wwPDB X-ray Structure Validation Summary Report (i)

Nov 14, 2023 – 12:06 AM JST

PDB ID	:	5YHW
Title	:	Crystal structure of Pig SAMHD1
Authors	:	Qin, X.H.; Kong, J.
Deposited on	:	2017-09-30
Resolution	:	2.70 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

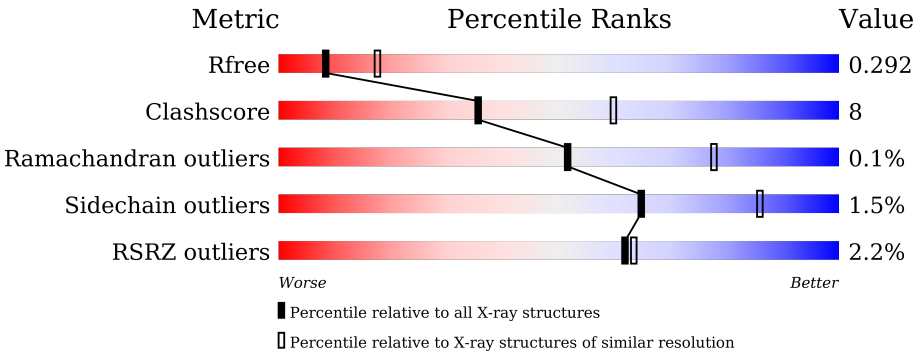
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	524	2% 71% 15% 14%
1	B	524	% 72% 14% 14%
1	C	524	2% 71% 15% 14%
1	D	524	3% 60% 13% • 26%
1	E	524	% 59% 14% • 26%
1	F	524	2% 72% 14% 14%

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Mol	Chain	Length	Quality of chain
1	G	524	2% 59% 14% 27%
1	H	524	2% 60% 12% 27%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DGT	G	706	-	-	X	-
3	MG	E	702	-	-	-	X
3	MG	G	705	-	-	-	X
3	MG	H	702	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 26957 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	453	Total	C	N	O	S	0	0	0
			3573	2292	623	638	20			
1	B	453	Total	C	N	O	S	0	0	0
			3549	2276	623	630	20			
1	C	453	Total	C	N	O	S	0	0	0
			3553	2279	624	630	20			
1	D	387	Total	C	N	O	S	0	0	0
			3006	1935	528	525	18			
1	E	387	Total	C	N	O	S	0	0	0
			3006	1935	529	524	18			
1	F	453	Total	C	N	O	S	0	0	0
			3578	2296	625	637	20			
1	G	381	Total	C	N	O	S	0	0	0
			2947	1891	520	518	18			
1	H	381	Total	C	N	O	S	0	0	0
			2942	1887	519	518	18			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	HIS	-	expression tag	UNP I3LG77
A	105	HIS	-	expression tag	UNP I3LG77
A	106	HIS	-	expression tag	UNP I3LG77
A	107	HIS	-	expression tag	UNP I3LG77
A	108	HIS	-	expression tag	UNP I3LG77
A	109	HIS	-	expression tag	UNP I3LG77
A	206	ARG	HIS	engineered mutation	UNP I3LG77
A	207	ASN	ASP	engineered mutation	UNP I3LG77
B	104	HIS	-	expression tag	UNP I3LG77
B	105	HIS	-	expression tag	UNP I3LG77
B	106	HIS	-	expression tag	UNP I3LG77
B	107	HIS	-	expression tag	UNP I3LG77
B	108	HIS	-	expression tag	UNP I3LG77

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Chain	Residue	Modelled	Actual	Comment	Reference
B	109	HIS	-	expression tag	UNP I3LG77
B	206	ARG	HIS	engineered mutation	UNP I3LG77
B	207	ASN	ASP	engineered mutation	UNP I3LG77
C	104	HIS	-	expression tag	UNP I3LG77
C	105	HIS	-	expression tag	UNP I3LG77
C	106	HIS	-	expression tag	UNP I3LG77
C	107	HIS	-	expression tag	UNP I3LG77
C	108	HIS	-	expression tag	UNP I3LG77
C	109	HIS	-	expression tag	UNP I3LG77
C	206	ARG	HIS	engineered mutation	UNP I3LG77
C	207	ASN	ASP	engineered mutation	UNP I3LG77
D	104	HIS	-	expression tag	UNP I3LG77
D	105	HIS	-	expression tag	UNP I3LG77
D	106	HIS	-	expression tag	UNP I3LG77
D	107	HIS	-	expression tag	UNP I3LG77
D	108	HIS	-	expression tag	UNP I3LG77
D	109	HIS	-	expression tag	UNP I3LG77
D	206	ARG	HIS	engineered mutation	UNP I3LG77
D	207	ASN	ASP	engineered mutation	UNP I3LG77
E	104	HIS	-	expression tag	UNP I3LG77
E	105	HIS	-	expression tag	UNP I3LG77
E	106	HIS	-	expression tag	UNP I3LG77
E	107	HIS	-	expression tag	UNP I3LG77
E	108	HIS	-	expression tag	UNP I3LG77
E	109	HIS	-	expression tag	UNP I3LG77
E	206	ARG	HIS	engineered mutation	UNP I3LG77
E	207	ASN	ASP	engineered mutation	UNP I3LG77
F	104	HIS	-	expression tag	UNP I3LG77
F	105	HIS	-	expression tag	UNP I3LG77
F	106	HIS	-	expression tag	UNP I3LG77
F	107	HIS	-	expression tag	UNP I3LG77
F	108	HIS	-	expression tag	UNP I3LG77
F	109	HIS	-	expression tag	UNP I3LG77
F	206	ARG	HIS	engineered mutation	UNP I3LG77
F	207	ASN	ASP	engineered mutation	UNP I3LG77
G	104	HIS	-	expression tag	UNP I3LG77
G	105	HIS	-	expression tag	UNP I3LG77
G	106	HIS	-	expression tag	UNP I3LG77
G	107	HIS	-	expression tag	UNP I3LG77
G	108	HIS	-	expression tag	UNP I3LG77
G	109	HIS	-	expression tag	UNP I3LG77
G	206	ARG	HIS	engineered mutation	UNP I3LG77

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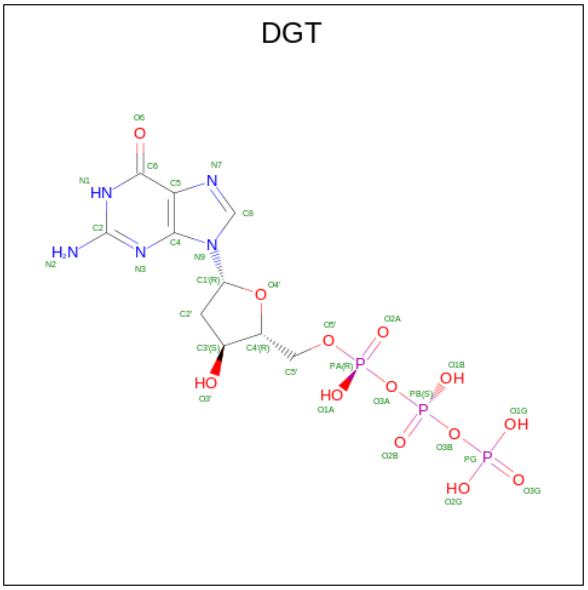
Chain	Residue	Modelled	Actual	Comment	Reference
G	207	ASN	ASP	engineered mutation	UNP I3LG77
H	104	HIS	-	expression tag	UNP I3LG77
H	105	HIS	-	expression tag	UNP I3LG77
H	106	HIS	-	expression tag	UNP I3LG77
H	107	HIS	-	expression tag	UNP I3LG77
H	108	HIS	-	expression tag	UNP I3LG77
H	109	HIS	-	expression tag	UNP I3LG77
H	206	ARG	HIS	engineered mutation	UNP I3LG77
H	207	ASN	ASP	engineered mutation	UNP I3LG77

- Molecule 2 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Mg 2 2	0	0
3	C	2	Total Mg 2 2	0	0
3	D	2	Total Mg 2 2	0	0
3	E	2	Total Mg 2 2	0	0
3	F	1	Total Mg 1 1	0	0
3	G	3	Total Mg 3 3	0	0
3	H	2	Total Mg 2 2	0	0

- Molecule 4 is water.

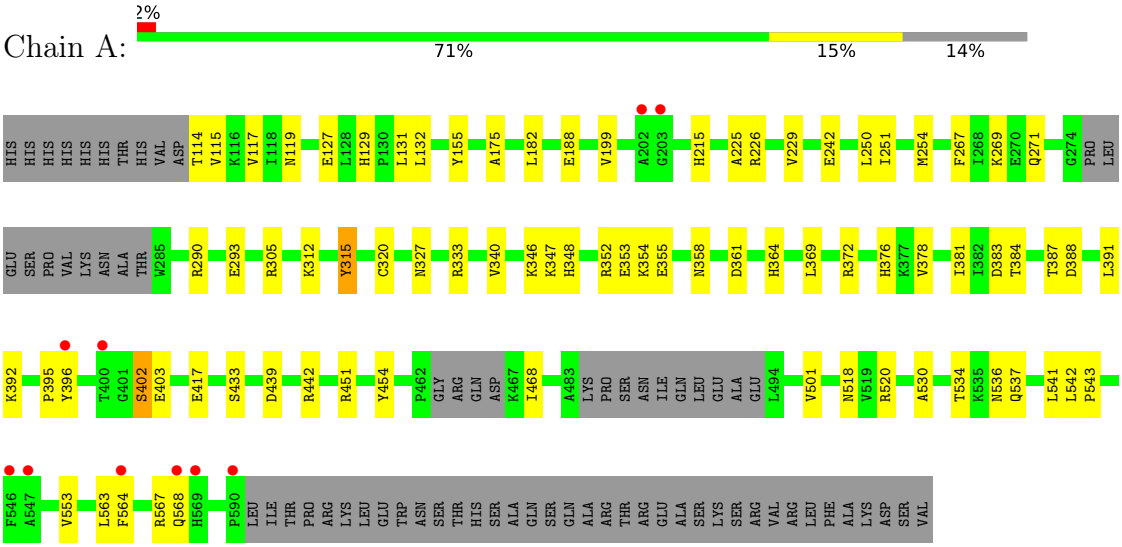
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	9	Total O 9 9	0	0
4	B	9	Total O 9 9	0	0
4	C	8	Total O 8 8	0	0
4	D	6	Total O 6 6	0	0
4	E	5	Total O 5 5	0	0
4	F	6	Total O 6 6	0	0

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.

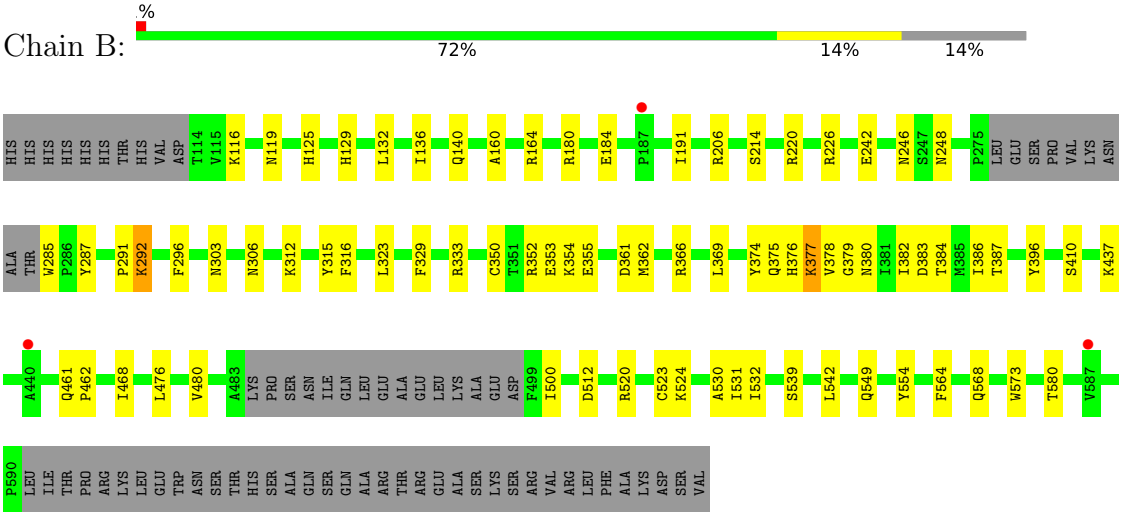
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain A:



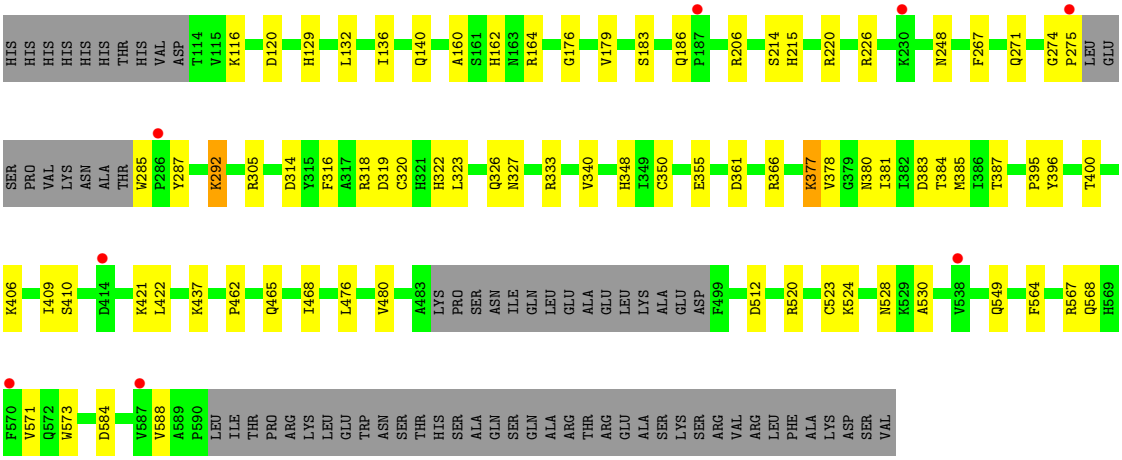
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain B:



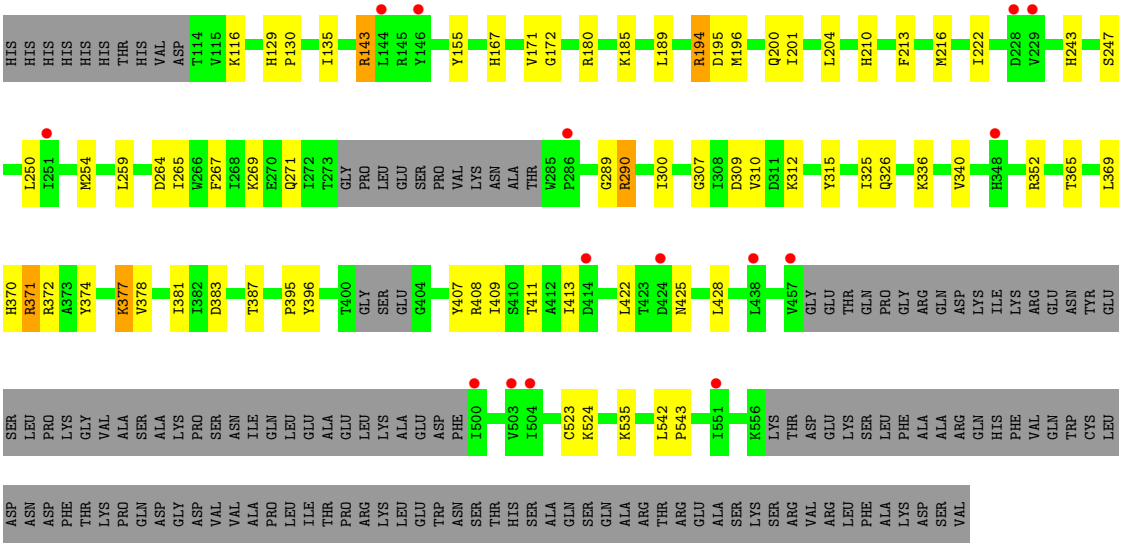
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain C:



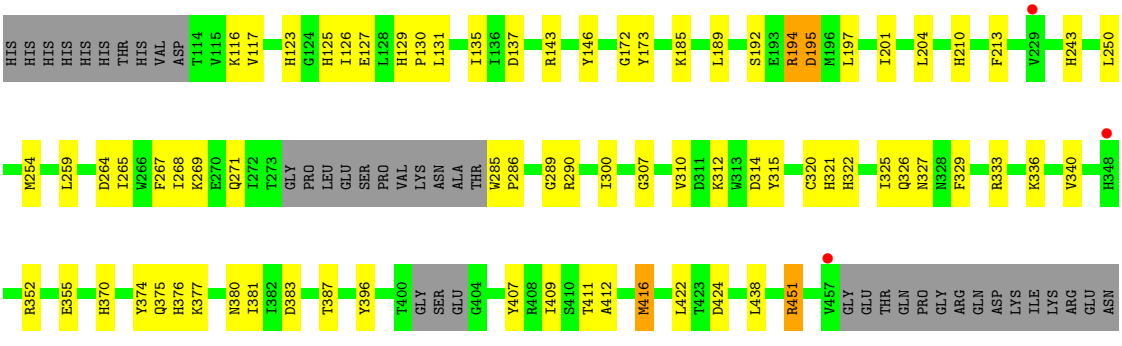
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

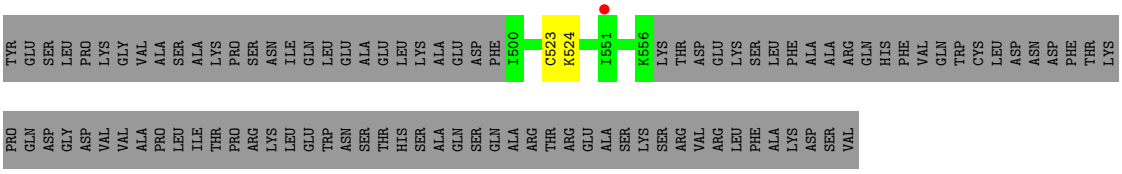
Chain D:



• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

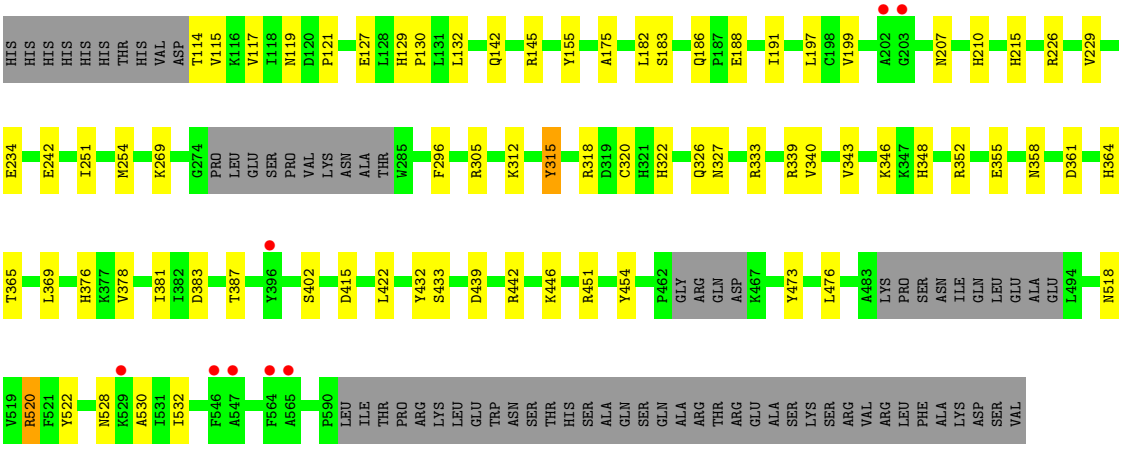
Chain E:





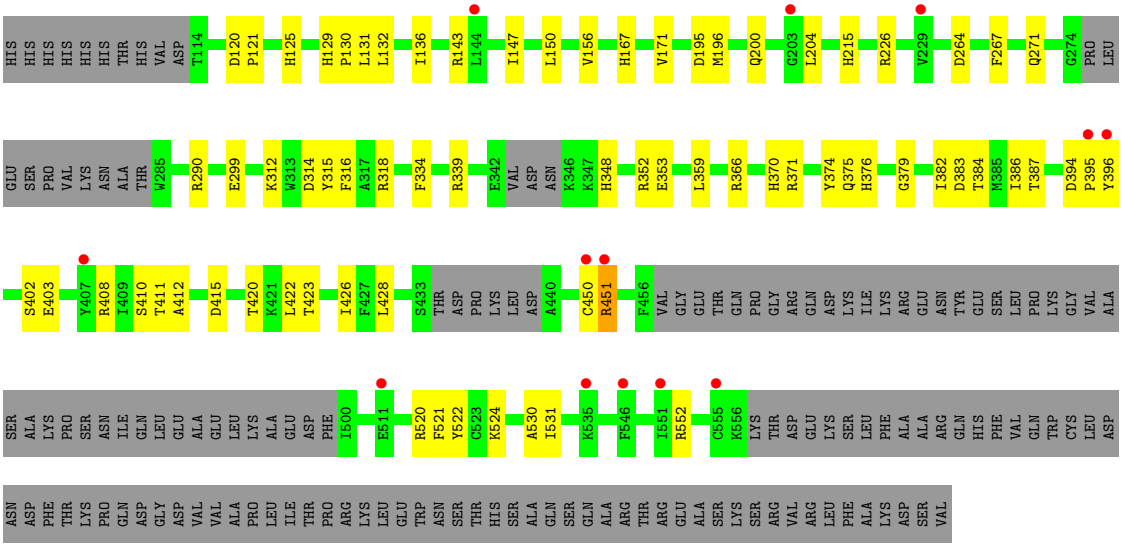
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain F:



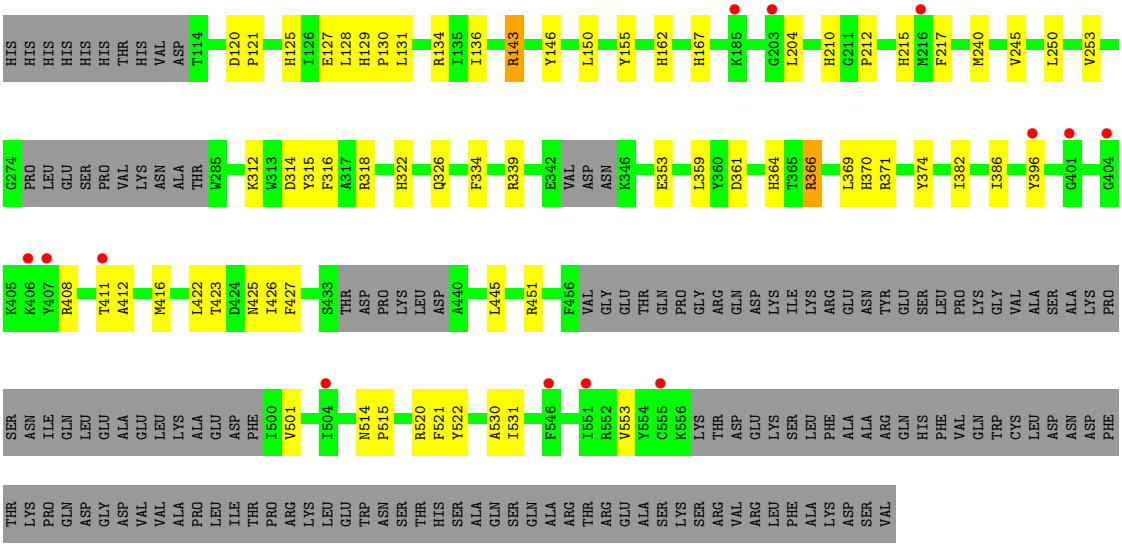
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain G:



• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain H:


HIS HIS HIS HIS HIS HIS THR HIS VAL ASP T114 D120 P121 H125 I126 E127 L128 H129 P130 L131 R134 I135 I136 R143 Y146 L150 Y155 H162 H167 K185 G203 L204 H210 G211 P212 H215 M216 F217 M240 V245 L250 V253
G274 PRO LEU GLU SER PRO VAL LYS ASN ALA THR W285 K312 W313 D314 Y315 F316 A317 R318 H322 Q326 F334 R339 E342 VAL ASP ASN K346 E353 L359 Y360 D361 H364 T365 R366 L369 H370 R371 Y374 I382 I386 Y396 G401 G404
K405 K406 Y407 R408 T411 A412 M416 L422 T423 D424 N425 I426 F427 S433 THR ASP PRO LYS LEU ASP A440 L445 R451 F456 VAL GLY GLU THR GLN PRO GLY ARG GLN ASP LYS ILE LYS ARG GLU ASN TYR GLU SER LEU PRO LYS GLY VAL ALA SER ALA LYS PRO
SER ASN ILE GLN LEU GLU ALA GLU LEU LYS ALA GLU ASP PHE I500 V501 I504 N514 P515 R520 F521 Y522 A530 I531 F546 I551 R552 V553 Y554 C555 K556 LYS THR ASP GLU LYS SER LEU PHE ALA ALA ARG GLN HIS PHE VAL GLN TRP CYS LEU ASP ASN ASP PHE
THR LYS PRO GLN ASP GLY ASP VAL VAL ALA ALA PRO LEU ILE THR PRO ARG LYS LEU GLU TRP ASN SER SER THR HIS SER ALA GLN SER GLN ALA ARG THR ARG GLU ALA SER LYS SER ARG VAL ARG LEU PHE ALA LYS ASP SER VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	86.54Å 95.91Å 130.75Å 78.66° 88.12° 82.68°	Depositor
Resolution (Å)	29.94 – 2.70 29.95 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.9 (29.94-2.70) 96.9 (29.95-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 2.68Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.263 , 0.290 0.265 , 0.292	Depositor DCC
R_{free} test set	1493 reflections (1.37%)	wwPDB-VP
Wilson B-factor (Å^2)	52.0	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 34.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	26957	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 97.73 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0370e-10. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: DGT, MG

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	0.30	0/3659	0.46	0/4959
1	B	0.30	0/3637	0.47	0/4932
1	C	0.29	0/3641	0.46	0/4936
1	D	0.29	0/3077	0.47	1/4173 (0.0%)
1	E	0.30	0/3077	0.46	0/4173
1	F	0.30	0/3664	0.45	0/4963
1	G	0.29	0/3015	0.46	0/4086
1	H	0.29	0/3010	0.46	0/4081
All	All	0.29	0/26780	0.46	1/36303 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	290	ARG	NE-CZ-NH1	-5.39	117.61	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3573	0	3430	59	0
1	B	3549	0	3387	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3553	0	3398	52	0
1	D	3006	0	2852	46	0
1	E	3006	0	2854	52	0
1	F	3578	0	3451	53	0
1	G	2947	0	2779	54	0
1	H	2942	0	2760	44	0
2	A	93	0	36	12	0
2	B	93	0	36	3	0
2	C	124	0	48	11	0
2	D	93	0	36	8	0
2	E	93	0	36	7	0
2	F	62	0	24	8	0
2	G	93	0	36	16	0
2	H	93	0	36	8	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	1	0	0	0	0
3	G	3	0	0	0	0
3	H	2	0	0	0	0
4	A	9	0	0	0	0
4	B	9	0	0	0	0
4	C	8	0	0	0	0
4	D	6	0	0	0	0
4	E	5	0	0	0	0
4	F	6	0	0	0	0
All	All	26957	0	25199	421	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 8.

