)
5	GTP	C	707	3	26,34,34	1.67	8 (30%)	32,54,54	1.82	11 (34%)
5	GTP	E	706	3	26,34,34	1.51	6 (23%)	32,54,54	2.53	14 (43%)
4	DZ4	E	708	3	29,32,32	1.60	7 (24%)	33,50,50	1.93	8 (24%)
5	GTP	D	707	3	26,34,34	1.24	2 (7%)	32,54,54	2.01	12 (37%)
4	DZ4	D	706	3,2	29,32,32	1.49	5 (17%)	33,50,50	1.81	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	DZ4	E	705	3,2	29,32,32	1.52	6 (20%)	33,50,50	1.73	7 (21%)
4	DZ4	H	701	3	29,32,32	1.41	4 (13%)	33,50,50	1.91	8 (24%)
4	DZ4	B	705	3,2	29,32,32	1.20	3 (10%)	33,50,50	1.37	3 (9%)
5	GTP	H	707	3	26,34,34	1.41	3 (11%)	32,54,54	1.63	9 (28%)
4	DZ4	C	708	3	29,32,32	1.54	6 (20%)	33,50,50	1.84	6 (18%)
5	GTP	G	707	3	26,34,34	1.91	5 (19%)	32,54,54	1.58	7 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DZ4	G	701	3	-	4/15/34/34	0/3/3/3
4	DZ4	F	706	3	-	2/15/34/34	0/3/3/3
4	DZ4	F	705	3,2	-	3/15/34/34	0/3/3/3
5	GTP	B	706	3	-	6/18/38/38	0/3/3/3
4	DZ4	G	706	3,2	-	1/15/34/34	0/3/3/3
4	DZ4	A	705	3,2	-	2/15/34/34	0/3/3/3
4	DZ4	C	706	3,2	-	2/15/34/34	0/3/3/3
5	GTP	E	707	3	-	8/18/38/38	0/3/3/3
4	DZ4	D	701	3	-	4/15/34/34	0/3/3/3
4	DZ4	H	706	3,2	-	2/15/34/34	0/3/3/3
4	DZ4	A	707	3	-	2/15/34/34	0/3/3/3
5	GTP	A	706	3	-	6/18/38/38	0/3/3/3
4	DZ4	C	701	3	-	2/15/34/34	0/3/3/3
5	GTP	C	707	3	-	7/18/38/38	0/3/3/3
5	GTP	E	706	3	-	9/18/38/38	0/3/3/3
4	DZ4	E	708	3	-	5/15/34/34	0/3/3/3
5	GTP	D	707	3	-	7/18/38/38	0/3/3/3
4	DZ4	D	706	3,2	-	1/15/34/34	0/3/3/3
4	DZ4	E	705	3,2	-	2/15/34/34	0/3/3/3
4	DZ4	H	701	3	-	4/15/34/34	0/3/3/3
4	DZ4	B	705	3,2	-	2/15/34/34	0/3/3/3
5	GTP	H	707	3	-	4/18/38/38	0/3/3/3
4	DZ4	C	708	3	-	5/15/34/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	G	707	3	-	8/18/38/38	0/3/3/3

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	706	DZ4	PA-O1A	7.61	1.58	1.46
4	A	705	DZ4	PB-O1B	6.99	1.57	1.46
4	H	706	DZ4	PB-O1B	6.83	1.57	1.46
5	B	706	GTP	O4'-C1'	6.34	1.49	1.41
4	H	706	DZ4	PB-O3B	-6.34	1.51	1.59
4	H	706	DZ4	PB-N3A	6.17	1.79	1.63
4	F	705	DZ4	PA-O1A	5.89	1.55	1.46
4	H	706	DZ4	PG-O2G	-5.87	1.32	1.54
4	A	705	DZ4	PA-O1A	5.73	1.55	1.46
4	F	705	DZ4	PB-O1B	5.62	1.55	1.46
5	G	707	GTP	O4'-C1'	5.21	1.48	1.41
5	G	707	GTP	C6-N1	-5.12	1.30	1.37
4	C	708	DZ4	PB-O3B	4.69	1.65	1.59
4	G	706	DZ4	PA-O1A	4.69	1.53	1.46
4	E	708	DZ4	PB-O3B	4.54	1.64	1.59
4	G	706	DZ4	PB-O1B	4.32	1.53	1.46
4	C	706	DZ4	PB-O1B	4.32	1.53	1.46
4	G	701	DZ4	PB-O1B	4.25	1.52	1.46
4	D	701	DZ4	PB-O3B	4.25	1.64	1.59
5	H	707	GTP	O4'-C1'	-4.18	1.35	1.41
4	A	707	DZ4	PB-O1B	3.93	1.52	1.46
4	E	705	DZ4	PA-O1A	3.92	1.52	1.46
4	H	701	DZ4	PB-O1B	3.79	1.52	1.46
4	D	706	DZ4	PA-O1A	3.72	1.52	1.46
4	F	706	DZ4	PA-O1A	3.69	1.52	1.46
5	C	707	GTP	C8-N7	-3.67	1.28	1.35
4	A	707	DZ4	PB-O2B	-3.66	1.46	1.56
4	D	706	DZ4	PB-O1B	3.65	1.51	1.46
4	D	701	DZ4	PB-O1B	3.64	1.51	1.46
4	E	705	DZ4	PB-O1B	3.63	1.51	1.46
4	H	706	DZ4	PG-O1G	3.47	1.61	1.50
4	C	706	DZ4	PA-O1A	3.37	1.51	1.46
4	E	708	DZ4	PB-O1B	3.31	1.51	1.46
4	C	708	DZ4	PB-O1B	3.28	1.51	1.46
4	C	701	DZ4	PB-O1B	3.21	1.51	1.46
4	G	701	DZ4	PA-O2A	-3.17	1.48	1.56
4	B	705	DZ4	PB-O1B	3.14	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	705	DZ4	PB-O2B	-3.11	1.48	1.56
5	E	707	GTP	O2'-C2'	3.11	1.50	1.43
4	A	707	DZ4	PA-O2A	-3.07	1.48	1.56
4	F	705	DZ4	PA-O2A	-3.07	1.48	1.56
5	C	707	GTP	C2'-C1'	-3.05	1.49	1.53
5	A	706	GTP	C6-N1	-3.05	1.33	1.37
4	H	701	DZ4	PB-O3B	3.02	1.62	1.59
4	D	706	DZ4	PB-O2B	-2.99	1.48	1.56
4	E	708	DZ4	PB-O2B	-2.99	1.48	1.56
4	H	701	DZ4	PA-O2A	-2.98	1.48	1.56
4	G	701	DZ4	PA-O1A	2.98	1.50	1.46
4	G	706	DZ4	PB-O2B	-2.94	1.48	1.56
5	C	707	GTP	C2-N1	-2.93	1.30	1.37
5	B	706	GTP	C3'-C4'	2.93	1.60	1.53
4	E	705	DZ4	C8-N7	-2.92	1.29	1.34
5	B	706	GTP	C4-N3	-2.92	1.30	1.37
5	E	706	GTP	PB-O2B	-2.92	1.41	1.55
4	F	706	DZ4	PB-O2B	-2.88	1.49	1.56
4	F	706	DZ4	PG-O2G	-2.87	1.43	1.54
5	G	707	GTP	O3'-C3'	-2.82	1.36	1.43
4	H	706	DZ4	C8-N7	-2.82	1.29	1.34
4	C	708	DZ4	PB-O2B	-2.81	1.49	1.56
4	D	706	DZ4	PB-O3B	2.79	1.62	1.59
5	G	707	GTP	O6-C6	2.77	1.28	1.23
4	D	701	DZ4	PA-O2A	-2.75	1.49	1.56
5	A	706	GTP	O4'-C1'	2.75	1.44	1.41
4	E	708	DZ4	PA-O1A	2.71	1.50	1.46
5	B	706	GTP	O6-C6	2.71	1.28	1.23
4	E	708	DZ4	PA-O2A	-2.70	1.49	1.56
5	E	706	GTP	PG-O1G	-2.69	1.41	1.50
5	C	707	GTP	C6-N1	-2.69	1.33	1.37
4	F	706	DZ4	PA-O2A	-2.66	1.49	1.56
4	E	705	DZ4	PA-O2A	-2.64	1.49	1.56
4	C	701	DZ4	PA-O2A	-2.60	1.49	1.56
4	G	706	DZ4	PG-O3G	-2.57	1.44	1.54
4	H	701	DZ4	PA-O1A	2.54	1.50	1.46
4	F	706	DZ4	PB-O1B	2.53	1.50	1.46
4	E	705	DZ4	PG-O3G	-2.49	1.45	1.54
5	E	706	GTP	C2'-C1'	-2.43	1.50	1.53
5	E	706	GTP	PA-O2A	-2.40	1.44	1.55
4	E	708	DZ4	C8-N7	-2.38	1.30	1.34
4	E	705	DZ4	PB-N3A	2.37	1.69	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	706	GTP	C2-N2	-2.37	1.28	1.34
4	C	708	DZ4	PG-O3G	-2.37	1.45	1.54
4	C	708	DZ4	PA-O2A	-2.31	1.50	1.56
5	C	707	GTP	PG-O1G	-2.30	1.43	1.50
4	G	701	DZ4	C2-N3	2.29	1.35	1.32
5	E	706	GTP	C5-C6	-2.29	1.42	1.47
5	G	707	GTP	PB-O2B	-2.29	1.44	1.55
5	C	707	GTP	O4'-C4'	-2.28	1.39	1.45
5	C	707	GTP	O3'-C3'	-2.28	1.37	1.43
4	G	701	DZ4	PG-O2G	-2.27	1.46	1.54
4	D	701	DZ4	PG-O3G	-2.27	1.46	1.54
5	D	707	GTP	PA-O5'	2.27	1.68	1.59
4	A	705	DZ4	PG-O2G	-2.26	1.46	1.54
4	C	701	DZ4	PG-O2G	-2.22	1.46	1.54
5	E	706	GTP	PG-O2G	-2.20	1.46	1.54
4	E	708	DZ4	PG-O2G	-2.19	1.46	1.54
4	C	708	DZ4	C2-N3	2.18	1.35	1.32
4	C	706	DZ4	PA-O2A	-2.17	1.50	1.56
5	H	707	GTP	PG-O1G	-2.17	1.43	1.50
4	B	705	DZ4	C8-N7	-2.17	1.30	1.34
4	B	705	DZ4	PA-O2A	-2.17	1.50	1.56
5	A	706	GTP	PB-O2B	-2.14	1.45	1.55
4	F	705	DZ4	PG-O3G	-2.12	1.46	1.54
4	C	706	DZ4	PB-O2B	-2.11	1.51	1.56
4	D	701	DZ4	PB-O2B	-2.11	1.51	1.56
5	D	707	GTP	PB-O2B	-2.10	1.45	1.55
4	C	701	DZ4	PA-N3A	2.09	1.68	1.63
5	H	707	GTP	PG-O3G	-2.07	1.46	1.54
4	C	701	DZ4	PB-O2B	-2.04	1.51	1.56
5	C	707	GTP	C2'-C3'	-2.02	1.47	1.53
5	B	706	GTP	PG-O2G	-2.01	1.47	1.54
4	D	706	DZ4	C8-N7	-2.00	1.31	1.34

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	701	DZ4	O1A-PA-N3A	-7.77	100.33	111.77
5	E	706	GTP	O5'-C5'-C4'	7.41	134.50	108.99
4	E	705	DZ4	O2B-PB-O1B	6.49	123.52	109.92
4	G	701	DZ4	O1B-PB-N3A	-6.28	102.52	111.77
4	A	707	DZ4	O1A-PA-N3A	-6.22	102.61	111.77
4	F	706	DZ4	O1A-PA-N3A	-6.02	102.91	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	708	DZ4	O1B-PB-N3A	-5.95	103.01	111.77
4	F	706	DZ4	O2B-PB-O1B	5.92	122.33	109.92
4	H	701	DZ4	O1A-PA-N3A	-5.42	103.79	111.77
4	H	706	DZ4	O2B-PB-O1B	5.37	121.18	109.92
4	C	706	DZ4	C5-C6-N6	5.31	128.42	120.35
4	F	705	DZ4	O2B-PB-O1B	5.27	120.97	109.92
4	D	701	DZ4	O2A-PA-O1A	5.25	120.92	109.92
4	F	706	DZ4	O1B-PB-N3A	-5.19	104.13	111.77
4	G	701	DZ4	O2B-PB-O1B	5.03	120.46	109.92
4	C	708	DZ4	O1B-PB-N3A	-5.00	104.40	111.77
4	G	701	DZ4	O2A-PA-O1A	4.93	120.26	109.92
4	B	705	DZ4	O2B-PB-O1B	4.90	120.20	109.92
4	F	705	DZ4	O2A-PA-O1A	4.90	120.19	109.92
4	G	701	DZ4	O1A-PA-N3A	-4.86	104.61	111.77
4	D	701	DZ4	O1B-PB-N3A	-4.86	104.61	111.77
4	A	707	DZ4	O2B-PB-O1B	4.84	120.07	109.92
4	H	701	DZ4	O2B-PB-O1B	4.79	119.97	109.92
4	C	706	DZ4	O1B-PB-N3A	-4.79	104.71	111.77
4	C	708	DZ4	O2A-PA-O1A	4.76	119.89	109.92
4	G	706	DZ4	O2B-PB-O1B	4.74	119.85	109.92
4	D	701	DZ4	O1A-PA-N3A	-4.72	104.82	111.77
4	E	708	DZ4	O2B-PB-O1B	4.63	119.62	109.92
5	E	706	GTP	O2G-PG-O3B	-4.61	89.16	104.64
4	D	701	DZ4	O2B-PB-O1B	4.58	119.52	109.92
4	H	706	DZ4	O2A-PA-O1A	4.49	119.34	109.92
5	E	706	GTP	O3B-PG-O1G	-4.43	86.64	111.19
4	A	705	DZ4	O2A-PA-O1A	4.40	119.14	109.92
4	H	706	DZ4	O5'-PA-O1A	-4.35	97.49	114.24
4	C	708	DZ4	O2B-PB-O1B	4.33	119.00	109.92
4	A	705	DZ4	O2B-PB-O1B	4.28	118.89	109.92
4	D	706	DZ4	O2B-PB-O1B	4.25	118.83	109.92
4	D	706	DZ4	O1A-PA-N3A	-4.24	105.52	111.77
4	H	701	DZ4	O2A-PA-O1A	4.21	118.75	109.92
5	C	707	GTP	PA-O3A-PB	-4.21	118.38	132.83
4	C	706	DZ4	O2A-PA-O1A	4.21	118.74	109.92
4	C	701	DZ4	O5'-PA-O1A	-4.16	98.23	114.24
4	F	706	DZ4	O2A-PA-O1A	4.14	118.59	109.92
4	A	707	DZ4	O2A-PA-O1A	4.10	118.53	109.92
5	B	706	GTP	C3'-C2'-C1'	4.08	107.13	100.98
4	D	706	DZ4	O2A-PA-O1A	4.06	118.43	109.92
4	D	706	DZ4	C5-C6-N6	3.94	126.33	120.35
5	D	707	GTP	O5'-C5'-C4'	3.88	122.36	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	706	GTP	O2B-PB-O1B	3.85	131.28	112.24
4	E	708	DZ4	O2A-PA-O1A	3.77	117.82	109.92
5	E	706	GTP	PA-O5'-C5'	3.77	143.77	121.68
5	E	706	GTP	O2G-PG-O1G	3.76	125.40	110.68
4	C	708	DZ4	O2A-PA-O5'	-3.76	96.55	106.75
4	C	706	DZ4	O2B-PB-O1B	3.71	117.70	109.92
5	E	706	GTP	O4'-C4'-C5'	-3.71	97.18	109.37
4	F	706	DZ4	O5'-PA-O1A	-3.69	100.06	114.24
5	E	707	GTP	O6-C6-N1	3.53	124.82	120.65
4	E	708	DZ4	O5'-PA-O1A	-3.50	100.80	114.24
5	E	707	GTP	O6-C6-C5	-3.47	117.60	124.37
4	G	706	DZ4	O1A-PA-N3A	-3.38	106.80	111.77
4	C	701	DZ4	O2B-PB-O1B	3.26	116.76	109.92
4	F	705	DZ4	O5'-PA-O1A	-3.24	101.79	114.24
4	C	701	DZ4	O2A-PA-O1A	3.23	116.70	109.92
4	E	705	DZ4	O2A-PA-O1A	3.22	116.67	109.92
5	A	706	GTP	O2A-PA-O1A	3.20	128.07	112.24
5	A	706	GTP	O6-C6-C5	-3.18	118.17	124.37
5	A	706	GTP	O3B-PG-O1G	-3.16	93.65	111.19
5	A	706	GTP	C5-C6-N1	3.15	119.52	113.95
5	H	707	GTP	C3'-C2'-C1'	3.12	105.68	100.98
4	E	705	DZ4	O3B-PB-N3A	-3.11	97.95	106.59
5	C	707	GTP	O3G-PG-O2G	3.09	119.43	107.64
5	D	707	GTP	O3G-PG-O2G	3.08	119.39	107.64
4	H	701	DZ4	O5'-PA-O1A	-3.06	102.47	114.24
5	H	707	GTP	O3G-PG-O2G	3.04	119.25	107.64
5	G	707	GTP	C8-N7-C5	3.01	108.73	102.99
5	D	707	GTP	C2-N1-C6	-3.01	119.56	125.10
5	A	706	GTP	PA-O3A-PB	-3.00	122.55	132.83
5	C	707	GTP	O3'-C3'-C4'	-2.99	102.41	111.05
5	G	707	GTP	PA-O3A-PB	-2.98	122.61	132.83
5	D	707	GTP	O3G-PG-O3B	2.97	114.60	104.64
5	D	707	GTP	N2-C2-N1	2.94	122.98	116.71
5	C	707	GTP	O2B-PB-O1B	2.93	126.72	112.24
5	D	707	GTP	N2-C2-N3	-2.91	114.08	119.74
5	B	706	GTP	O2G-PG-O3B	-2.89	94.95	104.64
4	G	706	DZ4	O2A-PA-O1A	2.89	115.97	109.92
4	G	701	DZ4	O5'-PA-O1A	-2.85	103.26	114.24
5	B	706	GTP	O5'-PA-O1A	-2.85	97.93	109.07
5	C	707	GTP	O5'-PA-O1A	-2.85	97.93	109.07
4	H	701	DZ4	O3B-PB-N3A	-2.82	98.76	106.59
4	G	706	DZ4	O1B-PB-N3A	-2.77	107.69	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	707	GTP	O5'-PA-O1A	-2.76	98.26	109.07
4	H	701	DZ4	O3G-PG-O2G	2.76	118.20	107.64
4	E	705	DZ4	O2A-PA-O5'	-2.73	99.34	106.75
4	E	708	DZ4	O3B-PB-N3A	-2.71	99.08	106.59
5	B	706	GTP	O6-C6-N1	2.70	123.83	120.65
4	H	701	DZ4	O3G-PG-O3B	-2.70	95.59	104.64
5	G	707	GTP	N2-C2-N3	-2.66	114.56	119.74
5	E	706	GTP	C3'-C2'-C1'	2.66	104.98	100.98
4	A	705	DZ4	O1A-PA-N3A	-2.63	107.89	111.77
4	H	706	DZ4	O2A-PA-O5'	-2.62	99.63	106.75
4	F	705	DZ4	O2A-PA-O5'	-2.60	99.69	106.75
5	G	707	GTP	O3'-C3'-C4'	-2.60	103.53	111.05
5	C	707	GTP	O5'-C5'-C4'	2.59	117.90	108.99
4	H	701	DZ4	O2A-PA-O5'	-2.57	99.78	106.75
5	H	707	GTP	C8-N7-C5	2.56	107.87	102.99
5	A	706	GTP	O3G-PG-O2G	2.56	117.42	107.64
5	G	707	GTP	O5'-C5'-C4'	2.55	117.76	108.99
4	D	706	DZ4	O1B-PB-N3A	-2.53	108.05	111.77
5	E	706	GTP	O2A-PA-O1A	2.53	124.74	112.24
4	E	708	DZ4	O2A-PA-O5'	-2.52	99.91	106.75
5	E	707	GTP	O2G-PG-O3B	-2.51	96.22	104.64
5	E	706	GTP	C8-N7-C5	2.49	107.74	102.99
5	A	706	GTP	C2-N1-C6	-2.49	120.52	125.10
5	E	706	GTP	O3G-PG-O3B	2.49	112.97	104.64
5	E	706	GTP	PA-O3A-PB	-2.47	124.36	132.83
5	D	707	GTP	C5-C6-N1	2.47	118.31	113.95
4	B	705	DZ4	O2A-PA-O1A	2.47	115.09	109.92
5	D	707	GTP	C3'-C2'-C1'	2.45	104.67	100.98
5	A	706	GTP	O3G-PG-O3B	2.44	112.83	104.64
5	D	707	GTP	O2A-PA-O1A	2.44	124.28	112.24
5	E	706	GTP	O2B-PB-O1B	2.43	124.27	112.24
5	D	707	GTP	PA-O3A-PB	-2.40	124.58	132.83
4	E	705	DZ4	C5-C6-N6	2.39	123.98	120.35
5	H	707	GTP	O2'-C2'-C1'	-2.38	102.06	110.85
5	H	707	GTP	O3G-PG-O1G	-2.38	101.38	110.68
5	E	707	GTP	N2-C2-N1	2.37	121.75	116.71
5	D	707	GTP	O2'-C2'-C1'	-2.36	102.14	110.85
4	A	705	DZ4	O3G-PG-O1G	2.35	119.89	110.68
5	E	706	GTP	O3G-PG-O2G	2.32	116.50	107.64
5	E	707	GTP	O2G-PG-O1G	2.31	119.73	110.68
5	H	707	GTP	C2-N1-C6	-2.31	120.85	125.10
5	H	707	GTP	O5'-PA-O1A	-2.30	100.08	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	706	GTP	N2-C2-N1	2.29	121.59	116.71
5	H	707	GTP	C5-C6-N1	2.29	118.00	113.95
5	G	707	GTP	C2'-C3'-C4'	2.29	107.09	102.64
4	B	705	DZ4	O1A-PA-N3A	-2.27	108.42	111.77
4	A	707	DZ4	O5'-PA-O1A	-2.27	105.52	114.24
4	E	708	DZ4	C4-C5-N7	2.26	111.75	109.40
4	C	701	DZ4	O1B-PB-N3A	-2.26	108.44	111.77
5	G	707	GTP	O6-C6-N1	2.23	123.28	120.65
4	D	706	DZ4	O5'-PA-O1A	-2.23	105.67	114.24
4	D	701	DZ4	C5-C6-N6	2.21	123.70	120.35
5	A	706	GTP	O5'-PA-O1A	-2.20	100.46	109.07
5	B	706	GTP	O2A-PA-O1A	2.18	123.00	112.24
5	B	706	GTP	O3G-PG-O1G	2.16	119.15	110.68
5	C	707	GTP	O2G-PG-O3B	-2.16	97.39	104.64
4	F	705	DZ4	C5-C6-N6	2.13	123.60	120.35
4	E	708	DZ4	O3G-PG-O3B	-2.13	97.48	104.64
5	B	706	GTP	O6-C6-C5	-2.13	120.22	124.37
5	C	707	GTP	O6-C6-N1	2.12	123.16	120.65
5	C	707	GTP	N2-C2-N3	-2.12	115.60	119.74
4	H	706	DZ4	O3B-PB-N3A	-2.12	100.72	106.59
5	B	706	GTP	O2'-C2'-C1'	-2.10	103.09	110.85
4	C	706	DZ4	O5'-PA-O1A	-2.08	106.23	114.24
4	H	706	DZ4	C5-C6-N6	2.08	123.51	120.35
4	C	708	DZ4	O2B-PB-O3B	-2.08	97.71	104.64
4	E	705	DZ4	O1B-PB-N3A	-2.07	108.72	111.77
4	E	705	DZ4	C5-C6-N1	-2.07	115.66	120.35
4	F	706	DZ4	O2A-PA-O5'	2.07	112.34	106.75
4	D	701	DZ4	O5'-PA-O1A	-2.07	106.30	114.24
5	C	707	GTP	O6-C6-C5	-2.06	120.34	124.37
5	E	707	GTP	C5-C6-N1	2.05	117.56	113.95
5	A	706	GTP	O2B-PB-O1B	2.04	122.35	112.24
5	C	707	GTP	C8-N7-C5	2.04	106.87	102.99
4	C	708	DZ4	O5'-PA-O1A	-2.02	106.45	114.24
4	D	706	DZ4	C5-C6-N1	-2.02	115.76	120.35
5	H	707	GTP	O6-C6-C5	-2.02	120.43	124.37

There are no chirality outliers.

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	705	DZ4	PA-N3A-PB-O1B
4	A	707	DZ4	PB-N3A-PA-O1A

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Mol	Chain	Res	Type	Atoms
4	A	707	DZ4	PA-N3A-PB-O1B
4	B	705	DZ4	PA-N3A-PB-O1B
4	C	701	DZ4	PA-N3A-PB-O1B
4	C	706	DZ4	PA-N3A-PB-O1B
4	C	708	DZ4	PB-N3A-PA-O1A
4	C	708	DZ4	PG-O3B-PB-O1B
4	C	708	DZ4	PG-O3B-PB-O2B
4	D	701	DZ4	PB-N3A-PA-O1A
4	D	701	DZ4	PA-N3A-PB-O1B
4	D	706	DZ4	PA-N3A-PB-O1B
4	E	705	DZ4	PA-N3A-PB-O1B
4	E	708	DZ4	PB-N3A-PA-O1A
4	E	708	DZ4	PG-O3B-PB-O1B
4	E	708	DZ4	PG-O3B-PB-O2B
4	F	705	DZ4	PA-N3A-PB-O1B
4	F	706	DZ4	PB-N3A-PA-O1A
4	G	701	DZ4	PB-N3A-PA-O1A
4	G	701	DZ4	PA-N3A-PB-O1B
4	G	701	DZ4	PG-O3B-PB-O1B
4	G	706	DZ4	PA-N3A-PB-O1B
4	H	701	DZ4	PA-N3A-PB-O1B
4	H	701	DZ4	PG-O3B-PB-O1B
4	H	701	DZ4	PG-O3B-PB-O2B
4	H	706	DZ4	PA-N3A-PB-O1B
5	A	706	GTP	C5'-O5'-PA-O2A
5	D	707	GTP	C5'-O5'-PA-O2A
5	E	706	GTP	PB-O3B-PG-O3G
5	E	706	GTP	C5'-O5'-PA-O3A
5	E	706	GTP	C5'-O5'-PA-O1A
5	E	706	GTP	C4'-C5'-O5'-PA
5	E	707	GTP	PB-O3B-PG-O3G
5	E	707	GTP	C5'-O5'-PA-O2A
5	H	707	GTP	PB-O3B-PG-O3G
5	E	706	GTP	O4'-C4'-C5'-O5'
5	E	706	GTP	C3'-C4'-C5'-O5'
5	C	707	GTP	PB-O3B-PG-O1G
5	E	707	GTP	PB-O3B-PG-O1G
5	G	707	GTP	PB-O3B-PG-O1G
5	B	706	GTP	C4'-C5'-O5'-PA
5	C	707	GTP	C4'-C5'-O5'-PA
5	G	707	GTP	C4'-C5'-O5'-PA
5	A	706	GTP	PB-O3B-PG-O1G

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Mol	Chain	Res	Type	Atoms
5	D	707	GTP	C4'-C5'-O5'-PA
5	B	706	GTP	PB-O3B-PG-O3G
5	C	707	GTP	PB-O3B-PG-O3G
5	G	707	GTP	PB-O3B-PG-O3G
5	C	707	GTP	C5'-O5'-PA-O3A
5	D	707	GTP	C5'-O5'-PA-O3A
5	G	707	GTP	C5'-O5'-PA-O3A
5	C	707	GTP	PG-O3B-PB-O1B
5	C	707	GTP	PB-O3A-PA-O2A
5	D	707	GTP	PG-O3B-PB-O1B
5	E	706	GTP	PB-O3A-PA-O2A
5	G	707	GTP	PG-O3B-PB-O1B
5	E	707	GTP	C4'-C5'-O5'-PA
4	C	708	DZ4	PA-N3A-PB-O3B
5	A	706	GTP	C4'-C5'-O5'-PA
5	B	706	GTP	PB-O3B-PG-O1G
5	D	707	GTP	PB-O3B-PG-O1G
5	A	706	GTP	PB-O3A-PA-O2A
5	B	706	GTP	PB-O3A-PA-O2A
5	D	707	GTP	PB-O3A-PA-O2A
5	E	707	GTP	PB-O3A-PA-O2A
5	G	707	GTP	PB-O3A-PA-O2A
5	H	707	GTP	PB-O3A-PA-O2A
5	H	707	GTP	C4'-C5'-O5'-PA
4	C	701	DZ4	PB-N3A-PA-O1A
4	C	708	DZ4	PA-N3A-PB-O1B
4	E	708	DZ4	PA-N3A-PB-O1B
4	H	701	DZ4	PB-N3A-PA-O1A
4	A	705	DZ4	C4'-C5'-O5'-PA
4	D	701	DZ4	PG-O3B-PB-O2B
4	G	701	DZ4	PG-O3B-PB-O2B
5	C	707	GTP	PB-O3A-PA-O1A
5	E	706	GTP	PB-O3A-PA-O1A
4	E	705	DZ4	C4'-C5'-O5'-PA
4	F	705	DZ4	C5'-O5'-PA-O2A
4	C	706	DZ4	C4'-C5'-O5'-PA
5	E	706	GTP	PB-O3B-PG-O1G
5	E	707	GTP	C5'-O5'-PA-O3A
5	A	706	GTP	PG-O3B-PB-O1B
5	A	706	GTP	PB-O3A-PA-O1A
5	B	706	GTP	PG-O3B-PB-O1B
5	B	706	GTP	PB-O3A-PA-O1A

