wwPDB X-ray Structure Validation Summary Report (i)

Jun 2, 2021 – 05:30 am BST

PDB ID	:	7A5Y
Title	:	Crystal structure of tetrameric human H215A-SAMHD1 (residues 109-626) with Rp-dGTP-alphaS (T8T) and Mg
Authors	:	Morris, E.R.; Kunzelmann, S.; Caswell, S.J.; Purkiss, A.; Taylor, I.A.
Deposited on	:	2020-08-24
Resolution	:	2.29 Å(reported)

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

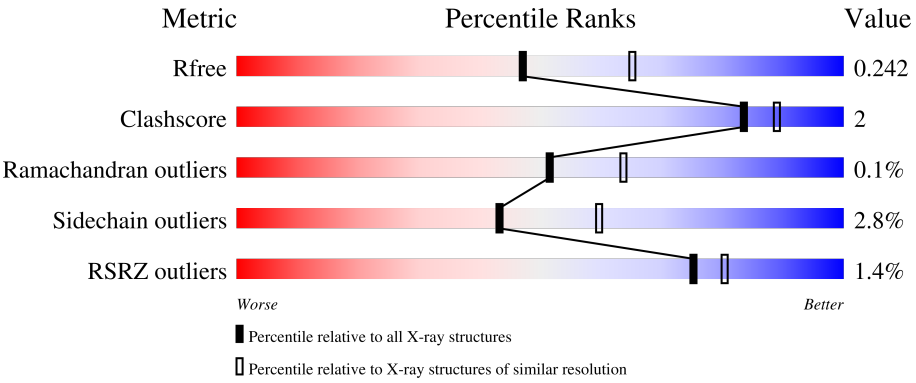
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.19
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.19

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.29 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	520	2% 78% 8% • 12%
1	B	520	% 79% 7% • 13%
1	C	520	% 81% 7% 12%
1	D	520	% 80% 7% 13%
1	E	520	% 80% 8% • 11%

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Mol	Chain	Length	Quality of chain
1	F	520	2% 79% 8% • 12%
1	G	520	% 80% 8% • 11%
1	H	520	% 77% 9% • 14%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30465 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	0	0	0
			3697	2369	640	668	20			
1	B	452	Total	C	N	O	S	0	0	0
			3637	2330	627	660	20			
1	C	459	Total	C	N	O	S	0	0	0
			3691	2364	641	666	20			
1	D	451	Total	C	N	O	S	0	0	0
			3631	2326	629	656	20			
1	E	462	Total	C	N	O	S	0	0	0
			3709	2376	642	671	20			
1	F	455	Total	C	N	O	S	0	0	0
			3653	2338	630	665	20			
1	G	464	Total	C	N	O	S	0	0	0
			3710	2370	640	680	20			
1	H	449	Total	C	N	O	S	0	0	0
			3618	2316	626	656	20			

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	4	Total Mg 4 4	0	0
3	B	3	Total Mg 3 3	0	0

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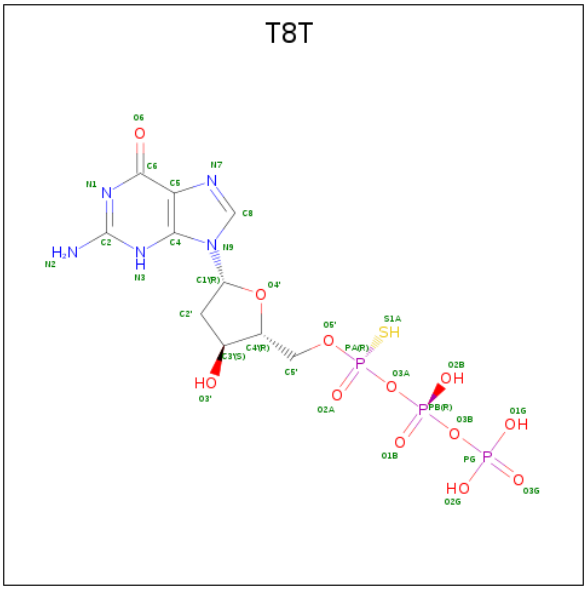
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	3	Total Mg 3 3	0	0
3	D	2	Total Mg 2 2	0	0
3	E	4	Total Mg 4 4	0	0
3	F	4	Total Mg 4 4	0	0
3	G	2	Total Mg 2 2	0	0
3	H	2	Total Mg 2 2	0	0

- Molecule 4 is 2'-deoxyguanosine-5'-O-(1-thiotriphosphate) (three-letter code: T8T) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P S 31 10 5 12 3 1	0	0
4	A	1	Total C N O P S 31 10 5 12 3 1	0	0
4	A	1	Total C N O P S 31 10 5 12 3 1	0	0
4	B	1	Total C N O P S 31 10 5 12 3 1	0	0
4	B	1	Total C N O P S 31 10 5 12 3 1	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	C	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	C	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	D	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	D	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	D	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	E	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	E	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	E	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	F	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	F	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	F	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	F	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	G	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	G	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	H	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	H	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	H	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

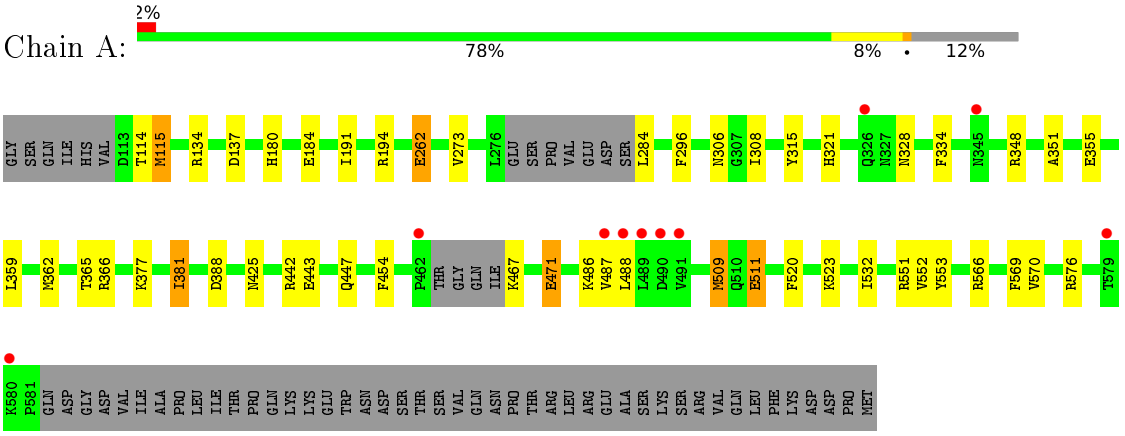
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	52	Total O 52 52	0	0
5	B	47	Total O 47 47	0	0
5	C	39	Total O 39 39	0	0
5	D	38	Total O 38 38	0	0
5	E	47	Total O 47 47	0	0
5	F	40	Total O 40 40	0	0
5	G	34	Total O 34 34	0	0
5	H	46	Total O 46 46	0	0

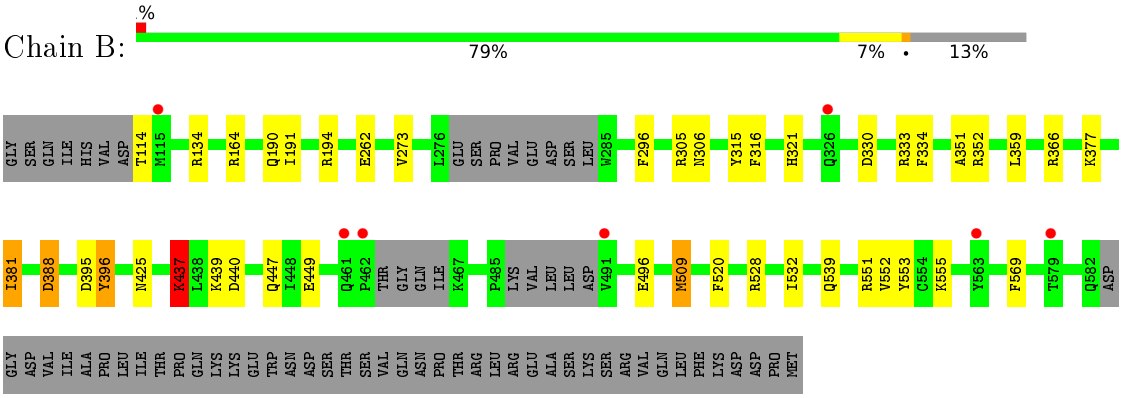
3 Residue-property plots (i)

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

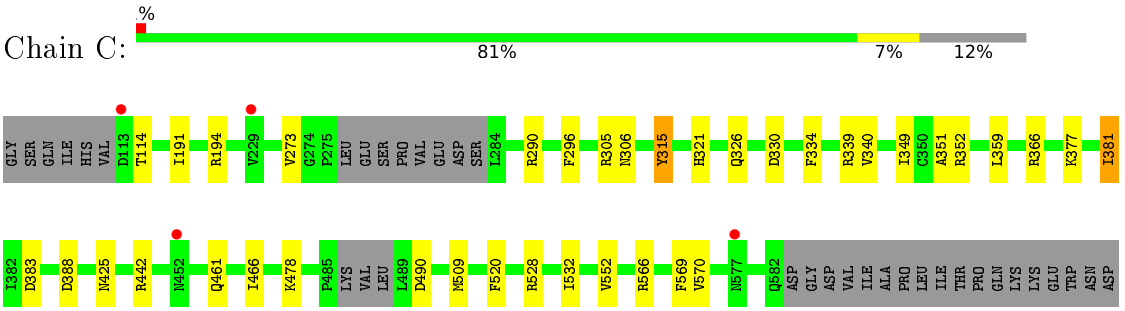
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

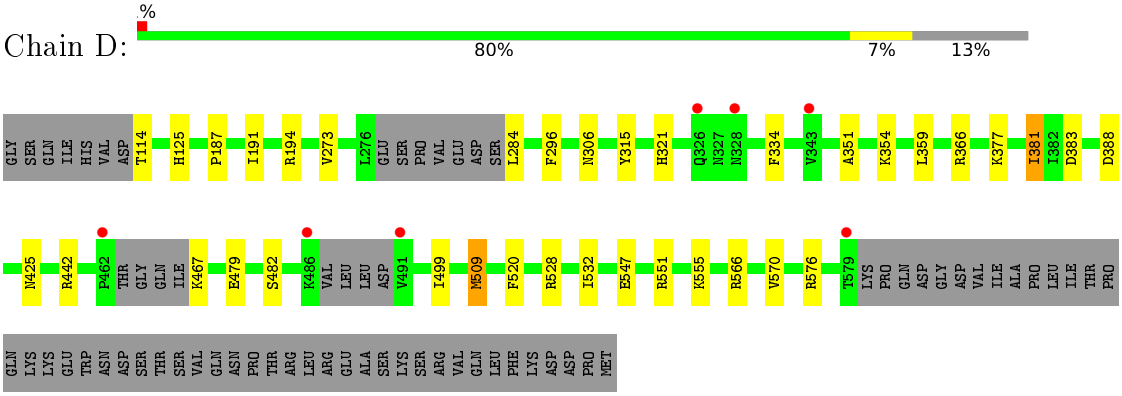


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



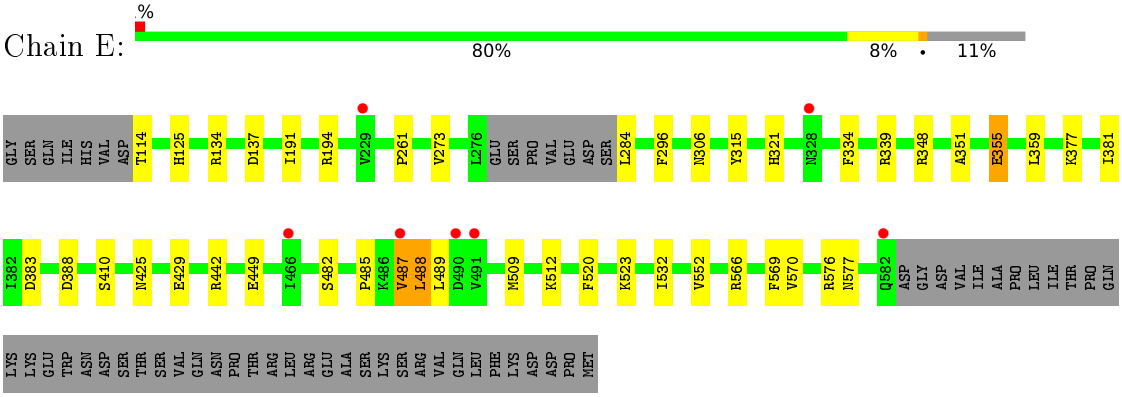
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain D:



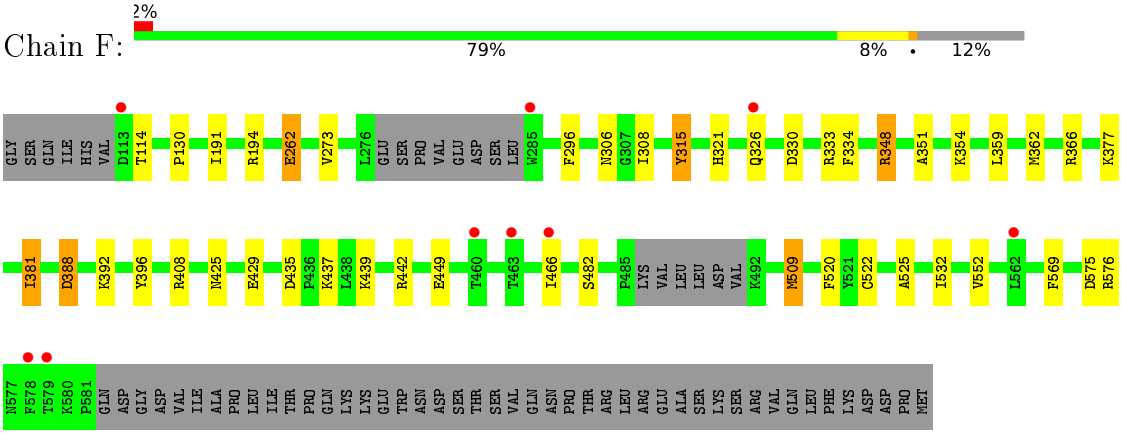
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain E:



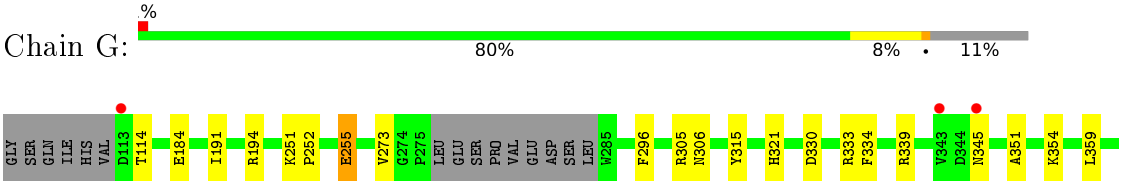
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

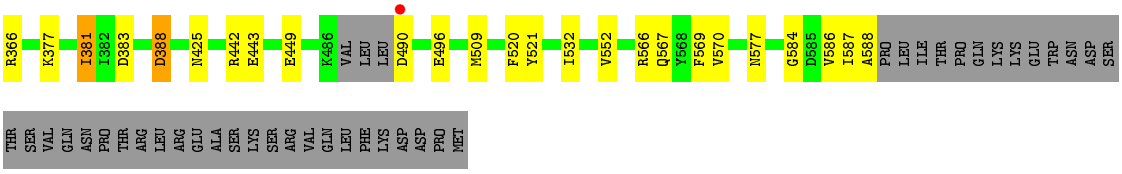
Chain F:



• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

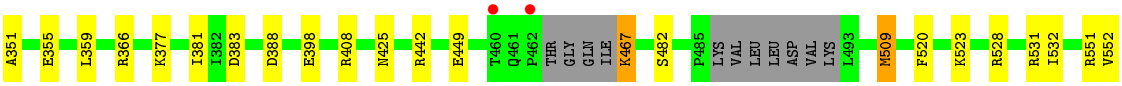
Chain G:

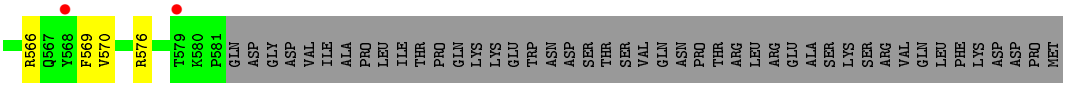




- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.19Å 181.26Å 286.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.15 – 2.29 153.15 – 2.29	Depositor EDS
% Data completeness (in resolution range)	77.2 (153.15-2.29) 77.2 (153.15-2.29)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.210 , 0.240 0.214 , 0.242	Depositor DCC
R_{free} test set	7326 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	30.7	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 38.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	30465	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, T8T, FE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.95	6/3784 (0.2%)	1.01	16/5116 (0.3%)
1	B	0.93	4/3723 (0.1%)	1.01	20/5034 (0.4%)
1	C	0.89	1/3778 (0.0%)	1.01	14/5108 (0.3%)
1	D	0.89	1/3716 (0.0%)	0.97	10/5024 (0.2%)
1	E	0.93	7/3797 (0.2%)	0.98	9/5139 (0.2%)
1	F	0.89	4/3740 (0.1%)	0.97	12/5060 (0.2%)
1	G	0.87	2/3797 (0.1%)	0.95	11/5140 (0.2%)
1	H	0.90	5/3704 (0.1%)	0.98	19/5009 (0.4%)
All	All	0.91	30/30039 (0.1%)	0.98	111/40630 (0.3%)

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

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

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	511	GLU	CD-OE2	8.93	1.35	1.25
1	E	355	GLU	CD-OE1	7.57	1.33	1.25
1	A	447	GLN	CG-CD	7.09	1.67	1.51
1	H	184	GLU	CG-CD	7.05	1.62	1.51
1	B	447	GLN	CG-CD	6.95	1.67	1.51

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	305	ARG	NE-CZ-NH1	-11.97	114.31	120.30
1	E	442	ARG	NE-CZ-NH1	10.43	125.52	120.30
1	B	528	ARG	NE-CZ-NH1	10.23	125.42	120.30
1	A	115	MET	CG-SD-CE	10.19	116.50	100.20
1	F	348	ARG	NE-CZ-NH1	9.00	124.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	396	TYR	Sidechain

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	3697	0	3628	20	0
1	B	3637	0	3546	25	0
1	C	3691	0	3618	16	0
1	D	3631	0	3546	16	0
1	E	3709	0	3626	15	0
1	F	3653	0	3554	21	0
1	G	3710	0	3593	25	0
1	H	3618	0	3524	22	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	4	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	2	0	0	0	0
3	E	4	0	0	0	0
3	F	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	2	0	0	0	0
3	H	2	0	0	0	0
4	A	93	0	38	1	0
4	B	124	0	51	1	0
4	C	62	0	25	2	0
4	D	93	0	38	0	0
4	E	93	0	38	0	0
4	F	124	0	51	3	0
4	G	62	0	25	1	0
4	H	93	0	38	0	0
5	A	52	0	0	0	0
5	B	47	0	0	0	0
5	C	39	0	0	0	0
5	D	38	0	0	0	0
5	E	47	0	0	1	0
5	F	40	0	0	0	0
5	G	34	0	0	0	0
5	H	46	0	0	0	0
All	All	30465	0	28939	142	0

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

The worst 5 of 142 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:E:355:GLU:OE2	5:E:801:HOH:O	1.80	0.98
1:A:328:ASN:ND2	1:A:365:THR:OG1	1.97	0.97
1:C:306:ASN:HA	1:C:509:MET:CE	2.05	0.87
1:E:306:ASN:HA	1:E:509:MET:CE	2.04	0.87
1:H:306:ASN:HA	1:H:509:MET:CE	2.04	0.87

There are no symmetry-related clashes.

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	452/520 (87%)	437 (97%)	14 (3%)	1 (0%)	47 58
1	B	444/520 (85%)	433 (98%)	11 (2%)	0	100 100
1	C	453/520 (87%)	441 (97%)	12 (3%)	0	100 100
1	D	443/520 (85%)	430 (97%)	13 (3%)	0	100 100
1	E	458/520 (88%)	442 (96%)	14 (3%)	2 (0%)	34 42
1	F	449/520 (86%)	438 (98%)	11 (2%)	0	100 100
1	G	458/520 (88%)	444 (97%)	13 (3%)	1 (0%)	47 58
1	H	441/520 (85%)	429 (97%)	12 (3%)	0	100 100
All	All	3598/4160 (86%)	3494 (97%)	100 (3%)	4 (0%)	51 64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	487	VAL
1	E	487	VAL
1	E	488	LEU
1	G	586	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	394/463 (85%)	380 (96%)	14 (4%)	35 49
1	B	386/463 (83%)	377 (98%)	9 (2%)	50 67
1	C	392/463 (85%)	384 (98%)	8 (2%)	55 72
1	D	385/463 (83%)	375 (97%)	10 (3%)	46 63
1	E	393/463 (85%)	383 (98%)	10 (2%)	47 65
1	F	387/463 (84%)	373 (96%)	14 (4%)	35 49
1	G	392/463 (85%)	383 (98%)	9 (2%)	50 67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	384/463 (83%)	372 (97%)	12 (3%)	40 55
All	All	3113/3704 (84%)	3027 (97%)	86 (3%)	43 60

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	348	ARG
1	G	388	ASP
1	F	381	ILE
1	G	114	THR
1	H	193	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	375	GLN
1	H	375	GLN
1	F	322	HIS
1	G	425	ASN
1	F	123	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 56 ligands modelled in this entry, 32 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	T8T	F	707	3,2	24,33,33	1.37	2 (8%)	30,52,52	2.00	10 (33%)
4	T8T	A	706	3	24,33,33	1.43	4 (16%)	30,52,52	1.66	6 (20%)
4	T8T	G	704	3,2	24,33,33	1.42	3 (12%)	30,52,52	1.63	4 (13%)
4	T8T	H	701	3	24,33,33	1.28	2 (8%)	30,52,52	1.70	6 (20%)
4	T8T	A	704	3,2	24,33,33	1.19	1 (4%)	30,52,52	1.67	6 (20%)
4	T8T	B	702	3	24,33,33	1.18	1 (4%)	30,52,52	1.64	7 (23%)
4	T8T	E	705	3,2	24,33,33	1.69	3 (12%)	30,52,52	1.70	6 (20%)
4	T8T	B	701	3	24,33,33	1.45	3 (12%)	30,52,52	1.69	6 (20%)
4	T8T	A	708	3	24,33,33	1.11	1 (4%)	30,52,52	1.88	8 (26%)
4	T8T	E	708	3	24,33,33	1.30	3 (12%)	30,52,52	1.79	7 (23%)
4	T8T	F	709	3	24,33,33	0.87	1 (4%)	30,52,52	1.50	6 (20%)
4	T8T	C	705	3,2	24,33,33	1.26	1 (4%)	30,52,52	1.68	7 (23%)
4	T8T	B	706	3,2	24,33,33	0.91	1 (4%)	30,52,52	1.93	9 (30%)
4	T8T	G	705	3	24,33,33	1.02	1 (4%)	30,52,52	1.94	8 (26%)
4	T8T	H	702	3	24,33,33	0.91	1 (4%)	30,52,52	1.83	9 (30%)
4	T8T	C	706	3	24,33,33	1.07	2 (8%)	30,52,52	1.91	8 (26%)
4	T8T	D	706	3,2	24,33,33	1.51	3 (12%)	30,52,52	1.74	6 (20%)
4	T8T	B	708	3	24,33,33	0.89	1 (4%)	30,52,52	1.43	5 (16%)
4	T8T	E	706	3	24,33,33	1.13	1 (4%)	30,52,52	1.86	8 (26%)
4	T8T	D	702	3	24,33,33	1.39	3 (12%)	30,52,52	1.58	5 (16%)
4	T8T	D	701	3	24,33,33	0.97	2 (8%)	30,52,52	1.78	6 (20%)
4	T8T	F	702	3	24,33,33	1.37	3 (12%)	30,52,52	1.53	5 (16%)
4	T8T	F	701	3	24,33,33	1.14	2 (8%)	30,52,52	1.75	7 (23%)
4	T8T	H	706	3,2	24,33,33	1.48	2 (8%)	30,52,52	1.92	8 (26%)

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	T8T	F	707	3,2	-	4/14/34/34	0/3/3/3
4	T8T	A	706	3	-	1/14/34/34	0/3/3/3
4	T8T	G	704	3,2	-	3/14/34/34	0/3/3/3
4	T8T	H	701	3	-	2/14/34/34	0/3/3/3
4	T8T	A	704	3,2	-	2/14/34/34	0/3/3/3
4	T8T	B	702	3	-	3/14/34/34	0/3/3/3
4	T8T	E	705	3,2	-	2/14/34/34	0/3/3/3
4	T8T	B	701	3	-	2/14/34/34	0/3/3/3
4	T8T	A	708	3	-	3/14/34/34	0/3/3/3
4	T8T	E	708	3	-	3/14/34/34	0/3/3/3
4	T8T	F	709	3	-	2/14/34/34	0/3/3/3
4	T8T	C	705	3,2	-	4/14/34/34	0/3/3/3
4	T8T	B	706	3,2	-	5/14/34/34	0/3/3/3
4	T8T	G	705	3	-	4/14/34/34	0/3/3/3
4	T8T	H	702	3	-	2/14/34/34	0/3/3/3
4	T8T	C	706	3	-	4/14/34/34	0/3/3/3
4	T8T	D	706	3,2	-	4/14/34/34	0/3/3/3
4	T8T	B	708	3	-	4/14/34/34	0/3/3/3
4	T8T	E	706	3	-	2/14/34/34	0/3/3/3
4	T8T	D	702	3	-	2/14/34/34	0/3/3/3
4	T8T	D	701	3	-	3/14/34/34	0/3/3/3
4	T8T	F	702	3	-	2/14/34/34	0/3/3/3
4	T8T	F	701	3	-	1/14/34/34	0/3/3/3
4	T8T	H	706	3,2	-	3/14/34/34	0/3/3/3

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	706	T8T	C6-N1	6.08	1.43	1.33
4	D	706	T8T	C6-N1	5.82	1.43	1.33
4	E	705	T8T	C6-N1	5.68	1.42	1.33
4	F	707	T8T	C6-N1	5.43	1.42	1.33
4	C	705	T8T	C6-N1	5.00	1.41	1.33

The worst 5 of 163 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	706	T8T	N3-C2-N1	-5.13	120.38	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	707	T8T	C2-N3-C4	5.08	121.16	115.36
4	A	706	T8T	N3-C2-N1	-5.05	120.48	127.22
4	E	705	T8T	N3-C2-N1	-4.91	120.67	127.22
4	D	706	T8T	N3-C2-N1	-4.91	120.68	127.22

There are no chirality outliers.

5 of 67 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	705	T8T	PB-O3A-PA-O2A
4	C	706	T8T	PB-O3B-PG-O1G
4	G	705	T8T	PB-O3B-PG-O1G
4	B	702	T8T	PA-O3A-PB-O1B
4	B	708	T8T	PA-O3A-PB-O1B

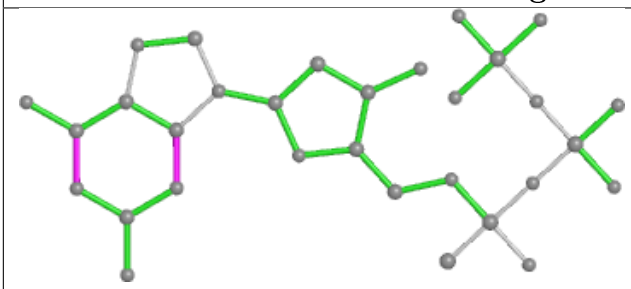
There are no ring outliers.

8 monomers are involved in 7 short contacts:

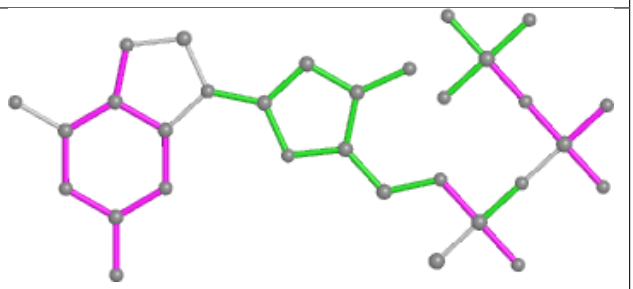
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	707	T8T	1	0
4	A	704	T8T	1	0
4	F	709	T8T	1	0
4	C	705	T8T	1	0
4	G	705	T8T	1	0
4	C	706	T8T	1	0
4	B	708	T8T	1	0
4	F	702	T8T	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

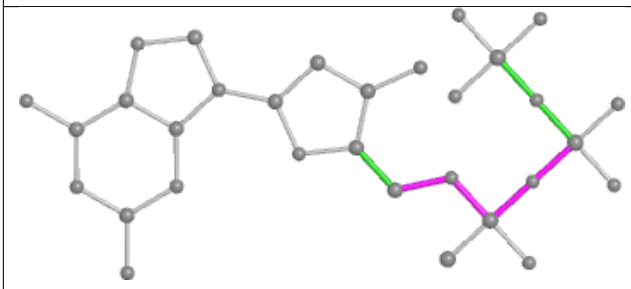
Ligand T8T F 707



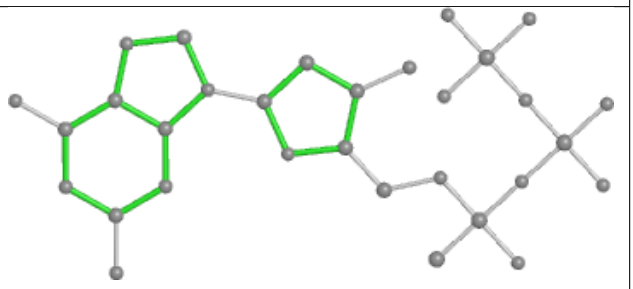
Bond lengths



Bond angles

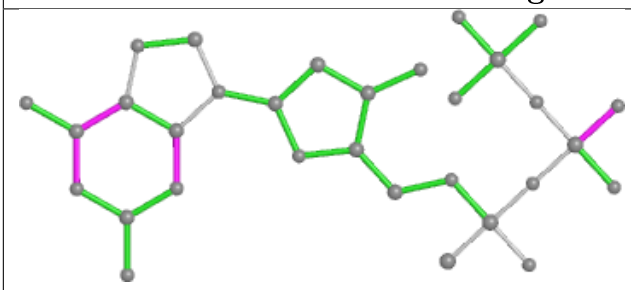


Torsions



Rings

Ligand T8T A 706



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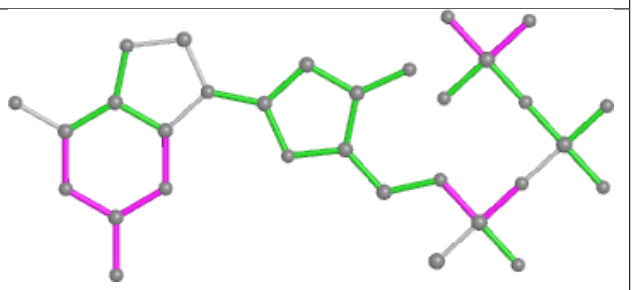

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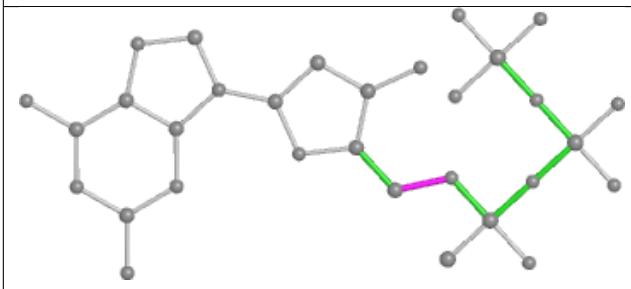

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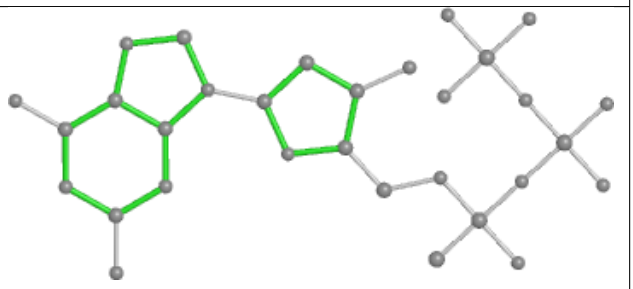
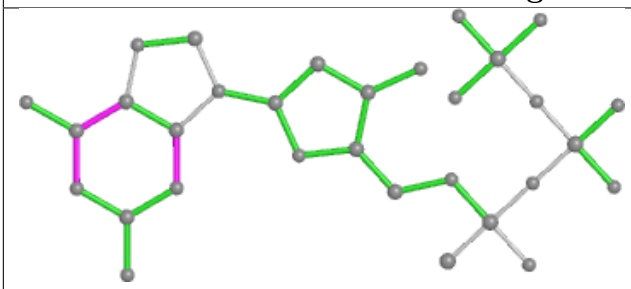