The worst 5 of 421 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)
2:A:703:DGT:O4'	2:A:703:DGT:C4'	1.65	1.28
2:C:705:DGT:O4'	2:C:705:DGT:C4'	1.65	1.27
1:G:451:ARG:NH1	2:G:706:DGT:N1	1.81	1.27
2:D:701:DGT:C4'	2:D:701:DGT:O4'	1.66	1.24
2:H:705:DGT:O4'	2:H:705:DGT:C4'	1.67	1.24

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	445/524 (85%)	426 (96%)	18 (4%)	1 (0%)	47 73
1	B	447/524 (85%)	431 (96%)	16 (4%)	0	100 100
1	C	447/524 (85%)	432 (97%)	15 (3%)	0	100 100
1	D	379/524 (72%)	362 (96%)	17 (4%)	0	100 100
1	E	379/524 (72%)	361 (95%)	18 (5%)	0	100 100
1	F	445/524 (85%)	427 (96%)	18 (4%)	0	100 100
1	G	371/524 (71%)	351 (95%)	19 (5%)	1 (0%)	41 66
1	H	371/524 (71%)	356 (96%)	15 (4%)	0	100 100
All	All	3284/4192 (78%)	3146 (96%)	136 (4%)	2 (0%)	51 78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	402	SER
1	G	403	GLU

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	369/467 (79%)	365 (99%)	4 (1%)	73 90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	362/467 (78%)	357 (99%)	5 (1%)	67 86
1	C	363/467 (78%)	357 (98%)	6 (2%)	60 84
1	D	300/467 (64%)	295 (98%)	5 (2%)	60 84
1	E	300/467 (64%)	295 (98%)	5 (2%)	60 84
1	F	371/467 (79%)	364 (98%)	7 (2%)	57 82
1	G	293/467 (63%)	289 (99%)	4 (1%)	67 86
1	H	291/467 (62%)	287 (99%)	4 (1%)	67 86
All	All	2649/3736 (71%)	2609 (98%)	40 (2%)	65 86

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	315	TYR
1	G	451	ARG
1	F	422	LEU
1	G	353	GLU
1	H	353	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	321	HIS
1	G	376	HIS
1	H	248	ASN
1	C	549	GLN
1	C	465	GLN

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 40 ligands modelled in this entry, 16 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	$\#\|Z\| > 2$
2	DGT	H	705	3	26,33,33	3.44	12 (46%)	32,52,52	1.40	5 (15%)
2	DGT	B	705	3	26,33,33	3.36	12 (46%)	32,52,52	1.50	8 (25%)
2	DGT	D	701	3	26,33,33	3.40	12 (46%)	32,52,52	1.48	5 (15%)
2	DGT	G	704	3	26,33,33	3.49	12 (46%)	32,52,52	1.50	6 (18%)
2	DGT	A	704	3	26,33,33	3.39	12 (46%)	32,52,52	1.43	5 (15%)
2	DGT	E	701	3	26,33,33	3.47	12 (46%)	32,52,52	1.47	6 (18%)
2	DGT	A	701	3	26,33,33	3.49	12 (46%)	32,52,52	1.48	7 (21%)
2	DGT	D	703	3	26,33,33	3.49	12 (46%)	32,52,52	1.49	5 (15%)
2	DGT	G	702	3	26,33,33	3.44	12 (46%)	32,52,52	1.49	6 (18%)
2	DGT	C	705	3	26,33,33	3.37	12 (46%)	32,52,52	1.46	6 (18%)
2	DGT	G	706	3	26,33,33	3.37	11 (42%)	32,52,52	1.61	9 (28%)
2	DGT	H	701	3	26,33,33	3.47	12 (46%)	32,52,52	1.41	6 (18%)
2	DGT	E	703	3	26,33,33	3.38	12 (46%)	32,52,52	1.50	7 (21%)
2	DGT	B	703	3	26,33,33	3.48	12 (46%)	32,52,52	1.40	7 (21%)
2	DGT	B	702	3	26,33,33	3.42	12 (46%)	32,52,52	1.40	5 (15%)
2	DGT	H	703	3	26,33,33	3.42	12 (46%)	32,52,52	1.46	8 (25%)
2	DGT	F	702	3	26,33,33	3.46	12 (46%)	32,52,52	1.42	7 (21%)
2	DGT	F	701	3	26,33,33	3.43	12 (46%)	32,52,52	1.39	5 (15%)
2	DGT	C	706	3	26,33,33	3.40	12 (46%)	32,52,52	1.42	5 (15%)
2	DGT	C	703	3	26,33,33	3.37	12 (46%)	32,52,52	1.53	7 (21%)
2	DGT	C	701	3	26,33,33	3.48	12 (46%)	32,52,52	1.41	6 (18%)
2	DGT	D	705	3	26,33,33	3.42	12 (46%)	32,52,52	1.45	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	DGT	E	704	3	26,33,33	3.42	12 (46%)	32,52,52	1.43	5 (15%)
2	DGT	A	703	3	26,33,33	3.39	12 (46%)	32,52,52	1.48	7 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DGT	H	705	3	-	2/18/34/34	0/3/3/3
2	DGT	B	705	3	-	2/18/34/34	0/3/3/3
2	DGT	D	701	3	-	2/18/34/34	0/3/3/3
2	DGT	G	704	3	-	8/18/34/34	0/3/3/3
2	DGT	A	704	3	-	6/18/34/34	0/3/3/3
2	DGT	E	701	3	-	8/18/34/34	0/3/3/3
2	DGT	A	701	3	-	4/18/34/34	0/3/3/3
2	DGT	D	703	3	-	8/18/34/34	0/3/3/3
2	DGT	G	702	3	-	2/18/34/34	0/3/3/3
2	DGT	C	705	3	-	5/18/34/34	0/3/3/3
2	DGT	G	706	3	-	3/18/34/34	0/3/3/3
2	DGT	H	701	3	-	7/18/34/34	0/3/3/3
2	DGT	E	703	3	-	5/18/34/34	0/3/3/3
2	DGT	B	703	3	-	6/18/34/34	0/3/3/3
2	DGT	B	702	3	-	2/18/34/34	0/3/3/3
2	DGT	H	703	3	-	3/18/34/34	0/3/3/3
2	DGT	F	702	3	-	6/18/34/34	0/3/3/3
2	DGT	F	701	3	-	3/18/34/34	0/3/3/3
2	DGT	C	706	3	-	4/18/34/34	0/3/3/3
2	DGT	C	703	3	-	2/18/34/34	0/3/3/3
2	DGT	C	701	3	-	7/18/34/34	0/3/3/3
2	DGT	D	705	3	-	4/18/34/34	0/3/3/3
2	DGT	E	704	3	-	1/18/34/34	0/3/3/3
2	DGT	A	703	3	-	1/18/34/34	0/3/3/3

The worst 5 of 287 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	703	DGT	O4'-C4'	10.03	1.67	1.45
2	F	701	DGT	O4'-C4'	9.97	1.67	1.45
2	G	704	DGT	O4'-C4'	9.95	1.67	1.45
2	H	705	DGT	O4'-C4'	9.93	1.67	1.45
2	B	703	DGT	O4'-C4'	9.93	1.67	1.45

The worst 5 of 150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	706	DGT	C5-C6-N1	3.85	120.75	113.95
2	D	701	DGT	C5-C6-N1	3.69	120.47	113.95
2	E	701	DGT	C5-C6-N1	3.69	120.46	113.95
2	B	702	DGT	C5-C6-N1	3.60	120.32	113.95
2	D	705	DGT	C5-C6-N1	3.56	120.24	113.95

There are no chirality outliers.

5 of 101 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	DGT	C3'-C4'-C5'-O5'
2	A	704	DGT	C5'-O5'-PA-O2A
2	C	701	DGT	PB-O3A-PA-O5'
2	C	705	DGT	PB-O3B-PG-O2G
2	C	706	DGT	PB-O3B-PG-O2G

There are no ring outliers.

24 monomers are involved in 69 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	705	DGT	1	0
2	B	705	DGT	1	0
2	D	701	DGT	4	0
2	G	704	DGT	3	0
2	A	704	DGT	5	0
2	E	701	DGT	1	0
2	A	701	DGT	3	0
2	D	703	DGT	1	0
2	G	702	DGT	2	0
2	C	705	DGT	4	0
2	G	706	DGT	11	0
2	H	701	DGT	3	0
2	E	703	DGT	3	0

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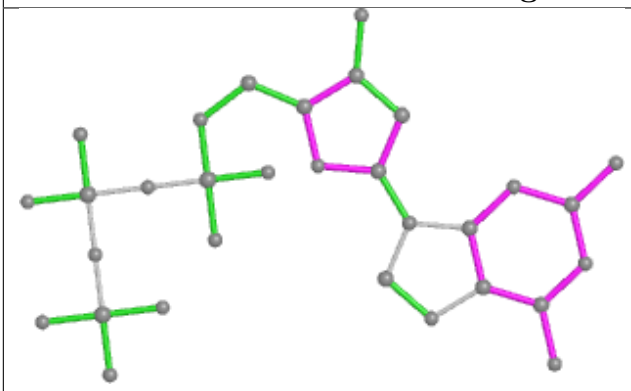
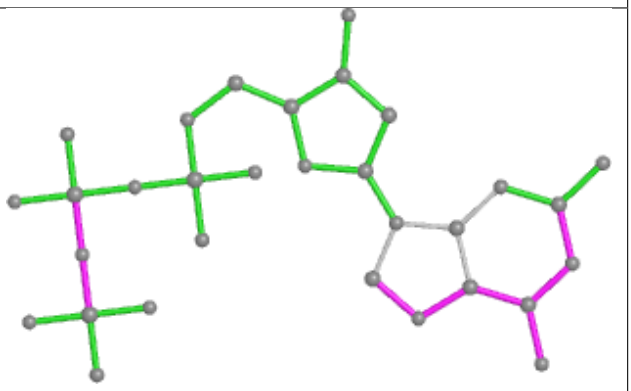
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	703	DGT	1	0
2	B	702	DGT	1	0
2	H	703	DGT	4	0
2	F	702	DGT	3	0
2	F	701	DGT	5	0
2	C	706	DGT	1	0
2	C	703	DGT	3	0
2	C	701	DGT	3	0
2	D	705	DGT	3	0
2	E	704	DGT	3	0
2	A	703	DGT	4	0

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.

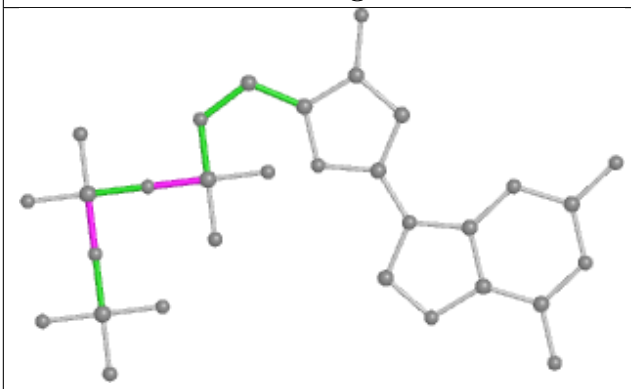
Ligand DGT H 705



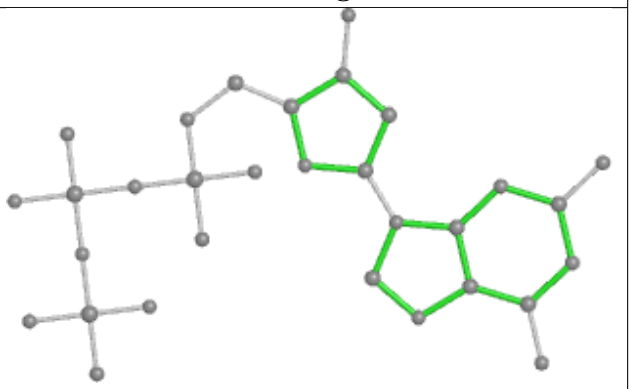
Bond lengths



Bond angles

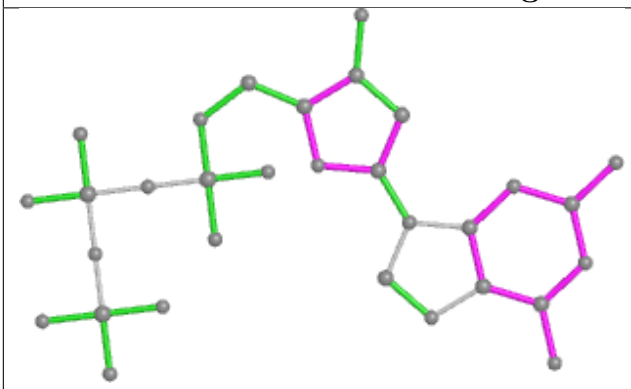


Torsions



Rings

Ligand DGT B 705



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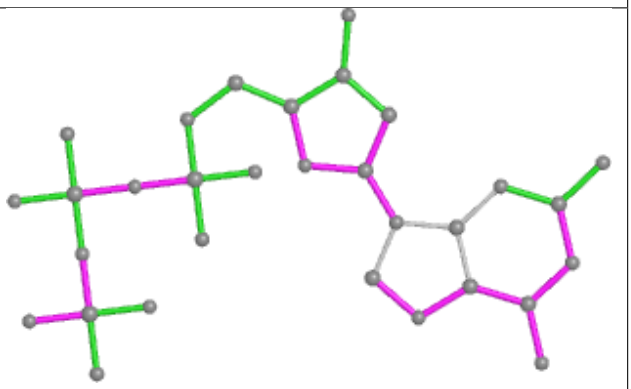

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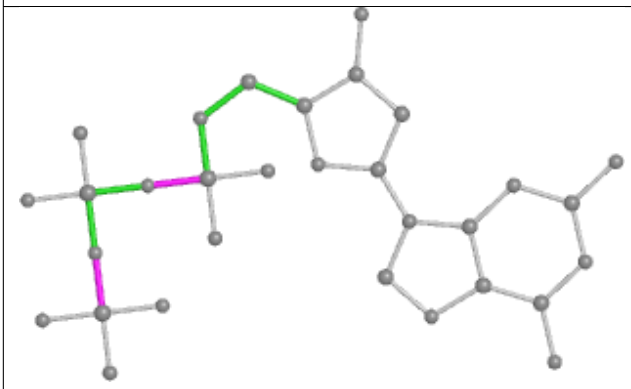
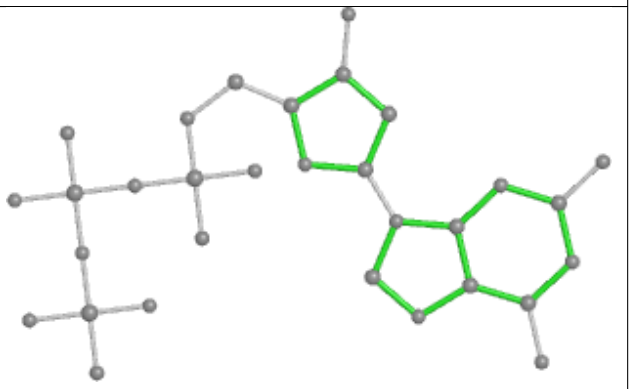
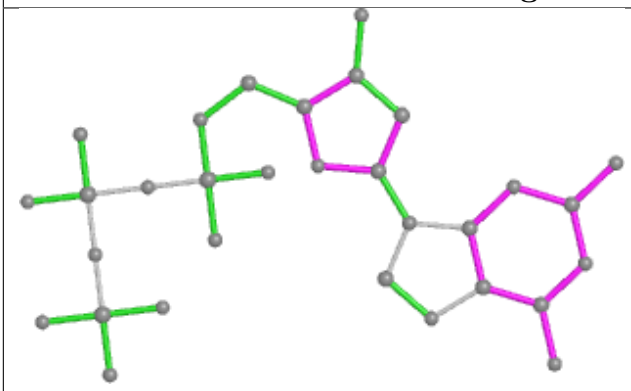


Torsions



Rings

Ligand DGT D 701



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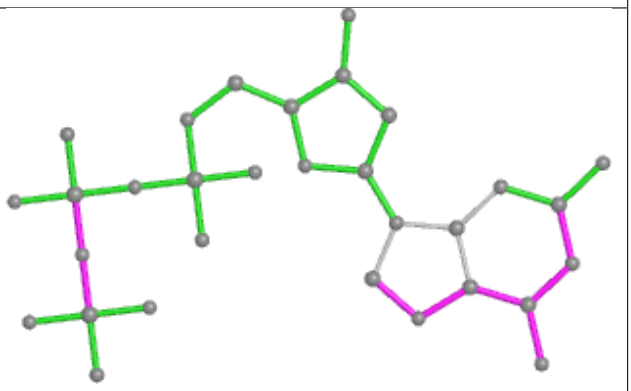
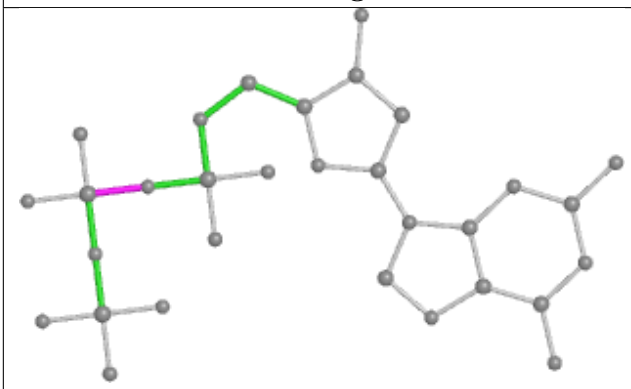


Bond angles



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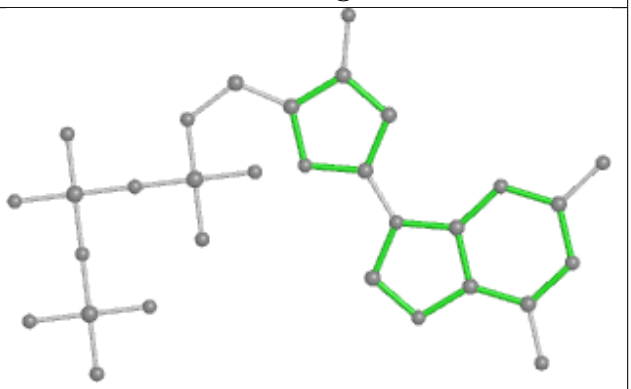
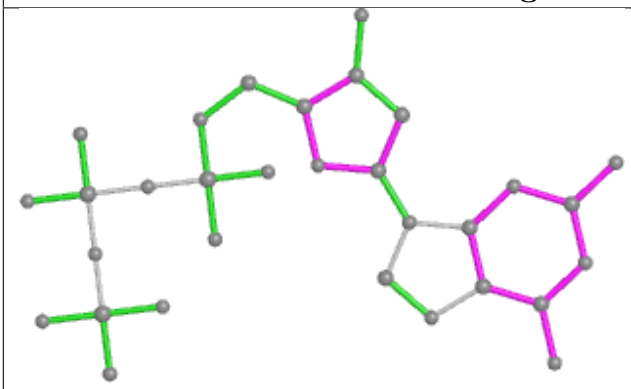


Rings

Ligand DGT G 704



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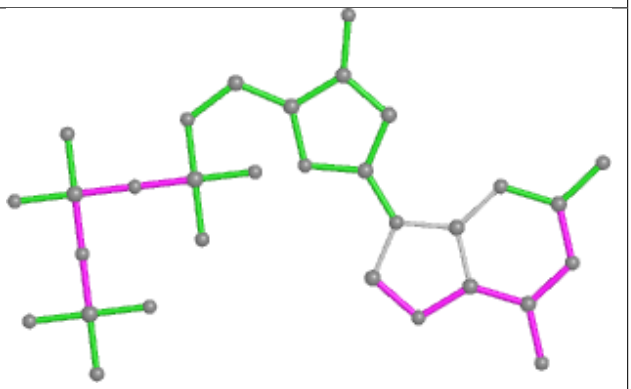

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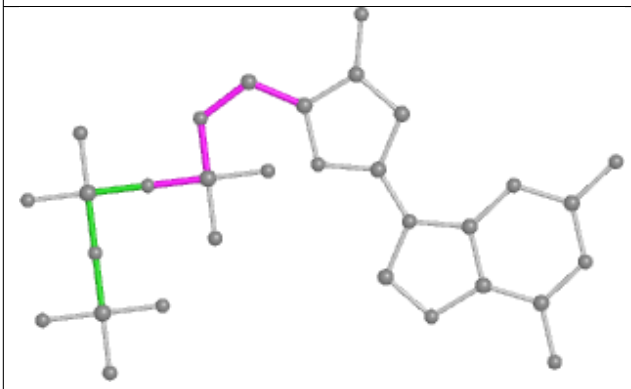

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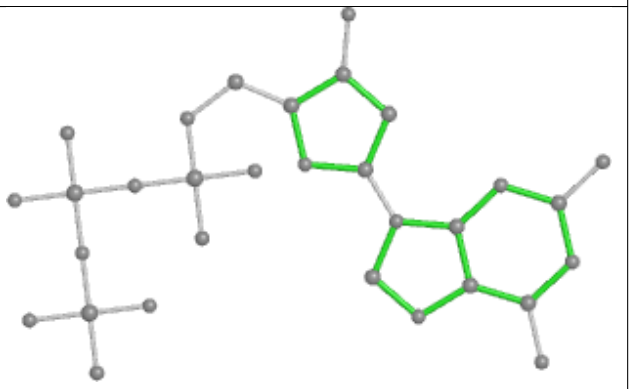
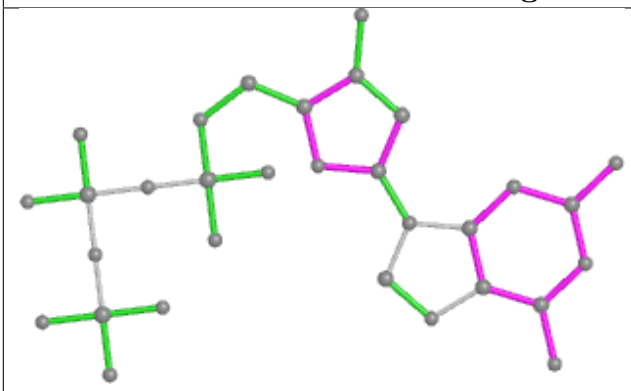
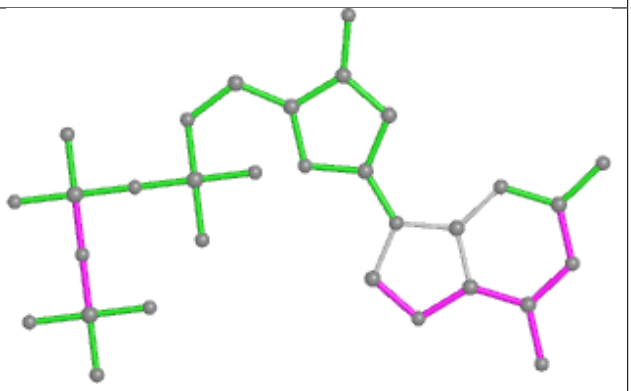


Rings

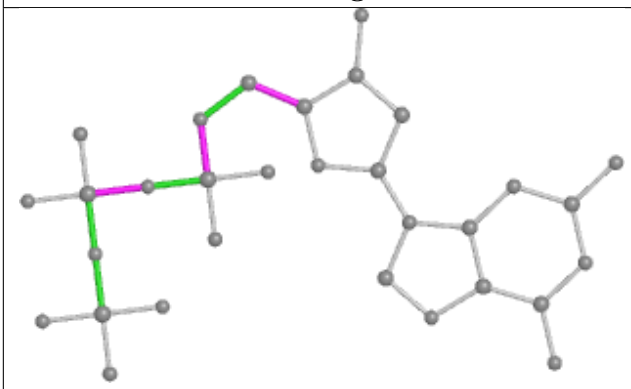
Ligand DGT A 704



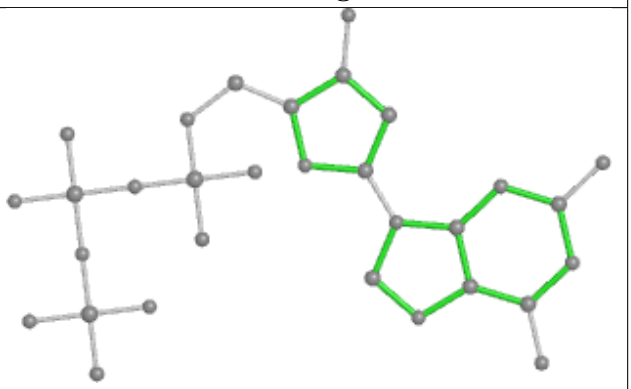
Bond lengths



Bond angles

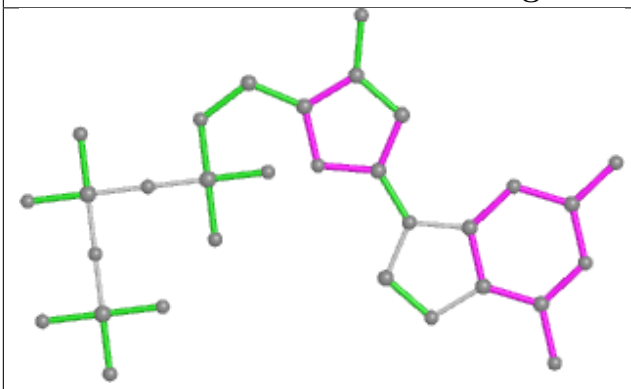


Torsions

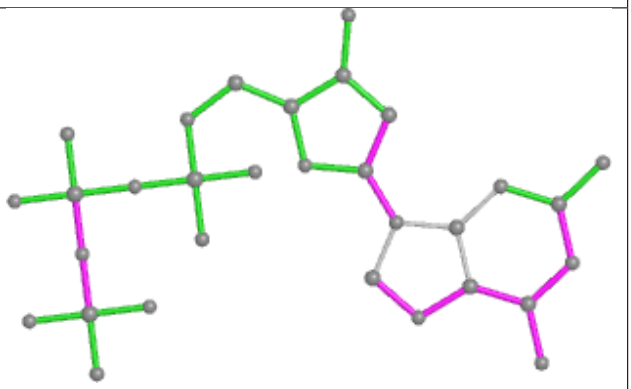


Rings

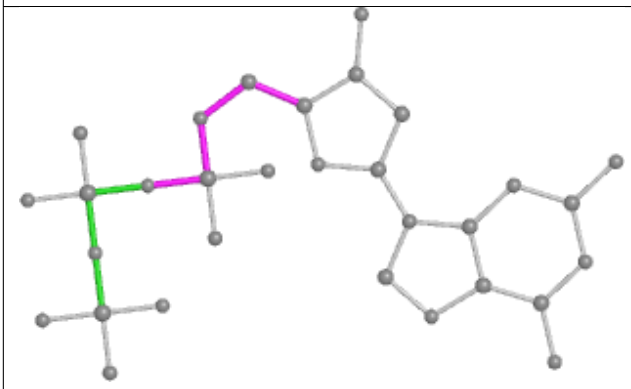
Ligand DGT E 701



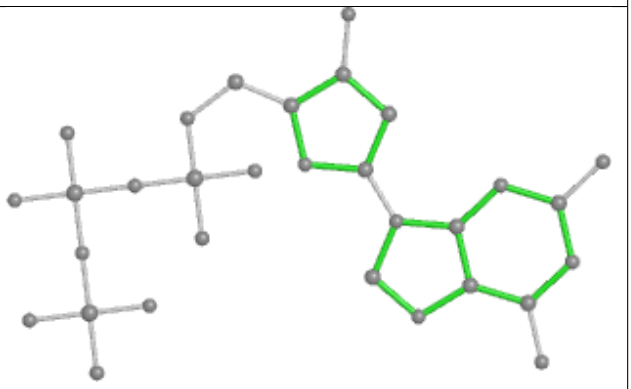
Bond lengths



Bond angles

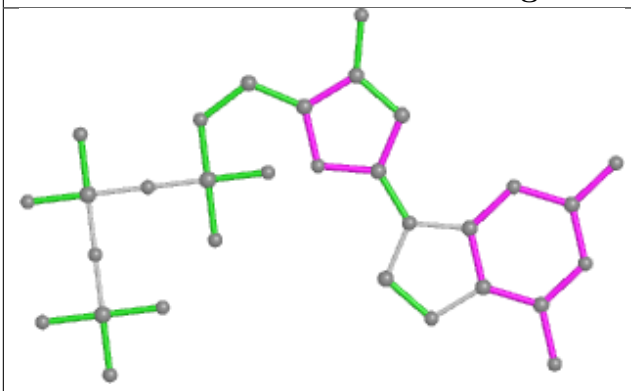


Torsions

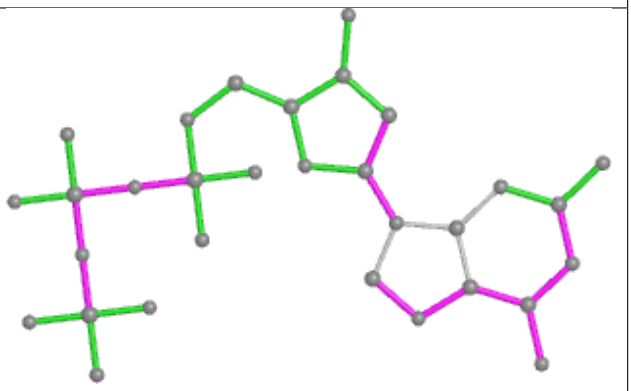


Rings

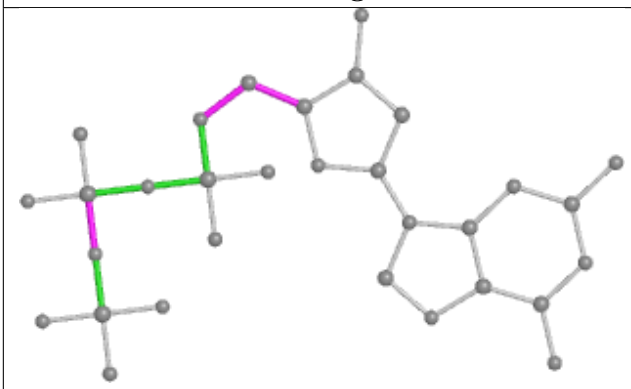
Ligand DGT A 701



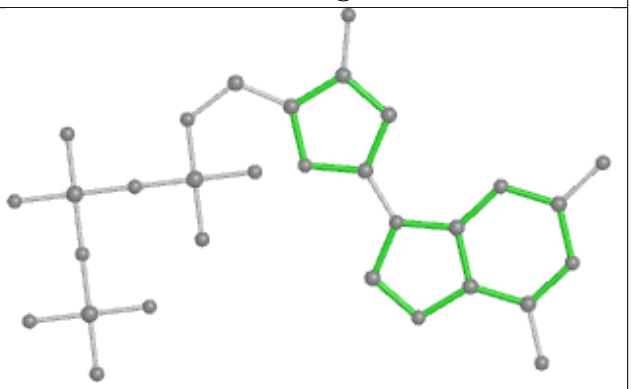
Bond lengths



Bond angles

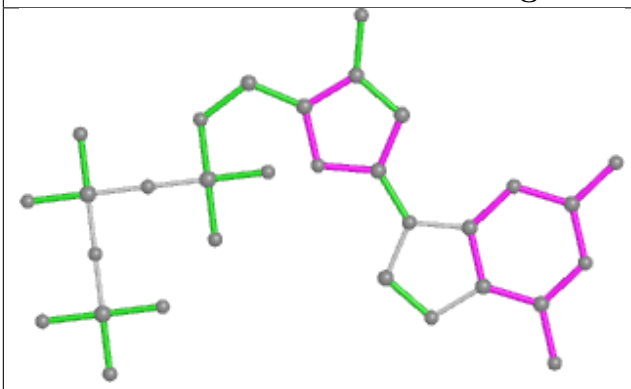


Torsions



Rings

Ligand DGT D 703



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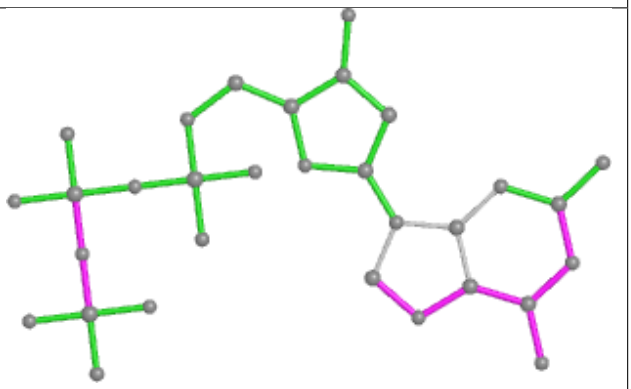
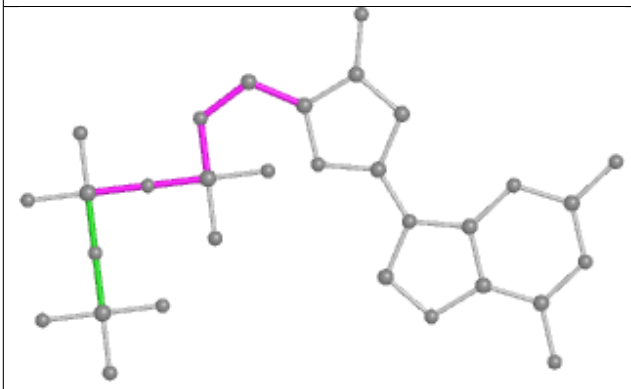