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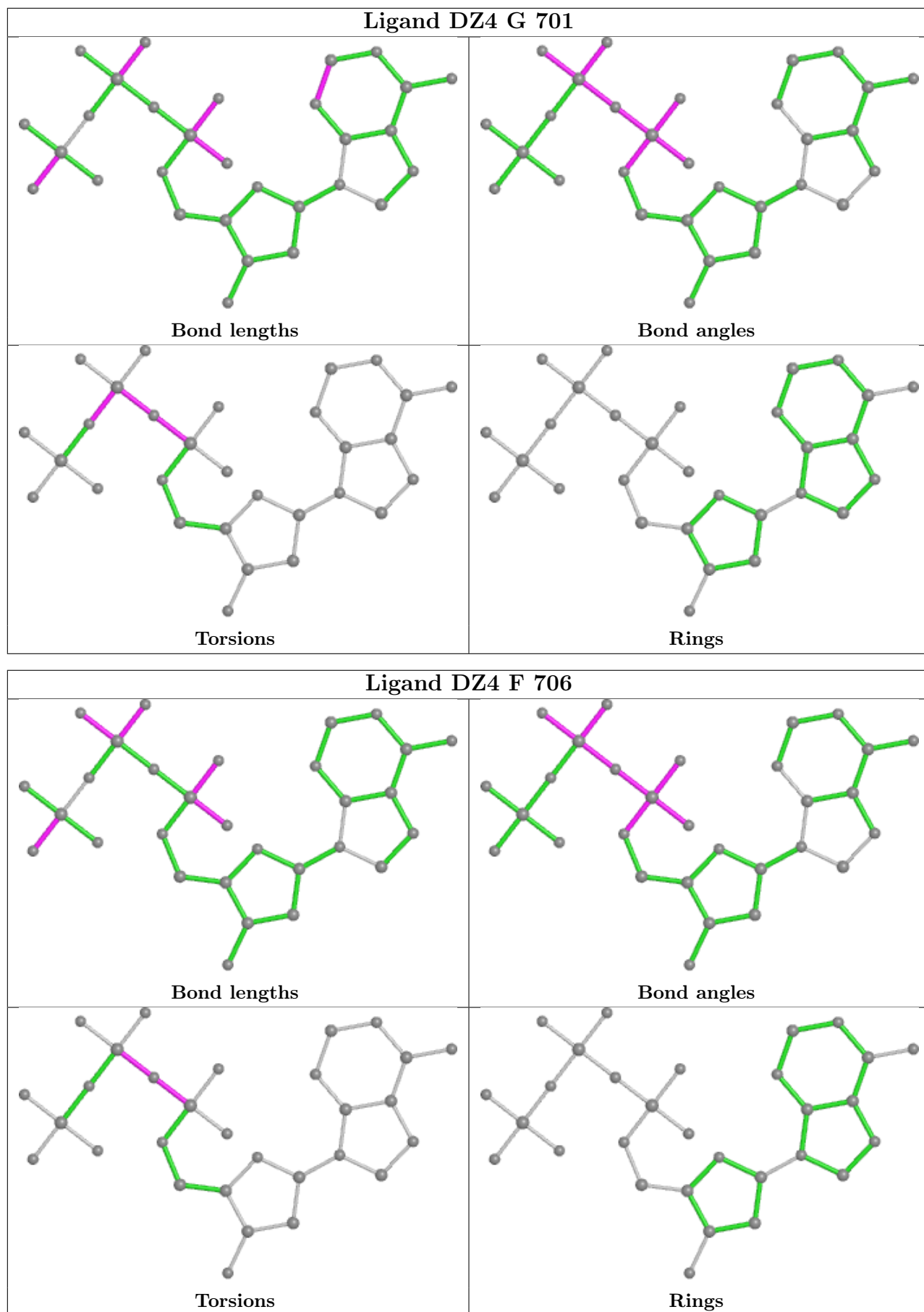
Mol	Chain	Res	Type	Atoms
5	E	707	GTP	PB-O3A-PA-O1A
5	G	707	GTP	PG-O3B-PB-O2B
5	G	707	GTP	PB-O3A-PA-O1A
5	H	707	GTP	PG-O3B-PB-O2B
4	B	705	DZ4	C4'-C5'-O5'-PA
4	H	706	DZ4	C4'-C5'-O5'-PA
5	D	707	GTP	C5'-O5'-PA-O1A
5	E	707	GTP	C5'-O5'-PA-O1A
4	D	701	DZ4	PA-N3A-PB-O3B
4	E	708	DZ4	PA-N3A-PB-O3B
4	F	706	DZ4	PA-N3A-PB-O3B
4	F	705	DZ4	C5'-O5'-PA-N3A

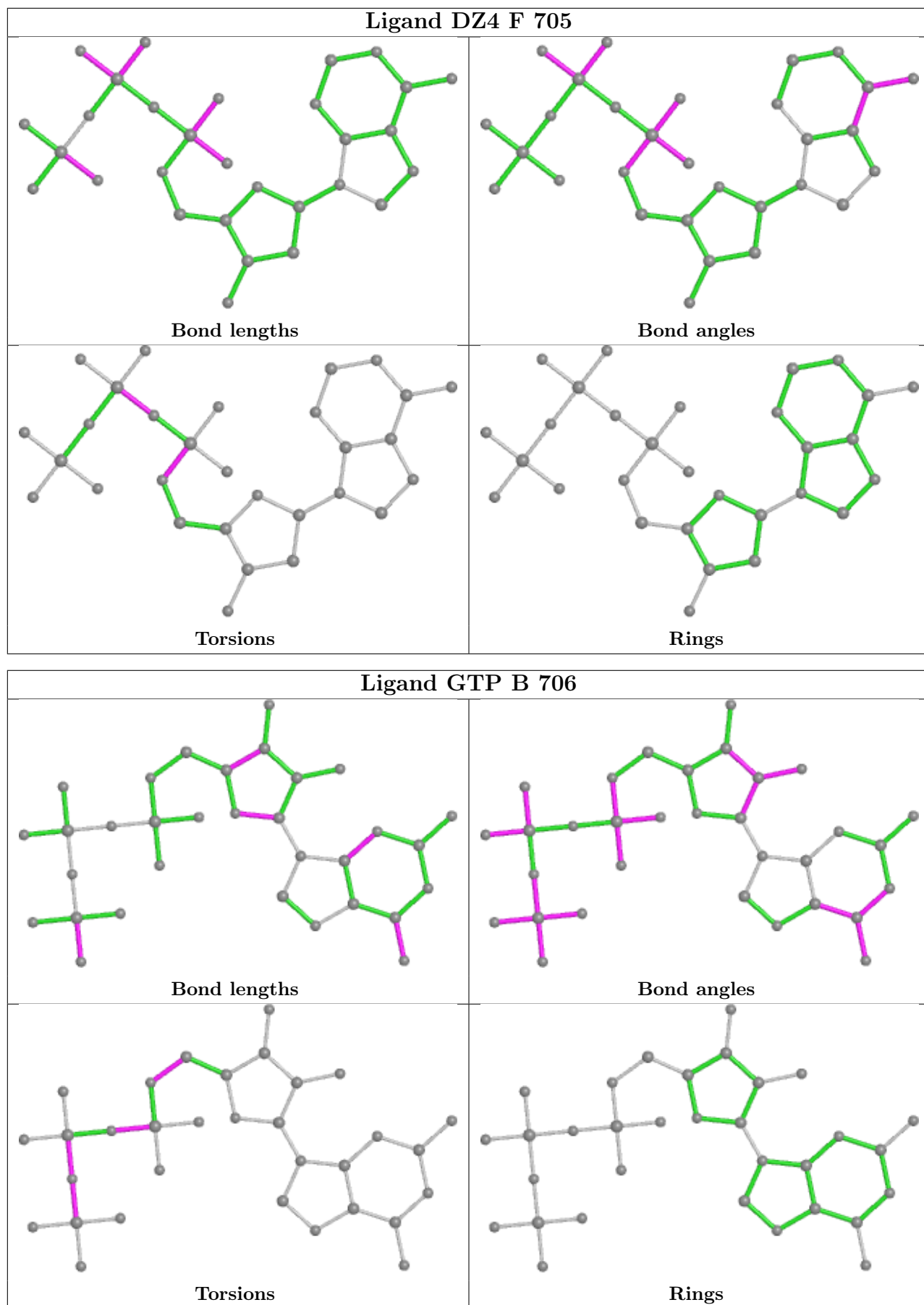
There are no ring outliers.

2 monomers are involved in 2 short contacts:

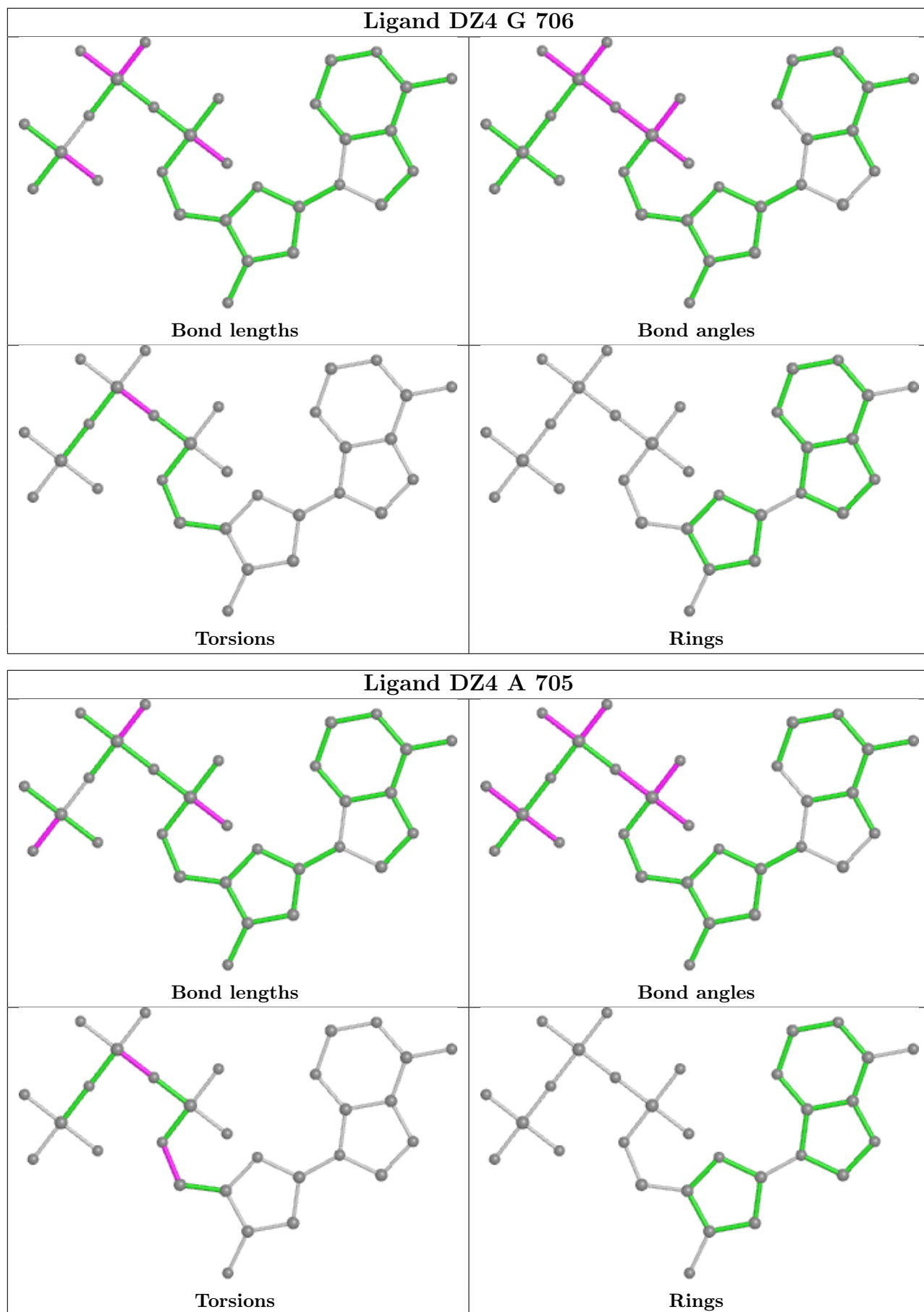
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	706	DZ4	1	0
5	D	707	GTP	1	0

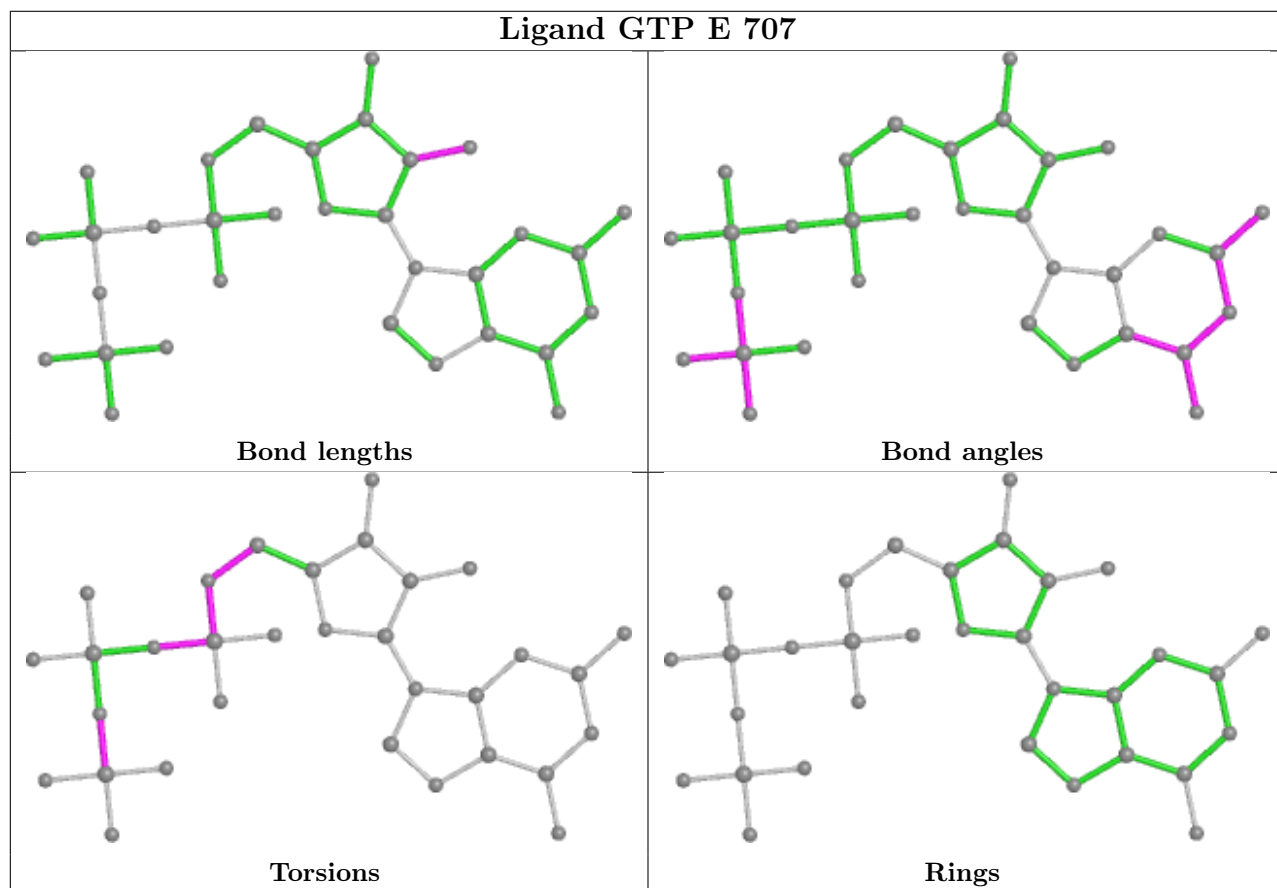
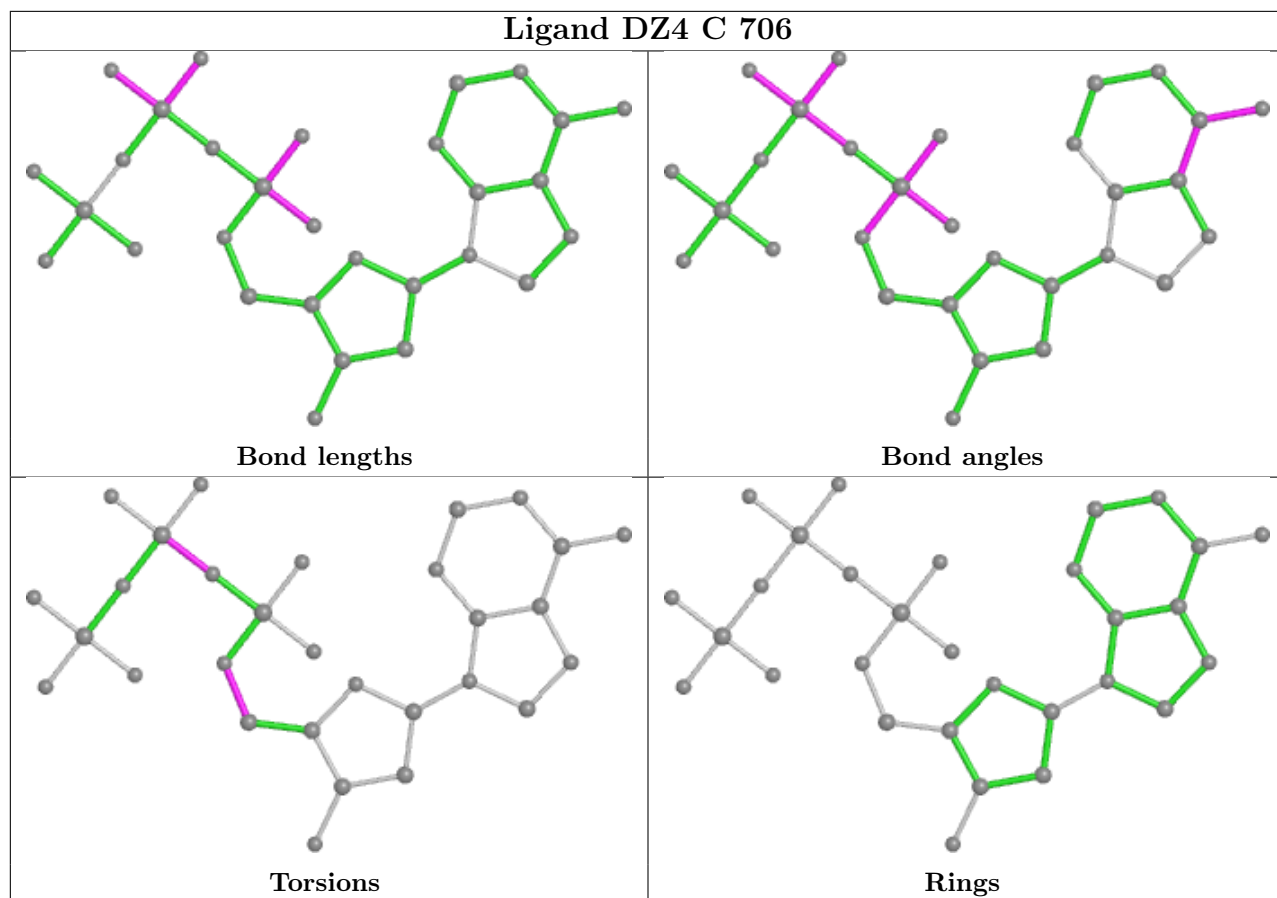
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