Rings

Ligand T8T G 704



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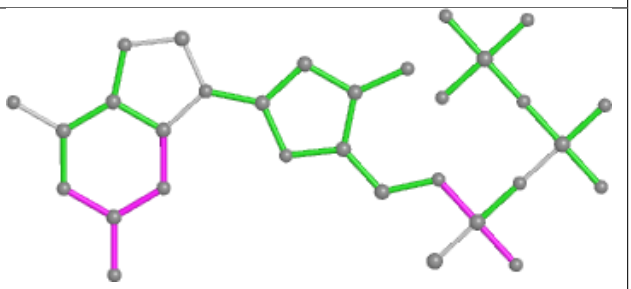
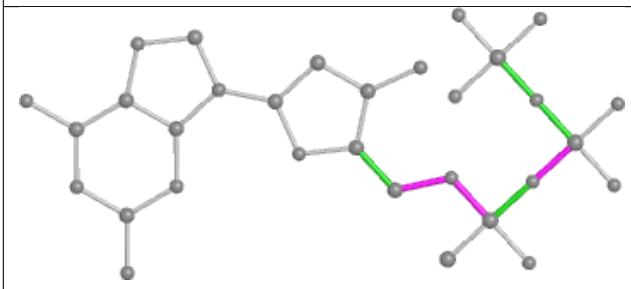


Bond angles



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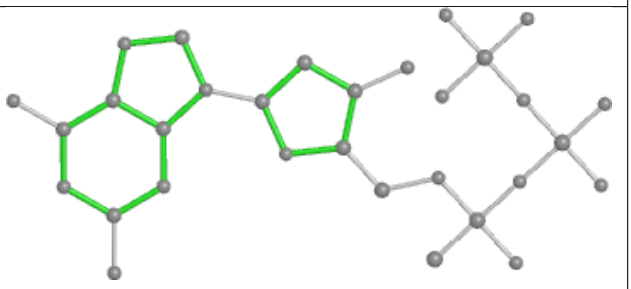
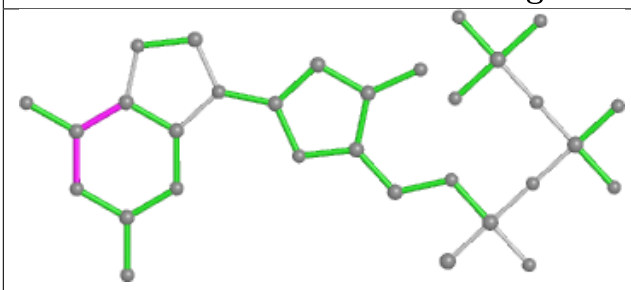


Rings

Ligand T8T H 701



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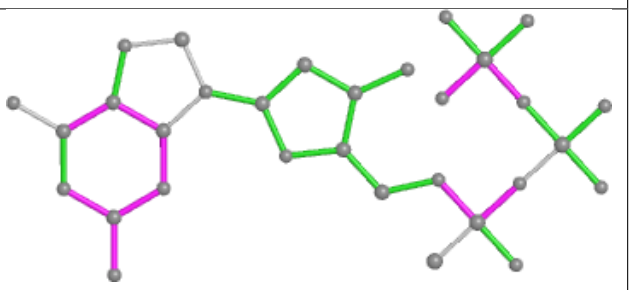

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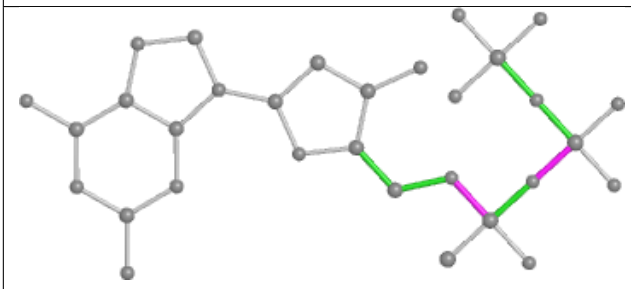

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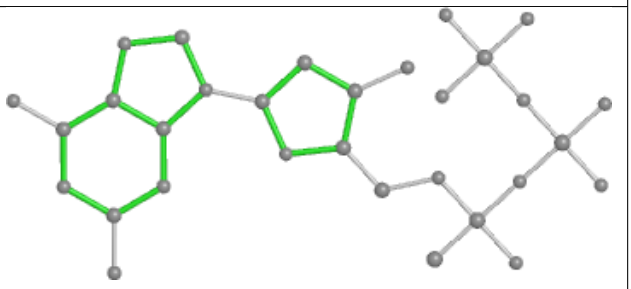
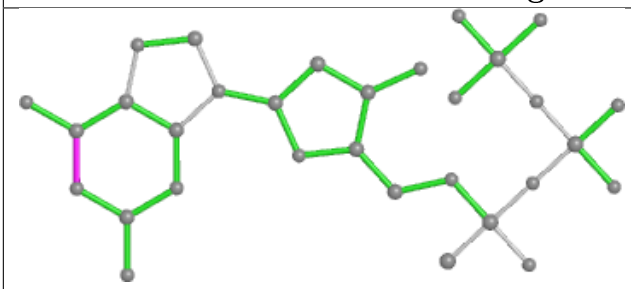


Rings

Ligand T8T A 704



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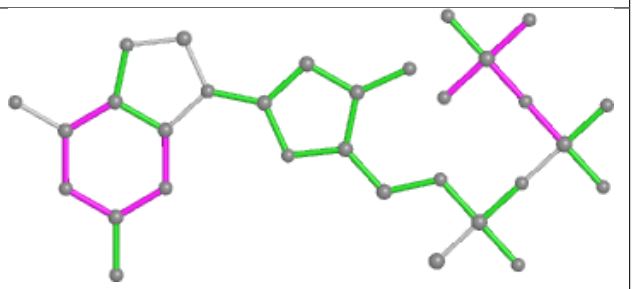
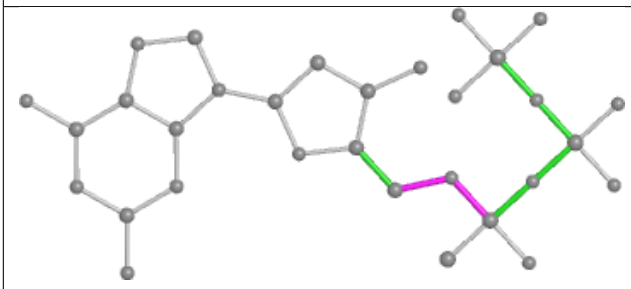


Bond angles



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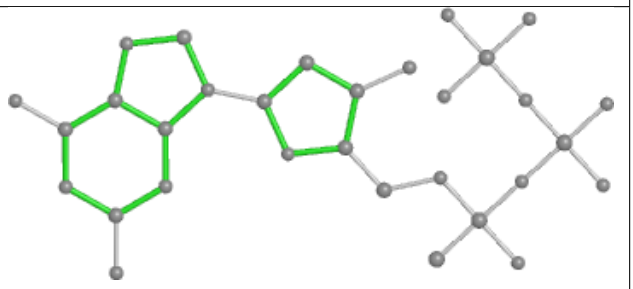
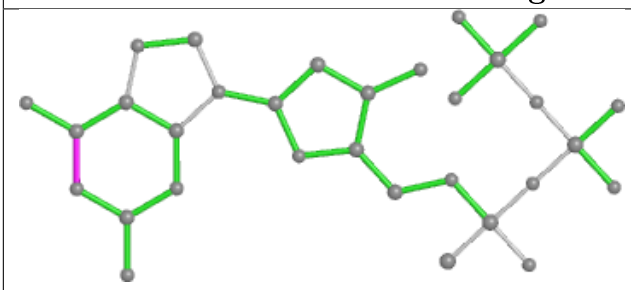
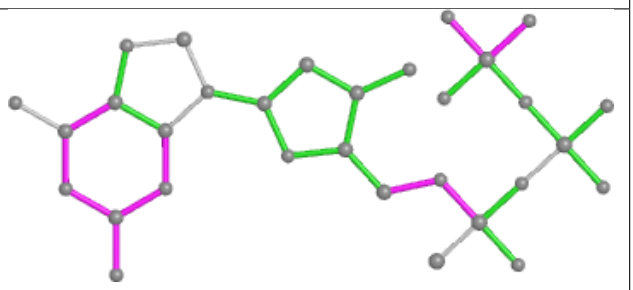


Rings

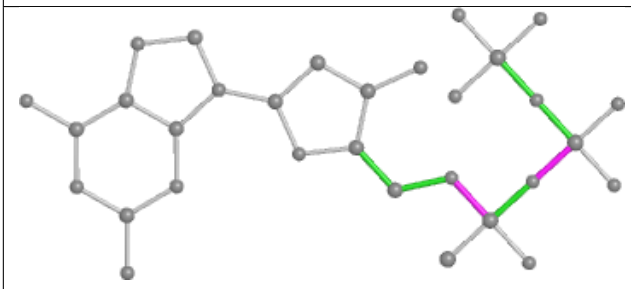
Ligand T8T B 702



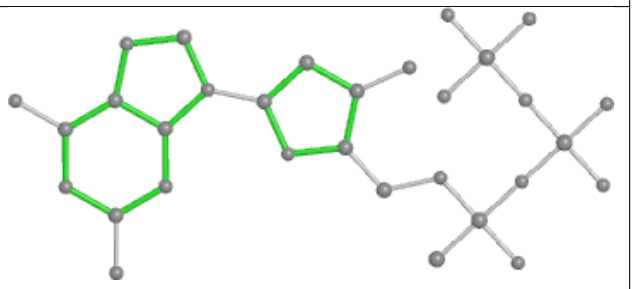
Bond lengths



Bond angles

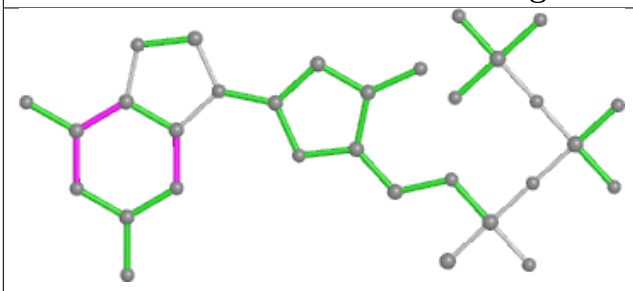


Torsions

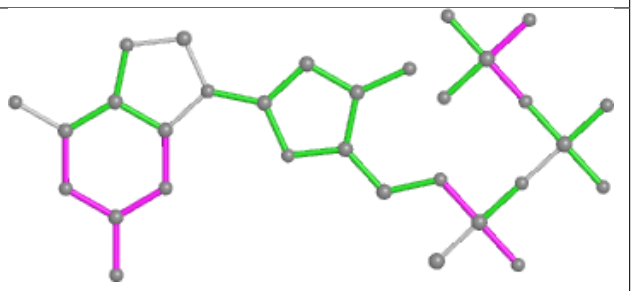


Rings

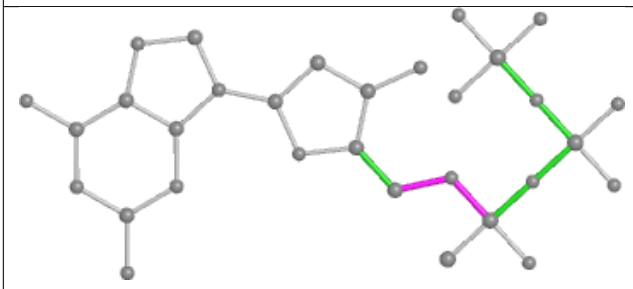
Ligand T8T E 705



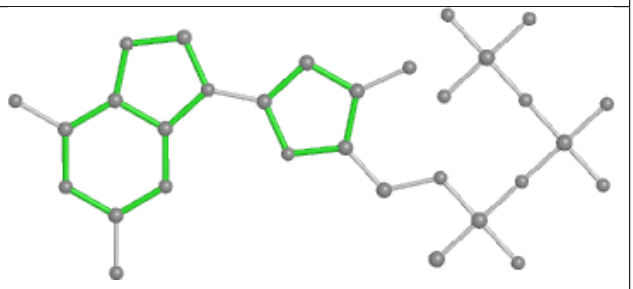
Bond lengths



Bond angles

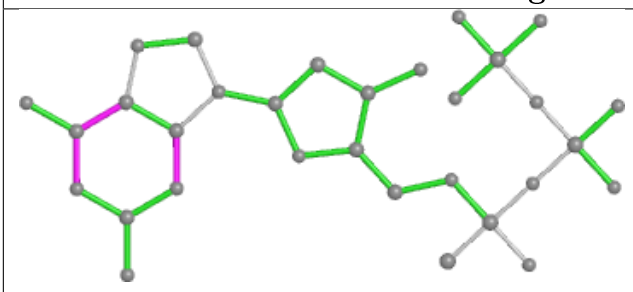


Torsions



Rings

Ligand T8T B 701



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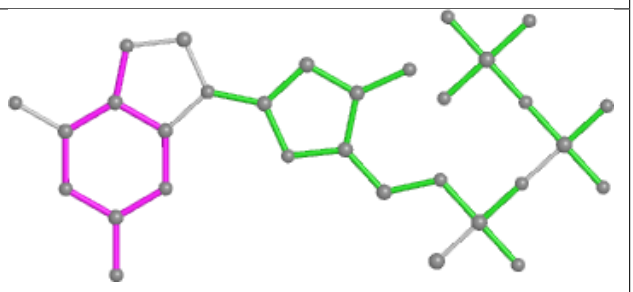
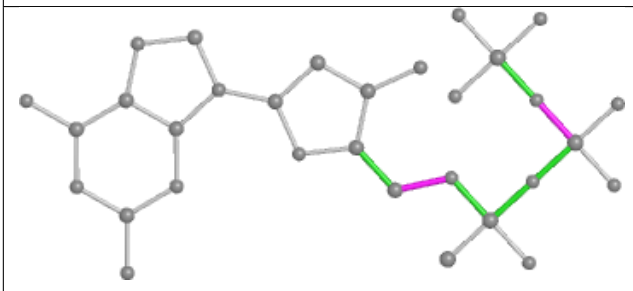
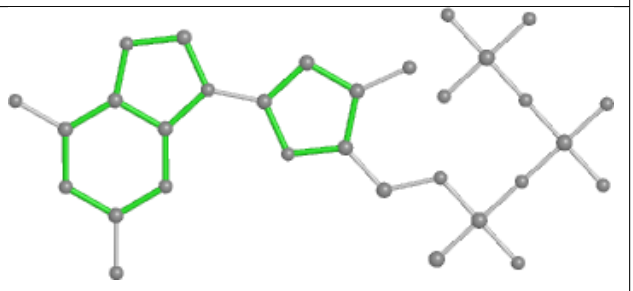


Bond angles

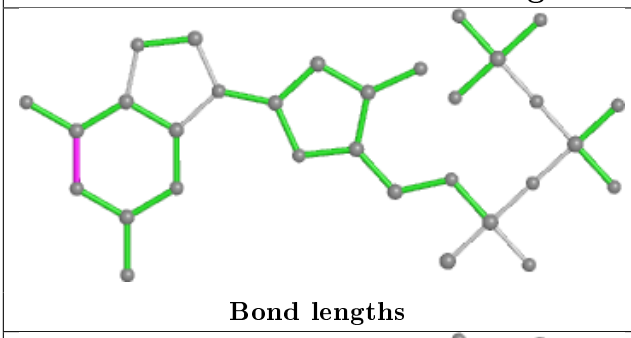


Torsions



Rings

Ligand T8T A 708



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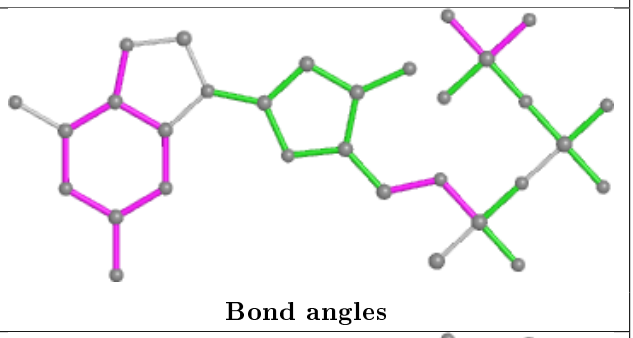
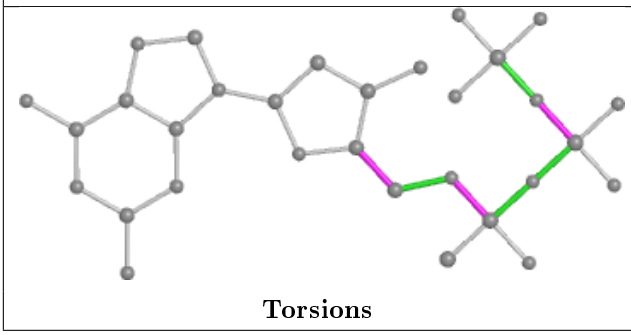
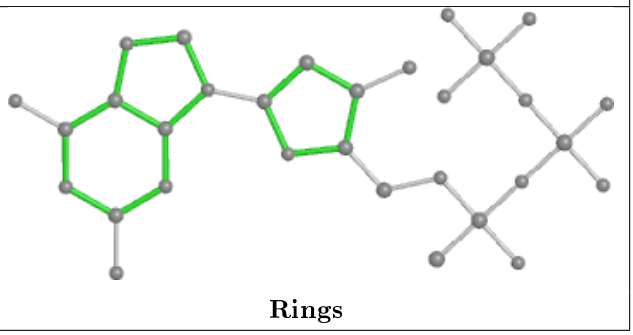


Bond angles

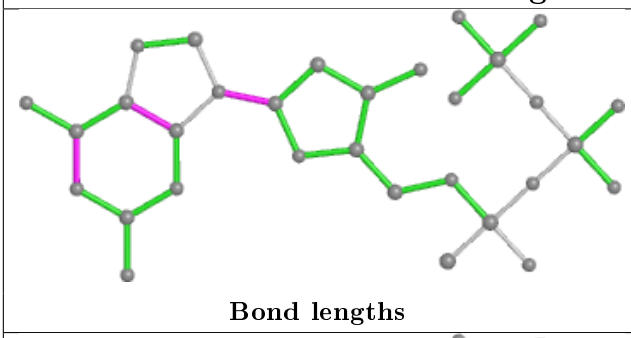


Torsions



Rings

Ligand T8T E 708



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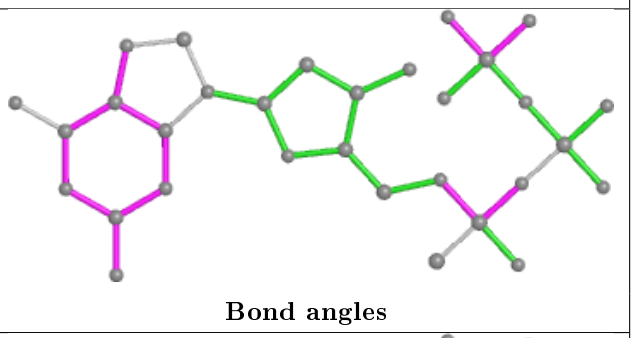
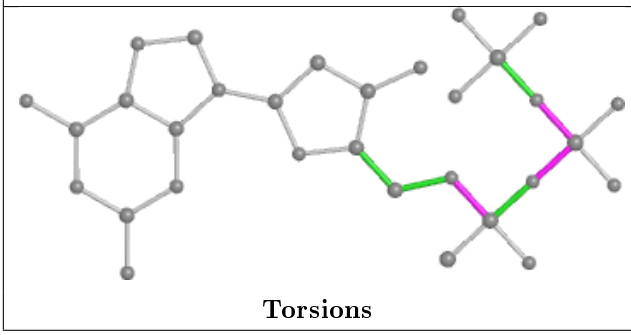
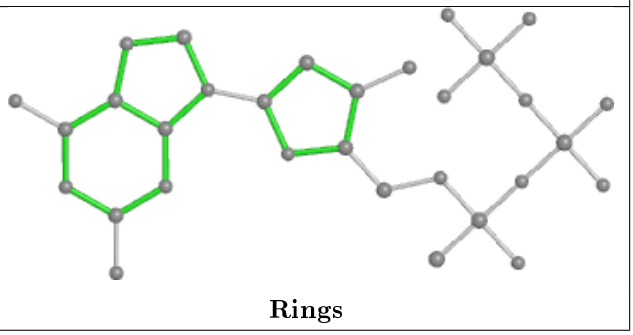


Bond angles

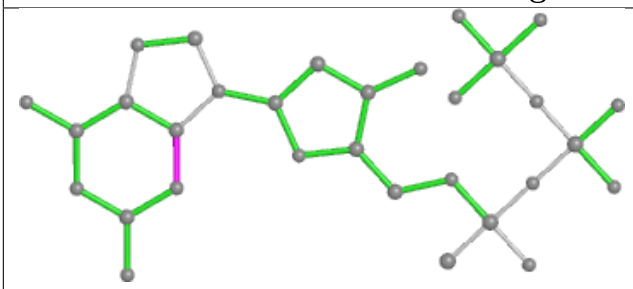


Torsions



Rings

Ligand T8T F 709



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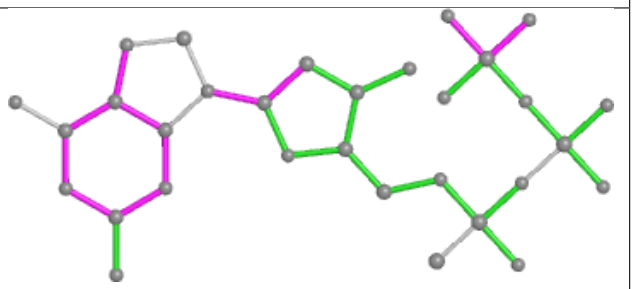
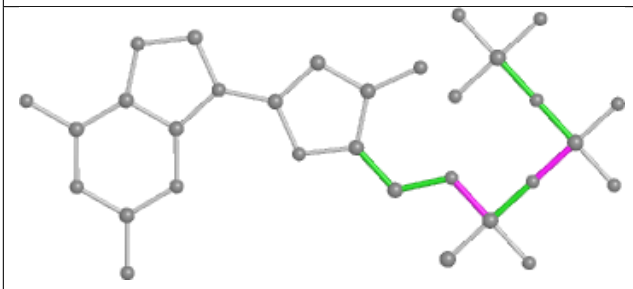


Bond angles



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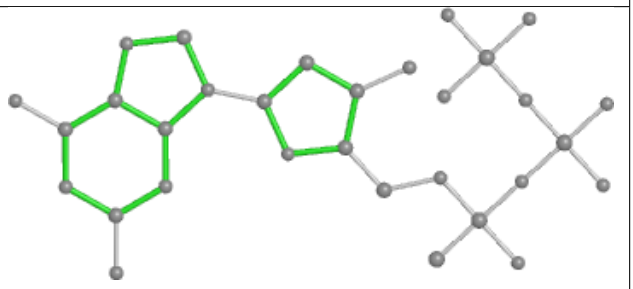
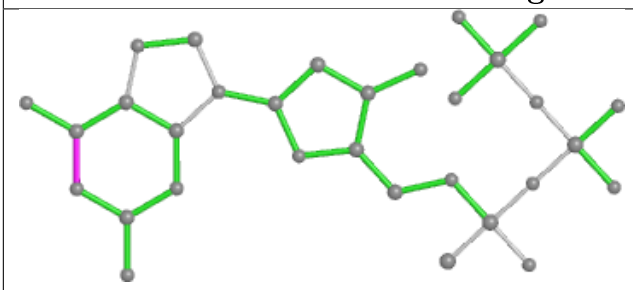


Rings

Ligand T8T C 705



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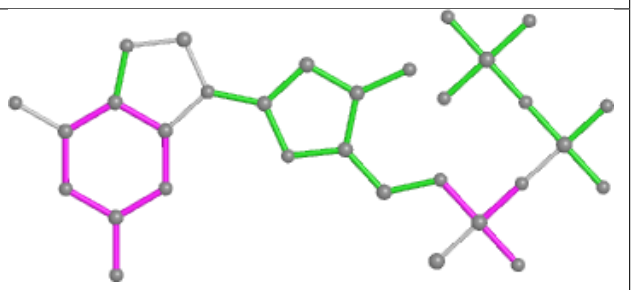
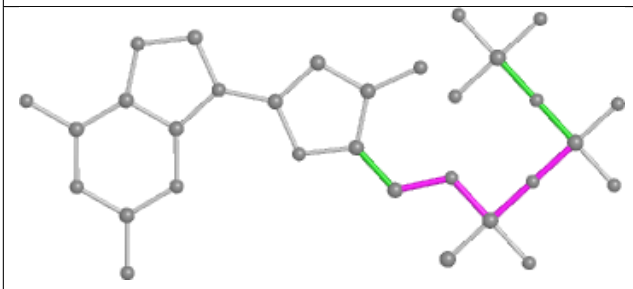


Bond angles



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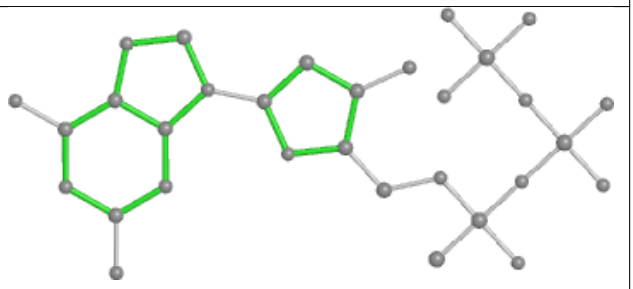
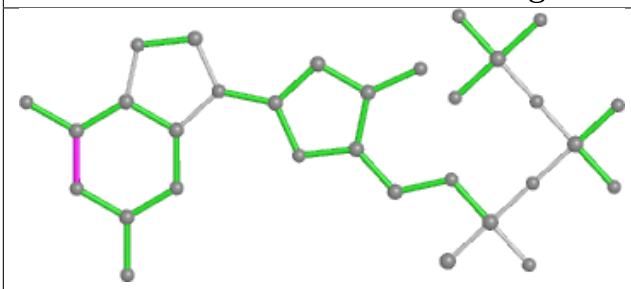


Rings

Ligand T8T B 706



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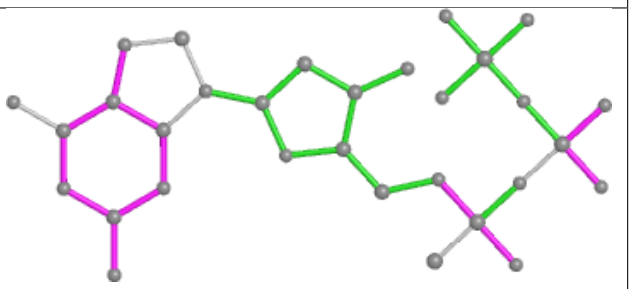
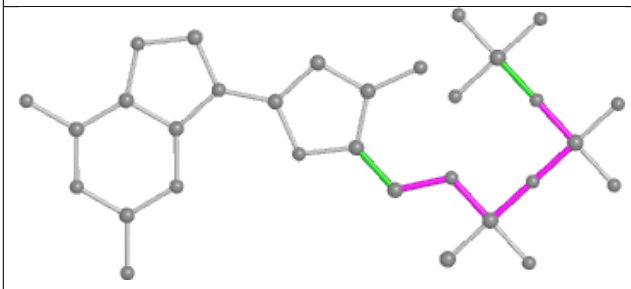


Bond angles



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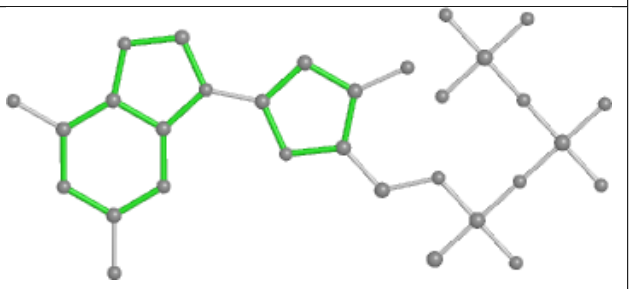
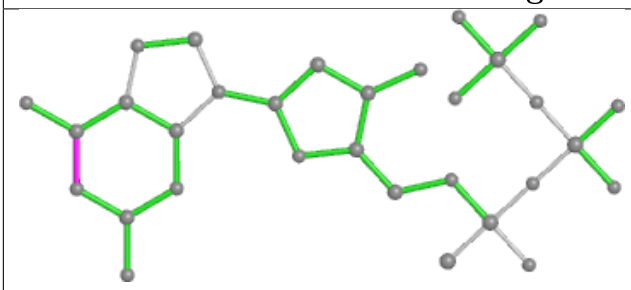


Rings

Ligand T8T G 705



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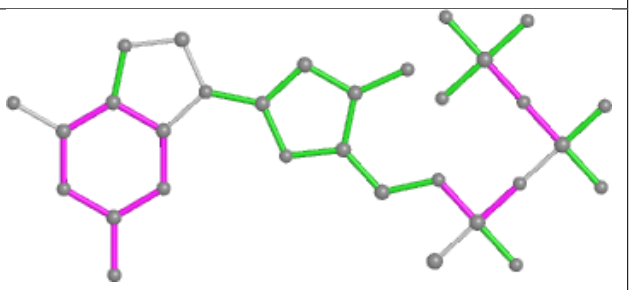

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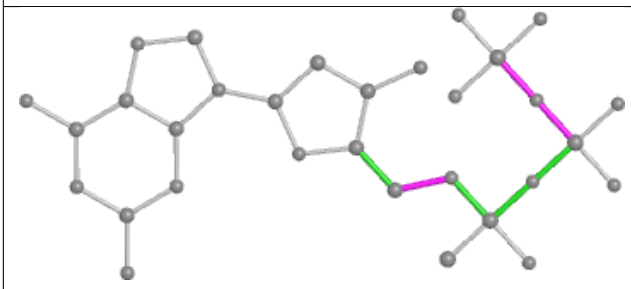

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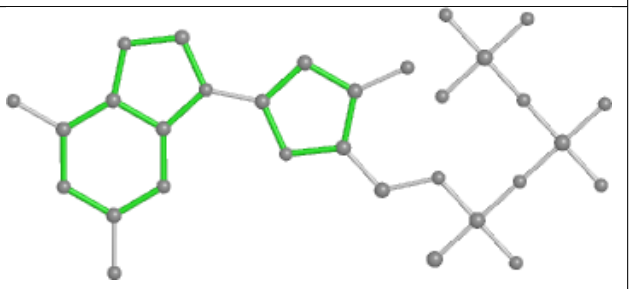
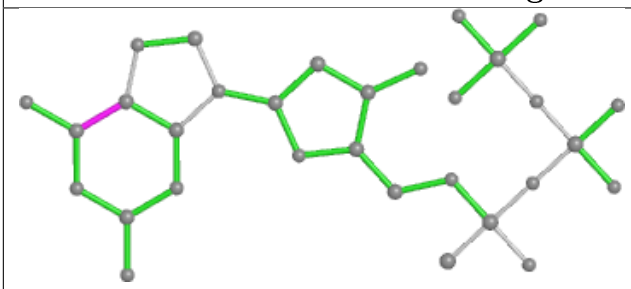


Rings

Ligand T8T H 702



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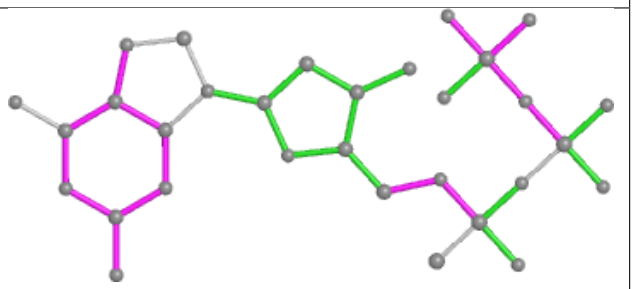
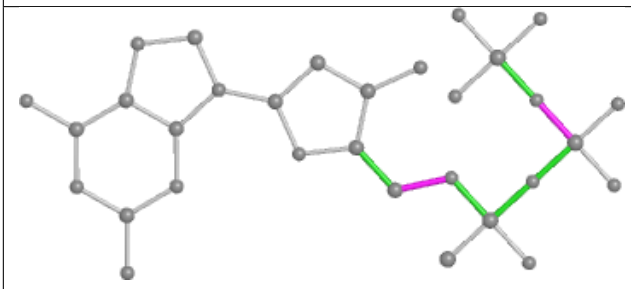