Bond angles



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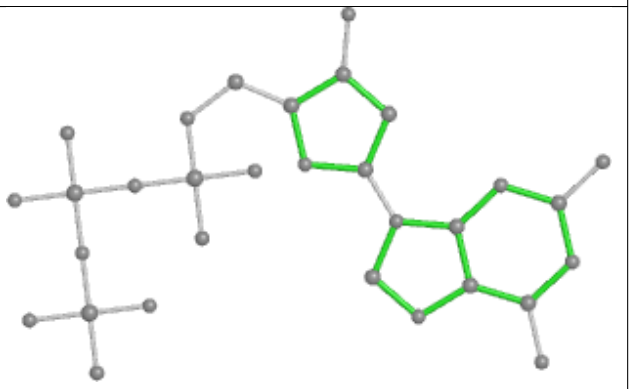
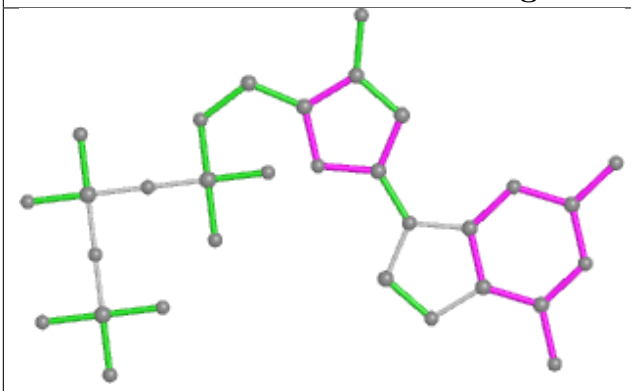


Rings

Ligand DGT G 702



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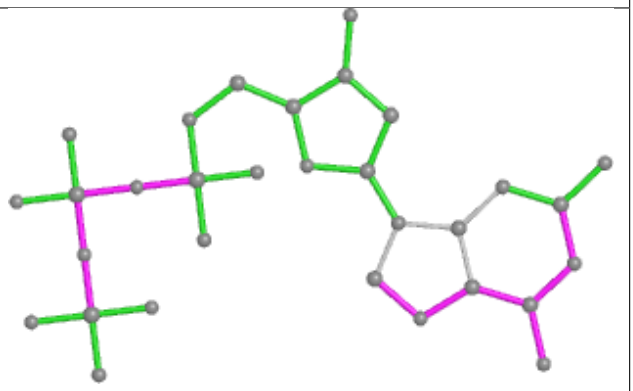
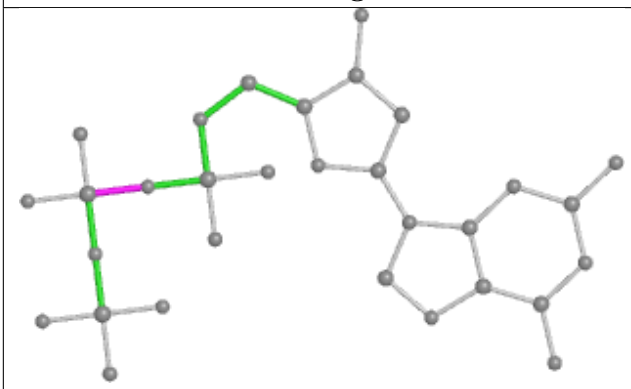


Bond angles



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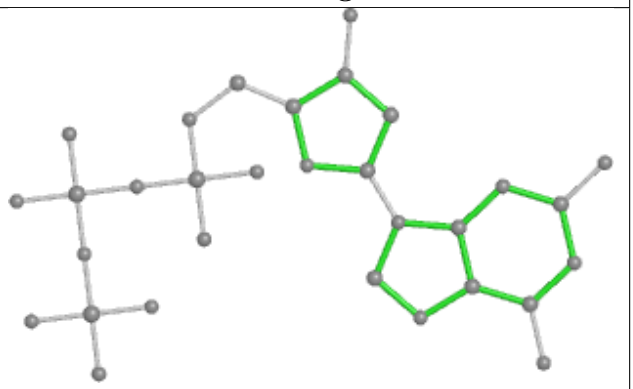
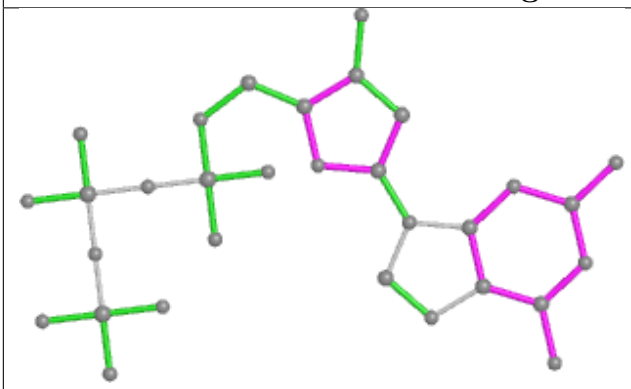


Rings

Ligand DGT C 705



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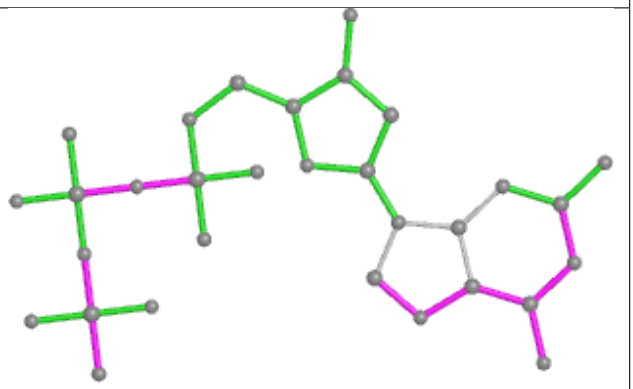
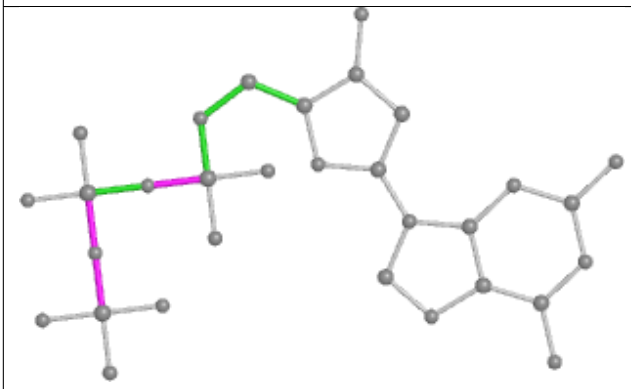


Bond angles



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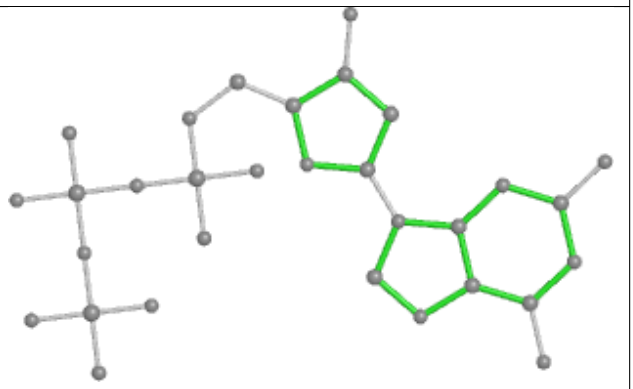
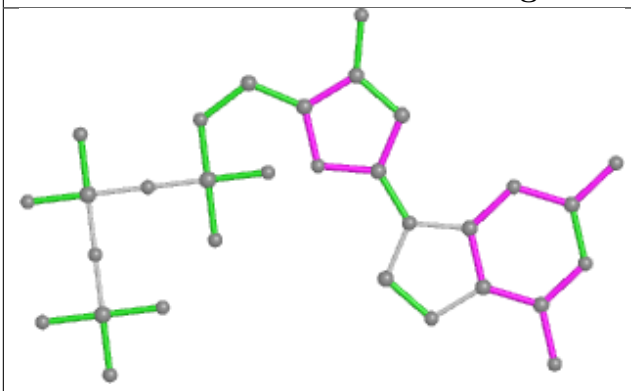


Rings

Ligand DGT G 706



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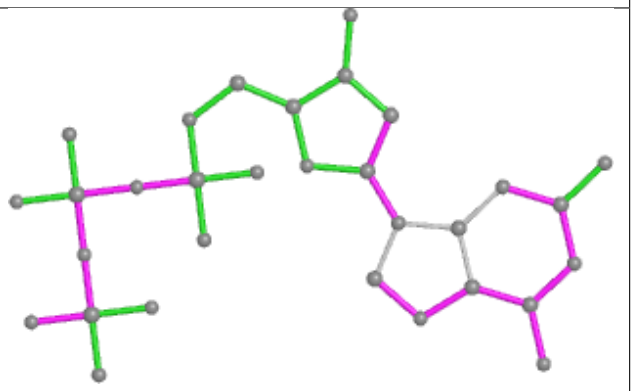
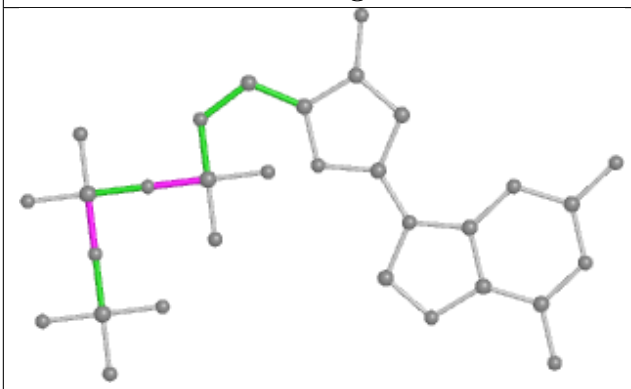


Bond angles



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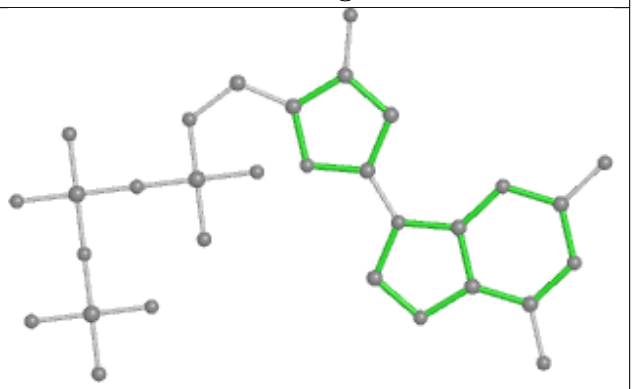
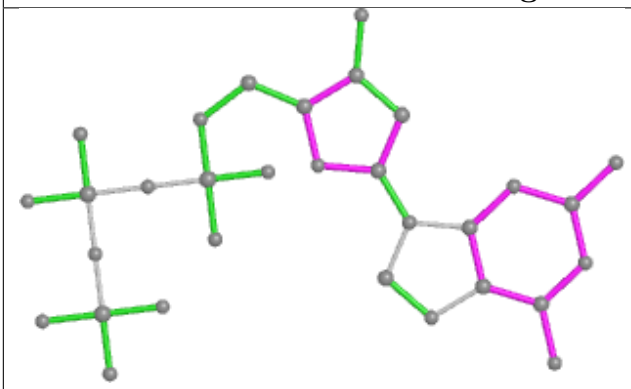


Rings

Ligand DGT H 701



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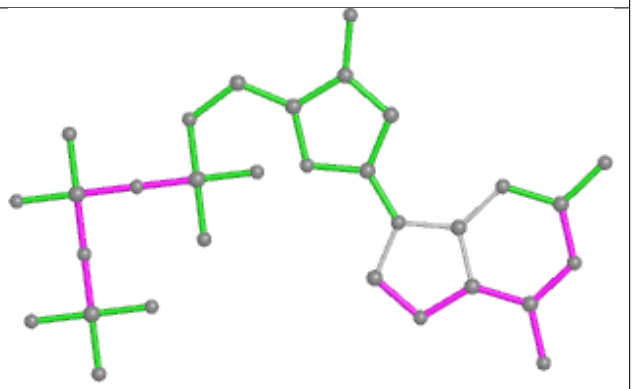

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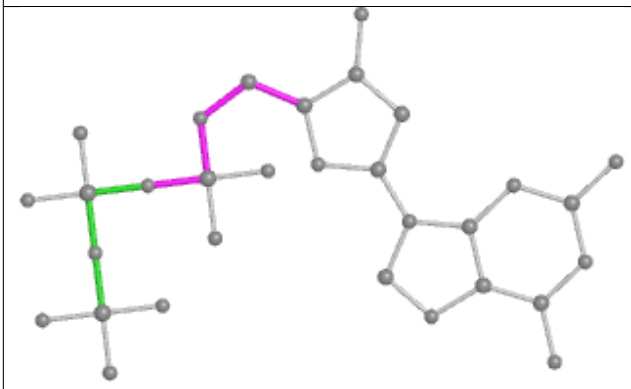

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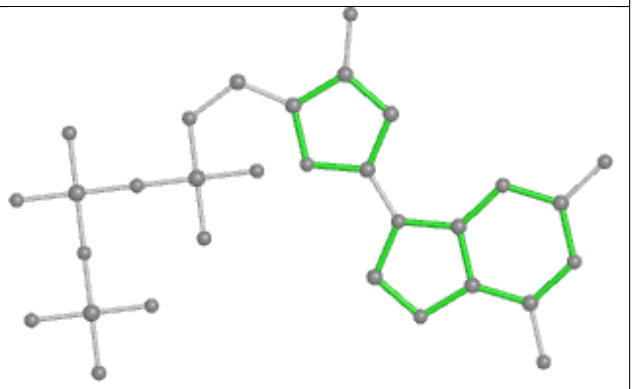
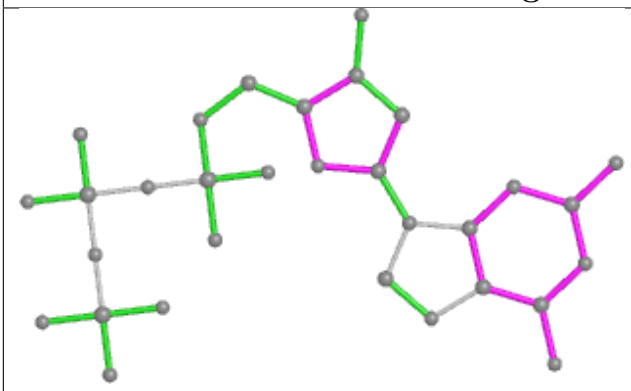


Rings

Ligand DGT E 703



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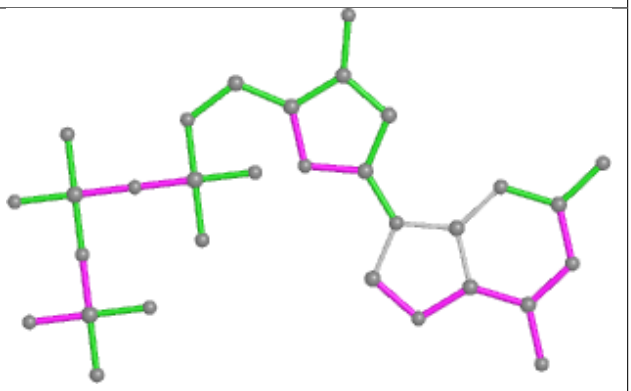
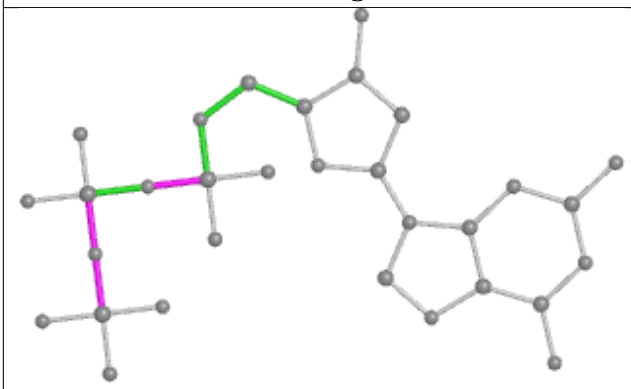


Bond angles



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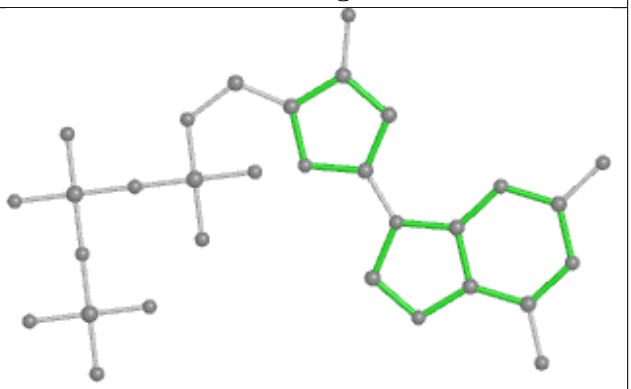
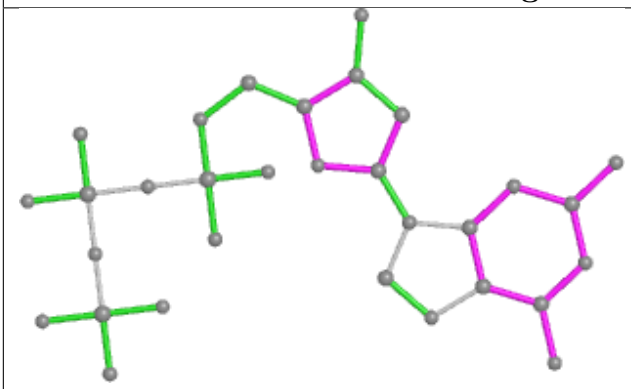


Rings

Ligand DGT B 703



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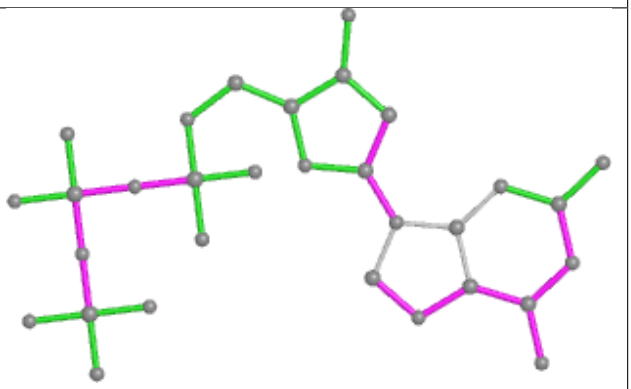

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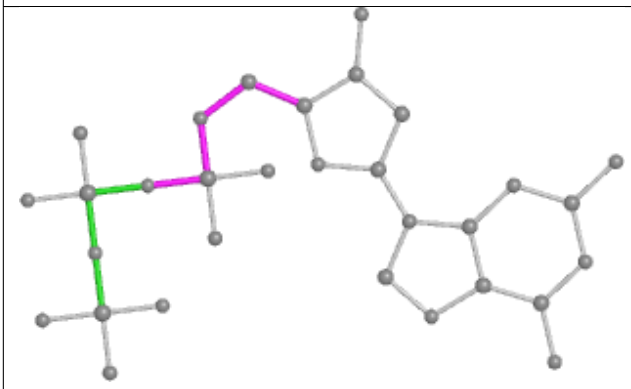

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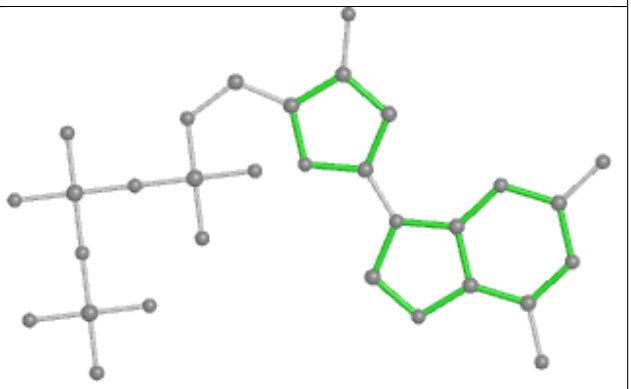
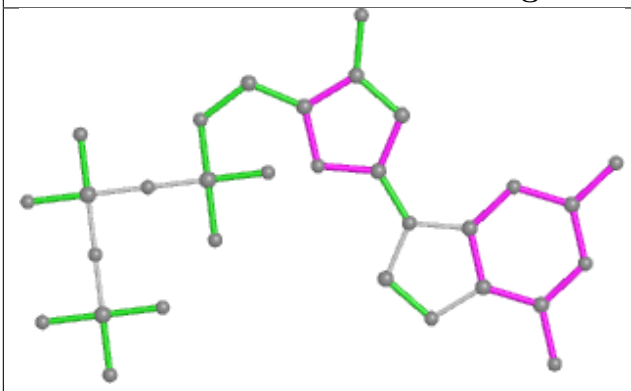


Rings

Ligand DGT B 702



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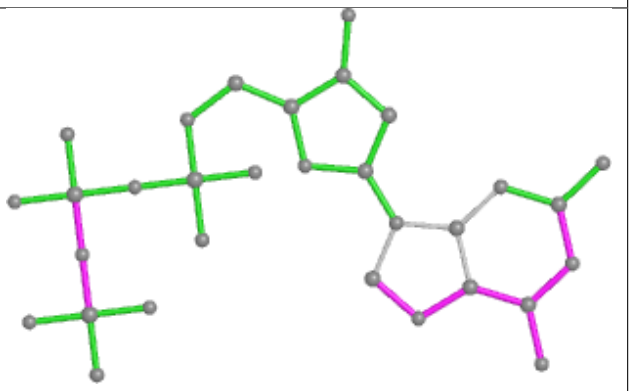
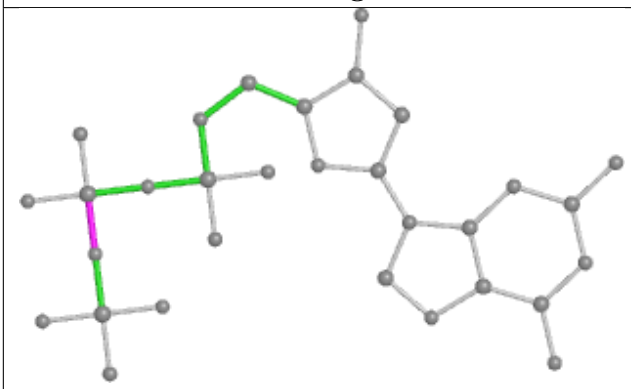


Bond angles



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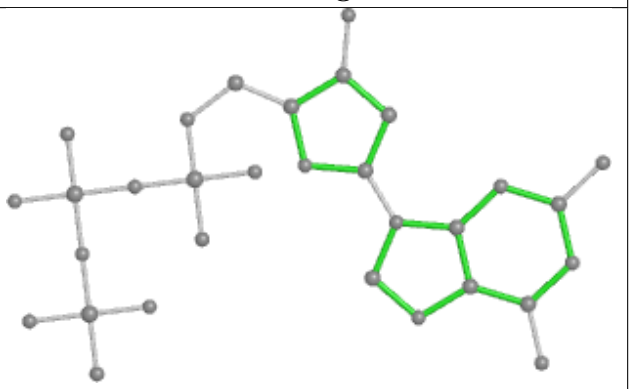
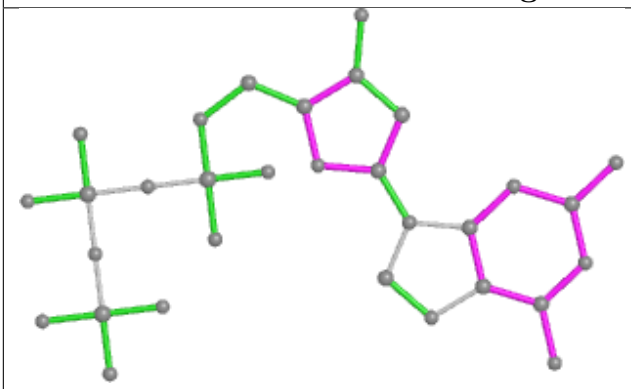