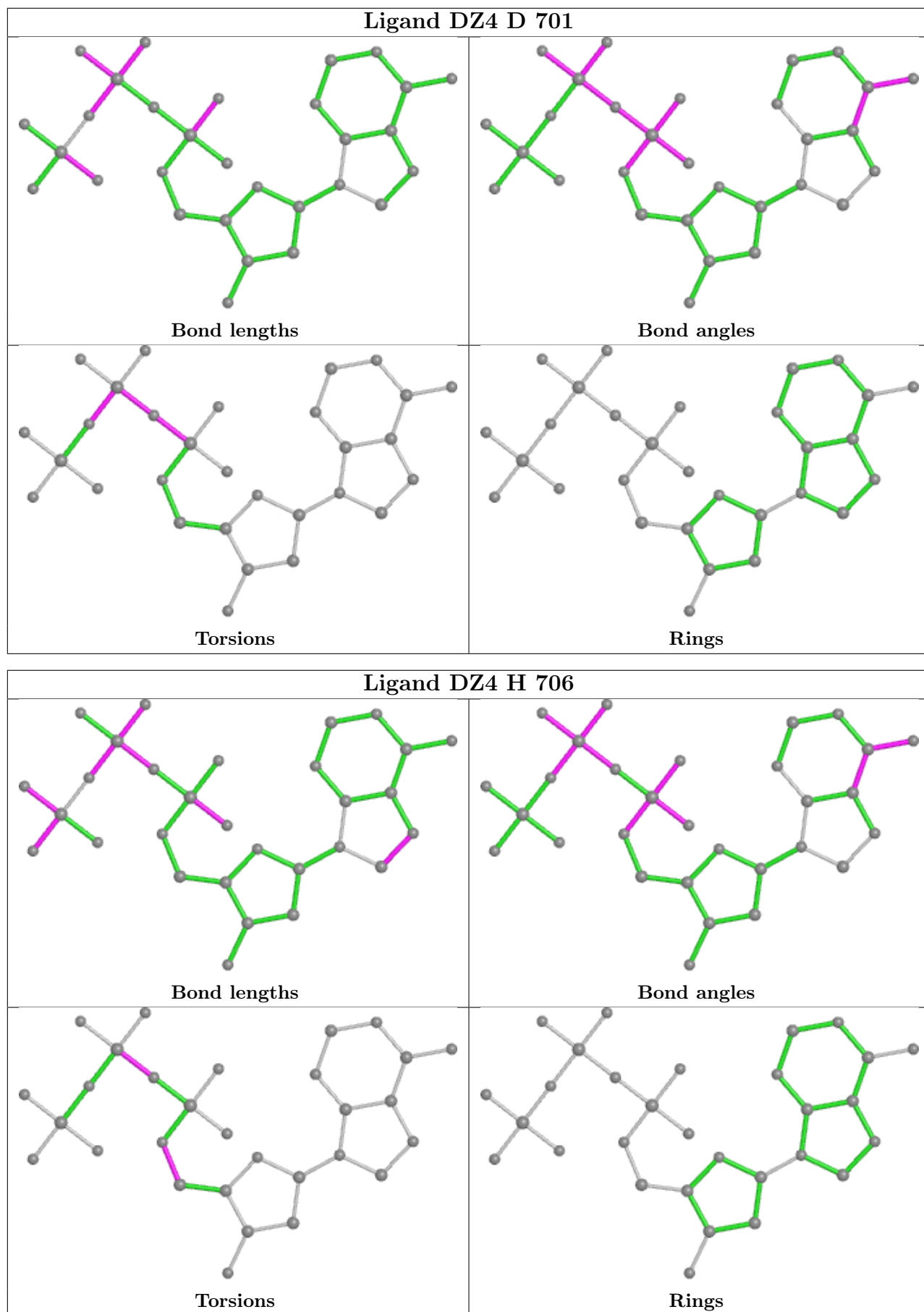


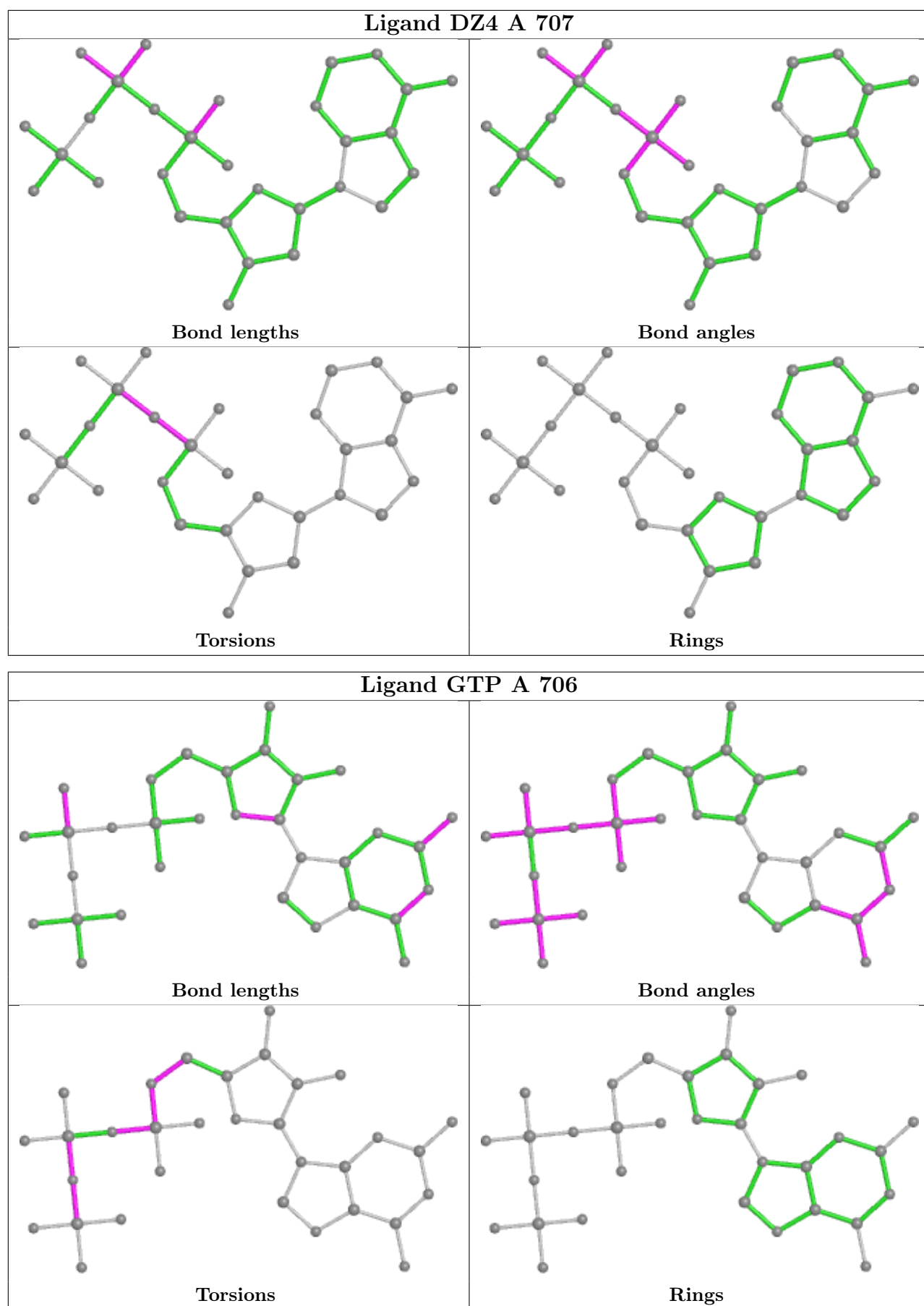


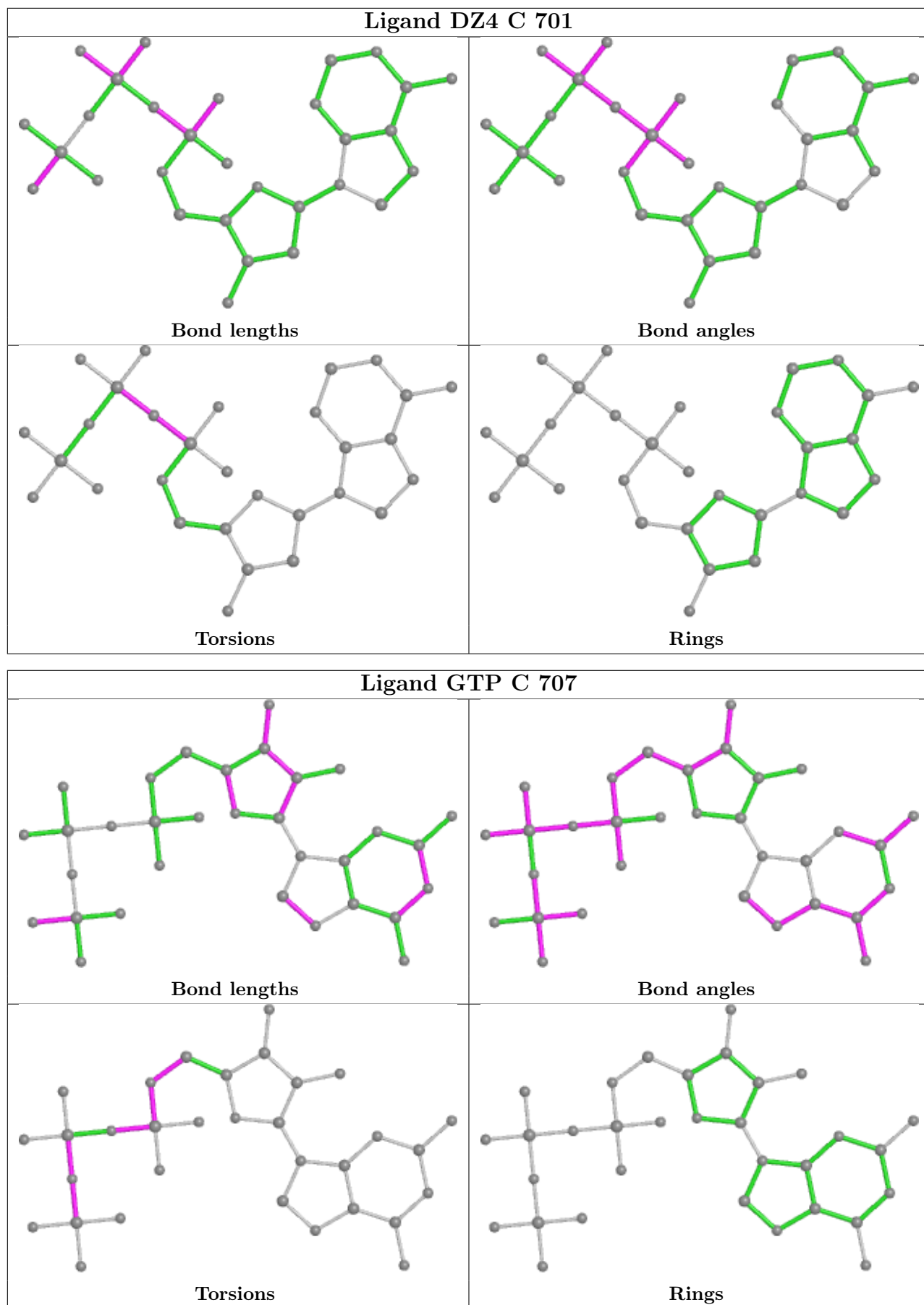


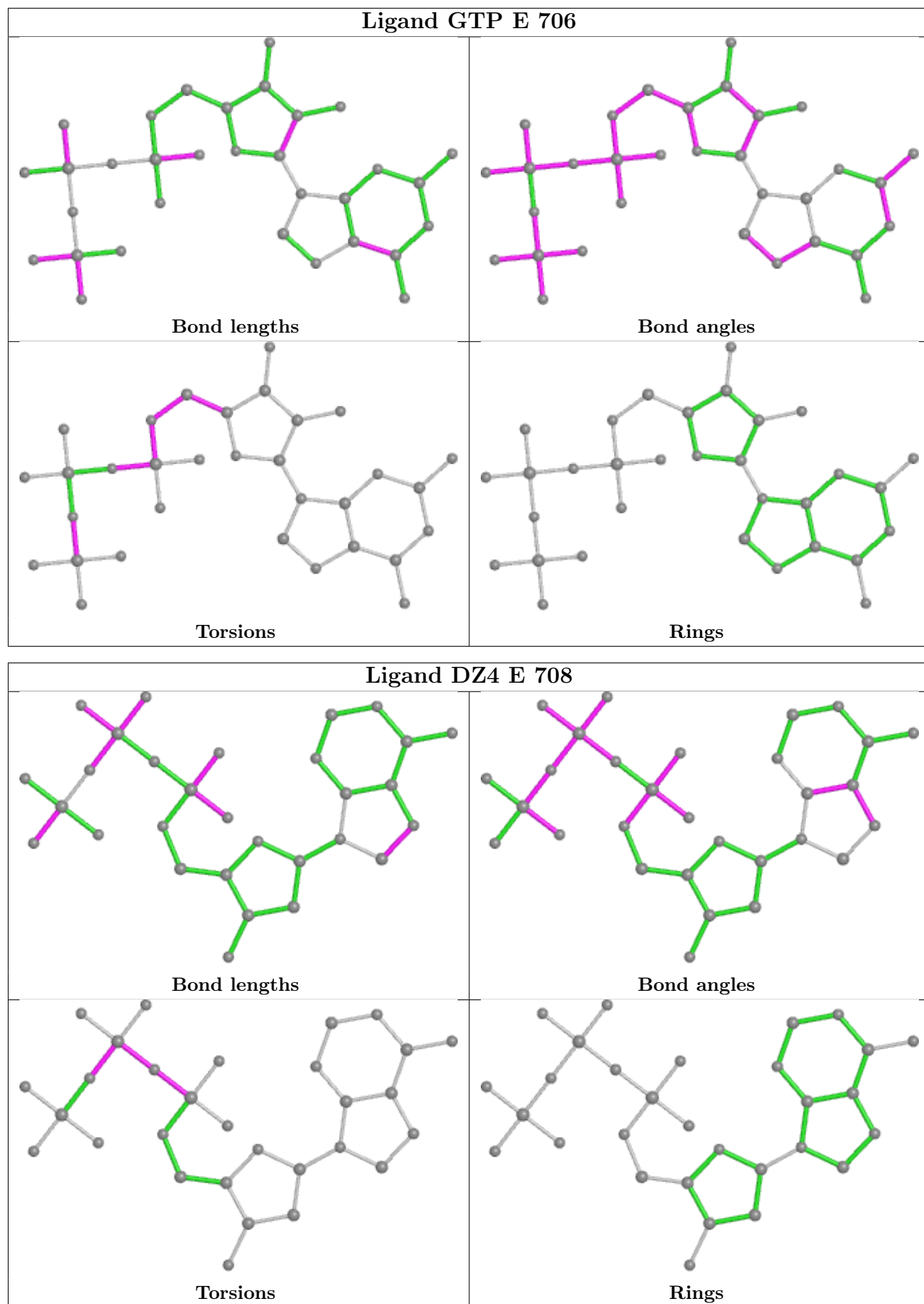


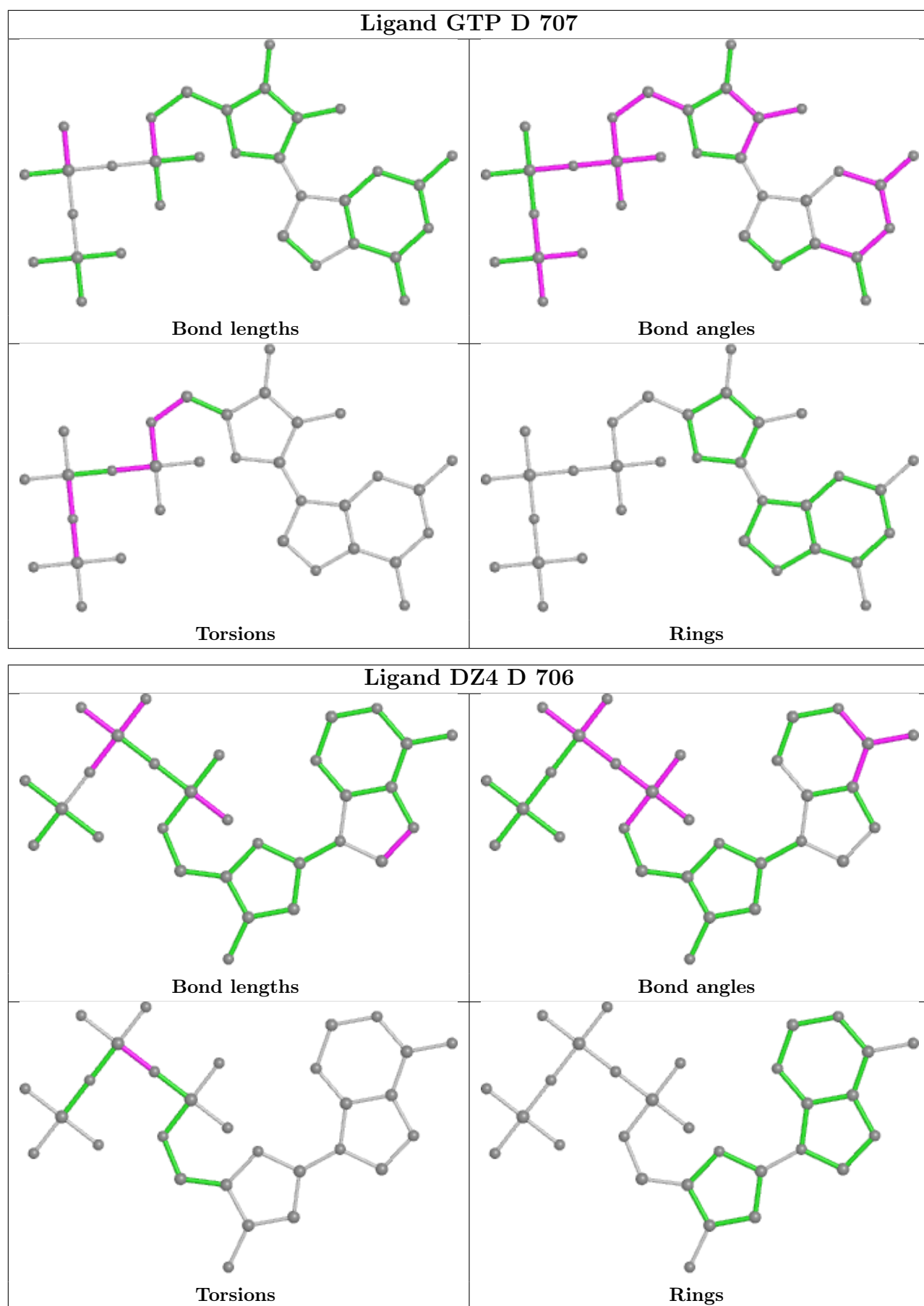


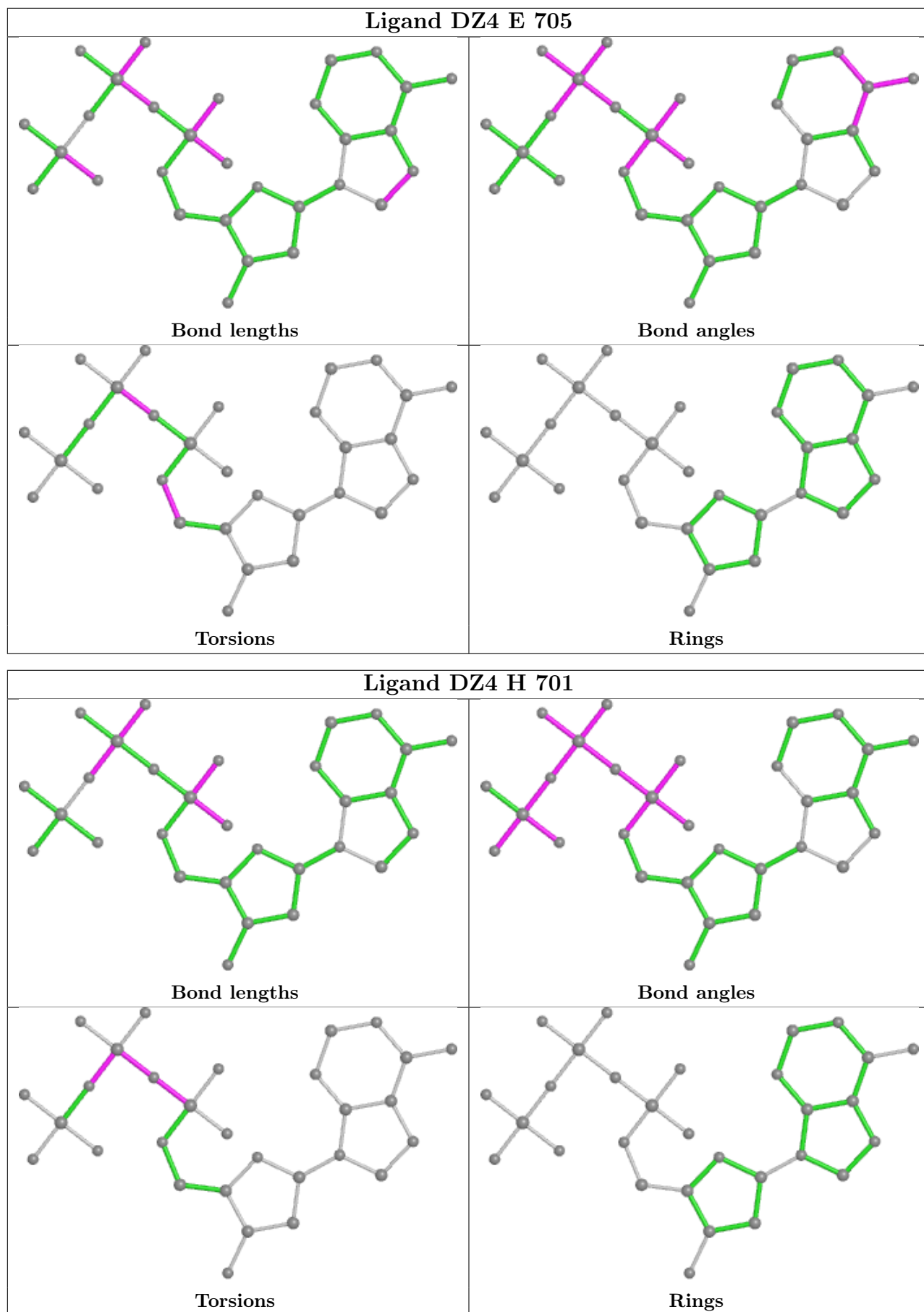




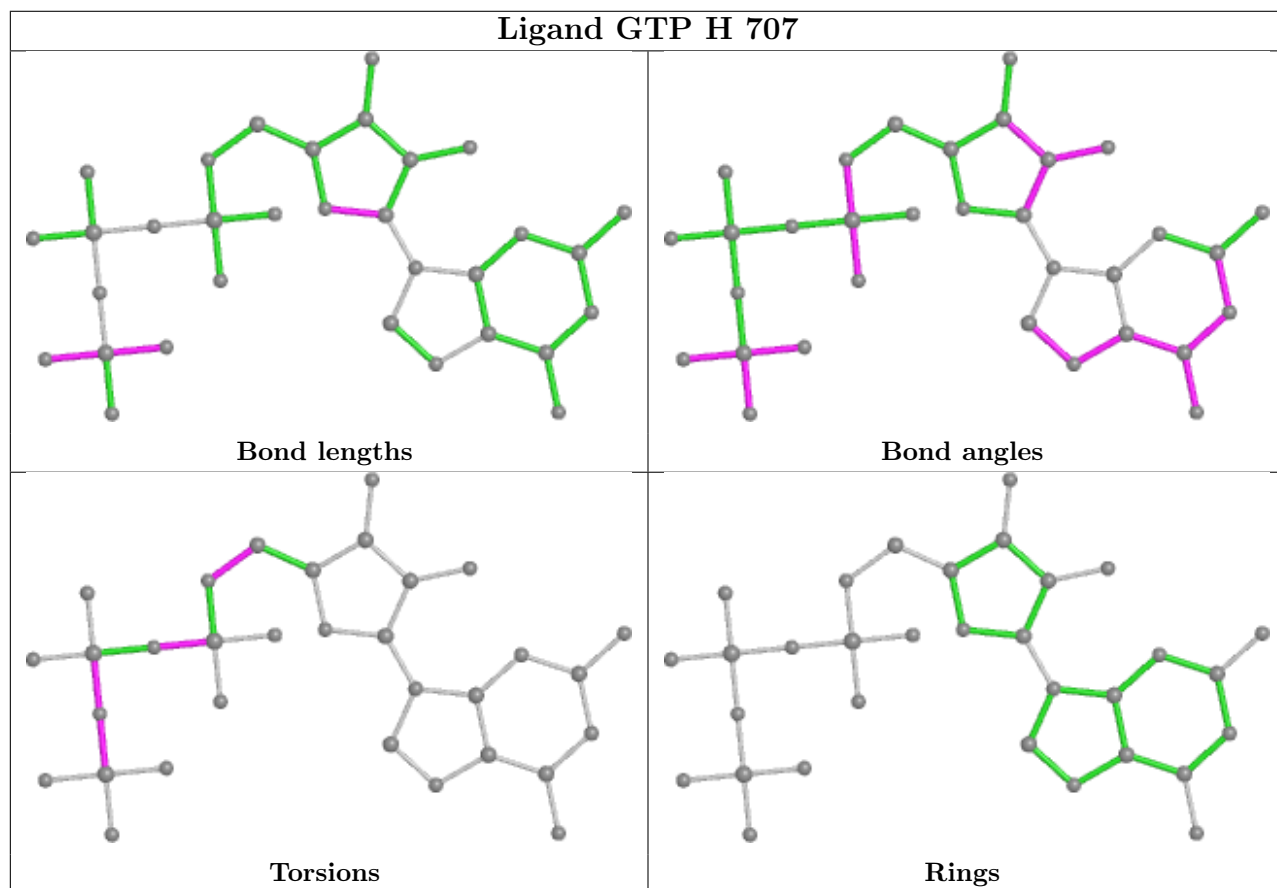
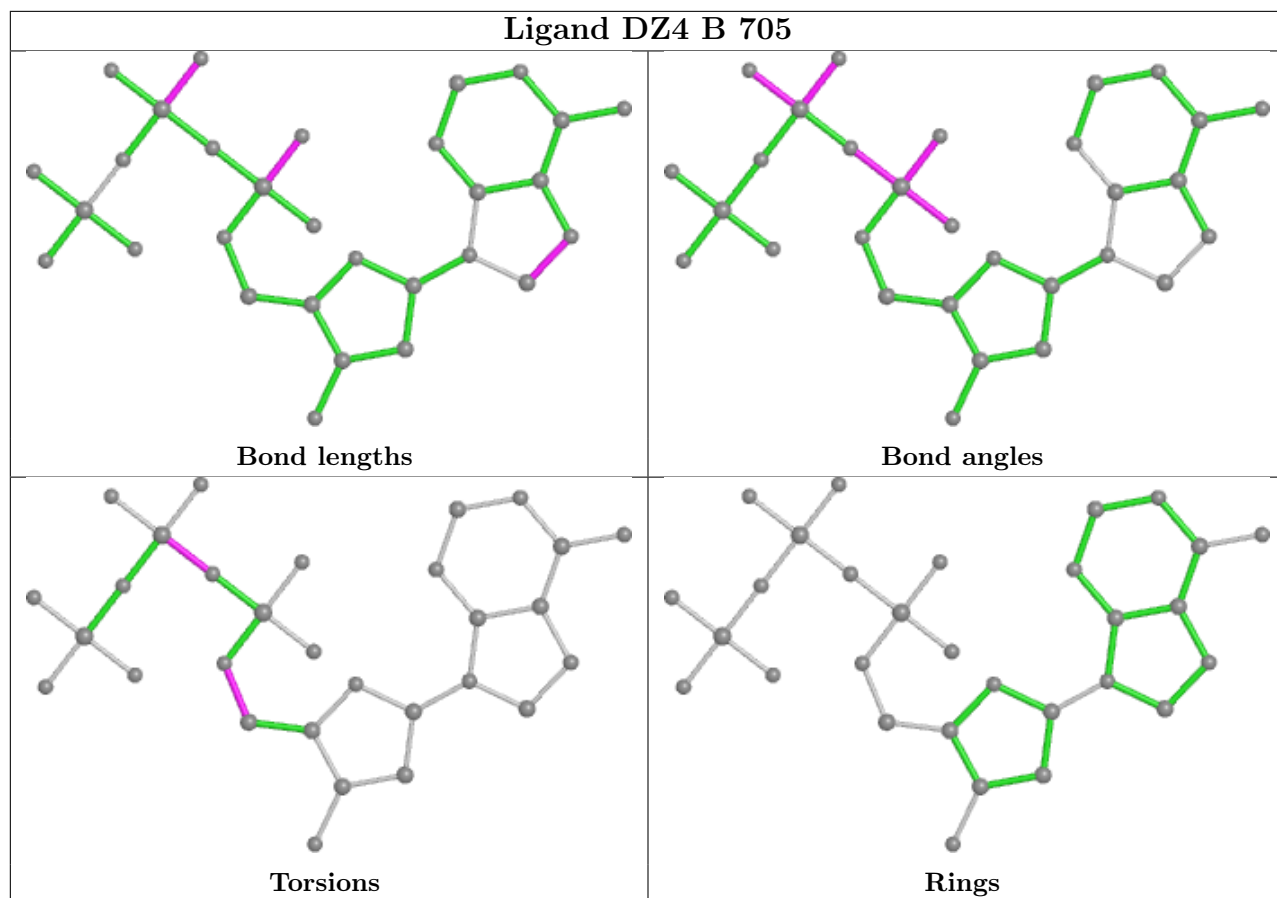


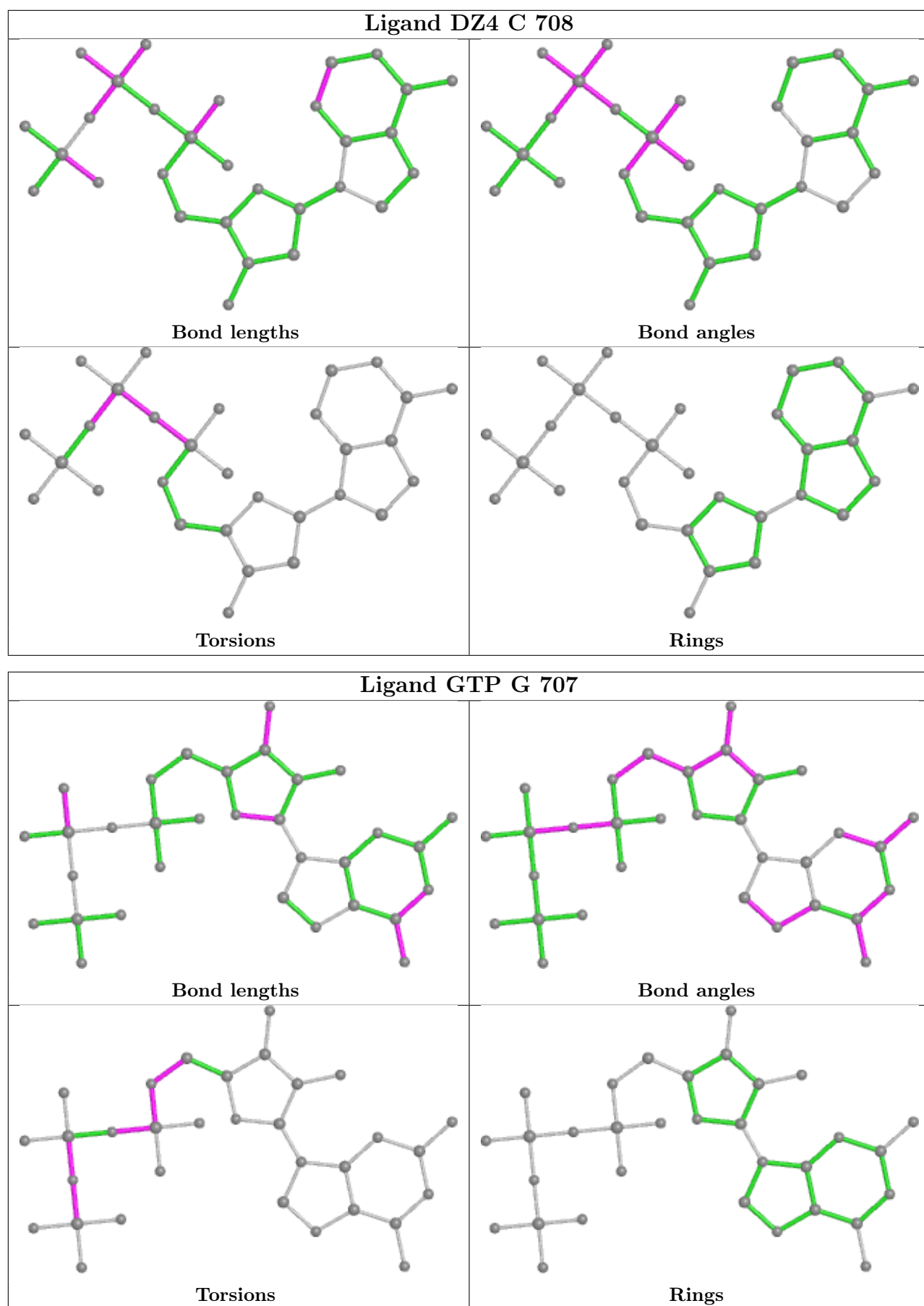












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	480/520 (92%)	-0.35	2 (0%) 92 91	12, 27, 59, 93	0
1	B	479/520 (92%)	-0.42	2 (0%) 92 91	12, 25, 53, 73	0
1	C	478/520 (91%)	-0.40	2 (0%) 92 91	12, 25, 57, 79	0
1	D	478/520 (91%)	-0.41	1 (0%) 95 94	13, 27, 54, 77	0
1	E	464/520 (89%)	-0.12	12 (2%) 56 53	14, 34, 70, 96	0
1	F	480/520 (92%)	-0.43	1 (0%) 95 94	11, 24, 47, 65	0
1	G	479/520 (92%)	-0.36	5 (1%) 82 81	13, 27, 56, 87	0
1	H	478/520 (91%)	-0.14	8 (1%) 70 68	17, 38, 75, 100	0
All	All	3816/4160 (91%)	-0.33	33 (0%) 84 83	11, 28, 60, 100	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	284	LEU	4.8
1	G	488	LEU	3.6
1	B	284	LEU	3.4
1	A	489	LEU	3.3
1	A	490	ASP	3.2
1	C	488	LEU	3.1
1	E	490	ASP	3.0
1	H	559	ARG	2.9
1	H	590	LEU	2.8
1	E	489	LEU	2.7
1	H	345	ASN	2.7
1	E	562	LEU	2.7
1	H	403	GLY	2.6
1	H	488	LEU	2.5
1	G	464	GLY	2.5
1	H	284	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	491	VAL	2.4
1	E	559	ARG	2.4
1	E	491	VAL	2.3
1	E	276	LEU	2.3
1	C	284	LEU	2.3
1	E	113	ASP	2.3
1	H	561	SER	2.3
1	E	563	TYR	2.3
1	D	488	LEU	2.2
1	B	113	ASP	2.2
1	G	599	ASN	2.2
1	G	490	ASP	2.1
1	E	326	GLN	2.1
1	F	114	THR	2.0
1	E	543	GLU	2.0
1	G	594	GLN	2.0
1	E	478	LYS	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	H	704	1/1	0.86	0.07	32,32,32,32	0
3	MG	D	708	1/1	0.89	0.07	38,38,38,38	0
3	MG	H	703	1/1	0.90	0.12	15,15,15,15	0
3	MG	G	705	1/1	0.95	0.06	36,36,36,36	0
3	MG	E	703	1/1	0.96	0.03	26,26,26,26	0
3	MG	B	704	1/1	0.96	0.06	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	DZ4	H	706	30/30	0.96	0.11	18,22,27,34	0
3	MG	F	703	1/1	0.97	0.05	15,15,15,15	0
3	MG	F	704	1/1	0.97	0.04	28,28,28,28	0
3	MG	B	703	1/1	0.97	0.03	16,16,16,16	0
3	MG	D	704	1/1	0.98	0.04	19,19,19,19	0
3	MG	D	705	1/1	0.98	0.05	18,18,18,18	0
3	MG	C	705	1/1	0.98	0.07	17,17,17,17	0
4	DZ4	A	707	30/30	0.98	0.09	13,15,18,20	0
4	DZ4	C	701	30/30	0.98	0.09	11,13,16,18	0
4	DZ4	E	708	30/30	0.98	0.10	20,23,32,33	0
4	DZ4	F	706	30/30	0.98	0.10	11,15,19,20	0
4	DZ4	H	701	30/30	0.98	0.09	20,23,28,29	0
3	MG	G	704	1/1	0.98	0.05	20,20,20,20	0
5	GTP	E	707	32/32	0.98	0.09	18,20,30,33	0
5	GTP	G	707	32/32	0.98	0.09	20,23,32,36	0
3	MG	E	702	1/1	0.99	0.09	15,15,15,15	0
3	MG	H	705	1/1	0.99	0.08	17,17,17,17	0
4	DZ4	A	705	30/30	0.99	0.09	13,15,19,21	0
3	MG	C	704	1/1	0.99	0.02	13,13,13,13	0
4	DZ4	B	705	30/30	0.99	0.10	12,14,16,16	0
3	MG	E	704	1/1	0.99	0.05	16,16,16,16	0
4	DZ4	C	706	30/30	0.99	0.10	13,14,16,17	0
4	DZ4	C	708	30/30	0.99	0.09	14,16,20,23	0
4	DZ4	D	701	30/30	0.99	0.09	13,15,19,19	0
4	DZ4	D	706	30/30	0.99	0.09	13,16,19,20	0
4	DZ4	E	705	30/30	0.99	0.09	17,21,23,24	0
3	MG	A	704	1/1	0.99	0.04	14,14,14,14	0
4	DZ4	F	705	30/30	0.99	0.10	12,13,15,16	0
3	MG	D	703	1/1	0.99	0.08	8,8,8,8	0
4	DZ4	G	701	30/30	0.99	0.10	12,15,19,20	0
4	DZ4	G	706	30/30	0.99	0.10	12,13,15,16	0
3	MG	G	703	1/1	0.99	0.09	11,11,11,11	0
3	MG	A	702	1/1	0.99	0.05	8,8,8,8	0
5	GTP	A	706	32/32	0.99	0.09	12,13,18,19	0
5	GTP	B	706	32/32	0.99	0.08	13,17,25,25	0
5	GTP	C	707	32/32	0.99	0.09	14,16,22,23	0
5	GTP	D	707	32/32	0.99	0.08	14,16,22,23	0
5	GTP	E	706	32/32	0.99	0.09	13,15,21,23	0
3	MG	A	703	1/1	0.99	0.05	14,14,14,14	0
3	MG	C	703	1/1	0.99	0.09	9,9,9,9	0
5	GTP	H	707	32/32	0.99	0.10	15,17,22,23	0
2	FE	A	701	1/1	1.00	0.11	14,14,14,14	0