Bond angles



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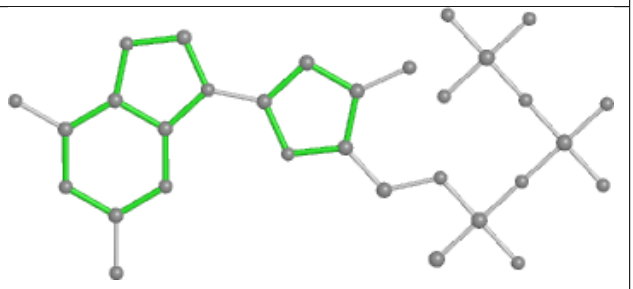
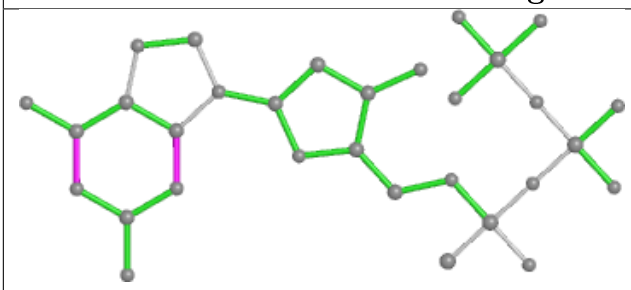


Rings

Ligand T8T C 706



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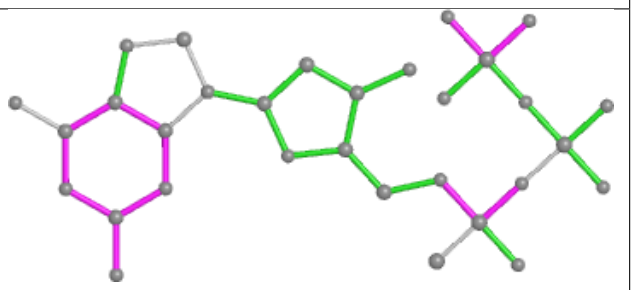
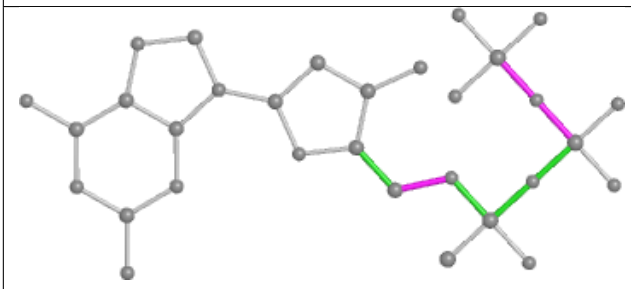


Bond angles



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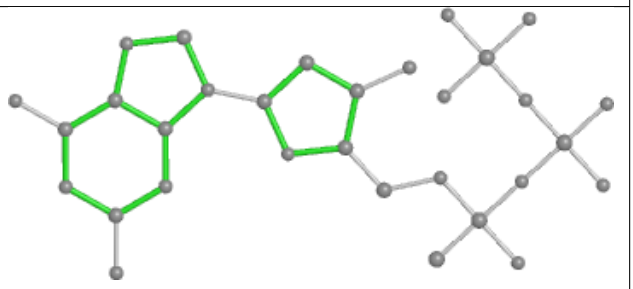
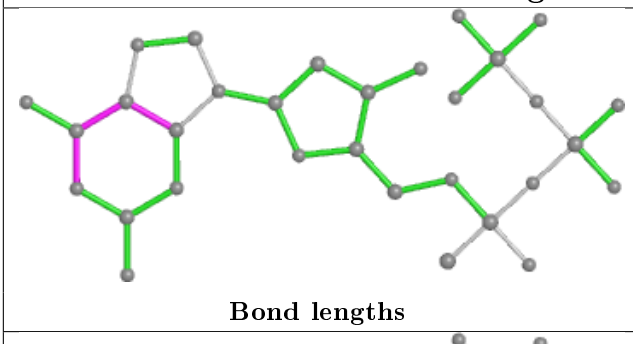


Rings

Ligand T8T D 706



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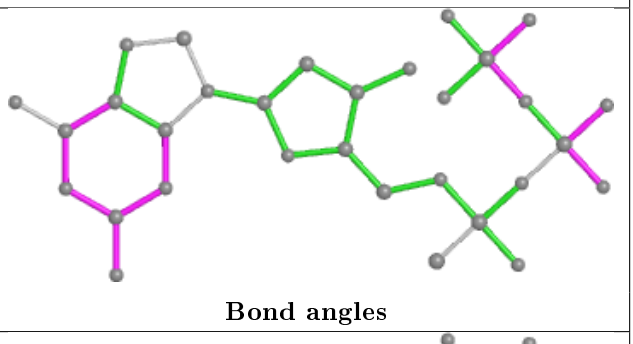

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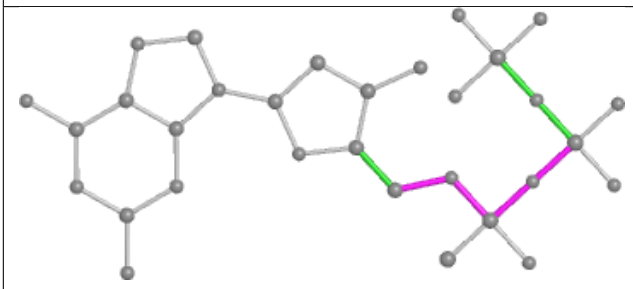

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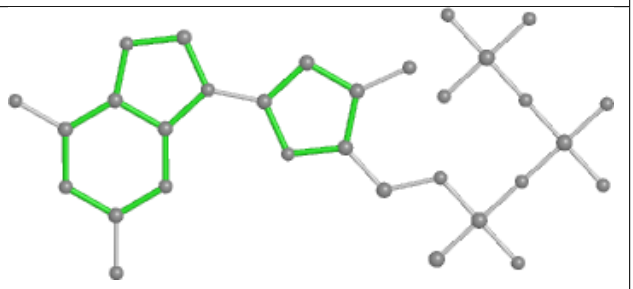
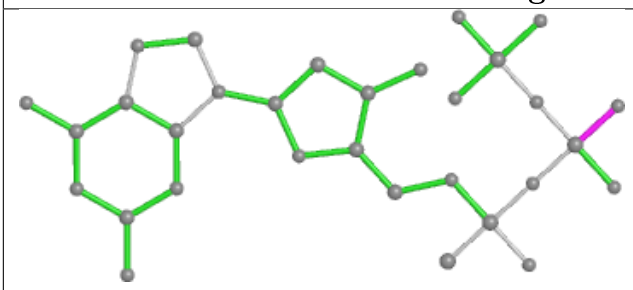


Rings

Ligand T8T B 708



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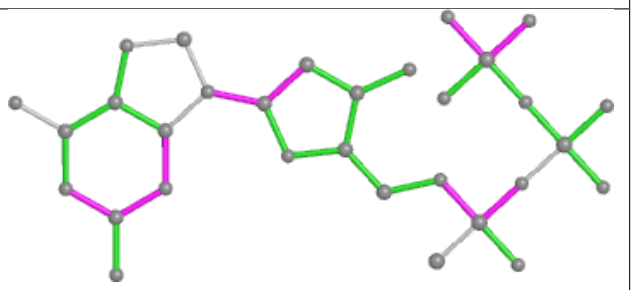
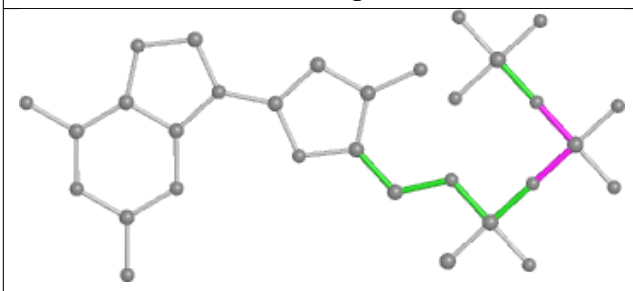


Bond angles



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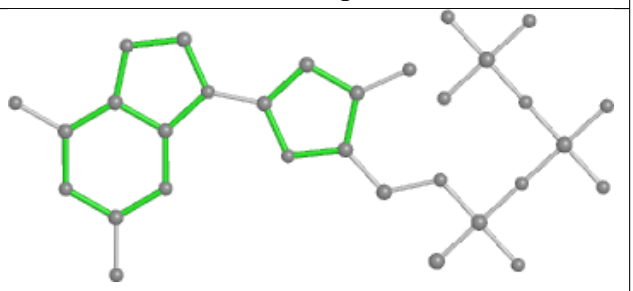
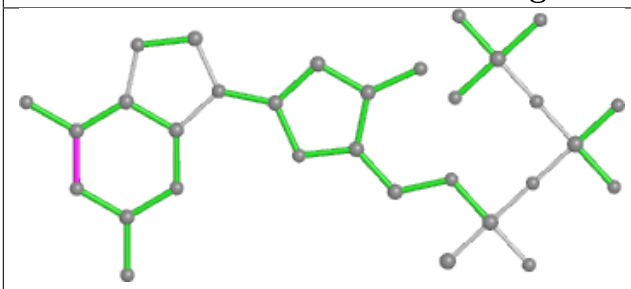


Rings

Ligand T8T E 706



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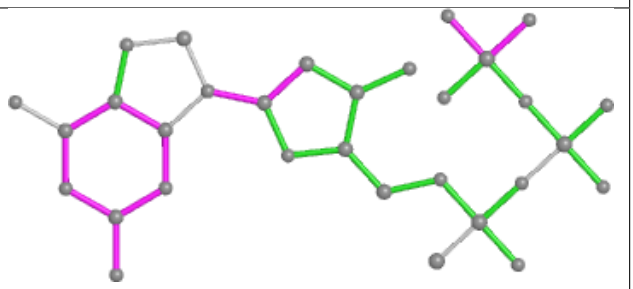
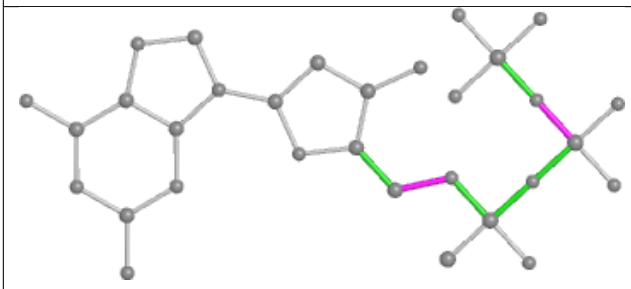


Bond angles



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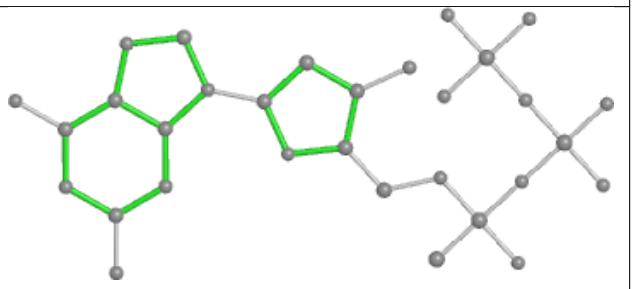
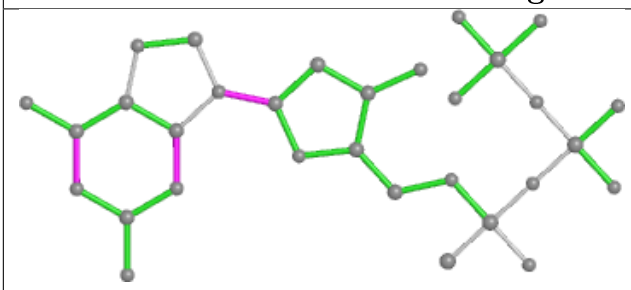


Rings

Ligand T8T D 702



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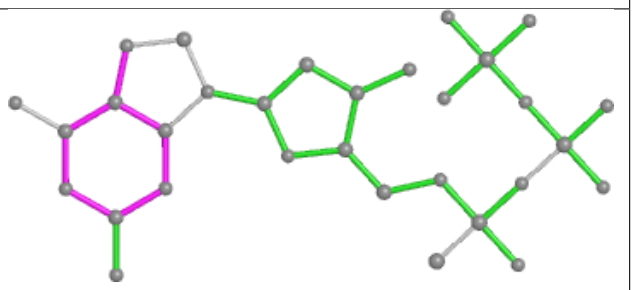
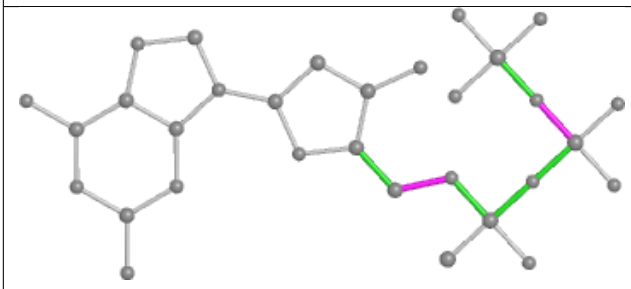
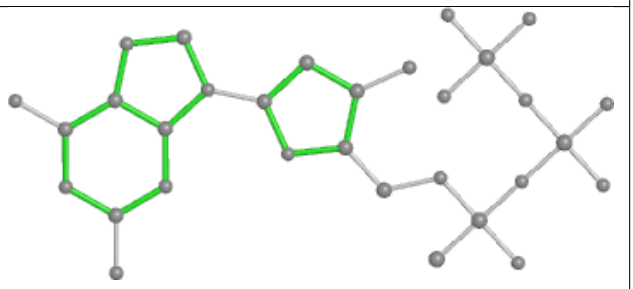


Bond angles

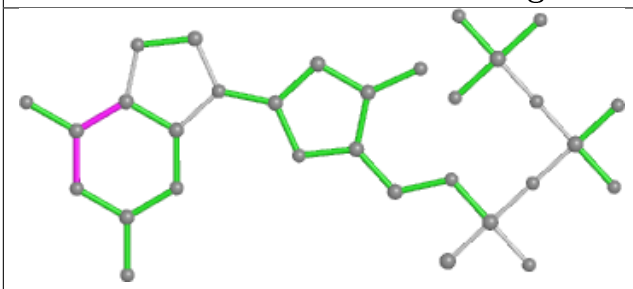


Torsions

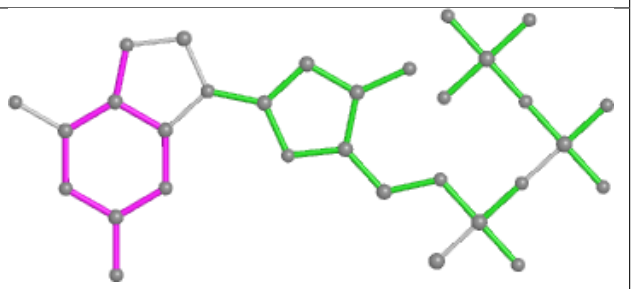


Rings

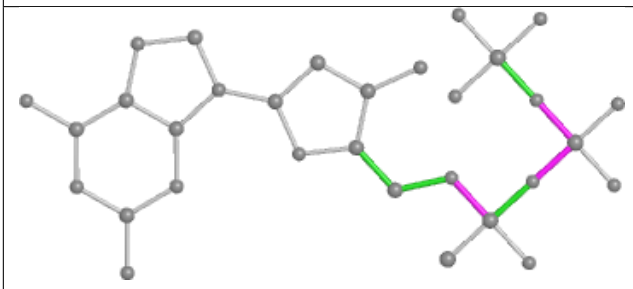
Ligand T8T D 701



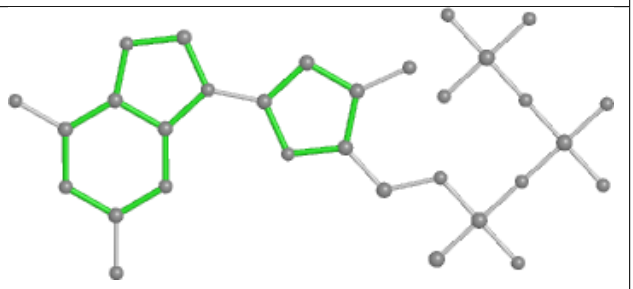
Bond lengths



Bond angles

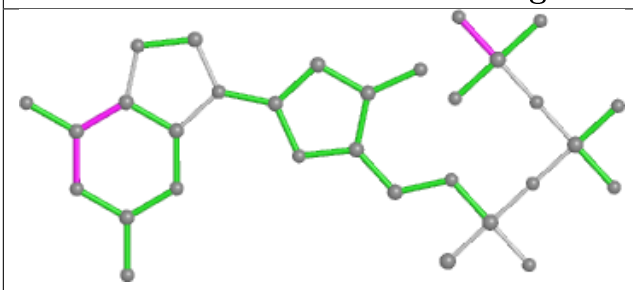


Torsions

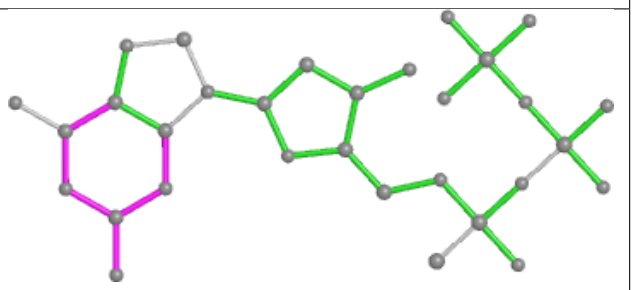


Rings

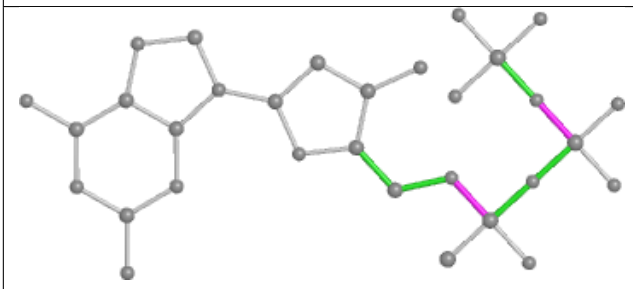
Ligand T8T F 702



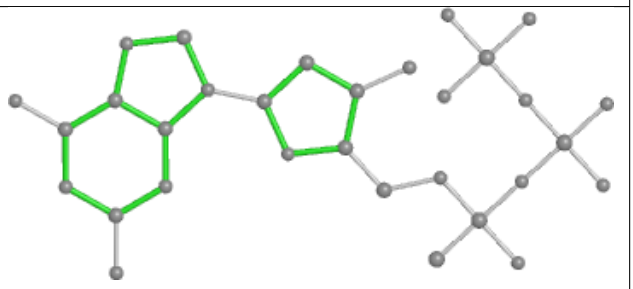
Bond lengths



Bond angles

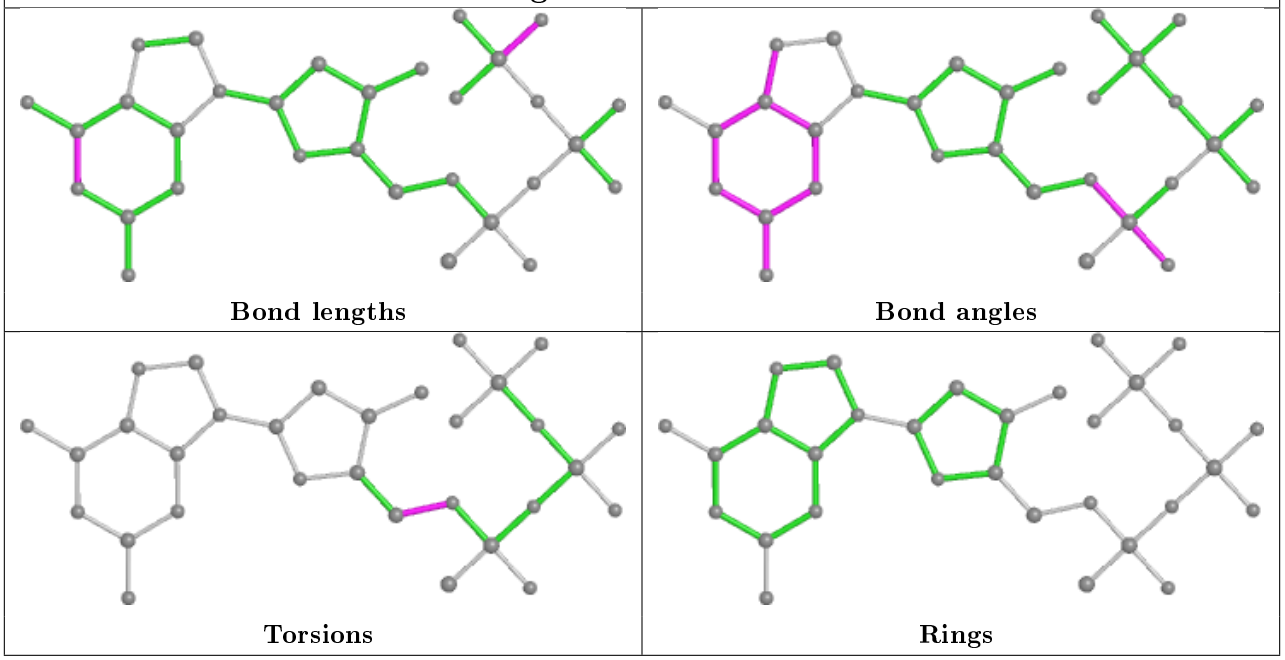


Torsions

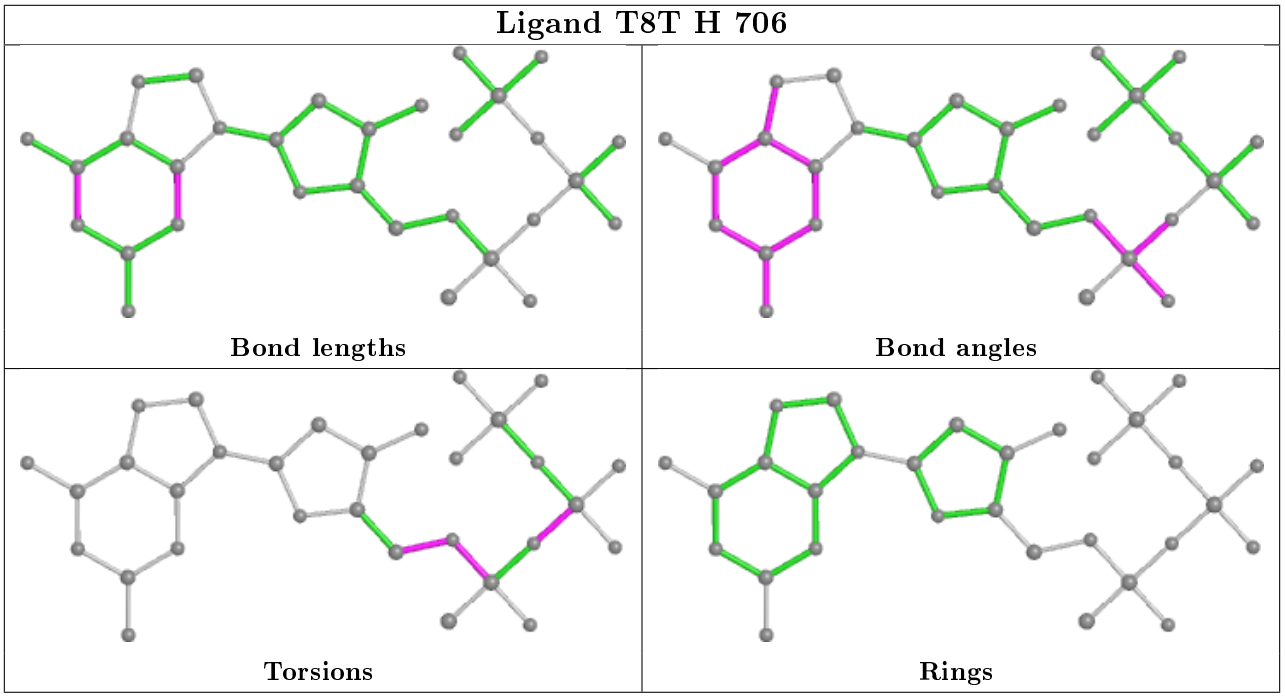


Rings

Ligand T8T F 701



Ligand T8T H 706



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	458/520 (88%)	0.01	10 (2%) 62 69	16, 35, 65, 96	0
1	B	452/520 (86%)	0.07	7 (1%) 73 79	17, 36, 77, 98	0
1	C	459/520 (88%)	-0.01	4 (0%) 84 88	17, 36, 59, 91	0
1	D	451/520 (86%)	-0.02	7 (1%) 72 77	16, 36, 62, 79	0
1	E	462/520 (88%)	-0.03	7 (1%) 73 79	16, 35, 66, 109	0
1	F	455/520 (87%)	0.08	9 (1%) 65 71	19, 39, 74, 91	0
1	G	464/520 (89%)	0.04	4 (0%) 84 88	19, 39, 62, 87	0
1	H	449/520 (86%)	0.00	4 (0%) 84 88	17, 35, 68, 87	0
All	All	3650/4160 (87%)	0.02	52 (1%) 75 80	16, 36, 67, 109	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	487	VAL	9.7
1	E	466	ILE	5.6
1	E	582	GLN	5.4
1	E	487	VAL	4.3
1	F	466	ILE	4.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	E	703	1/1	0.83	0.06	35,35,35,35	0
3	MG	A	705	1/1	0.96	0.07	20,20,20,20	0
3	MG	B	704	1/1	0.96	0.07	32,32,32,32	0
3	MG	D	705	1/1	0.96	0.03	21,21,21,21	0
3	MG	A	703	1/1	0.96	0.04	30,30,30,30	0
3	MG	H	705	1/1	0.96	0.02	26,26,26,26	0
4	T8T	B	702	31/31	0.96	0.12	20,23,27,27	0
4	T8T	B	708	31/31	0.96	0.12	22,24,29,30	0
3	MG	G	702	1/1	0.97	0.09	30,30,30,30	0
3	MG	B	705	1/1	0.97	0.06	23,23,23,23	0
4	T8T	F	702	31/31	0.97	0.12	20,24,27,29	0
4	T8T	F	709	31/31	0.97	0.11	23,25,30,31	0
4	T8T	A	704	31/31	0.98	0.10	21,22,25,26	0
4	T8T	A	706	31/31	0.98	0.10	20,22,29,30	0
4	T8T	A	708	31/31	0.98	0.10	18,22,26,27	0
4	T8T	B	701	31/31	0.98	0.11	20,23,26,26	0
3	MG	F	706	1/1	0.98	0.05	24,24,24,24	0
4	T8T	B	706	31/31	0.98	0.10	18,22,25,27	0
3	MG	C	701	1/1	0.98	0.06	23,23,23,23	0
4	T8T	C	705	31/31	0.98	0.10	22,25,26,28	0
4	T8T	C	706	31/31	0.98	0.10	21,23,27,29	0
4	T8T	D	701	31/31	0.98	0.11	17,20,28,29	0
4	T8T	D	702	31/31	0.98	0.11	23,24,28,30	0
4	T8T	D	706	31/31	0.98	0.10	17,20,23,23	0
4	T8T	E	705	31/31	0.98	0.09	19,23,25,25	0
4	T8T	E	708	31/31	0.98	0.11	20,21,25,26	0
4	T8T	F	701	31/31	0.98	0.10	18,23,28,29	0
3	MG	G	703	1/1	0.98	0.04	26,26,26,26	0
4	T8T	F	707	31/31	0.98	0.11	20,23,26,27	0
3	MG	E	704	1/1	0.98	0.04	29,29,29,29	0
4	T8T	G	704	31/31	0.98	0.10	25,28,31,33	0
4	T8T	G	705	31/31	0.98	0.10	24,26,28,29	0
4	T8T	H	701	31/31	0.98	0.11	20,22,28,29	0
4	T8T	H	702	31/31	0.98	0.11	24,26,29,30	0
4	T8T	H	706	31/31	0.98	0.09	18,20,25,26	0
3	MG	C	704	1/1	0.99	0.02	23,23,23,23	0
3	MG	H	704	1/1	0.99	0.05	21,21,21,21	0

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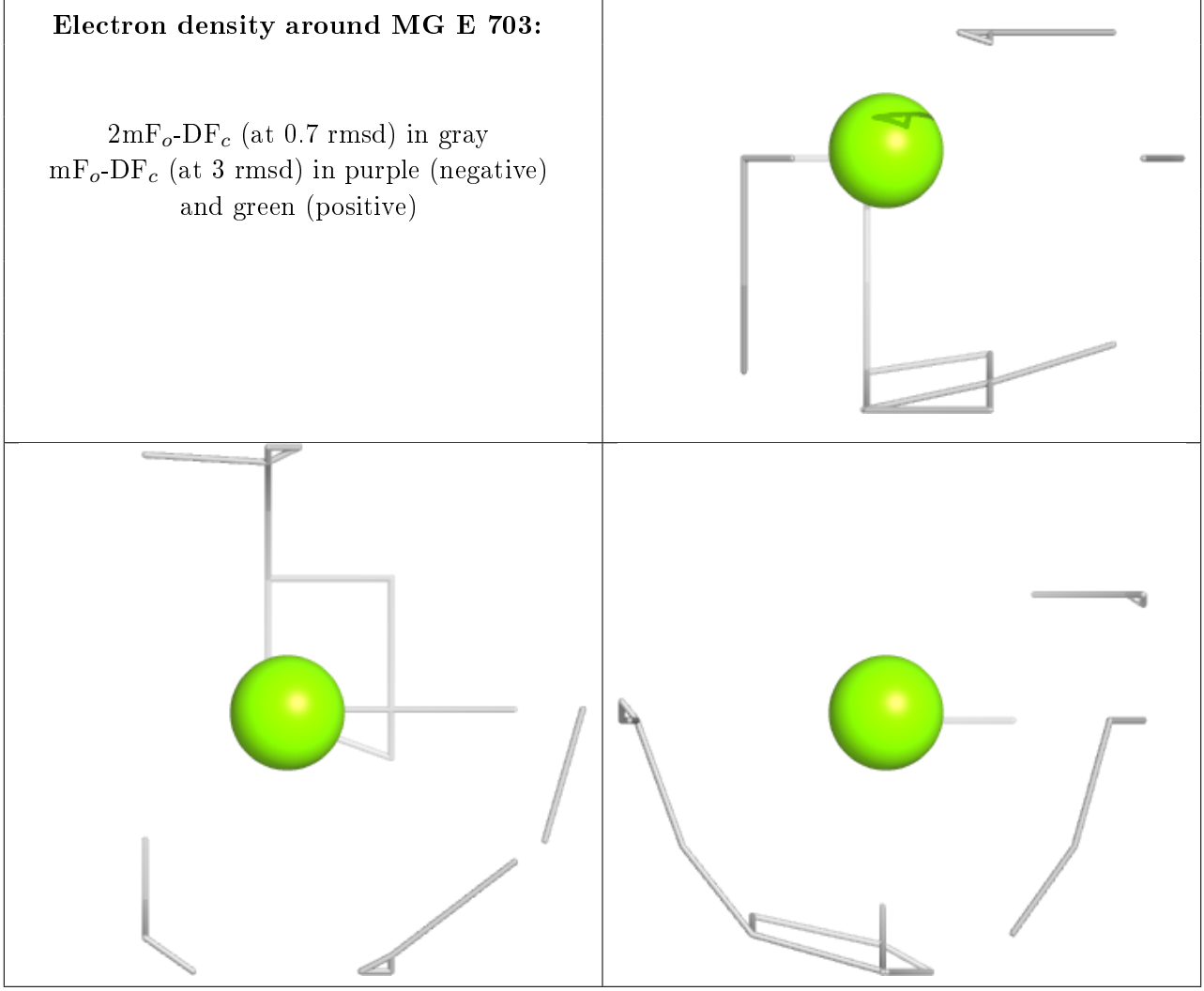
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	D	704	1/1	0.99	0.04	26,26,26,26	0
4	T8T	E	706	31/31	0.99	0.10	23,24,27,27	0
3	MG	A	707	1/1	0.99	0.07	20,20,20,20	0
3	MG	E	702	1/1	0.99	0.06	24,24,24,24	0
3	MG	A	702	1/1	0.99	0.05	22,22,22,22	0
2	FE	A	701	1/1	0.99	0.11	21,21,21,21	0
3	MG	E	707	1/1	0.99	0.04	27,27,27,27	0
3	MG	F	704	1/1	0.99	0.05	33,33,33,33	0
3	MG	F	705	1/1	0.99	0.06	21,21,21,21	0
3	MG	B	707	1/1	0.99	0.05	24,24,24,24	0
3	MG	F	708	1/1	0.99	0.04	21,21,21,21	0
2	FE	H	703	1/1	0.99	0.10	23,23,23,23	0
2	FE	C	702	1/1	1.00	0.08	23,23,23,23	0
2	FE	D	703	1/1	1.00	0.10	22,22,22,22	0
3	MG	C	703	1/1	1.00	0.05	23,23,23,23	0
2	FE	E	701	1/1	1.00	0.11	18,18,18,18	0
2	FE	F	703	1/1	1.00	0.10	18,18,18,18	0
2	FE	G	701	1/1	1.00	0.09	23,23,23,23	0
2	FE	B	703	1/1	1.00	0.10	18,18,18,18	0