Rings

Ligand DGT H 703



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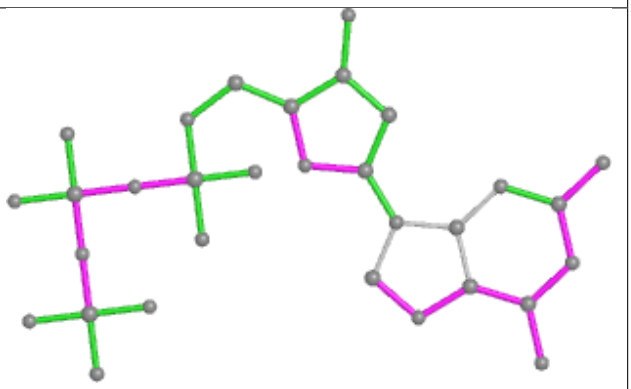
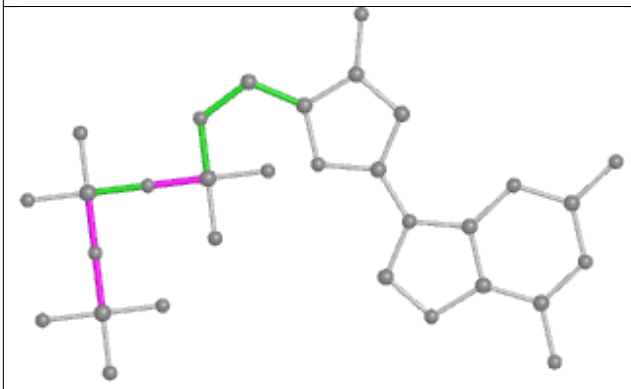


Bond angles



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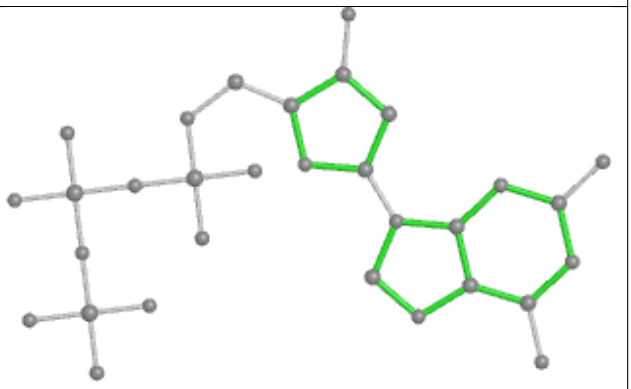
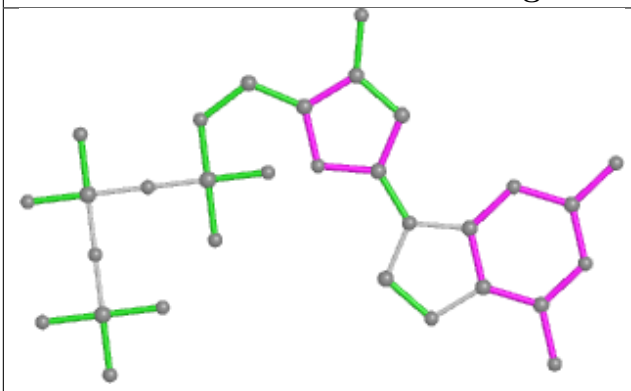


Rings

Ligand DGT F 702



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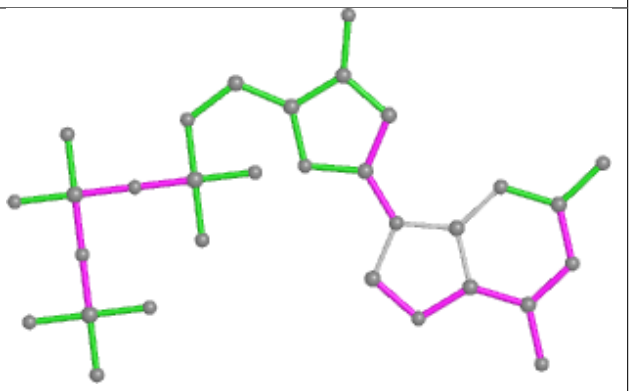
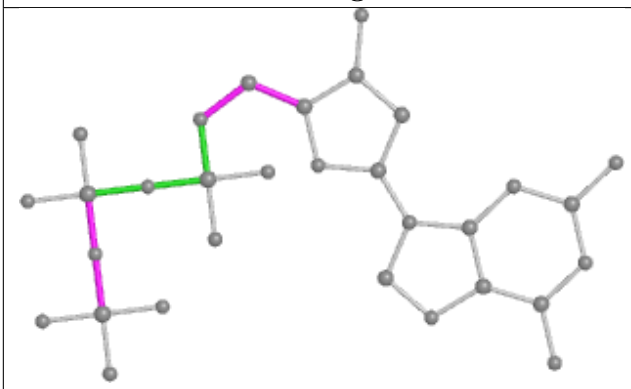


Bond angles



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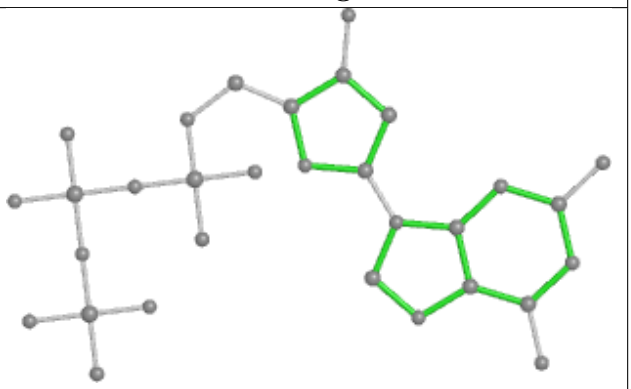
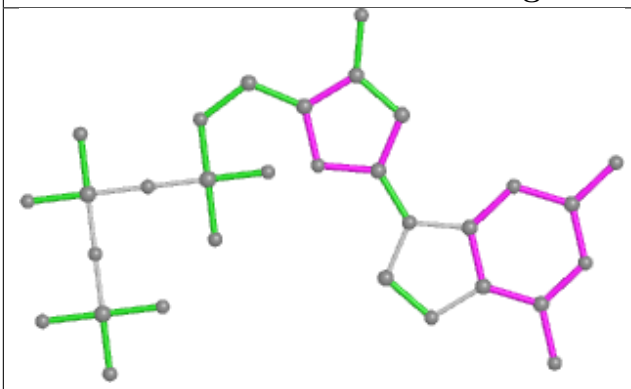


Rings

Ligand DGT F 701



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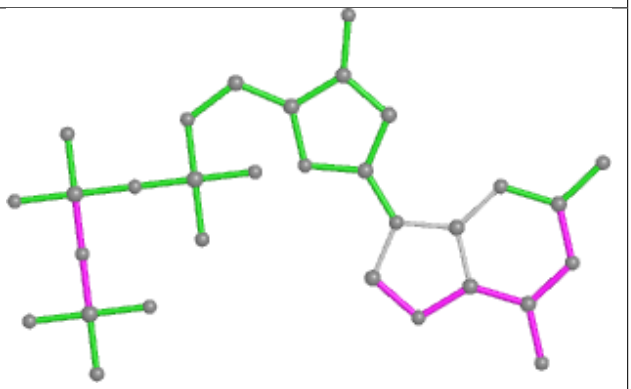
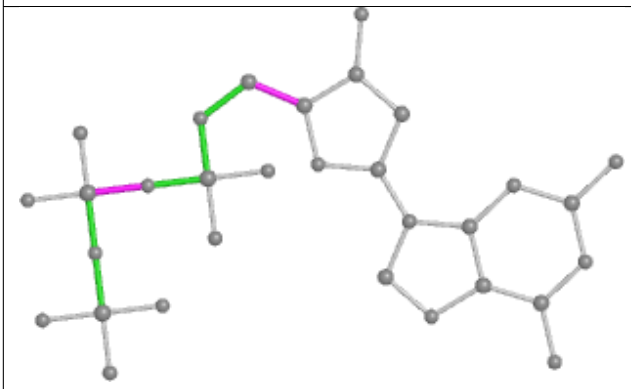


Bond angles



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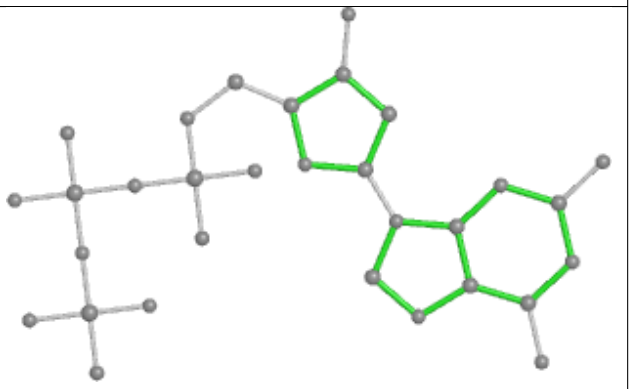
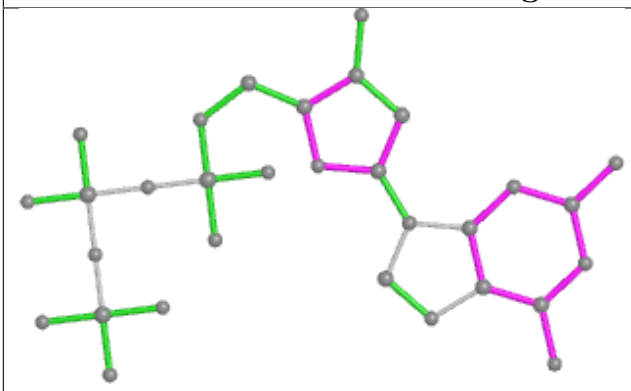
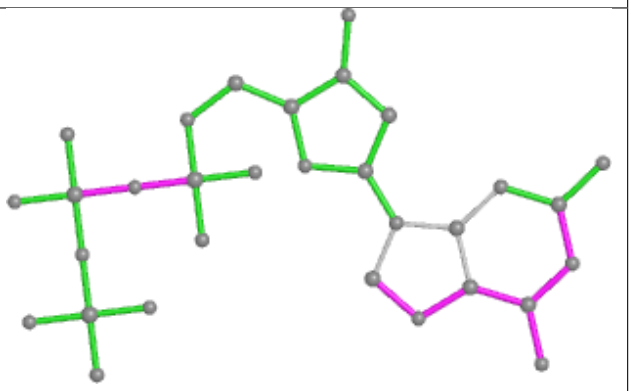


Rings

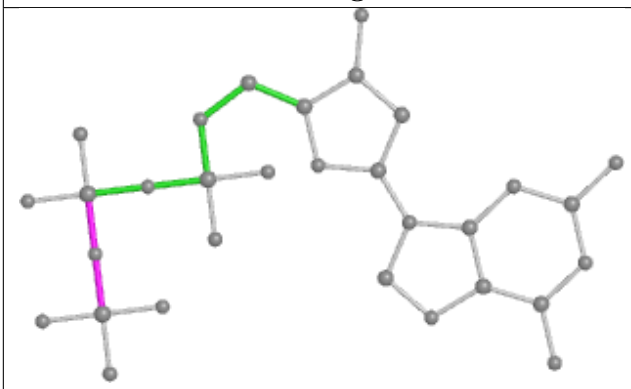
Ligand DGT C 706



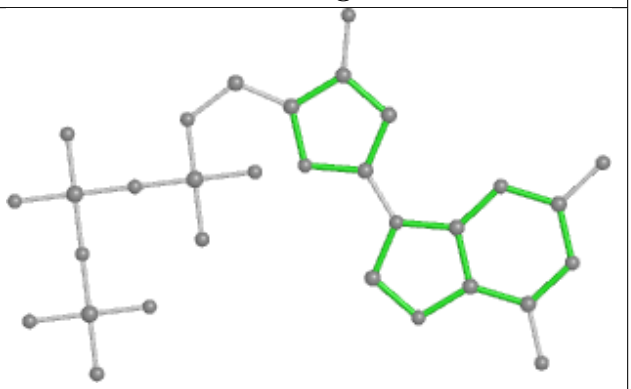
Bond lengths



Bond angles

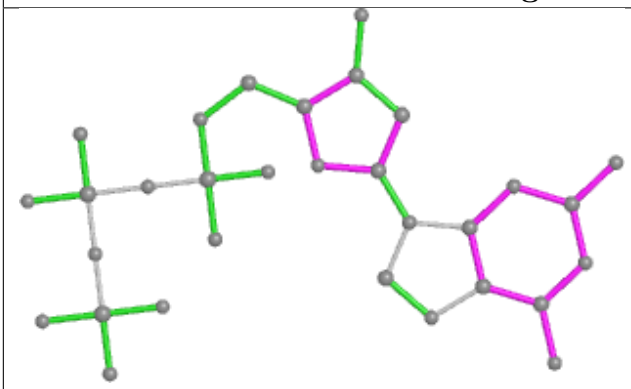


Torsions



Rings

Ligand DGT C 703



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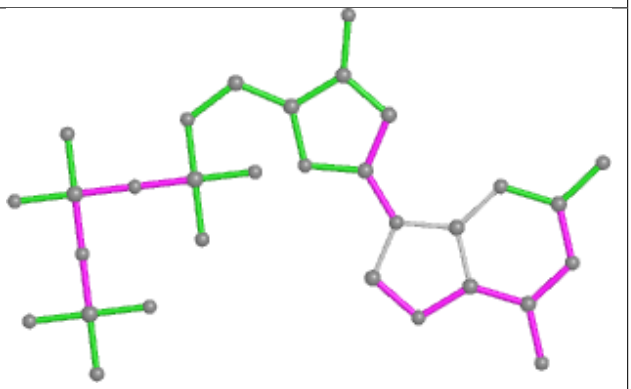
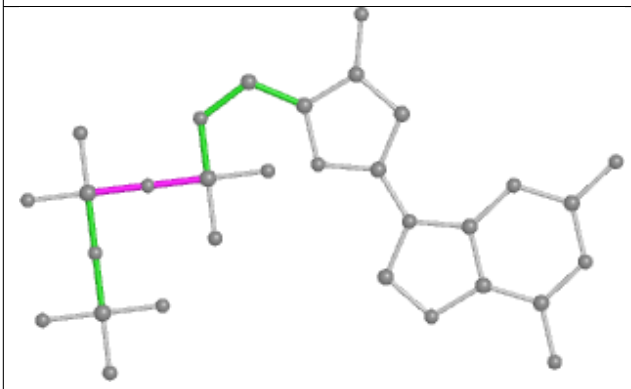
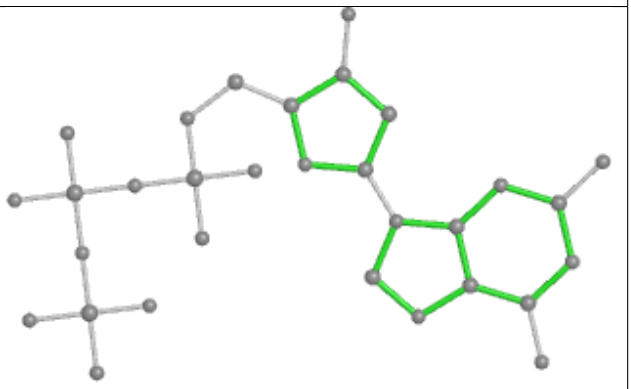


Bond angles

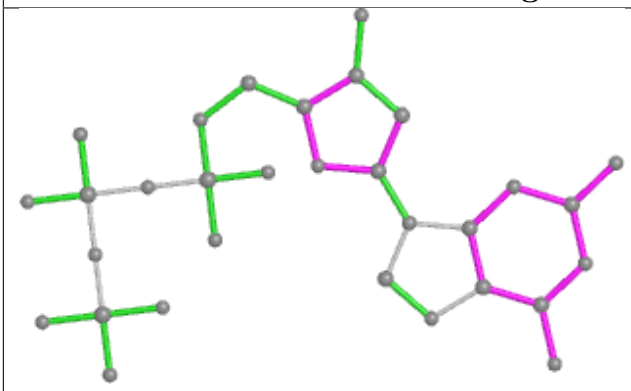


Torsions

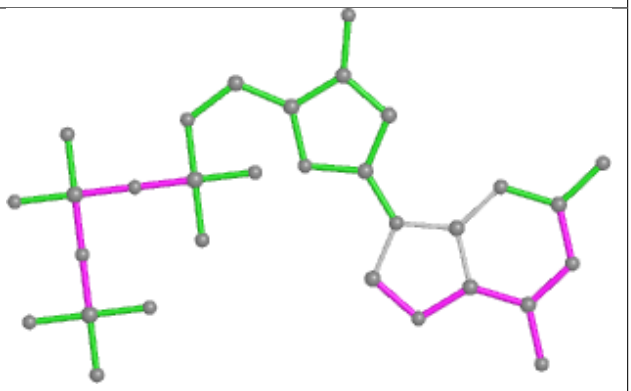


Rings

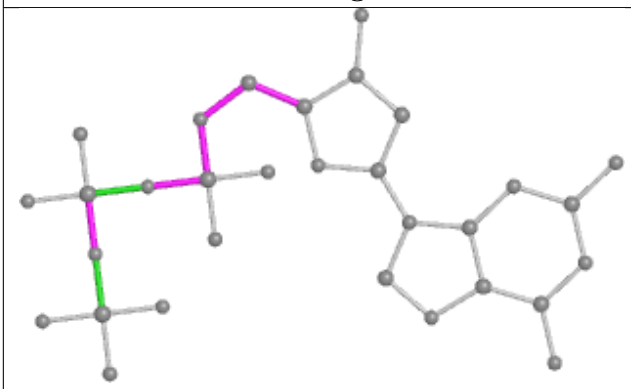
Ligand DGT C 701



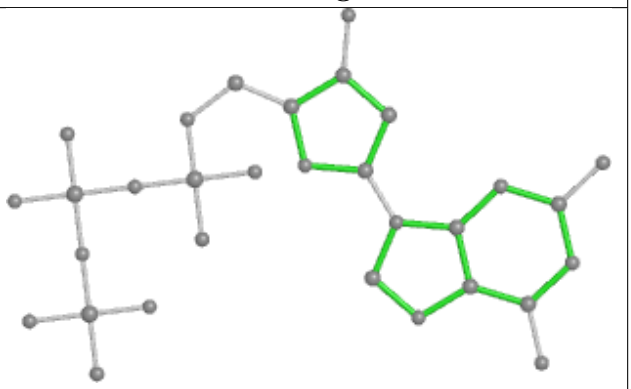
Bond lengths



Bond angles

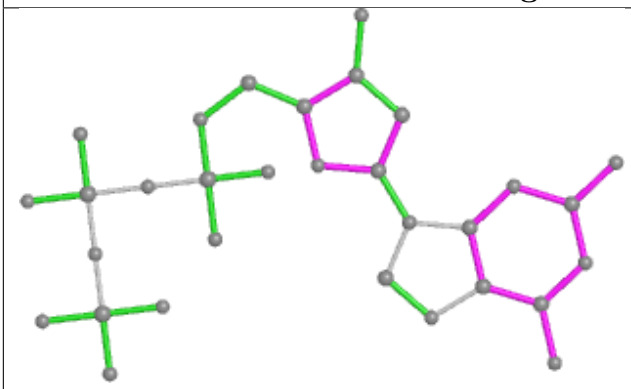


Torsions

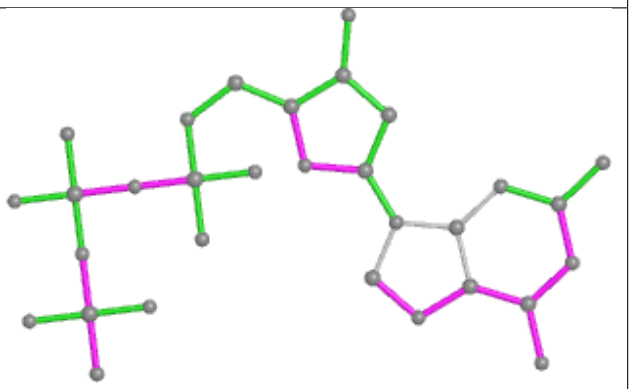


Rings

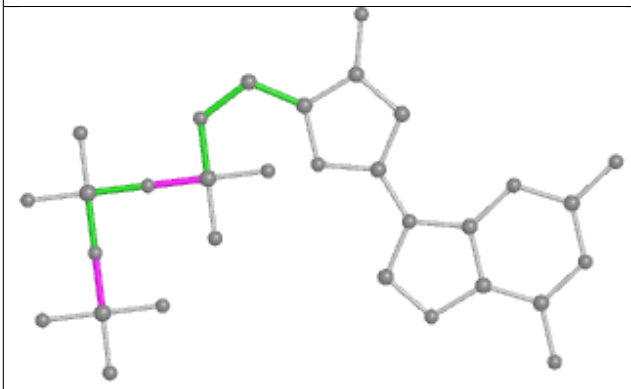
Ligand DGT D 705



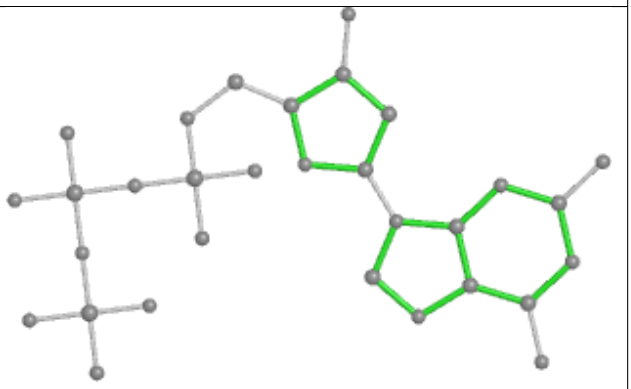
Bond lengths



Bond angles

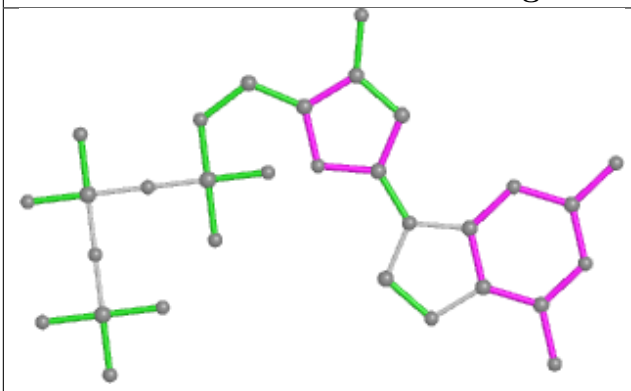


Torsions

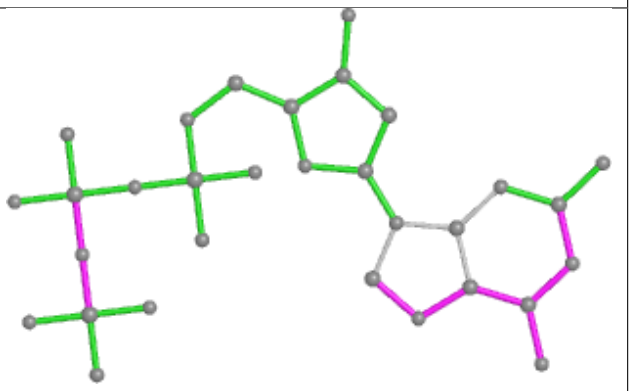


Rings

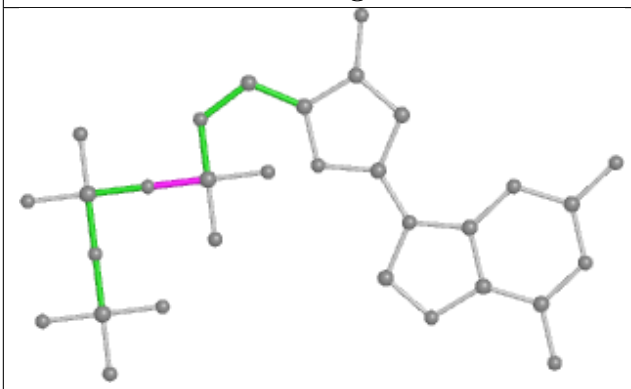
Ligand DGT E 704



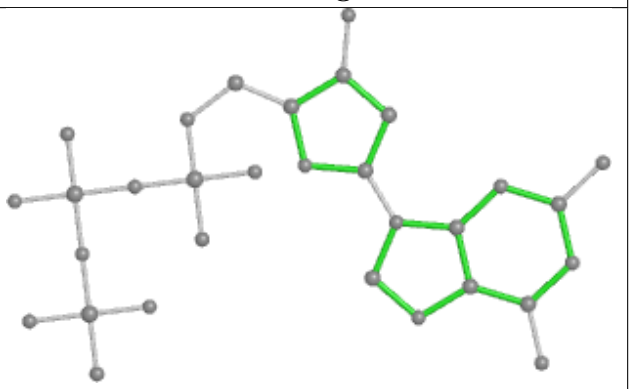
Bond lengths



Bond angles

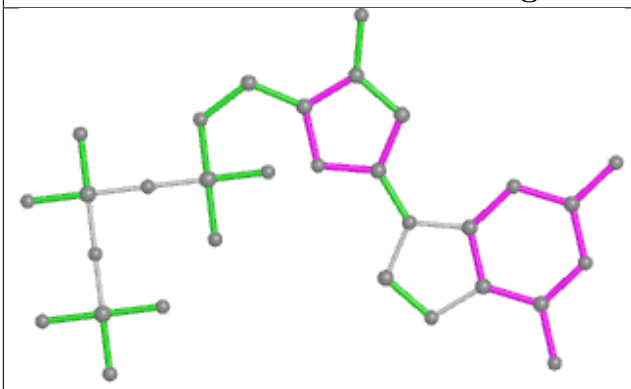


Torsions

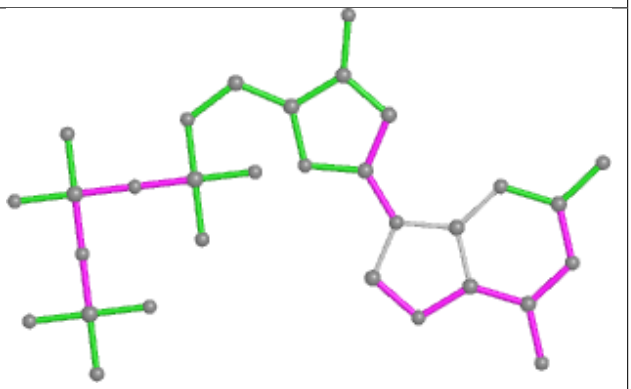


Rings

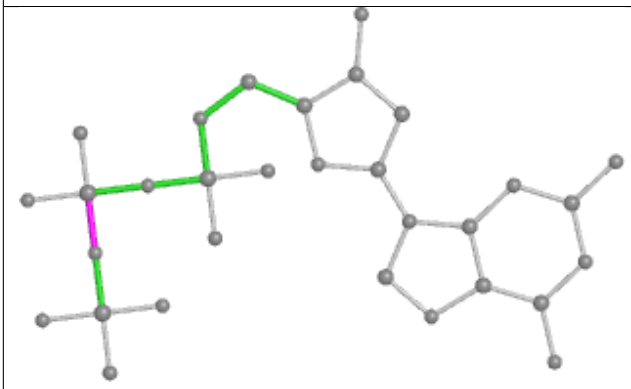
Ligand DGT A 703



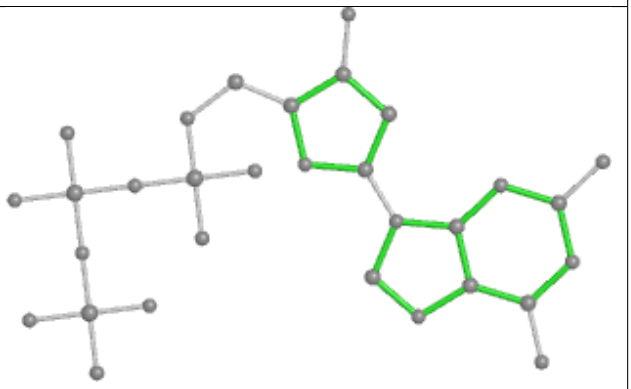
Bond lengths



Bond angles



Torsions



Rings

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	453/524 (86%)	0.01	10 (2%)	62	63	33, 51, 72, 94	0
1	B	453/524 (86%)	0.05	3 (0%)	87	89	38, 54, 79, 92	0
1	C	453/524 (86%)	0.04	8 (1%)	68	70	34, 50, 71, 81	0
1	D	387/524 (73%)	0.21	15 (3%)	39	38	37, 58, 74, 92	0
1	E	387/524 (73%)	0.09	4 (1%)	82	83	40, 60, 80, 93	0
1	F	453/524 (86%)	0.01	8 (1%)	68	70	37, 56, 82, 97	0
1	G	381/524 (72%)	0.15	13 (3%)	45	45	36, 58, 76, 92	0
1	H	381/524 (72%)	0.23	13 (3%)	45	45	43, 62, 83, 94	0
All	All	3348/4192 (79%)	0.09	74 (2%)	62	63	33, 56, 78, 97	0