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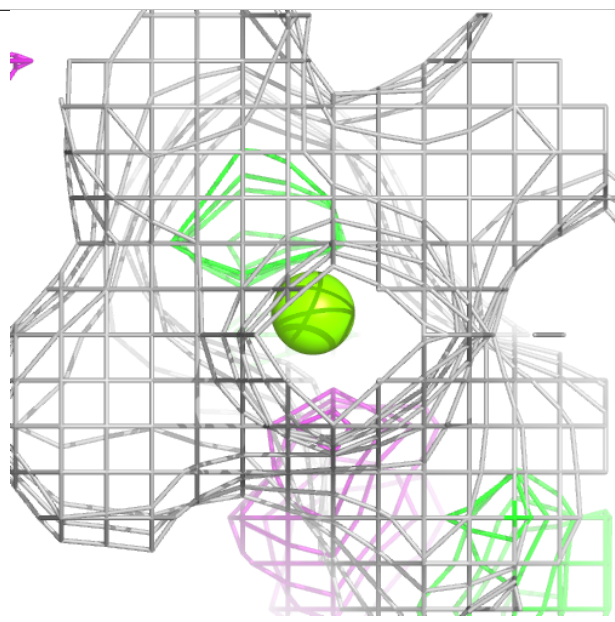
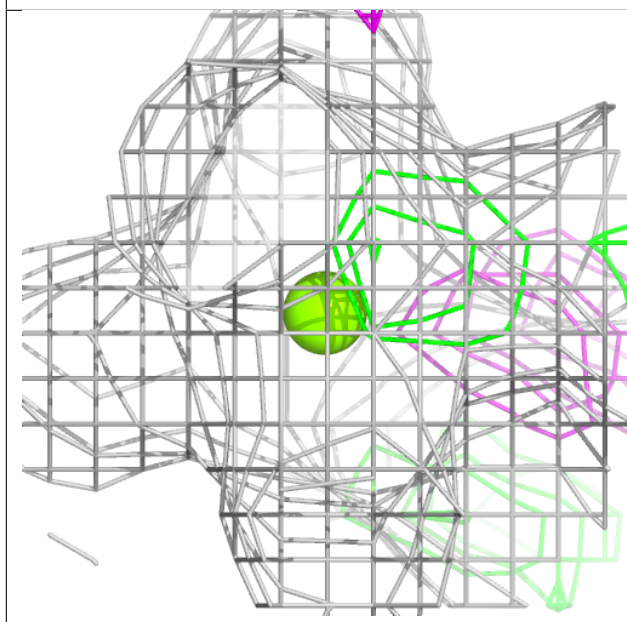
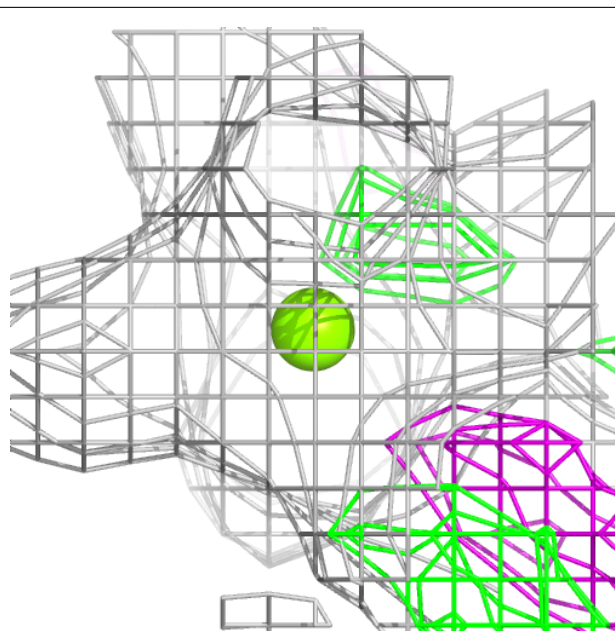
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FE	B	701	1/1	1.00	0.09	13,13,13,13	0
2	FE	C	702	1/1	1.00	0.10	13,13,13,13	0
3	MG	B	702	1/1	1.00	0.05	9,9,9,9	0
2	FE	D	702	1/1	1.00	0.10	15,15,15,15	0
2	FE	E	701	1/1	1.00	0.11	17,17,17,17	0
2	FE	F	701	1/1	1.00	0.09	14,14,14,14	0
3	MG	F	702	1/1	1.00	0.11	9,9,9,9	0
2	FE	G	702	1/1	1.00	0.10	13,13,13,13	0
2	FE	H	702	1/1	1.00	0.10	20,20,20,20	0

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

**Electron density around MG H 704:**

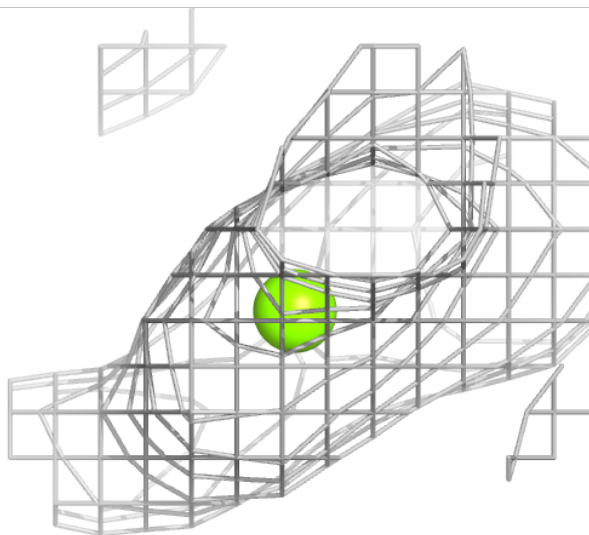
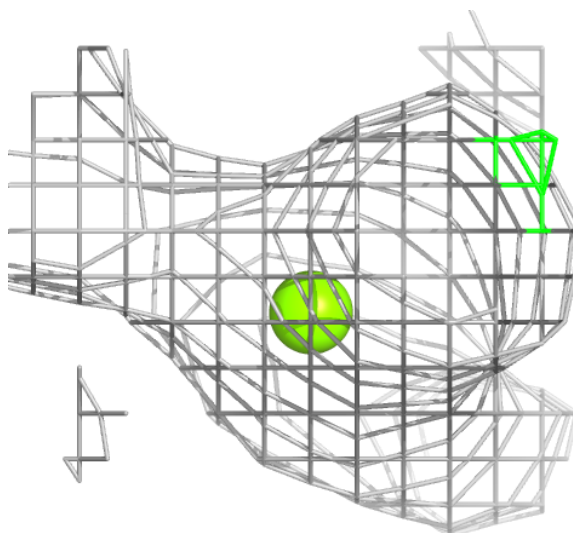
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





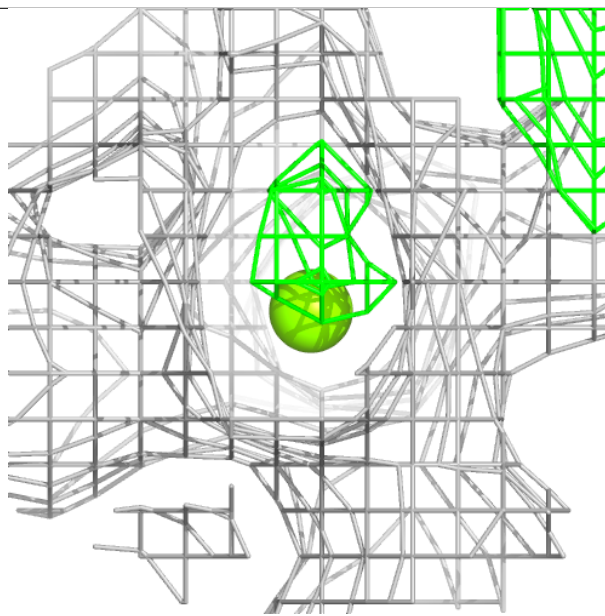
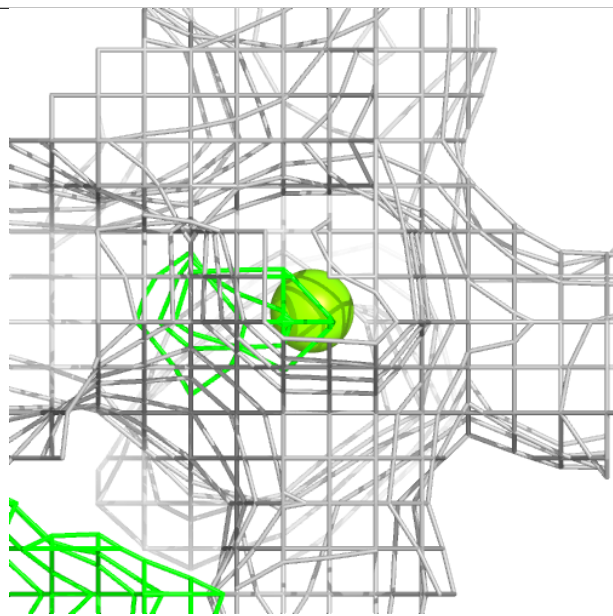
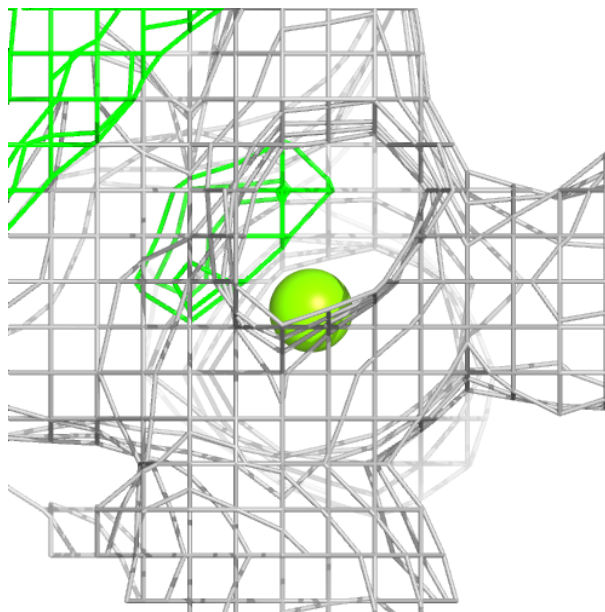
**Electron density around MG D 708:**

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and green (positive)



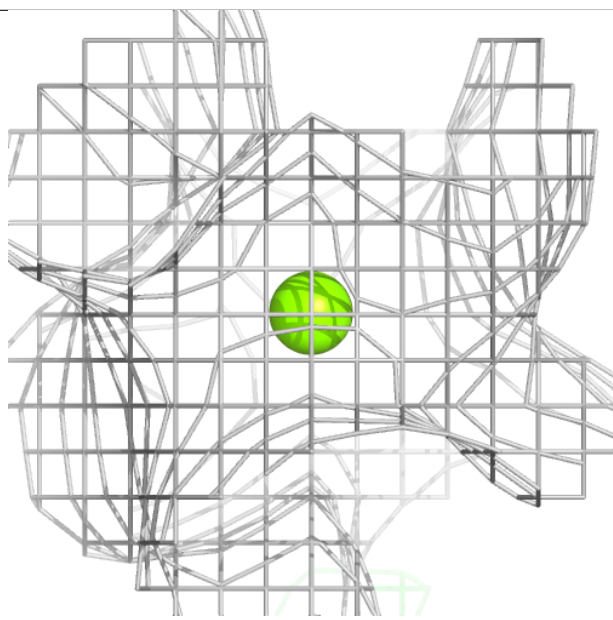
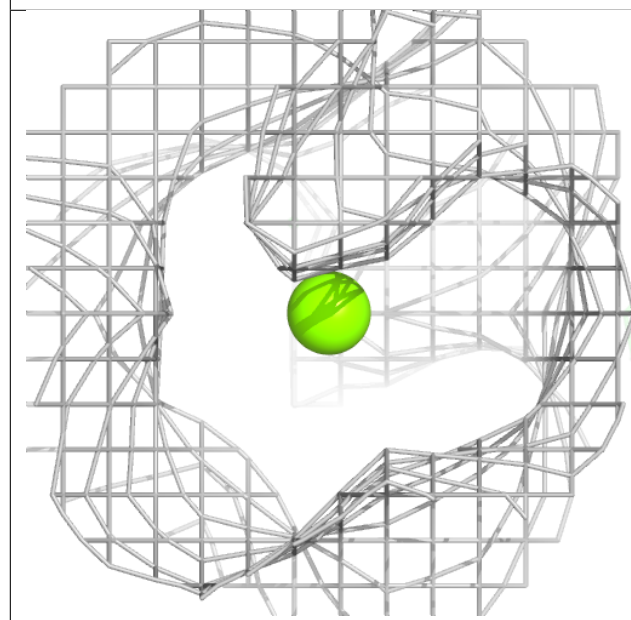
**Electron density around MG H 703:**

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



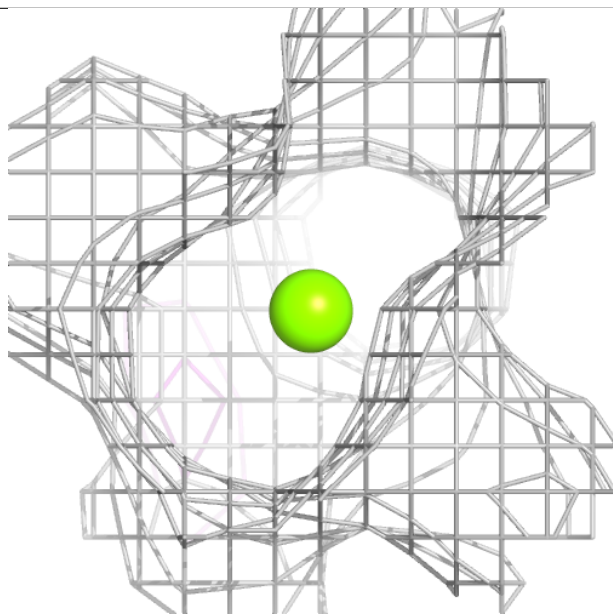
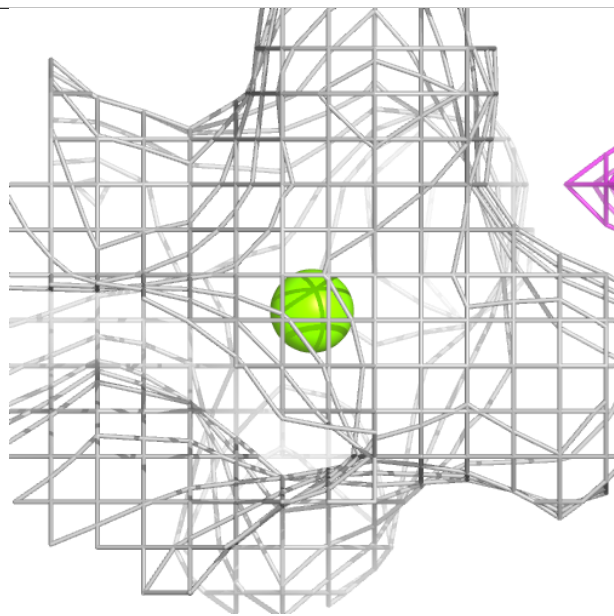
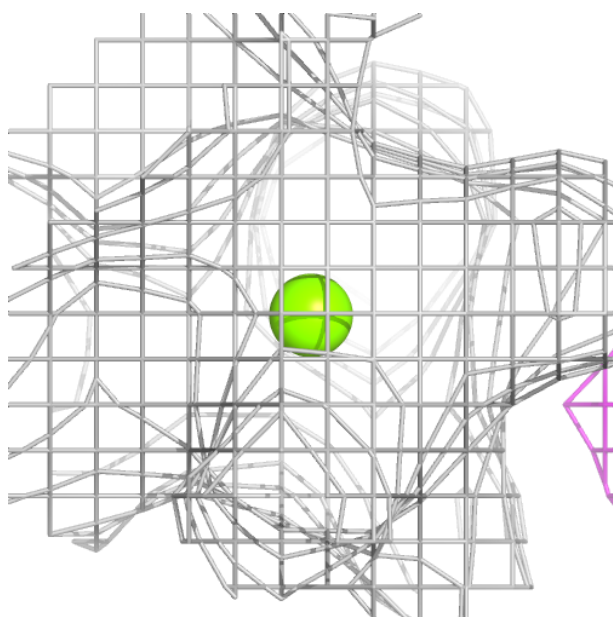
**Electron density around MG G 705:**

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



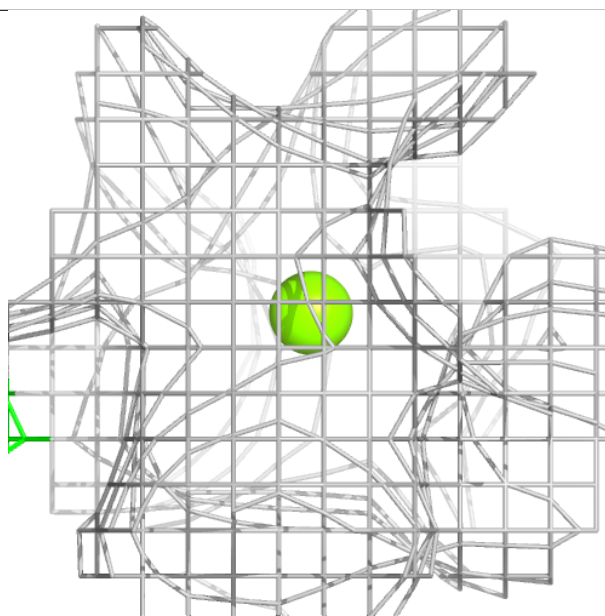
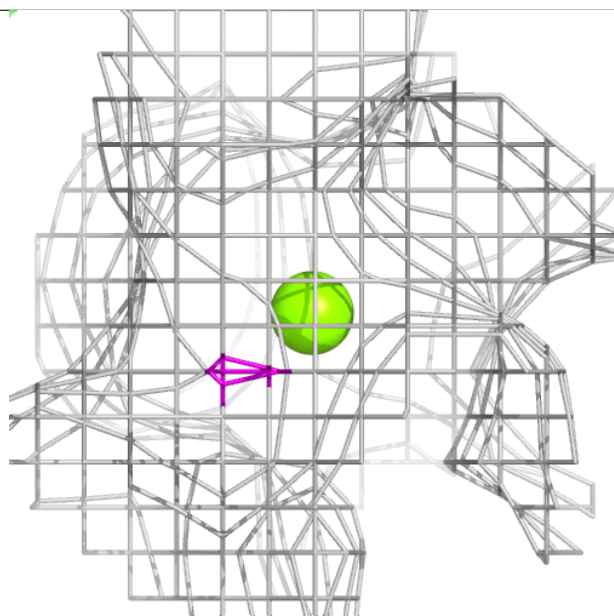
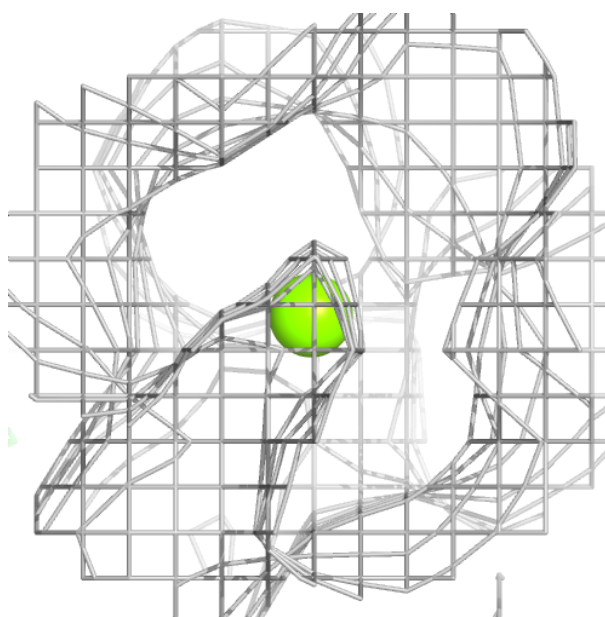
**Electron density around MG E 703:**

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



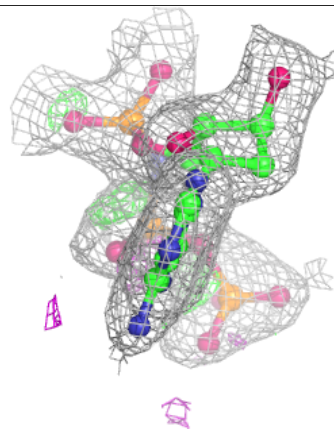
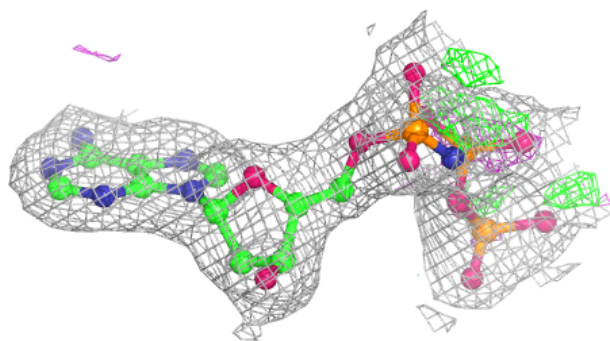
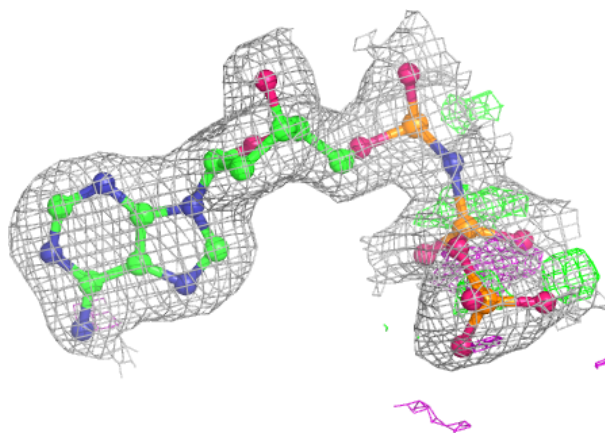
**Electron density around MG B 704:**

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



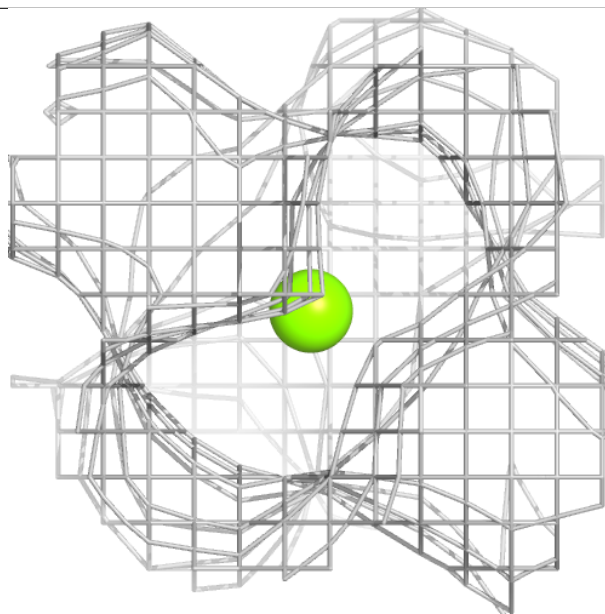
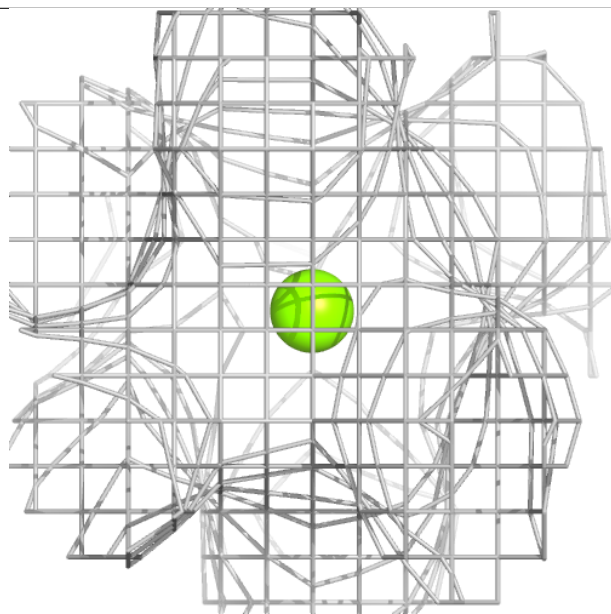
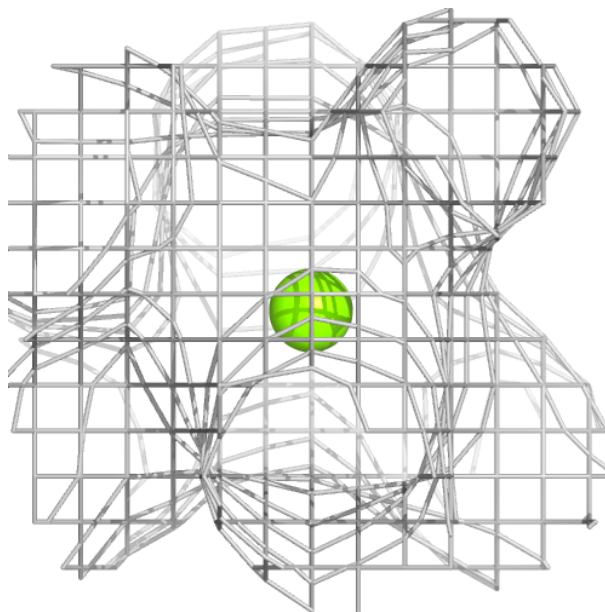
**Electron density around DZ4 H 706:**

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



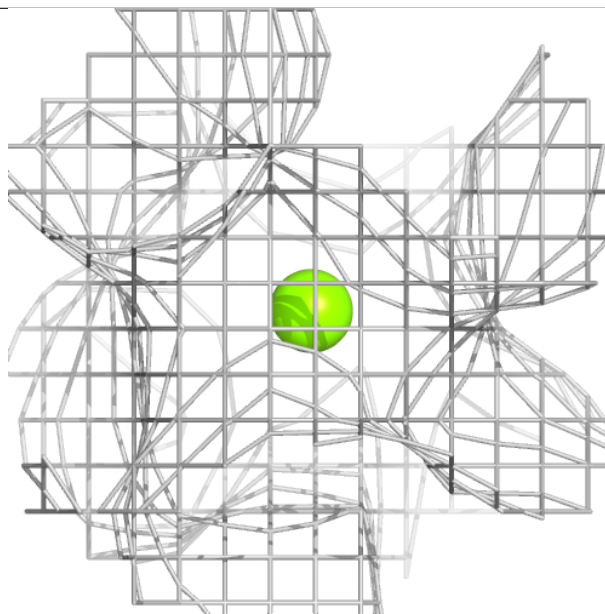
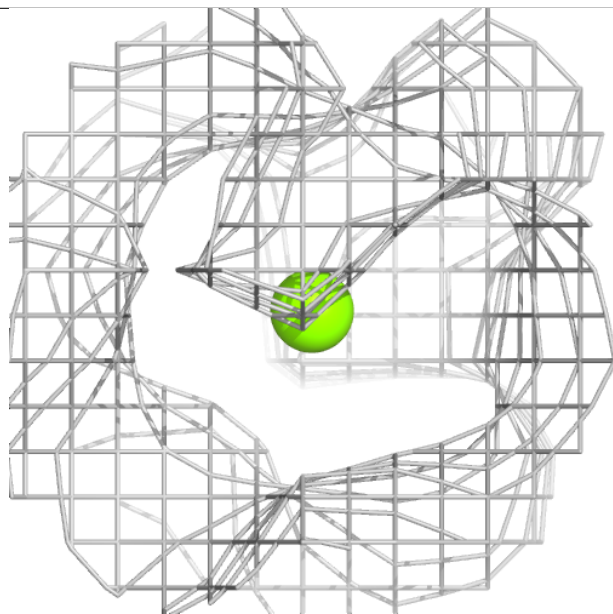
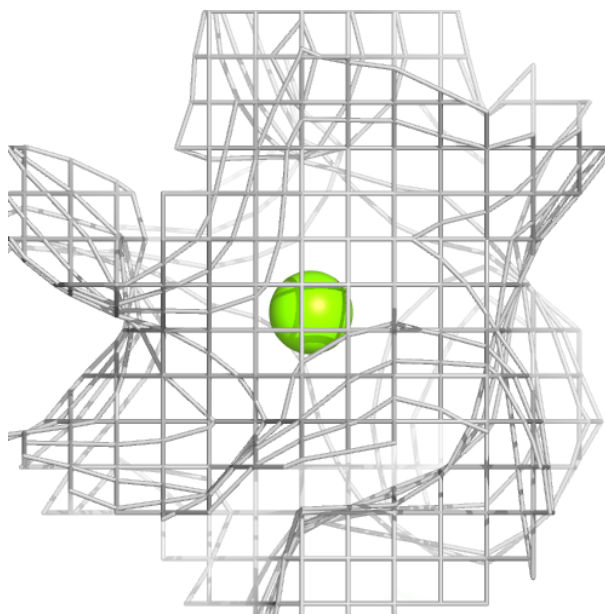
**Electron density around MG F 703:**

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



**Electron density around MG F 704:**

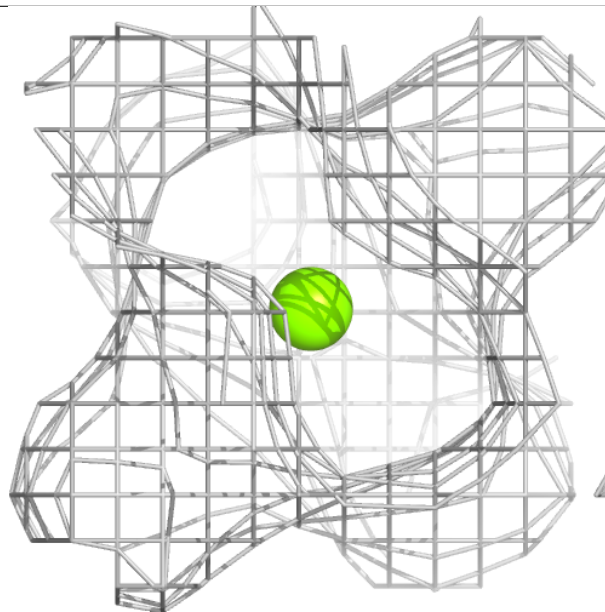
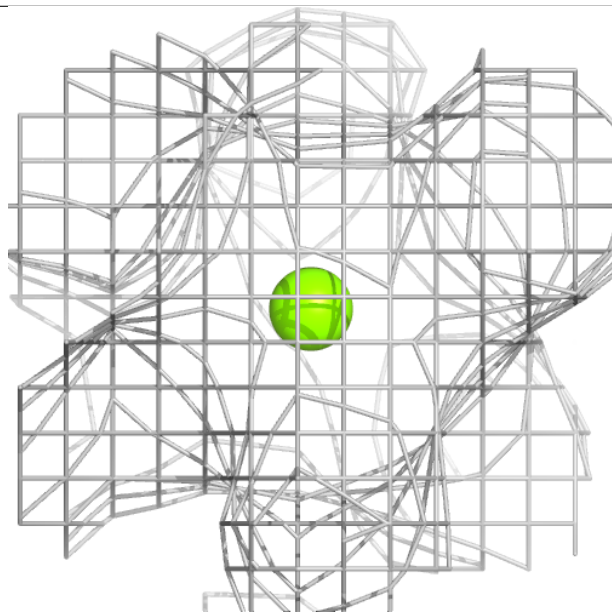
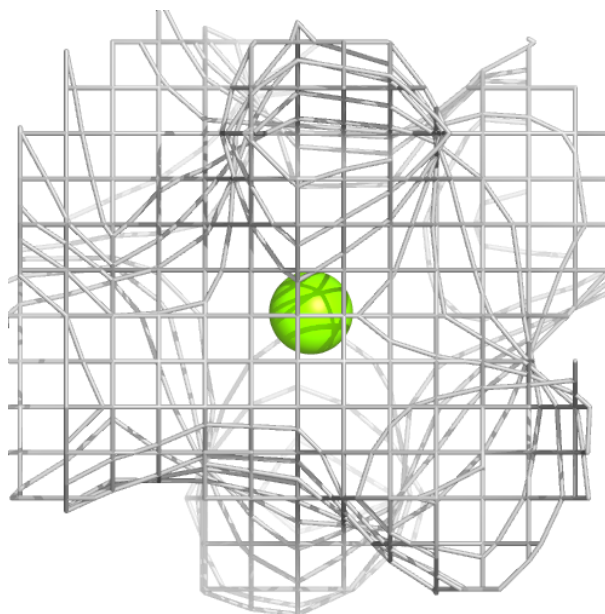
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