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

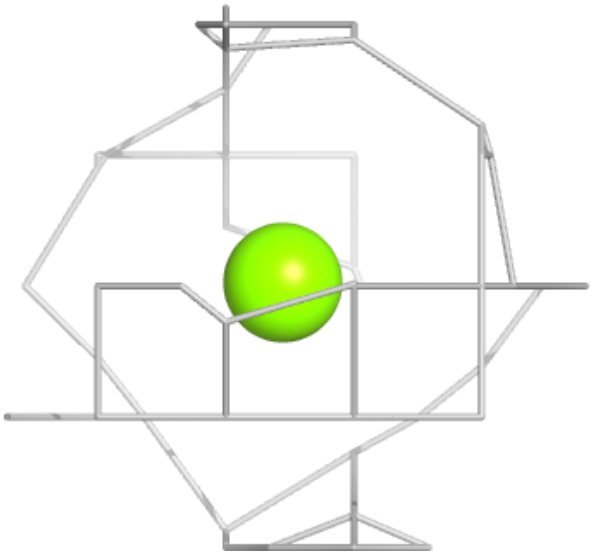
Electron density around MG E 703:

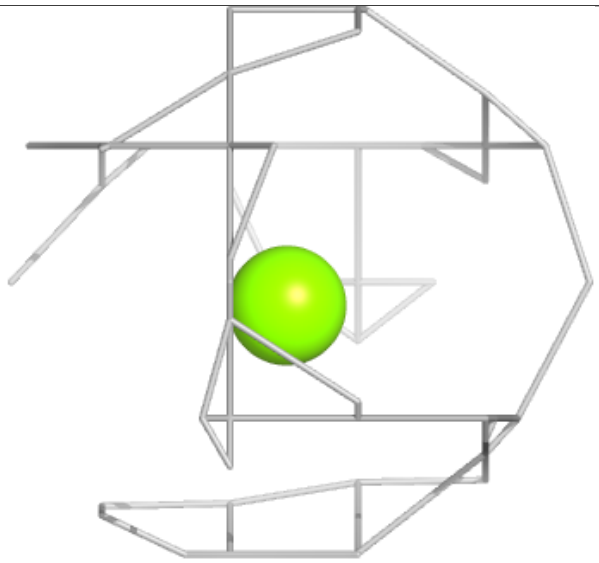
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

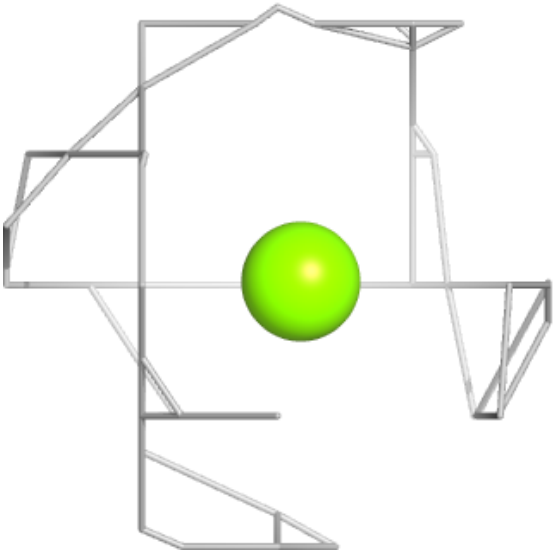


Electron density around MG A 705:

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

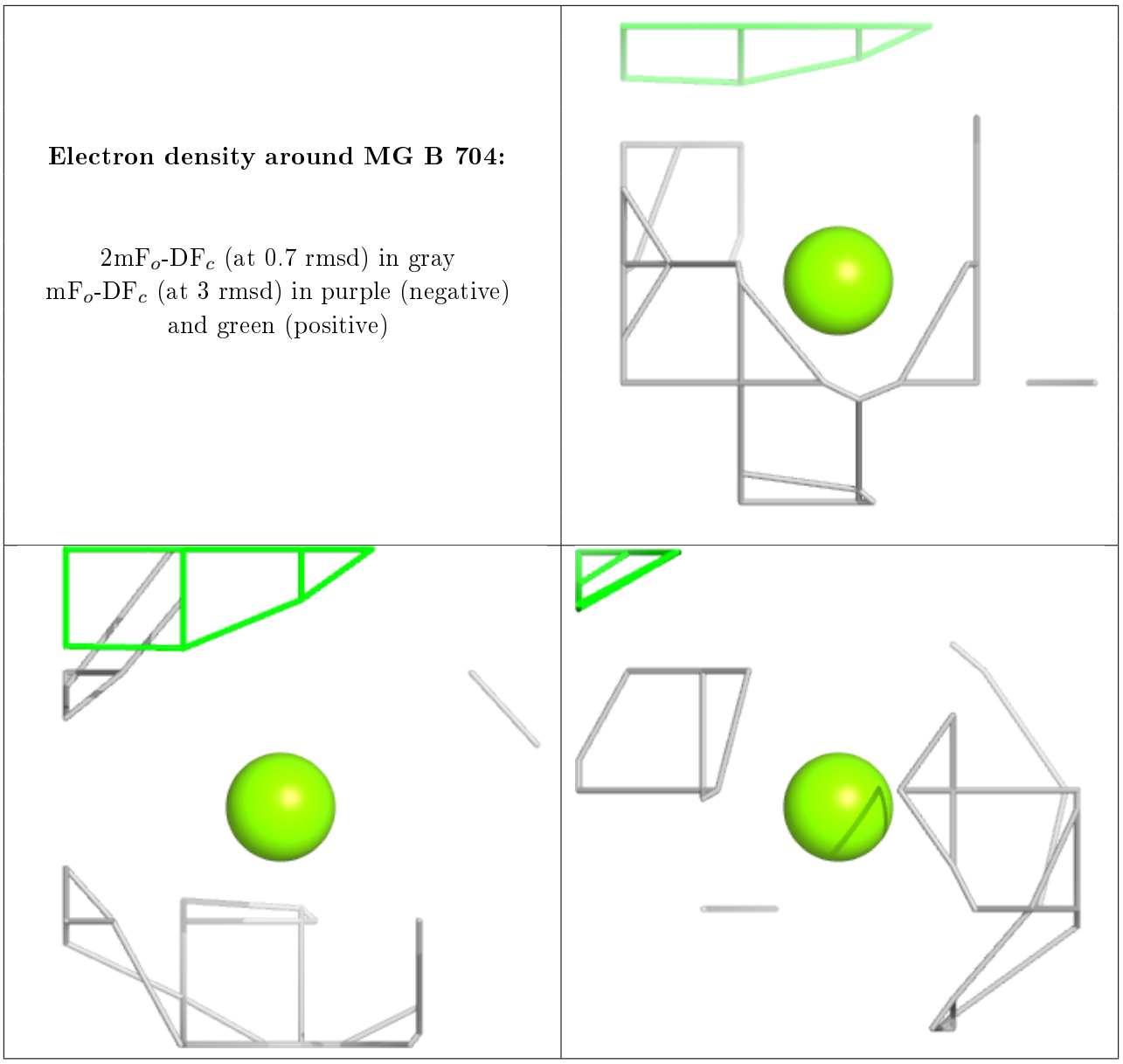






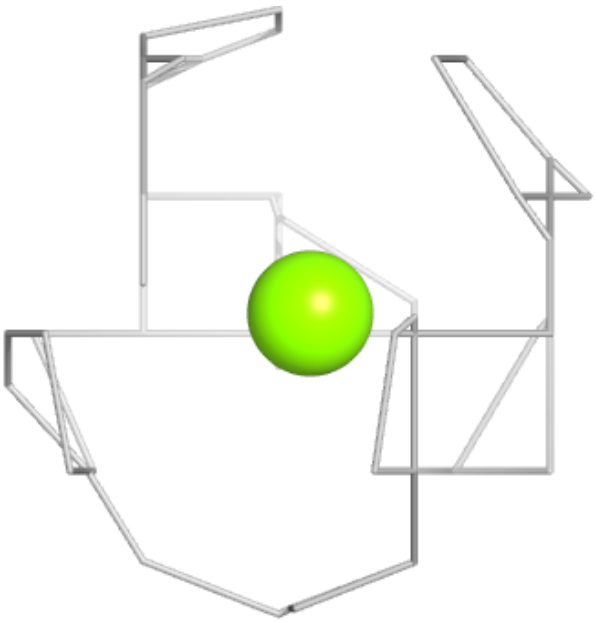
Electron density around MG B 704:

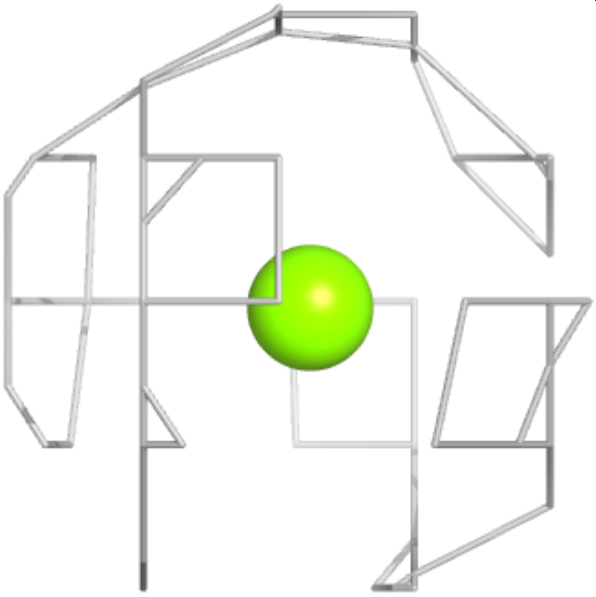
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

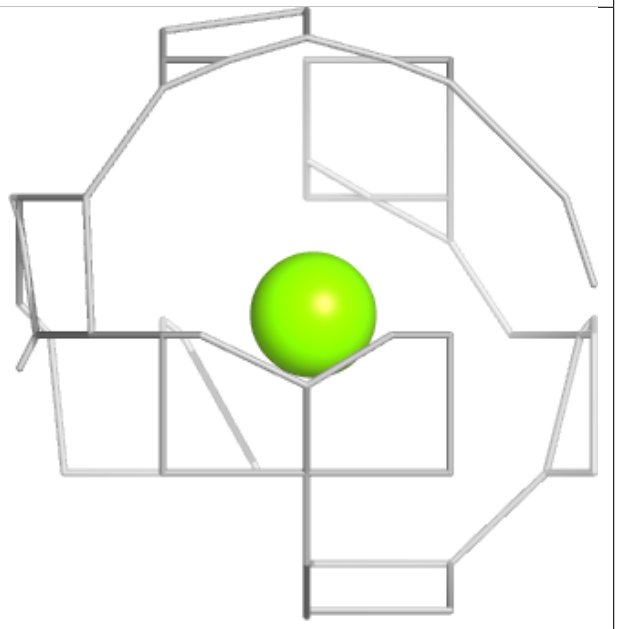


Electron density around MG D 705:

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

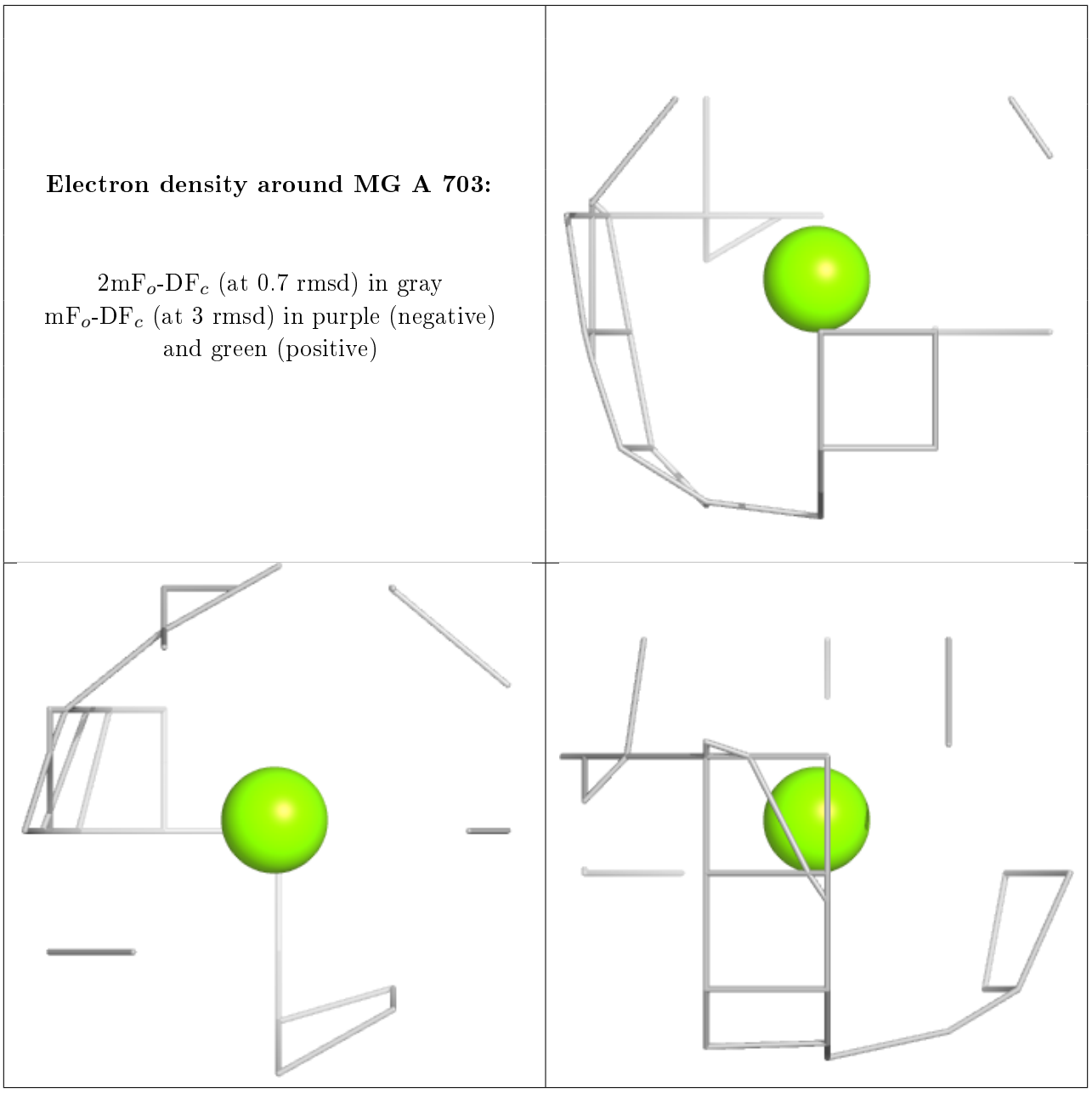






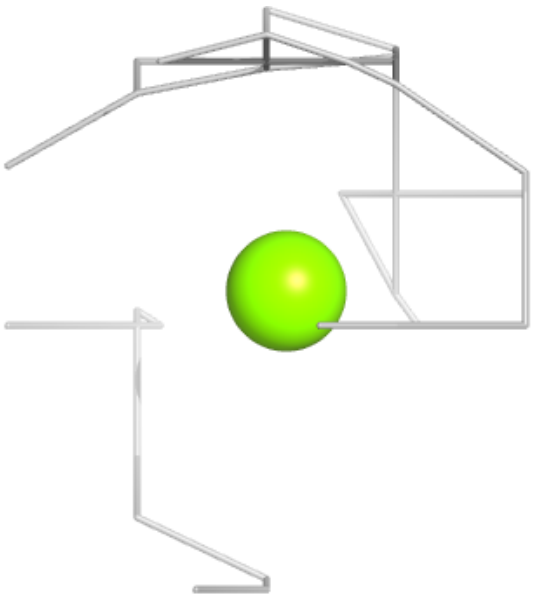
Electron density around MG A 703:

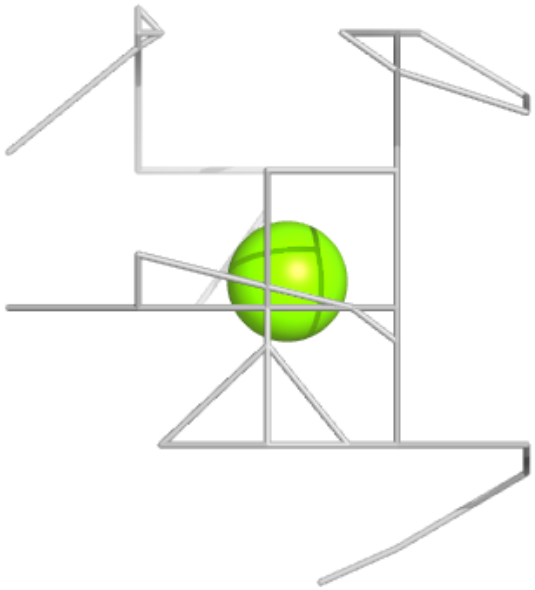
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

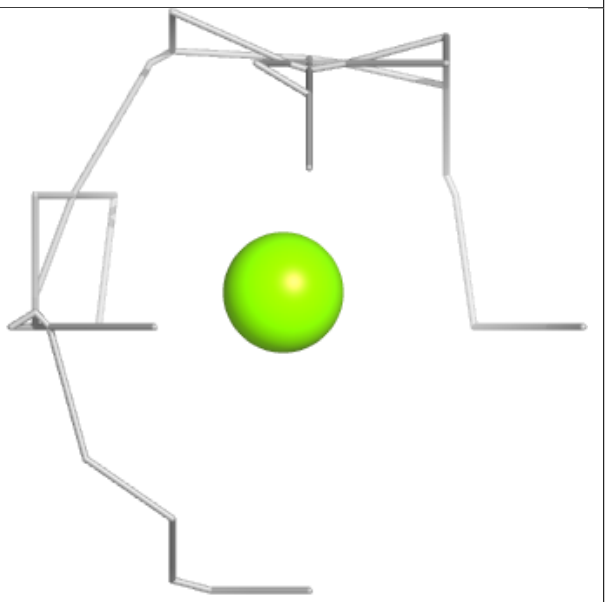


Electron density around MG H 705:

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

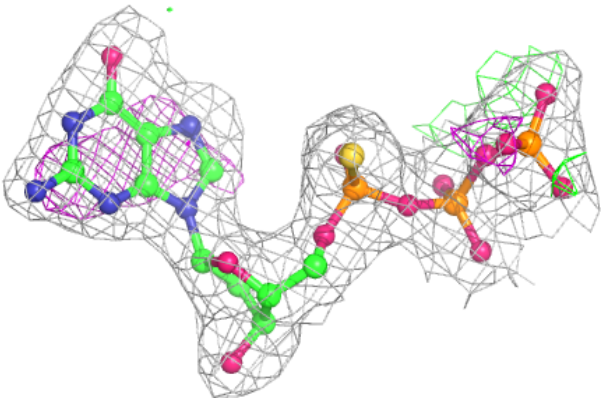


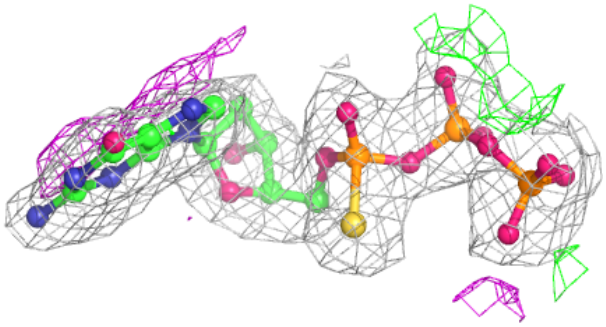


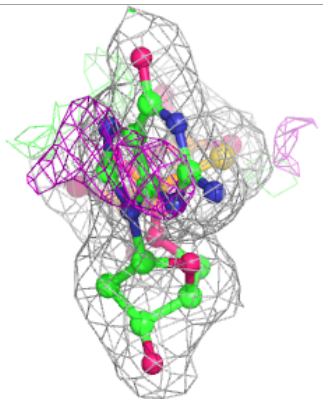


Electron density around T8T B 702:

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

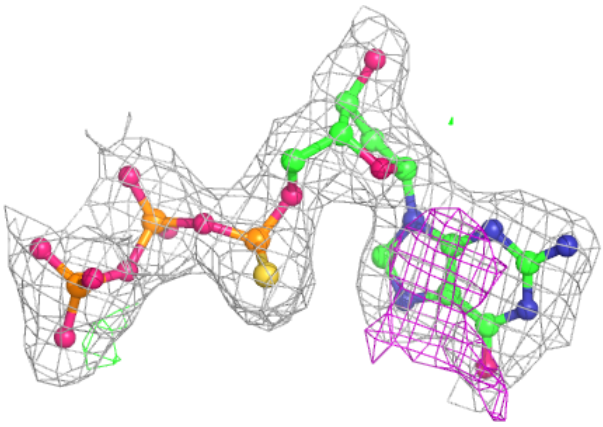


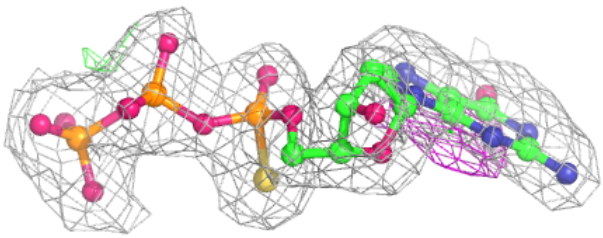


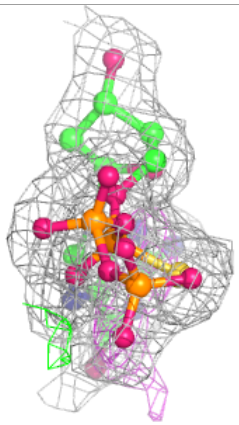


Electron density around T8T B 708:

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

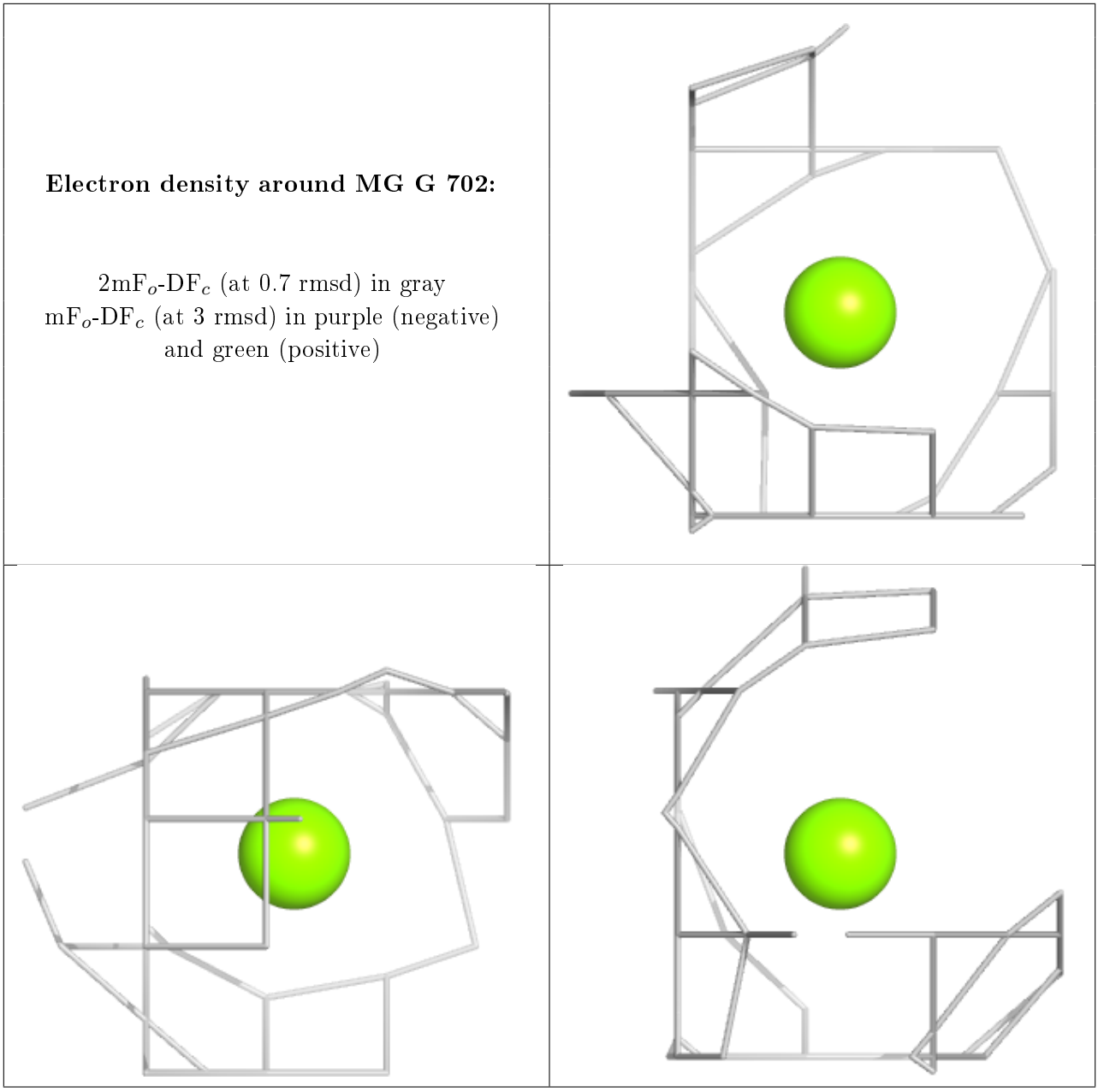






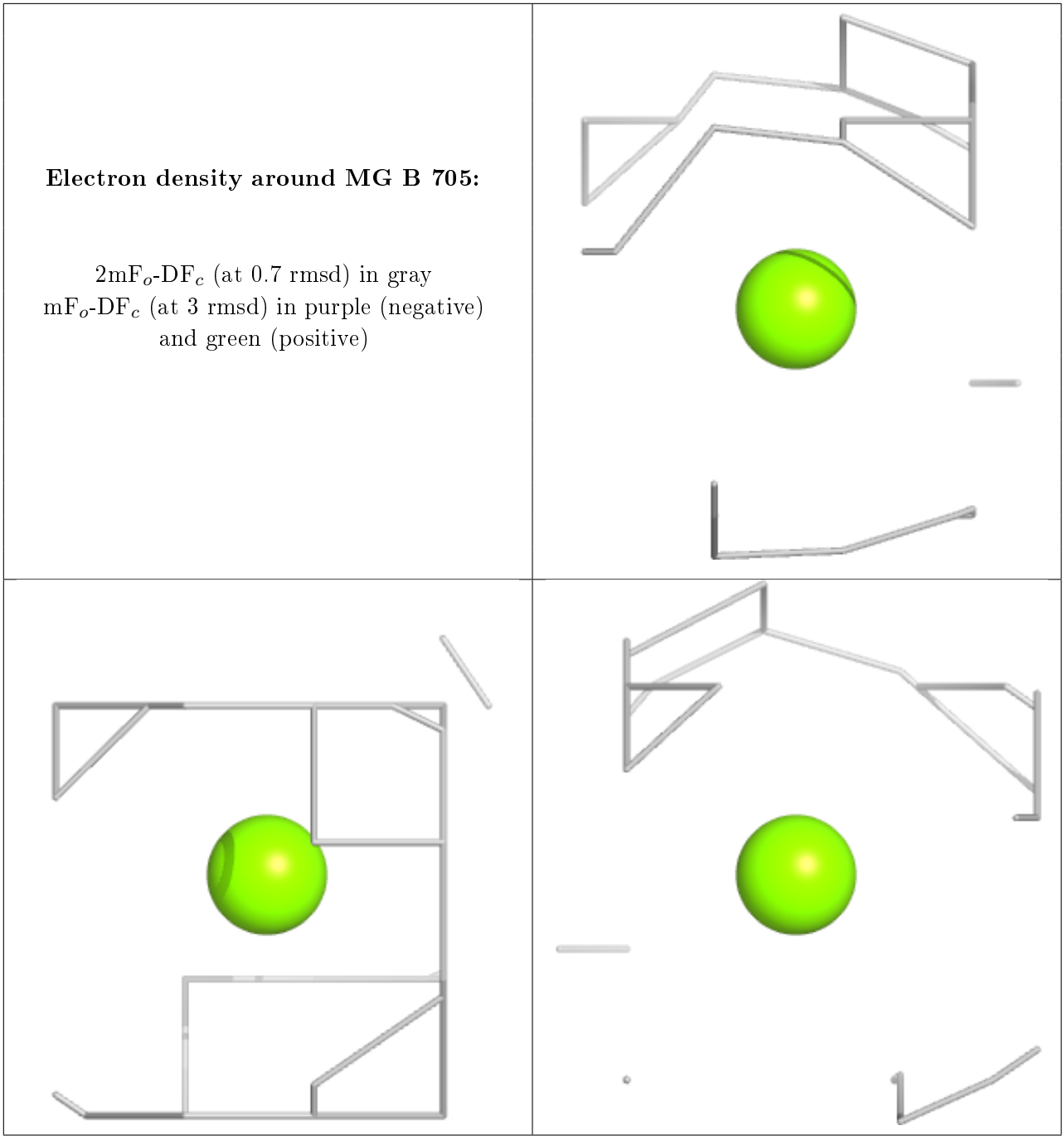
Electron density around MG G 702:

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



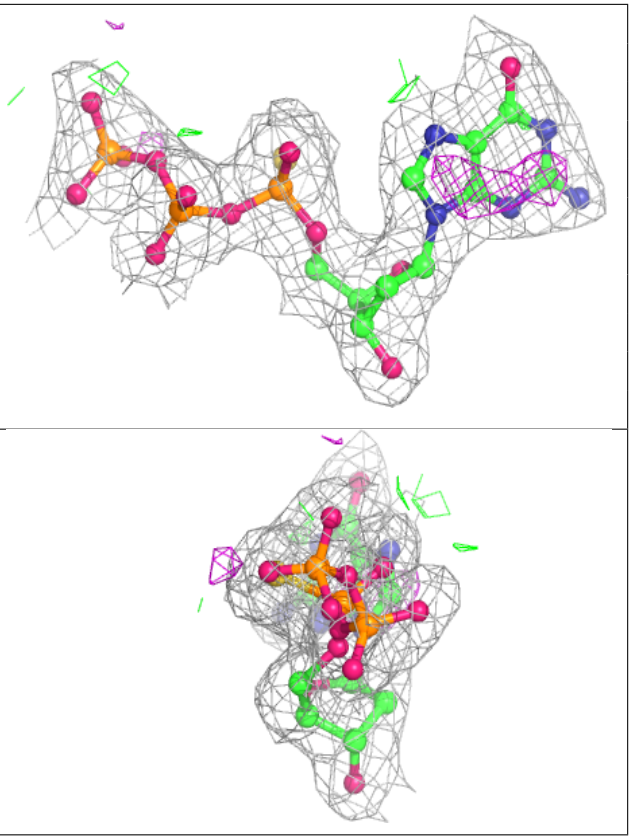
Electron density around MG B 705:

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



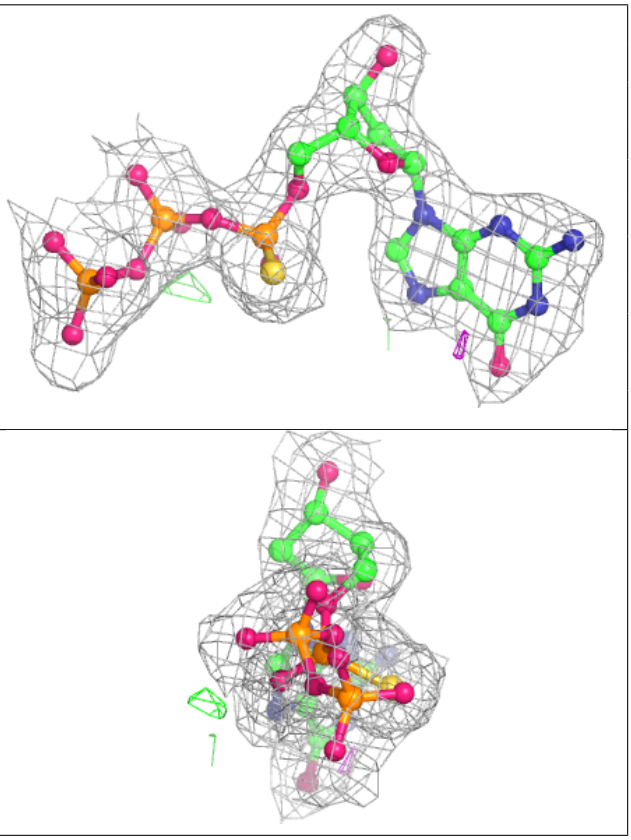
Electron density around T8T F 702:

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



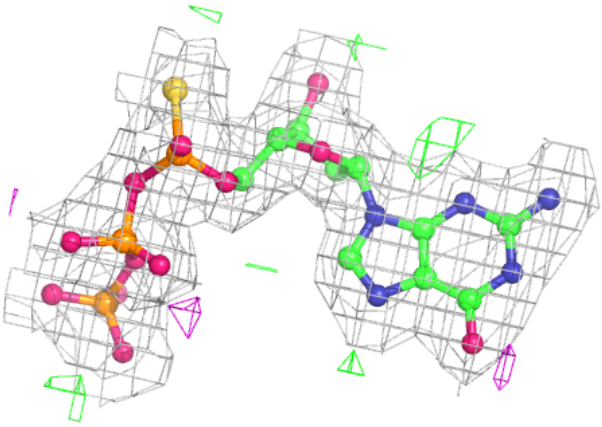
Electron density around T8T F 709:

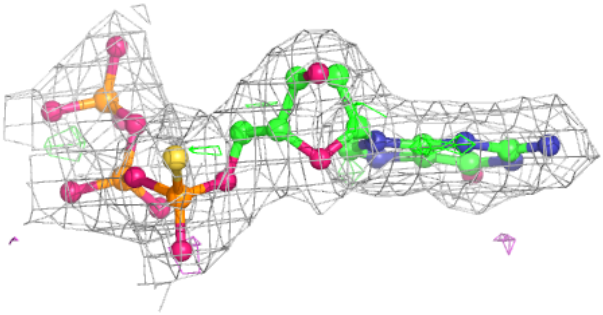
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around T8T A 704:

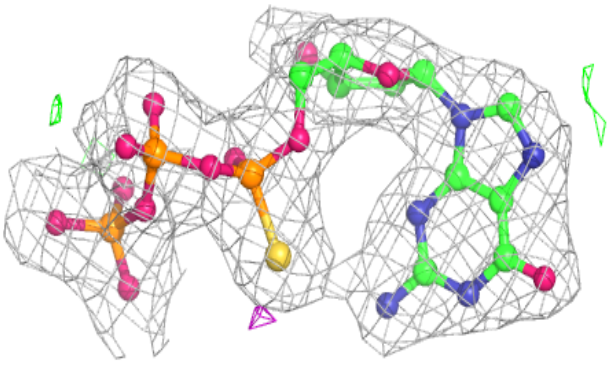
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

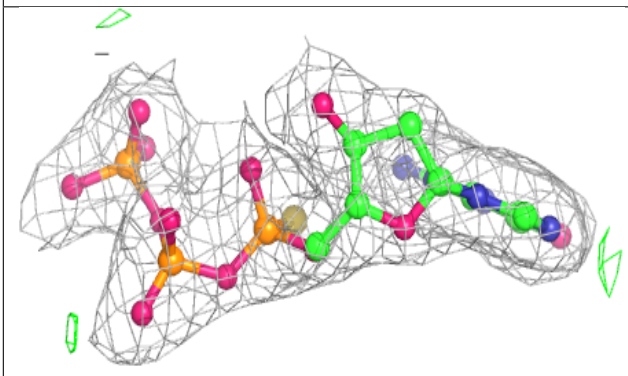


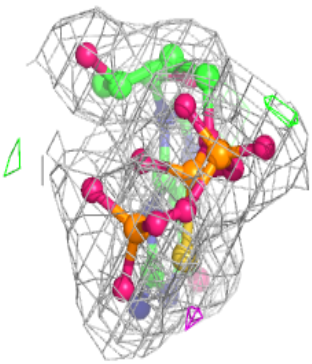


Electron density around T8T A 706:

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

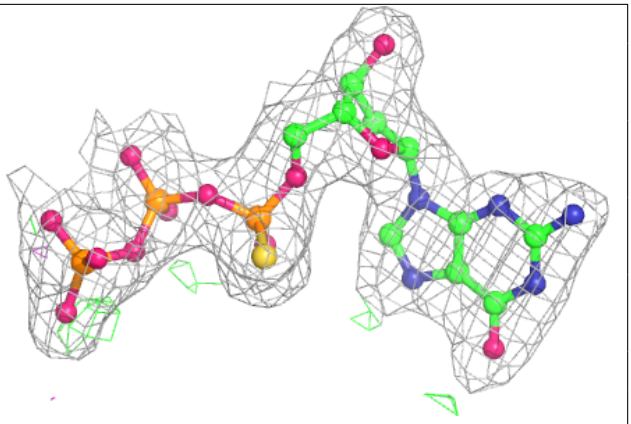


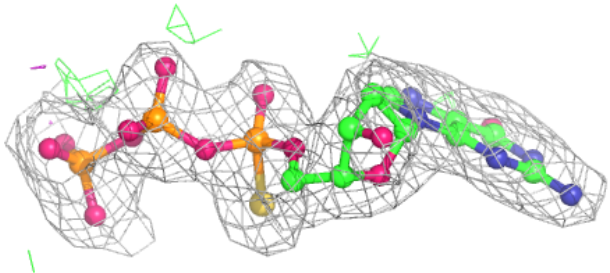




Electron density around T8T A 708:

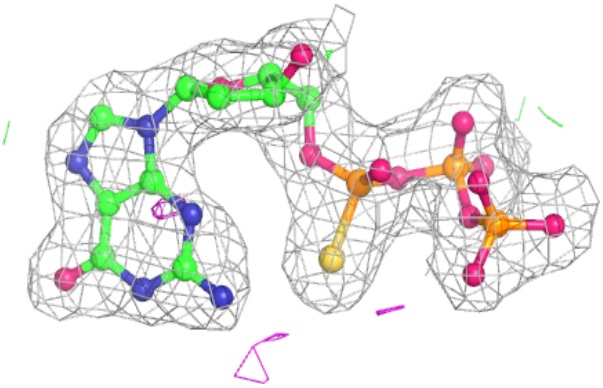
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

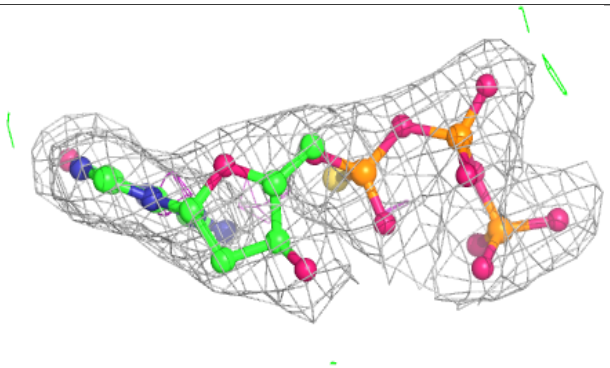


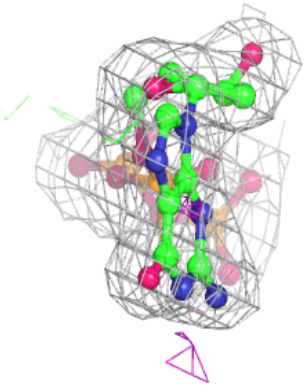


Electron density around T8T B 701:

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

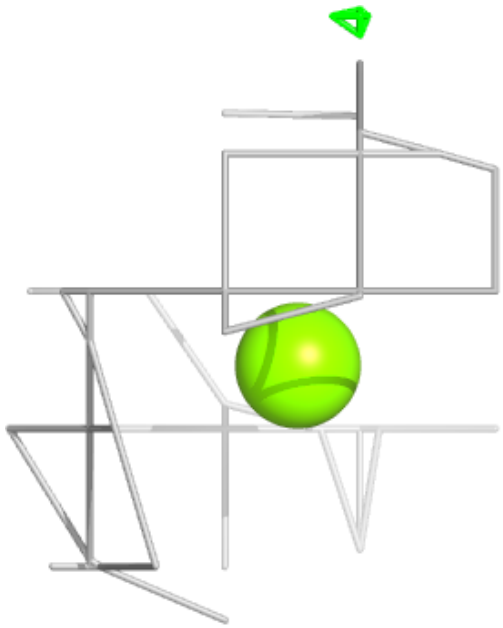


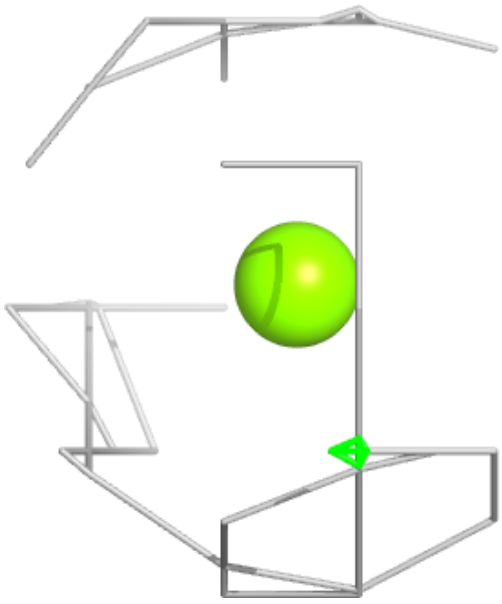


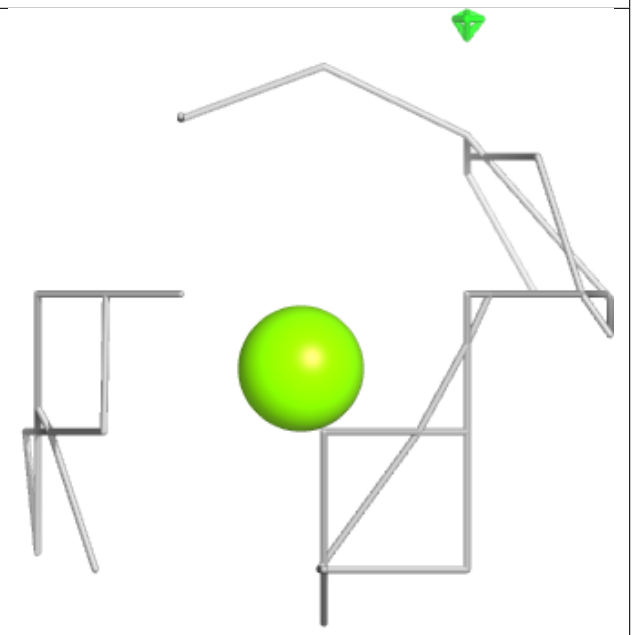


Electron density around MG F 706:

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

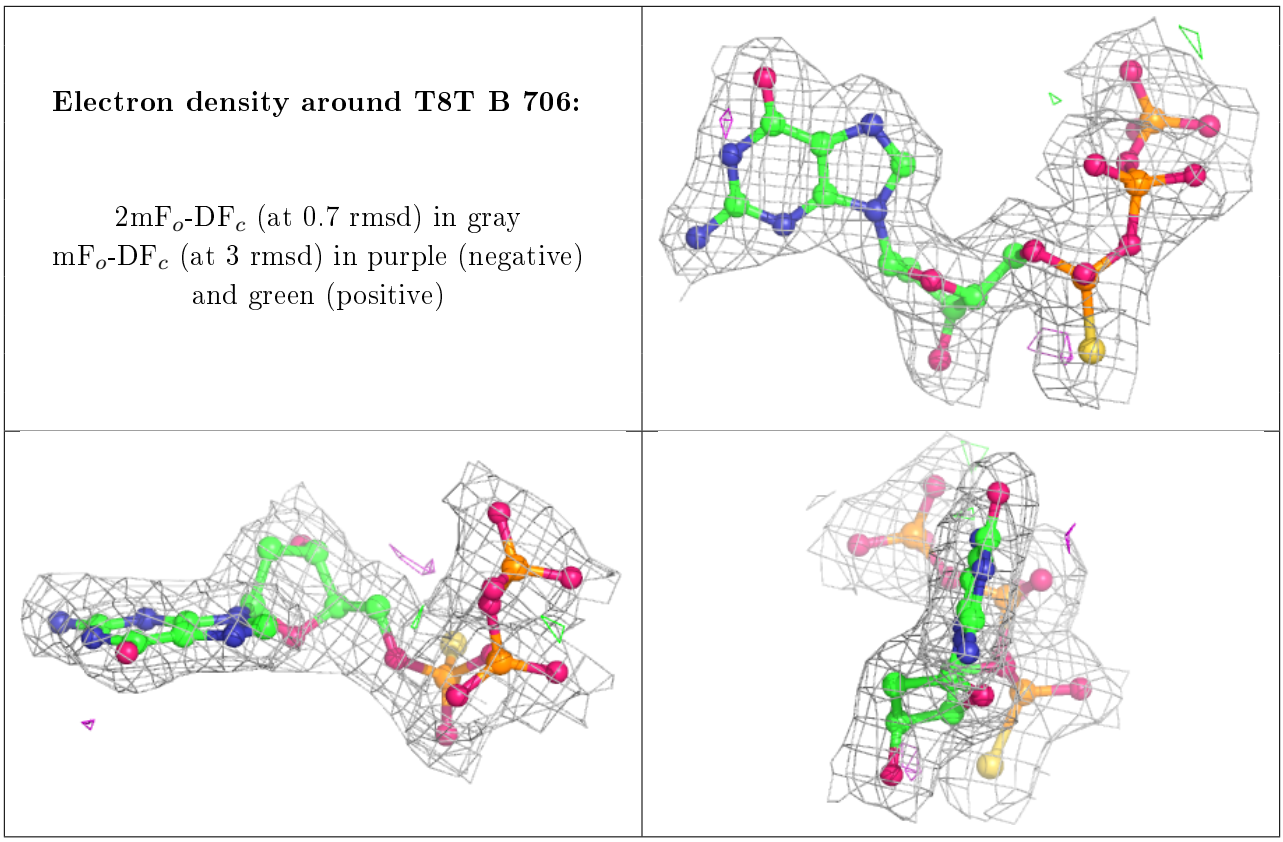






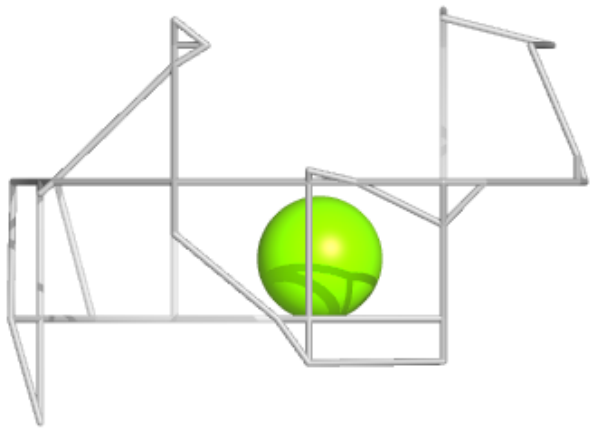
Electron density around T8T B 706:

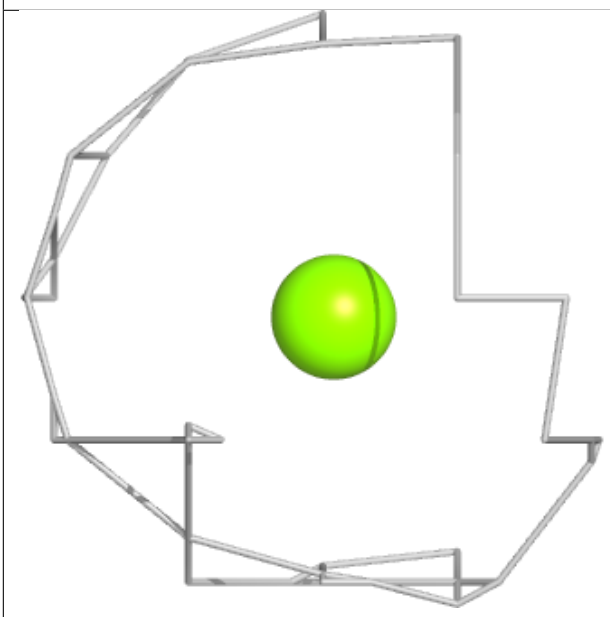
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

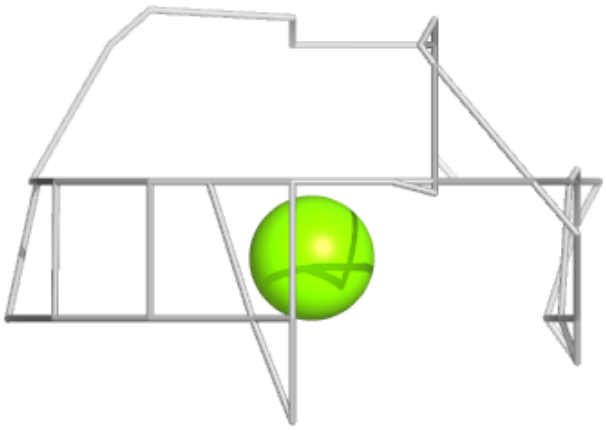


Electron density around MG C 701:

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

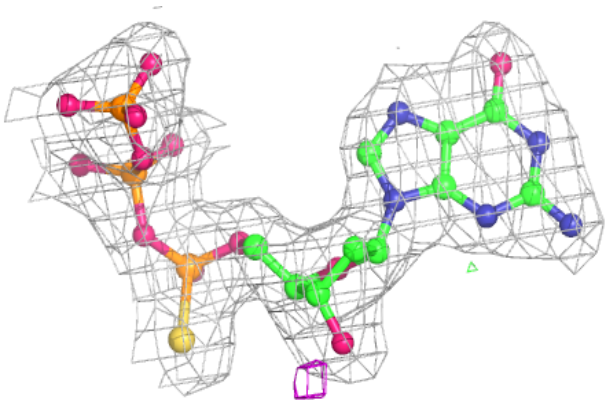


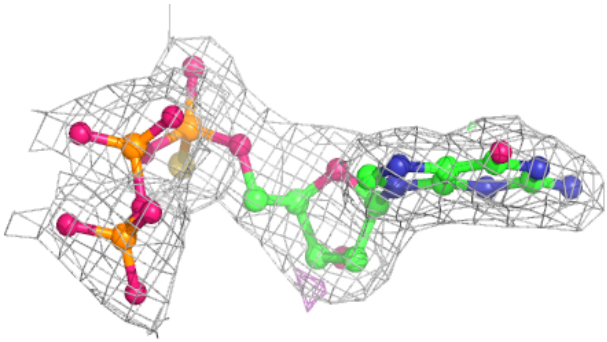


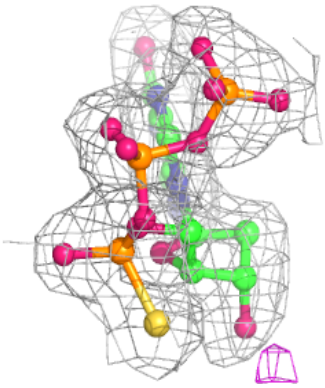


Electron density around T8T C 705:

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

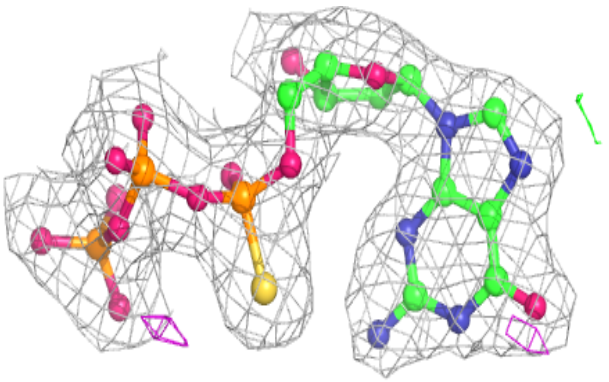


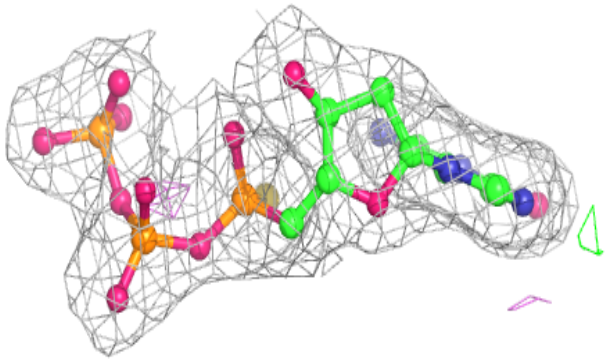


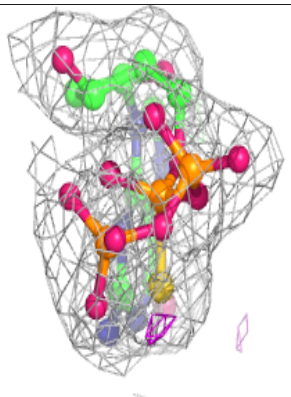


Electron density around T8T C 706:

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

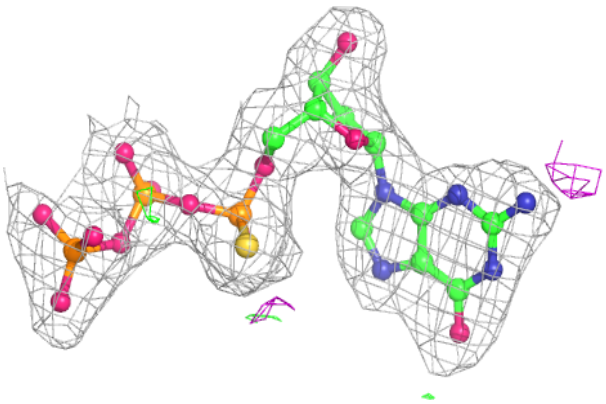


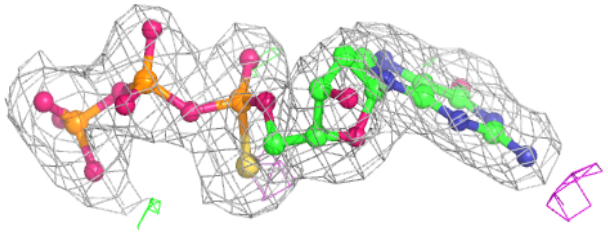


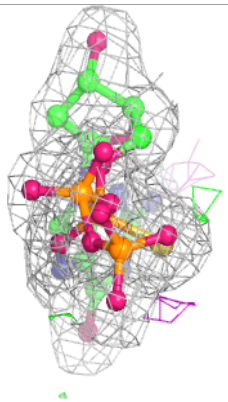


Electron density around T8T D 701:

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

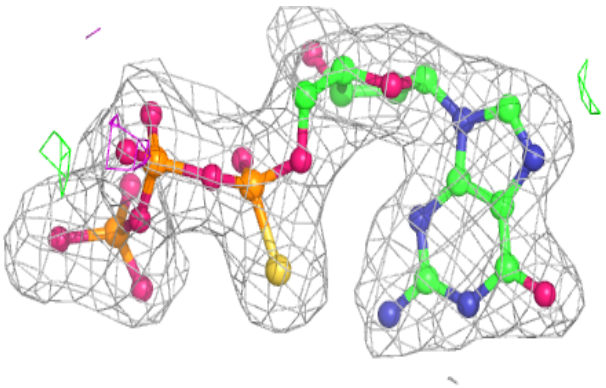


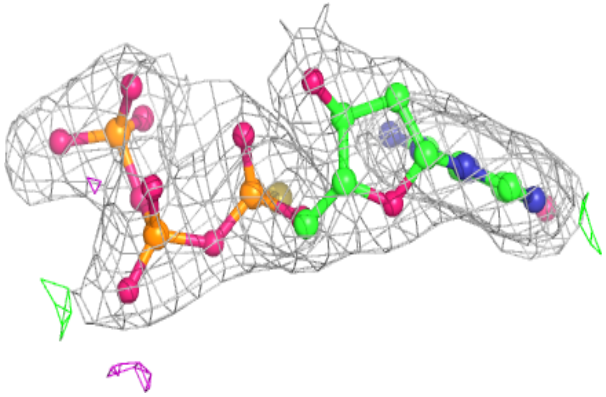


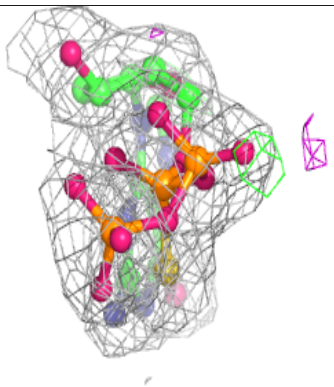


Electron density around T8T D 702:

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

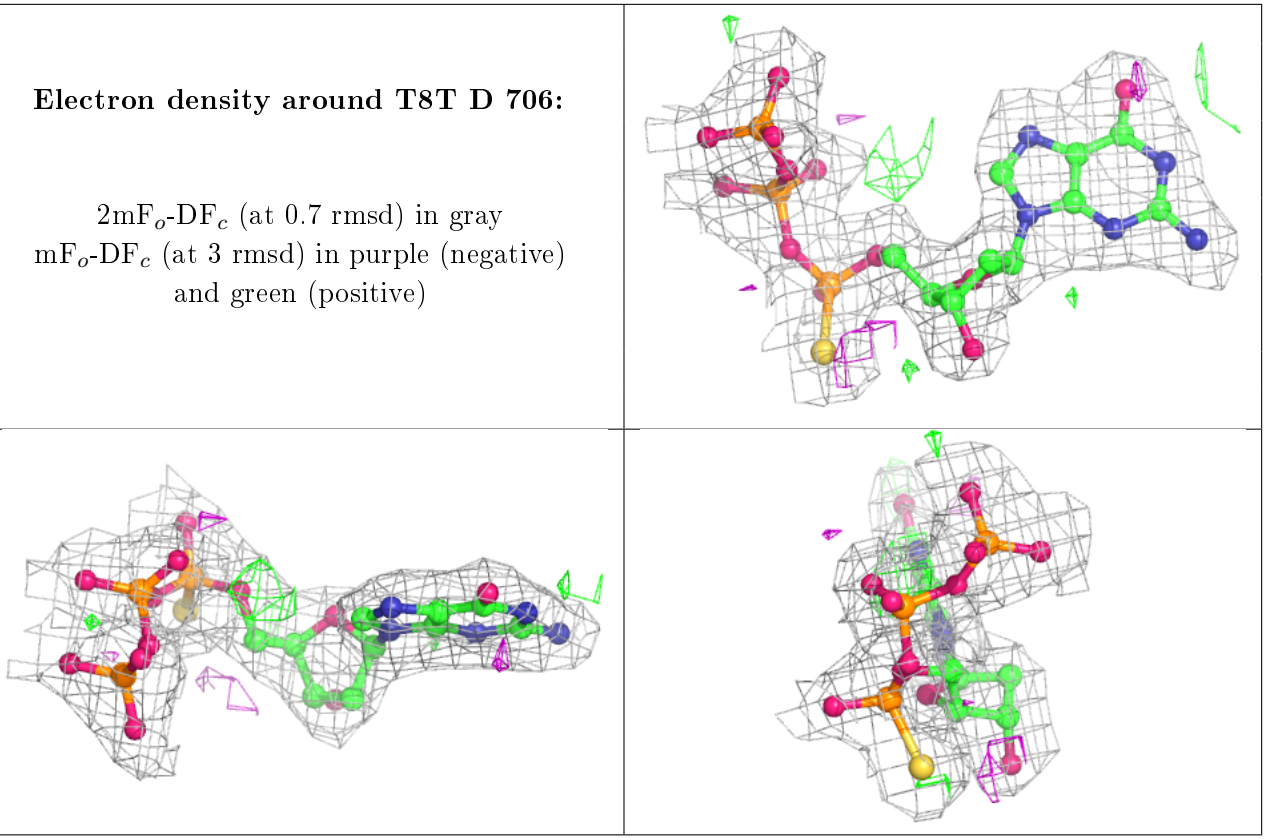






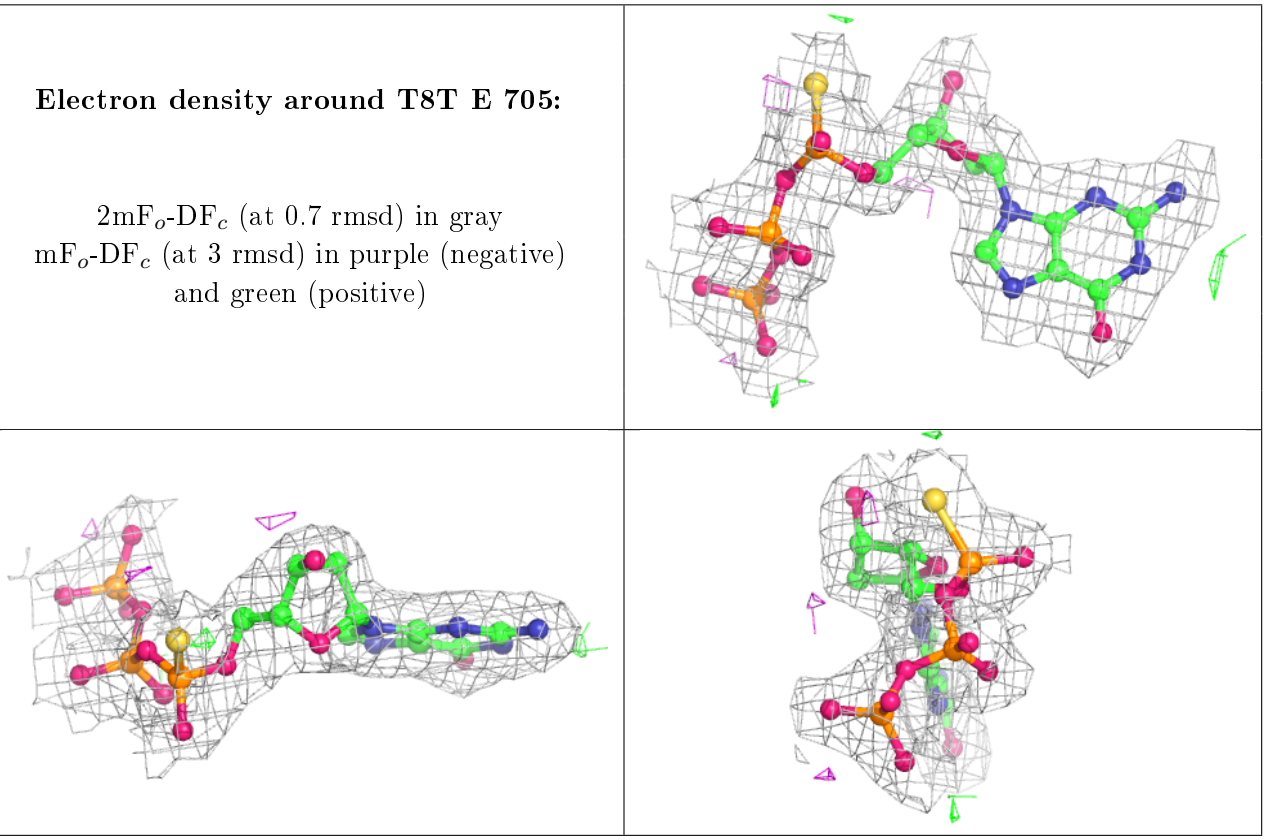
Electron density around T8T D 706:

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



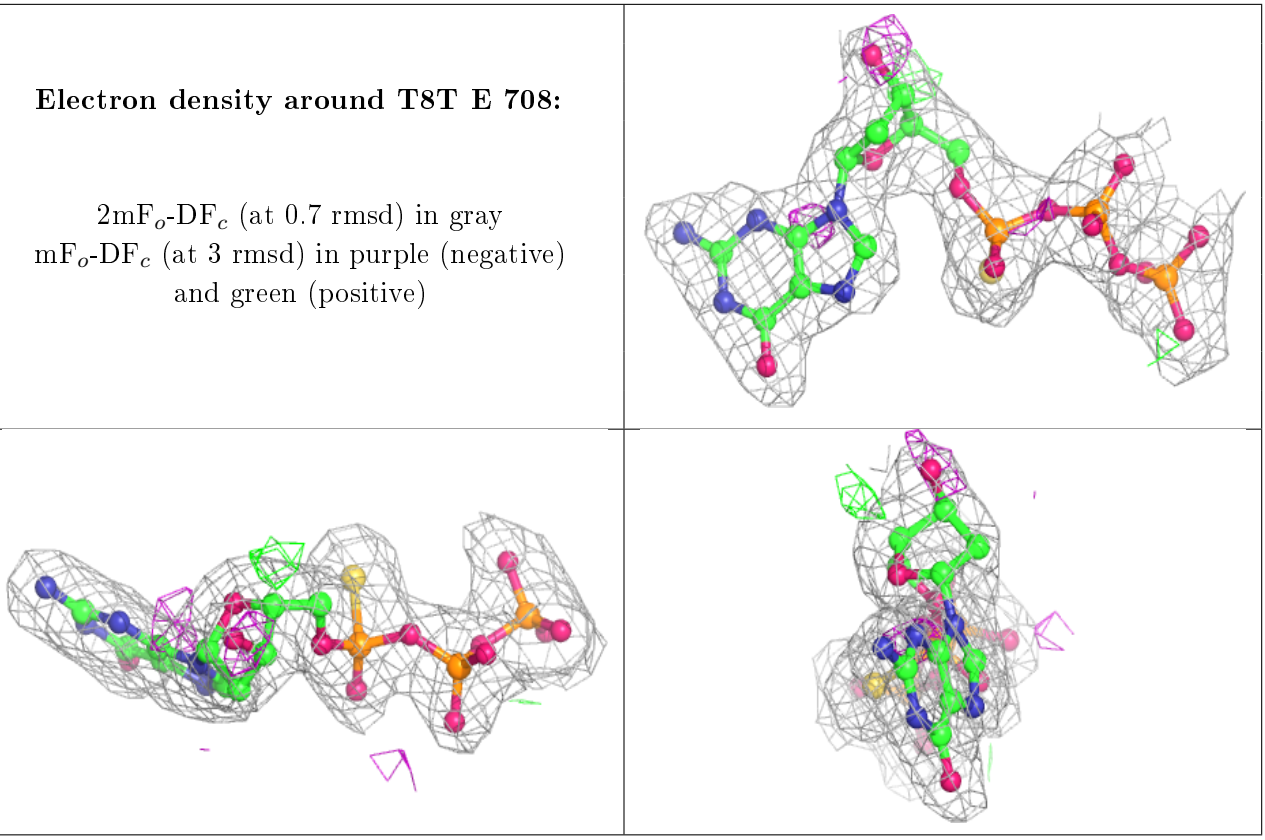
Electron density around T8T E 705:

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



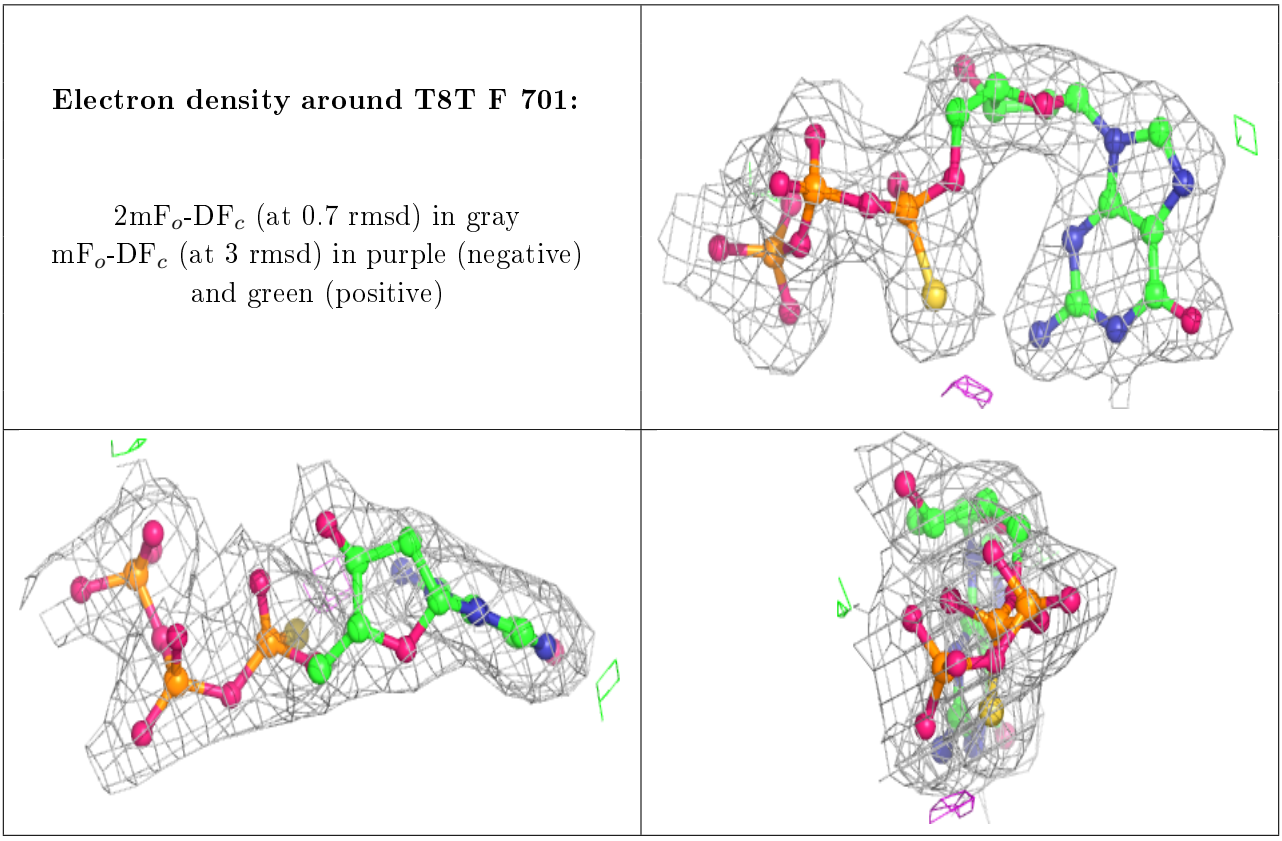
Electron density around T8T E 708:

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



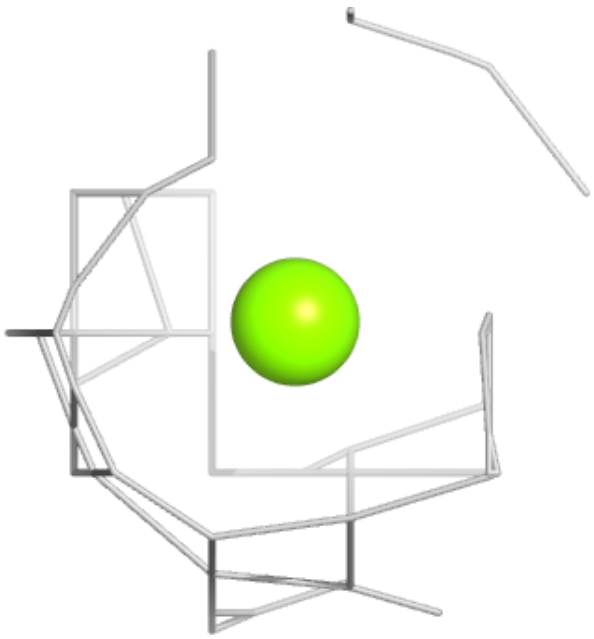
Electron density around T8T F 701:

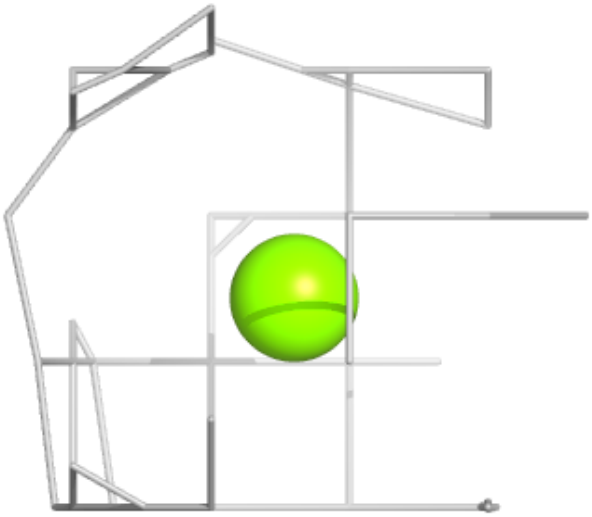
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

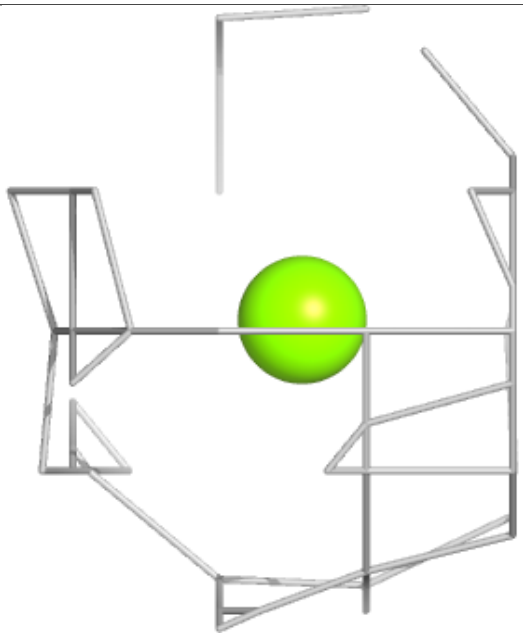


Electron density around MG G 703:

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

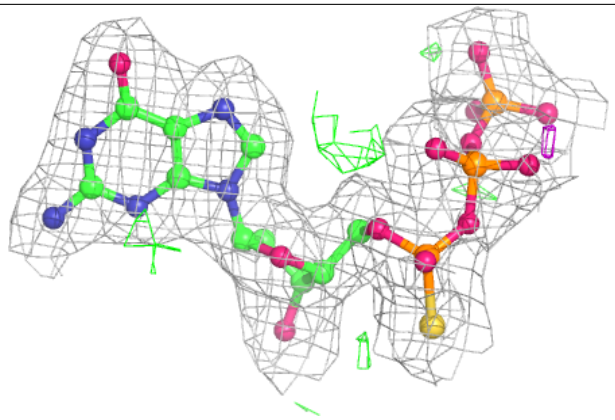


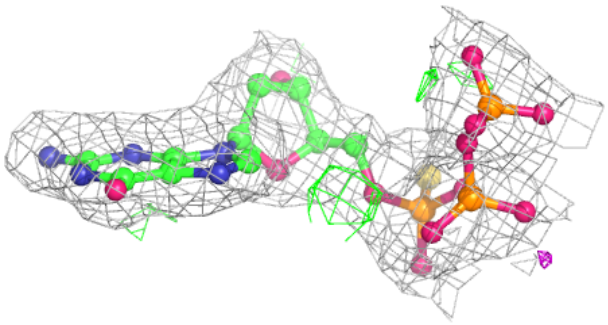


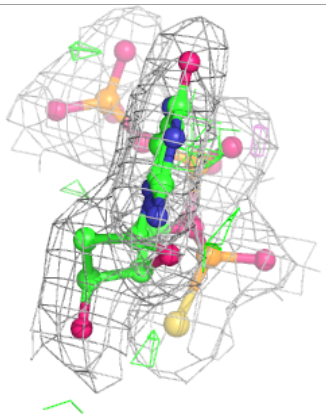


Electron density around T8T F 707:

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

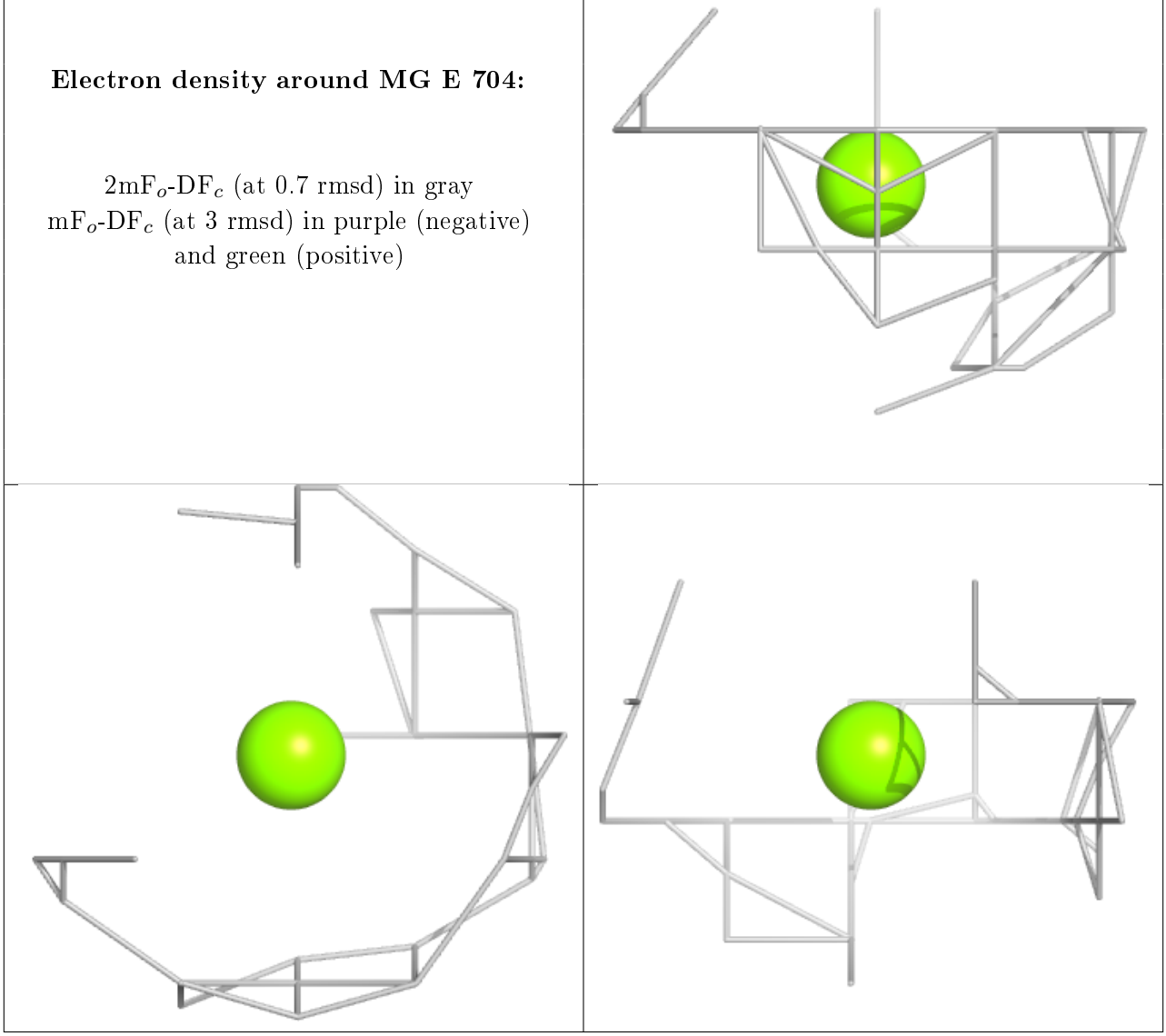






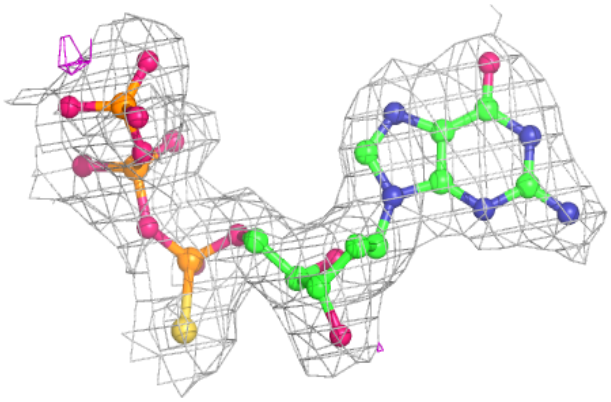
Electron density around MG E 704:

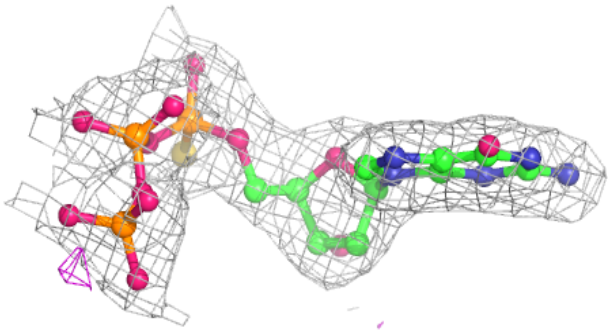
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

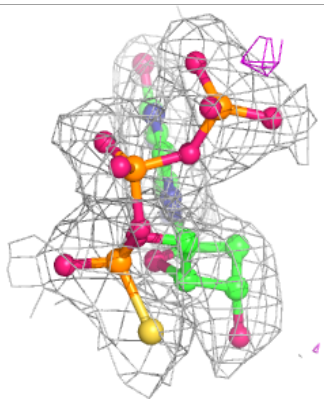


Electron density around T8T G 704:

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

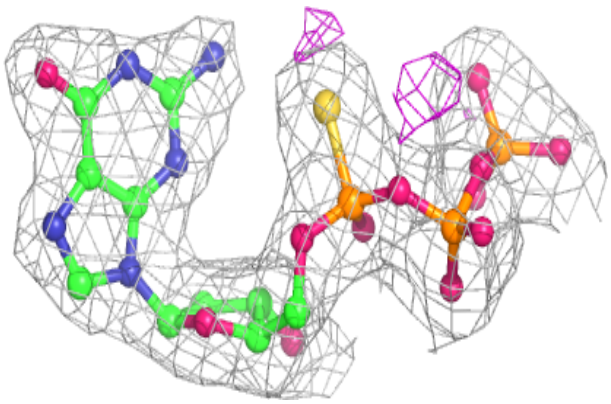


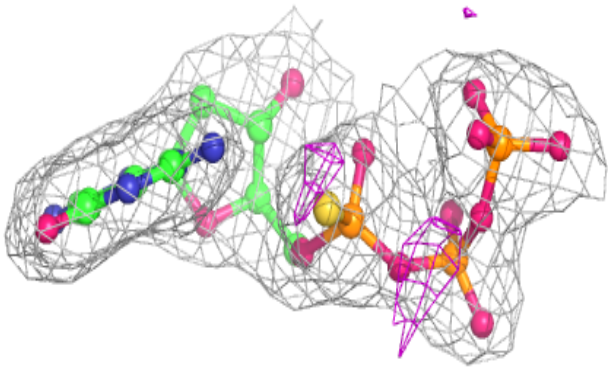


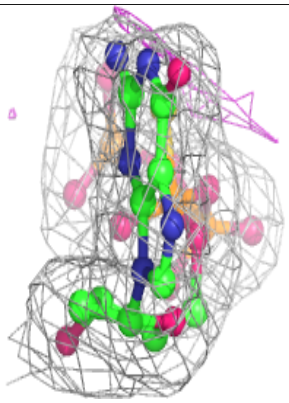


Electron density around T8T G 705:

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

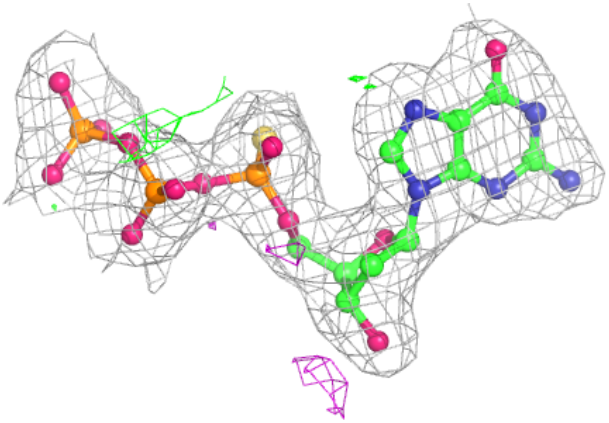


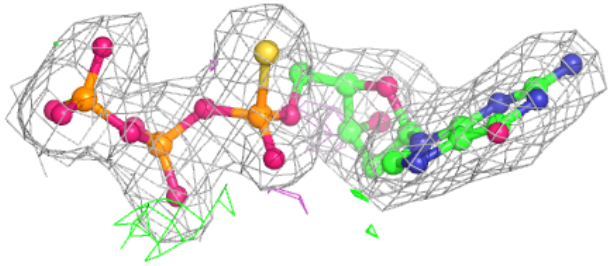


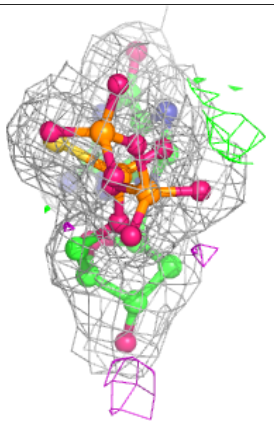


Electron density around T8T H 701:

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

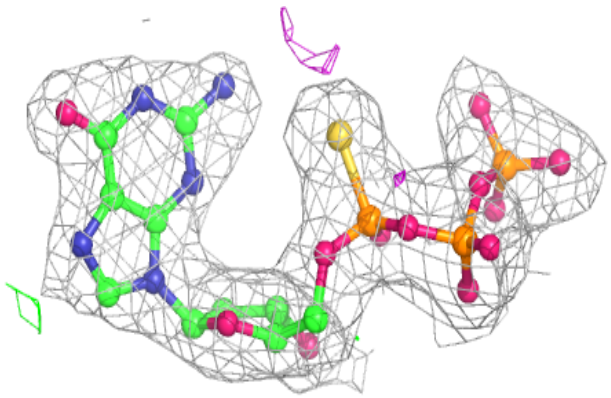


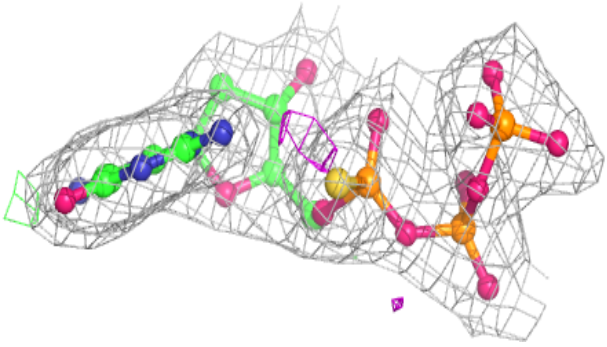


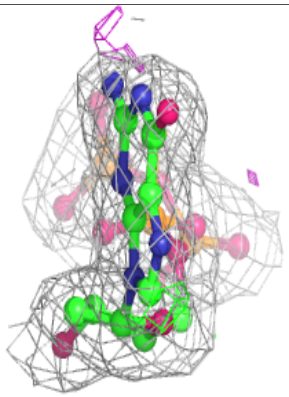


Electron density around T8T H 702:

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

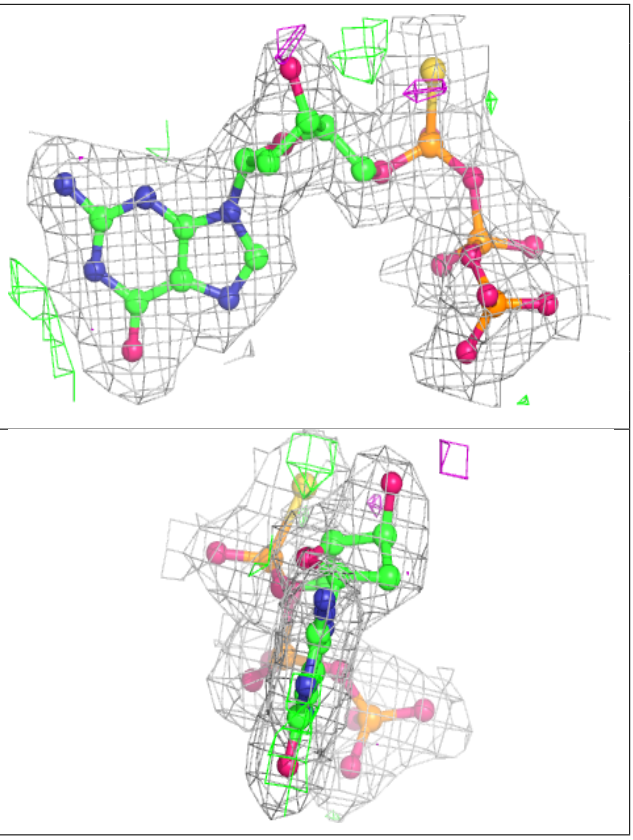






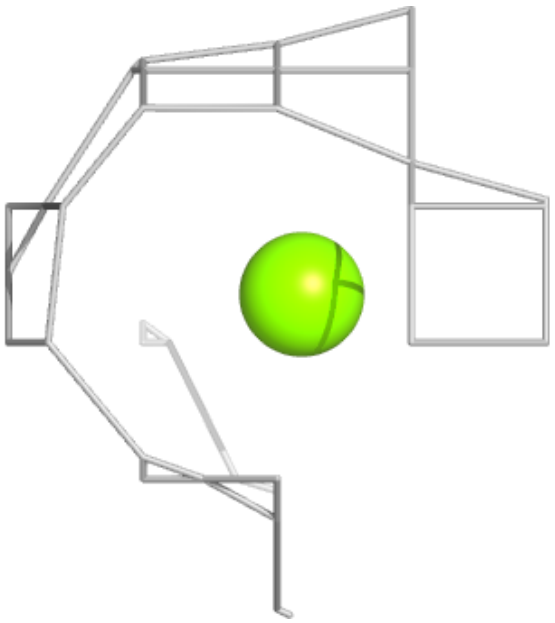
Electron density around T8T H 706:

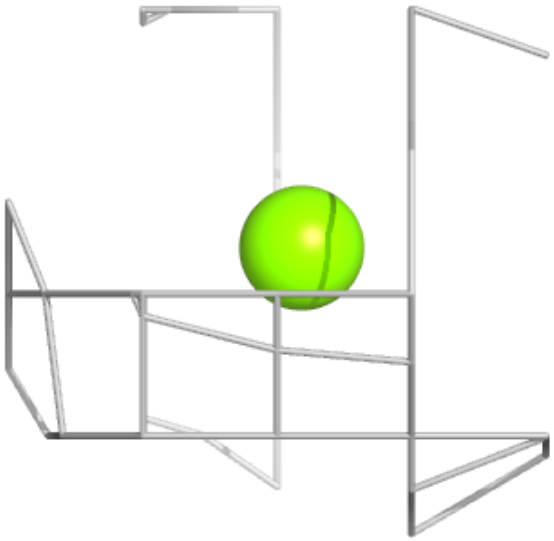
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

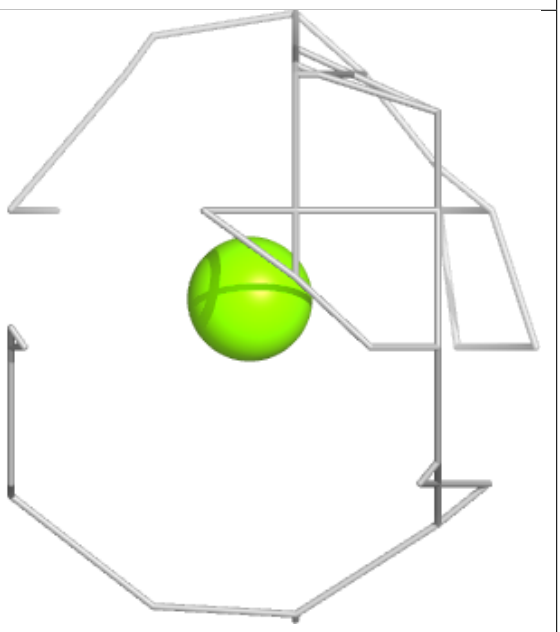


Electron density around MG C 704:

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

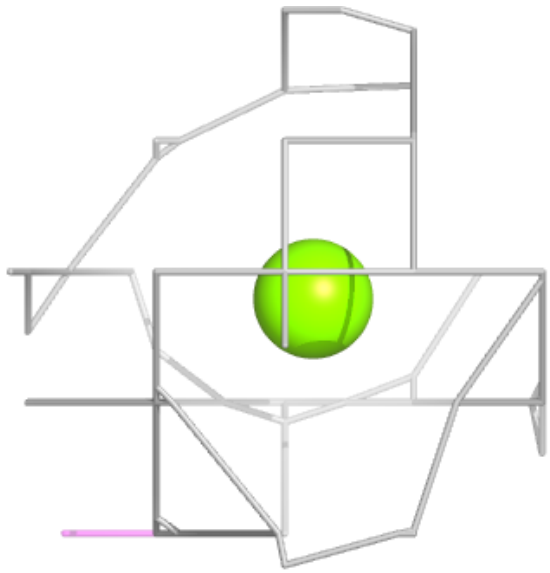


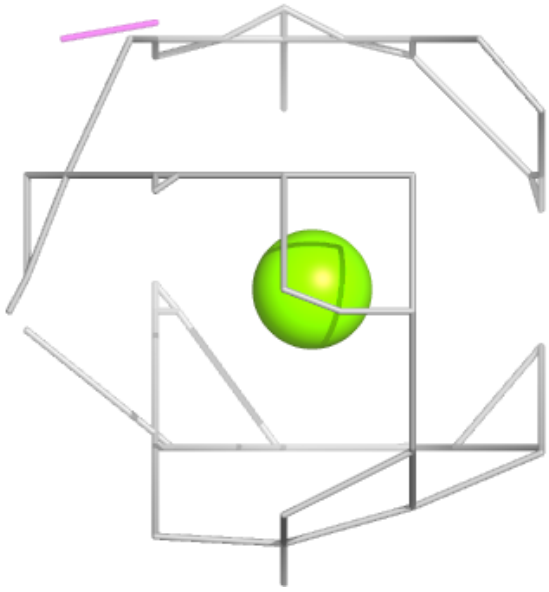


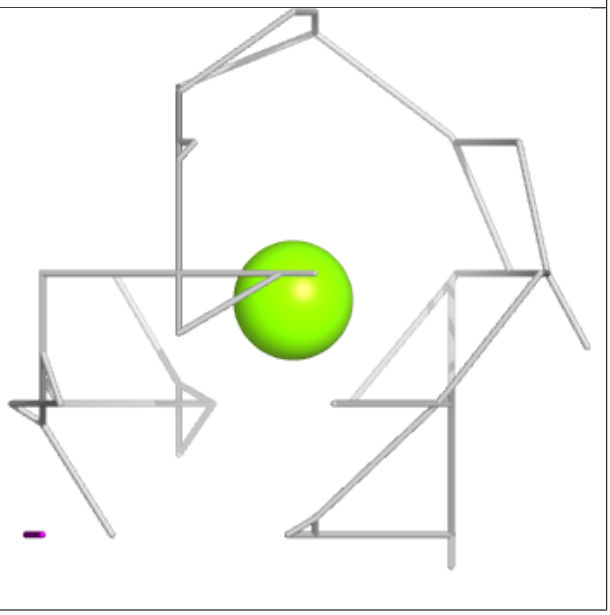


Electron density around MG H 704:

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

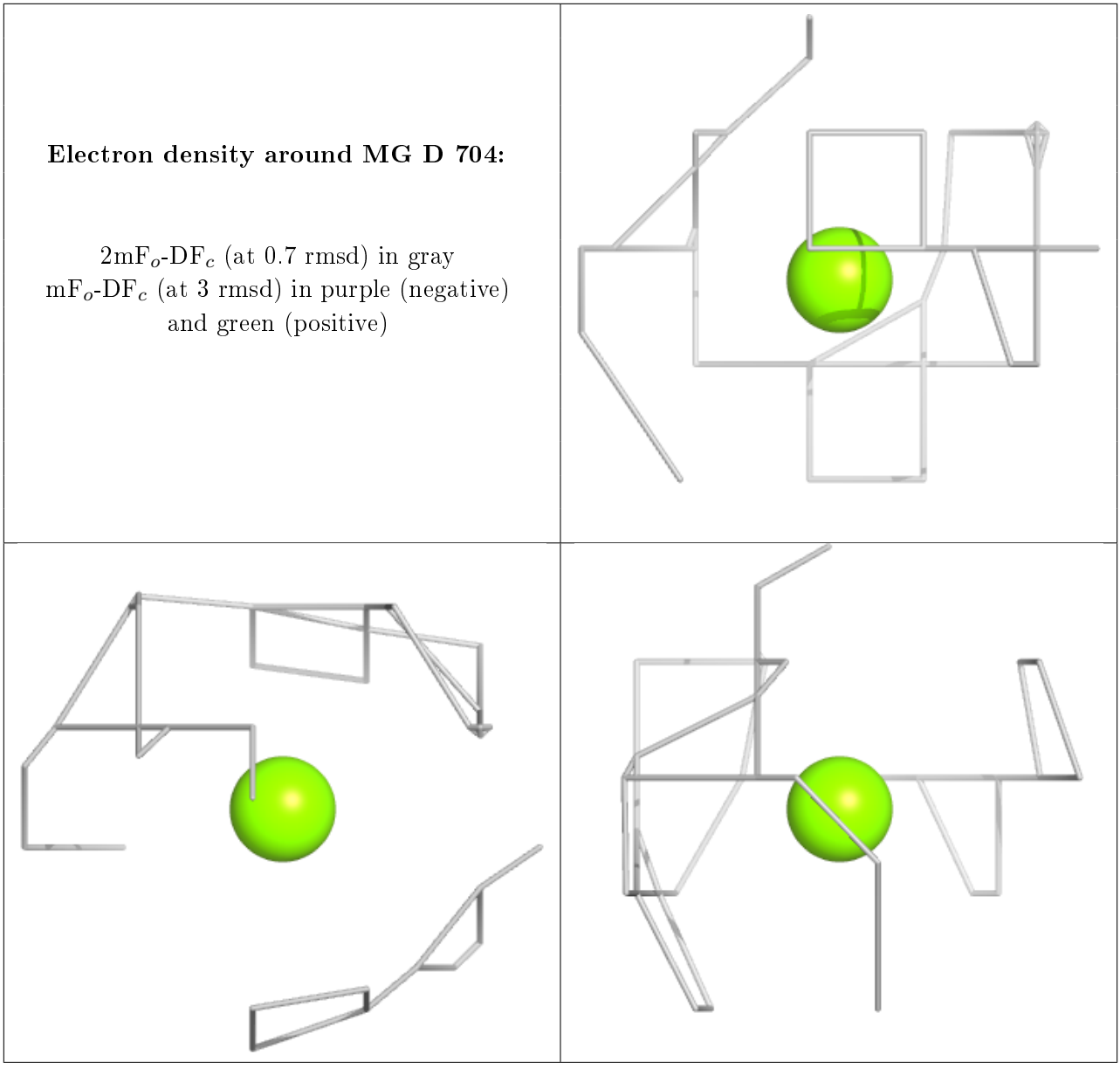






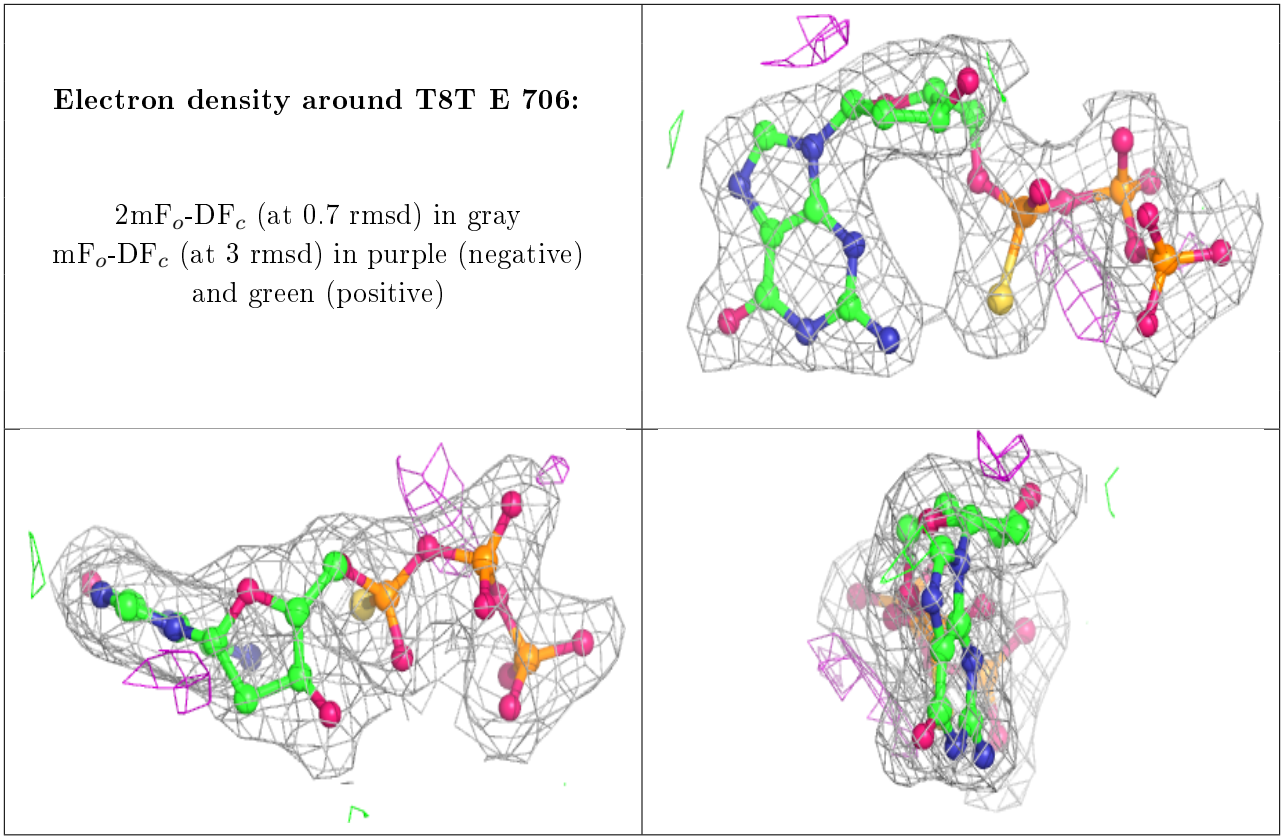
Electron density around MG D 704:

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



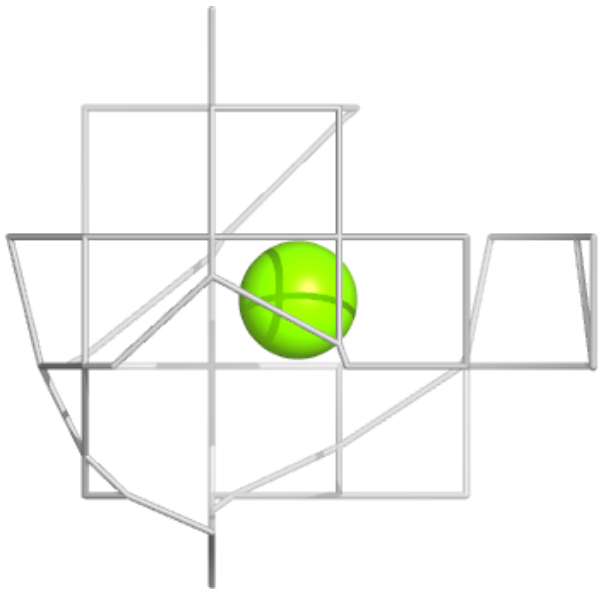
Electron density around T8T E 706:

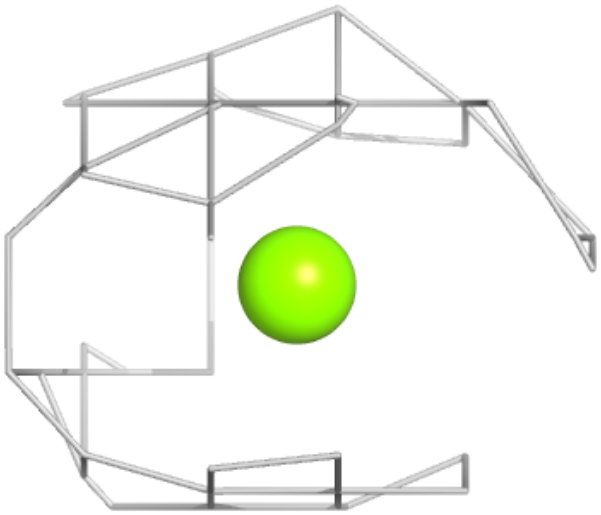
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

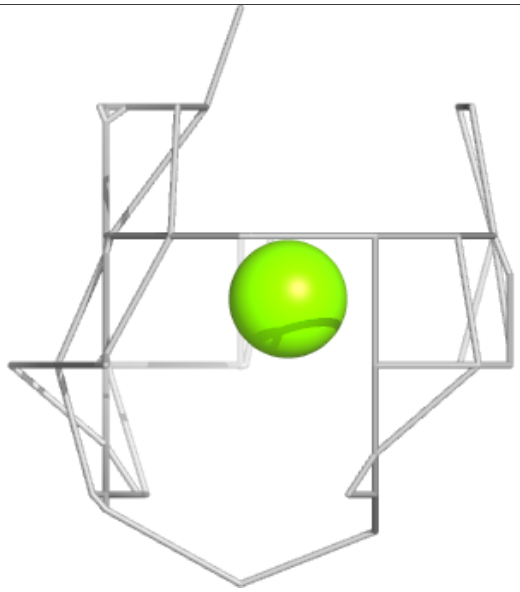


Electron density around MG A 707:

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

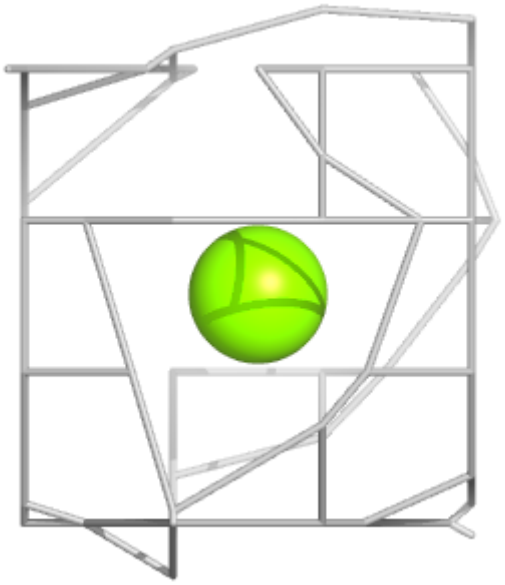


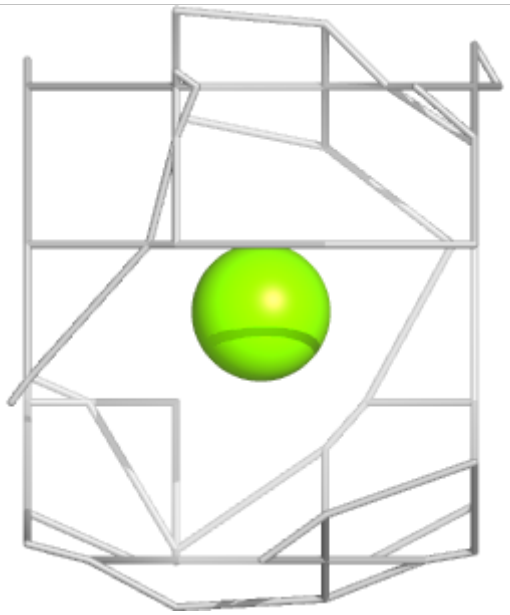


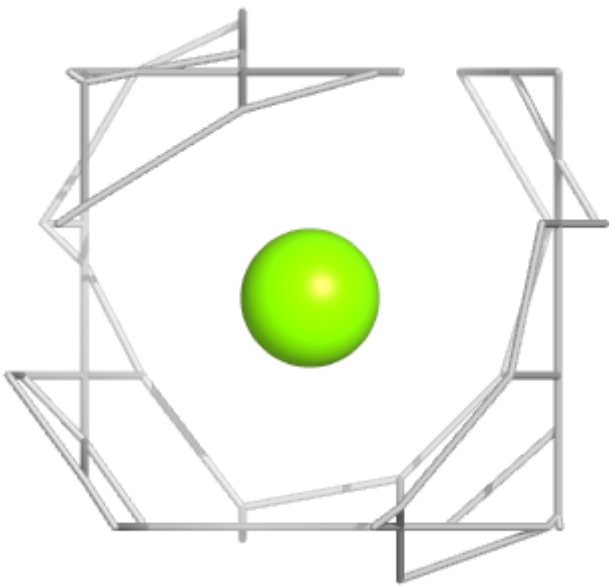


Electron density around MG E 702:

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

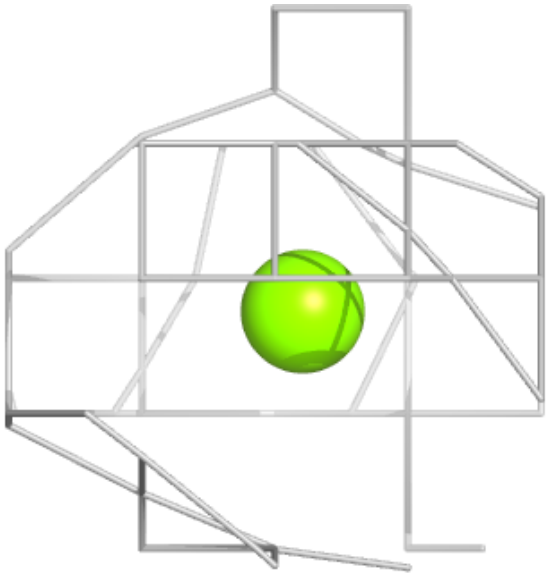


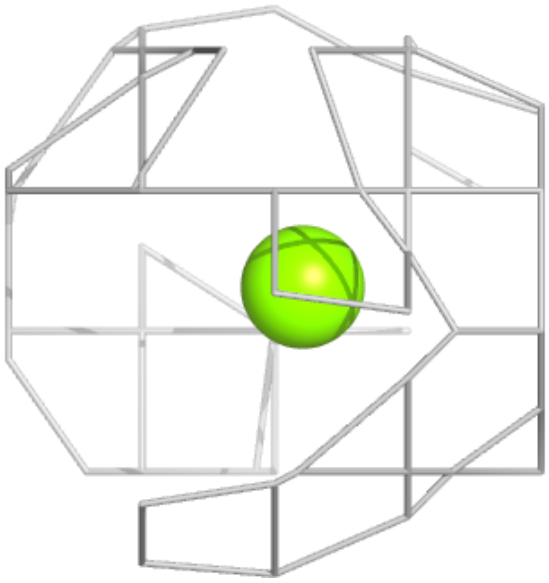


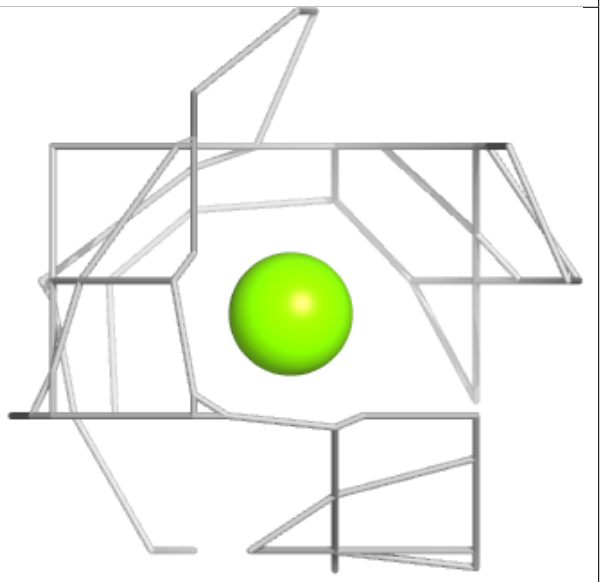


Electron density around MG A 702:

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

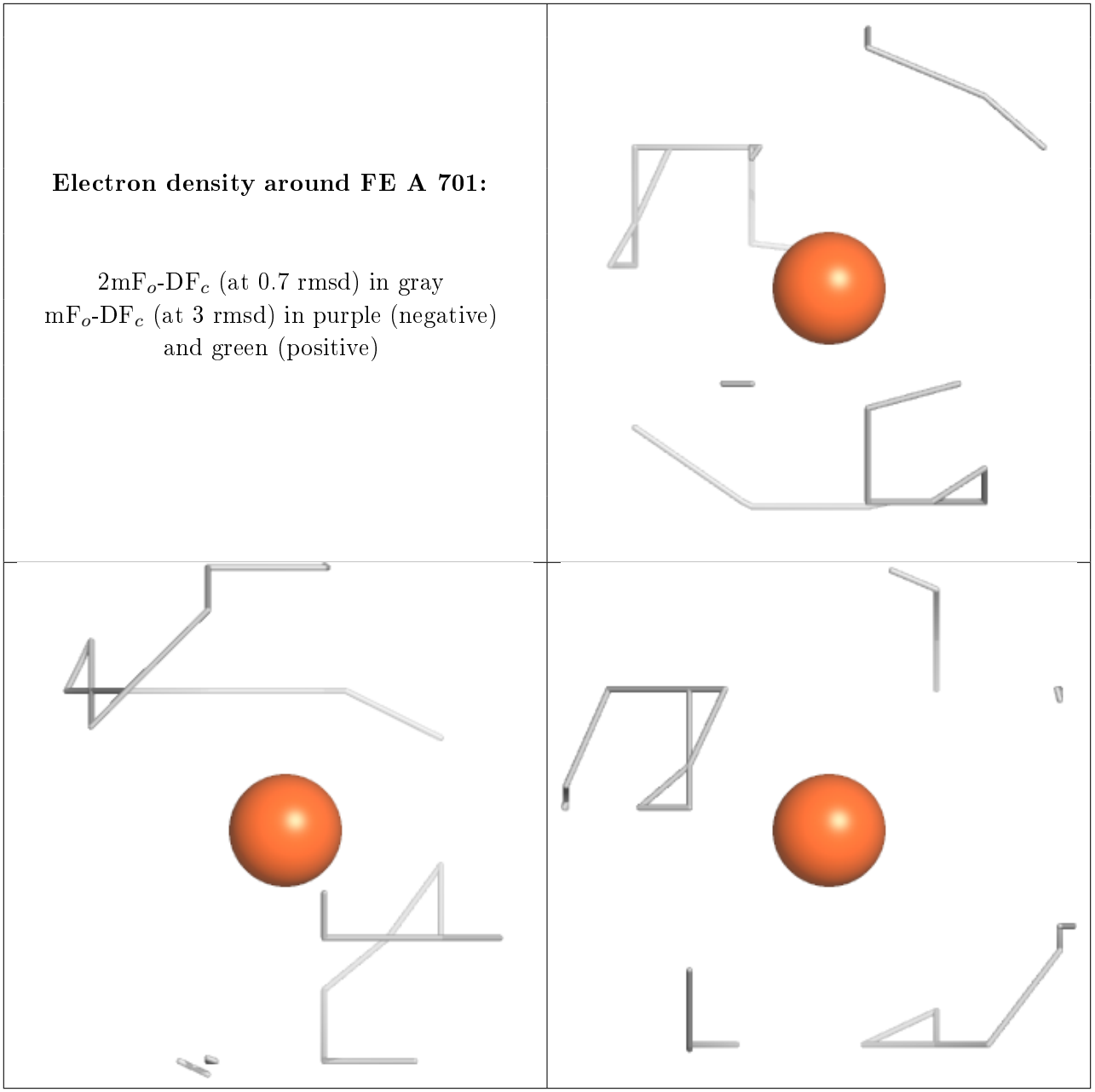






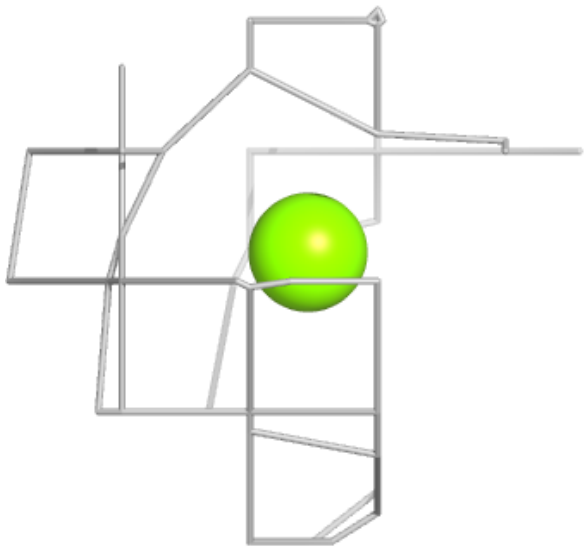
Electron density around FE A 701:

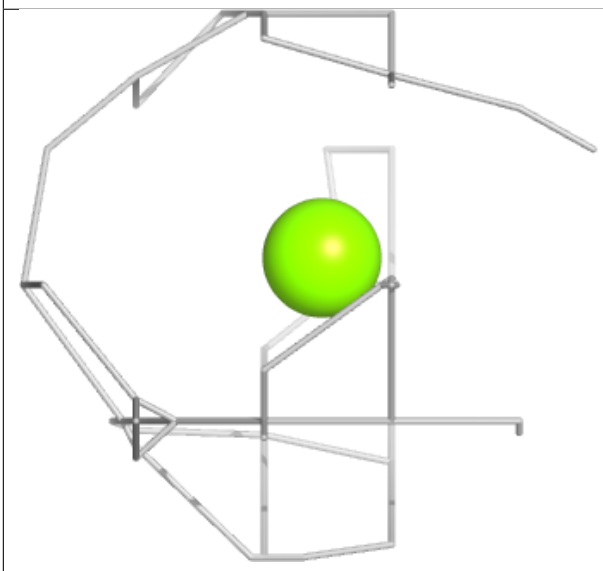
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

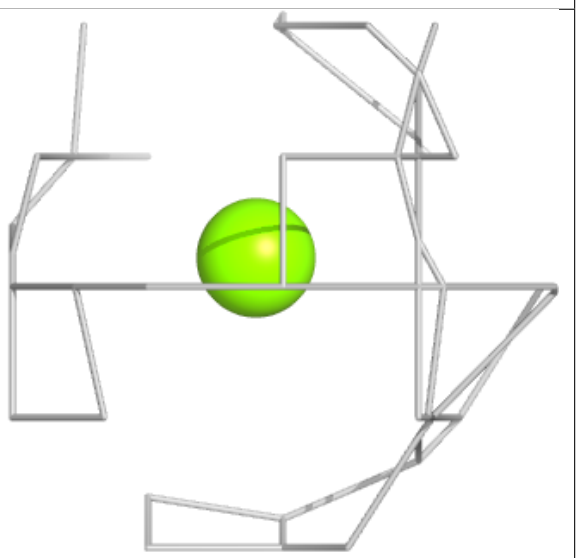


Electron density around MG E 707:

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

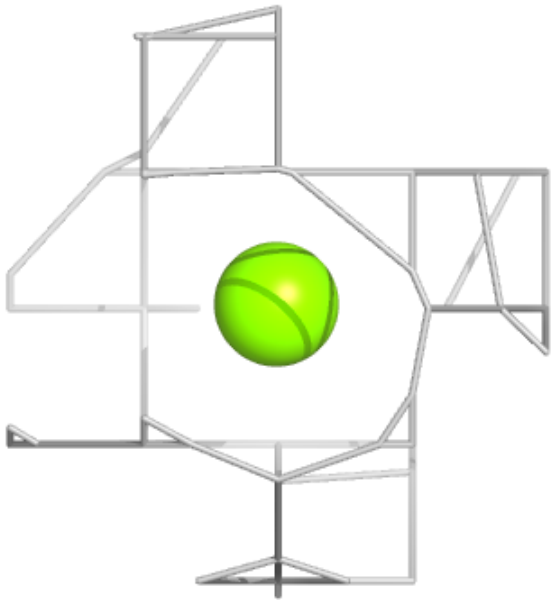


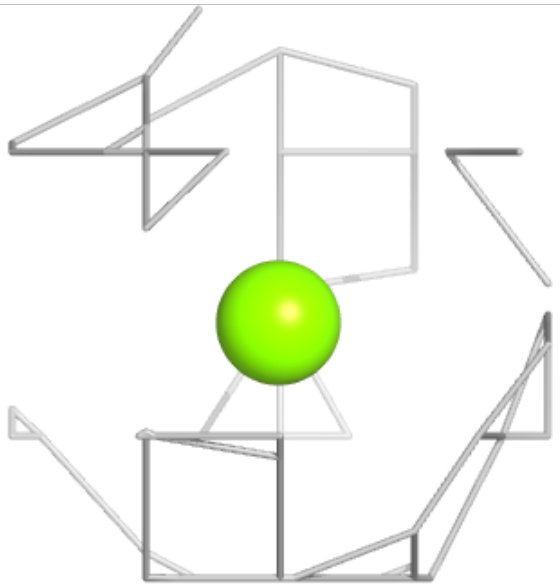


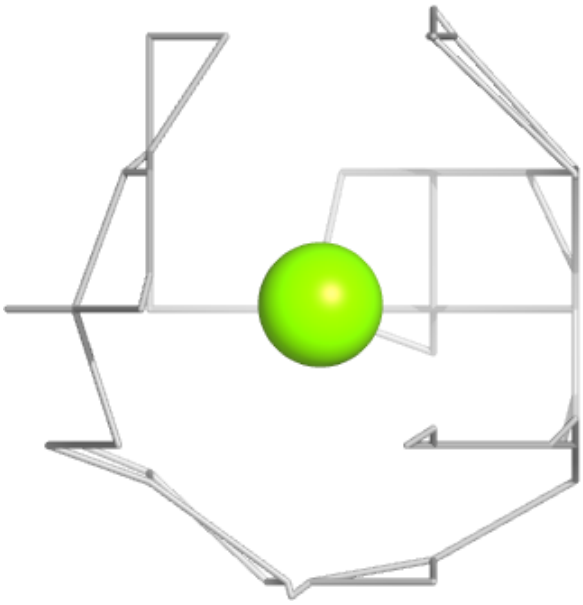


Electron density around MG F 704:

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

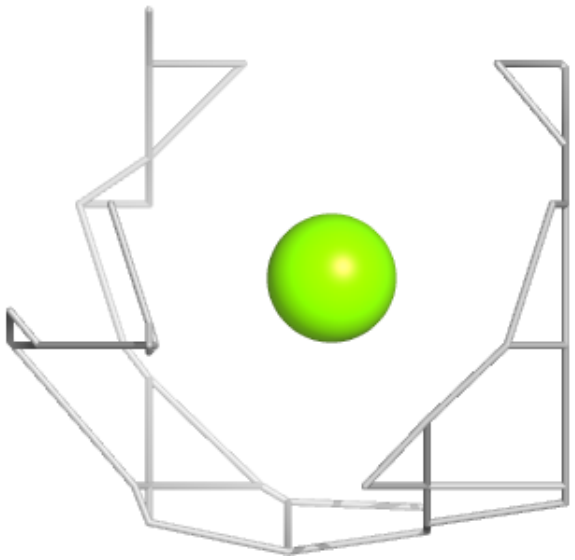


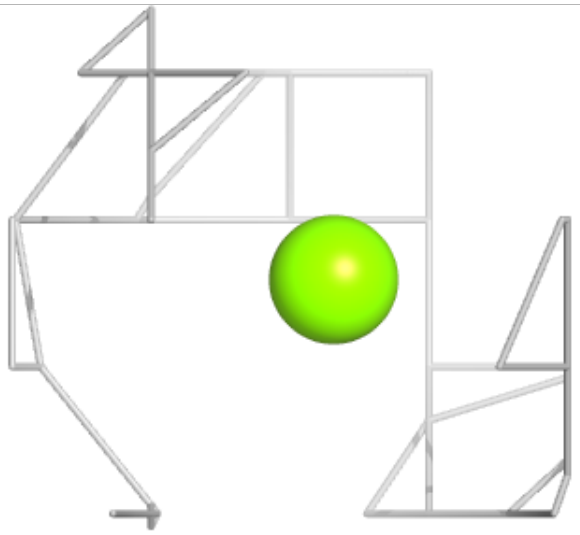


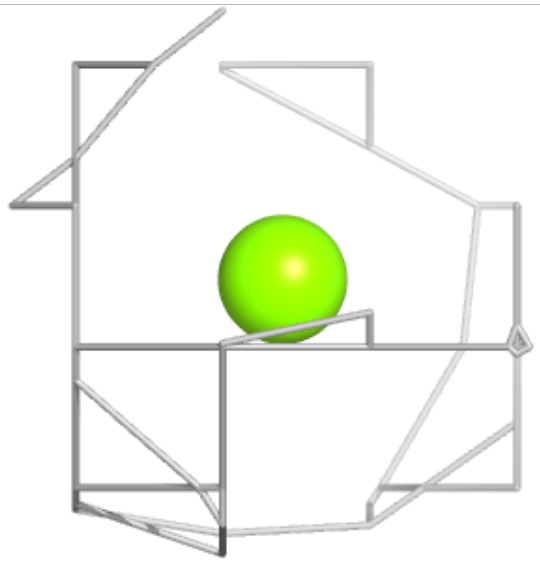


Electron density around MG F 705:

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

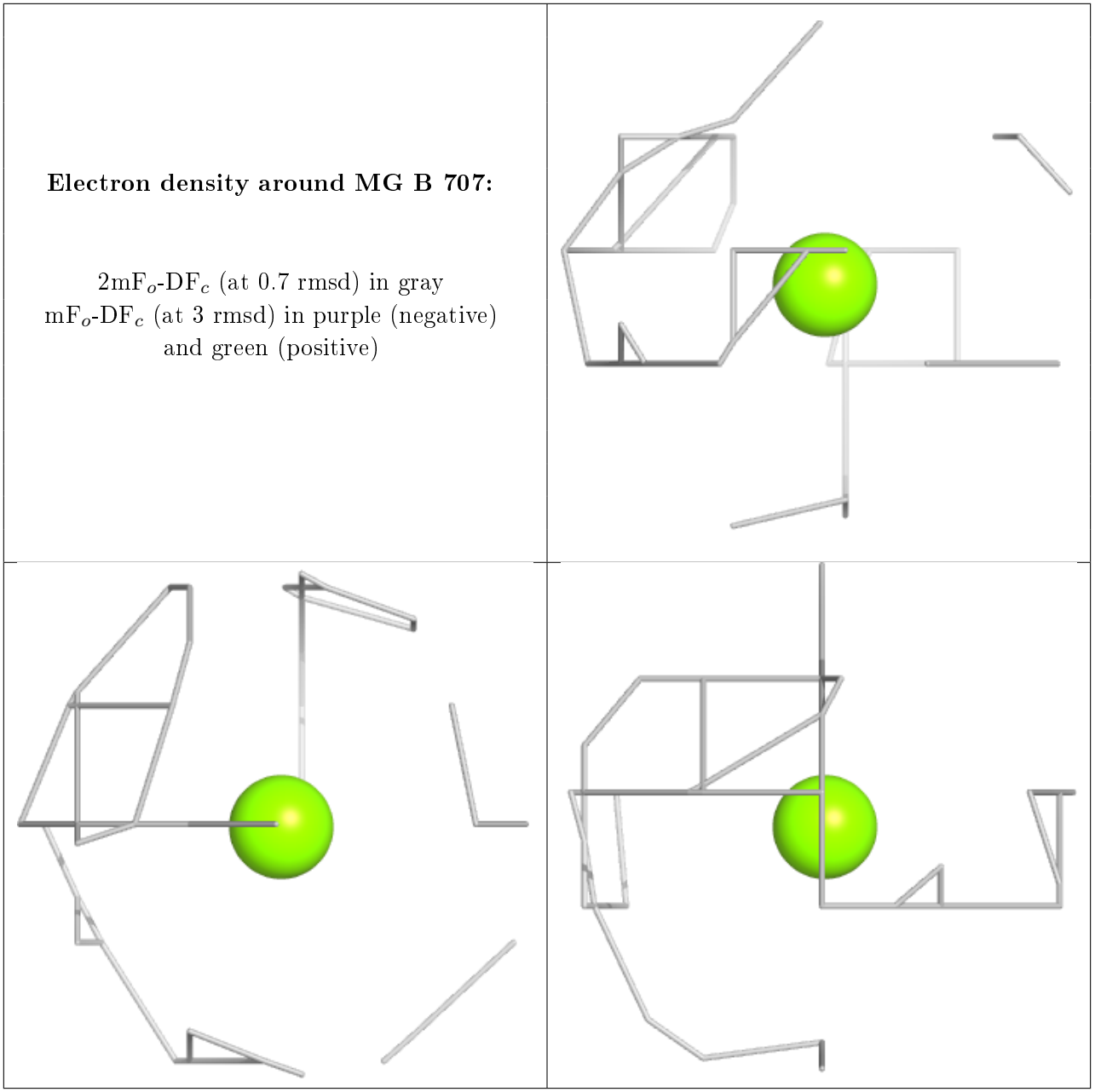






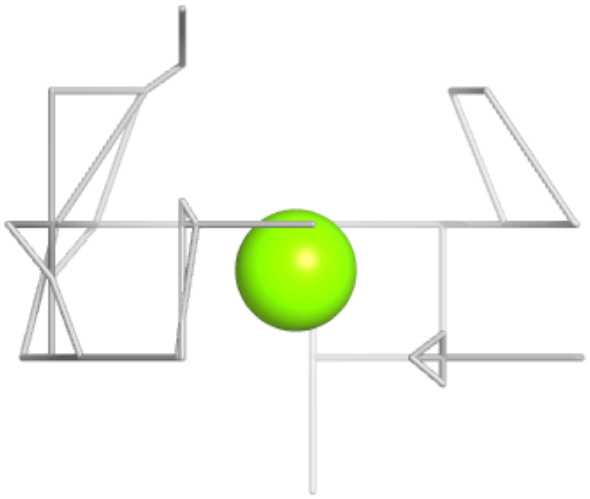
Electron density around MG B 707:

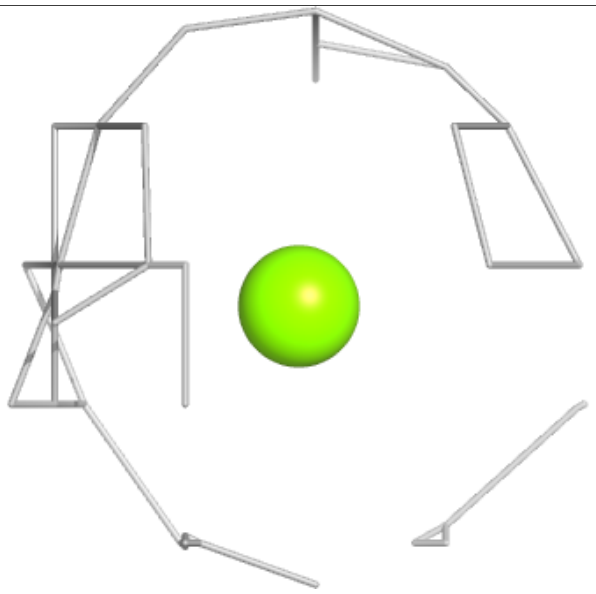
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

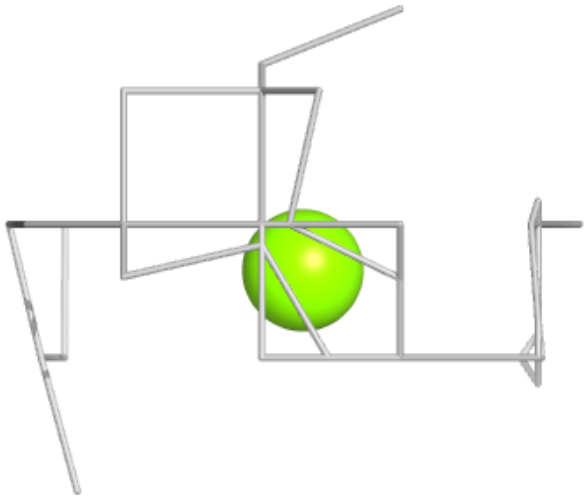


Electron density around MG F 708:

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

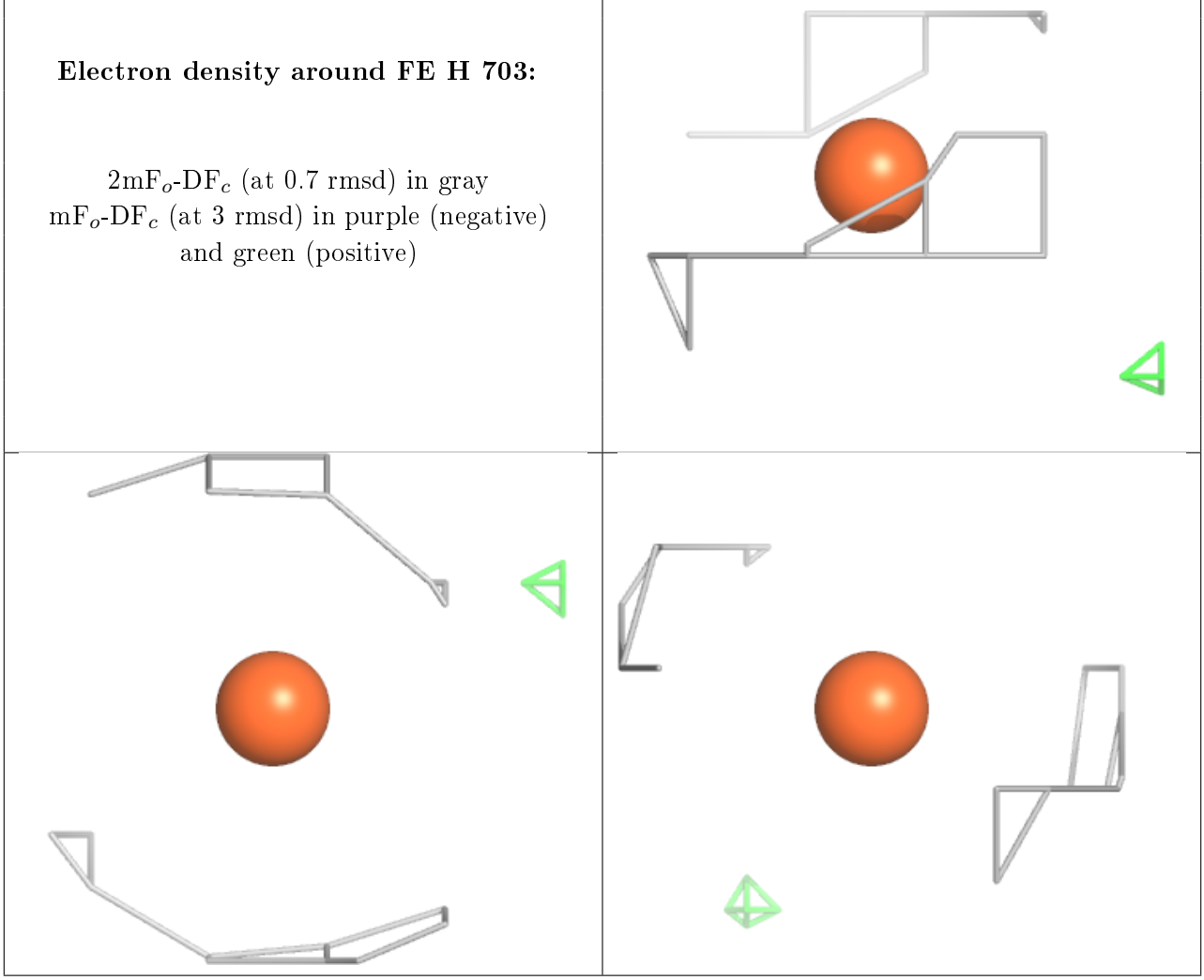






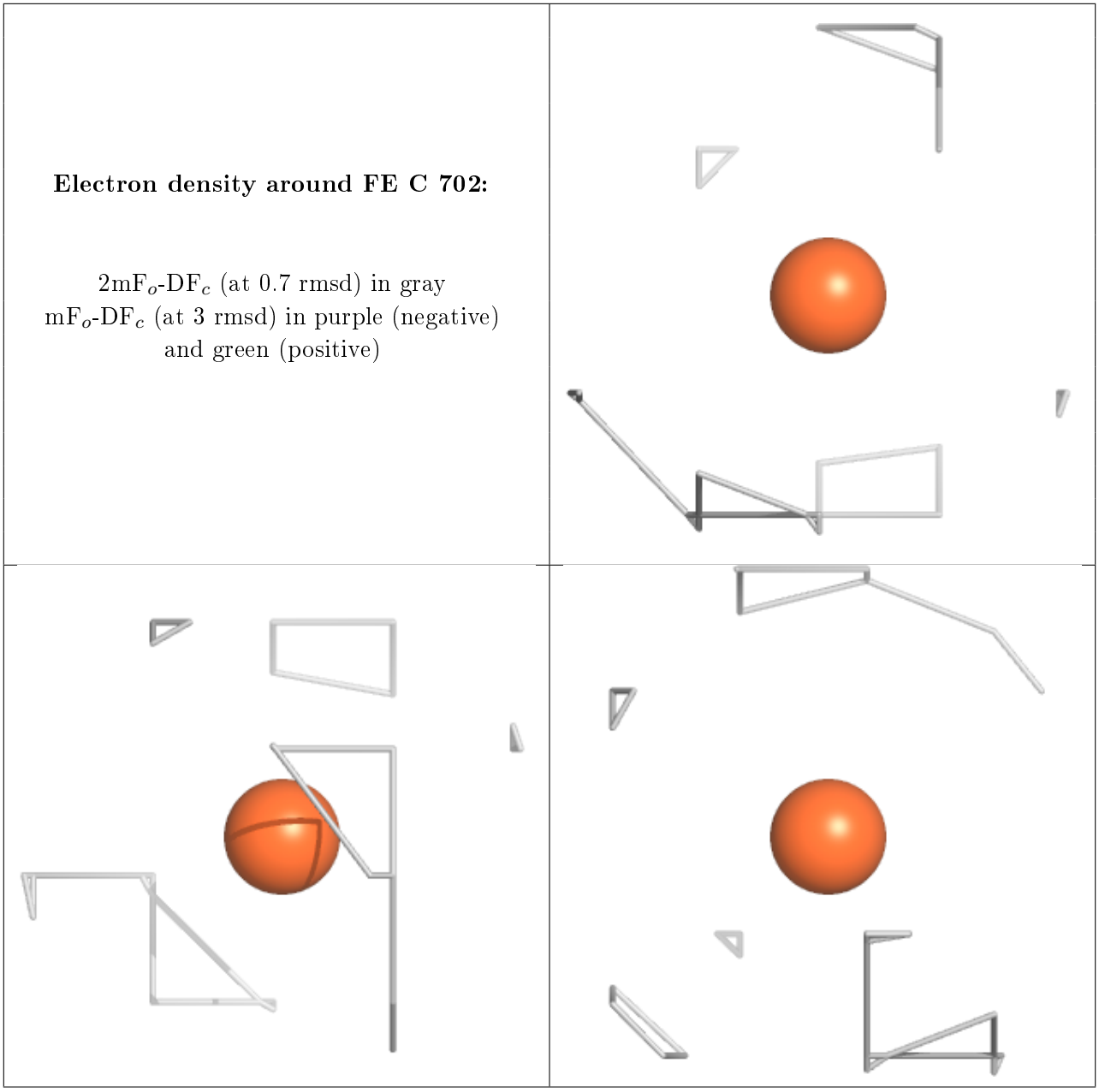
Electron density around FE H 703:

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



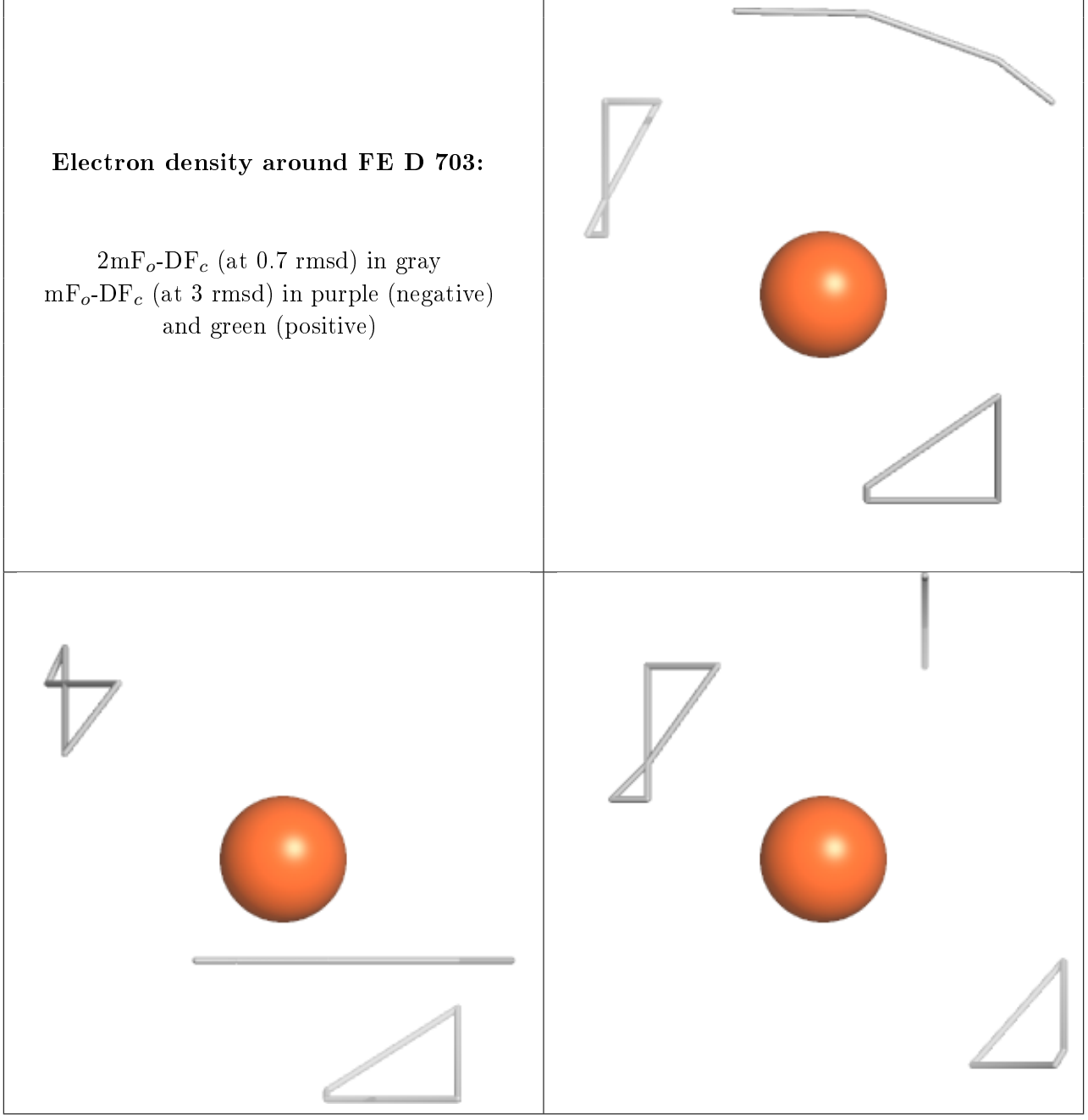
Electron density around FE C 702:

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



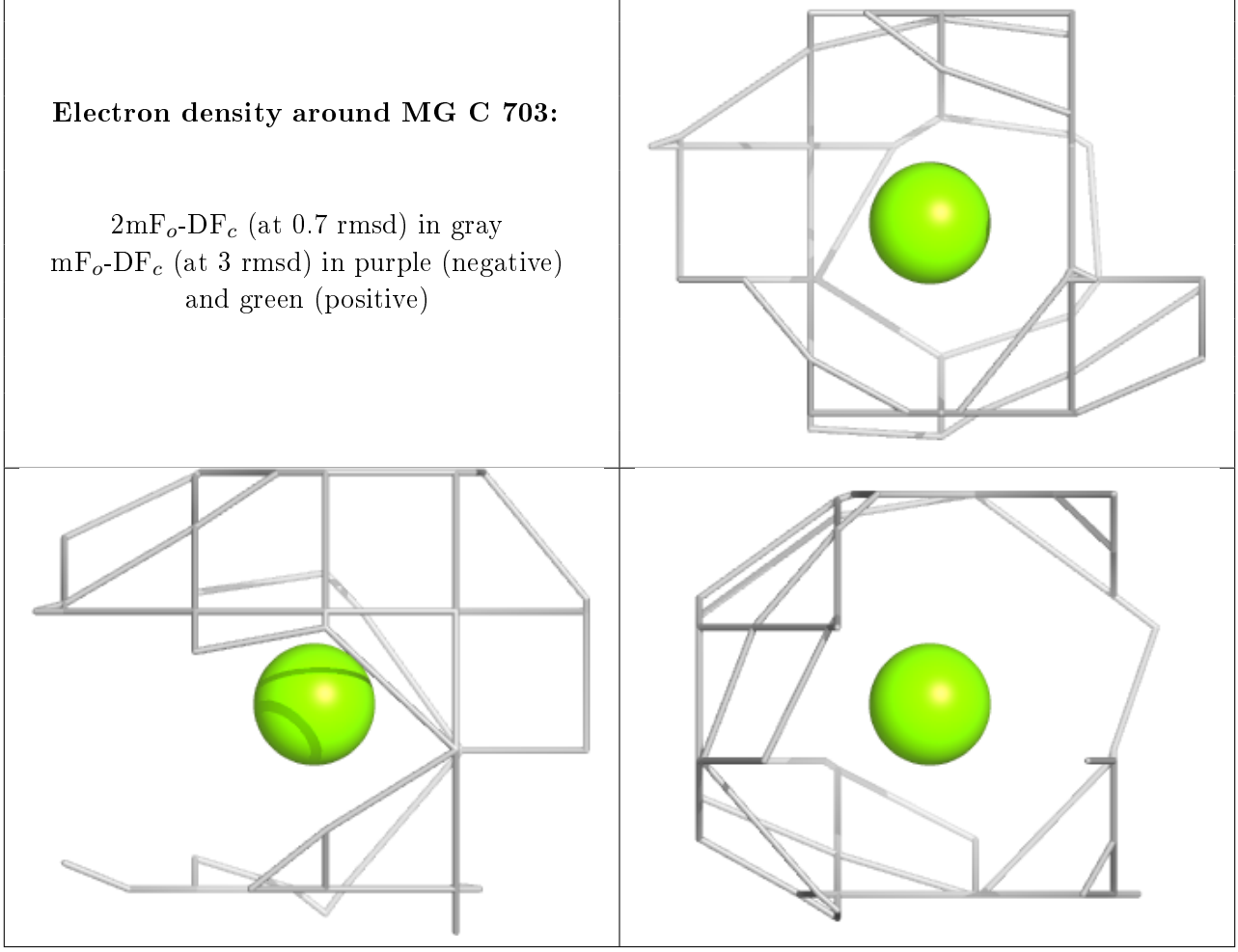
Electron density around FE D 703:

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



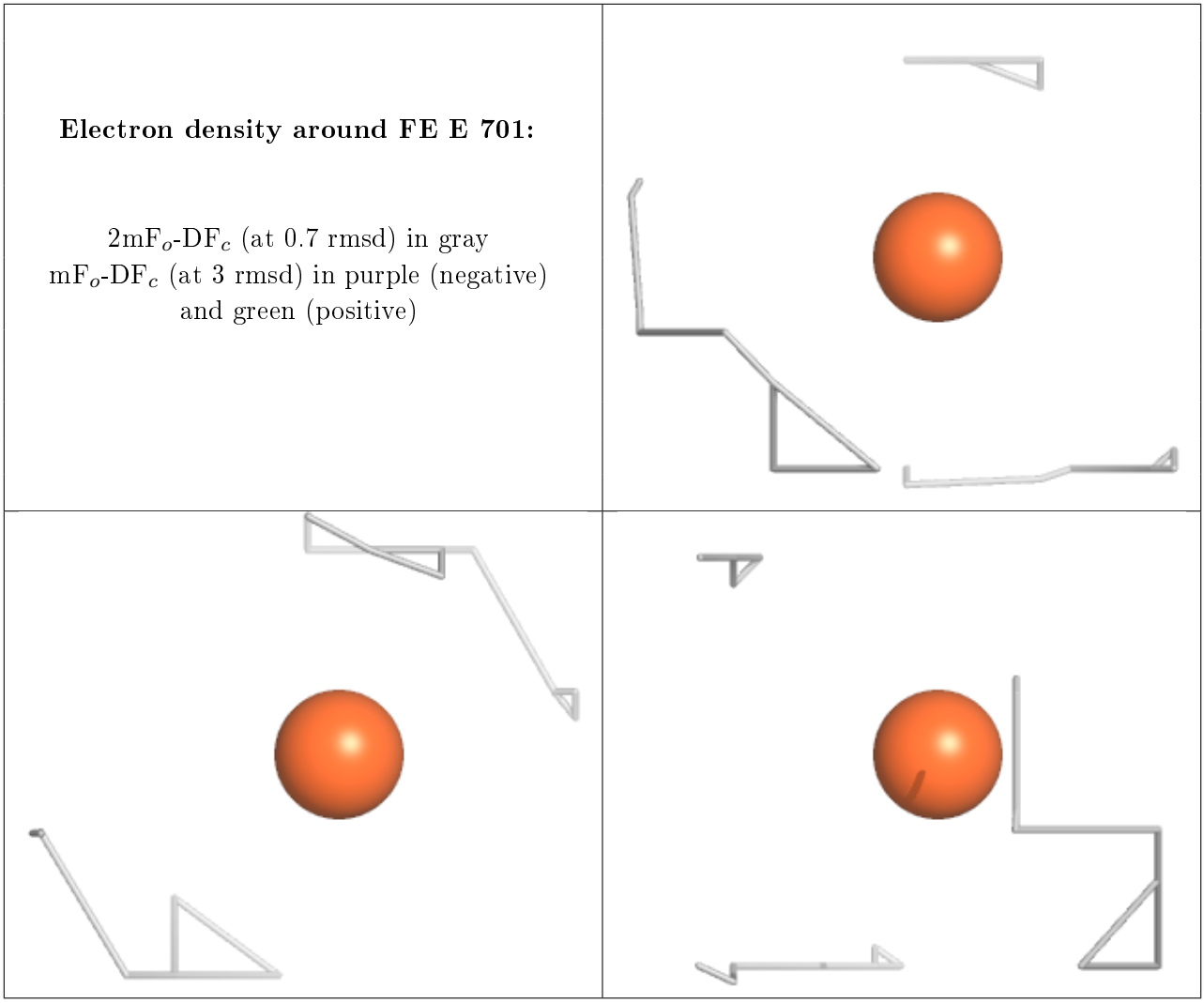
Electron density around MG C 703:

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



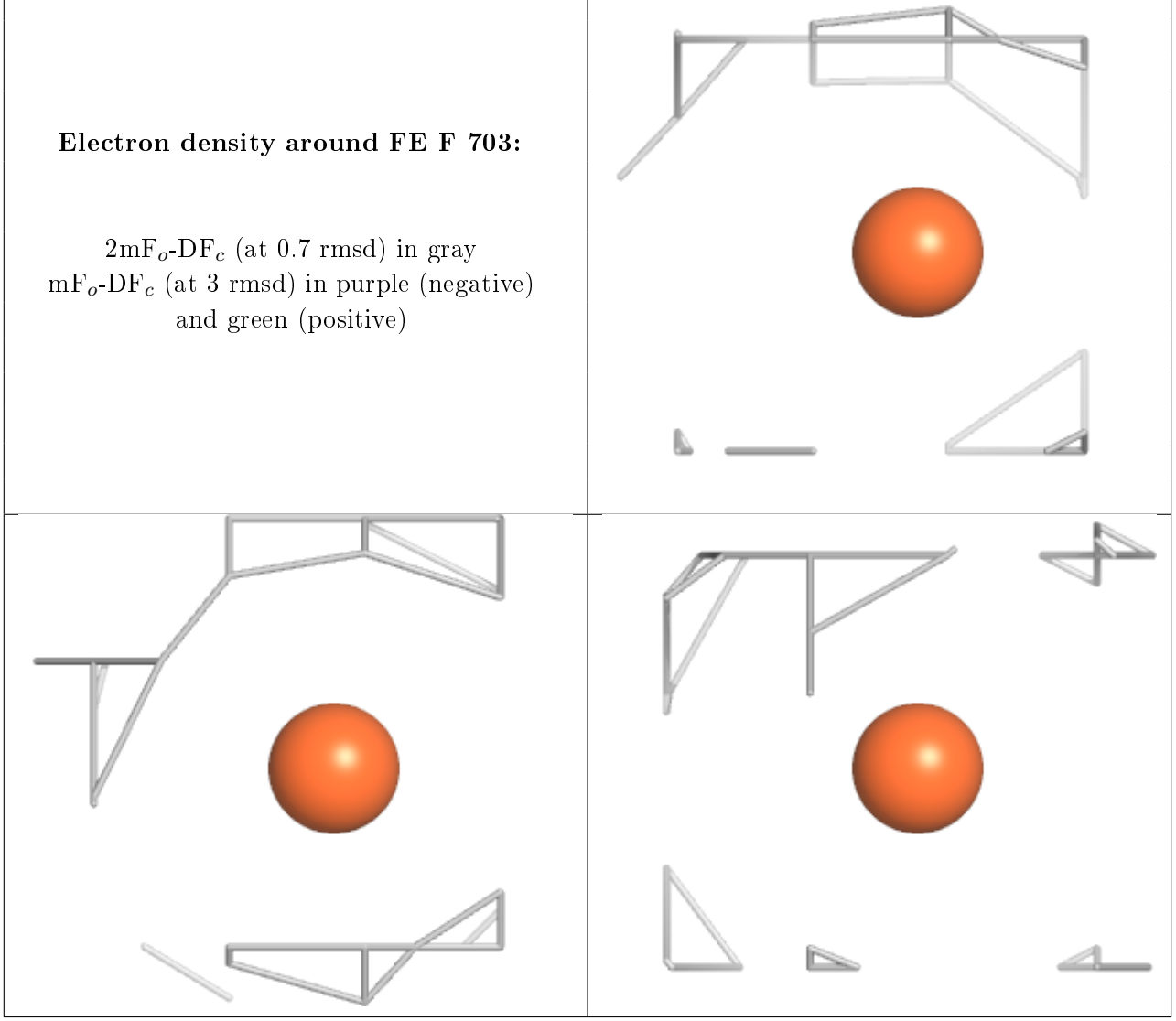
Electron density around FE E 701:

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



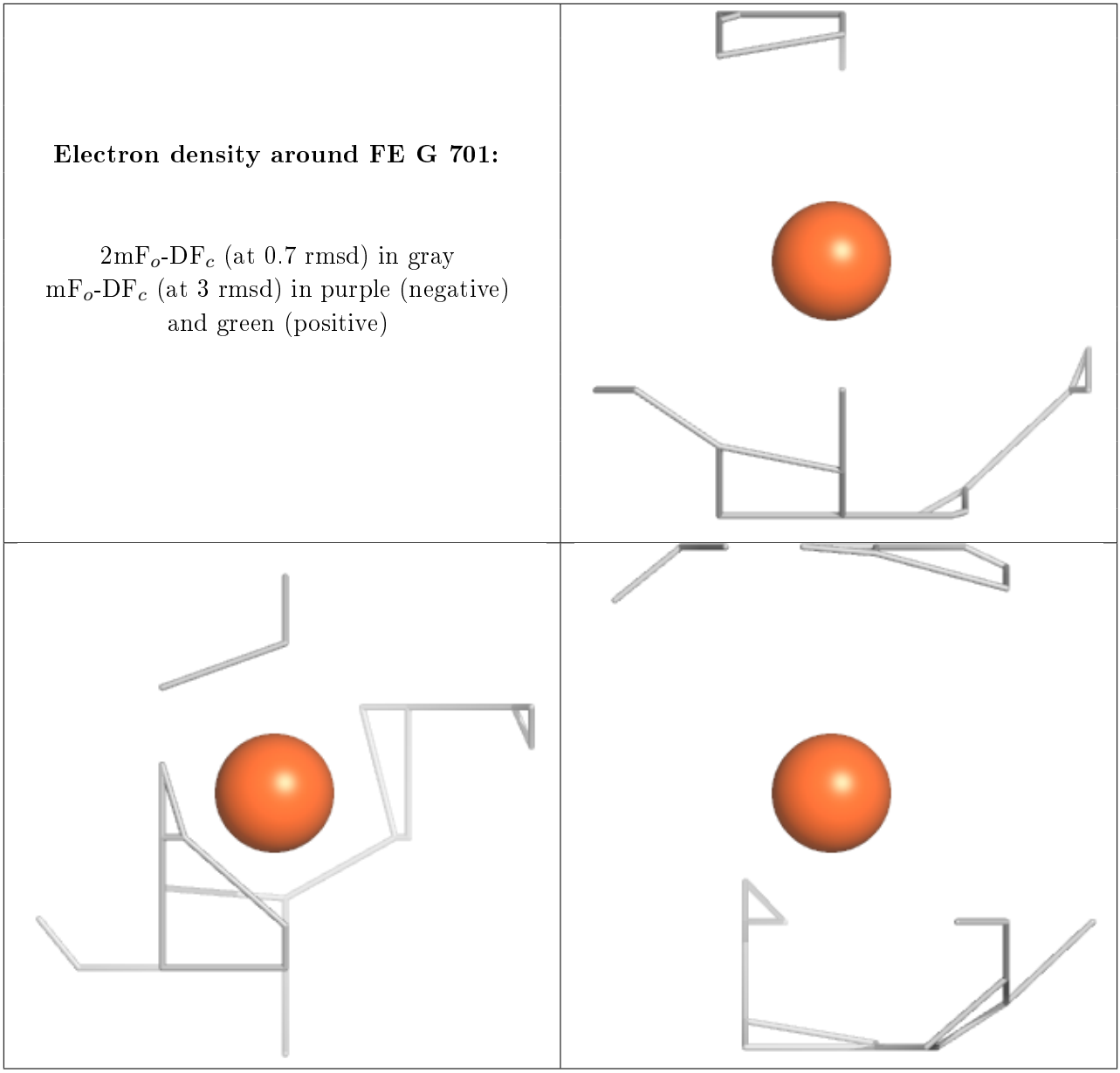
Electron density around FE F 703:

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



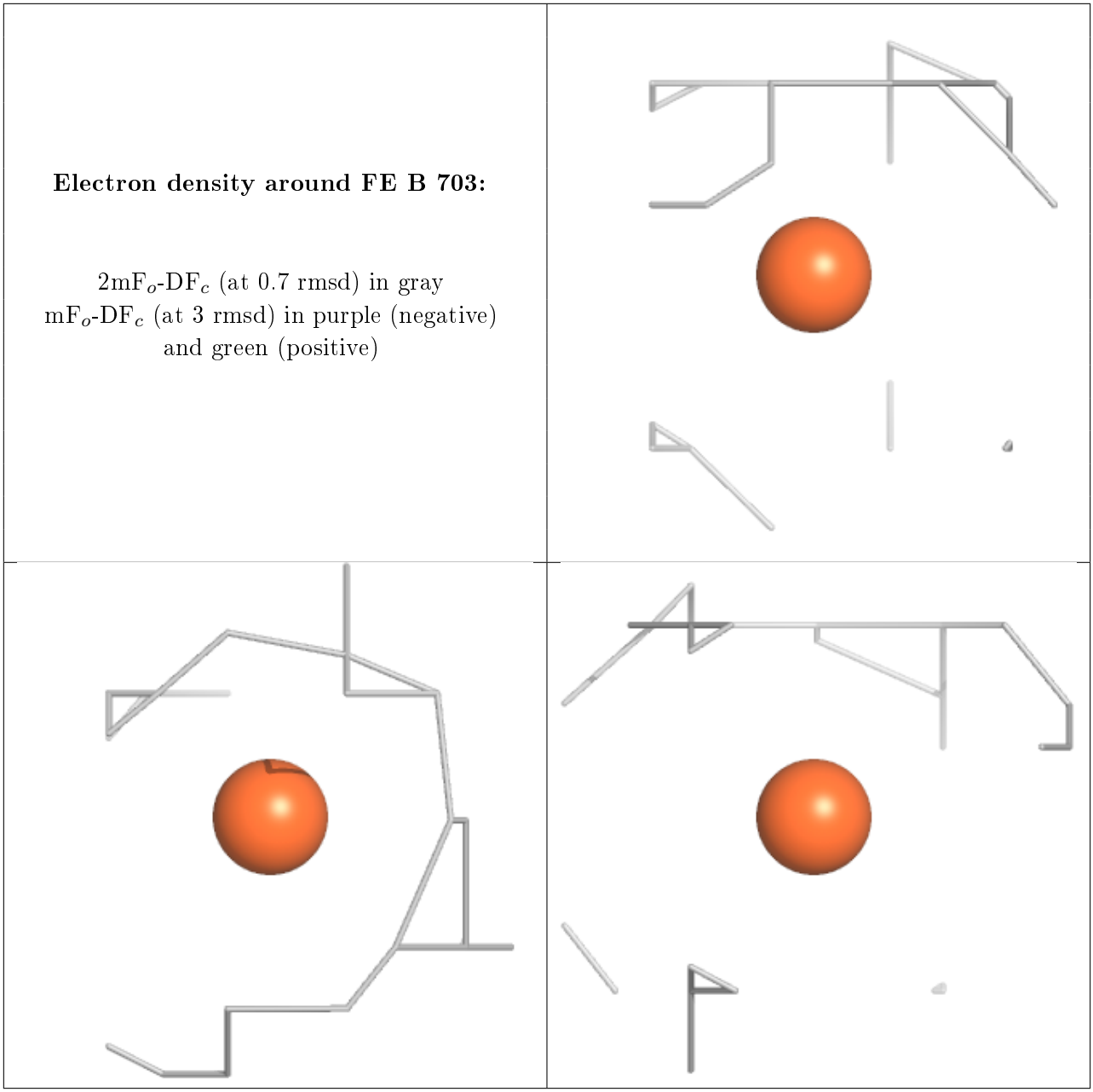
Electron density around FE G 701:

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



Electron density around FE 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)



6.5 Other polymers

There are no such residues in this entry.