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	551	ILE	4.6
1	G	396	TYR	4.2
1	H	551	ILE	4.1
1	D	457	VAL	3.8
1	C	587	VAL	3.8

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	G	705	1/1	0.63	0.66	76,76,76,76	0
3	MG	E	702	1/1	0.64	0.46	84,84,84,84	0
3	MG	H	702	1/1	0.68	0.73	88,88,88,88	0
3	MG	B	701	1/1	0.70	0.08	50,50,50,50	0
2	DGT	A	701	31/31	0.91	0.16	58,61,63,64	0
2	DGT	H	701	31/31	0.91	0.16	59,63,68,68	0
3	MG	C	704	1/1	0.92	0.11	55,55,55,55	0
2	DGT	F	702	31/31	0.92	0.15	61,64,70,71	0
2	DGT	A	703	31/31	0.92	0.29	88,91,96,98	0
2	DGT	D	703	31/31	0.92	0.16	64,70,73,75	0
2	DGT	B	703	31/31	0.93	0.17	59,62,70,71	0
2	DGT	G	704	31/31	0.93	0.16	66,68,69,70	0
2	DGT	G	706	31/31	0.93	0.15	51,55,59,59	0
3	MG	E	705	1/1	0.93	0.16	57,57,57,57	0
2	DGT	E	701	31/31	0.93	0.15	60,63,67,68	0
3	MG	A	702	1/1	0.93	0.20	57,57,57,57	0
3	MG	H	704	1/1	0.93	0.09	54,54,54,54	0
3	MG	D	704	1/1	0.94	0.33	61,61,61,61	0
2	DGT	H	703	31/31	0.94	0.16	57,59,63,64	0
2	DGT	C	701	31/31	0.94	0.13	52,56,59,60	0
2	DGT	D	705	31/31	0.95	0.19	71,73,76,77	0
3	MG	F	703	1/1	0.95	0.23	58,58,58,58	0
2	DGT	D	701	31/31	0.95	0.12	35,37,39,41	0
2	DGT	F	701	31/31	0.95	0.16	46,48,54,55	0
3	MG	A	705	1/1	0.95	0.15	60,60,60,60	0
2	DGT	B	705	31/31	0.96	0.25	59,64,70,71	0
2	DGT	B	702	31/31	0.96	0.19	63,66,68,69	0
3	MG	G	703	1/1	0.96	0.31	49,49,49,49	0
2	DGT	C	703	31/31	0.96	0.11	36,38,42,43	0
2	DGT	C	705	31/31	0.96	0.20	60,64,70,71	0
2	DGT	A	704	31/31	0.96	0.12	39,42,44,45	0
2	DGT	C	706	31/31	0.97	0.11	46,49,52,53	0
2	DGT	E	703	31/31	0.97	0.14	61,63,67,68	0
3	MG	B	704	1/1	0.97	0.44	53,53,53,53	0
2	DGT	G	702	31/31	0.97	0.13	34,36,38,40	0
2	DGT	H	705	31/31	0.97	0.28	60,64,69,71	0
2	DGT	E	704	31/31	0.97	0.25	59,62,69,70	0

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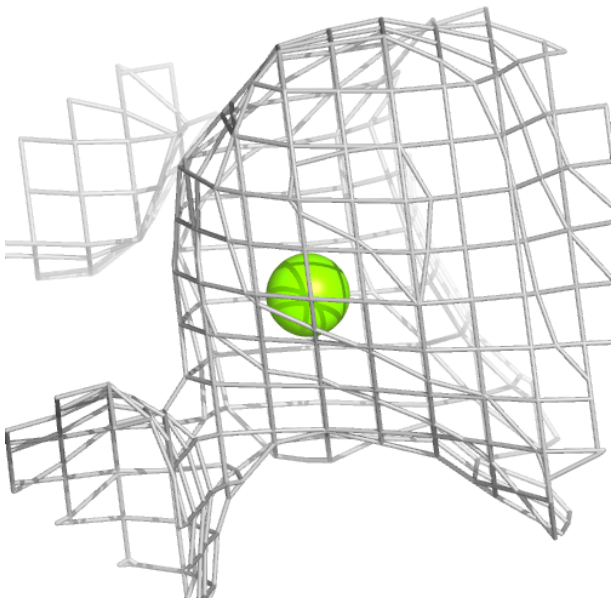
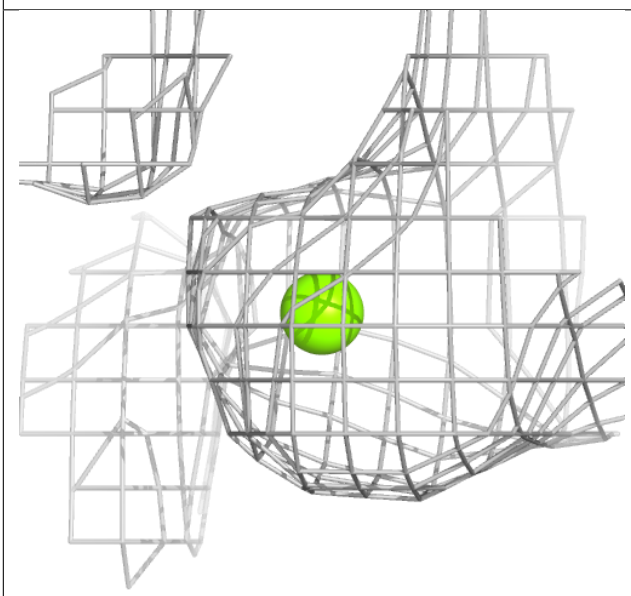
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	D	702	1/1	0.98	0.07	59,59,59,59	0
3	MG	G	701	1/1	0.98	0.15	59,59,59,59	0
3	MG	C	702	1/1	0.98	0.21	56,56,56,56	0

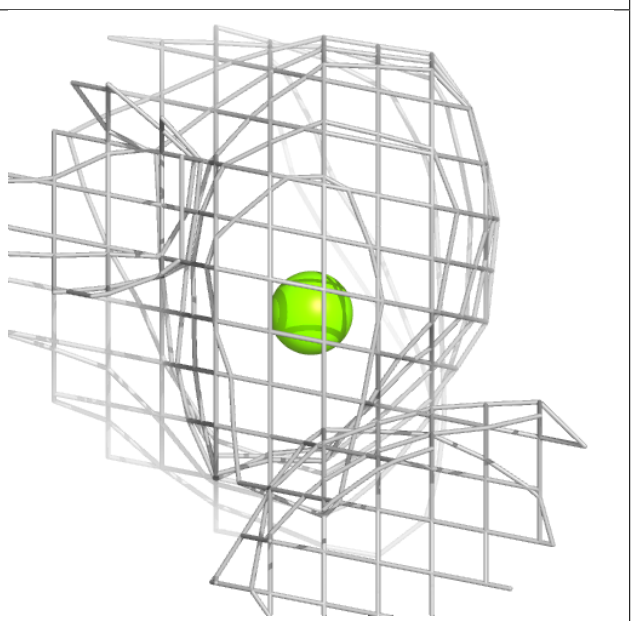
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MG G 705:

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

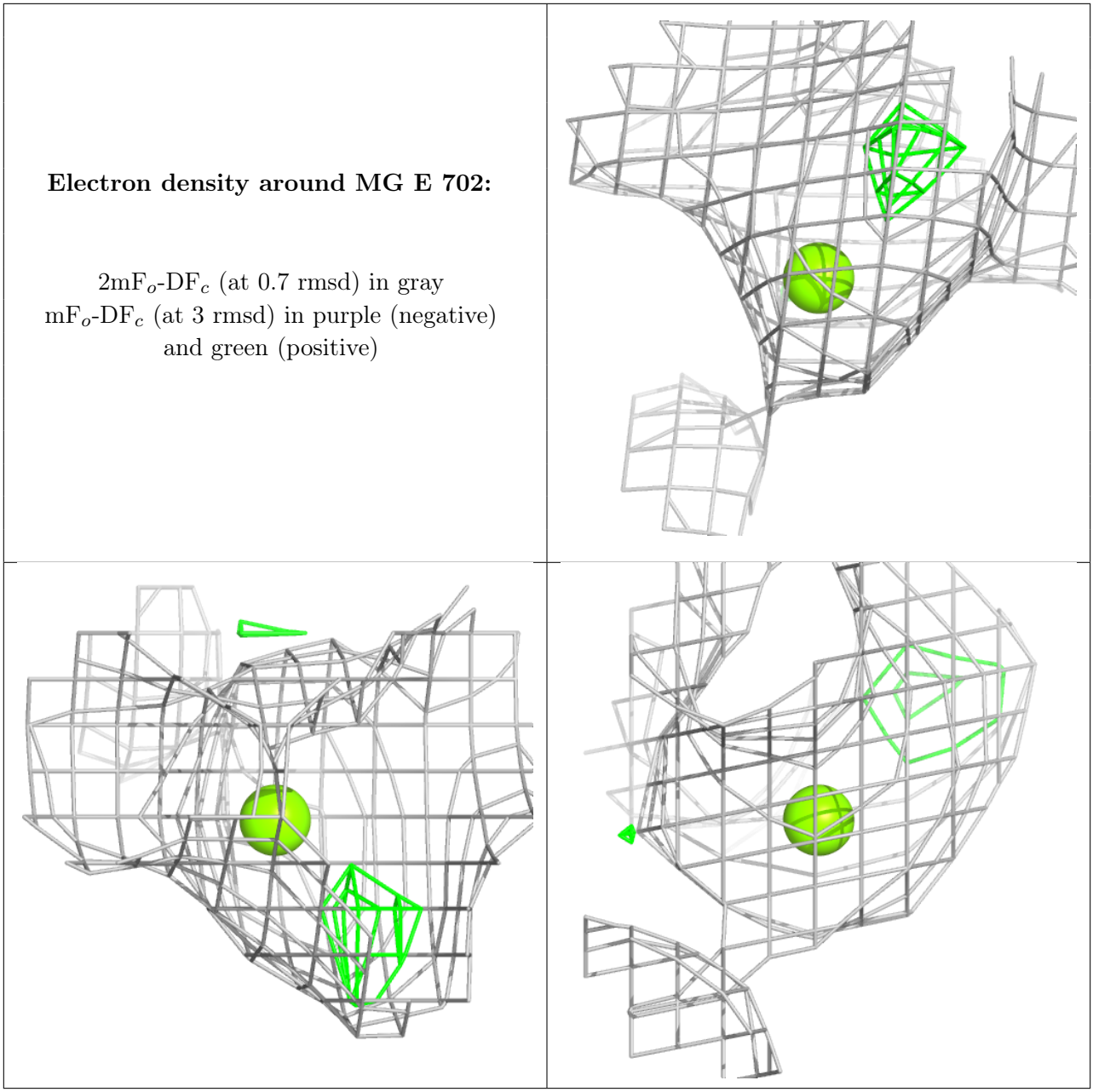






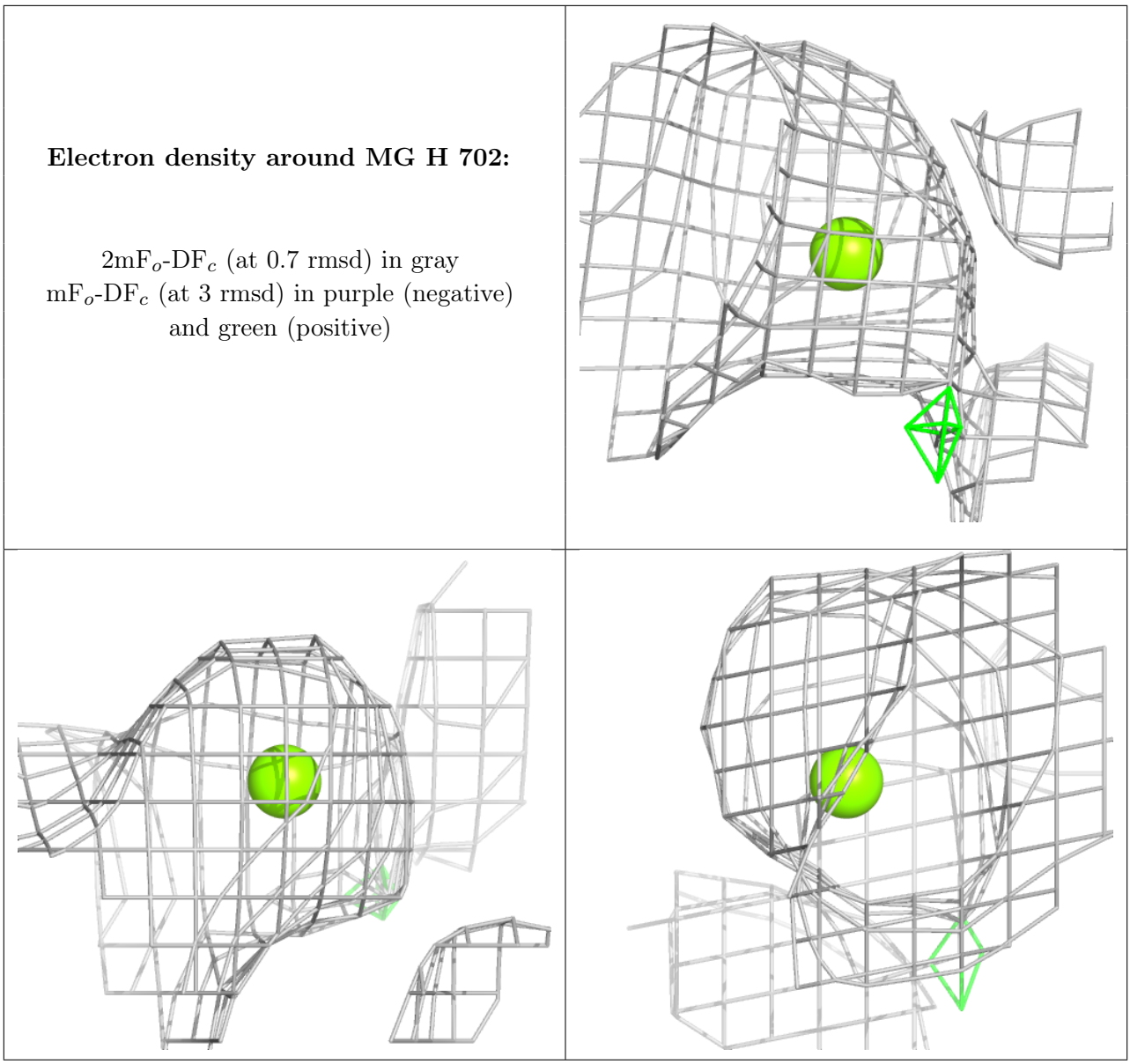
Electron density around MG E 702:

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



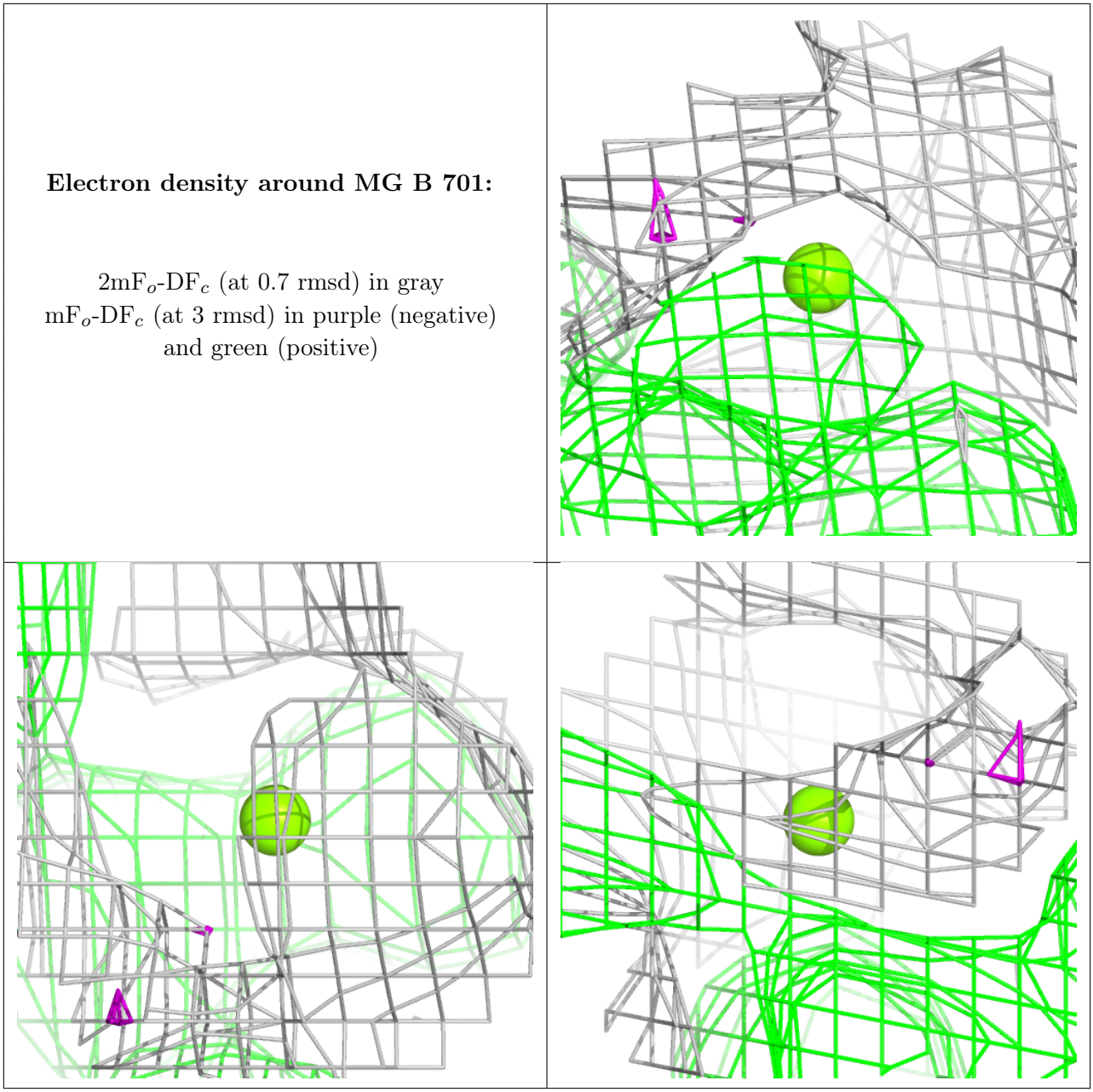
Electron density around MG H 702:

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



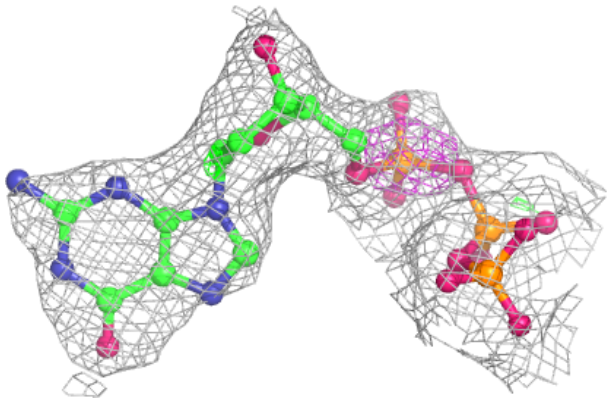
Electron density around MG B 701:

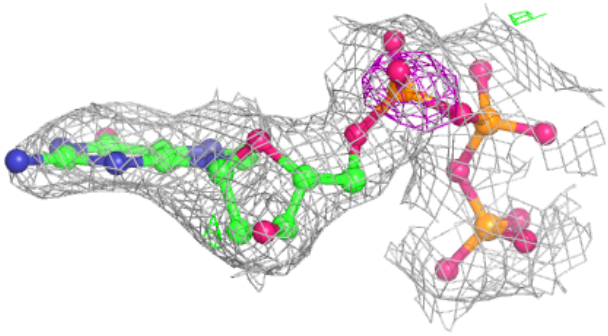
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

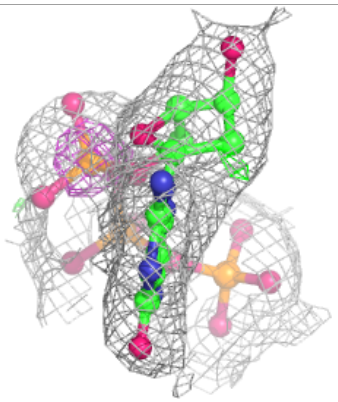


Electron density around DGT A 701:

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

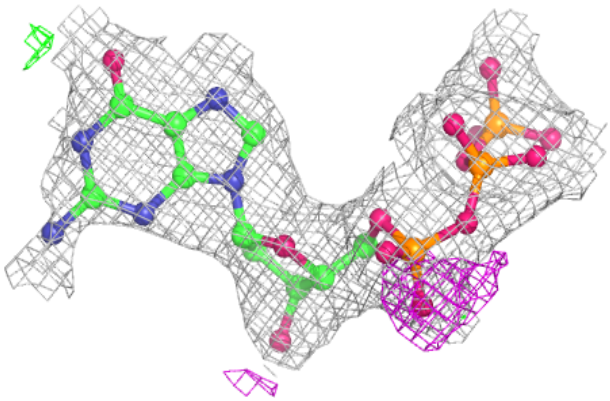


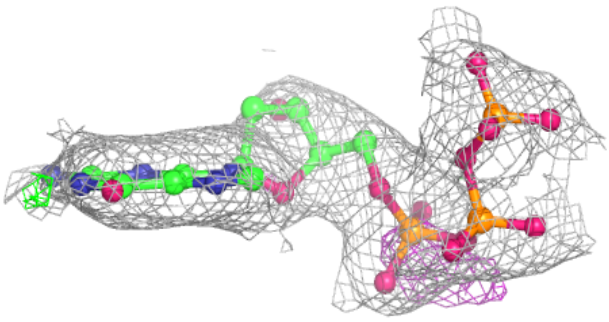


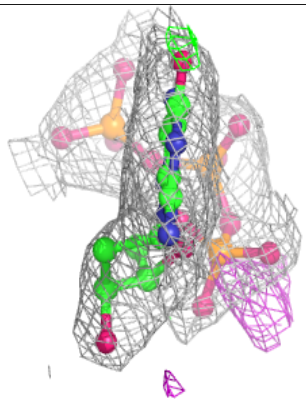


Electron density around DGT H 701:

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

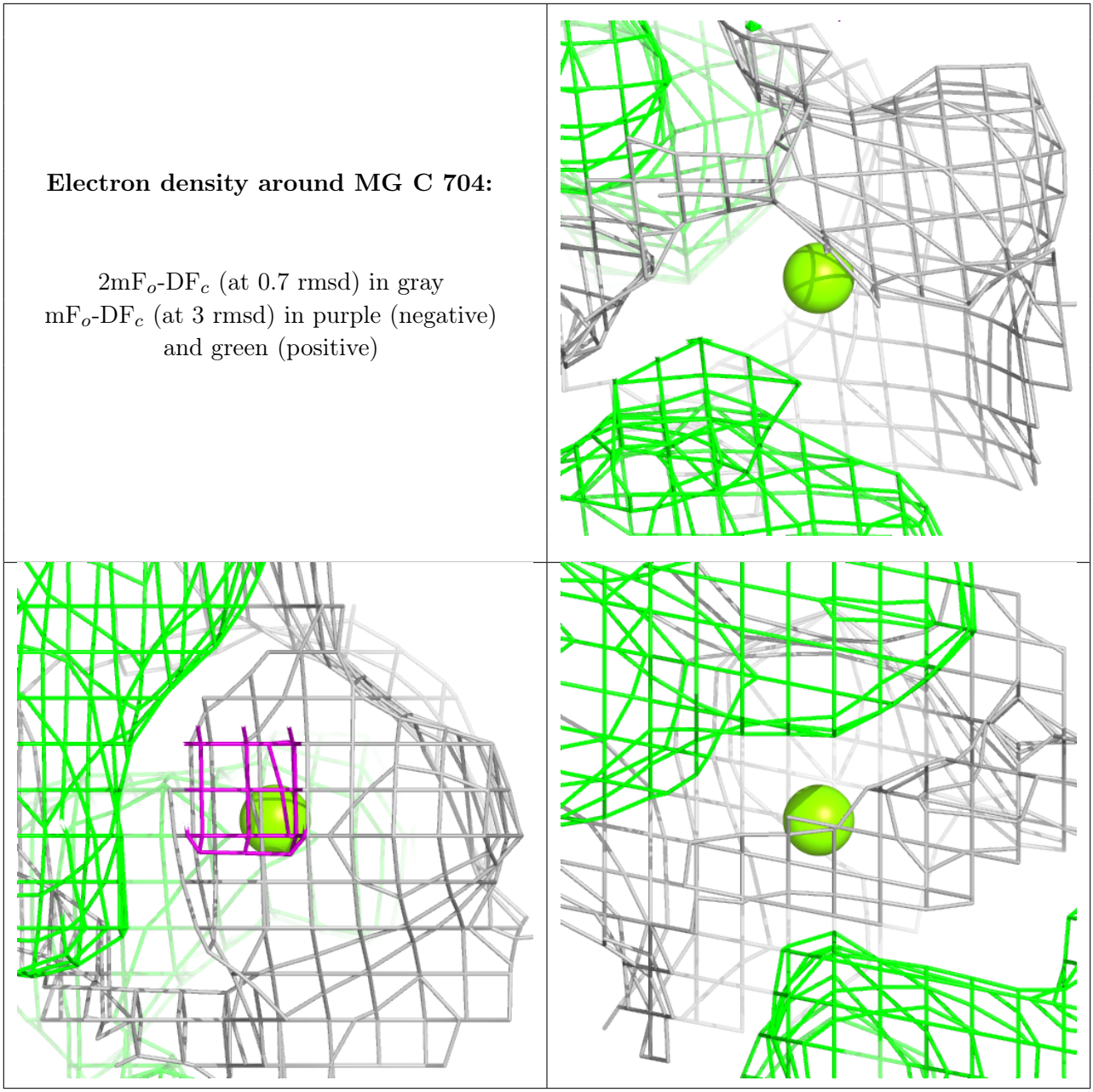






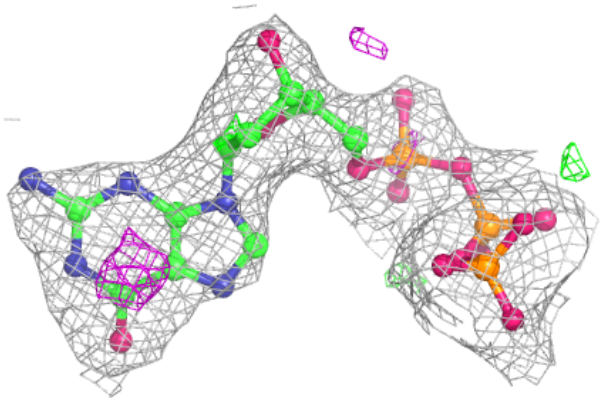
Electron density around MG C 704:

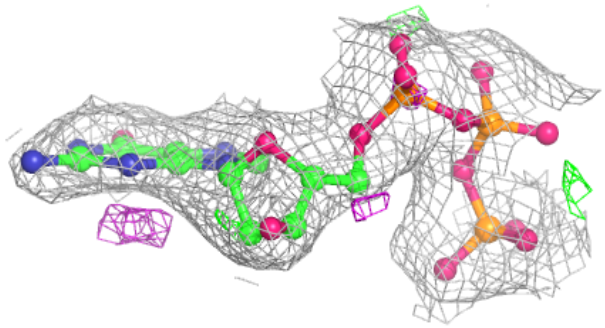
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

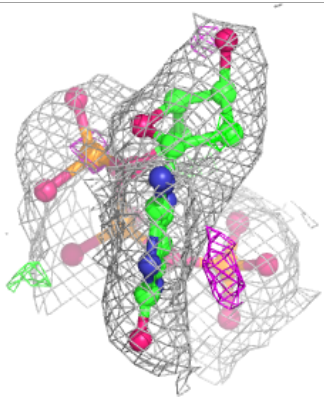


Electron density around DGT F 702:

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

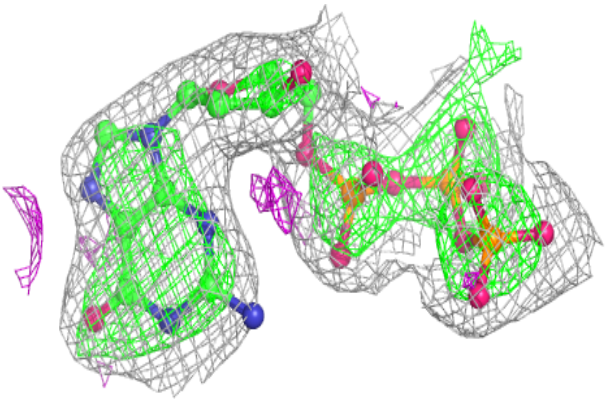


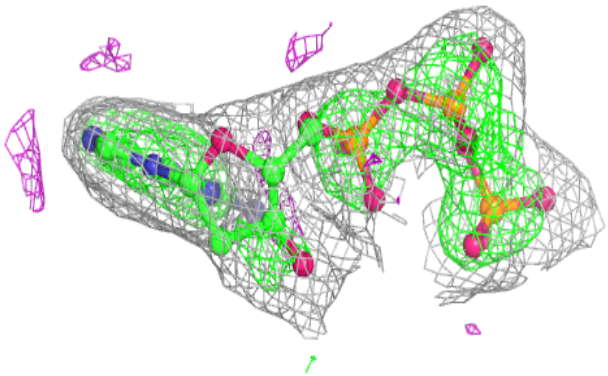


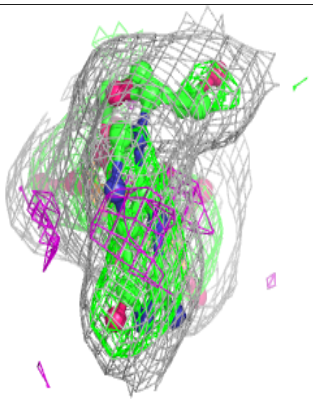


Electron density around DGT A 703:

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

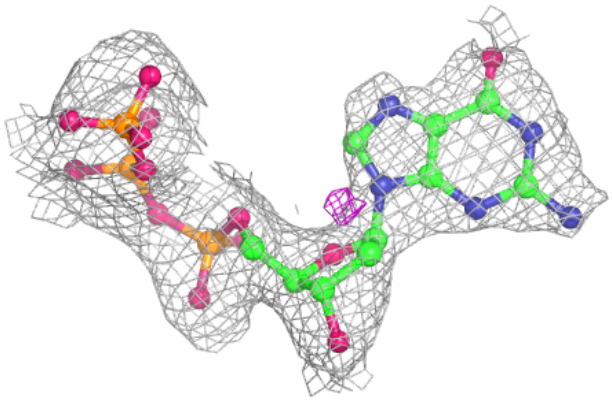


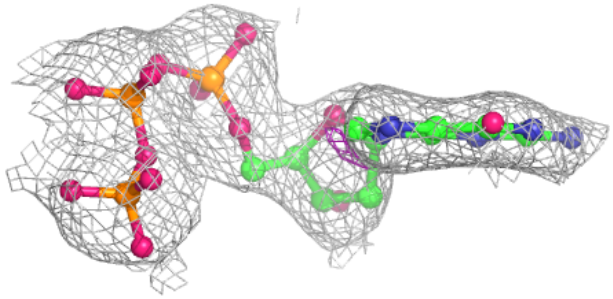


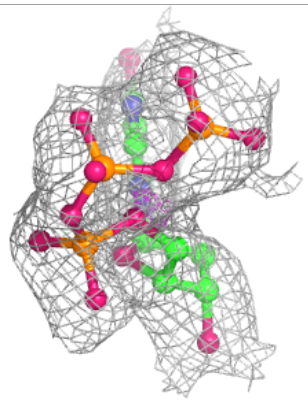


Electron density around DGT D 703:

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

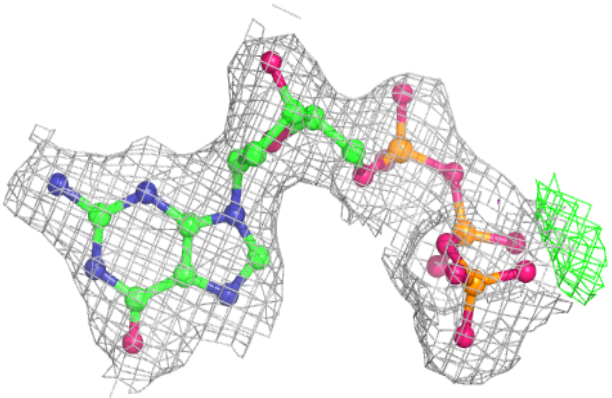


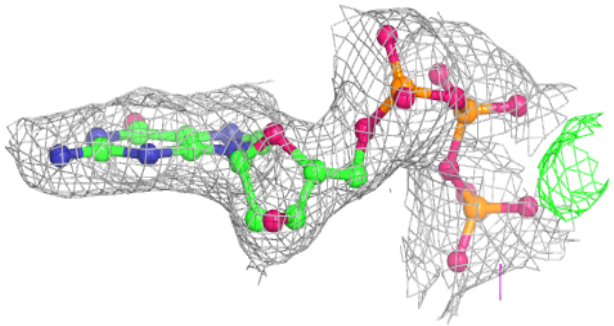


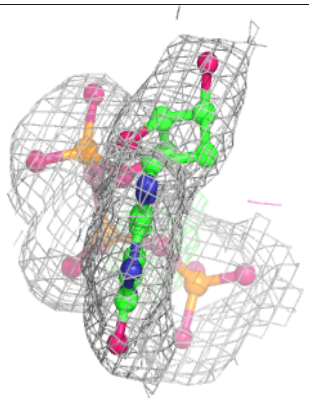


Electron density around DGT B 703:

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

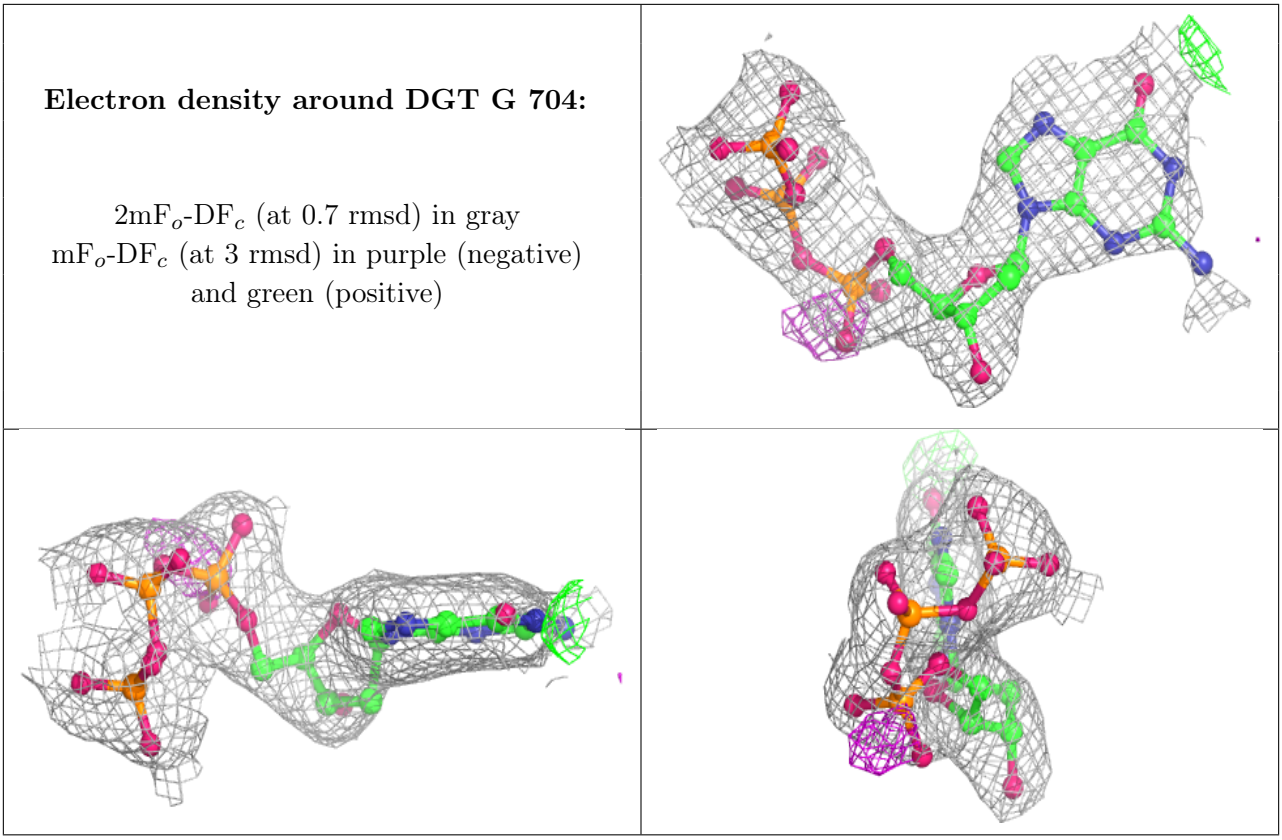






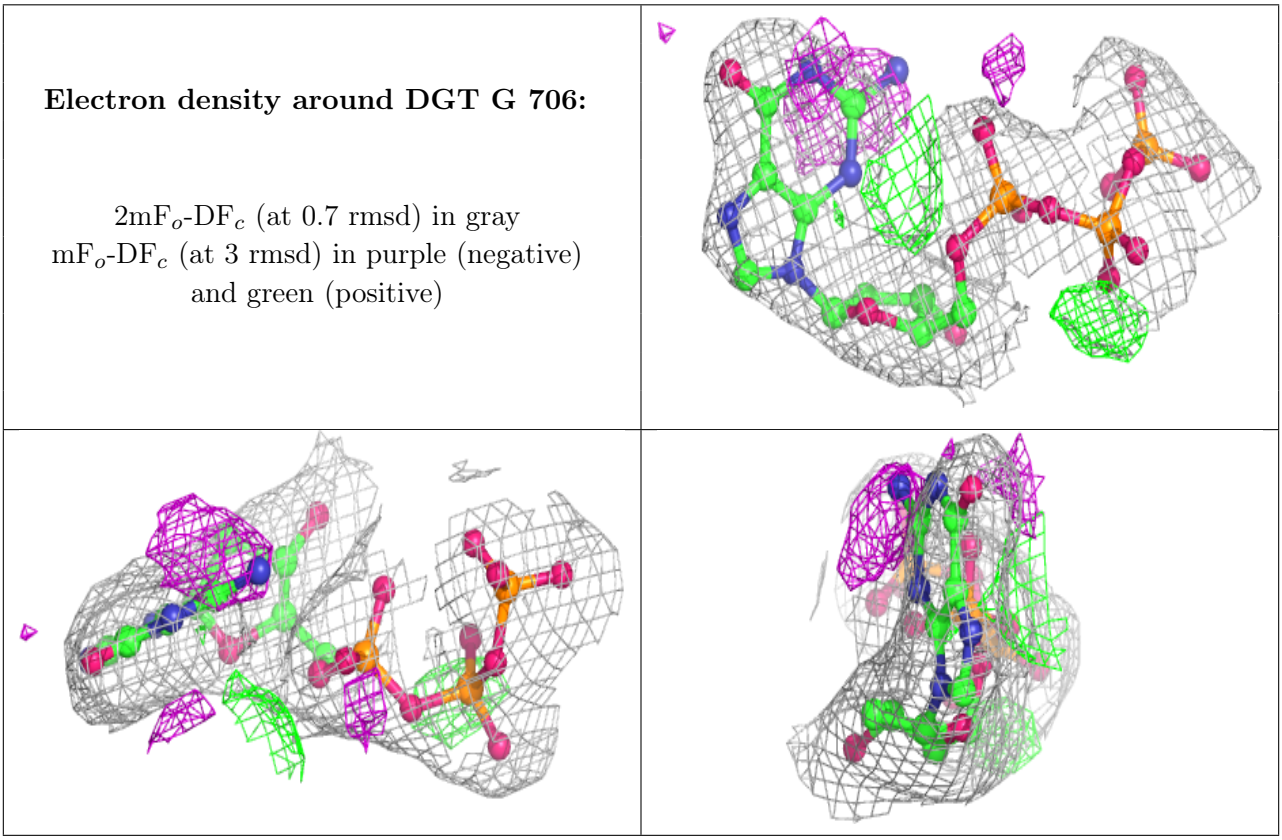
Electron density around DGT G 704:

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



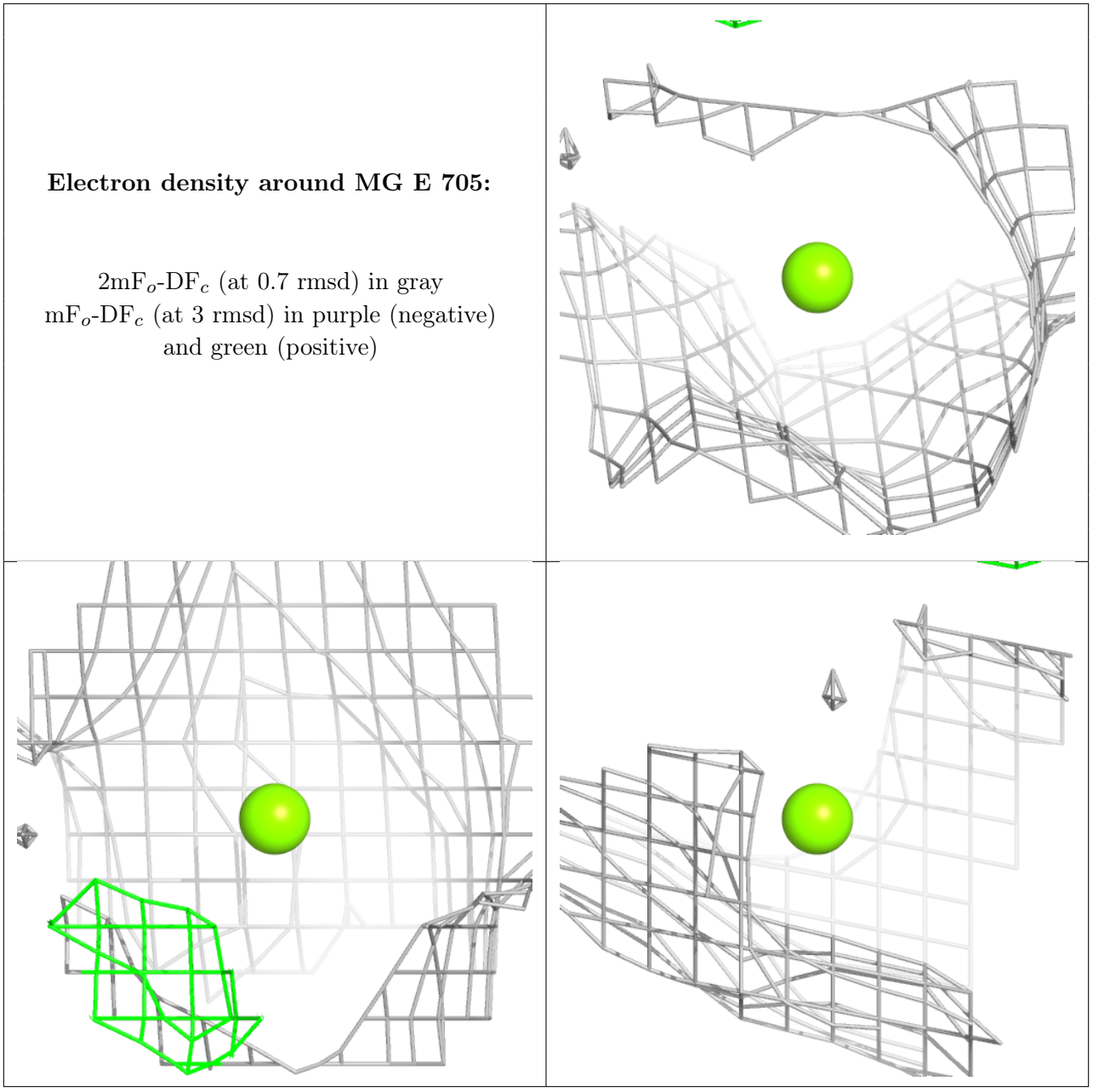
Electron density around DGT G 706:

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



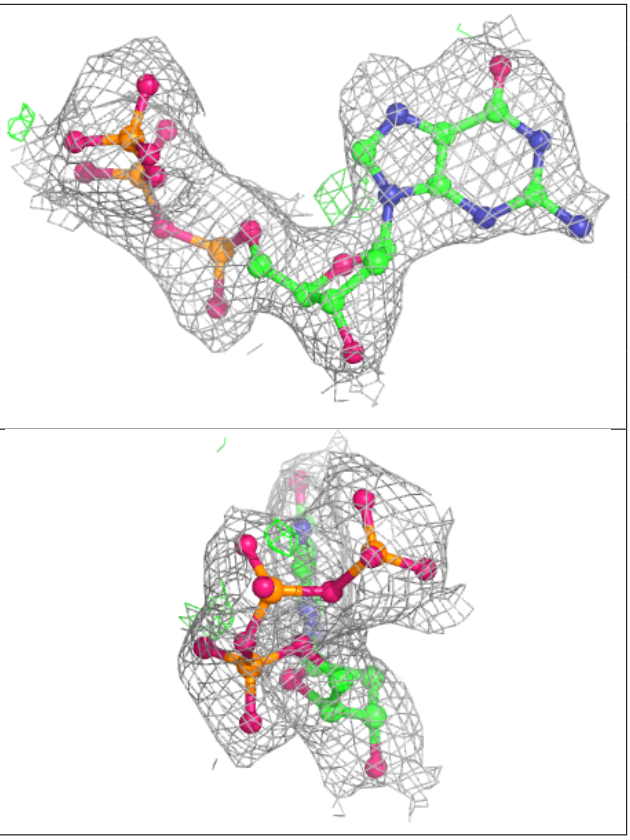
Electron density around MG E 705:

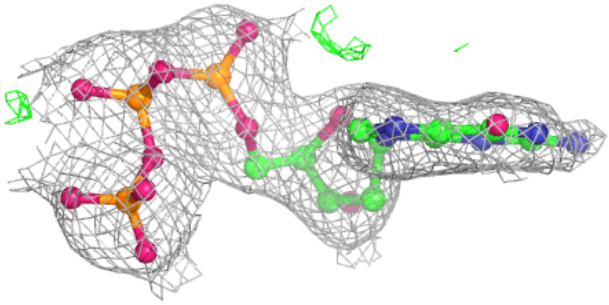
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around DGT E 701:

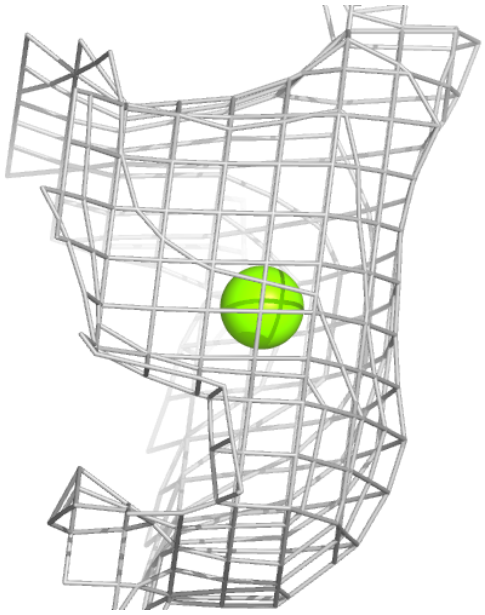
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

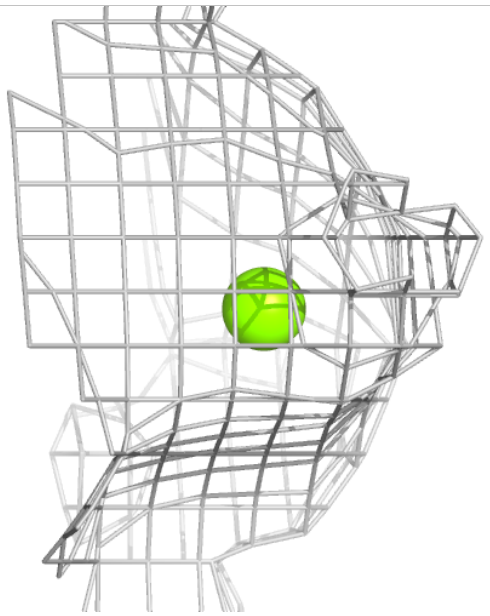


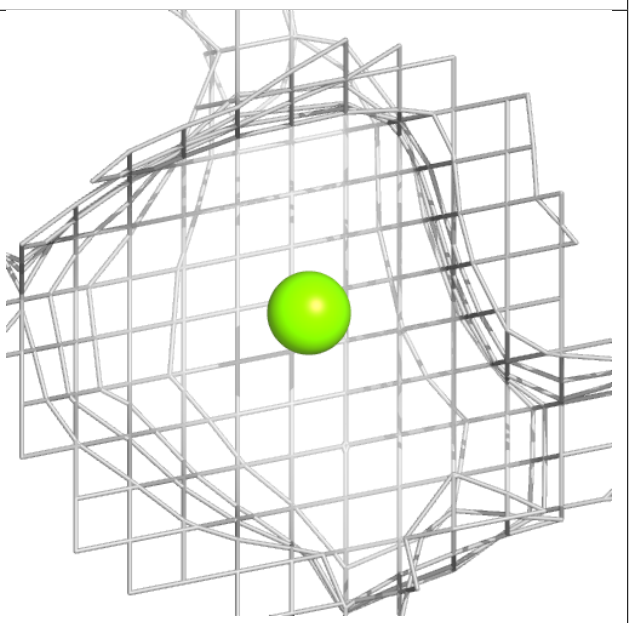


Electron density around MG A 702:

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

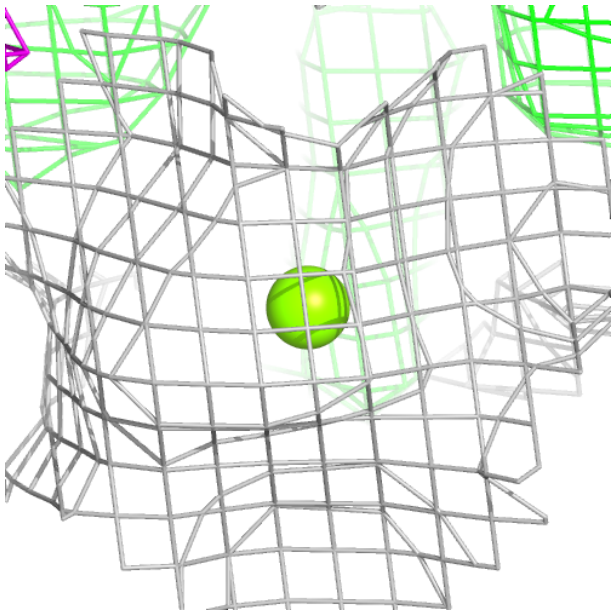


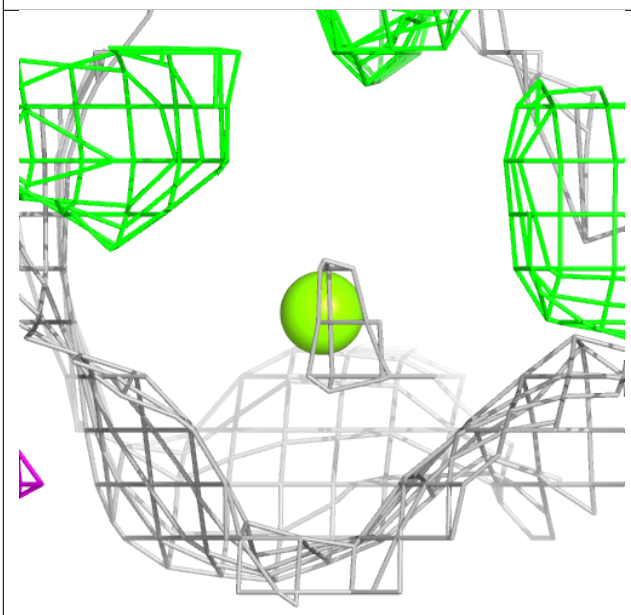


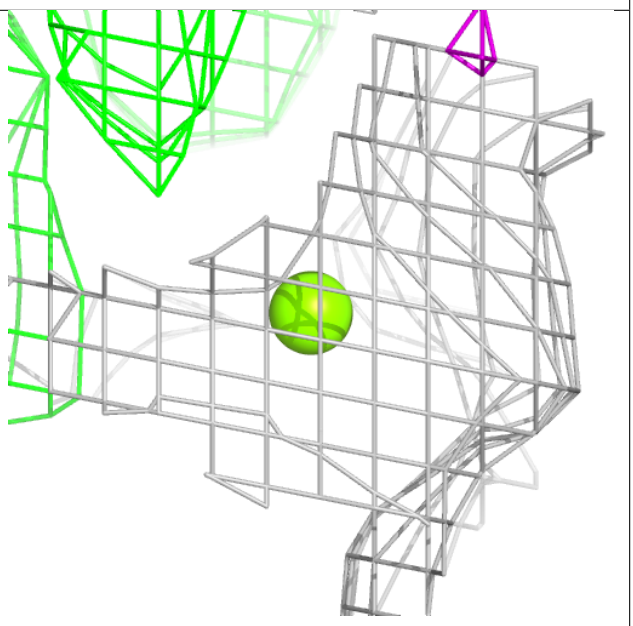


Electron density around MG H 704:

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

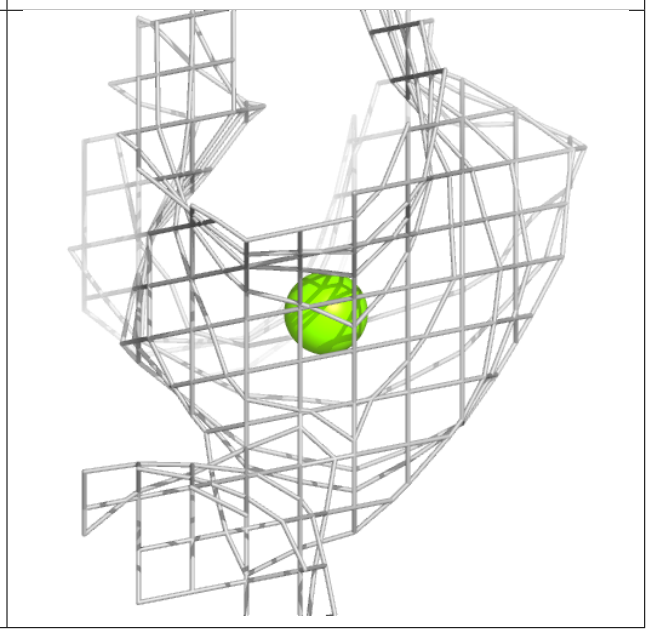






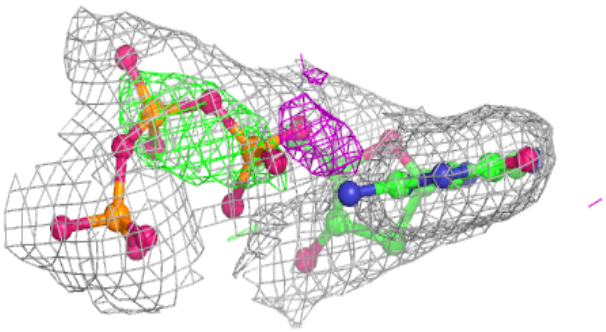
Electron density around MG D 704:

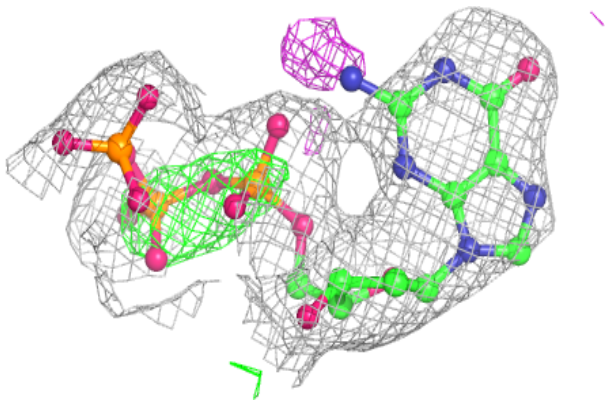
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