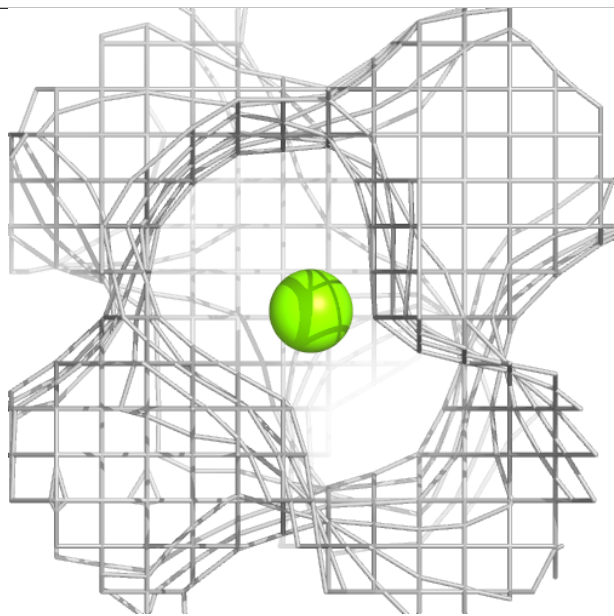
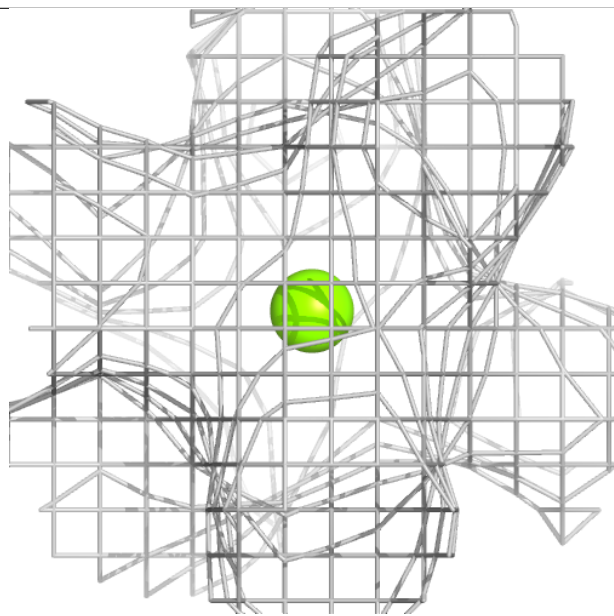
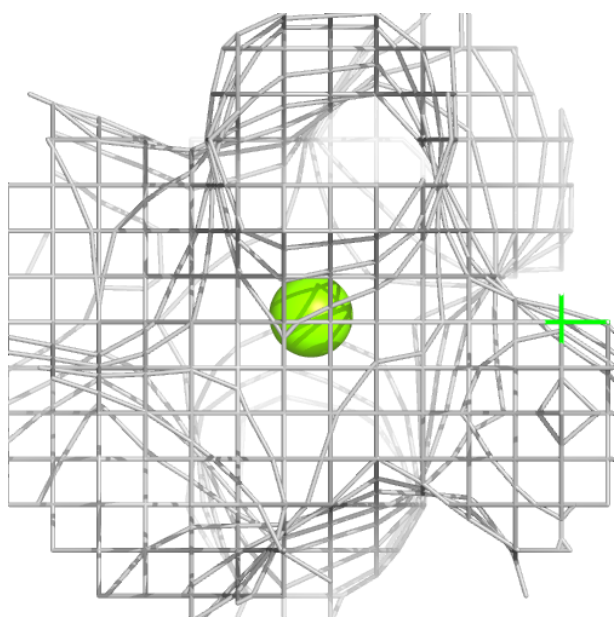
**Electron density around MG B 703:**

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



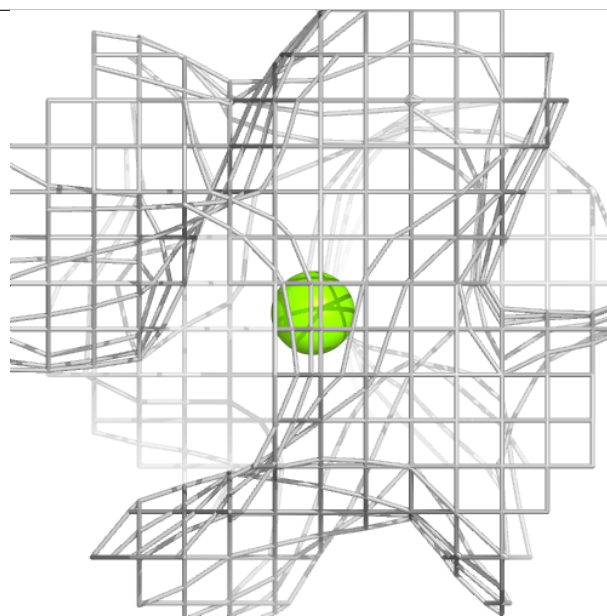
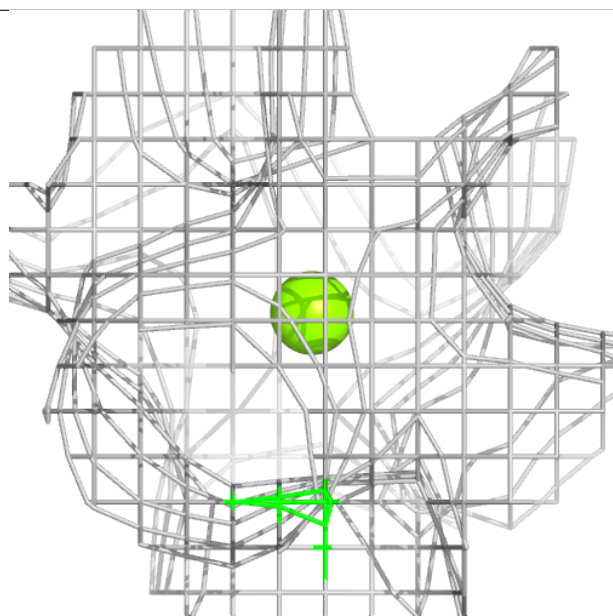
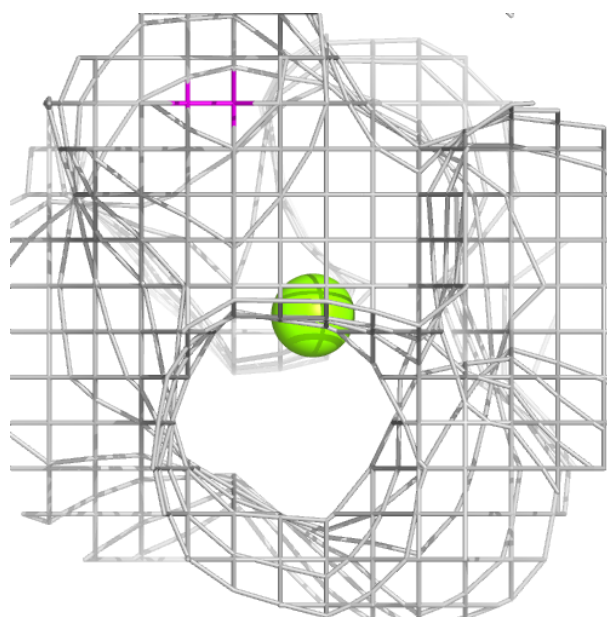
**Electron density around MG D 704:**

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



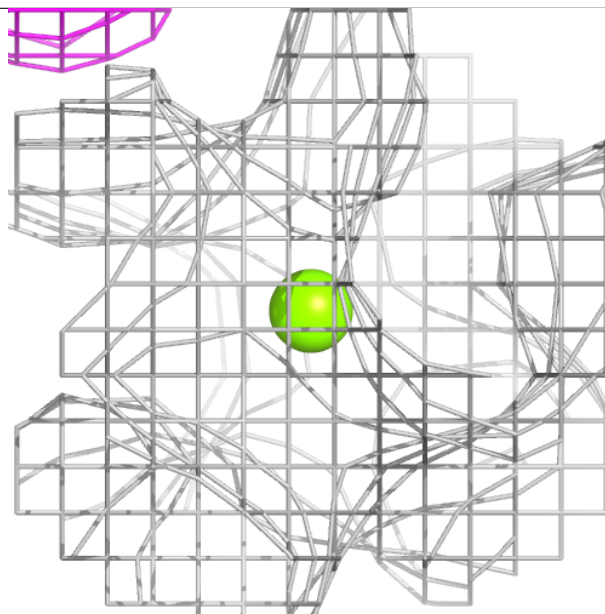
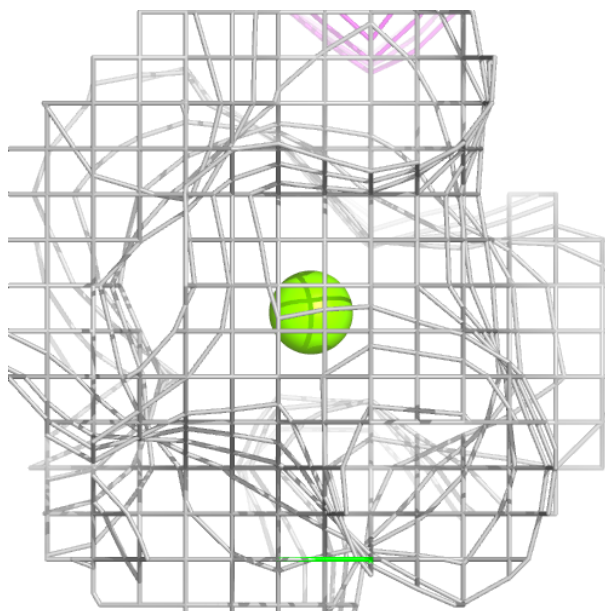
**Electron density around MG D 705:**

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



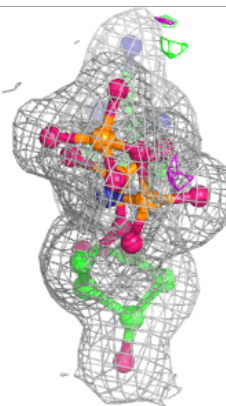
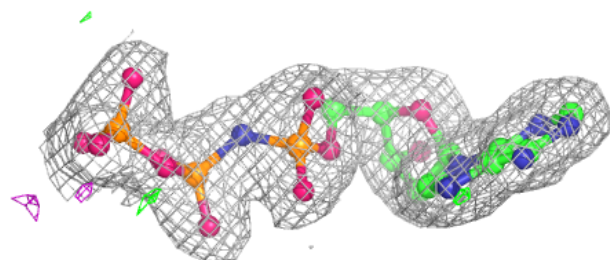
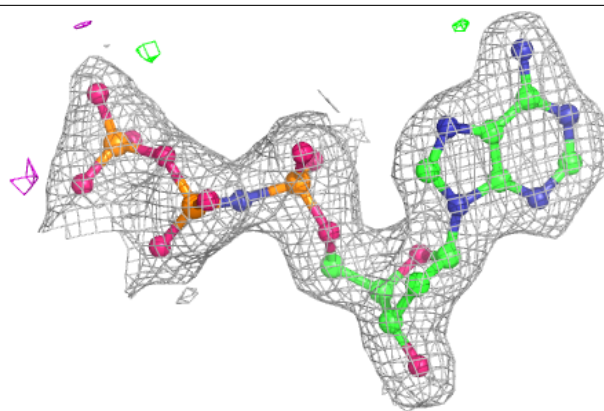
**Electron density around MG C 705:**

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

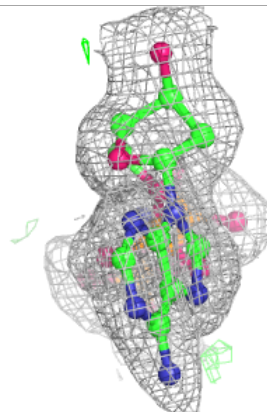
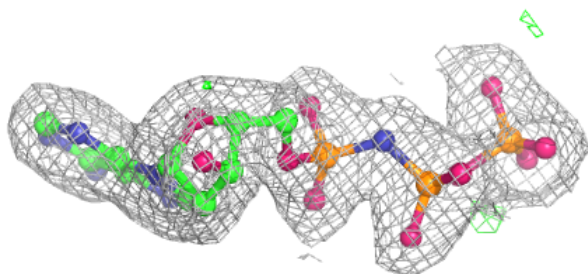
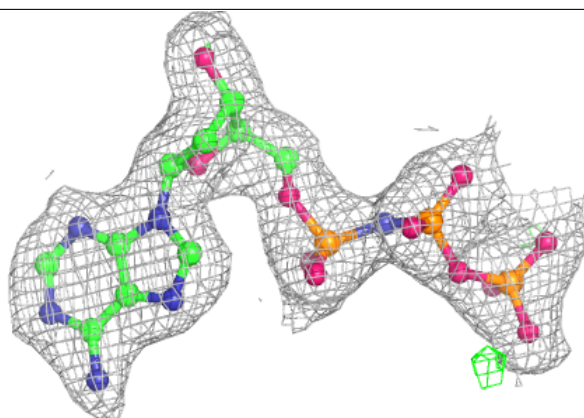


**Electron density around DZ4 A 707:**

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

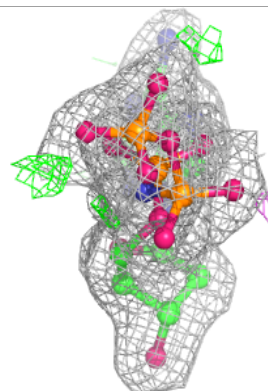
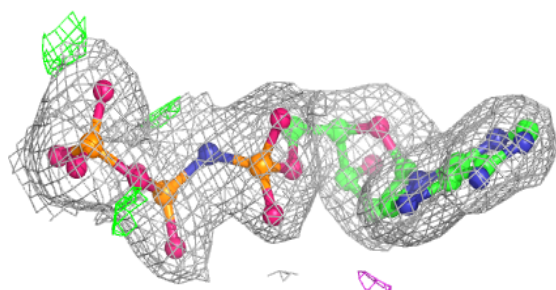
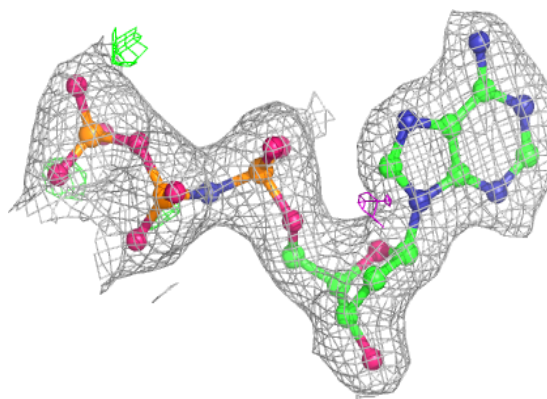
**Electron density around DZ4 C 701:**

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

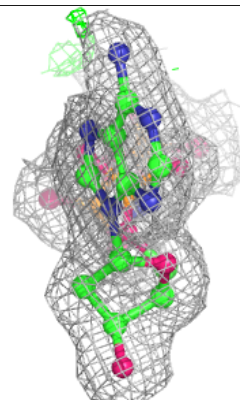
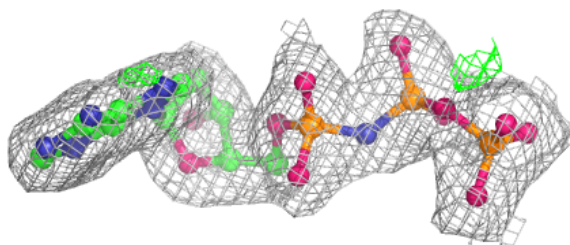
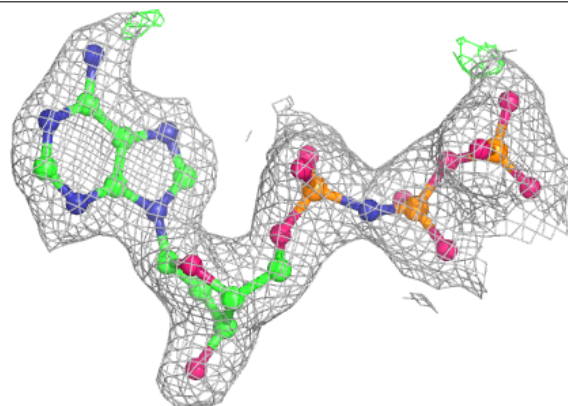


**Electron density around DZ4 E 708:**

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

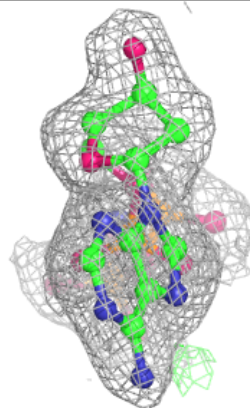
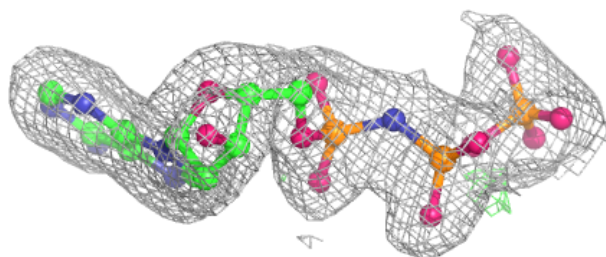
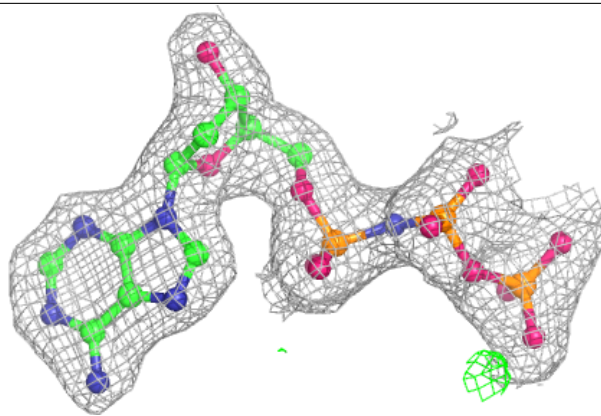
**Electron density around DZ4 F 706:**

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



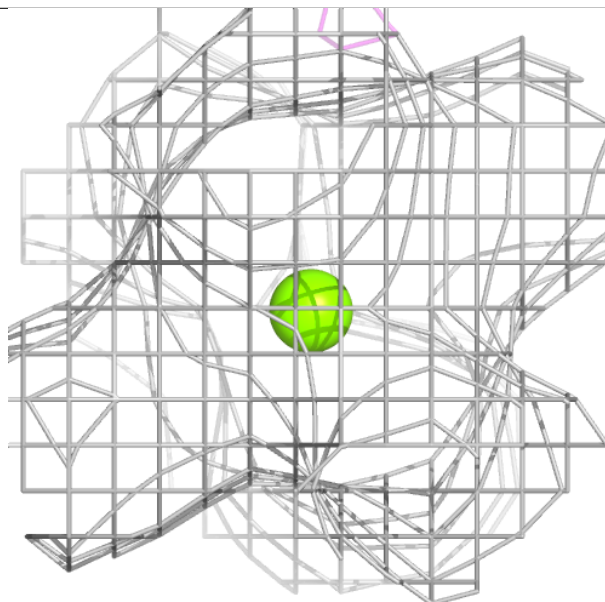
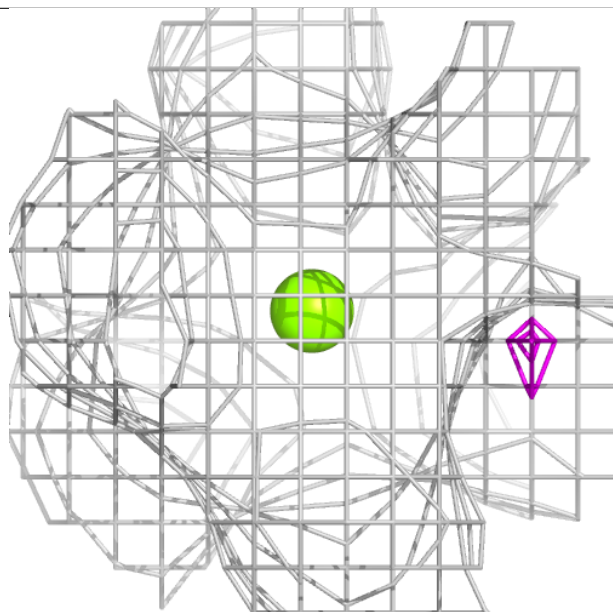
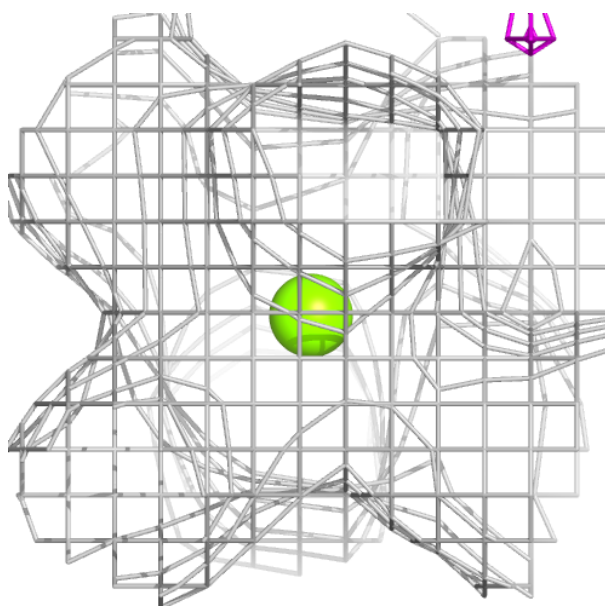
**Electron density around DZ4 H 701:**

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



**Electron density around MG G 704:**

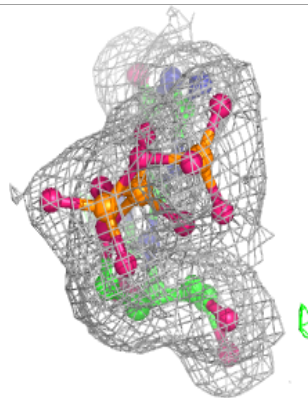
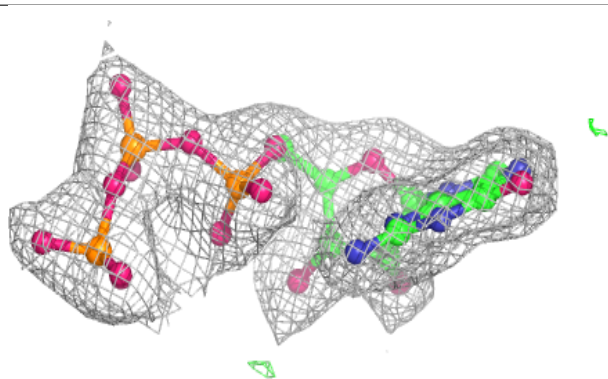
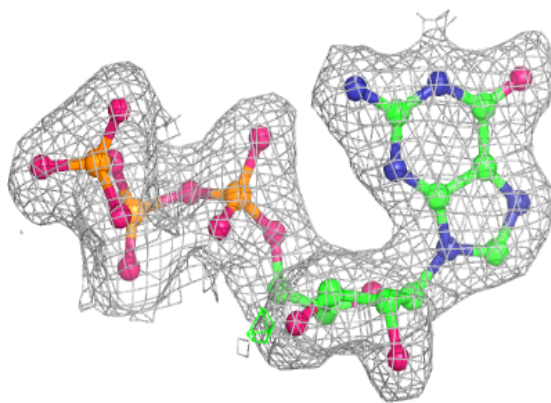
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



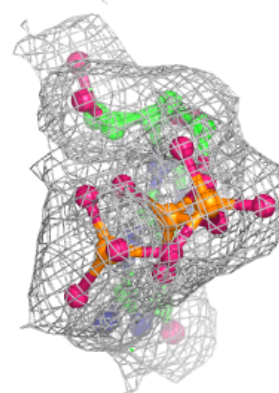
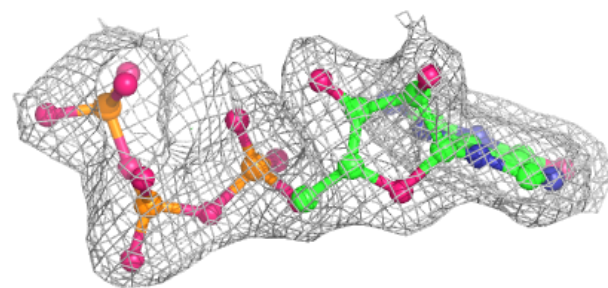
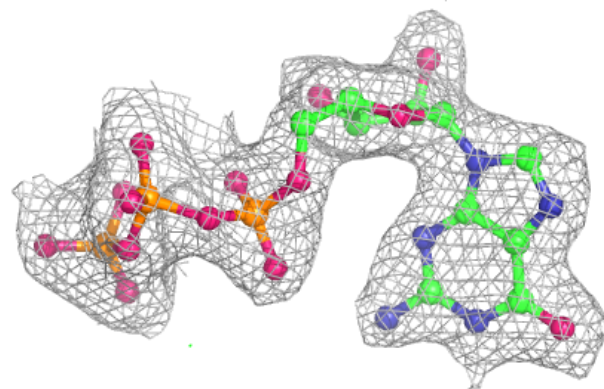


**Electron density around GTP E 707:**

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

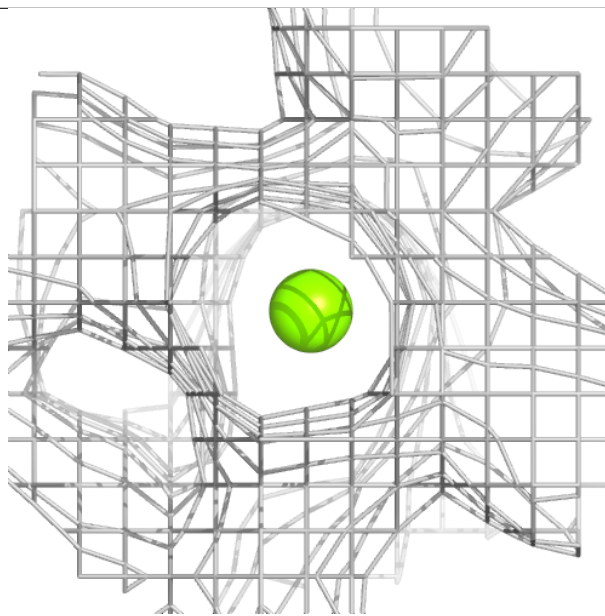
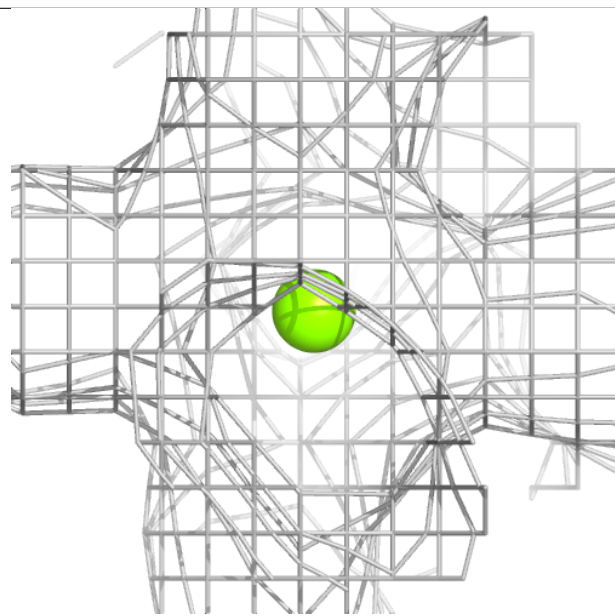
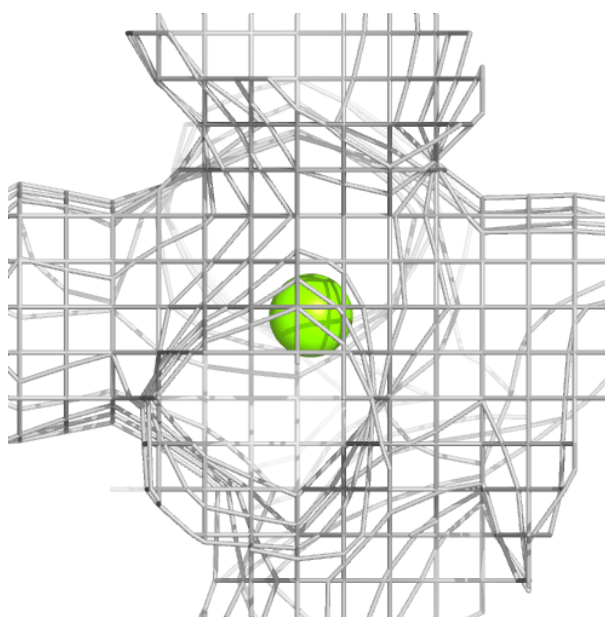
**Electron density around GTP G 707:**

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



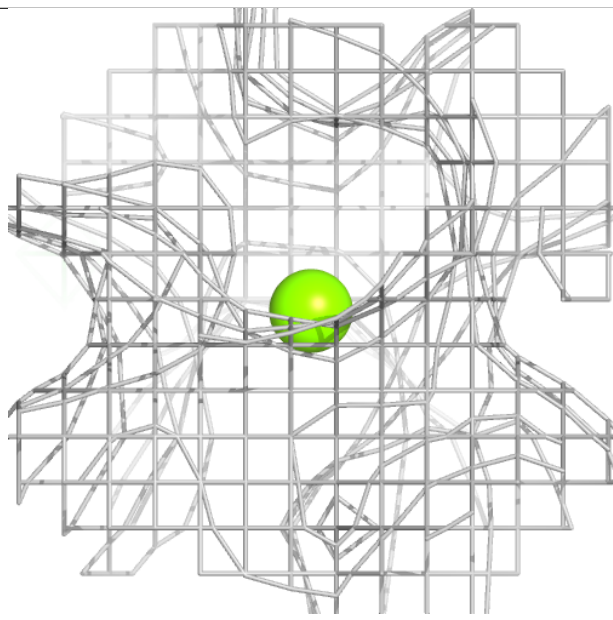
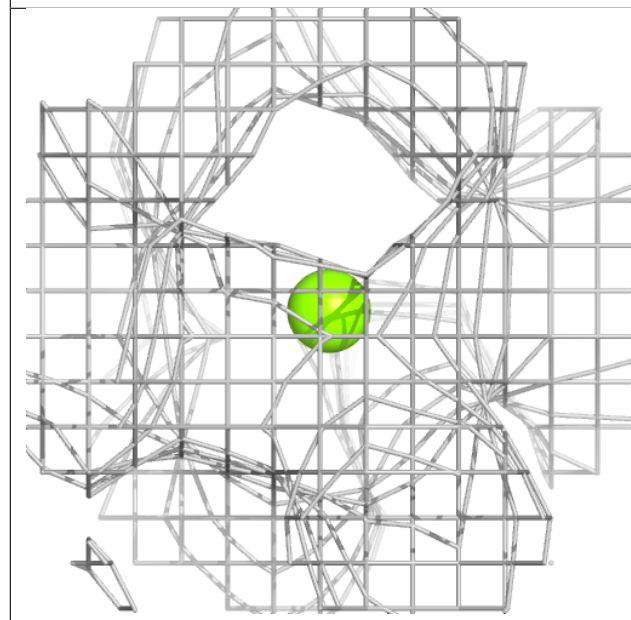
**Electron density around MG E 702:**

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



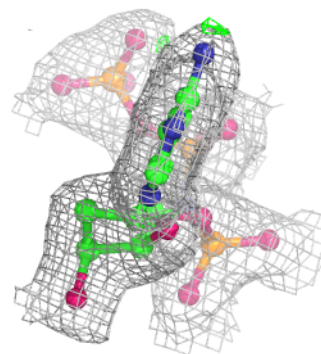
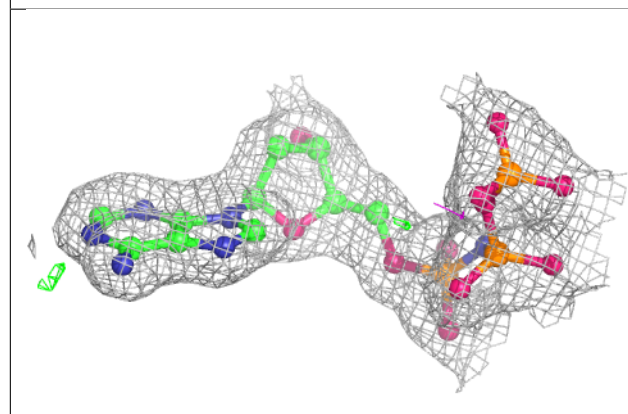
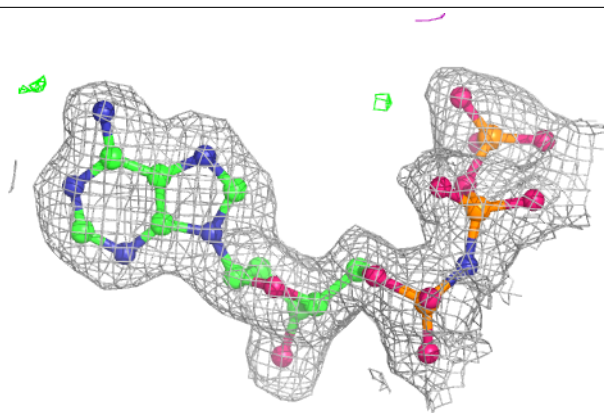
**Electron density around MG H 705:**

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



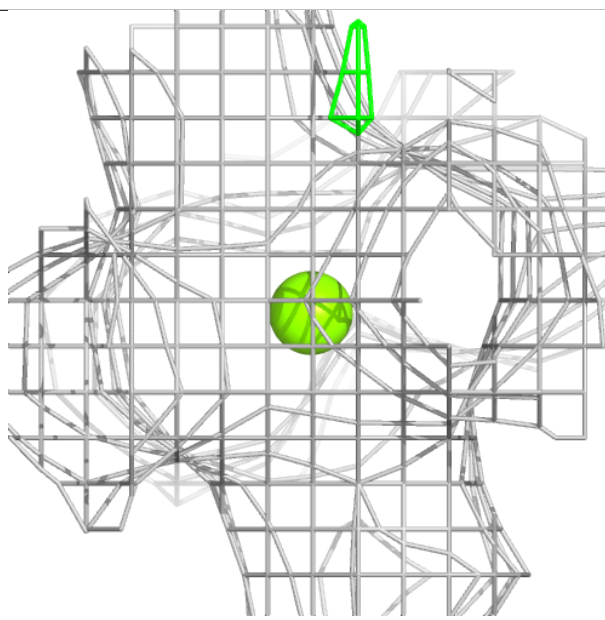
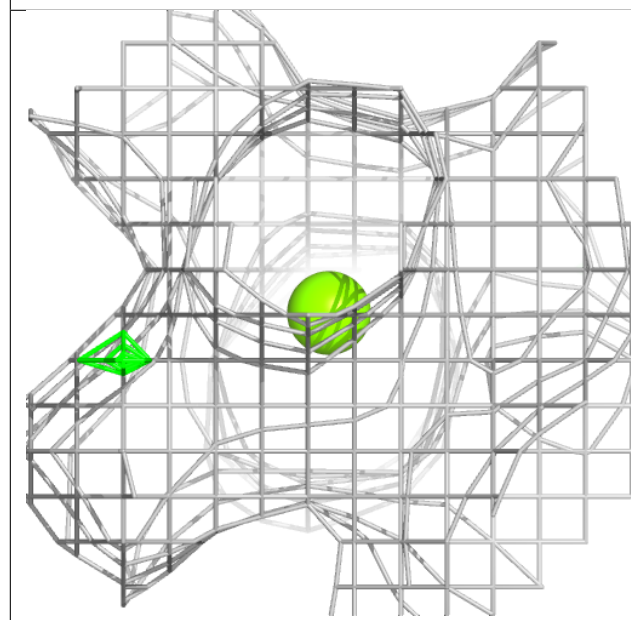
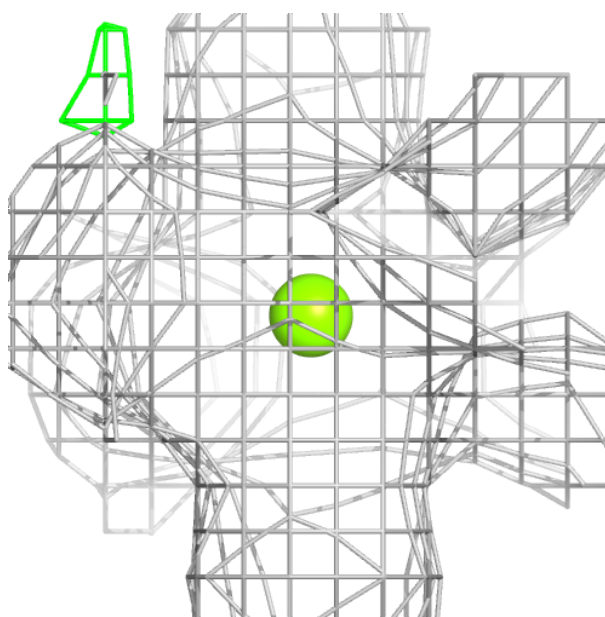
**Electron density around DZ4 A 705:**

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



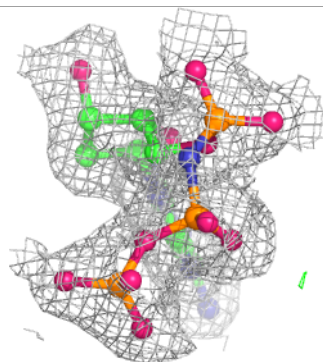
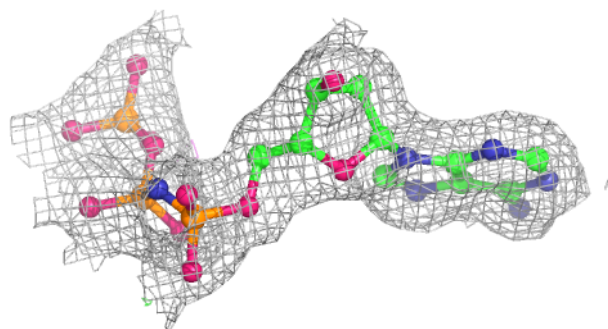
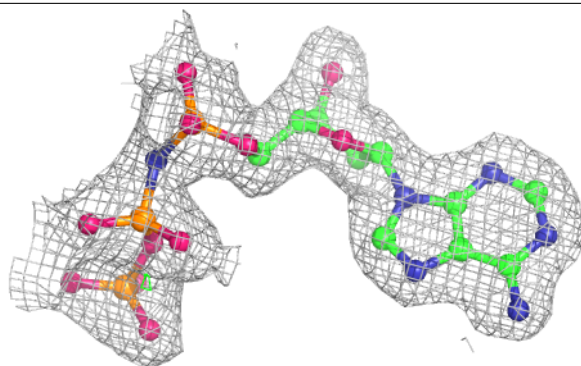
**Electron density around MG C 704:**

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



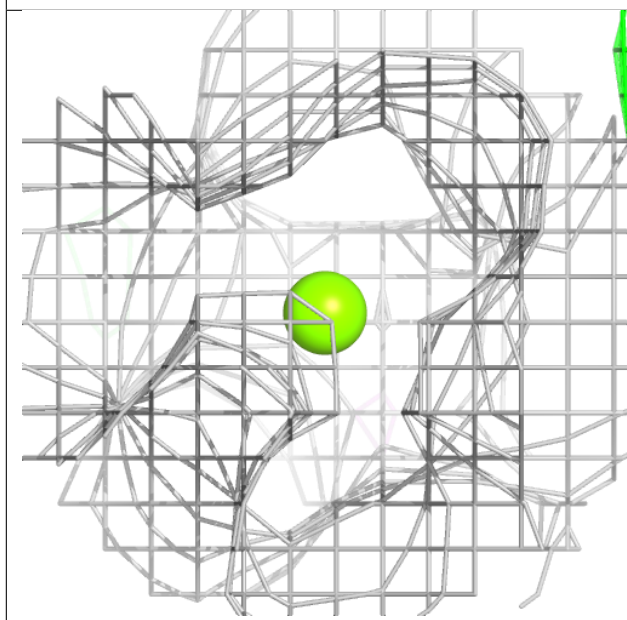
**Electron density around DZ4 B 705:**

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



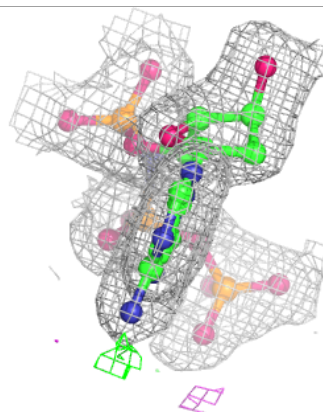
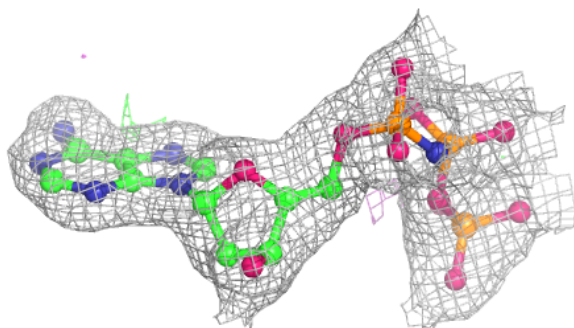
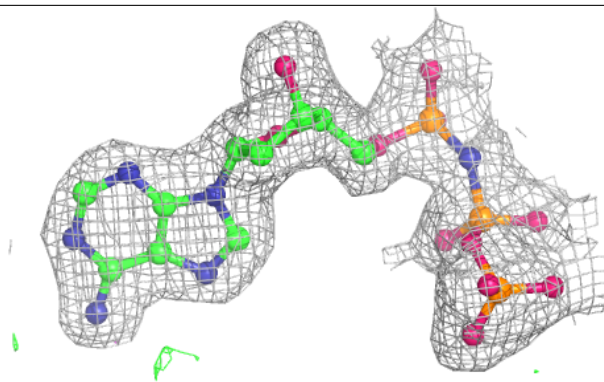
**Electron density around MG E 704:**

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

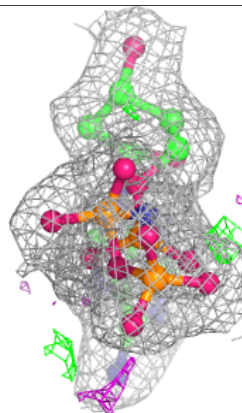
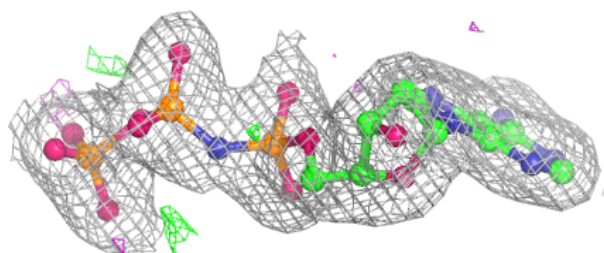
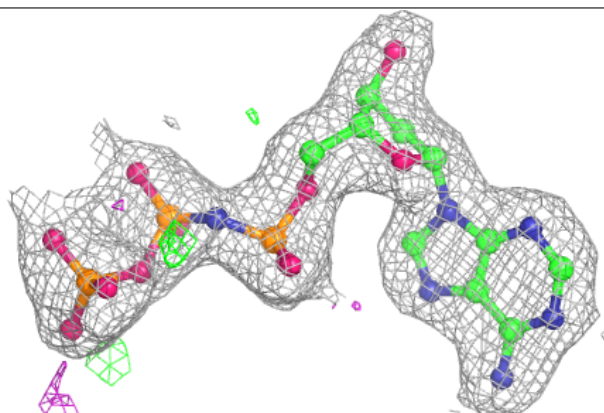


**Electron density around DZ4 C 706:**

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

**Electron density around DZ4 C 708:**

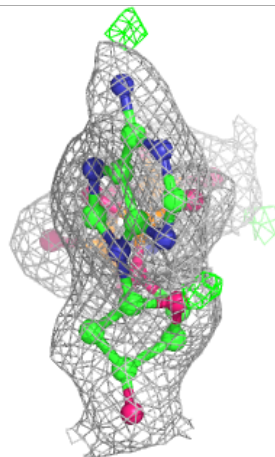
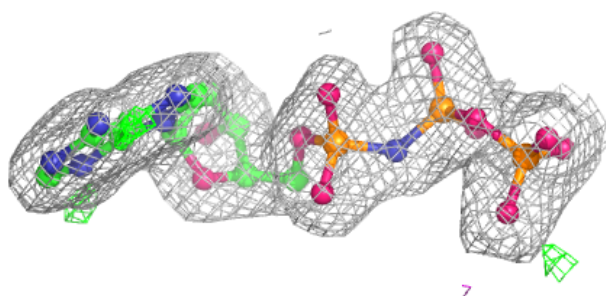
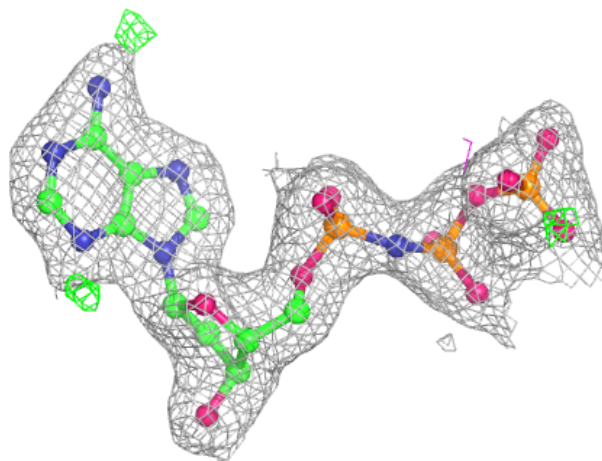
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





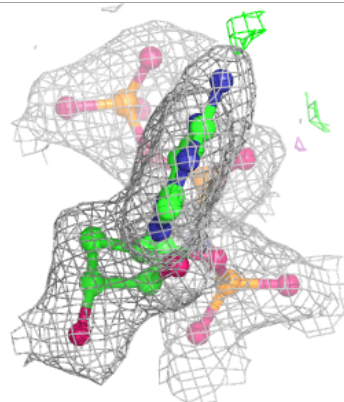
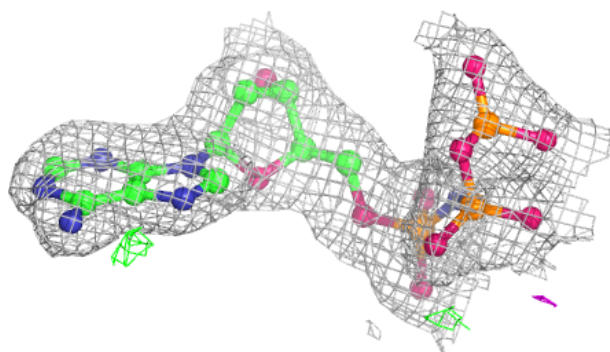
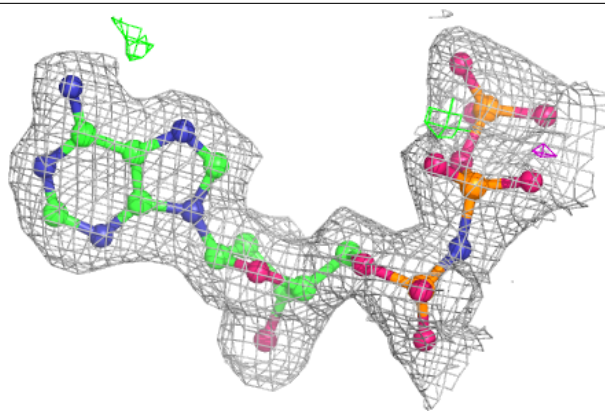
**Electron density around DZ4 D 701:**

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

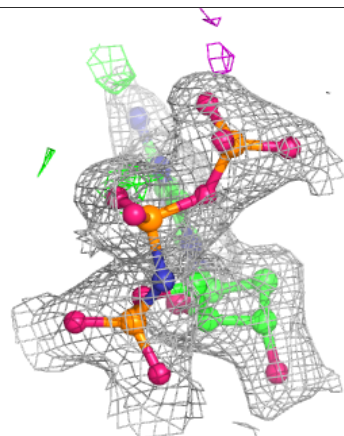
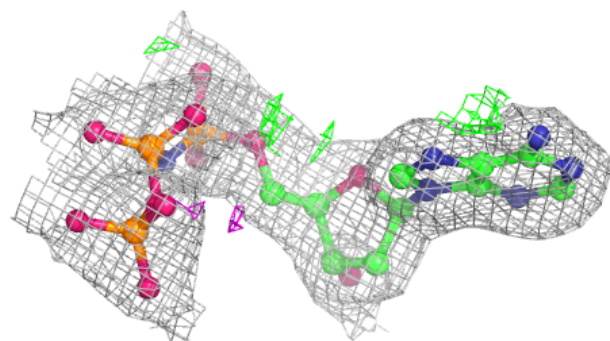
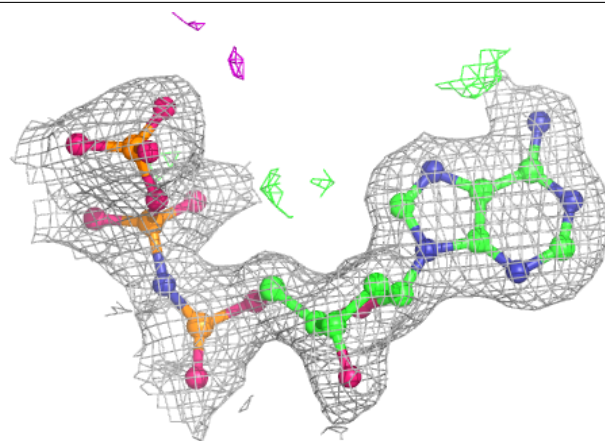


**Electron density around DZ4 D 706:**

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

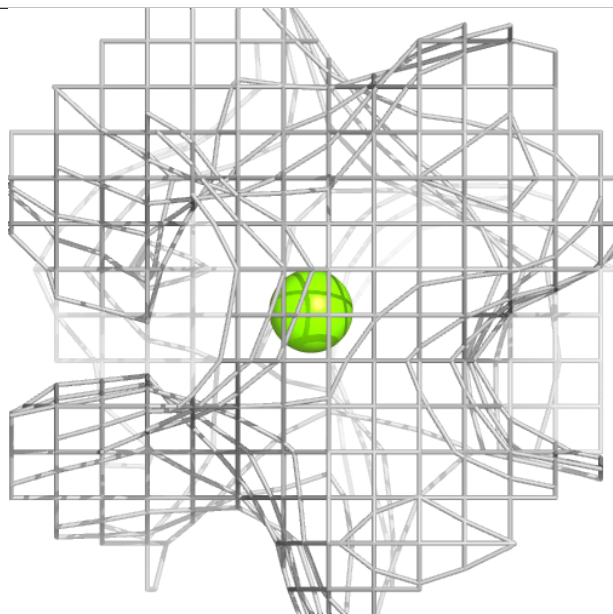
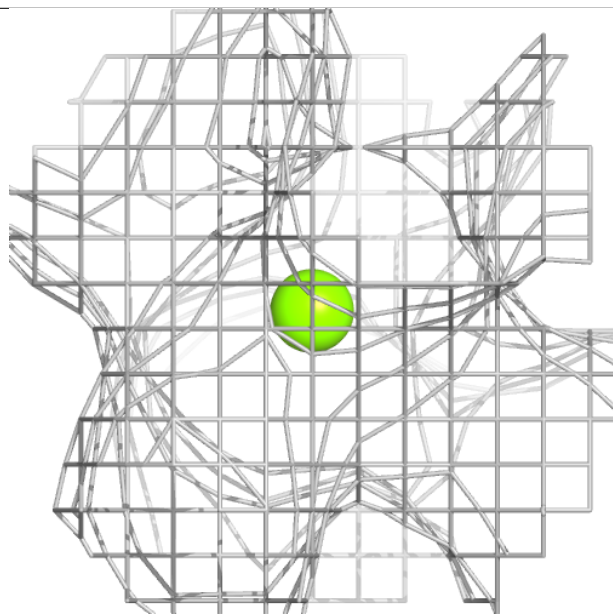
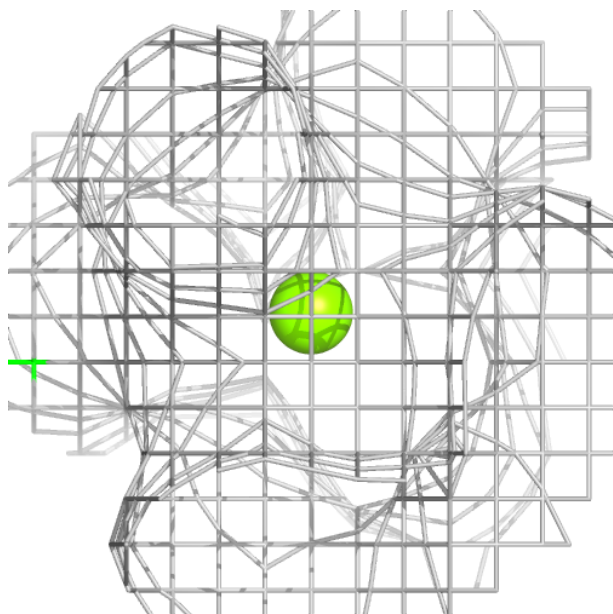
**Electron density around DZ4 E 705:**

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



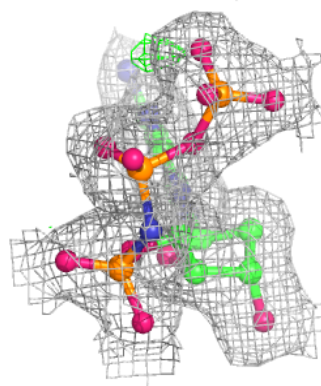
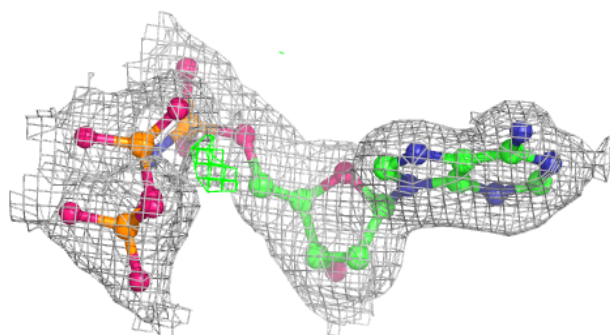
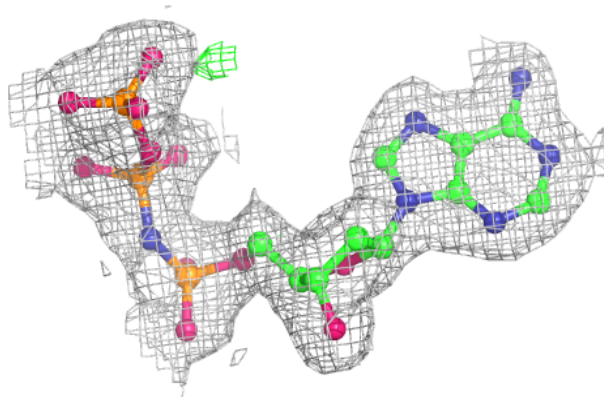
**Electron density around MG A 704:**

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



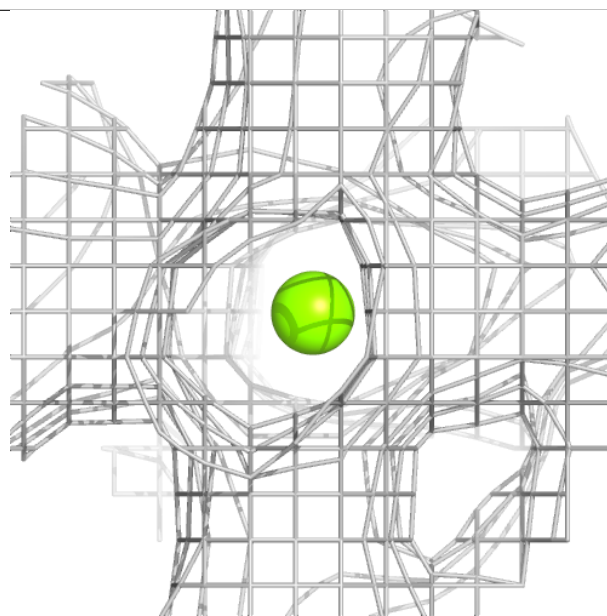
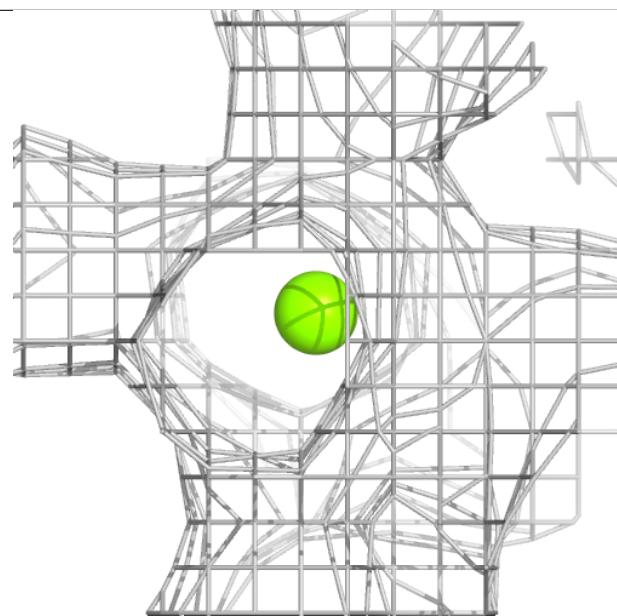
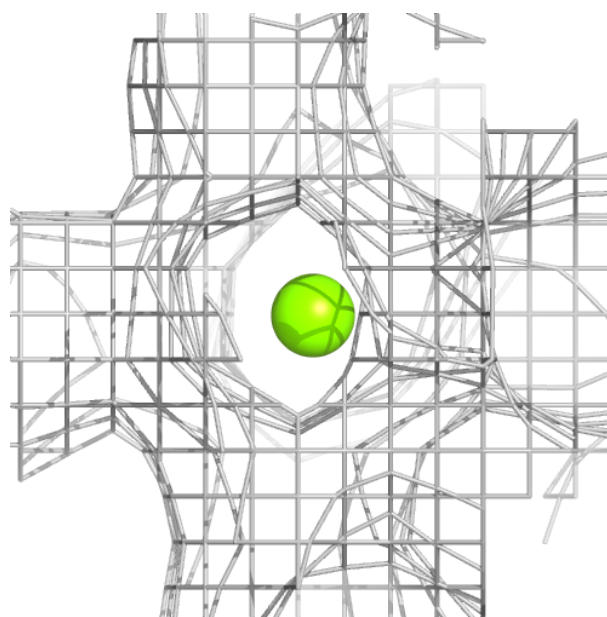
**Electron density around DZ4 F 705:**