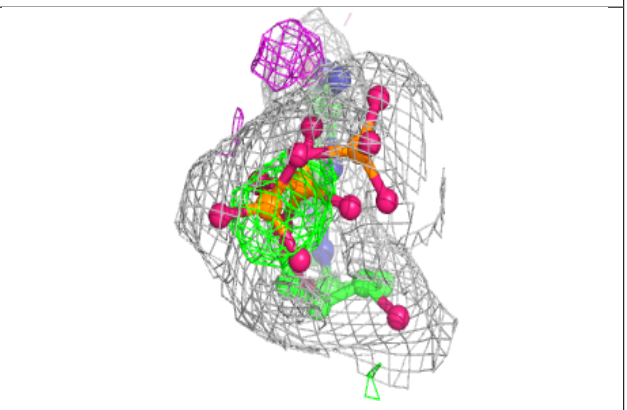


Electron density around DGT H 703:

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

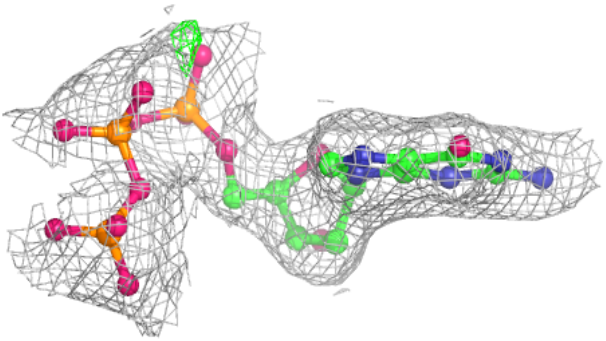


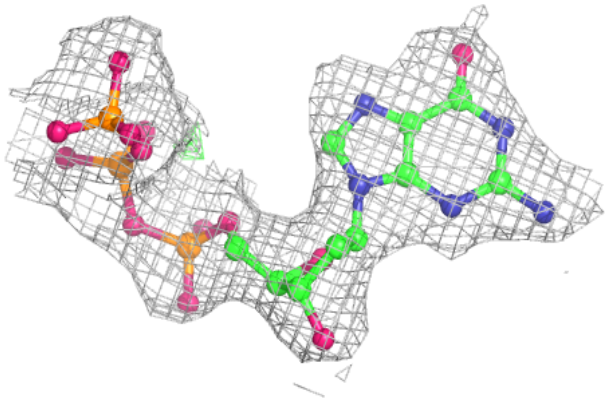


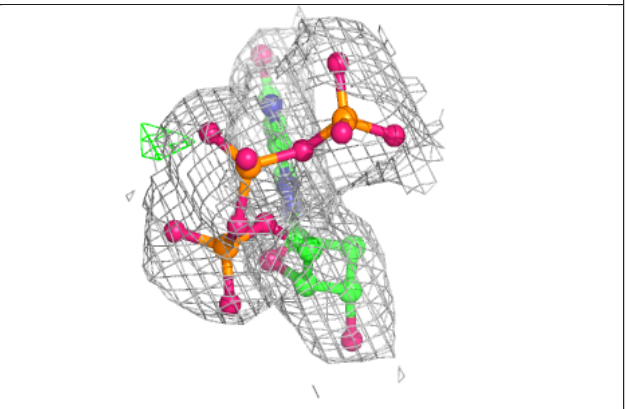


Electron density around DGT C 701:

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

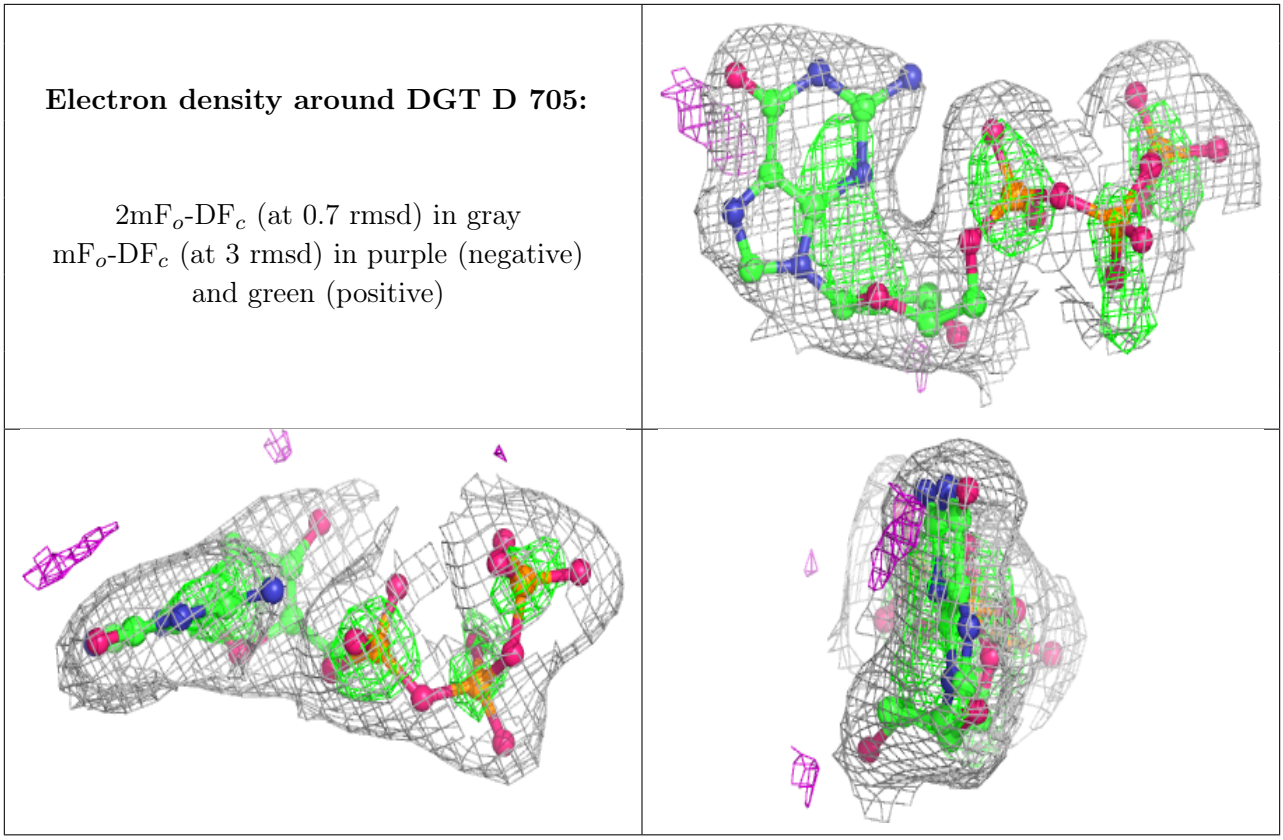






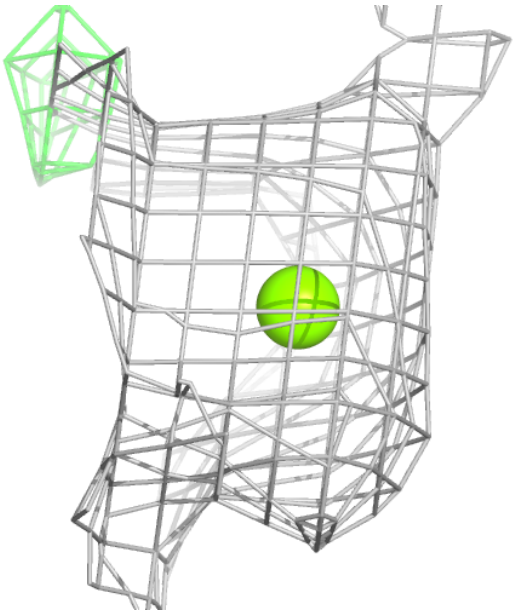
Electron density around DGT D 705:

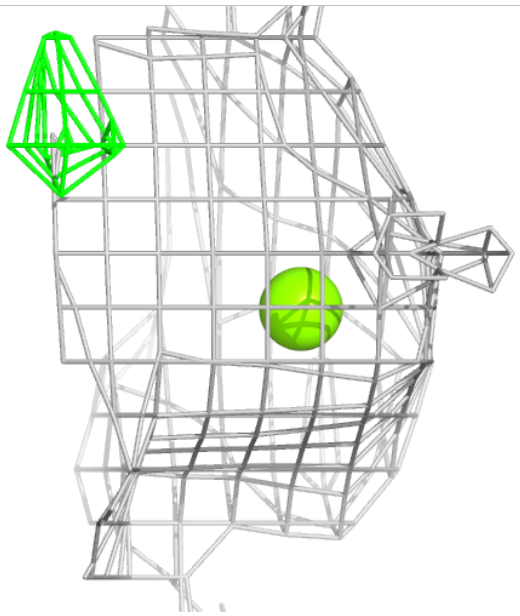
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

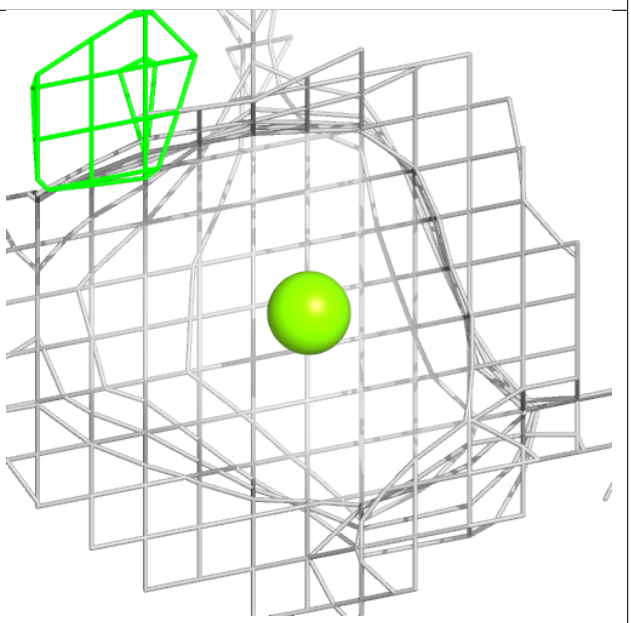


Electron density around MG F 703:

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

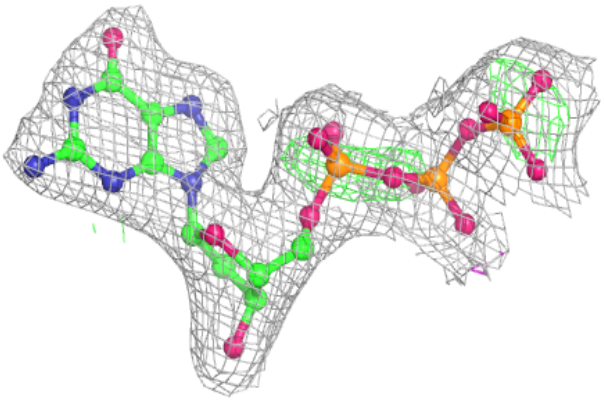


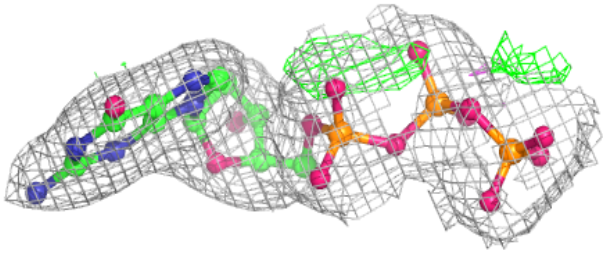


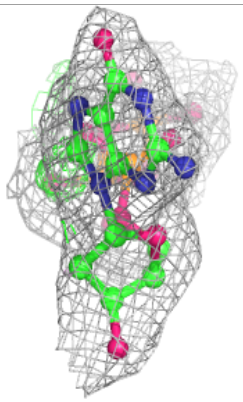


Electron density around DGT D 701:

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

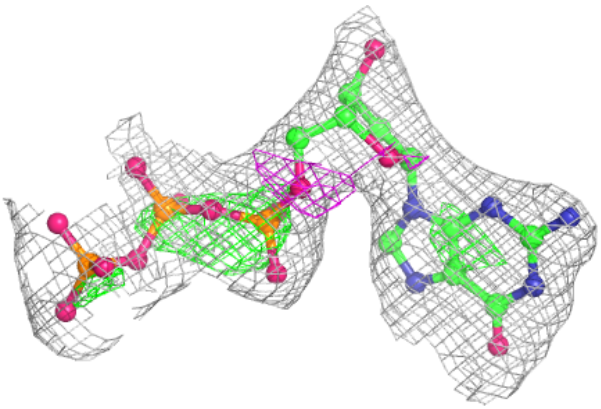


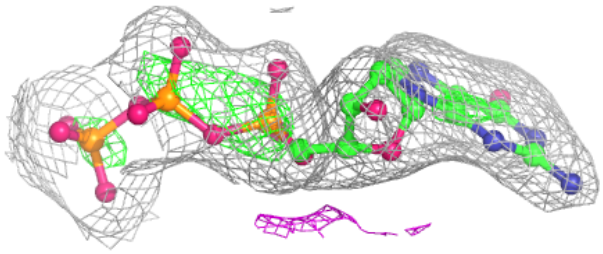


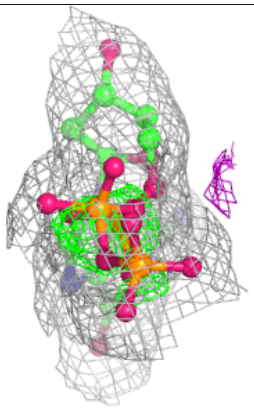


Electron density around DGT F 701:

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

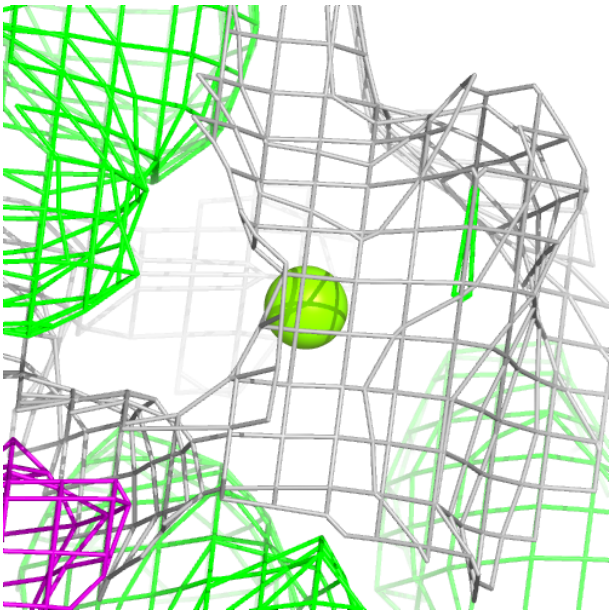


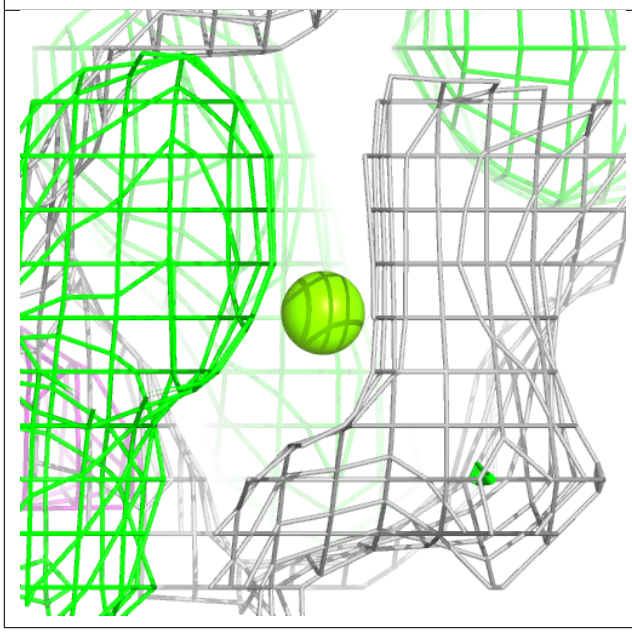


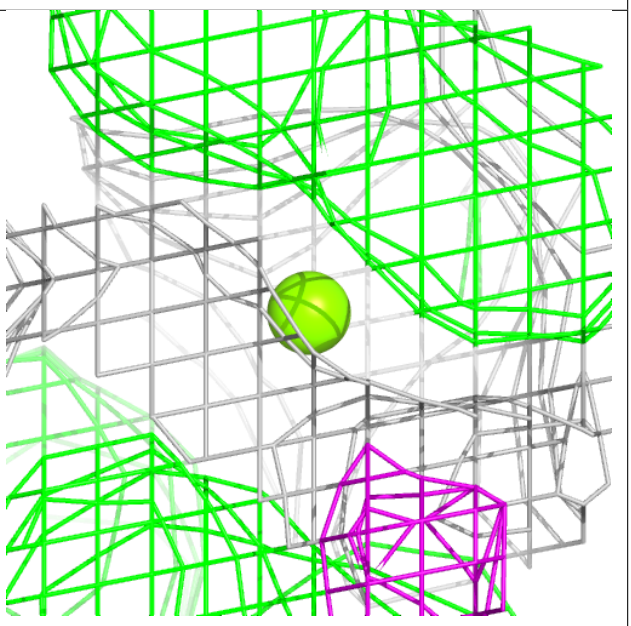


Electron density around MG A 705:

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

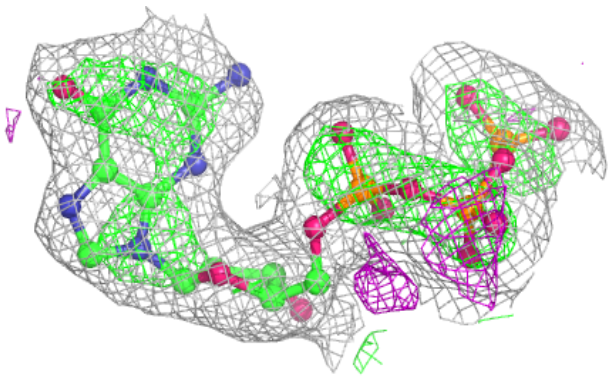


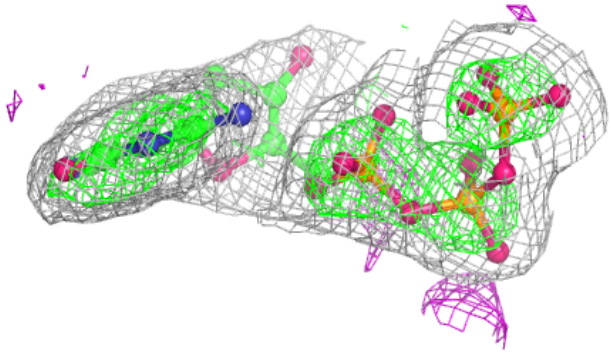


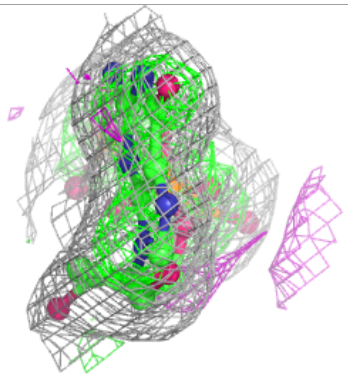


Electron density around DGT B 705:

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

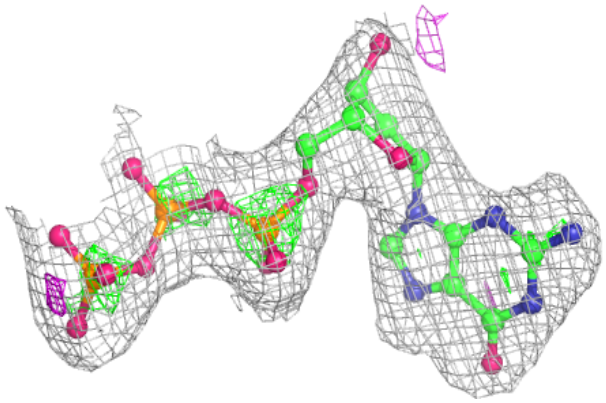


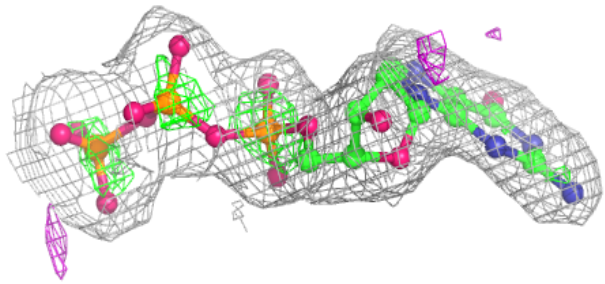


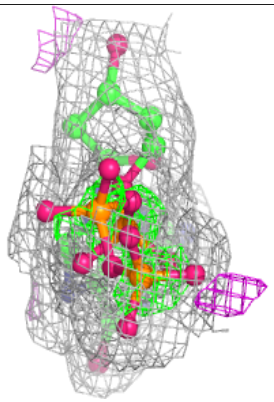


Electron density around DGT B 702:

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

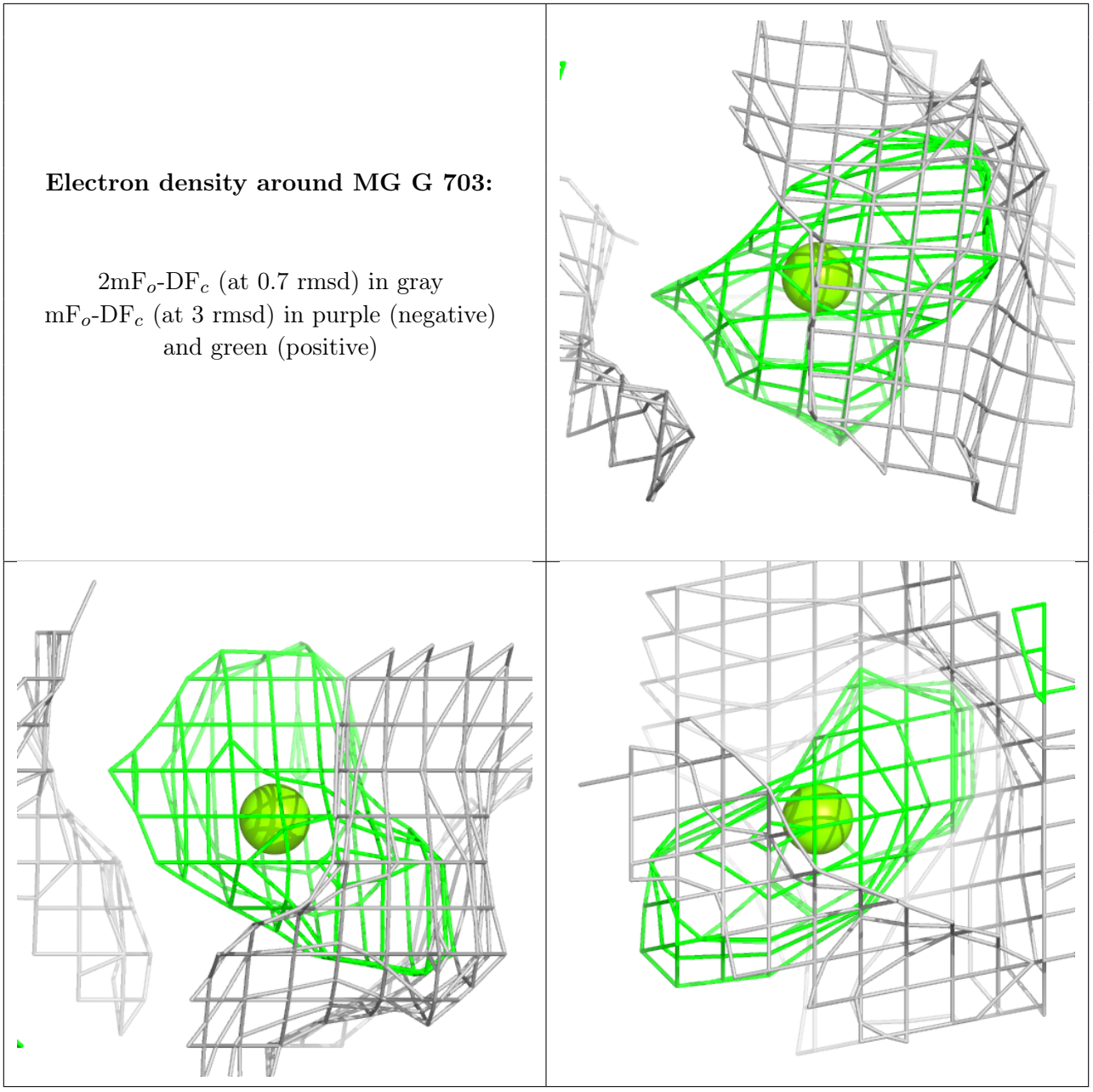






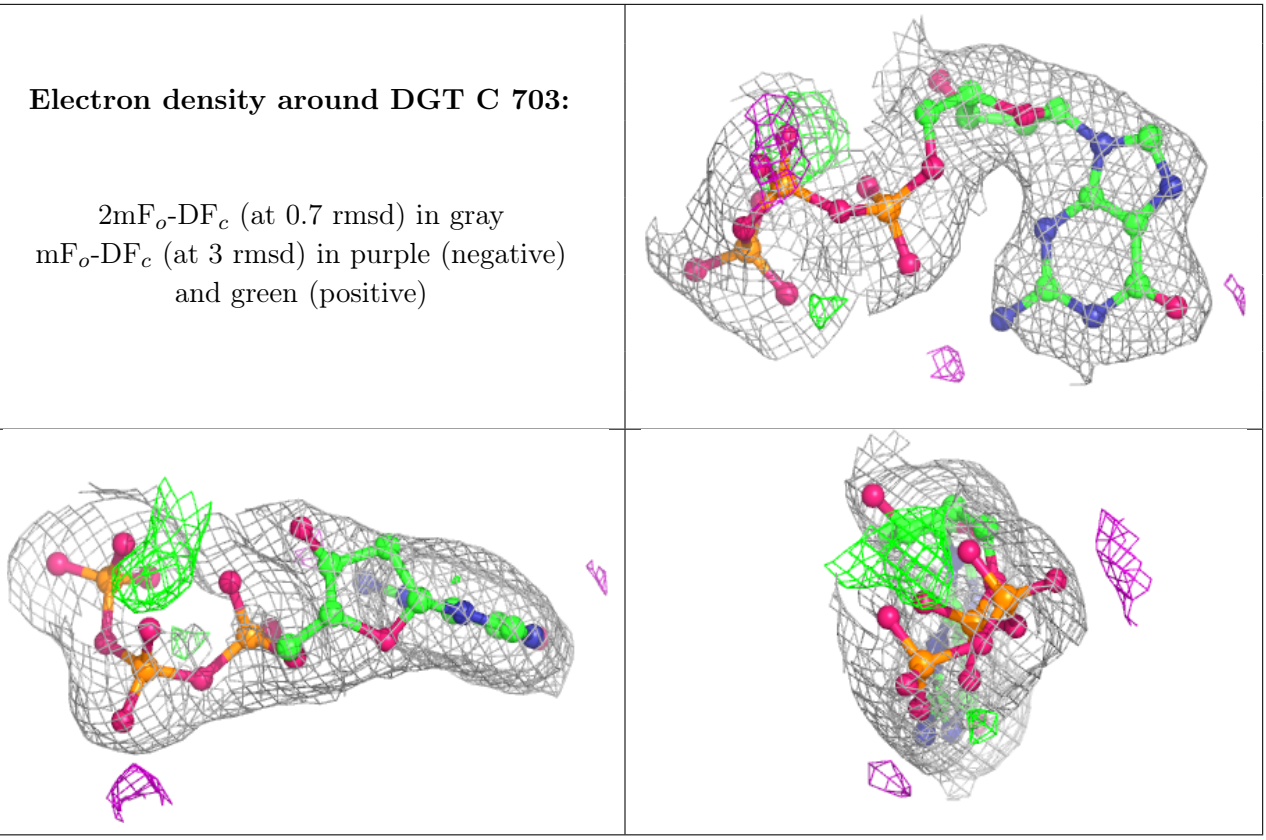
Electron density around MG G 703:

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



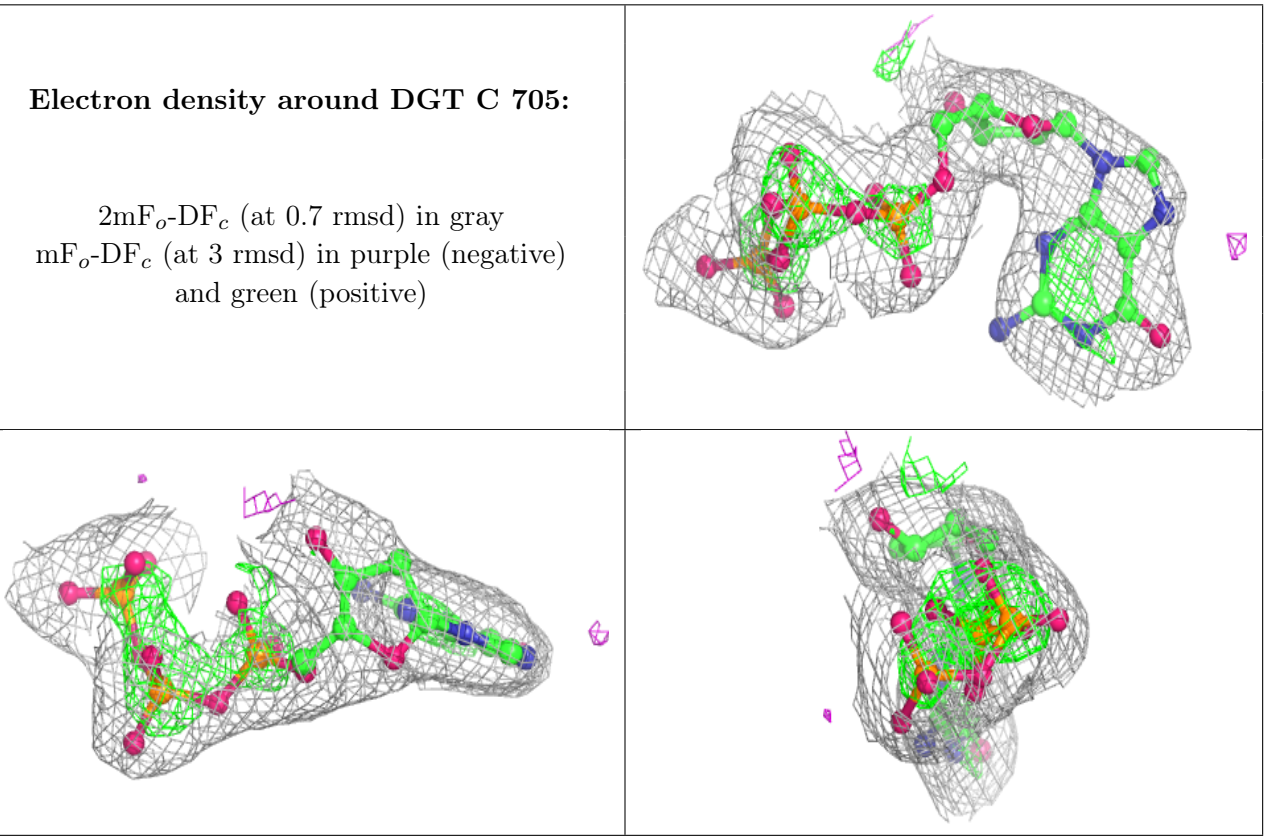
Electron density around DGT C 703:

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



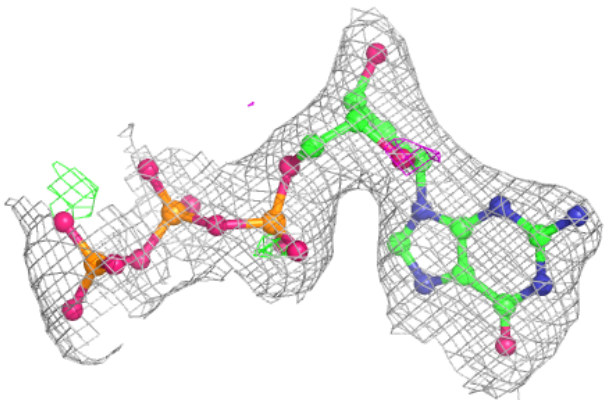
Electron density around DGT C 705:

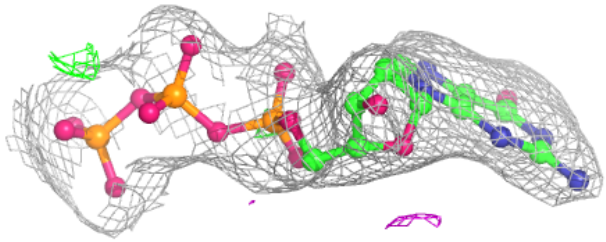
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

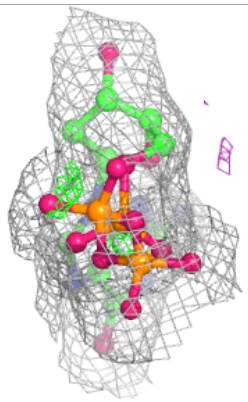


Electron density around DGT A 704:

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

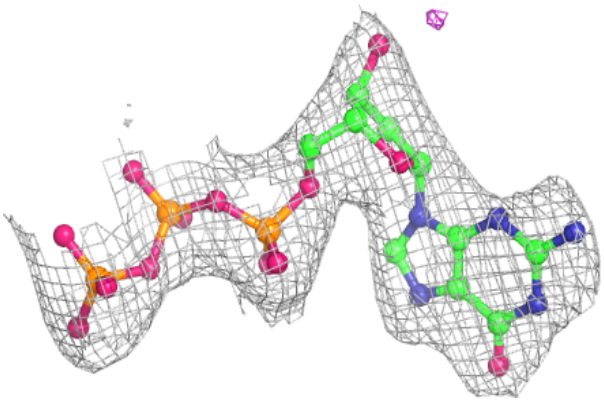


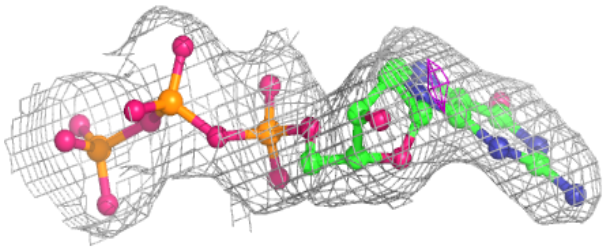


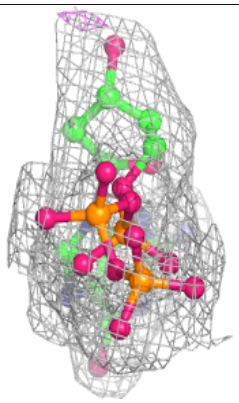


Electron density around DGT C 706:

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

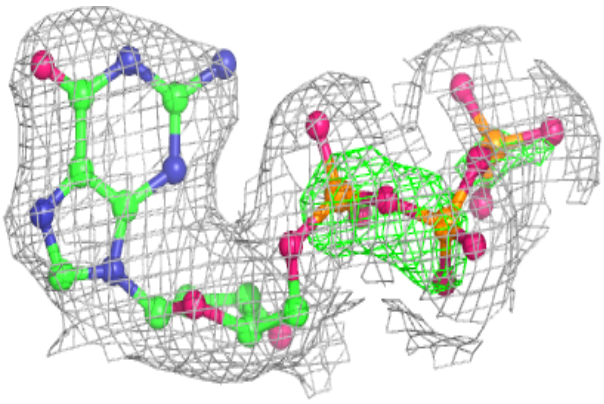


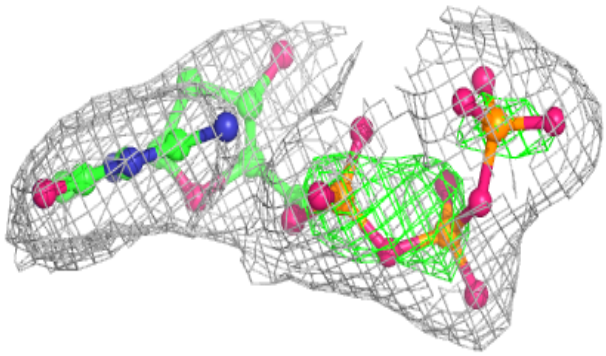


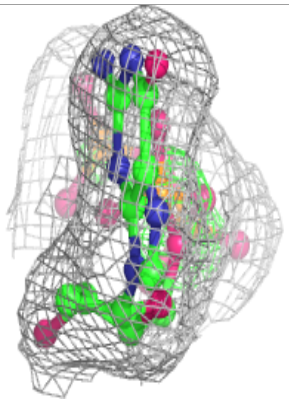


Electron density around DGT E 703:

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

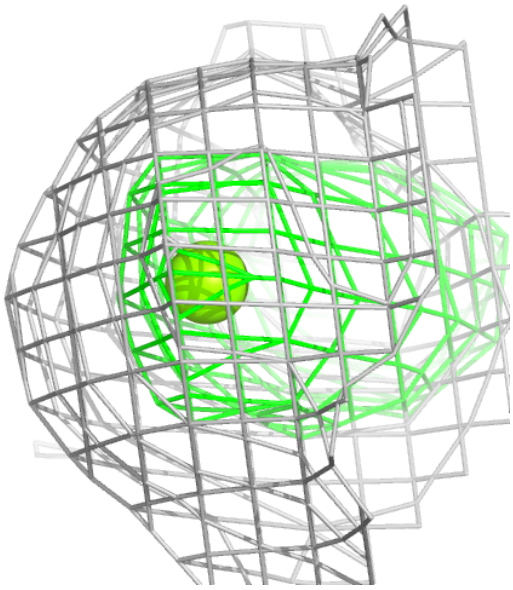


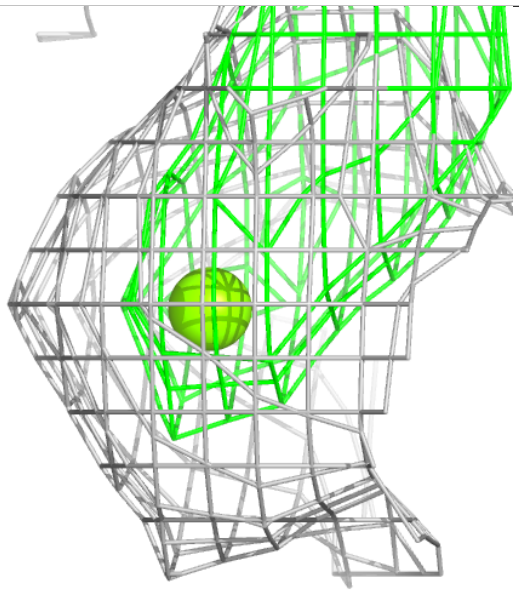


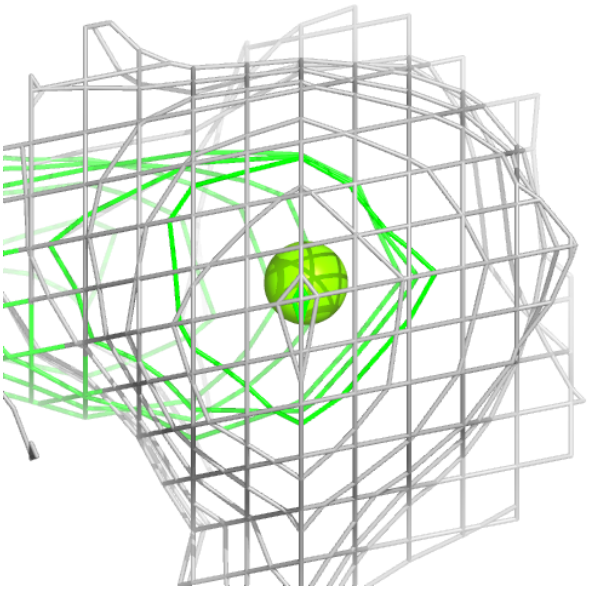


Electron density around MG B 704:

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

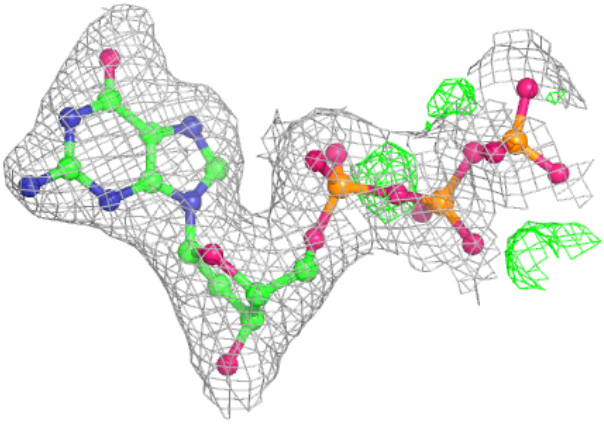


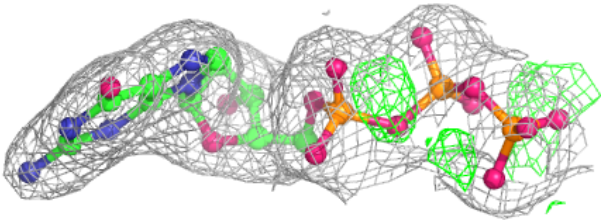


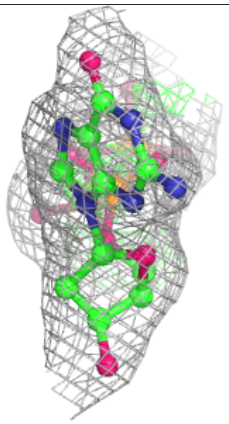


Electron density around DGT G 702:

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

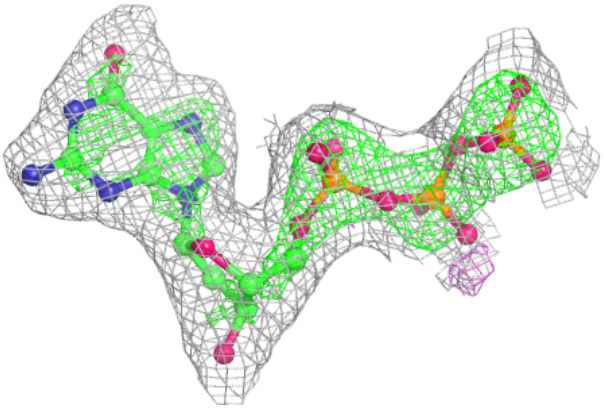


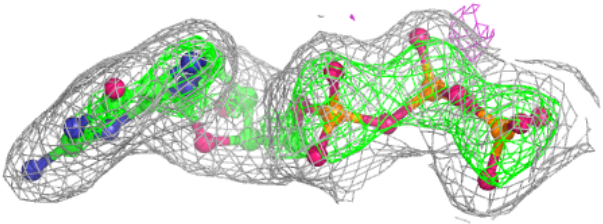


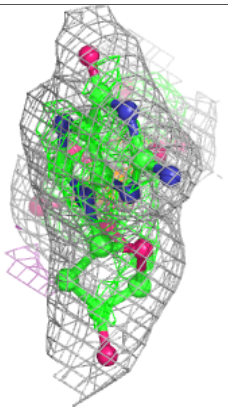


Electron density around DGT H 705:

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

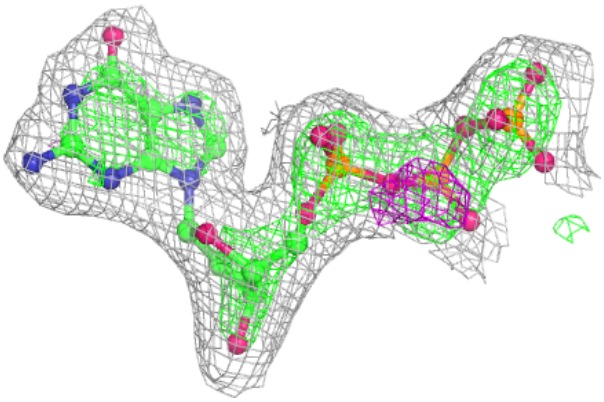


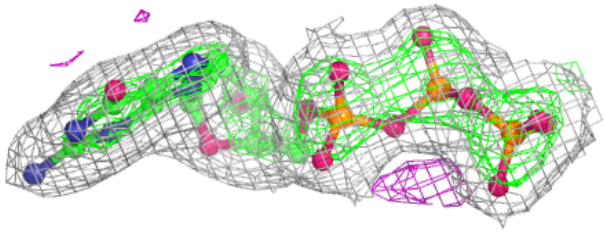


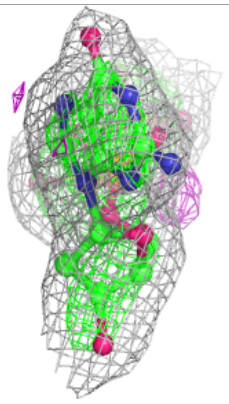


Electron density around DGT E 704:

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

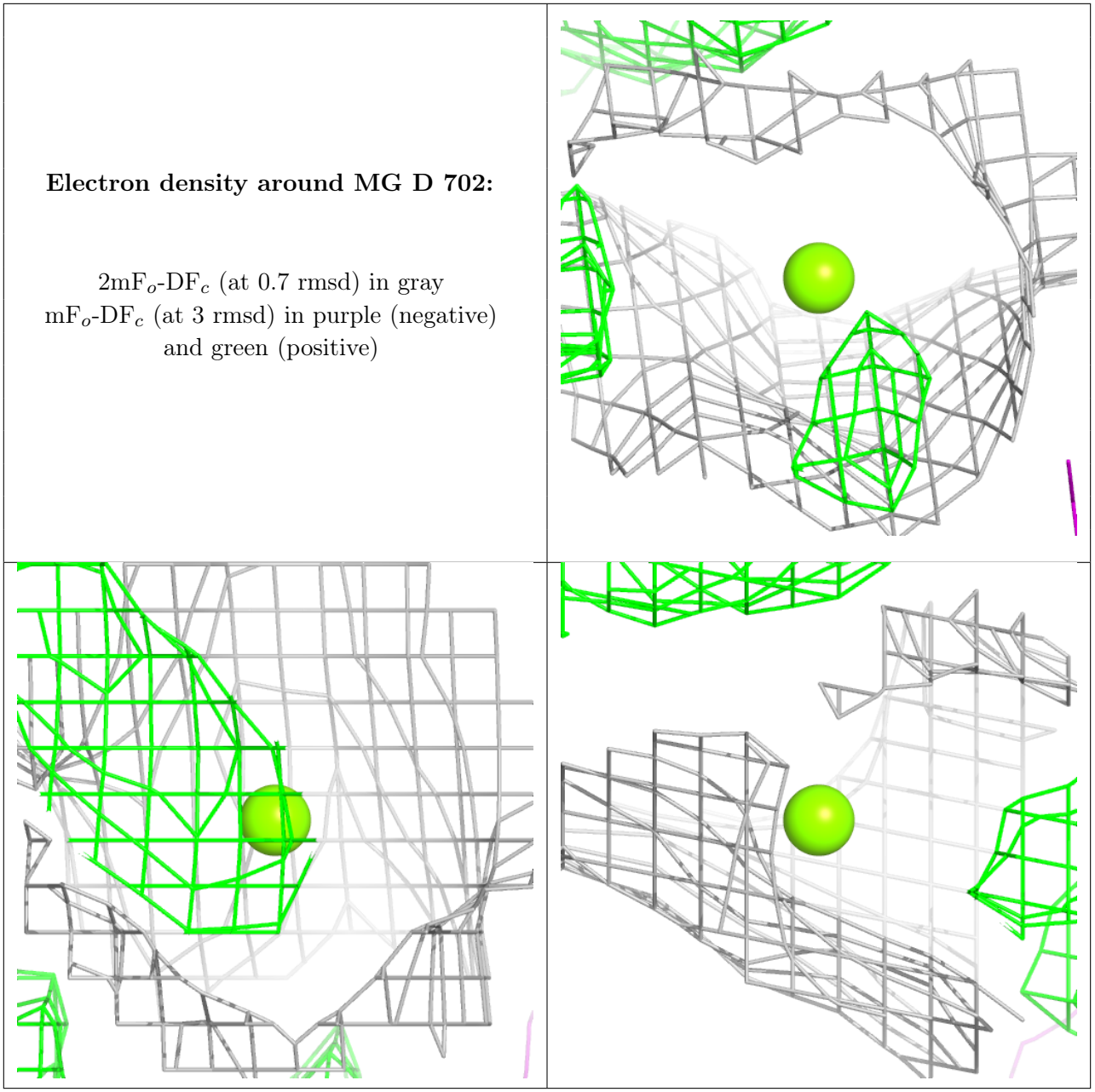






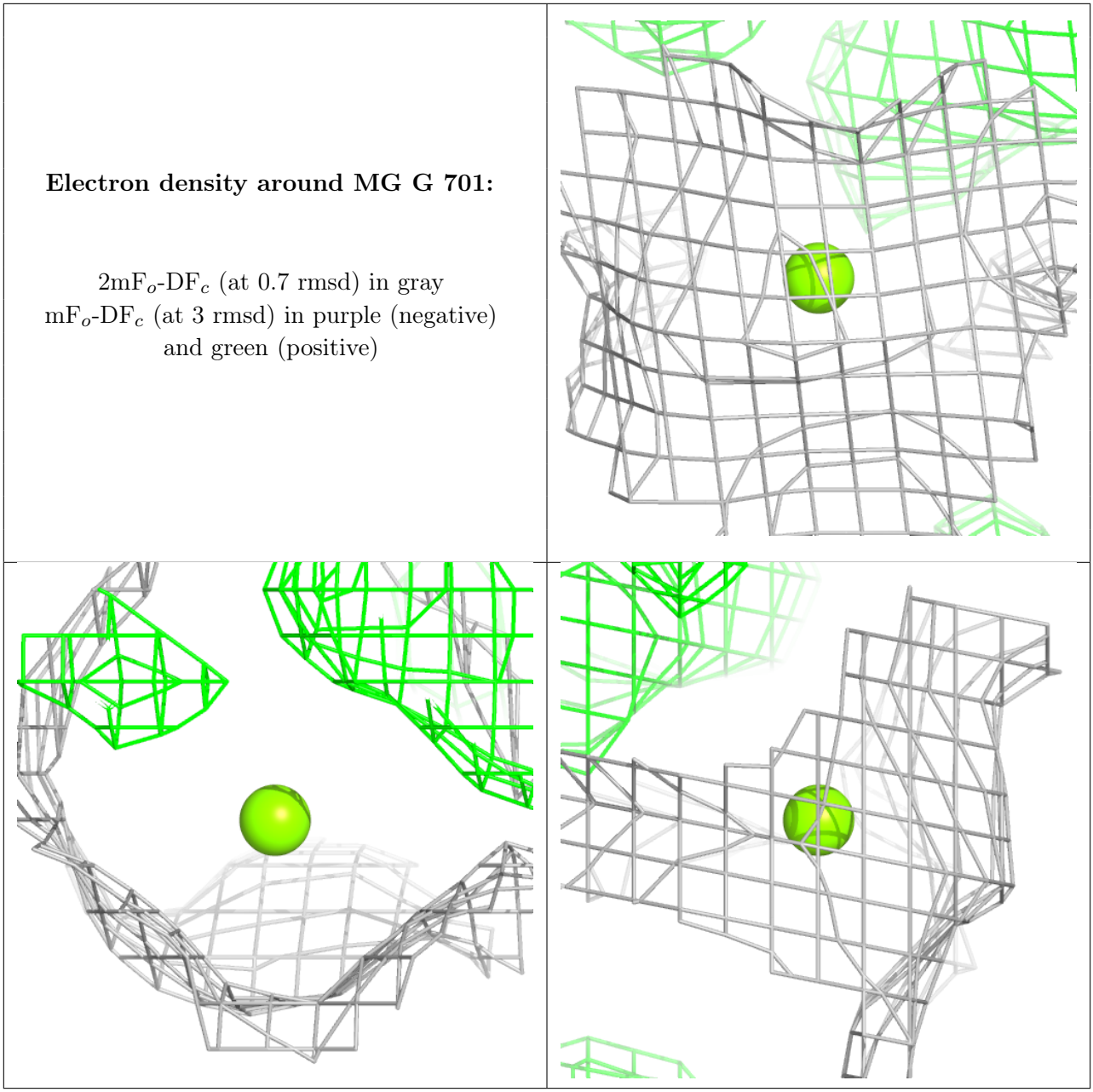
Electron density around MG D 702:

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



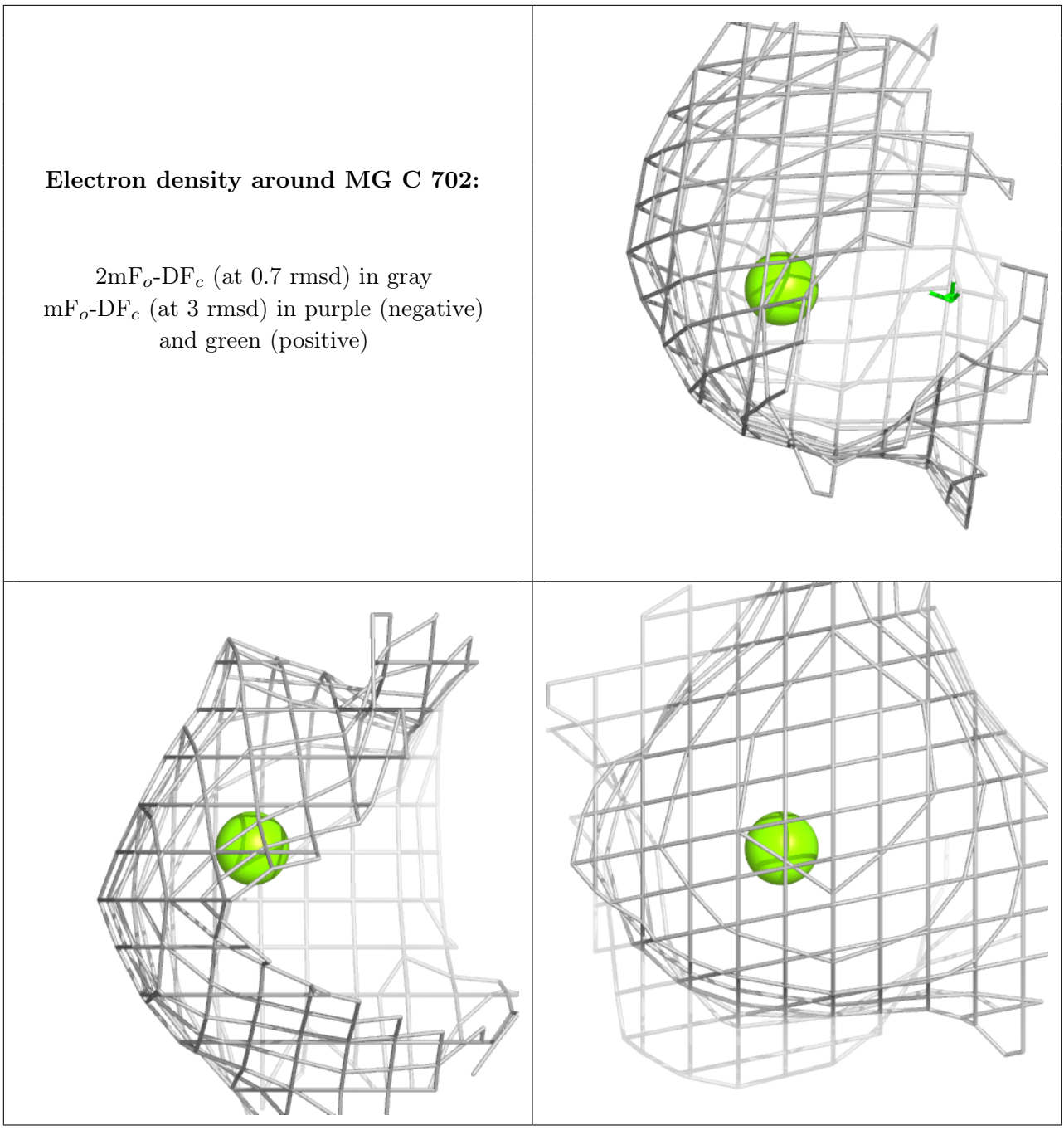
Electron density around MG G 701:

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



Electron density around MG 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)



6.5 Other polymers (i)

There are no such residues in this entry.