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



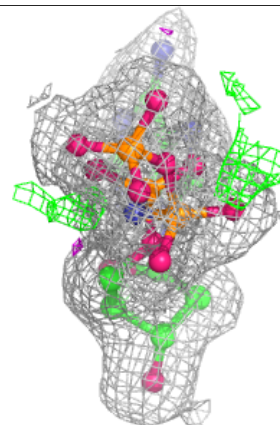
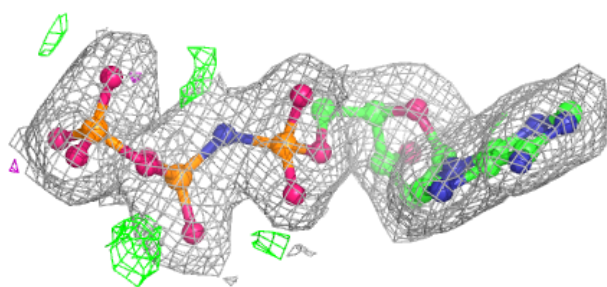
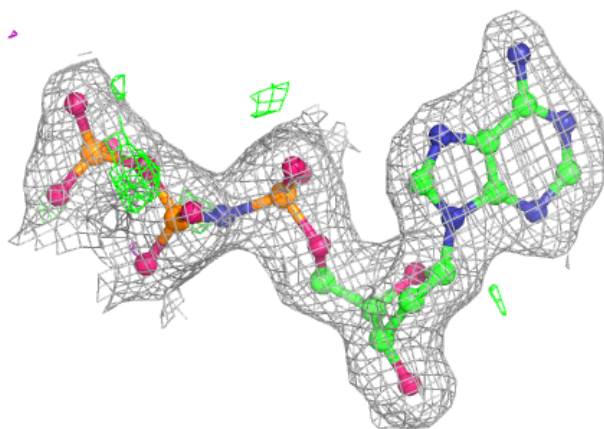
**Electron density around MG D 703:**

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

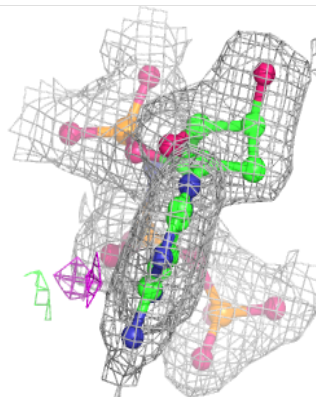
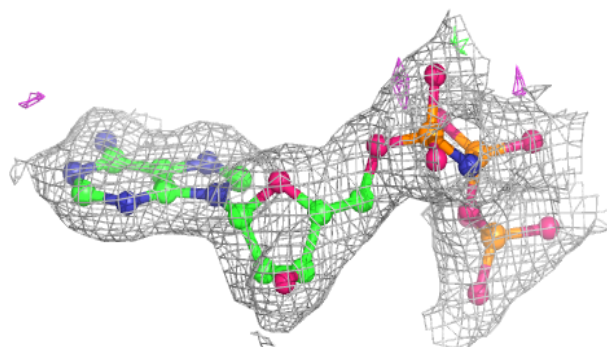
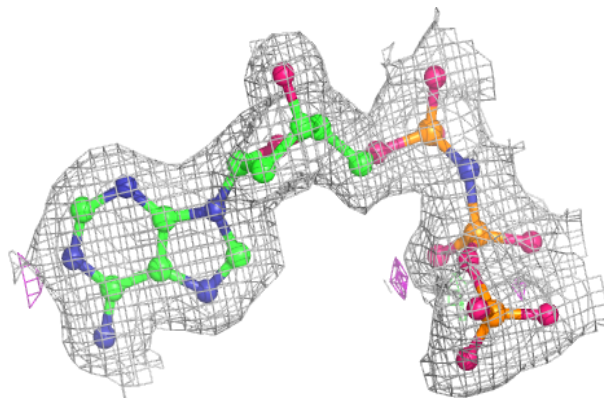


**Electron density around DZ4 G 701:**

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

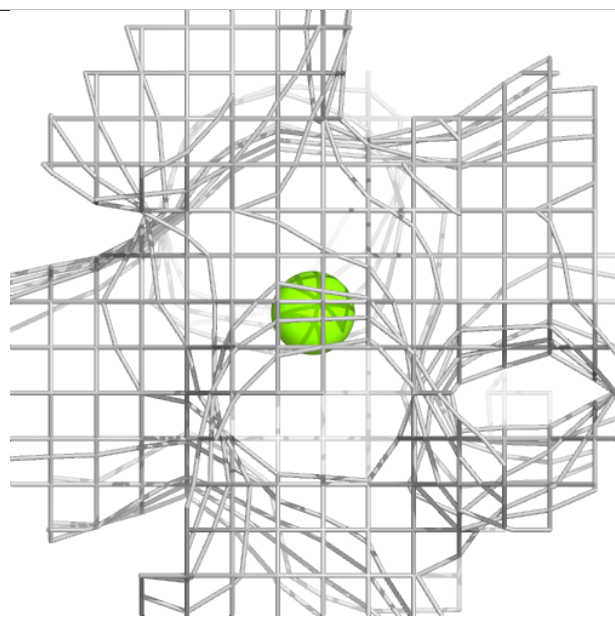
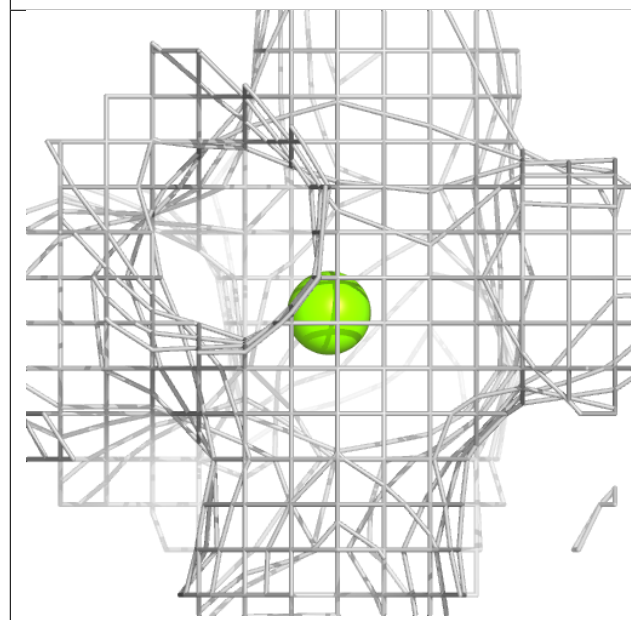
**Electron density around DZ4 G 706:**

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



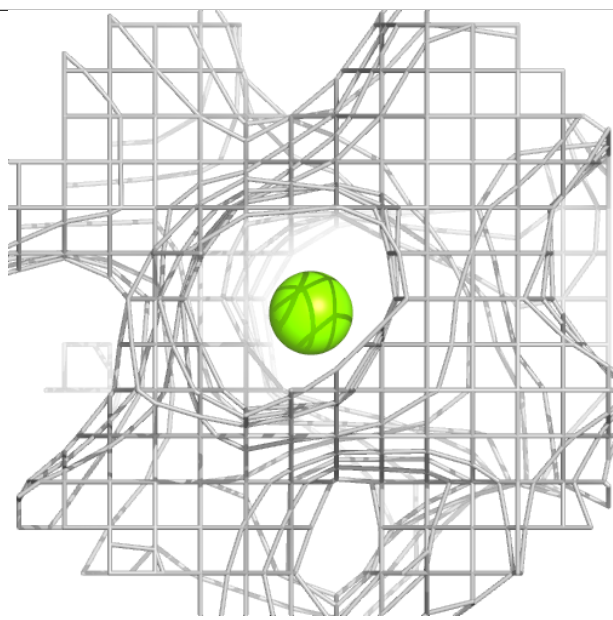
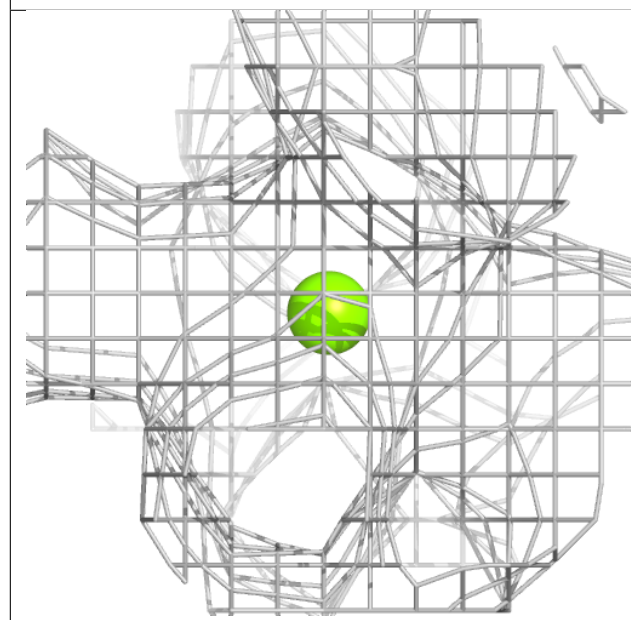
**Electron density around MG G 703:**

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

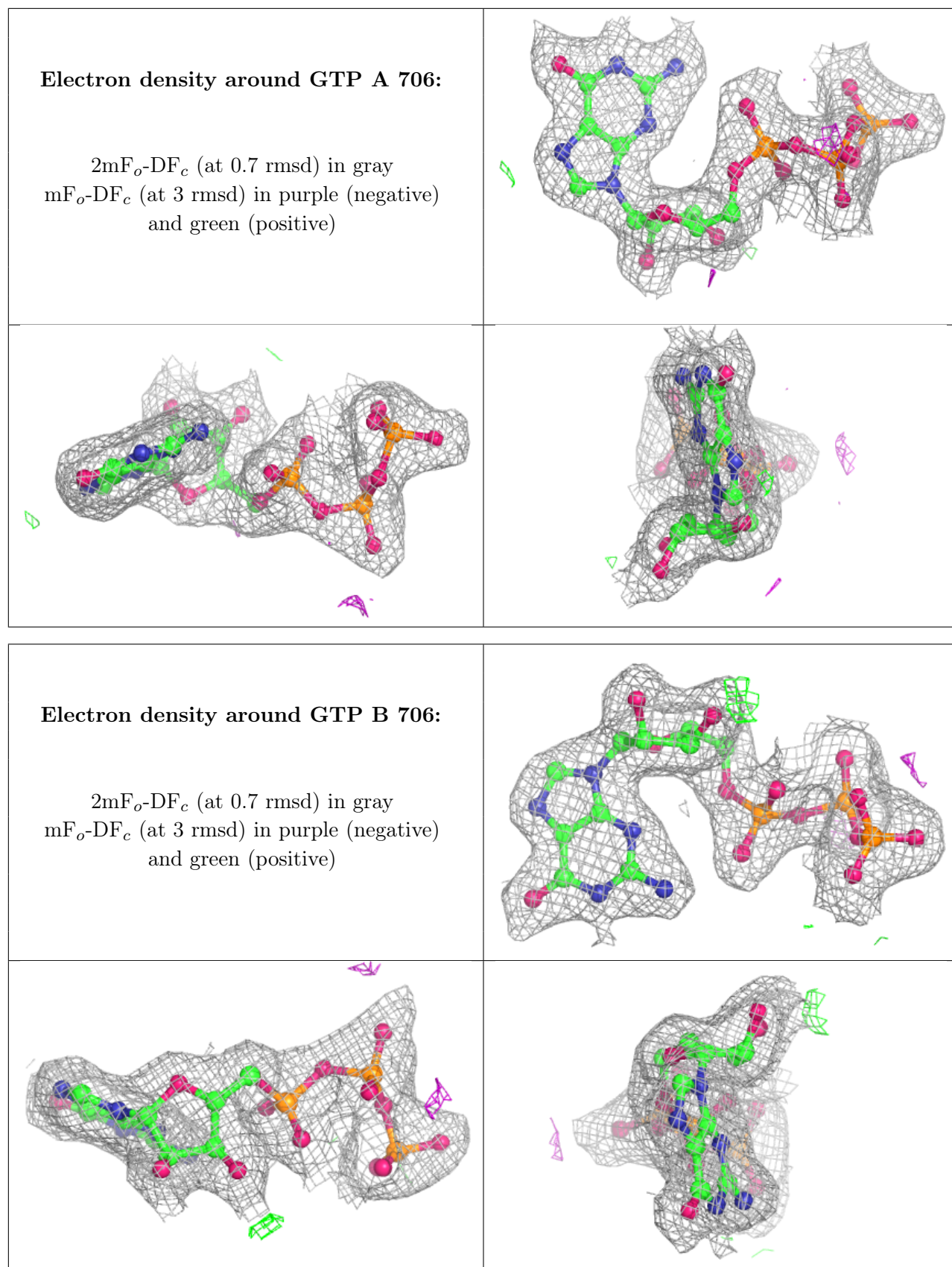


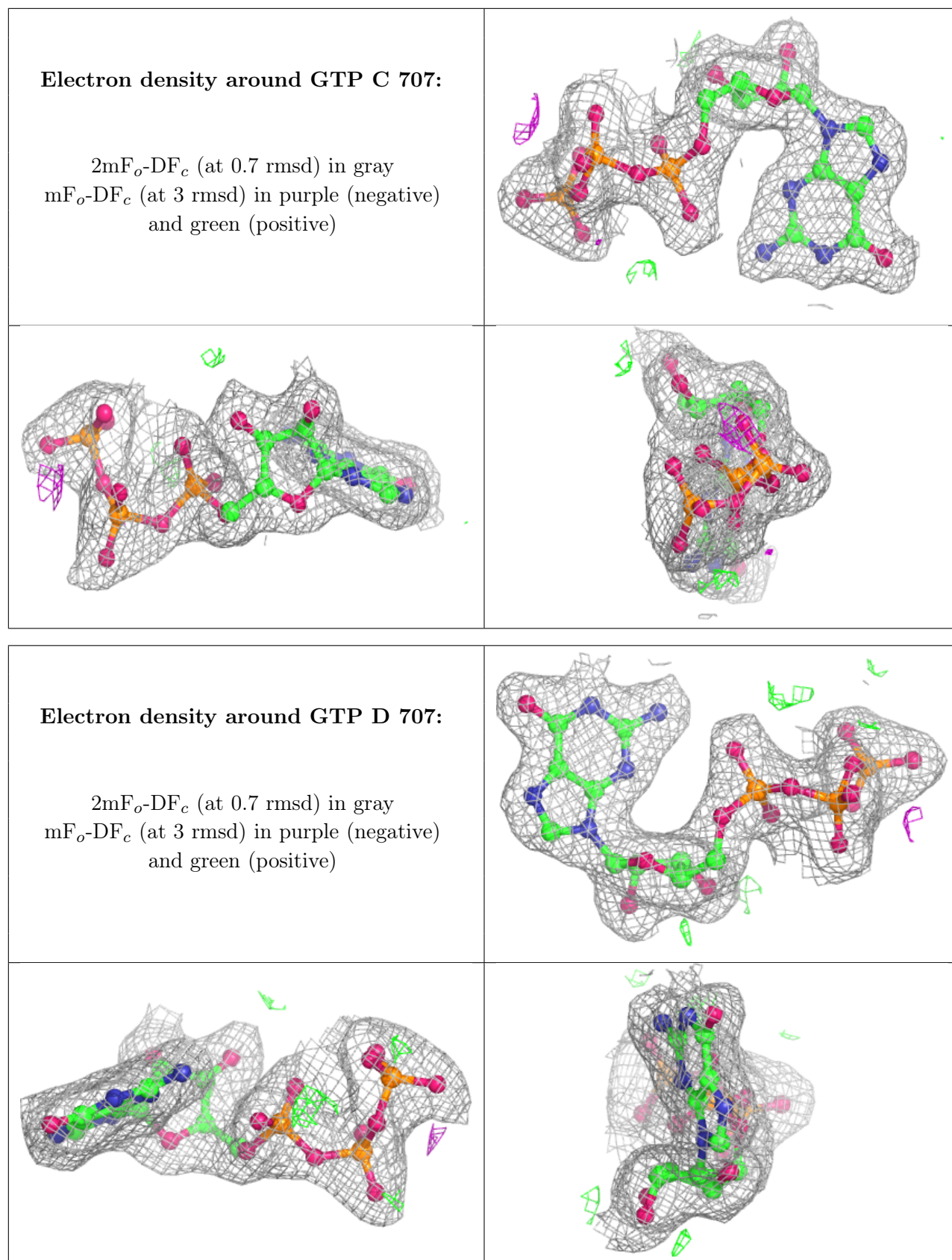
**Electron density around MG A 702:**

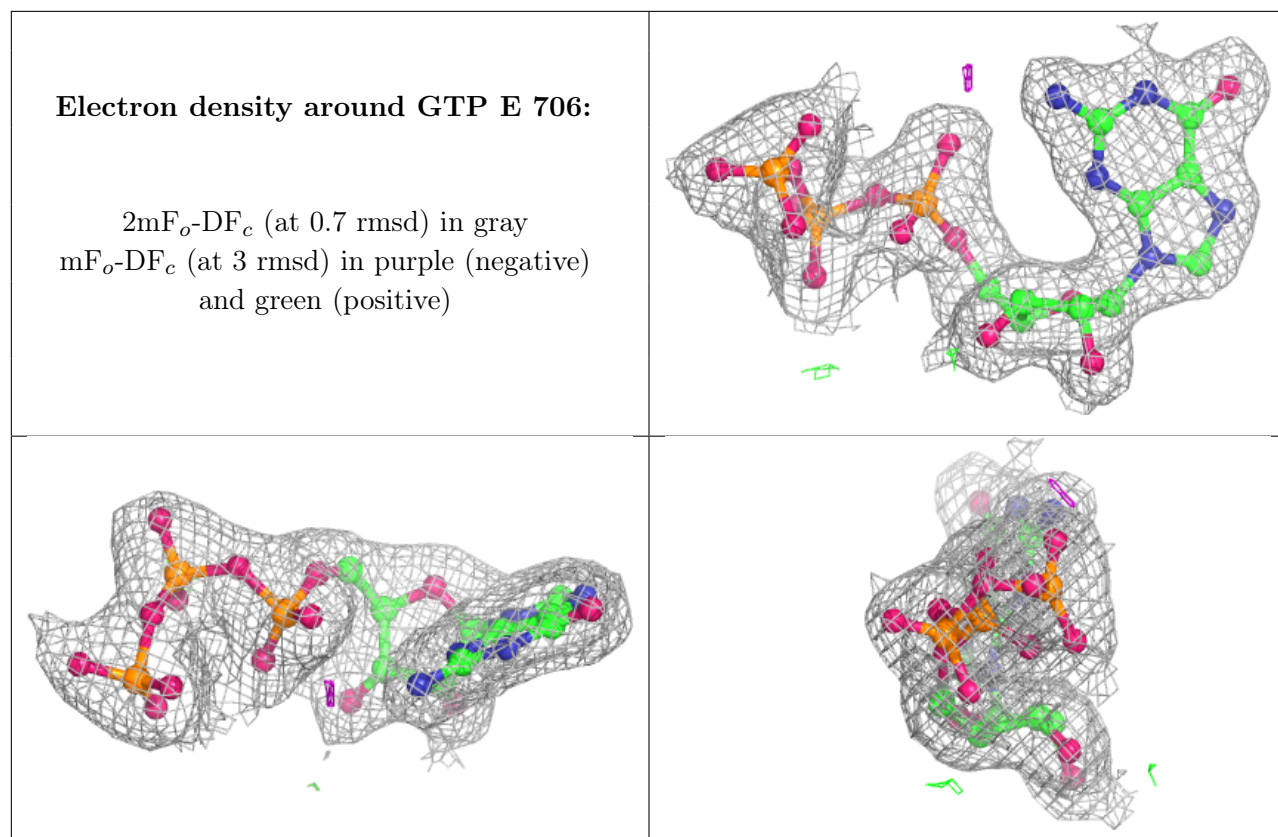
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





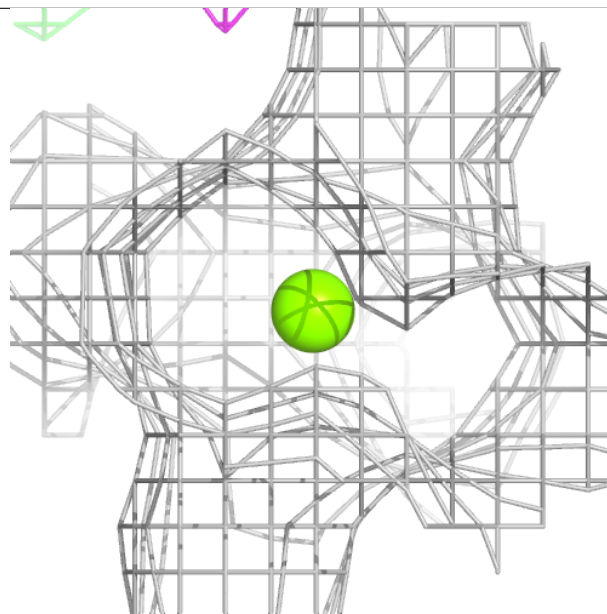
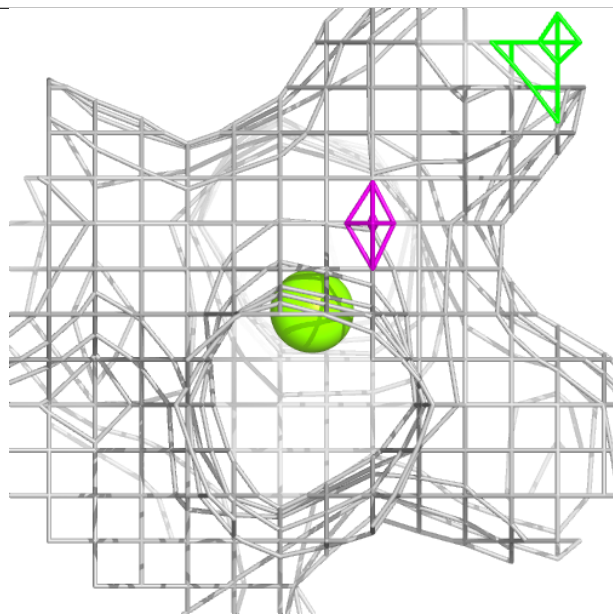
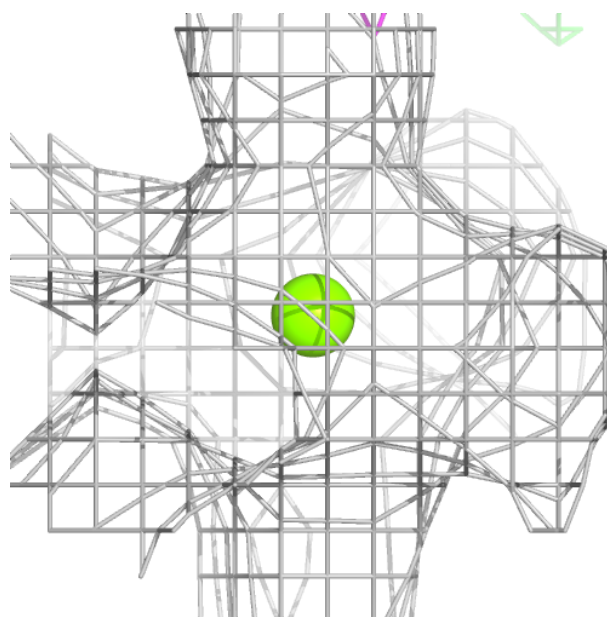






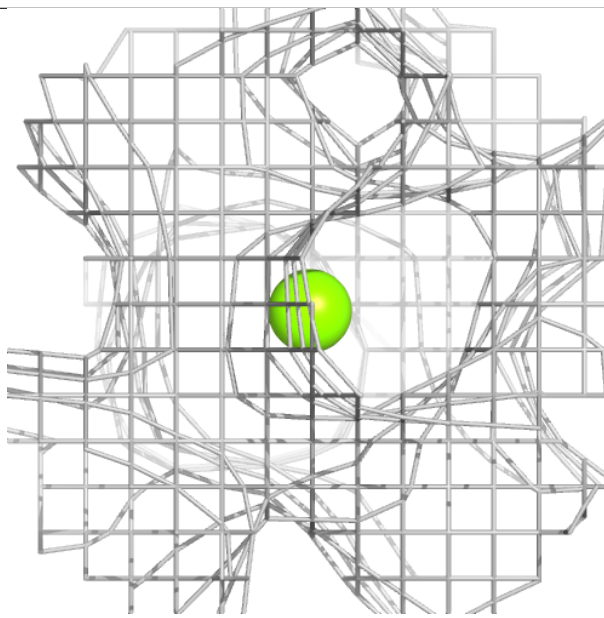
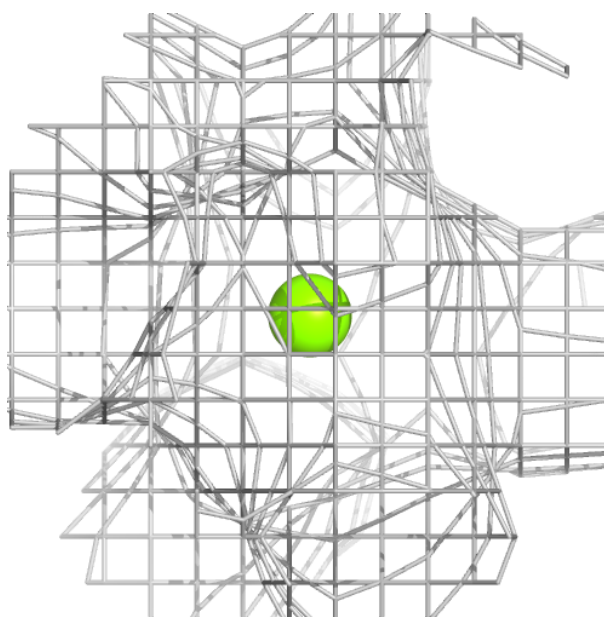
**Electron density around MG A 703:**

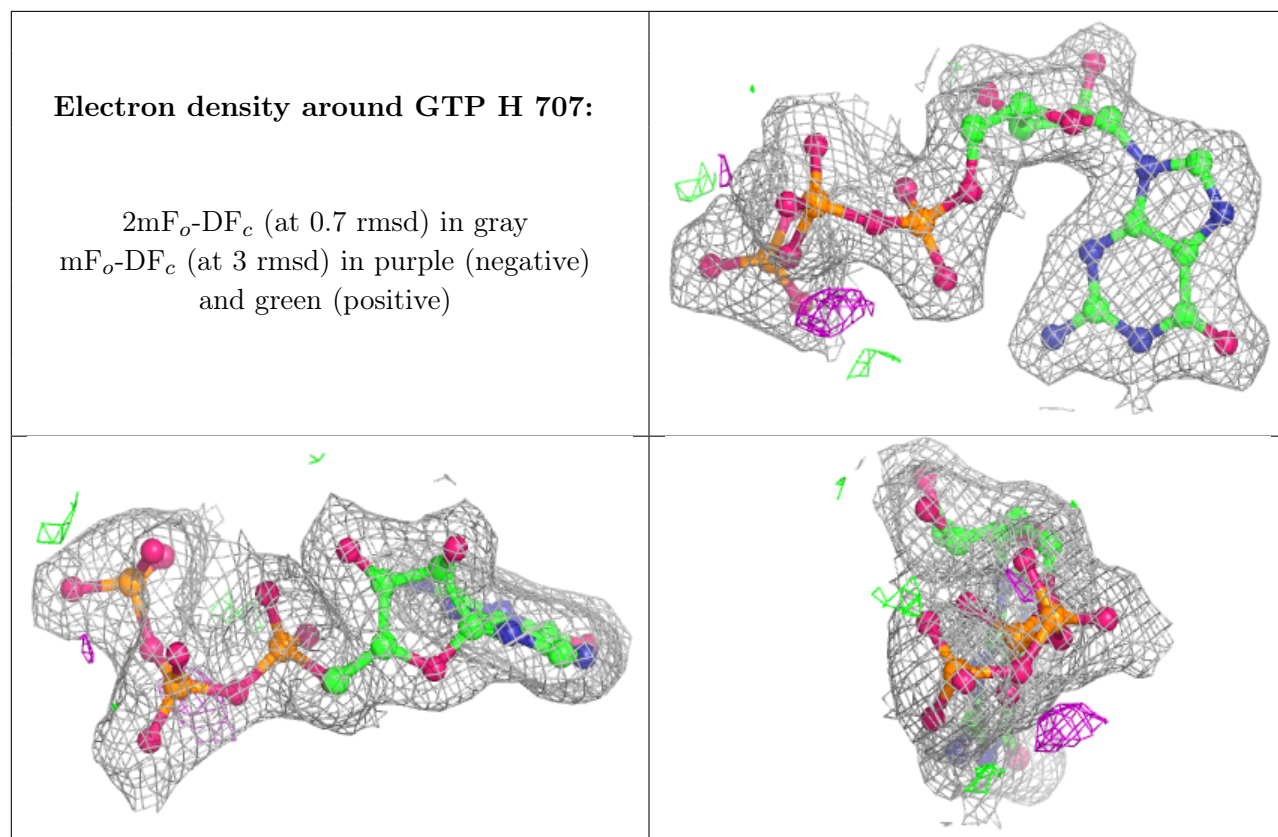
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around MG C 703:**

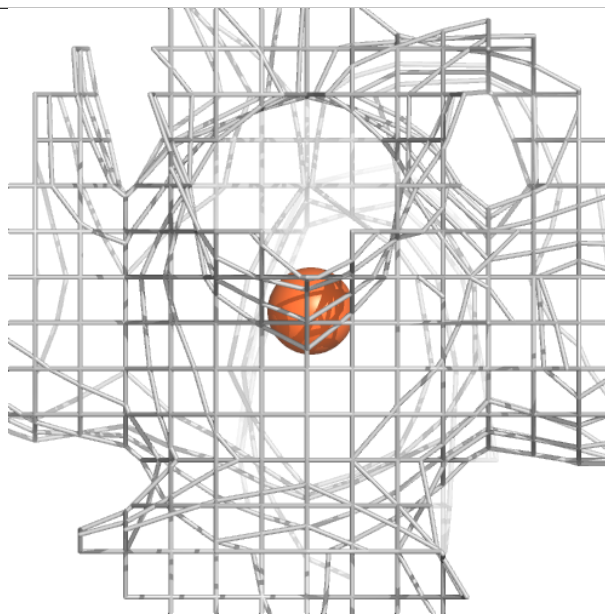
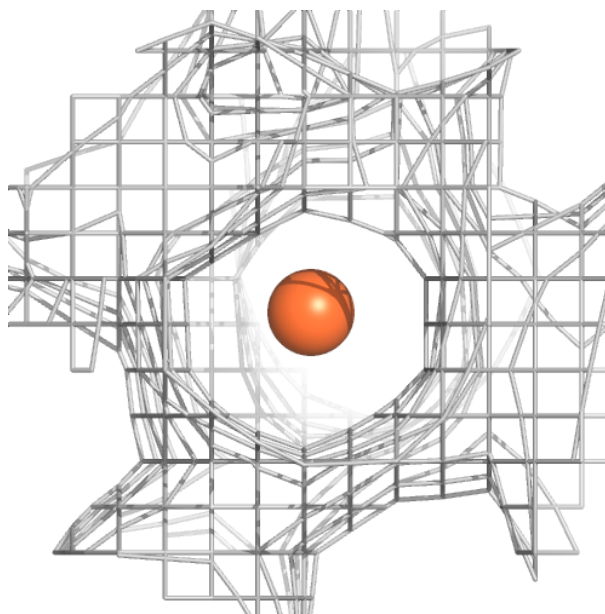
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





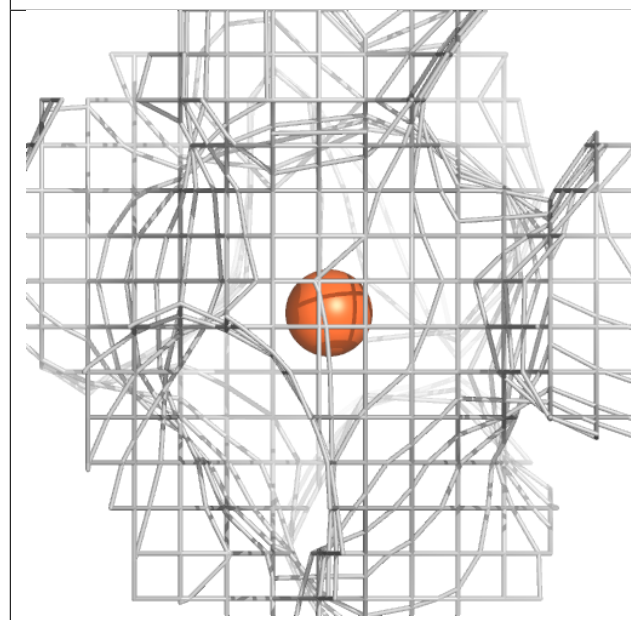
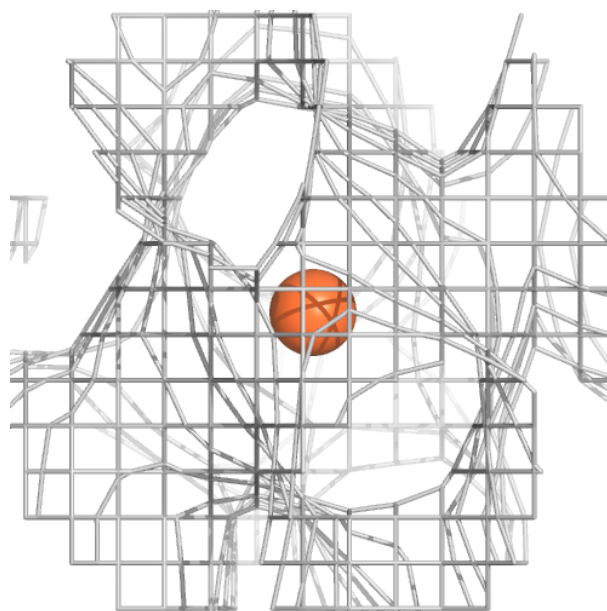
**Electron density around FE A 701:**

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



**Electron density around FE B 701:**

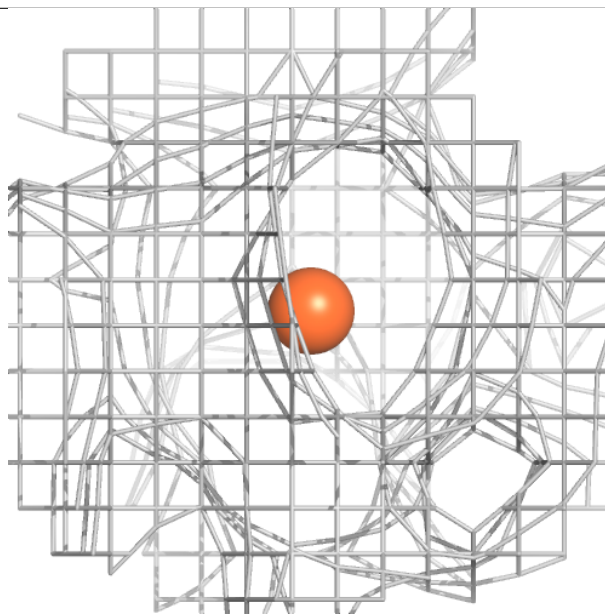
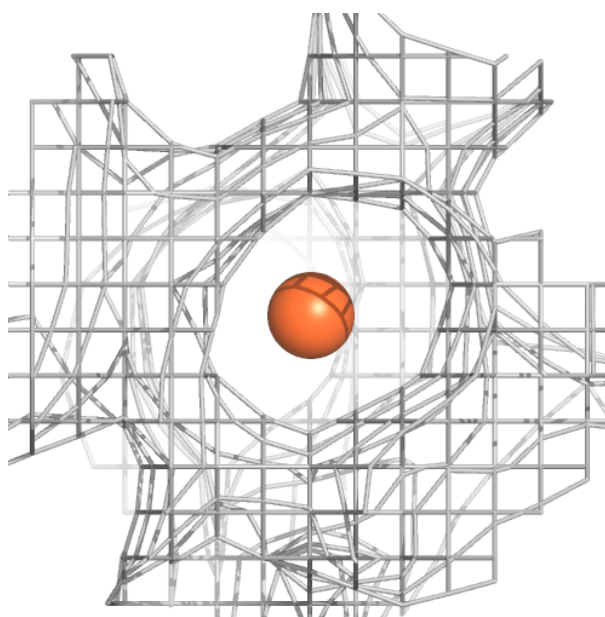
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





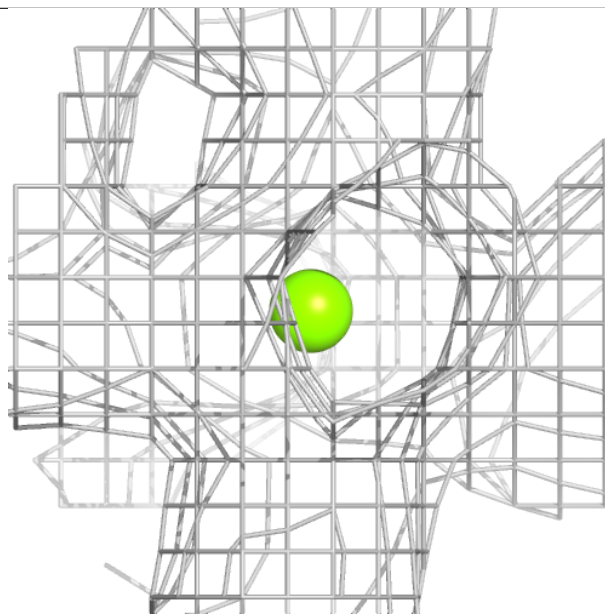
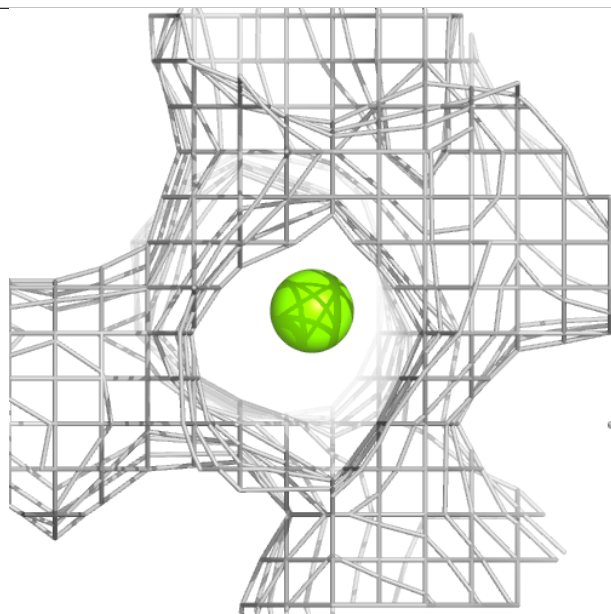
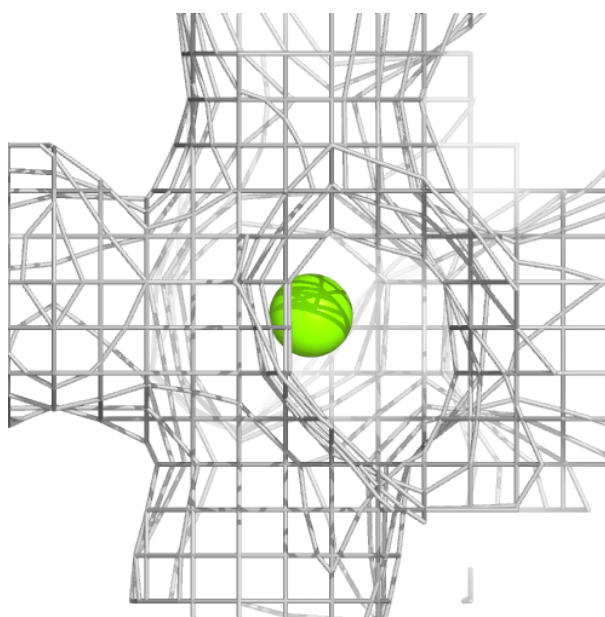
**Electron density around FE C 702:**

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



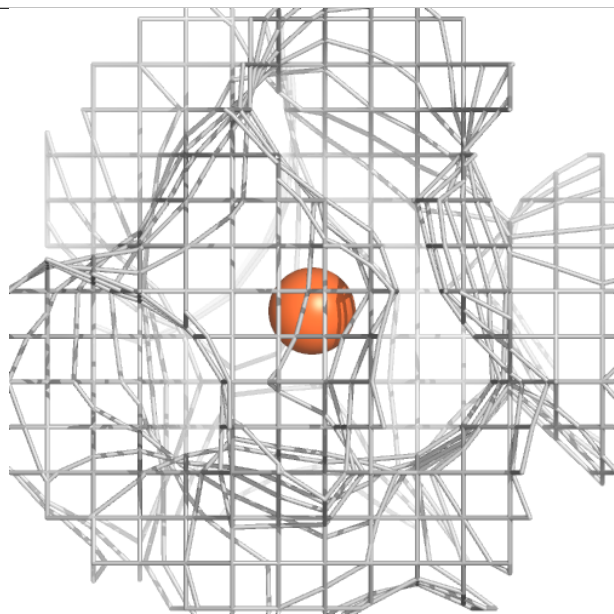
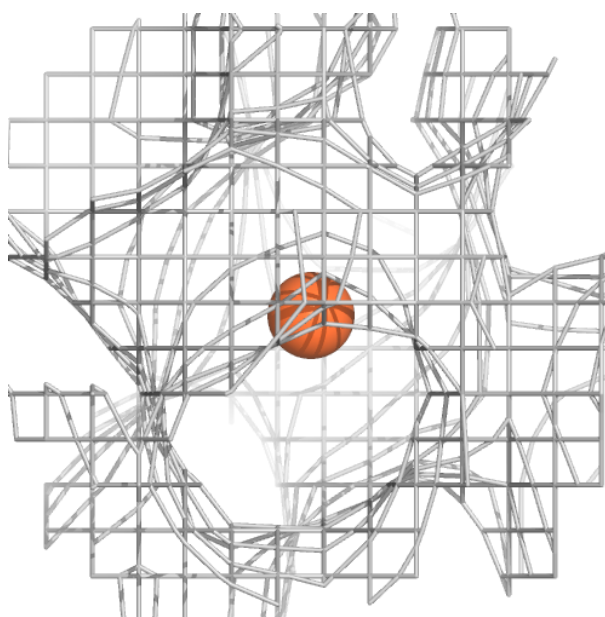
**Electron density around MG B 702:**

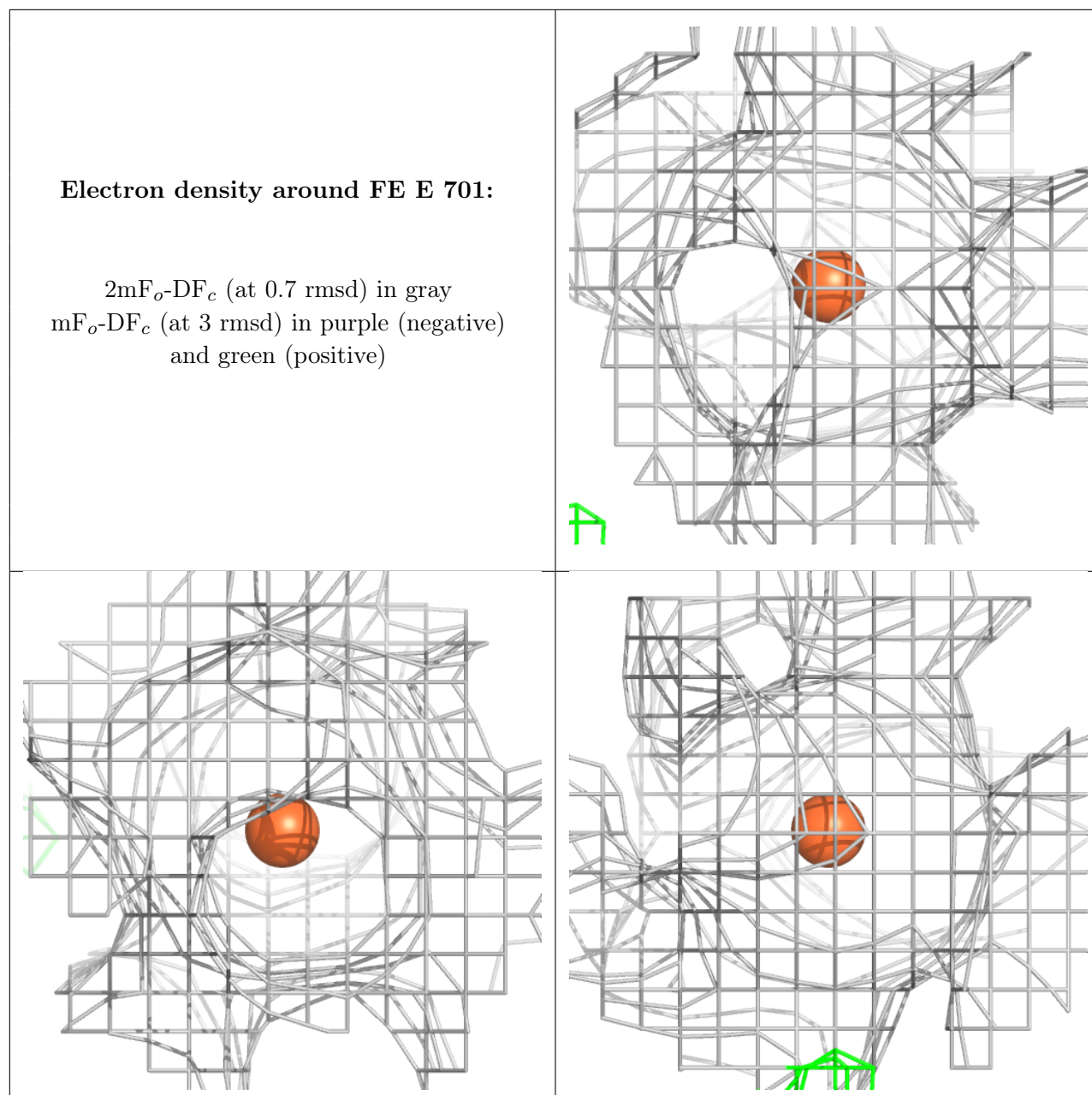
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

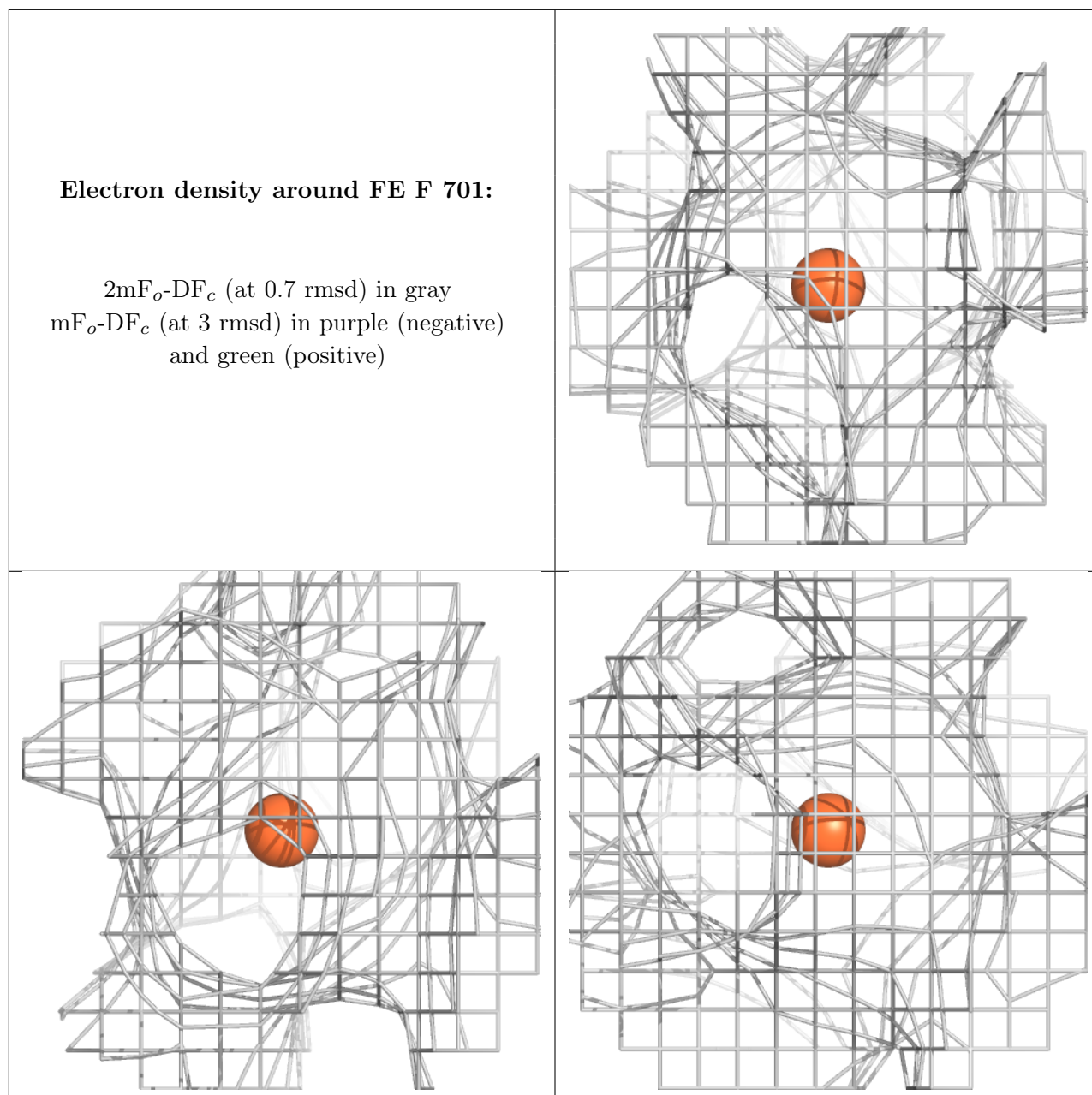


**Electron density around FE D 702:**

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

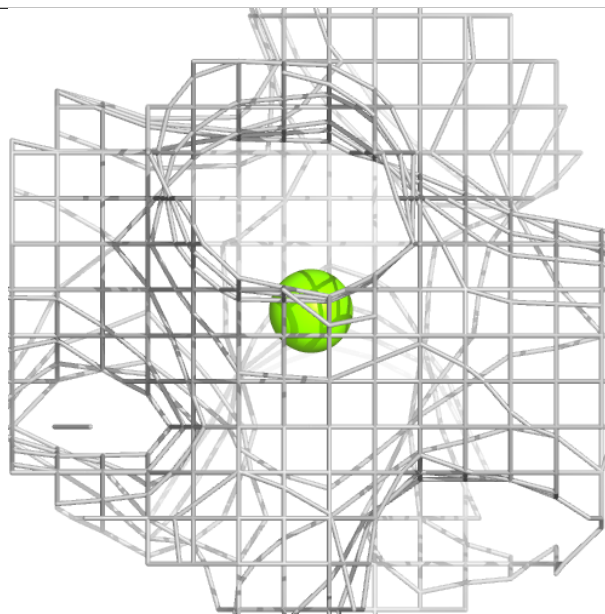
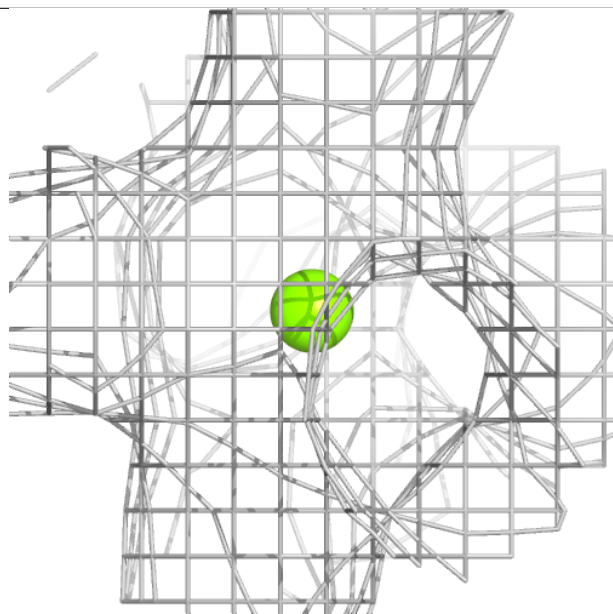
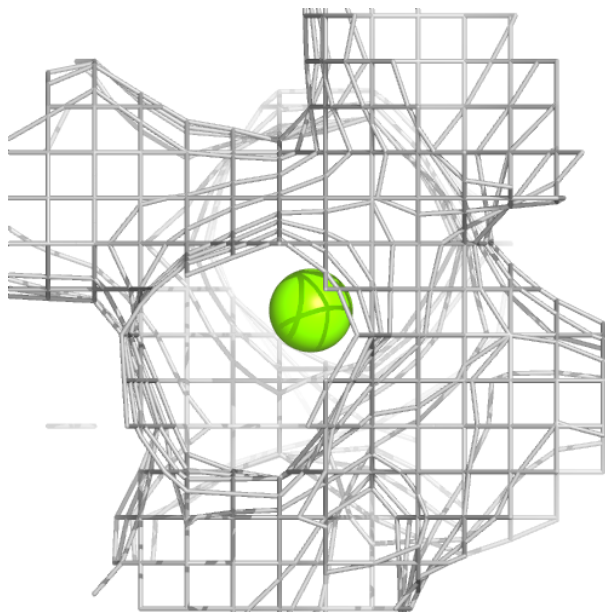






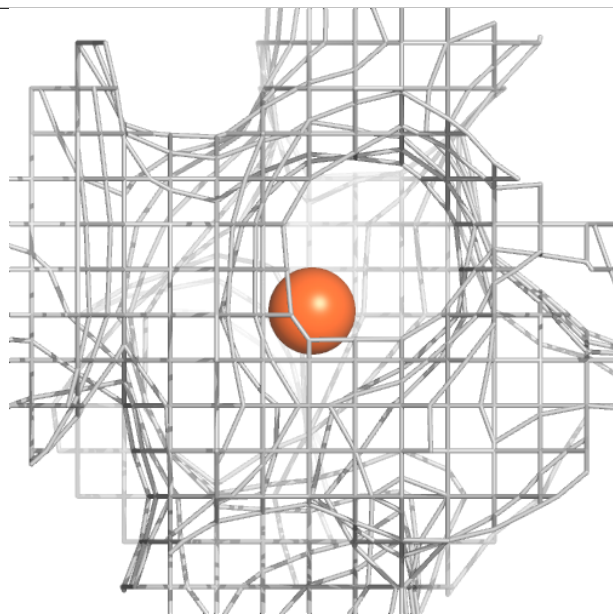
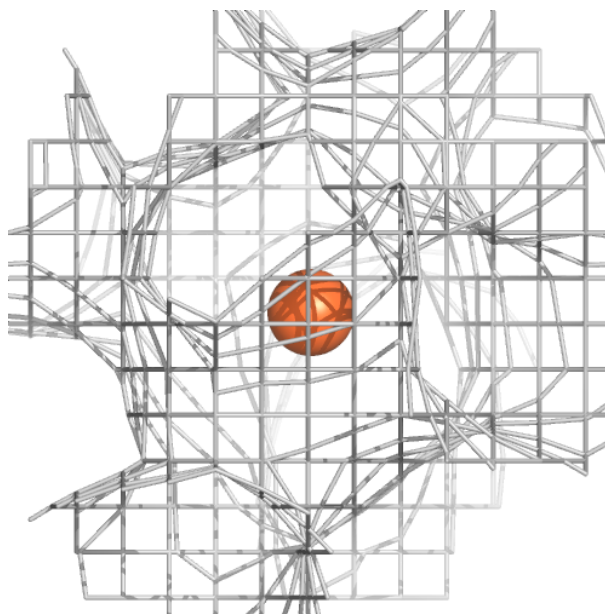
**Electron density around MG F 702:**

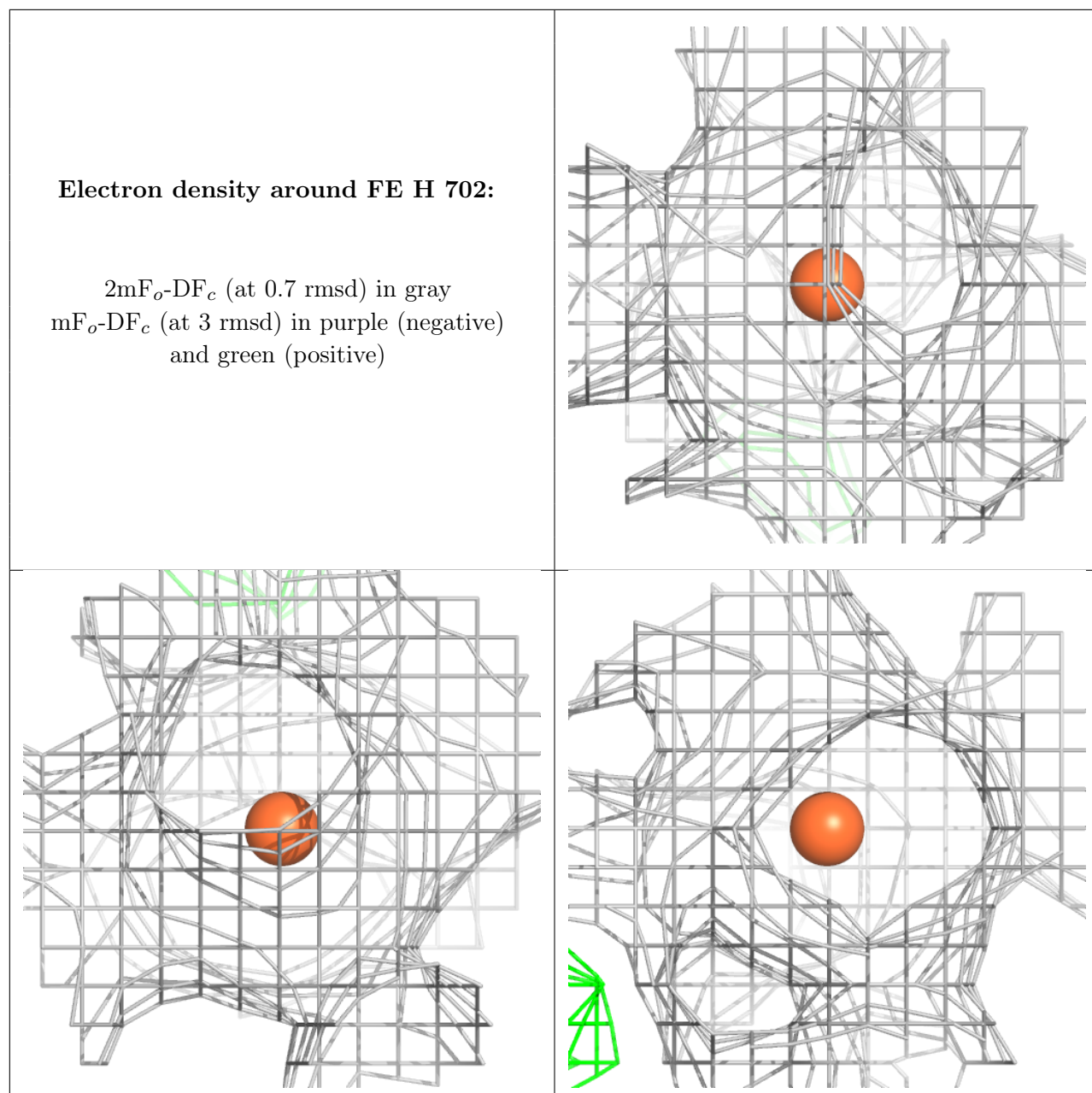
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FE 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.